Sparse inverse problems for Fourier imaging: applications to Optical Interferometry and Diffusion Magnetic Resonance Imaging
To my dear uncle
Many natural images have low intrinsic dimension (a.k.a. sparse), meaning that they can be represented with very few coefficients when expressed in an adequate domain. The recent theory of Compressed Sensing exploits this property offering a powerful framework for sparse signal recovery from undetermined linear systems.

In this thesis, we deal with two different applications of remote Fourier sensing, for which the available measurements relate to the Fourier coefficients of our concerned signal: optical interferometry and diffusion Magnetic Resonance Imaging (dMRI). In both applications, we face challenging problems due to a restricted number of available measurements and the nonlinearity of the direct model for the data. Inspired by the Compressed Sensing framework, our strategy to solve these nonlinear and ill-posed problems resorts to reformulating them as linear inverse problems and propose novel priors to leverage the intrinsic low dimensionality of the solution.

The first part of this thesis is devoted to image reconstruction from optical interferometry data. State-of-the-art methods are nonconvex due to the intrinsic data nonlinearity and are therefore known to suffer from a strong sensitivity to initialization. We reformulate the problem as a tensor completion problem, where the aim is to recover a tensor from which we have information through some linear mapping. We propose two different alternatives to solve it, one being a purely convex approach. An original nonconvex alternate minimization method has also been explored. We present results on synthetic data and compare pros and cons for both approaches. Our original formulation can be seen as a generalization of the Phase Lift approach and can potentially be applied to other partial phase retrieval problems.

In the second part, we tackle the problem of fiber reconstruction in dMRI. dMRI exploits the anisotropy of the water diffusion in the brain to study the organization of its tissue. Particularly, the goal of our work is to recover the local properties of the axon tracts, i.e. their orientation and microstructural features in every voxel of the brain. We resort to a reweighting scheme to leverage the structured sparsity of the solution, where
the structure originates from the spatial coherence of the fiber characteristics between neighbor voxels. Imposing this original prior promotes a powerful regularization that guarantees a strong robustness to undersampling. Due to a time-consuming measuring process, this ability to solve the imaging problem from few dMRI data points is crucial to guarantee the feasibility of this technique in a clinical context. We present results on real and simulated data and compare our approach to other state-of-the-art methods. We also discuss how our novel approach can actually be applied in a more generic framework for multiple correlated sparse signal recovery.

**Keywords:** inverse problems, compressed sensing, sparsity, structured sparsity, convex optimization, optical interferometry, diffusion MRI, spherical deconvolution, HARDI, microstructure imaging.
Beaucoup d’images naturelles ont une dimension intrinsèque bien réduite (alias par-cimonieuses), signifiant qu’elles peuvent être représentées avec un nombre limité de coefficients si elles se trouvent exprimées dans une base adéquate. La récente théorie de l’échantillonnage compressif (compressed sensing) exploite cette propriété en offrant un cadre très solide pour la récupération des signaux parcimonieux à partir de systèmes linéaires incomplets.

Dans cette thèse, nous traitons deux applications différentes de détection de Fourier à distance, pour lesquelles les mesures qui nous sont accessibles sont liées aux coefficients de Fourier du signal qui nous intéresse : l’interférométrie optique et l’Imagerie par Résonance Magnétique de diffusion (IRMd). Dans les deux cas, nous nous trouvons face à des problèmes qui représentent un gros défi dû à la non-linéarité du modèle et à l’accessibilité à un nombre très restreint de mesures. Inspirés par la théorie de l’échantillonnage compressif, notre stratégie pour résoudre ces problèmes inverses mal posés et non-linéaires recourt à les ré-exprimer comme des problèmes inverses linéaires et à proposer des nouvelles informations à priori afin d’exploiter la petite dimension intrinsèque à la solution.

La première partie de cette thèse est consacrée à la reconstruction des images à partir des données d’interférométrie optique. Dans ce domaine, les méthodes de pointe sont non-convexes dû à la non-linéarité des données et, par conséquent, sont très sensibles à leur initialisation. Nous reformulons ce problème comme un problème de remplissage de tenseurs, avec le but de récupérer un tenseur duquel on obtient information à travers une conversion linéaire. Nous proposons deux alternatives différentes pour le résoudre, dont l’une est purement convexe. Nous avons aussi exploré une nouvelle méthode de minimisation alternée non-convexe. Nous présentons des résultats avec des données synthétiques et on compare les avantages et désavantages des deux approches. Notre formulation originale peut être vue comme une généralisation de l’approche PhaseLift et peut potentiellement être appliquée à d’autres problèmes de récupération de phase.

Dans la deuxième partie, nous abordons le problème de reconstruction des fibres en
IRMd. IRMd exploite l'anisotropie de la diffusion de l'eau dans le cerveau pour étudier l'organisation de ses tissus. En particulier, le but de notre travail est de récupérer les propriétés locales des voies axonales, i.e. leur orientation et microstructure pour chaque voxel du cerveau. Nous recourons à un schéma de repondération itérative afin d'exploiter la parcimonie structurée de la solution, structure qui a lieu grâce à la cohérence spatiale des fibres entre les voxels voisins. En imposant cette nouvelle information a priori nous promouvons une régularisation solide qui assure la reconstruction dans des régimes fortement sous-échantillonnés. À cause d’un processus de mesure de longue durée, le fait d’être capable de résoudre le problème avec très peu de données IRMd est crucial afin de garantir la faisabilité de cette technique dans un contexte clinique. Nous présentons des résultats avec des données autant simulées que réelles que nous comparons à l’état-de-l’art. Nous discutons aussi comment notre nouvelle méthode peut être appliquée à la récupération de multiples signaux parcimonieux corréls dans un cadre plus générique.

**Mots-clefs** : problèmes inverses, échantillonnage compressif, parcimonie, parcimonie structurée, optimisation convexe, interférométrie optique, IRM de diffusion, déconvolution sphérique, HARDI, imagerie de la microstructure.
Pursuing a PhD is like running a long-distance race. Hereafter, I would like to take the opportunity to thank many people around me who have helped me to get to the finish line since, surely, I would have never gotten there on my own.

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Lausanne, 22 March 2017
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<tr>
<td>2D</td>
<td>2-dimensional</td>
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<tr>
<td>3D</td>
<td>3-dimensional</td>
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<tr>
<td>ADD</td>
<td>Axonal Diameter Distribution</td>
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<td>CS</td>
<td>Compressed Sensing</td>
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<td>CSF</td>
<td>Cerebrospinal Fluid</td>
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<td>DSI</td>
<td>Diffusion Spectrum Imaging</td>
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<td>DTI</td>
<td>Diffusion Tensor Imaging</td>
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<tr>
<td>DWI</td>
<td>Diffusion Weighted Imaging</td>
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<tr>
<td>EAP</td>
<td>Ensemble Average Propagator</td>
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<tr>
<td>FOD</td>
<td>Fiber Orientation Distribution</td>
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<td>GM</td>
<td>Grey Matter</td>
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<tr>
<td>HARDI</td>
<td>High-Angular Resolution Diffusion Imaging</td>
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<td>ODF</td>
<td>Orientation Diffusion Function</td>
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<td>OTF</td>
<td>Optical Transfer Function</td>
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<td>SD</td>
<td>Spherical Deconvolution</td>
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<td>SVD</td>
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Chapter 1

Preface

1.1 Context

When we have a physical system we can build mathematical models to predict the outcome of a certain measurement process. For instance, the weather forecast predicts the curve of temperatures or the quantity of rain at a certain location based on a particular model. These kinds of problems are commonly known as forward problems. Conversely, inverse problems are concerned with determining the causes for an observed effect. Inverse problems became very popular by the end of last century being increasingly used for applications in science and engineering. As an example, the restoration of a signal or an image from its “degraded” versions can be cast as an inverse problem and is the basis of many imaging modalities that involve remote sensing, such as medical, astronomical, radar, sonar, etc. In these contexts usually only a limited number of noisy observations is available and this limitation leads to ill-posed inverse problems, meaning that their solution either is not unique or does not exists or is not stable. As a consequence, to ensure a plausible solution, the problem needs to be regularized by injecting some prior information either on the physical model or on the unknown signal itself.

Many natural signals are sparse in some adequate transformed domain, meaning that they can actually be described with very few coefficients when expressed in a suitable basis (i.e. they have low intrinsic dimension). For instance, wavelet techniques provide a multi-scale representation of natural signals characterized by a sparse structure. Therefore, functions that promote the sparsity of the signal of interest appear as very good candidates to regularize ill-posed inverse problems.

Among inverse problems in general, linear inverse problems (l.i.p.) have been widely studied and the theory of regularization methods in the linear case is very well developed. One of the nice properties that makes l.i.p very attractive is that they can be efficiently solved by using fast and versatile convex optimization methods. The theory of Compressed Sensing (CS)* can actually be framed in the context of ill-posed linear sensing. CS builds a framework where a sparse signal can be recovered from very few measurements, beyond

*Also known as compressive sensing or compressed/ive sampling. Throughout this manuscript the reader will find these terms used indistinctly.
the requirements of the Nyquist sampling theorem, by exploiting the sparsity of the signal and cleverly designing adequate sensing matrices.

In this thesis, we deal with sparse, ill-posed and nonlinear inverse problems that arise from two applications of Fourier sensing: optical interferometry and diffusion Magnetic Resonance Imaging (dMRI). In what we call Fourier sensing, not directly the signal of interest is retrieved but a set of measurements that are related to the Fourier coefficients of the object of interest. In both applications, we deal with undersampled problems, for which the number of available measurements is smaller than the dimension of the signal. Nevertheless, the nature of the ill-posedness stems from different origins, depending on the application. In optical interferometry the undersampling is due to an highly-limited number of sensing devices (i.e. telescopes). Otherwise, in the field of diffusion MRI the measuring process is so time consuming that undersampling is the only way to guarantee the feasibility of the technique in a clinical context.

We tackle these originally nonlinear inverse problems by reformulating them as linear problems, so that we can take advantage of all the flexibility of convex optimization methods to easily inject prior information and efficiently solve them. Our formulations to solve sparse linear inverse problems are built on the CS framework, even if in this work we do not explore explicitly the design of sensing matrices. The strategies that have been implemented to move from a nonlinear to a linear formulation, as well as the chosen regularization methods to leverage the appropriate sparse structure of the signal, vary depending on the application. The reader can find an overview of all of them in the next subsection, devoted to describe our contributions and the organization of the manuscript.

1.2 Contributions and organization of the manuscript

In the following lines I present a brief summary of each of the parts of this manuscript:

Chapter 2 includes a review on general linear inverse problems and describes the theory of Compressed Sensing (CS) for sparse signals. From the formulation perspective, it addresses the problem of sparse signal recovery based on CS ideas. Regarding the reconstruction, it revises convex optimization and proximal splitting methods. This part is meant to provide the reader with the background required to understand subsequent parts of the thesis and does not include any original contribution.

In part I, I detail the work we have done on image reconstruction from Optical Interferometry data. Optical interferometers are now the state-of-the-art to reach the best resolution in the optical spectrum. Nevertheless, their output is not directly an image and tools for image reconstruction are, therefore, required. Image recovery in optical interferometry is an ill-posed problem arising from incomplete power spectrum and bispectrum
measurements. Consequently, the direct model of the data happens to be highly nonliner, inducing nonconvexity in the problem. So far, all state-of-the-art methods perform local optimization, which (i) does not provide a global solution and (ii) makes them highly dependent on the initialization. We generalize the Phase Lift approach [2] and reformulate the problem as a tensor completion problem, where the aim is to recover a tensor from which we have information through some linear mapping. In order to regularize it, we propose a novel prior to account for low-rankness of the tensor, trying to exploit the specific conditions of our problem. For the sake of comparison, an original nonconvex gauss-seidel alternate minimization approach has also been explored. We present results on synthetic data and discuss pros and cons of both approaches. This work has been published in [3, 4].

In part II, I describe the work we have done on fiber reconstruction from diffusion Magnetic Resonance Imaging (dMRI) data, in the domain of brain imaging. dMRI exploits the random diffusional property (Brownian motion) of the water molecules to try to infer features of the body tissue. In particular, it has become popular in brain imaging to recover axons orientation and microstructure. In chapter 4 we give some background information on the field and cite the main state-of-the-art local modeling methods to explain the dMRI signal in each voxel of the brain.

Chapter 5 addresses the problem of fiber orientation estimation. The direct forward model that explains the dMRI signal as a Gaussian mixture is actually nonlinear and estimating its parameters directly resorts to nonlinear fitting. However, the problem can be discretized and reformulated using a linear dictionary made of a concatenation of ”response functions” in the framework of spherical deconvolution [5, 6]. In this framework, we take advantage of the versatility of convex optimization to include a novel prior that imposes spatial regularization directly on the fiber space. We present results on real and simulated data and compare our approach to other state-of-the-art methods. This work has been published in [7, 8].

Chapter 6 is concerned with assessing the microstructure of the fibers. Most micros-tucture imaging techniques recover the microstructure properties by modeling the dMRI signal in different tissue compartments. Similarly as in chapter 5, the direct nonlinear routines usually employed to fit these models are computationally very intensive and cause practical problems for their application in clinical studies. Our novel approach is based on the framework of AMICO\(^\dagger\) that reformulates these microstructure imaging techniques as linear systems [9]. Again, thanks to the flexibility of convex optimization, we generalize its formulation to enable microstructure estimation and fiber orientation recovery simultaneously. Besides, we adapt the novel prior defined in chapter 5 to the problem of microstructure recovery to impose spatial coherence on the solution. We show preliminary results on simulated data and discuss general open questions in the field of microstructure imaging. Part of this work has been published in [10, 11, 12, 13].

\(^\dagger\)Accelerated Microstructure Imaging via Convex Optimization
Finally, conclusions and future perspectives are presented in Chapter 7.
2.1 Introduction

Many natural signals have low intrinsic dimension (a.k.a. sparse), meaning that most of their coefficients vanish when expressed in a suitable basis. As a consequence, the concept of sparsity has become very popular in many signal processing problems, such as deconvolution, denoising and deblurring. Sparsity of the signal can appear in different domains: besides classical sparsity, TV-sparse signals (i.e. signals whose gradient has few significant coefficients) or low-rank matrices can also be considered sparse objects since they have much less degrees of freedom than their actual dimension.

Sparsity is therefore a good candidate to be injected as a prior to regularize ill-posed inverse problems. Precisely, the recent theory of Compressive Sensing (CS) resorts to $\ell_1$-norm minimization to promote sparse solutions. In this chapter we address the problem of sparse signal recovery from both, formulation and reconstruction perspective.

The chapter is organized as follows: our notation and some useful mathematical definitions are presented in section 2.2. In section 2.3 the reader can find a short reminder on linear inverse problems and regularization strategies. Section 2.4 is devoted to the formulation of convex minimization problems for the recovery of sparse signals based on Compressive Sensing ideas. Low-rank matrix recovery is also addressed, seen as an extension of the original CS framework. In section 2.5 we revise fundamental notions on convex optimization. We present, as well, the group of proximal splitting methods that appear as reconstruction algorithms particularly convenient to solve the convex problems previously proposed. We conclude in section 2.6 reviewing the background context presented in this chapter and linking it with the novel contributions that will be introduced further in this thesis.

2.2 Notation and basic definitions

Throughout this thesis, we use $\mathbb{R}$ to denote the set of real numbers and $\mathbb{C}$ for the complex set. $\mathbb{R}_+$ denotes the set of non-negative real numbers. We denote vectors with bold lower case letters, matrices with upper case letters and tensor with italic ones. We denote
the $i$-th element of a vector $x \in \mathbb{R}^N$ (or alternatively $\mathbb{C}^N$) for any index $i \in \{1, \ldots, N\}$. Let $x, z \in \mathbb{R}^N, z \in \mathbb{C}^N$ be two $N$-dimensional real and complex vectors, respectively. $x^\top$ stands for the simple transpose vector whereas $z^\dagger$ stands for the conjugate-transpose vector.

Let $x, y \in \mathbb{R}^N$ be two $N$-dimensional vectors. The standard inner product on $\mathbb{R}^N$ is given by $\langle x, y \rangle = x^\top y$. The $\ell_2$ norm, the Euclidean norm, of a vector $x \in \mathbb{R}^N$ is defined as $\|x\|_2 = \sqrt{x^\top x} = \sqrt{\sum_{i=1}^N x_i^2}$. More generally, the $\ell_p$ norm ($p \geq 1$) of a vector is defined as:

$$\|x\|_p = \left(\sum_{i=1}^N |x_i|^p\right)^{1/p}. \quad (2.1)$$

In particular, for the case $p = 1$, the well-known $\ell_1$ norm corresponds to the sum of the absolute values of the signal. The $\ell_0$ pseudo-norm of a vector is a cardinality function which corresponds to the number of its nonzero coefficients:

$$\|x\|_0 = \#(i|x_i \neq 0). \quad (2.2)$$

For matrices $X, Y \in \mathbb{R}^{M \times N}$, the standard inner product is given by:

$$\langle X, Y \rangle = \text{tr}(X^\top Y) = \sum_{i=1}^M \sum_{j=1}^N X_{ij} Y_{ij}, \quad (2.3)$$

where tr denotes the trace of a matrix (i.e., the sum of the elements of its diagonal). $X$ can be factored as

$$X = U\Sigma V^\top, \quad (2.4)$$

where $U \in \mathbb{R}^{M \times r}$ satisfies $UU^\top = I$ (being $I$ the identity matrix), $V \in \mathbb{R}^{N \times r}$ satisfies $VV^\top = I$ and $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_r)$ with

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq 0. \quad (2.5)$$

Factorization (2.4) is known as the singular value decomposition (SVD) of $X$ and $\sigma_i$ are the singular values. The rank $r$ of a matrix denotes the number of its nonzero singular values. The nuclear norm of a matrix $\| \cdot \|_*$ is equal to the sum of its singular values:

$$\|X\|_* = \sum_{i=1}^r \sigma_i(X), \quad (2.6)$$

for a matrix $X$ of rank$(X) = r$. Note that the rank of a matrix actually corresponds to the $\ell_0$ norm of its vector of singular values, whereas the nuclear norm of a matrix is equivalent
to the $\ell_1$ norm of its vector of singular values.

A symmetric matrix $Z \in \mathbb{R}^{N \times N}$ (or more generally $\in \mathbb{C}^{N \times N}$) is called \textit{positive definite} if for all $x \neq 0$, $xZx^\top \geq 0$ (or $zZz^\dagger \geq 0$) and we denote $Z > 0$. The \textit{negative definite}, \textit{positive semidefinite}, and \textit{negative semidefinite} matrices are defined analogously, requiring the expression $zZz^\dagger$ to be always negative, nonnegative, and nonpositive, respectively.

The order (or number of dimensions, ways or modes) of a tensor $X \in \mathbb{C}^{N_1 \times \ldots \times N_d}$ with components $X_{i_1, \ldots, i_d}$ is the number $d$ of the indices characterizing its components. For the sake of simplicity, we present the following notation only for tensors of order 3.

A 3-way tensor $X \in \mathbb{C}^{N_1 \times N_2 \times N_3}$ is rank-1 if it can be written as the outer product of 3 vectors, i.e. $X = a \circ b \circ c$, or component-wise $X_{ijk} = a_ib_jc_k$.

The rank of a tensor, rank($X$), is defined as the smallest number of rank-1 tensors that generate $X$ as their sum. In other words, if $X$ can be expressed as

\begin{equation}
X = \sum_{r=1}^{R} a_r \circ b_r \circ c_r,
\end{equation}

then $\text{rank}(X) \leq R$. The notion of rank when applied to a tensor is analogue to the matrix rank though most of the common properties of the latter do not hold when dealing with objects of a dimension higher than 2. One of the main differences is that there is no algorithm to compute the rank of a given tensor. In fact the problem is NP-hard [14].

The well-known method to find a rank-$k$ approximation of a matrix through the largest $k$ values of its SVD [15] does not apply or have an equivalent for the case of high-dimension tensors.

\textit{Matricization} is the process of transforming a tensor into a matrix. The mode-$n$ matricization of a tensor $X$ is denoted by $X_{(n)}$ and results from unfolding all its modes but the mode $n$ into the rows of a matrix. The $n$-rank of a tensor follows as

\begin{equation}
n\text{-rank}(X) = (\text{rank}(X_{(1)}), \text{rank}(X_{(2)}), \text{rank}(X_{(3)})).\end{equation}

In contrast to the rank function, it is easier to handle, since the problem is reduced to calculations with matrices which are already well-known objects with nice properties. The reader can refer to [16] for a more detailed explanation on different notions of tensor rank and their associated decomposition methods.

A tensor is called cubical if every mode has the same size, i.e. $X \in \mathbb{R}^{N \times N \times N}$. A cubical tensor $X$ is called supersymmetric if its entries are invariant under permutation of their indices: $X_{ijk} = X_{ikj} = X_{jik} = X_{jki} = X_{kij} = X_{kji}$. 

2.2. Notation and basic definitions 7
2.3 Linear inverse problems

A typical linear inverse problem aims to solve a linear system of equations of the form

\[ y = \Phi x + \eta, \]  

(2.9)

where \( \Phi \in \mathbb{R}^{M \times N} \) and \( y \in \mathbb{R}^M \) are known, \( \eta \) is some noise or perturbation of the measurement vector \( y \) and \( x \in \mathbb{R}^N \) represents the true signal to be recovered. The least squares (LS) approach to solve problem (2.9) chooses to minimize the data discrepancy by solving

\[ \hat{x} = \min_x \| \Phi x - y \|^2. \]  

(2.10)

However, in many applications, matrix \( \Phi \) is ill-conditioned, implying that small changes in the input argument \( x \) can result in large changes on the output value of the measurements, making (2.9) a very unstable system, extremely sensitive to noise.

Regularization methods overcome this challenge by replacing the original ill-posed problem by a well-conditioned problem with solution

\[ \hat{x} = \min_x \| \Phi x - y \|^2 + \lambda f_r(x). \]  

(2.11)

In (2.11) the role of the regularization function \( f_r(\cdot) \) is to improve the ill-conditioned nature of the original problem by injecting some prior knowledge on the required solution. The so-called regularization parameter \( \lambda \) controls the compromise between accuracy and stability of the solution. Actually, the whole "art" of regularizing relies on wisely tuning this compromise [17]. To mention a simple example, one popular strategy, known as Tikhonov regularization, corresponds to choosing \( f_r(\cdot) = \| \cdot \|_2^2 \), the quadratic penalty of the unknown:

\[ \hat{x} = \min_x \| \Phi x - y \|^2 + \lambda \| x \|^2_2. \]  

(2.12)

In (2.12), the quadratic term that is added to the initial objective function helps stabilizing the problem by controlling the norm of the solution. In this case, \( \lambda \) can be read off as a trade-off between data fidelity and noise sensitivity. Problem (2.11) has also an equivalent constrained form that reads:

\[ \hat{x} = \min_x f_r(x) \quad \text{s.t.} \quad \| \Phi x - y \|^2 \leq \epsilon, \]  

(2.13)

for some value of \( \epsilon \) acting as a bound on the noise level.

In the following section, we focus on the design of minimization problems, i.e. the choice of relevant regularization functions, for sparse signal recovery.
2.4 Sparse signal model

2.4.1 Review on Compressed Sensing

It is known that a large variety of natural signals are sparse or compressible in multiscale dictionaries, such as wavelet bases. By definition, a signal is *sparse* in some orthonormal basis $\Psi \in \mathbb{C}^{N \times N}$ if its expansion $\alpha \in \mathbb{C}^N$, with $x \equiv \Psi \alpha$, contains only a small number $K \ll N$ of nonzero coefficients $\alpha_i$. More generally, it is *compressible* if its expansion only contains a small number of significant coefficients, i.e. if a large number of its coefficients bear a negligible value. In figure 2.1, we show an example of an image and its sparse representations in two different bases.

![Figure 2.1: Sparsity of Lena in two different basis](image)

The Compressed Sensing (CS) theory [18, 19, 20] builds a framework where a signal can be recovered with very high probability from fewer measurements $M \propto K \ll N$ than what it had used to be considered sufficient, beyond the traditional Nyquist paradigm [21]. The signal is assumed to be probed by $M$ linear measurements denoted by a vector $y \in \mathbb{C}^M$ in some orthonormal sensing basis and identified by the sensing matrix $\Phi \in \mathbb{C}^{N \times M}$ and possibly affected by i.i.d. Gaussian noise $\eta \in \mathbb{C}^M$. Therefore the following linear inverse problem in matrix form holds:

$$y \equiv \Theta \alpha + \eta, \quad \text{with} \quad \Theta \equiv \Phi \Psi \in \mathbb{C}^{M \times N} \quad (2.14)$$
One popular strategy for the signal recovery resorts to solving the associated minimization problem and regularizing the originally ill-posed inverse problem by an explicit sparsity or compressibility prior on the signal. Knowing that the representation of signal $\alpha$ is sparse or compressible and considering a set of measurements $y$ corrupted by some bounded noise, the first natural approach to recover $x$ would be by solving an optimization problem like:

$$
\min_{\hat{\alpha} \in \mathbb{C}^N} \|\hat{\alpha}\|_0 \quad \text{subject to} \quad \|y - \Theta \hat{\alpha}\|_2 \leq \epsilon,
$$

(2.15)

where $\epsilon$ represents a bound on the $\ell_2$ norm of the residual noise, $\eta \equiv y - \Theta \hat{\alpha}$. Unfortunately, the $\ell_0$ norm is a nonconvex function and it is known that finding a minimum for (2.15) is NP-hard.

One common approach to recover $x$ from $y$ is to replace the nonconvex $f_r(\cdot) = \|\cdot\|_0$ in (2.15) by its convex approximation, the $\ell_1$ norm, and solve the following convex problem:

$$
\min_{\hat{\alpha} \in \mathbb{C}^N} \|\hat{\alpha}\|_1 \quad \text{subject to} \quad \|y - \Theta \hat{\alpha}\|_2 \leq \epsilon.
$$

(2.16)

In (2.16), the $\ell_1$ norm of the coefficients of the signal in the sparsity basis $\alpha \equiv \Psi^\dagger x$ is minimized under a constraint on the $\ell_2$ norm of the residual noise. This $\ell_1$ minimization approach formulates the CS problem of recovering sparse signals in the powerful framework of convex optimization, for which there exists a number of efficient numerical solvers and algorithms (refer to section 2.5). A simple illustrated example meant to provide an understanding on how the $\ell_1$ norm induces sparsity on the solution can be found in Figure 2.2. In the illustration, dashed lines represent an $\ell_1$ ball and an $\ell_2$ ball in $\mathbb{R}^2$ (set of vectors with the same $\ell_1$ or $\ell_2$ norm, respectively) and line $A$ represents a linear data constraint. The constrained line intersects the $\ell_1$ ball on the axis, thus resulting in a sparse solution.

**Figure 2.2:** Illustration of the $\ell_p$ approximation $\hat{x}$ of a point $x \in \mathbb{R}^2$ by a one-dimensional space $A$. Dashed lines represent an $\ell_1$ ball and an $\ell_2$ ball (set of vectors with the same $\ell_1$ or $\ell_2$ norm, respectively). Illustration taken from [22]. Image used with permission.

The theory of CS performs an analysis of problem (2.16) and provides recovery guarantees under certain conditions on the signal and the sensing matrix [23]. However, convex
optimization is particularly versatile and can account for variations in the formulation of the problem. For instance, the unconstrained version of the $\ell_1$ minimization problem can also be considered, i.e.,

$$\min_{\hat{\alpha} \in \mathbb{C}^N} \frac{1}{2} \| y - \Theta \hat{\alpha} \|_2^2 + \lambda \| \hat{\alpha} \|_1.$$  \hspace{1cm} (2.17)

For some value of $\lambda$, this optimization problem will yield the same result as the formulation (2.16). Another possible variation implies optimizing the signal $x$ itself (analysis-based formulation), instead of solving the minimization problem for the representation vector $\hat{\alpha}$ and then recovering the signal through $\hat{x} \equiv \Psi \hat{\alpha}$ (synthesis-based methods). Note that in the case of $\Psi$ being an orthonormal basis the two approaches are equivalent.

### 2.4.2 Beyond $\ell_1$: iterative reweighted $\ell_1$ minimization

In this subsection, we present a reweighted iterative algorithm that in many situations finds the good solution for (2.14) but with less measurement requirements than considering the $\ell_1$ surrogate [24]. In this approach, the $\ell_0$ norm in (2.15) is substituted by a weighted $\ell_1$ norm defined as $\| w\alpha \|_1 = \sum_i w_i |\alpha_i|$, for positive weights $w_i$. A reweighted scheme algorithm is defined, alternating between solving a problem of the form:

$$\hat{\alpha}^{(t)} = \min_{\alpha \in \mathbb{C}^N} \| W^{(t)} \hat{\alpha} \|_1 \text{ subject to } \| y - \Theta \hat{\alpha} \|_2 \leq \epsilon,$$  \hspace{1cm} (2.18)

and updating the weights $w_i$. In (2.18), matrix $W^{(t)} \in \mathbb{R}^N$ represents a diagonal matrix with coefficients $\{ w_1, \ldots, w_N \}$ in the main diagonal and superindex $t$ indexes the iteration number.

In this kind of scheme, large weights tend to discourage nonzero entries whereas small weights promote nonzero entries in the solution. Therefore, as it is extensively discussed in [24], the weights need to relate to the inverse of the associated element of the solution at the previous iteration, so as to lead to an $\ell_0$-norm prior at convergence. In [24], the authors propose to update the weights as follows:

$$w_i^{(t+1)} = \frac{1}{|x_i^{(t)}| + \tau}$$  \hspace{1cm} (2.19)

and terminate either on convergence or when $t$ reaches a maximum-allowed number of iterations. The parameter $\tau$ that appears in the definition of the weights has the role of providing stability and ensuring that all weights are well defined, even for zero coefficients.

With this definition (2.19), the weights compensate the fact that simple $\ell_1$ minimization does not treat all coefficients evenly. Indeed, when minimizing the convex $\ell_1$ norm to promote sparsity, larger coefficients are actually more penalized than the smaller ones, whereas they would be equally treated if one was directly minimizing the original $\ell_0$ pseudo-norm.
The reweighted $\ell_1$ minimization outperforms plain $\ell_1$ minimization in a variety of setups and since the number of iterations is typically very low, its additional computational cost is affordable [24]. Illustration 2.3 provides an visual example of a situation where the (unweighted) $\ell_1$ minimization fails to recover the correct solution whereas the weighted-$\ell_1$ minimization, does not. In this simple 3D situation, the feasible set intersects the interior of the $\ell_1$ ball centered in the origin with a radius equal to $\|x_0\|_1$, and therefore minimizing the $\ell_1$ norm does not find the correct solution (situation (b) in Figure 2.3). However, *weighting* the $\ell_1$ ball with appropriate weights provokes a “sharpening” effect on the shape of the ball, avoiding its intersection with the linear constraint and leading the weighted problem to find the correct solution.

![Figure 2.3: Visual example of sparse signal recovery using a weighted $\ell_1$ norm.](image)

- (a): The linear constraint $y = \Phi x$ and the $\ell_1$ ball containing the sparse signal to be recovered $x_0$ are shown.
- (b): $x \neq x_0$ with $\|x\|_1 < \|x_0\|_1$ exists.
- (c): Weighted $\ell_1$ ball. No $x$ such that $\|Wx\|_1 < \|Wx_0\|_1$ exists.

*Illustration taken from [24]. Image used with permission.*

### 2.4.3 Low-rank matrix recovery

The problem of recovering a matrix from some sample of its entries, or from fewer linear functionals about the matrix, is known as the matrix completion problem [25, 26, 27]. Mathematically, it can as well be formulated as a linear inverse problem

$$y = A(X) + \eta,$$

where the unknown would be a matrix $X \in \mathbb{R}^{N_1 \times N_2}$ and $A$ a linear operator acting on the space of $N_1 \times N_2$ matrices. Note that matrix $X$ is represented by $N_1 \cdot N_2$ numbers but it only has $(2N - r) \cdot r$ degrees of freedom, with $N = \max(N_1, N_2)$ and $r = \text{rank}(X)$. When the rank is small, this is notably smaller than $N_1 \cdot N_2$.

Analogously to the vector case, the assumption that the unknown has low dimension (low rank) makes the search of solutions feasible. Consequently, one would like to solve...
the following optimization problem:

$$\min_{X \in \mathbb{R}^{N_1 \times N_2}} \text{rank}(X) \quad \text{subject to} \quad \|y - A(X)\|_2 \leq \epsilon.$$  \hspace{1cm} (2.21)

However, even if (2.21) appears as the most natural problem to solve, it is actually NP-hard.

A popular alternative to problem (2.21) resorts to minimizing the nuclear norm of the unknown, i.e. $f_r(\cdot) = \|\cdot\|_*$ [27], leading to the following formulation:

$$\min_{X \in \mathbb{R}^{N_1 \times N_2}} \|X\|_* \quad \text{subject to} \quad \|y - A(X)\|_2 \leq \epsilon.$$  \hspace{1cm} (2.22)

Interestingly, the nuclear norm is a convex functional and therefore (2.22) can be solved efficiently using convex optimization methods (see section 2.5). Note that, as already mentioned in section 2.2, whereas the nonconvex function $\text{rank}(X)$ corresponds to the $\ell_0$ norm of the vector of singular values of $X$, $\|X\|_*$ can be seen as its $\ell_1$ norm. This creates a strong analogy between the $\ell_1$ prior in (2.16), appearing as the convex surrogate for the natural $\ell_0$ minimization, and the nuclear norm of a matrix appearing as a convex alternative to its rank in (2.22).

This formulation is used in the so-called Phase Lift approach [28]. In that framework, quadratic measurements of the form $|\langle x, a_i \rangle|^2$ for given projection vectors $a_i$, are seen as linear measurements on the rank-1 matrix $X = xx^\dagger$ representing the outer product of the signal with itself.

### 2.5 Convex optimization and proximal splitting methods

A real valued function $f(x)$, from $\mathbb{R}^N$ to $\mathbb{R}$, is called convex if

$$f((1 - \beta)x_1 + \beta x_2) \leq (1 - \beta)f(x_1) + \beta f(x_2)$$  \hspace{1cm} (2.23)

for any $x_1, x_2 \in \mathbb{R}^N$ and any $\beta \in [0, 1]$. Optimization problems including convex objective functions and convex constraints, called convex optimization problems, have many attractive properties, in particular the essential property that any local minimum must be a global minimum, which comes directly from the definition of a convex function. Also, convex problems can be efficiently solved, both in theory (i.e., via algorithms with worst-case polynomial complexity) and in practice [29].

Among the broad range of convex optimization methods, proximal splitting methods, exhaustively reviewed in [30], offer great flexibility and are shown to capture and extend several well-known algorithms in a unifying framework. Examples of proximal splitting algorithms include Douglas-Rachford, iterative thresholding, projected Landweber, projected gradient, forward-backward, alternating projections, alternating direction method
Figure 2.4: Projection onto a convex set.

of multipliers and alternating split Bregman [30]. They solve optimization problems of the form

\[
\min_{x \in \mathbb{R}^N} f_1(x) + \ldots + f_K(x),
\]

(2.24)

where \(f_1(x), \ldots, f_K(x)\) are convex lower semicontinuous functions from \(\mathbb{R}^N\) to \(\mathbb{R}\). In the case of convex constrained problems, they can be reformulated as unconstrained problems by using the indicator function of the convex constraint set as one of the functions in (2.24), i.e. \(f_k(x) = i_C(x)\) where \(C\) represents the convex constraint set. The indicator function, defined as \(i_C(x) = 0\) if \(x \in C\) or \(i_C(x) = +\infty\) otherwise, belongs to the class of convex lower semicontinuous functions. Note that complex-valued vectors are treated as real-valued vectors with twice the dimension accounting for real and imaginary parts [31].

Proximal splitting methods proceed by splitting the contribution of the functions \(f_1(x), \ldots, f_K(x)\) individually so as to yield an easily implementable algorithm. They are called proximal because each function in (2.24) is involved by its proximity operator, which can be seen as a generalization of a convex projection operator.

Let \(f\) be a convex lower semicontinuous function from \(\mathbb{R}^N\) to \(\mathbb{R}\), then the proximity operator of \(f\) is defined as:

\[
\text{prox}_f(x) = \arg\min_{z \in \mathbb{R}^N} f(z) + \frac{1}{2}\|x - z\|^2.
\]

(2.25)

In the case of indicator functions of convex sets, the proximity operator is the projection operator onto the set (see figure 2.4):

\[
\mathcal{P}_C(x) = \arg\min_{z \in \mathbb{R}^N} i_C(z) + \frac{1}{2}\|x - z\|^2.
\]

(2.26)

The proximity operator of the \(\ell_1\) norm is well-known as the soft-thresholding operator, or shrinkage:

\[
\text{prox}_{\lambda\|\cdot\|_1}(x) = \max\{|x| - \lambda, 0\} \cdot \text{sign}(x) \triangleq \text{soft}(x, \lambda).
\]

(2.27)

soft\((x, \lambda)\) sends all components \(x_i \leq \lambda\) to zero and shrinks the rest and consequently, it
induces sparsity to $x$. Figure 2.5 shows the soft-thresholding function for one of the components $x_i$ of a vector $x$ and can help the reader to intuitively see how the $\ell_1$ regularization induces sparsity.

Most proximal splitting algorithms reach a solution to (2.24) by alternately applying the proximity operator associated with each function. For example, in the case that all functions in (2.24) are indicator functions, the algorithm reduces to the classical projection onto convex sets algorithm [29], which performs alternate projections to reach the solution. An important feature of proximal splitting methods is that they offer a powerful framework for solving convex problems in terms of speed and scalability of the techniques to very high dimensions. Hereafter two of the most popular proximal splitting methods, the forward-backward algorithm and the Douglas-Rachford algorithm, are described in detail since they are referred to in parts I and II of the manuscript. See [30] for a complete review of proximal splitting methods and their applications in signal and image processing.

### 2.5.1 Forward-Backward algorithm

This algorithm solves optimization problems of the form:

$$\min_{x \in \mathbb{R}^N} f_1(x) + f_2(x),$$

with $f_1$ being a lower semicontinuous convex function from $\mathbb{R}^N$ to $\mathbb{R}$ and such that $\text{dom} f \neq \emptyset$, $f_2 : \mathbb{R}^N \to \mathbb{R}$ being convex with a $\beta$-Lipschitz continuous gradient $\nabla f_2$, i.e.

$$\|\nabla f_2(x) - \nabla f_2(y)\| \leq \beta \|x - y\|, \quad \forall (x, y) \in \mathbb{R}^N \times \mathbb{R}^N, \beta > 0,$$

and assuming that $f_1(x) + f_2(x) \to +\infty$ as $\|x\| \to +\infty$.

Starting from an initial point $x_0 \in \mathbb{R}^N$, for a chosen step-size parameter $\gamma \in (0, \min\{1, 1/\beta\})$ and iterating as follows:
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\[ x_{n+1} = \text{prox}_{\gamma f_1} \left( x_n - \gamma \nabla f_2(x_n) \right), \quad (2.30) \]

A sequence \((x_n)_{n \geq 0}\) is generated that converges to a solution to problem (2.28) [30]. Equation (2.30) summarizes the forward-backward algorithm, that requires one single proximal step at each iteration.

### 2.5.2 Douglas-Rachford algorithm

This algorithm provides solutions for problems of the form (2.28) where the Lipschitz-differenciability condition on \(f_2\) is relaxed. Starting from \(y_0 \in \mathbb{R}^N\) and choosing parameters \(\gamma > 0, \epsilon \in (0, 1)\), the Douglas-Rachford algorithm can be summarized in the following 2-steps proximal scheme:

1. \(x_n = \text{prox}_{\gamma f_2} y_n\)

2. \(y_{n+1} = y_n + \text{prox}_{\gamma f_1}(2x_n - y_n) - x_n\)

The Douglas-Rachford algorithm can be seen as a generalization of the forward-backward algorithm since it does not require the functions involved to be Lipschitz-differenciable. However, it is numerically more complex than the latter since it involves two proximal steps at each iteration.

### 2.6 Conclusion

In this chapter, we have presented an overview on linear inverse problems since the theory of regularization methods is very well studied for them and they can be easily solved using the versatile framework of convex optimization. We have focused on sparse inverse problems, since most of the natural signals are known to be sparse or compressible in a suitable domain. The theory of Compressed Sensing offers a powerful framework for sparse signal recovery. We have reviewed its main results and formulated different convex minimization problems that leverage some kind of sparsity or low dimensionality of the signal. At the reconstruction level, we have given some notions on convex optimization and have revised two popular proximal splitting methods that we will use further in this thesis.

Before concluding, we want to highlight that convex optimization is an extremely adaptable framework that enables to easily include prior information about the signal, such as positivity, as long as it is formulated as a convex constraint. Therefore, different minimization problems, other than the ones described in this chapter, can be straightforwardly defined for the recovery. For example, a TV norm\(^*\) may also be substituted for the

\(^*\)The TV norm of a signal is simply defined as the \(\ell_1\) norm of the magnitude of its gradient
\ell_1 \text{ norm in (2.16) for signals with sparse or compressible gradients. All this flexibility in the definition of the optimization problem is an important manifestation of the versatility of the convex optimization scheme and, as the reader will see, we take advantage of it when designing the novel algorithms that we present in subsequent chapters. In particular, in chapter 3 we propose a generalization of the Phase Lift approach (2.4.3) for tensor recovery. In chapters 5 and 6, we have designed novel reweighting schemes to minimize a weighted \ell_1 \text{ norm (2.4.2) that induces structure on the sparsity of the solution thanks to a specific definition of the weights.}

Part of this chapter was published in [3].
Part I

Optical Interferometry
3.1 Introduction

In interferometry, electromagnetic waves are superposed to retrieve information from their emitting sources that otherwise would not be easily accessible. An astronomical interferometer consists of an array of telescopes that brings together their signals, offering a much higher resolution (approximately equivalent to that of a telescope of diameter equal to the largest separation between its individual elements).

The measurements associated with a given pair of telescopes \((j_1, j_2)\) at one instant of observation \(t\) are known as the complex visibilities, \(V_{j_1,j_2}(t)\). These measurements correspond to the Fourier transform of the image of interest at a spatial frequency \(\nu_{j_1,j_2,m}(t) = \frac{\vec{B}}{\lambda} \equiv (u, v)\), where vector \(\vec{B}\) indicates the projection onto the plane of the sky of the baseline between the pair of telescopes \((j_1, j_2)\) and \(\lambda\) denotes the wavelength. The two-dimensional space of spatial frequencies is commonly known as the \((u, v)\)-plane.

What an interferometer actually measures are the complex visibilities averaged during a finite exposure duration:

\[
\langle V_{j_1,j_2}(t) \rangle_m \approx G_{j_1,j_2,m} \hat{I}(\nu_{j_1,j_2,m}).
\] (3.1)

In (3.1), \(\nu_{j_1,j_2,m}\) denotes to the spatial frequency sampled by the pair of telescopes \((j_1, j_2)\), averaged over the \(m\)th exposure. \(G_{j_1,j_2,m}\) indicates the effective optical transfer function (OTF) and \(\hat{I}(\nu)\) corresponds to the Fourier transform of \(I(\theta)\), the brightness distribution of the observed object under a view angle \(\theta\). The reader can find a visual representation of an optical interferometer and its main associated parameters in figure 3.1.

At radio wavelengths, the OTF is nonnegligible \((G_{j_1,j_2,m} \neq 0)\) and the visibilities in (3.1) are indeed accessible, thereby setting a sparse Fourier inverse problem in the perspective of image recovery. When the OTF can be calibrated, the problem boils down to a deconvolution problem with sparse Fourier data. Several methods have been proposed to solve such an ill-posed problem, for instance, the standard CLEAN algorithm operates by local iterative removal of the convolution kernel associated with the partial Fourier
coverage [33]. Alternatively, convex optimization methods regularizing the inverse problem through sparsity constraints have recently been proposed in the framework of the recent theory of compressive sampling [34, 35, 36, 37, 38, 39, 40].

At optical wavelengths though, atmospheric turbulence induces a random phase delay that drives $G_{j_1,j_2,m} \approx 0$, implying a systematic cancellation of the visibility values. To overcome this challenge current optical interferometers can retrieve power spectrum information:

$$S_{j_1,j_2,m} = \langle |V_{j_1,j_2}(t)|^2 \rangle_m \approx H_{j_1,j_2,m}|\hat{I}(\nu_{j_1,j_2,m})|^2. \quad (3.2)$$

In this case, $H_{j_1,j_2,m}$ becomes a nonzero transfer function that can be easily estimated. Since the power spectrum measurements do not provide any phase information, the bispectrum of the complex visibilities for a triplet of telescopes $(j_1, j_2, j_3)$ can also be measured [32, 41, 42]:

$$B_{j_1,j_2,j_3,m} = \langle V_{j_1,j_2}(t)V_{j_2,j_3}(t)V_{j_3,j_1}(t) \rangle_m \approx J_{j_1,j_2,j_3,m}\hat{I}(\nu_{j_1,j_2,m})\hat{I}(\nu_{j_2,j_3,m})\hat{I}(\nu_{j_3,j_1,m}). \quad (3.3)$$

The transfer function $J_{j_1,j_2,j_3,m}$ in (3.3) can also be easily estimated and, since it takes real values, has no effect on the phase of the bispectrum, the so-called phase closure. Note that the phase closure actually corresponds to the sum of three phases around a closed triangle of baselines and indeed is a very robust measure insensitive to atmosphere-induced phase shifts [43]. However, for any number of telescopes, there are always less independent Fourier phases, among all the possible phase closures that can be measured, than the actual number of phases we would like to determine [43]. These considerations apply both to aperture masking interferometry on a single telescope [44, 45, 46], as well
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As a result, the problem of image recovery in optical interferometry represents a very challenging ill-posed nonlinear Fourier inverse problem with incomplete phase information. The simplified version of this problem, with calibrated and debiased power spectrum and bispectrum measurements, reads as:

\[
S_{j_1,j_2,m} = |\hat{I}(\nu_{j_1,j_2,m})|^2 + S_{j_1,j_2,m}^{err}, \\
B_{j_1,j_2,j_3,m} = \hat{I}(\nu_{j_1,j_2,m})\hat{I}(\nu_{j_2,j_3,m})\hat{I}(\nu_{j_3,j_1,m}) + B_{j_1,j_2,j_3,m}^{err},
\]

(3.4)

where \(S_{j_1,j_2,m}^{err}\) and \(B_{j_1,j_2,j_3,m}^{err}\) correspond to noise terms.

To solve (3.4), the state-of-the-art MiRA method [47] takes a maximum a posteriori (MAP) approach where the image is the solution of an optimization problem with an objective function \(f(x) = f_{data}(x) + \ell f_{prior}(x)\), for some arbitrary parameter \(\ell\) to be tuned, and with additional positivity and total flux constraints. Sparsity priors have in particular been promoted [47, 48]. The data nonlinearity induces nonconvexity of the objective function. The adopted strategy is to perform only local optimization, in the context of which the solution depends not only on the data and on the priors but also strongly on the initial image and on the path followed by the local optimization method. The WISARD alternative [49] takes a two-step alternate minimization self-calibration approach. Firstly, the missing Fourier phases are recovered on the basis of a current estimate and phase closure information enabling to build pseudocomplex visibilities. Secondly, the image is recovered from the pseudocomplex visibilities as in radio interferometry. While the second step is convex and leads to a unique image independently of the initialization, the first step is not. The overall procedure remains nonconvex and the final solution depends on the initial guess. In summary, state-of-the-art methods are nonconvex due to the intrinsic data nonlinearity [32], and therefore known to suffer from a strong sensitivity to initialization.

The approaches proposed in this work stem from a different perspective. We firstly formulate a linear version of the problem for the real and positive supersymmetric rank-1 order-3 tensor \(X = \mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x}\) formed by the tensor product of the size-\(N\) vector \(\mathbf{x}\) representing the image under scrutiny\(^1\) with itself. This allows us to pose a linear convex problem for recovery of a size-\(N^3\) tensor \(X\) with built-in supersymmetry. We regularize the inverse problem through a nuclear norm relaxation of a low-rank constraint, also enforcing reality, positivity and optionally sparsity constraints. We also study a different nonlinear nonconvex approach with built-in rank-1 constraint but where supersymmetry is relaxed, formulating the problem for the tensor product \(\mathbf{u}_1 \circ \mathbf{u}_2 \circ \mathbf{u}_3\) of 3 size-\(N\) vectors. In contrast with the state of the art though, only linear convex minimization subproblems are solved,

\(^{*}\)www.eso.org/sci/facilities/paranal/telescopes/vlti/

\(^{1}\)The image \(\mathbf{x}\) correspond to the vector of coefficients of the brightness distribution in a representation basis. In this work we always represent the image in real space, therefore \(\mathbf{x}\) corresponds directly to the unfolding of \(I\).
alternately and iteratively for the vectors, also enforcing reality and positivity\(^\dagger\). While the former approach is much heavier than the latter in terms of memory requirements and computation complexity due to the drastically increased dimensionality of the unknown, the underlying convexity ensures essential properties of convergence to a global minimum of the objective function and independence to initialization, justifying a comparative analysis.

For numerical experiments, we consider a generic discrete measurement setting where measurements identify with triple products of discrete Fourier coefficients of \(x\). These triple products are selected randomly according to a variable-density scheme sampling more densely low spatial frequencies, and are affected by simple additive Gaussian noise.

The rest of the chapter is organized as follows: In subsection 3.2.1, we introduce our generic discrete data model and describe our new linear tensor formulation of the optical-interferometric imaging problem. In subsections 3.2.2 and 3.2.3, the new AM, NM and NM-RW approaches are discussed. Our simulation setting for comparison of these two methods and corresponding results are presented in section 3.3. Section 3.4 concludes this chapter with a reminder of our contributions as well as a mention to future work.

### 3.2 Materials and Methods

#### 3.2.1 Data model and tensor formulation

For the sake of simplicity, we adopt a discrete setting where the intensity image of interest is represented by the real and positive vector \(x \in \mathbb{R}_+^N\) with components \(x_i\). Its 2D discrete Fourier transform is denoted \(\hat{x} \in \mathbb{C}^N\) with components \(\hat{x}_i\). By abuse of notation, we denote \(\hat{x}_{-i}\) the component of \(\hat{x}\) at the opposite spatial frequency to that associated with \(\hat{x}_i\). Signal reality implies \(\hat{x}_{-i} = \hat{x}_i^*\), where * stands for complex conjugation.

The optical interferometry inverse problem is simplified considering a generic discrete measurement setting where the closure constraint is relaxed and optical-interferometric measurements take the generic form of a triple product of Fourier coefficients of the image: \(\hat{x}_i\hat{x}_j\hat{x}_k\). Power spectrum measurements follow with \(j = -i\), and \(k = 0\) (\(\hat{x}_0\) stands for the Fourier coefficient at zero frequency), and explicit bispectrum measurements would follow from the constraint that the spatial frequencies associated with \(\hat{x}_i\), \(\hat{x}_j\), and \(\hat{x}_k\) sum to zero. In this context, measurements are performed on the frequencies of a discrete grid in the Fourier plane, the so-called frequels. In a real scenario the Fourier transform should be evaluated at (non-equispaced) continuous frequencies [31]. We write the measurement equation in compact form as

\[
y = V(x) + n, \tag{3.5}
\]

where \(V\) is a nonlinear operator providing an undersampled set of triple products of Fourier

\(^\dagger\)We also attempted an alternative nonconvex approach consisting in solving the nonlinear problem directly for \(x\), using the nonconvex projected gradient method proposed by [50]. First simulations did not produce any meaningful reconstruction and this approach was discarded.
coefficients of $\mathbf{x}$. The measurement vector $\mathbf{y} \in \mathbb{C}^M$, with components $y_a$ ($1 \leq a \leq M$) is assumed to be affected by a simple noise vector $\mathbf{n} \in \mathbb{C}^M$ with i.i.d. Gaussian components $n_a$. The number of measurements is typically smaller than the signal dimension: $M < N$. Finally, we assume that the total flux is measured independently and consider a normalized signal such that $\sum_i x_i = \hat{x}_0 = 1$. This flux normalization is approximately enforced by adding the data point $\hat{x}_0^3 = 1$.

In what follows, we show how to bring the linearity of the measurement scheme by lifting the image model from a vector to a tensor formulation. The reader can review some tensor definitions and notations in section 2.2. The measurement model (3.5) can be recast as the following linear model for the real and positive supersymmetric rank-1 order-3 tensor $\mathbf{X} = \mathbf{x} \circ \mathbf{x} \circ \mathbf{x} \in \mathbb{R}^{N \times N \times N}$:

$$\mathbf{y} = \mathcal{T}(\mathbf{X}) + \mathbf{n}, \quad (3.6)$$

where the linear operator $\mathcal{T}$ consists in performing a 2D discrete Fourier transform along each of the 3 dimensions, identified by an operator $\mathcal{F}$, followed by a selection and vectorization operator $\mathcal{M}$ providing variable-density undersampling in this 6D Fourier space: $\mathcal{T} = \mathcal{MF}$. The unit flux measurement is also included in the mask as a measurement on the “triple-zero frequency”. Note that this formulation is a generalization of the Phase Lift approach for the well-known phase retrieval problem [28]. In that framework, quadratic measurements of the form $|\langle \mathbf{x}, \mathbf{a}_i \rangle|^2$ for given projection vectors $\mathbf{a}_i$, are seen as linear measurements on the rank-1 matrix $\mathbf{X} = \mathbf{x} \mathbf{x}^\dagger$ representing the outer product of the signal with itself.

We note however that the rank-1 and supersymmetry properties are not explicitly built-in in the tensor formulation (3.6), which thereby presents a drastically increased dimensionality, $N^3$, of the unknown $\mathbf{X}$ compared to the original $\mathbf{x}$ of size $N$ in (3.5). In the following sections, we discuss our two different regularization schemes for tensor recovery. We firstly study a nonconvex alternate minimization (AM) approach where the rank-1 constraint is built-in, and subsequently move to a convex nuclear minimization (NM) scheme with built-in supersymmetry.

### 3.2.2 Rank-1 alternate minimization (AM)

#### 3.2.2.1 Algorithm formulation

We consider the following explicit rank-1 formulation of (3.6), where supersymmetry is relaxed:

$$\mathbf{y} = \mathcal{T}(\mathbf{u}_1 \circ \mathbf{u}_2 \circ \mathbf{u}_3) + \mathbf{n}. \quad (3.7)$$

The measurements can now be understood as an undersampled set of products of Fourier coefficients of $\mathbf{u}_1$, $\mathbf{u}_2$, and $\mathbf{u}_3$, thus bringing back nonlinearity. We consider the following
nonconvex minimization problem for tensor recovery:

\[
\min_{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3 \in \mathbb{R}_+^N} \| \mathcal{T}(\mathbf{u}_1 \circ \mathbf{u}_2 \circ \mathbf{u}_3) - \mathbf{y} \|_2^2.
\]  \hspace{1cm} (3.8)

A priori this problem seems as nonlinear and nonconvex as the initial problem (3.5). Thanks to the nonsupersymmetric relaxation though, an alternate minimization algorithm can be designed, solving sequentially for each variable ($\mathbf{u}_1$, $\mathbf{u}_2$ or $\mathbf{u}_3$) while keeping the other two fixed, and iterating until convergence. At each iteration, the 3 linear and convex subproblems

\[
\min_{\mathbf{u}_p \in \mathbb{R}_+^N} \| \mathcal{T}_{(\mathbf{u}_q \mathbf{u}_s)} \mathbf{u}_p - \mathbf{y} \|_2^2,
\]  \hspace{1cm} (3.9)

are therefore solved sequentially for $1 \leq p \neq q \neq s \leq 3$, where the linear operators $\mathcal{T}_{(\mathbf{u}_q \mathbf{u}_s)}$ are defined by $\mathcal{T}_{(\mathbf{u}_q \mathbf{u}_s)} \mathbf{u}_p \equiv \mathcal{T}(\mathbf{u}_p \circ \mathbf{u}_q \circ \mathbf{u}_s)$. In each subproblem the linear operator is computed using the values of the fixed variables at the current step. The final AM algorithm is depicted in Algorithm 3. The algorithm is initialized with the same random vector for each of the 3 subproblems. The algorithm is stopped when the relative variation between the objective function in (3.8) evaluated at successive solutions is smaller than some predefined bound or after the maximum number of iterations allowed is reached. At convergence, the tensor solution takes the form of 3 vectors $\mathbf{u}_1$, $\mathbf{u}_2$, and $\mathbf{u}_3$. We have no guarantee that the 3 solution vectors are identical and heuristically choose the final solution to be their mean as shown in step 8 of Algorithm 3\(^5\).

\[\text{Algorithm 1 AM algorithm}\]

1: Initialize $k = 1$, $\mathbf{u}_1^{(0)}$, $\mathbf{u}_2^{(0)}$, $\mathbf{u}_3^{(0)} \in \mathbb{R}_+^N$.  
2: while not converged do  
3: \hspace{0.5cm} $\mathbf{u}_1^{(k)} = \arg \min_{\mathbf{u}_1} \| \mathcal{T}_{(\mathbf{u}_2^{(k-1)} \mathbf{u}_3^{(k-1)})} \mathbf{u}_1 - \mathbf{y} \|_2^2.$ 
4: \hspace{0.5cm} $\mathbf{u}_2^{(k)} = \arg \min_{\mathbf{u}_2} \| \mathcal{T}_{(\mathbf{u}_1^{(k)} \mathbf{u}_3^{(k-1)})} \mathbf{u}_2 - \mathbf{y} \|_2^2.$ 
5: \hspace{0.5cm} $\mathbf{u}_3^{(k)} = \arg \min_{\mathbf{u}_3} \| \mathcal{T}_{(\mathbf{u}_1^{(k)} \mathbf{u}_2^{(k)})} \mathbf{u}_3 - \mathbf{y} \|_2^2.$ 
6: \hspace{0.5cm} $k \leftarrow k + 1$ 
7: end while  
8: $\mathbf{x}_{\text{AM}} = \frac{1}{3}(\mathbf{u}_1^{(k)} + \mathbf{u}_2^{(k)} + \mathbf{u}_3^{(k)})$  
9: return $\mathbf{x}_{\text{AM}}$

\(^5\)Note that [51] prove that this alternate minimization approach converges to a critical point of the objective function (3.8), provided that terms of the form $\gamma \| \mathbf{u}_p - \bar{\mathbf{u}}_p \|_2^2$ controlling the distance between the current unknown $\mathbf{u}_p$ with respect to its value at the previous iteration $\bar{\mathbf{u}}_p$ are added to the objective function in (3.9), for any $\gamma > 0$. Simulations in the context of the setting described in Section 3.3 show that the algorithm converges to the same solution for $\gamma \neq 0$ and $\gamma = 0$. Other simulations also show that starting the minimization of the three variables with the same random initial point leads to very similar solutions for the 3 vectors, or for their mean, both in terms of signal-to-noise ratio and visual quality.
3.2.2.2 Optimization details

To solve each of the subproblems in Algorithm 3 (steps 3–5) we resort to a forward-backward (projected gradient) algorithm [30]. The forward-backward algorithm solves (3.9) using a two-step procedure: a gradient descent step (forward step) to minimize the quadratic function in (3.9), and a projection step (backward step) to bring back the current update to the constraint set. The algorithm uses the following recursion:

$$u_p^{(t+1)} = \text{prox}_{iC} \left( u_p^{(t)} + \mu_p^{(t)} T(u_q u_s) \left( y - T(u_q u_s) u_p^{(t)} \right) \right),$$

(3.10)

where $t$ denotes the iteration variable, $C = \mathbb{R}_+^N$ and $\mu_p^{(t)}$ is a variable step size that controls the gradient descent update. The step size is adapted using a backtracking line-search procedure [52]. The proximity operator $\text{prox}_{iC}$ is nothing but the projector onto the positive orthant $\mathbb{R}_+^N$, i.e., setting the imaginary part and the negative values of the real part to zero [29].

The memory requirement to solve this minimization problem is dominated by the storage of the 3 vectors, which is of size $O(N)$. In terms of computation time, the algorithm is dominated at each iteration by the application of the operator $T$ which computes 3 2D FFTs of size $N$, with an asymptotic complexity of order $O(N \log N)$. This approach is computationally efficient. In contrast with the state-of-the-art approaches such as MiRA and WISARD, it brings convexity to the subproblems. But the global problem remains nonconvex and the solution may still depend on the initialization. One can easily identify convergence to a local minimum through large residual values of the objective function. With the aim to mitigate the dependence to initialization, and as suggested by [53], we propose to run the algorithm $n_{ri}$ times with random initializations, choosing a posteriori the solution with minimum objective function value.

3.2.3 Supersymmetric nuclear minimization (NM)

3.2.3.1 Algorithm formulation

Tensor supersymmetry can be embedded in various ways. One approach is to formulate the inverse problem (3.6) only for the subset of variables $X_{ijk}$ with $i \leq j \leq k$. The collection of these values define the “subtensor” $X_s$, which can be related to $X$ by an operator $R$ replicating tensor components over all permutations for each triplet $(i,j,k)$: $X = R(X_s)$. The inverse problem would thus read $y = [T R](X_s) + n$. We adopt an alternative and equivalent approach consisting in substituting the original measurement vector $y$ by its replicated version $R(y)$, and using a symmetrized version $M_s$ of the selection mask, ensuring that all permutations of a triplet $(i,j,k)$ are assumed to be measured. We will see below why a symmetrized data vector together with a symmetrized measurement operator represent a sufficient condition to impose the tensor symmetry at each step of the algorithm in our approach, and in particular supersymmetry of the solution. The modified
inverse problem thus reads as:
\[ y_s = T_s(X) + n_s, \]  
(3.11)

with \( y_s = \mathcal{R}(y), \ n_s = \mathcal{R}(n) \) and \( T_s = M_s T \) denoting the symmetrized versions of the measurement vector, noise vector and measurement operator, respectively. Without loss of generality, we assume that the initial selection operator \( M \) contains no redundant measurements, i.e. \( i \leq j \leq k \). This ensures that \( \mathcal{R} \) is well-defined. Also note that the noise statistics remains unaltered and only concerns the entries before replication.

Low-rankness, reality and positivity will be imposed as regularization priors in the convex minimization problem to be defined. As pointed out, the rank of a tensor is difficult to handle since the problem of finding rank(\( X \)) is NP-hard. Computing the rank of different matricization of the tensor is an easier task. The unfoldings of a rank-1 tensor are actually rank-1 matrices, so that a low \( n \)-rank constraint can be used as a proxy for low-rankness. The rank of a matrix is however a nonconvex function. The nuclear norm, defined as the \( \ell_1 \)-norm of its singular values, is a well-known convex relaxation of the rank function that was recently promoted in matrix recovery theory [25]. Building on those results, [54] tackle the low-\( n \)-rank tensor recovery problem through the minimization of the sum of the nuclear norms of the mode-\( n \) matricizations \( X_{(n)} \) for all \( n \). In the supersymmetric case, the mode-\( n \) matricizations are all identical and denoted \( X_{(n)} = U(X) \in \mathbb{C}^{N \times N \times N} \), where \( U \) stands for the unfolding operator. We propose here to exploit the symmetry of the tensor under scrutiny, together with the signal normalization, to promote a computationally more efficient low-rank prior. Relying on these properties, we note that summations over one index of a tensor of the form \( x \circ x \circ x \) with \( \sum_i x_i = 1 \) leads to the order-2 tensor \( x \circ x \), which is real, positive, symmetric, as well as rank-1 and positive-semidefinite. We define \( C \) as the operator performing the summation over one dimension. Once more supersymmetry ensures that the resulting matrix is independent of the choice of the dimension along which components are summed up: \( C(X) \in \mathbb{C}^{N \times N} \) with \( [C(X)]_{ij} = \sum_k X_{ijk} \). A low-rank constraint on \( C(X) \) will be promoted, through a nuclear norm minimization, as a convex proxy for the low-rankness of \( X \). Positive-semidefiniteness of \( C(X) \), i.e. positivity of the eigenvalues, which are then identical to the singular values, may also be explicitly added as a convex prior, denoted \( C(X) \succeq 0 \), together with the convex reality and positivity constraints of \( X \): \( X \in \mathbb{R}_+^{N \times N \times N} \). This summation approach is a priori computationally significantly more efficient given the reduced matrix size of \( C(X) \) compared to that of the unfolded matrix \( U(X) \).

The resulting convex nuclear norm minimization problem (NM) for \( X \) thus reads as:
\[
\min_{X} \|C(X)\|_* \quad \text{subject to} \quad \|y_s - T_s(X)\|_2 \leq \epsilon,
\]
(3.12)

where \( S = S_1 \cap S_2 \), with \( S_1 = \mathbb{R}_+^{N \times N \times N} \) and \( S_2 = \{ X \mid C(X) \succeq 0 \} \). Recalling that the measurements \( y \) are assumed to be corrupted with simple i.i.d. complex Gaussian noise with
3.2. Materials and Methods

variance \( \sigma_n^2 \) on real and imaginary parts, the residual estimator \( \| y - T(x) \|^2 \) follows a \( \chi^2 \) distribution with \( 2M \) degrees of freedom, with expectation \( 2M \) and standard deviation is \( (4M)^{1/2} \). For a large number of degrees of freedom the distribution is extremely peaked around its expectation value. This fact is related to the well-known phenomenon of the concentration of measure [38]. The value \( \chi_0^2 = (2M + 4\sqrt{M})\sigma_n^2/2 \), i.e. 2 standard deviations above the expectation, represents a high percentile of the distribution (in practice extremely close to \( 2M \)), and consequently a likely bound for \( \| n \|^2_2 \). An equivalent bound for the symmetrized residual noise term \( \| y_s - T_s(x) \|^2 \) may simply be inferred as \( \varepsilon^2 \simeq \alpha \chi_0^2 \), where \( \alpha \) is simply the ratio of number of components in \( y_s \) and \( y \). We take the value \( \alpha = 6 \) as the relative number of \((i, j, k)\) triplets with repeated indices in the mask is very small. Note that this last consideration only arises from the discrete setting adopted.

Once the tensor solution \( X_{NM} \) is recovered, the problem of extracting the sought signal \( x_{NM} \) remains. If the tensor solution was actually a real positive rank-1 supersymmetric tensor whose elements sum up to unity, the retrieval of \( x_{NM} \) could be done in different ways, such as directly extracting the first eigenvector of matrix \( \mathcal{E}(X_{NM}) \) or simply performing a sum over two dimensions \( \sum_{jk} [X_{NM}]_{ijk} \). The nuclear norm minimization approach however does not guarantee that the final solution is indeed rank-1. We therefore resort to the generic algorithm proposed in [55] to find the best rank-1 supersymmetric approximation \( \mathcal{P}_1(X_{NM}) \) of a supersymmetric tensor \( X_{NM} \) in the least square sense. This algorithm is a generalization for the tensor case of the power method applied to find the dominant eigenvector of matrices [56]. It boils down to determining a unitary vector \( x \) and a scalar \( \lambda \), such that \( \| X - \lambda x \circ x \circ x \| \) is minimized, where \( \| \cdot \| \) indicates simply the sum of the square of the components of the tensor. We denote the resulting solution as

\[
x_{NM} = [\mathcal{E}\mathcal{P}_1](X_{NM}), \tag{3.13}
\]

where \( \mathcal{E} \) formally represents the operator retrieving from a supersymmetric rank-1 order-3 tensor its underpinning vector. Note that this vector extraction problem is not convex.

The final NM algorithm is shown in Algorithm 2. To solve the complex optimization problem in (3.12) we use the Douglas-Rachford splitting algorithm, which is tailored to solve problems of the form in (2.24) with \( K = 2 \). The problem in (3.12) can be reformulated as in (2.24) by setting \( f_1(x) = \| \mathcal{E}(x) \|_* + i_{S}(x) \) and \( f_2(x) = i_{C_{\varepsilon}}(x) \), where \( C_{\varepsilon} = \{ x \in \mathbb{C}^{N \times N \times N} : \| y_s - T_s(x) \|_2 \leq \varepsilon \} \). The main recursion of the Douglas-Rachford algorithm is detailed in steps 3-4 of Algorithm 2, where \( \nu > 0 \) and \( \tau_k \in (0,2) \) are convergence parameters. The sequence \( \{ X^{(k)} \} \) generated by the recursion in Algorithm 2 converges to a solution of the problem (3.12) [30]. The algorithm is stopped when the relative variation between successive solutions, \( \| X^{(k)} - X^{(k-1)} \| / \| X^{(k-1)} \| \), is smaller than some

\*Note that in [55] a proof of convergence of their algorithm only for even-order tensors is provident. Simulations in the context of the setting described in Section 3.3 show that the this procedure systematically converges for our order-3 tensors, and provides significantly better results than a heuristic procedure based on extracting the first eigenvector of \( \mathcal{E}(X_{NM}) \) or performing a sum over two dimensions \( \sum_{jk} [X_{NM}]_{ijk} \).
bound $\xi \in (0, 1)$, or after the maximum number of iterations allowed, $T_{\text{max}}$, is reached. In our implementation we use the values $\tau_t = 1$, $\forall t$, $\xi = 10^{-3}$ and $\nu = 10^{-1}$. In the following subsection we detail the computation of the proximity operators for $f_1$ and $f_2$.

**Algorithm 2** NM algorithm

1: Initialize $k = 1$, $\mathcal{X}^{(1)} \in \mathbb{R}^{N \times N \times N}$, $\tau_k \in (0, 2)$ and $\nu > 0$.
2: while not converged do
3:     $\mathcal{Z}^{(k)} = \text{prox}_{\nu f_2} (\mathcal{X}^{(k)})$.
4:     $\mathcal{X}^{(k+1)} = \mathcal{X}^{(k)} + \tau_k \left( \text{prox}_{\nu f_1} \left( 2\mathcal{Z}^{(k)} - \mathcal{X}^{(k)} \right) - \mathcal{Z}^{(k)} \right)$.
5:     $k \leftarrow k + 1$
6: end while
7: $x_{\text{NM}} = [\mathcal{E} \mathcal{P}_1](\mathcal{X}^{(k)})$.
8: return $x_{\text{NM}}$

### 3.2.3.2 Optimization details

The computation of the proximal operator of $f_1$, which includes the nuclear norm prior, as well as the positive-semidefiniteness, reality and positivity constraints, is itself a complicated optimization problem. Therefore the dual forward-backward algorithm [30] is used at each iteration of the Douglas-Rachford recursion to compute the proximal operator of $f_1$. We can decompose $f_1$ as $f_1(\mathcal{X}) = g_1(\mathcal{X}) + g_2(\mathcal{X})$, where $g_1(\mathcal{X}) = \|\mathcal{C}(\mathcal{X})\|_* + iS_1(\mathcal{X})$ and $g_2(\mathcal{X}) = iS_2(\mathcal{X})$. Let $Q^{(0)} \in \mathbb{C}^{N \times N}$ and $S^{(0)} \in \mathbb{C}^{N \times N \times N}$ be the all zero matrix and the all zero tensor respectively. The dual forward-backward algorithm uses the following recursion to compute $\text{prox}_{\nu f_1}(\mathcal{X})$:

\[
Q^{(t+1)} = (I - \text{prox}_{\nu g_1}) \left( Q^{(t)} + \gamma_t \mathcal{E}(S^{(t)}) \right)
\]

\[
S^{(t+1)} = \text{prox}_{\nu g_2} \left( \mathcal{X} - \mathcal{C}^*(Q^{(t+1)}) \right),
\]

where $I \in \mathbb{R}^{N \times N}$ is the identity operator and $\gamma_t \in (0, 2)$ is a step size. The sequence \{$S^{(t)}$\} converges linearly to $\text{prox}_{\nu f_1}(\mathcal{X})$.

The computation of $\text{prox}_{\nu g_1}$ and $\text{prox}_{\nu g_2}$ are very simple operations. We start by computing $\text{prox}_{\nu g_1}$. Let $Q \in \mathbb{C}^{N \times N}$ be a symmetric matrix and suppose it has an eigenvalue decomposition $U \Lambda U^\dagger$, where $U$ is the orthogonal matrix of eigenvectors and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_N)$ is the diagonal matrix with the eigenvalues. Then, the proximity operator of $\nu g_1$ is computed as:

\[
\text{prox}_{\nu g_1}(Q) = U \tilde{\Lambda}_{\nu} U^\dagger,
\]

where $\tilde{\Lambda}_{\nu} = \text{diag}((\lambda_1 - \nu)^+, \ldots, (\lambda_N - \nu)^+)$ and $(a)^+ = \max(0, a)$ denotes the positive part of $a$. The operator $\tilde{\Lambda}_{\nu}$ performs a soft thresholding on the eigenvalues of $Q$, to minimize
the nuclear norm, and also preserves only the positive eigenvalues, to project onto the set of positive-semidefinite matrices [57, 58]. The proximal operator of $\nu g_2$ is the projector onto the set of positive tensors in $\mathbb{R}^{N \times N \times N}$ which is computed by setting the imaginary part and the negative values of the real part of the input tensor to zero, i.e.

$$\text{prox}_{\nu g_2} (S) = \{ (\text{Re}(S_{i,j,k}))^+ \}_{1 \leq i,j,k \leq N},$$

(3.16)

where $\text{Re} (\cdot)$ denotes the real part of a complex number [29].

The proximal operator of $f_2$ is the projector operator onto the set $C_\epsilon$, which is computed as:

$$\text{prox}_{\nu f_2} (X) = X + T_s^\dagger (\mathcal{P}_\epsilon (T_s(X) - y_s) - T_s(X) + y_s),$$

(3.17)

where $\mathcal{P}_\epsilon (r) = \min (1, \epsilon/\|r\|_2) r$. All the operations done in the computation of the proximal operators of $f_1$ and $f_2$ preserve tensor symmetry, provided that the symmetrized version $T_s$ of the measurement operator and a symmetrized data vector are used. These two are sufficient conditions to impose supersymmetry at each iteration of Algorithm 2, and consequently for the final tensor solution.

The memory requirement to solve this NM problem is dominated by the storage of the tensor, which is of size $O(N^3)$. In terms of computation time, the algorithm is dominated at each iteration by the application of the operator $T_s$ which computes $N^2$ 2D FFTs of size $N$ along each of the three dimensions, with an asymptotic complexity of $O(N^3 \log N)$. These orders of magnitude obviously stand in stark contrast with those for the AM approach.

While the NM approach is much heavier than the AM approach in terms of memory requirements and computation complexity due to the drastically increased dimensionality of the unknown, the underlying convexity at the tensor level ensures essential properties of convergence to a global minimum of the objective function and independence to initialization, justifying a comparative analysis.

### 3.2.3.3 Nuclear minimization with sparsity

Following the lines of recent evolutions in radio interferometry [34, 35, 38] and in optical interferometry [32, 48], we decided to study the inclusion of a sparsity prior for the NM approach. As a first proof of concept we have chosen to promote the simplest sparsity – in image space – of the signal $x$ of interest, as this can be done simply through adopting a sparsity prior directly on the full tensor $X$. While $\ell_0$-minimization would promote sparsity explicitly, we adopt the common convex relaxation relying on the $\ell_1$ norm. Note that a nonweighted $\ell_1$ norm is not a meaningful prior function as the tensor values are positive and sum up to unity. In that scenario, we resort to a reweighting scheme consisting in approaching both $\ell_0$-minimization on $X$ and rank minimization on $\mathcal{C}(X)$ by solving a
sequence of weighted $\ell_1$ and nuclear norm minimization [24, 59], each of which is initialized with the solution of the previous problem (see sections 2.4.2 and 2.4.3).

The weighted-$\ell_1$ and nuclear-norm minimization problem (NM-RW) thus reads as:

$$\min_{X \in S} \|C(X)\|_{s,w} + \lambda \|X\|_{1,w} \quad \text{s. t.} \quad \|y_s - T_s(X)\|_2 \leq \epsilon,$$

where $S$ denotes the same set as in (3.12) and $\|\cdot\|_{s,w}$ and $\|\cdot\|_{1,w}$ denote weighted nuclear and $\ell_1$ norms respectively. Notice that the weights for the nuclear and the $\ell_1$ norm are defined in a different form. In both weighted norms, each element of the vector to be reweighted should essentially be divided by its absolute value in the previous iteration. A stabilization parameter, $\delta$, is necessary to define the weights properly, even when the signal value is zero. In the weighted $\ell_1$ norm, each weight is defined as $w_{ijk} = \delta(t) / (\delta(t) + \lambda^{(t-1)}_{ijk})$, where $t$ indicates the iteration of the reweighting process. $\lambda$ is set to zero at the first iteration to avoid the use of a nonweighted $\ell_1$ norm as a prior, as previously mentioned.

In the following iterations, we heuristically set $\lambda(t) = \alpha \|X^{(t-1)}\|_\infty$, where $\|\cdot\|_\infty$ denotes the maximum absolute value of the tensor and $0 < \alpha < 1$ is a parameter to be tuned. In order to approximate the rank function through the weighted nuclear norm — i.e. the weighted $\ell_1$ norm of the singular values $\sigma_i, i \in \mathbb{R}_+^N$ —, each weight is computed as the inverse of the singular value of $C(X)$ at the previous iteration, $w_i = \delta(t) / (\delta(t) + \sigma_{i(t-1)}^{(t-1)})$.

The reweighting process stops when the relative variation between successive solutions $\|X^{(t)} - X^{(t-1)}\|_2 / \|X^{(t-1)}\|_2$ is smaller than some bound or after the maximum number of iterations allowed is reached. Finally, the signal is extracted from the tensor using the rank-$1$ approximation algorithm [55], as mentioned in Section 3.2.3.1.

### 3.3 Simulations and results

In this section we evaluate the performance of the AM, NM and NM-RW algorithms through numerical simulations. Our optimization code\footnote{Code and test data are available at \url{https://github.com/basp-group/co-oi}.} was implemented in MATLAB and run on a standard 2.4 GHz Intel Xeon processor. Given the expected large memory requirements and long reconstructions time for the NM formulation, we consider small-size images with $N = 16^2 = 256$ for which the image vector occupies the order of 4 KB in double precision, while the size-$N^3$ tensor variable already takes the order of 100 MB. The memory requirement for the simple tensor variable would already rise to the order of 8 GB for a $32^2 = 1024$ image size.

For what the measurement setting is concerned, we assume random variable-density sampling in the 6D Fourier space, where low spatial frequencies are more likely to be sampled than high frequencies. In practice the sampling pattern is obtained by sampling frequencies independently along each of the 3 tensor dimensions from a bidimensional random Gaussian profile in the corresponding Fourier plane, associating the originally continuous
3.3. Simulations and results

Figure 3.2: Example of variable-density sampling pattern in the discrete 6D Fourier space of $X$ of dimension $N^3$, for a $N = 16^2$ image size and an undersampling regime of $M/N = 0.75$.

random points with the nearest discrete frequency. The sampling is carried out progressively, noting that if a product is sampled twice the result is discarded and repeating this procedure until $M$ samples are obtained. Again this consideration only arises from the discrete setting adopted. Figure 3.2 presents a typical sampling pattern.

In all experiments we define the input signal-to-noise ratio as $\text{ISNR} = -10 \log(\sigma_n^2/e_y^2)$ where $e_y^2 = (1/M) \sum_a |y_a|^2$. The signal-to-noise ratio of a reconstruction $\bar{x}$ is defined as $\text{SNR} = -10 \log(\|\bar{x} - x\|^2/\|x\|^2)$. With this definition, the higher the SNR, the closer the recovered signal $\bar{x}$ is from the original $x$.

3.3.1 AM vs NM comparison

As a preliminary experiment, we provide a comparison of the performance of the NM approach defined in (3.12), with the equivalent minimization problem where the summation operator $\mathcal{C}$ is replaced by the unfolding operator $\mathcal{U}$ in the nuclear norm and where the positive-semidefiniteness constraint is discarded as it does not apply for non-square matrices. Both algorithms were tested on images constructed from 32 random spikes, with ISNR = 30dB. The positive spike values are taken uniformly at random and normalized to get unit flux, while positions are drawn at random from a Gaussian profile centered on the image. The graphs in Figure 3.3 represent the SNR and timing curves as a function of undersampling in the range $[0.25, 1]$. A total of 10 simulations per point are performed, varying the signal, as well as the sampling and noise realizations. Both approaches provide similar reconstruction qualities, with a smaller variability of the component summation approach, which is also slightly superior at low undersamplings. The component summation approach, running in the order of $10^3$ seconds, is as expected significantly faster than the unfolding approach, running on average more than 10 times more slowly in the range $[0.5, 1]$. We therefore discard further consideration of the latter.

Having validated our NM approach in comparison with alternative state-of-the-art low tensor rank approaches, we compare its performance with that of the AM scheme. Firstly, we evaluate the reconstruction quality on images constructed from 32 and 64 randomly located spikes. The AM approach is also evaluated for varying reinitialization numbers: $n_{ri} \in \{1, 5, 10\}$. The graphs in Figure 3.4 represent the SNR curves as a function of undersampling in the range $[0.25, 1]$. A total of 50 and 10 simulations per point are performed for AM and NM respectively, varying the signal, as well as the sampling and
Chapter 3. Tensor optimization for optical-interferometric imaging

Figure 3.3: Reconstruction quality and timing comparison between the NM approach defined in (3.12), with the equivalent minimization problem where the summation operator $\mathcal{C}$ is replaced by the unfolding operator $\mathcal{U}$. Tests done on $N = 16^2$ images with 32 randomly located spikes and ISNR = 30dB, for undersampling ratios $M/N$ in the range $[0.25, 1]$. The SNR curves (left panel) represent average values over 10 simulations and corresponding 1-standard-deviation error bars. The timing curves (right panel) represent average values over 10 simulations and min-max error bars.

Figure 3.4: Reconstruction quality results for synthetic images of size $N = 16^2$ with randomly distributed spikes and ISNR = 30dB for undersampling ratios $M/N$ in the range $[0.25, 1]$. Left panel: 64 spikes. Right panel: 32 spikes. The curves represent the average SNR values over multiple simulations (50 for AM and 10 for NM) and corresponding 1-standard-deviation error bars.

noise realizations. The results show a clear superiority of AM relative to NM in terms of average reconstruction quality. Both approaches exhibit nonnegligible variability. The dependency of the nonconvex AM approach to initialization is clearly illustrated by the $n_{ri} = 1$ and $n_{ri} = 5$ curves, confirming the importance of the multiple reinitializations. We also observe a saturation between $n_{ri} = 5$ and $n_{ri} = 10$. As expected from asymptotic complexity considerations, AM runs significantly faster than NM, with reconstructions in the order of $10^2$ seconds for $n_{ri} = 5$, approximately 10 times faster than NM.

Secondly, simulations are performed in an identical setting on realistic images representing low-resolution versions of the Eta Carinae star system, of a simulated rapidly rotating star, and of the M51 Galaxy∗∗. The multiple simulations per point are performed by varying the sampling and noise realizations. The graphs in Figures 3.5, 3.6, and 3.7 present the SNR curves as a function of undersampling in the range $[0.25, 1]$ (AM only reported for $n_{ri} = 5$), confirming the previous results on random images. Reconstructed

∗∗Images from [48], downloaded from the JMMC service at apps.jmmc.fr/oidata/shared/srenard/.
images are also reported, providing visual confirmation of the superiority of AM relative to
NM over the full undersampling range. In both approaches, the visual quality difference
between the reconstructions with, respectively, best and median SNR values illustrates
the variability of the reconstruction quality. The NM approach suffers from a significantly
larger visual degradation of median SNR value at $M = 0.25N$ than AM. This degradation
appears at larger sampling ratios for M51.

Let us highlight that, while only 5 reinitializations are necessary in the AM approach
in low dimension to reach saturation, additional experimental tests on random signals of
size $N = 64^2$ show that $n_{ri} = 20$ or larger is necessary for a meaningful reconstruction,
thereby emphasizing the convergence problem due to nonconvexity in higher dimension.
Also, computation time scales linearly with $n_{ri}$ and can rapidly blow up in this context.

3.3.2 NM vs NM-RW comparison

To compare the performance of the linear NM-RW and NM approaches, we first evalu-
ate the reconstruction quality on sparse images made of 8 and 16 randomly located spikes.
The SNR curves in Figure 3.8 are built from 10 simulations per point, varying the signal,
the sampling and noise realizations. The results show a clear improvement on the SNR
when accounting for sparsity. In Figure 3.9, the effect of the reweighting scheme can be ap-
preciated on an illustration representing a sparsified version of Galaxy M51**. Reweighted
images (second row) are less blurred and their support is clearly better defined.

3.4 Conclusion

We have proposed a novel linear formulation of the optical-interferometric imaging
problem in terms of the supersymmetric rank-1 order-3 tensor formed by the tensor prod-
uct of the vector representing the image sought with itself. In this context, we proposed a
linear convex approach for tensor recovery with built-in supersymmetry, and regularizing
the inverse problem through nuclear norm minimization. We have also studied a non-
linear nonconvex alternate minimization approach where supersymmetry is relaxed while
the rank-1 constraint is built-in. While the former approach is associated with drastically
increased dimensionality of the unknown, the underlying convexity ensures essential prop-
erties of convergence to a global minimum of the objective function and independence
to initialization, justifying its analysis. Simulation results in low dimension show that
the AM scheme provides significantly superior imaging quality than the NM approach,
in addition to be much lighter in its memory requirements and computation complexity.
Another set of results in higher dimension however suggests that the number of necessary
reinitializations for the nonconvex AM scheme rapidly increases with $N$. This state of
things clearly calls for further considerations of a purely convex approach. As a first step
in this direction, we have studied the inclusion of a sparsity prior in the convex formulation.
Figure 3.5: Eta Carinae star system illustration ($N = 16^2$, ISNR = 30dB). Top row: original image and SNR graph. The curves represent the average SNR values over multiple simulations (50 for AM and 10 for NM) and corresponding 1-standard-deviation error bars. Second and third rows: NM (second) and AM for $n_{ri} = 5$ (third) reconstructions with best SNR for $M = N$ (left), $M = 0.75N$ (center) and $M = 0.25N$ (right). Fourth and bottom rows: NM (fourth) and AM for $n_{ri} = 5$ (bottom) reconstructions with median SNR for $M = N$ (left), $M = 0.75N$ (center) and $M = 0.25N$ (right).
Figure 3.6: Rapidly rotating star illustration \((N = 16^2, \text{ISNR} = 30\text{dB})\). Top row: original image and SNR graph. The curves represent the average SNR values over multiple simulations (50 for AM and 10 for NM) and corresponding 1-standard-deviation error bars. Second and third rows: NM (second) and AM for \(n_{ri} = 5\) (third) reconstructions with best SNR for \(M = N\) (left), \(M = 0.75N\) (center) and \(M = 0.25N\) (right). Fourth and bottom rows: NM (fourth) and AM for \(n_{ri} = 5\) (bottom) reconstructions with median SNR for \(M = N\) (left), \(M = 0.75N\) (center) and \(M = 0.25N\) (right).
Figure 3.7: M51 Galaxy illustration ($N = 16^2$, ISNR = 30dB). Top row: original image and SNR graph. The curves represent the average SNR values over multiple simulations (50 for AM and 10 for NM) and corresponding 1-standard-deviation error bars. Second and third rows: NM (second) and AM for $n_{ri} = 5$ (third) reconstructions with best SNR for $M = N$ (left), $M = 0.75N$ (center) and $M = 0.25N$ (right). Fourth and bottom rows: NM (fourth) and AM for $n_{ri} = 5$ (bottom) reconstructions with median SNR for $M = N$ (left), $M = 0.75N$ (center) and $M = 0.25N$ (right).
3.4. Conclusion

Figure 3.8: Reconstruction quality results for synthetic images of size $N = 16^2$ with randomly distributed spikes and ISNR $= 30\text{dB}$ for undersampling ratios $M/N$ in the range $[0.25, 1]$. Left panel: 8 spikes. Right panel: 16 spikes. The curves represent the average SNR values over 10 simulations and corresponding 1-standard-deviation error bars.

Figure 3.9: Sparsified version of M51 Galaxy illustration ($N = 16^2$, ISNR $= 30\text{dB}$). Top row: original image and SNR graph. The curves represent the average SNR values over 10 simulations and corresponding 1-standard-deviation error bars. Second and third rows: NM (second) and NM-RW (bottom) reconstructions with best SNR for $M = N$ (left), $M = 0.75N$ (center) and $M = 0.25N$ (right).

and, in that setting, numerical simulations confirm a clear improvement in the quality of the reconstruction of sparse images. We point out though, that in the present investigations only the simplest case of sparsity – sparsity in image space – has been considered, as a proof of concept. Future work should investigate the effects of assuming different kinds
of sparsity priors, as suggested in recent approaches for radio interferometry [60].

Our approaches should also be studied in a more realistic setting with exact power
spectrum and bispectrum measurements in the continuous domain and for different noise
statistics, and explicitly compared to existing MiRA and WISARD implementations. The
linear approaches NM and NM-RW are extremely exacting from a computational stand-
point so that software and hardware optimization should also be studied to solve the
problem for higher dimension images, e.g. using graphics processing units [61]. Recent
results studying the uniqueness of the solution of the phase retrieval problem for sparse sig-
nals are presented in [62]. Further research should also analyze our results and formulation
in full view of this new theoretical framework.

The work presented in this chapter has been published in [3, 4]. We highlight that in
[63], the authors enhance the present work by further study of the AM approach. They
propose an algorithm that accounts for sparsity and presents convergence guarantees,
missing in our original formulation. Numerical simulations in [63] show that the inclusion
of a sparsity prior improves significantly the quality of their reconstructions, analogously
to what we observe for the NM approach. Furthermore, they successfully extend the
current model to hyperspectral imaging and demonstrate the superiority of their global
approach compared to single-channel reconstruction.
Part II

Diffusion Magnetic Resonance Imaging
Chapter 4

Background on diffusion MRI

4.1 Introduction

Diffusion Magnetic Resonance Imaging (dMRI) is sensitive to the Brownian motion of water molecules, i.e. its random displacement in a fluid due to thermal energy. This erratic movement is described in statistical terms by a displacement distribution indicating the proportion of molecules that have been displaced a specific distance in a specific direction. Typically, the displacement distribution for free water is a Gaussian function. However, in organs with ordered structures, such as the brain, water does not diffuse equally in all directions [64]. This phenomenon, known as anisotropic diffusion, is exploited to study the structure of spatial order in living organs in a non-invasive way.

This chapter aims to familiarize the reader with the principles of dMRI applied to brain imaging and it does not contain any original contribution. The chapter is organized as follows: Section 4.2 explains the principles behind this imaging modality and how the diffusion process is characterized. Section 4.3 describes how and why dMRI can be used in brain imaging to recover the properties of its fiber bundles (i.e. axon tracts), from both neuroscientific and clinical perspectives. Sections 4.4 and 4.5 review the main state-of-the-art methods for fiber reconstruction (orientation and microstructure recovery, respectively). The take-home messages of this chapter are summarized in Section 4.6.

4.2 Principles of diffusion Magnetic Resonance Imaging

Thanks to Stejskal and Tanner’s experiments and proofs [65], a methodology was defined to measure diffusion with MRI. They introduced the Pulse Gradient Spin Echo (PGSE) sequence that makes MR imaging sequences sensitive to diffusion by inserting two additional magnetic field gradient pulses subsequently besides the standard ones used for spatial encoding. This protocol allows a clear distinction between the encoding time $\delta$ (pulse duration) and the diffusion time $\Delta$ (time between the two gradient pulses). After applying the first gradient, protons’ phase changes along the direction of the gradient. When then, a second gradient of opposite magnitude (with the same direction and time period) is applied, the phase-shift induced by the first gradient can be reversed. If the
protons moved in between the application of the gradients the net phase accumulation cannot be exactly zero. As a result, in each voxel, we get a distribution of phase-shifts which results in a loss of coherence and therefore to a decrease of the signal amplitude (Figure 4.1). The wider the spread of displacements, the larger the signal damping. Thus, by applying a pair of gradient pulses before the data acquisition we make the resultant image sensitive to motional processes, such as diffusion.

![Diagram of a PGSE sequence and visual understanding of signal loss due to the dephasing of spins.](image)

**Figure 4.1:** Diagram of a PGSE sequence and visual understanding of signal loss due to the dephasing of spins. *Part of the illustration is taken from [66]. Image used with permission.*

Each diffusion gradient is represented as a 3D vector $q$, oriented in its direction and with a magnitude $q$ proportional to its strength. The new 3D-space determined by the coordinates of $q$ is commonly named after $q$-space. The $b$-value, most commonly used when characterizing the gradient, is proportional to the product of the square of the gradient strength $q$ and the diffusion time interval ($b \propto q^2 \cdot \Delta$). A single application of the PGSE sequence produces one brain image with a given diffusion weighting that corresponds to one point of the $q$-space. The resulting has already some diffusion information: where the main diffusion direction is aligned with the applied diffusion gradient, the intensity of the signal is markedly decreased, and the region therefore appears darker on the image (see figure 4.4 A). This is the principle behind the simplest diffusion imaging technique, known as Diffusion Weighted Imaging (DWI). Multiple repetitions of the sequence, each with a different diffusion weighting, are necessary if we want to characterize the entire diffusion process.

The diffusion process is represented by a 3D probability density function (pdf) of diffusion displacements at every point, i.e. for each voxel. This function $p(r) \in \mathbb{R}^3$ is known as the Ensemble Average Propagator (EAP) for every $r$ coordinate vector in real
space and it relates to the diffusion signal $S(q)$ through a 3D Fourier transform [67], as follows:

$$ \text{EAP} \equiv p(r) = \int_{\mathbb{R}^3} dq S(q) e^{-2\pi i q \cdot r}. \quad (4.1) $$

Equation (4.1) defines a relationship between the propagator (or real) space, with coordinates $r$, and the signal (or Fourier) space, the $q$-space, through a Fourier transform.

### 4.3 dMRI in the brain

dMRI can provide very useful information about the organization of the tissue in the brain. In fact, the grey matter (GM) does not have an ordered fiber structure. Therefore, GM and the cerebrospinal fluid (CSF), that can be found in the ventricles, are typically isotropic media. However, high anisotropy can be observed in the white matter (WM), made of axons also called tracts. Experimental evidences point at the cell membrane as the main tissue component responsible for this anisotropy of molecular diffusion in the WM (see Figure 4.2). The degree of myelination of the individual axons and the density of cellular packing seem to merely modulate the anisotropy as measured with dMRI, with microtubules and neurofilaments playing only a minor role [64].

![Figure 4.2](image-url)

**Figure 4.2:** (A) Random motion of water molecules (free diffusion). (B) Water diffusion in the brain is mainly restricted by the membranes of the axons. (C) Inside the axons, water diffuses mainly along the axis of the axon. *Part of the illustration is taken from [68]. Image used with permission.*

Assessing the direction(s) with maximal diffusion remains one of the main interests of the study of the WM using dMRI. Thus, the Orientation Distribution Function (ODF) is defined to integrate the angular content of the EAP (4.1). The ODF gathers this angular information through radial integration, as follows:

$$ \text{ODF} \equiv o(\hat{r}) = \int_{\mathbb{R}^+} dr r^2 p(r, \hat{r}), \quad (4.2) $$

where $r$ and $\hat{r}$ correspond to the angular and radial components of $r$. An ODF can be computed in every voxel, providing a better visualization of the diffusion at that position. The ODF can also be interpreted as a convolution on the sphere of a fiber response function or kernel with a Fiber Orientation Distribution function (FOD). The FOD is a real-valued function.
function on the unit sphere ($S^2$) that indicates the orientation and the volume fractions of the fiber populations in a voxel (see Figure 4.3).

**Figure 4.3:** The propagator EAP (left) is a 3D pdf that indicates the probability of water displacements. The ODF (middle) is a function on $S^2$ that represents the probability of diffusion along a given direction. The FOD (right), also a function on $S^2$, can be interpreted as a probability of having a fiber along a given direction. *Part of the illustration is taken from [68]. Image used with permission.*

The structural neuronal connectivity of the brain can be mapped in a non-invasive way thanks to the anisotropy of diffusion in the WM. The study of this connectivity is of major importance in a fundamental neuroscience perspective – for developing our understanding of the brain – but also in a clinical perspective, with particular applications for the understanding of stroke, schizophrenia, or Parkinson’s disease. Note that a precise mapping of the connectivity is commonly performed by so-called fiber-tracking or tractography algorithms. These algorithms produce trajectories capturing coherent orientations of maximal diffusion that are likely to represent real axonal fibers. Therefore they heavily rely on the quality of the fiber orientation recovery in each voxel.

More recently, the anisotropy of diffusion in the brain has started to be exploited to characterize the microstructural properties of the WM, like axon diameter and density. These features are related to conduction velocity [69] and play an important role in the performance of the WM tracts. Also, the microstructure organization of specific areas of the brain changes in subjects affected by certain pathologies, such as multiple sclerosis [70]. As a consequence, assessing both the orientation of the WM tracts and their microstructure characteristics through diffusion MR imaging in vivo represents today a fundamental tool for neuroscience as well as from the clinical point of view.

A great variety of approaches have been proposed to tackle the problem of intra-voxel fiber estimation from dMR measurements. In what follows, we cover in detail the main state-of-the-art dMR imaging techniques so that their strengths as well as their limitations can be understood. We distinguish two groups of local reconstruction techniques: those mainly concerned to recover the orientation of the fiber bundles in each voxel (section 4.4) and those that go a step further and aim to recover the microstructure configuration of

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*Of course, there are several orders of magnitude between the resolution of the MR acquisitions and the diameter of the axons. Therefore, a single reconstructed trajectory has to be thought of as representative of a huge coherent set of real anatomical fibers.*
4.4 Fiber orientation reconstruction

Many methods have been proposed to assess the orientation of the main fiber bundles voxelwise. Hereafter we present in detail the three of them that appear more relevant in the context of this thesis: Diffusion Tensor Imaging, Diffusion Spectrum Imaging and Spherical Deconvolution methods. We name and refer to others in section 5.1.

4.4.1 Diffusion Tensor Imaging, DTI

The Diffusion Tensor Imaging (DTI) technique was one of the first approaches proposed to provide a unified description of the diffusion process from a series of DWI images. It was introduced by Basser in 1994 [71]. The DT model is based on the hypothesis that the diffusion follows a Gaussian damping with \( q \), or equivalently, exponential in \( b \). In an isotropic medium, the attenuation of the MRI signal can be described as \( A = e^{-bD} \), where \( D \), the diffusion coefficient, is a scalar. However, a tensor \( D \) is required to describe the diffusion process along the three directions of our reference frame when it takes place in an anisotropic medium. To fully determine the diffusion tensor, diffusion-weighted images along several gradient directions must be collected. As the diffusion tensor is symmetric, measurements along only six directions are mandatory -instead of nine- (Figure 4.4 B), along with an image acquired without diffusion weighting \( b = 0 \). Once the set of DW images is acquired, linear regression techniques can be used to estimate the full tensor \( D \). Its largest eigenvalue and corresponding eigenvector describe the intensity and the principal direction of diffusion, which are then associated with the orientation of the underlying fiber bundle.

Figure 4.4: (A) Illustration of a DWI image from sampling the signal at a single \( q \)-point. (B) In DTI, the \( q \)-space is sampled at least at 6 \( q \)-points. (C) In DSI, the \( q \)-space is densely sampled, each \( q \)-point corresponding to a different gradient orientation and strength. Part of the illustration is taken from [68]. Image used with permission.

The diffusion tensor is normally visualized as an ellipsoid with the principal axes along the eigenvectors of \( D \), and with the length of these axes proportional to the corresponding eigenvalues. These eigenvalues can be considered as unidimensional diffusion coefficients,
or diffusivities, in the main directions of diffusion in the medium, so for instance, the eccentricity of the ellipsoid gives us information about the degree of anisotropy.

The Tensor Model assumes gaussian diffusion and gaussian functions have only one maximum. In voxels with presence of multiple fiber orientations (fiber crossings or branching), DTI will recover a single fiber orientation, corresponding to the mean of the true underlying directions. Consequently, the DT model is not valid in regions of the brain where there are fiber crossings. In such areas, other methods providing a higher angular resolution are needed.

4.4.2 Diffusion Spectrum Imaging, DSI

DSI is a model-free imaging technique that samples densely the q-space from which the displacement distribution can be later recovered directly exploiting the Fourier relationship described in (4.1). It therefore requires the acquisition of many DW images, each of them corresponding to a different q-point distributed in a Cartesian grid (Figure 4.4).

With this imaging technique, fiber orientations are also associated with directions of maximum diffusion, but since there is no restriction on one single diffusion direction, it appears as a more suitable approach to detect fiber crossings. DSI provides very good angular resolution when sampling densely the q-space. Nevertheless, the main drawback of DSI strongly relates to its complexity. Measuring the complete 3-dimensional diffusion function requires long acquisition times and thus it is not appropriate for all clinical applications.

4.4.3 Methods based on spherical deconvolution

Spherical deconvolution (SD) methods [5, 72, 73] reformulate the imaging problem from dMR data as a deconvolution problem on the sphere under the following two assumptions:

(i) There is no exchange of water between different fiber bundles over the time of a dMR measurement, meaning that the signal attenuation in a voxel with the presence of $N$ fiber populations can be expressed as $S = \sum_{i} f_i S_i$, where $f_i$ is the volume fraction of the $i$th bundle and $S_i$ its corresponding signal damping.

(ii) All fiber bundles in the brain share the same diffusion attenuation profile, i.e. if there is any difference among them it must be due to a partial-volume effect.

Under conditions (i) and (ii), the diffusion signal in every voxel can be expressed as a convolution over the unit sphere of a response function and the FOD:

$$S(q) = S_0 \int_{S^2} K(q, \hat{u}) f(\hat{u}) d\hat{u}. \tag{4.3}$$

In (4.3), $S_0$ corresponds to the signal without diffusion weighting, $K$ represents the kernel or response function, $f$ stands for the FOD and $\hat{u} \in S^2$ is a unitary vector. Assuming
4.5. Microstructure imaging techniques

Most microstructure imaging techniques describe the brain tissue using multi-compartment models distinguishing, for instance, axons, glial cells and extra-axonal space. Subsequently, the microstructure properties are recovered by modeling the signal decay in each of the considered tissue compartments and assuming the measured signal as a combination of all of them (see Figure 4.5).

\[ S_{\text{voxel}} = f_h S_h + f_r S_r + f_f S_f + f_s S_s \]

**Figure 4.5:** Schematic representation of the tissue multi-compartment model for ActiveAx [1]. In every voxel, the signal decay \( S_{\text{voxel}} \) is expressed as the weighted sum of the contributions of each compartment. \( f_r, f_h, f_f \) and \( f_s \) represent the volume fractions corresponding to the restricted, hindered, free and stationary compartments, respectively. *Part of the illustration is taken from [74]. Image used with permission.*

The main differences between different microstructure imaging methods depend on the number of tissue compartments they consider, the chosen model for the diffusion
in each compartment and whether they assume water exchange between them or not. The reader can find an exhaustive survey on many of the state-of-the-art microstructure imaging techniques in [75]. We have summarized their principal characteristics in Table 4.6, indicating for each image modality the signal model used in each compartment and the features it estimates. In Table 4.6, we borrow Panagiotaki’s taxonomy [75] to refer to the diverse signal models. We briefly describe them hereafter and we refer the reader to [75] for further study:

- **Intra-axonal** refers to the signal decay due to water diffusion inside the axons. Subsequently we also refer to it as restricted compartment.
  - *stick*: provides the signal decay that would correspond to diffusion inside an idealized 0-radius cylinder.
  - *cylinder*: indicates the signal corresponding to diffusion inside a cylinder.
  - *GDRCylinders*: indicates the signal decay corresponding to diffusion inside a group of cylinders whose radii are drawn from a Γ-distribution.

- **Extra-axonal** refers to the signal decay due to water diffusion outside and between axons. Subsequently we also refer to it as hindered compartment. The different models express hindered diffusion as gaussian tensors, with different degrees of freedom.
  - *ball*: corresponds to isotropic diffusion with a single diffusivity parameter.
  - *zeppelin*: stands for an anisotropic cylindrically-symmetric tensor with two diffusivity parameters: \( d_{\parallel} \), parallel to the principal direction of the tensor and \( d_{\perp} \), perpendicular to it.
  - *tensor*: stands for an anisotropic tensor with three diffusivity parameters: \( d_{\parallel} \), parallel to the principal direction of the tensor and \( d_{\perp 1}, d_{\perp 2} \), perpendicular to it.

- **Stationary** refers to the signal decay due to water trapped in other cellular structures, such as glial cells.
  - *sphere*: models the water diffusion inside bodies with spherical boundaries.
  - *dot*: refers to a 0-radius sphere and is intend to model water that does not move.

- **Free** refers to the signal decay due to free water in a non-restrictive environment, such as CSF.

The microstructure parameters that can be estimated with each technique depend on its chosen tissue/signal model. When interpreting Table 4.6, consider that a specific
feature is estimated by a particular technique if a green tick appears in the corresponding row. A red cross indicates that the referred technique does not estimate that particular parameter, either because it is meaningless according to the chosen signal model or because it is fixed \textit{a priori}. In general they can all be related either to the orientation, the size or the packing density of the axons; hereafter we list those mentioned on Table 4.6:

- Fiber bundle main \textbf{orientation}.

- \textbf{Volume fractions} corresponding to every considered compartment.

- \textbf{Diffusivities}: each technique chooses to fix some (or all) of the diffusivity parameters to biologically-plausible values characteristic to the medium and to estimate the rest from the data\textsuperscript{†}. In most cases, they are related to the intra-axonal volume fraction through a tortuosity model [76].

- \textbf{Axon Diameter Distribution (ADD)}.

- \textbf{Axon Diameter Index}: It is a single summary statistics that corresponds to the diameter that would produce the signal decay best matching the average signal decay over the distribution. Since large axons contain more water than the small ones, they also contribute “more” to the diffusion signal. Therefore, this diameter index correlates to a \textit{weighted mean} axonal diameter, in which the contribution of each axon to the total signal is proportional to the square of its diameter [1].

- \textbf{Orientation dispersion} around the mean fiber orientation.

All microstructure imaging techniques mentioned in Table 4.6 require computationally very expensive nonlinear procedures to fit their models to the data [9]. Moreover, they are only valid in regions with one single fiber population, which makes them inappropriate to characterize the microstructure of the majority of voxels in the brain. In the next subsection, we present a general framework in which any of the existing techniques can potentially be reformulated into a linear problem that can be easily and very rapidly solved using convex optimization.

4.5.1 The AMICO framework

In [9], the authors define a flexible framework for microstructure imaging named after AMICO, Accelerated Microstructure Imaging via Convex Optimization. The authors get inspired by spherical deconvolution methods that formulate the problem of fiber orientation recovery in a voxel as a linear inverse problem, provided the response function of a

\textsuperscript{†}In the table we do not specify which are the fixed/estimated diffusivities for every model since it appears out of the scope of this thesis. A red cross indicates that the method does not estimate any diffusivity and a green tick, some of them. The reader can refer to the original papers for more details.
**Figure 4.6:** Summary-table of the main features of the following microstructure imaging techniques: Stick and Ball [77], CHARMED [78, 79], AxCaliber [80], extended AxCaliber [74], ActiveAx [1, 81], NODDI [82], Stainsz [83].

A single fiber can be estimated (see section 4.4.3). To extend this idea to microstructure imaging, in AMICO the original problem is decoupled into two independent subproblems:

(i) estimation the main orientation \( (\mu \in \mathbb{S}^2) \) of the fiber population under study, and

(ii) estimation of its main microstructure features.

Assuming the presence of a single fiber population in the voxel, step (i) is easily performed using DTI [71]. Once \( \mu \) is known, the microstructure mapping problem is expressed in terms of a linear formulation, as follows:

\[
y = \Phi_\mu x + \eta,
\]

being \( y \in \mathbb{R}^m \) the vector of diffusion measurements, \( x \in \mathbb{R}^n \) the coefficients to be estimated and \( \eta \) the acquisition noise. In (4.5), \( \Phi_\mu \) is a linear operator or dictionary that accounts for the signal decay from different compartments (oriented along direction \( \mu \)) and therefore, it is designed according to the imaging modality that is meant to reformulate. In [9], the authors demonstrate the linearization of ActiveAx [1] and NODDI [82], even if the AMICO framework can be also applied to other microstructure imaging models. Hereafter, we exemplify this linearization process by detailing the construction of the dictionary for ActiveAx.

ActiveAx as a linear system is built from different sub-matrices:

\[
\Phi_\mu = [\Phi_\mu^r | \Phi_\mu^h | \Phi_\mu^i].
\]
In equation (6.6), sub-matrices $\Phi_r^{\mu} \in \mathbb{R}^{m \times N_r}$, $\Phi_h^{\mu} \in \mathbb{R}^{m \times N_h}$ and $\Phi_i^{\mu} \in \mathbb{R}^m$ model, respectively, the intra-axonal, extra-axonal and isotropic contributions to the diffusion signal along the direction $\mu$. Each atom in sub-matrices $\Phi_r^{\mu}$ models the diffusion signal corresponding to water molecules restricted within parallel cylinders of a specific diameter. Alternatively, the atoms in sub-matrices $\Phi_h^{\mu}$ describe the hindered space between the axons and a single atom in $\Phi_i^{\mu}$ accounts for any isotropic contribution. $N_r$ and $N_h$ represent, respectively, the number of different axon radii and hindered environments considered to build the dictionary ($n = N_r + N_h + 1$).

Equation (4.5) is then solved as a Tikhonov-regularized least-squares problem as follows:

$$\min_{x \geq 0} \frac{1}{2} ||\Phi_\mu x - y||_2^2 + \lambda \frac{1}{2} ||x||_2^2,$$  \hspace{1cm} (4.7)

where $|| \cdot ||_2$ is the standard $\ell_2$ norm and parameter $\lambda > 0$ controls the trade-off between data and regularization terms. Equation (4.7) can be solved using fast convex optimization methods and therefore, AMICO provides an acceleration factor of several orders of magnitude in the intrinsic fitting time with respect to the original microstructure imaging techniques [9]. Moreover, AMICO guarantees convergence to a global minimum without any initialization procedure since its formulation is convex.

### 4.6 Conclusion

In this chapter, we have presented some background information on diffusion MRI, an MR technique that can measure the diffusion of water in biological tissue.

We have focused on applications of dMRI in the brain, where the anisotropy of diffusion in the white matter can be exploited 1) to map the neural connectivity in the brain through assessing the main orientation(s) of the fiber tracts voxelwise and 2) to characterize the microstructural properties of the white matter, like axon diameter and density. We have presented the state-of-the-art approaches to tackle both problems, providing the reader with an overview of their strengths and their main limitations.
5.1 Introduction

In this chapter, we propose a novel formulation to solve the problem of intra-voxel reconstruction of the fiber orientation distribution function (FOD) in each voxel of the white matter of the brain from diffusion MRI data.

A great variety of approaches have been proposed to tackle the problem of intra-voxel fiber orientation estimation (see chapter 4). Diffusion Tensor Imaging (DTI) [71] is one of the simplest and fastest reconstruction techniques since it only requires sampling 6 points of the $q$-space. However, it is by construction unable to model multiple fiber populations within a voxel and thus it is not valid in regions with crossings. Diffusion Spectrum Imaging (DSI) [84], on the other hand, is a model-free imaging technique known to provide good imaging quality. Yet, it requires strong magnetic field gradients and long acquisition times, needing typically 256 samples for a good reconstruction. As a consequence, it generally becomes too time-consuming to be of real interest in a clinical perspective. Accelerated acquisitions, relying on as few sampling points as possible while still sensitive to fiber crossings represent thus a major goal in the field.

In the last years, spherical deconvolution (SD) methods [5, 72, 73] have become very popular in the framework of local reconstruction since they can recover the fiber configuration with a relatively small number of points, typically from 30 up to 60. They consider that both anisotropy and magnitude of water diffusion in white matter (WM) are constant in the whole volume. Under this assumption, SD methods acknowledge the fact that the diffusion signal can be expressed as the convolution of a response function, or kernel, with the fiber orientation distribution function (FOD). The FOD is a real-valued function on the unit sphere that indicates the orientation and the volume fraction of the fiber populations in a voxel. The Constrained Spherical Deconvolution approach [5, 73] represents the first attempt to solve the ill-posed SD problem. It applies Tikhonov regularization, introducing a constraint on the $\ell_2$ norm of the FOD, specially to ensure its positivity. Apart from the aforementioned work, most of the state-of-the-art methods to solve SD problems promote sparse regularization based on $\ell_1$ minimization [6, 85, 86], where the
The $\ell_1$ norm is defined, for any real vector, as the sum of the absolute value of its coefficients. Yet, in [87] the authors acknowledge that $\ell_1$ minimization is formally inconsistent with the fact that the volume fraction sum up to unity, and demonstrate the superiority of $\ell_0$-norm minimization. All these local reconstruction methods solve the FOD recovery problem for each voxel independently and thus, do not exploit the spatial coherence of the fiber tracts in the brain. A number of approaches have addressed this shortcoming by formulating the problem globally (simultaneously for all voxels) to be able to exploit the correlation between the different volumes. Some of them decouple the problem and propose a global denoising of the diffusion data prior to reconstruction [88, 89]. Another group of methods present a joint scheme for reconstruction and spatial regularization on the diffusion images at each $q$-space point. For instance, [90] propose a variational formulation to jointly estimate and regularize DTI to account for the effect of Rician noise in low SNR regimes, while the standard state-of-the-art minimization of the total variation (TV) semi-norm [91] of the diffusion images is used to denoise in [86, 92].

In this chapter, we propose a formulation that solves the fiber configuration of all voxels of interest simultaneously and imposes spatial regularization directly on the fiber space. This reconstruction allows us to exploit information from the neighboring voxels that cannot be taken into account by the existing state-of-the-art methods that approach fiber reconstruction independently in each voxel. The natural smoothness of the anatomical fiber tracts through the brain can be translated in a certain spatial coherence of the FOD in neighboring voxels. Accordingly, in the aim of recovering the global FOD field in all voxels, the present work leverages a reweighted $\ell_1$-minimization scheme to promote a spatially structured sparsity prior imposing spatial coherence. While the spatial regularization schemes proposed in [86, 90, 92] enforce sparsity of the images at each $q$-space point, our spatial regularization relates to the fundamental coherence between fiber directions – the FOD – in neighbor voxels, thus adding anatomically driven constraints. Our code is available at https://github.com/basp-group/co-dmri and it is distributed open-source.

The rest of the chapter is organized as follows: In section 5.2 we recall the framework for local FOD reconstruction through spherical deconvolution. We firstly introduce the local $\ell_0$ algorithm in [87] and secondly propose a nonlocal method which solves for the FOD in all voxels simultaneously introducing spatial coherence of the fiber bundles orientation in neighboring voxels. We report and discuss results on both synthetic and real data in section 5.3. Conclusions and further work to be considered are examined in section 5.4.
5.2 Materials and Methods

5.2.1 dMRI framework for recovery of FOD via spherical deconvolution

In the SD framework, the intra-voxel structure estimation can be expressed through the FOD recovery problem in terms of the following linear formulation:

\[ y = \Phi x + \eta, \]  

(5.1)

where \( x \in \mathbb{R}_+^n \) stands for the FOD, \( y \in \mathbb{R}_+^m \) is the vector of measurements, \( \Phi \) is the linear measurement operator and \( \eta \) is the acquisition noise. The reader can refer to [85] for a more detailed overview on SD methods and the formal equations describing the relationship between the FOD and the diffusion signal. We consider a dictionary \( \Phi \) that spans a set of the Diffusion Basis Functions introduced in [6]. Each of these basis functions is generated by applying a different rotation to a kernel, which corresponds to the diffusion signal response to a single fiber. The set of available orientations represents a discretization of half of the unit sphere (\( S^2 \)), assuming antipodal symmetry in the diffusion signal. The diffusion signal can then be expressed as a linear combination of these basis functions, also referred to as the atoms of our dictionary \( \Phi \).

Prior constraints are essential to regularize a deconvolution problem like (5.1) in order to find a unique solution from an originally ill-posed problem. In the framework of the recently developed theory of compressed sensing (CS) [18, 20] sparsity priors are commonly used as regularizers to recover a signal from a set of undersampled measurements (see chapter 2). In formulation (5.1) the sparsity can directly be inferred from the small number of fiber directions of interest, in correspondence with the FOD coefficients. In this work, the method proposed in [87] is taken as the state-of-the-art algorithm in the framework of SD local methods for FOD recovery. For the sake of completeness, it is described in detail hereafter.

In [87], the authors propose to resort explicitly to the nonconvex \( \ell_0 \) prior to solve for the FOD rather than to its convex \( \ell_1 \) relaxation. A convex optimization problem for FOD reconstruction can be defined through a constrained formulation between adequate sparsity prior and data, also making use of a reweighted sparse deconvolution. The proposed minimization problem reads as:

\[
\min_{x \geq 0} \| \Phi x - y \|^2_2 \quad \text{s.t.} \quad \| x \|_0 \leq k.
\]  

(5.2)

In (5.2), \( \| \cdot \|_0 \) represents the \( \ell_0 \) norm (number of nonzero coefficients) and \( k \) acts as a bound on the expected number of fiber populations in a voxel. Since the \( \ell_0 \) norm is nonconvex, a reweighted \( \ell_1 \)-minimization scheme [24] is used in order to approach \( \ell_0 \) minimization by
a sequence of convex weighted-$\ell_1$ problems of the form:

$$\min_{x \geq 0} \|\Phi x - y\|_2^2 \quad \text{s.t.} \quad \|x\|_{w,1} \leq k.$$  \hfill (5.3)

In (5.3), the $\ell_0$ norm has been substituted by a weighted-$\ell_1$ norm defined as $\|x\|_{w,1} = \sum_i w_i |x_i|$. The algorithm alternates between estimating the solution at iteration $t$, $x^{(t)}$, and redefining the weights essentially as the inverse of the values of the solution at the previous iteration $w_i^{(t+1)} \approx 1/x_i^{(t)}$ (see section 2.4.2). The use of these weights allows the algorithm to iteratively better estimate the nonzero locations and induces that, at convergence, the weighted-$\ell_1$ norm mimics the $\ell_0$ norm. Hence, formulation (5.2) promotes sparsity through a sequence of problems (5.3). Hereafter we will refer to this voxel-by-voxel method based on $\ell_2$ and $\ell_0$ priors as L2L0.

In the next subsection we describe an algorithm, inspired by L2L0, that exploits the anatomical coherence of the fiber tracts of the brain by promoting a structured sparsity prior on the FOD field. We show evidence that taking into account neighboring information through an appropriate prior directly on the object of interest improves significantly the results in comparison with solving for all voxels independently or using indirect spatial regularization schemes.

### 5.2.2 Spatial regularization through structured sparsity

In the aim of exploiting the spatial coherence of the fibers in the brain when recovering the local fiber configuration, we formulate a problem to solve the ensemble FOD field for all voxels simultaneously. To emphasize the fact that the minimization problem (5.2) is formulated separately for each voxel of the brain, we can rewrite it using the following notation:

$$\min_{x^{(v)} \geq 0} \|\Phi x^{(v)} - y^{(v)}\|_2^2 \quad \text{s.t.} \quad \|x^{(v)}\|_0 \leq k,$$  \hfill (5.4)

where $x^{(v)} \in \mathbb{R}^n_+$ represents the real-valued FOD in the particular voxel indexed $v$. By concatenating all vectors $x^{(v)}$ columnwise, one can build a matrix $X \in \mathbb{R}^{n \times N}_+$, whose columns correspond to the FOD in each particular voxel. The elements of matrix $X$ will be indexed as $X_{dv}$, each row $d$ being associated with the atom of the dictionary oriented in direction indexed $d$, each column $v$ being associated with voxel indexed $v$, $X_v = x^{(v)}$, as represented in Figure 5.3. $N$ denotes the total number of voxels we want to recover the fiber configuration from. The rows of $\Phi X$ represent the modeled diffusion images at each $q$-space point.

In our proposed formulation, a global data term is minimized adding a sparsity constraint that simultaneously promotes spatial coherence of the solution. Inspired by formulation (5.3), we adopt a procedure that consists in solving a sequence of problems of the
5.2. Materials and Methods

form:
\[
\min_{X \in \mathbb{R}^{n \times N}} \| \Phi X - Y \|_2^2 \quad \text{s.t.} \quad \|X\|_{W,1} \leq K,
\]  

where the matrix \( Y \in \mathbb{R}^{m \times N} \) is formed by the concatenation of all \( N \) measurement column vectors: \( Y_v = y^{(v)} \in \mathbb{R}^m \). The sensing matrix \( \Phi \) is exactly the same as in (5.4) and \( \| \cdot \|_{W,1} \) stands for a weighted \( \ell_1 \) norm of a matrix defined as:

\[
\|X\|_{W,1} = \sum_{d,v} W_{dv} |X_{dv}|.
\]  

The following paragraphs are devoted to describe in detail the reweighting scheme and define the weighting matrix \( W \).

In a reweighted-\( \ell_1 \) scheme, large weights will progressively tend to discourage nonzero entries whereas small weights will promote nonzero entries in the solution. The weighting matrix \( W \) has the same dimension as \( X \) and each of its entries acts as a weight for the corresponding entry of \( X \). The weights should still represent the inverse value of the associated entry at the previous iteration, so as to lead to an \( \ell_0 \)-norm prior at convergence. However, a strong spatial coherence prior can actually be promoted by adapting the computation of the weights as follows. Our definition of the weights is driven by the underlying anatomical assumption that fiber bundles in neighboring voxels should have very close orientations as the trajectories are smooth (schematically represented in Figure 5.1). In terms of the FOD, this premise implies that neighbor voxels should bear similar directions.

![Figure 5.1: Synthetic FOD field in a representative 2D slice, which consists of two crossing fiber bundles. Due to the natural smoothness of the bundles, FODs in neighboring voxels are expected to contain similar peaks, as highlighted in the figure. Figure published in [7].](image)
both $N(d)$ and $N(v)$ is shown in Figure 5.2. For convenience, we define $\overline{N(d)} = d \cup N(d)$ and $\overline{N(v)} = v \cup N(v)$, the neighborhoods that include the central element. We then define the neighborhood of an element $X_{d,v}$ as the entries of $X$ at the intersection of rows $d$ and all its neighbor directions, and columns $v$ and all its neighbor voxels: $\overline{N(d,v)} = \{(d',v'); d' \in \overline{N(d)}, v' \in \overline{N(v)}\}$, as it is schematically represented in Figure 5.3.

At each iteration, every element of the weighting matrix $W_{d,v}$ is set as the inverse of an average of the absolute values that $X$ takes in the neighborhood of $X_{d,v}$ in the previous iteration:

$$W_{d,v}^{(t+1)} = \left[ \tau(t) + \frac{1}{|\overline{N(v)}|} \sum_{d',v' \in \overline{N(d,v)}} |X_{d',v'}^{(t)}| \right]^{-1}. \tag{5.7}$$

Consequently, at each iteration $t$, the weighting matrix $W^{(t)}$ represents a blurred version of the current estimation of the solution $X^{(t)*}$. In (5.7), we average over voxels, but sum over directions as all values in neighbor directions are interpreted as contributing to a single true local direction, in particular because the true direction does in general not coincide exactly to one of the discrete points of the sphere identifying our orientation dictionary.

$^*$The values of the final solution are influenced by their weights, however they are not directly identified with them.
This helps to stabilize the regularization and prevent the appearance of spurious peaks: fiber contributions are usually spread over a small angular support while spurious peaks are associated with isolated directions. To avoid infinite values for null averages, we add a stability parameter $\tau$ in the definition of the weights. We apply an homotopy strategy [94] and use a decreasing sequence $\{\tau^{(t)}\}$ in such a way that $\tau^{(t)} \to 0$ when $t \to \infty$. In the absence of any spatial constraint, $W^{(0)}$ corresponds to the matrix of all 1s and thus, the weighted $\ell_1$ norm is the standard $\ell_1$ norm of a matrix, $\|X\|_{W,1} = \|X\|_{1,1}$.

The specific computation of the weights described in the former paragraphs encourages that neighbor voxels present the same or very close (neighbor) directions, imposing structured sparsity of the solution. Indeed, all entries corresponding to the neighborhood of an element contribute to its weight. Therefore those orientations that are “supported” by the surrounding voxels are reinforced, since they will be given a small weight compared to isolated directions that are not coherent with their environment. At convergence, our definitions (5.6) and (5.7) thus implement a spatially coherent version of the matrix $\ell_0$ norm, i.e. the sum of the $\ell_0$ norms of its columns. This reweighting scheme promotes a regularization that takes into account the true anatomy of the brain accounting for the fact that fiber populations present a coherent trajectory across voxels close to each other in the brain volume. This prior constitutes a powerful constraint that cannot be exploited when solving the problem independently for each voxel, like in (5.4).

The main steps of the reweighting scheme are reported in algorithm 3; in the remaining of the manuscript we will refer to it as L2L0NW, in reference to the described neighbor weighted scheme. The reweighting process stops when the relative variation between successive solutions $\|X^{(t)} - X^{(t-1)}\|_2 / \|X^{(t-1)}\|_2$ is smaller than some bound or after the maximum number of iterations allowed is reached.
Algorithm 3  Reweighted $\ell_1$ minimization for global reconstruction of the FOD

Require: $Y \in \mathbb{R}^{m \times N}$; $\Phi \in \mathbb{R}^{n \times m}$; $K$; $\tau_{\text{thr}}$; $N_{\text{max}}$; $N(d)$, $d = 1, \ldots, n$; $N(v)$, $v = 1, \ldots, N$

Ensure: FOD $X \in \mathbb{R}_{+}^{n \times N}$

Initialize $t \leftarrow 0$; $X^{(0)} = 0$; $W^{(0)} \leftarrow 1$

while $\rho > \nu$ and $t < N_{\text{max}}$ do

Solve: $X^{(t)} \leftarrow \min_{X \in \mathbb{R}^{n \times N}} \|\Phi X - Y\|_2^2$ s.t. $\|X\|_{W,1} \leq K$

Update $W^{(t+1)}$

Update $\rho = \|X^{(t)} - X^{(t-1)}\|_2 / \|X^{(t-1)}\|_2$

$t \leftarrow t + 1$

end while

$X \leftarrow X^{(t-1)}$

5.2.3 Implementation details

To generate the dictionary $\Phi$ in our experiments, we estimated two different Gaussian kernels that model the diffusion signal in the regions of the brain corresponding to (i) white matter (WM) and (ii) partial volume with grey matter or cerebrospinal fluid (CSF). Modeling each kernel actually corresponds to estimating the three eigenvalues of the diffusion tensor. Grey matter and CSF are typically isotropic media. Consequently, their representative kernel is spherical – a tensor with three equal eigenvalues – and not sensitive to rotations. On the other hand, the kernel corresponding to the WM is anisotropic. Its response function was first estimated by fitting a tensor from the diffusion signal in those voxels with the highest fractional anisotropy (as expected to contain only one fiber population) and subsequently it was rotated in 200 different directions equally distributed on the sphere. Therefore, the final number of atoms of the dictionary used for this reconstruction is 201: 200 atoms corresponding to WM plus 1 isotropic atom modeling partial volume with CSF and grey matter.

Each weighted-$\ell_1$ problem of the form (5.5) is solved using a forward-backward algorithm [95] in the context of proximal splitting theory (see chapter 2). To set a meaningful bound $K$ we have followed the criterion that at convergence the weighted-$\ell_1$ norm of a matrix, as defined in section 5.2.2, mimics the $\ell_0$ norm – as in formulation (5.3) –. $K$ is then heuristically fixed as $K = 3N$, as it represents a conservative bound on the total number of fiber orientations to be identified, computed as the number of voxels $N$ times an average bound on the number of fiber orientation per voxel. We initialize $\tau^{(0)}$ as the variance of the solution after the first iteration $X^{(0)}$ and, in subsequent iterations, we update $\tau^{(t+1)} = \beta \tau^{(t)}$ with $\beta = 10^{-1}$. Ideally $\tau^{(t)}$ should decrease to 0 but we heuristically fix a lower bound $\tau_{\text{thr}} = 10^{-7}$, above which significant signal components could be identified. Experiments show that for a convergence bound $\nu = 10^{-3}$ the reweighting process stops after a relatively small number of iterations, typically 4 or 5. In our simulations, $\nu$ is set to $10^{-3}$ and $N_{\text{max}}$ to 10.

To extract the final fiber directions from the solution to algorithm 3 in every voxel
we perform a search for local maxima among all directions within a cone of 15° around every direction. In this entire process, we disregard the directions with contributions (i.e. coefficients) smaller than 10% of the maxima in order to filter out spurious peaks.

5.2.4 Phantom data

We perform our experiments using the phantom data used for the HARDI reconstruction Challenge 2012 [96]. The public results in [96] allow us to compare the performance of L2L0NW with other methods using different spatial regularization schemes – such as TV regularization mentioned above – with no need for their explicit implementation. The dataset is a 16 × 16 × 5 volume that comprises 5 different fiber bundles that result in voxels with bending, crossing and kissing tracts. The response function of each bundle has been generated with a fractional anisotropy between 0.75 and 0.90 and the diffusion properties are constant along all its trajectory. More details on its geometry can be found in [96].

The signal is contaminated with Rician noise [97] as follows:

\[ S_{\text{noisy}} = \sqrt{(S + \xi_1)^2 + (\xi_2)^2}, \]

with \( \xi_1, \xi_2 \sim N(0, \sigma^2) \) and \( \sigma = S_0/\text{SNR} \) corresponding to a given signal-to-noise ratio (SNR) on the \( S_0 \) image. The quality of the reconstructions has been evaluated as a function of three different noise levels, i.e. \( \text{SNR} = 10, 20, 30 \) and 5 different \( q \)-space acquisition schemes (30, 20, 15, 10 and 6 samples), evenly spaced on half of the unit sphere.

5.2.5 Real Data

One HARDI\(^\dagger\) dataset was acquired at \( b = 3000 \text{ s/mm}^2 \) using 256 directions uniformly distributed on half of the unit sphere (as described in [98]), \( \text{TR/TE} = 7000/108 \text{ ms} \) and spatial resolution = 2.5 × 2.5 × 2.5 mm. To assess the robustness of L2L0NW to different undersampling rates, the dataset has been retrospectively undersampled and three additional datasets have been created, consisting of only 30, 20 and 10 diffusion directions selected in order to be evenly spaced on half of the unit sphere using the tool subsetpoints which is available in the camino toolbox\(^\ddagger\). We will refer to these four data sets as hardi\(_{256} \), hardi\(_{30} \), hardi\(_{20} \) and hardi\(_{10} \), respectively. The actual SNR in the \( b = 0 \) images, computed as the ratio of the mean value in a region-of-interest placed in the WM and the standard deviation of the noise estimated in the background, was about 30.

To evaluate the reconstructions from the undersampled real datasets, the metrics described in subsection 5.2.6 are computed considering the fully-sampled hardi\(_{256} \) as the

\(^\dagger\)High-Angular Resolution Diffusion Imaging

\(^\ddagger\)www.camino.org.uk
golden truth, as it is suggested in [99].

5.2.6 Evaluation criteria

To evaluate the quality of the reconstructions we have focused on the performance of each method in both correctly assessing the number of fiber populations in each voxel and the angular accuracy in their orientation. In this work we adopted a set of metrics that was used to evaluate and compare all methods participating in the HARDI reconstruction Challenge 2012 [96]. For consistency we have kept their notation to design the different quality indices. The success rate ($SR_\angle$) corresponds to the proportion of voxels in which a reconstruction algorithm correctly estimates the number of fiber populations. A fiber is considered to be correctly identified when an estimated fiber falls within a tolerance cone around a true fiber. To compare our results with different algorithms evaluated in [96], in this work the tolerance was set to 20°. False positive and negative rates ($n_+^\angle$ and $n_-^\angle$, respectively) are an average over all voxels of the number of over-/underestimated fiber populations per voxel.

The angular accuracy is measured through the mean angular error $\bar{\theta}$ (in degrees) averaged over all true fiber directions, where the angular error associated with each true fiber is formally defined as:

$$\theta = \frac{180}{\pi} \arccos(|d_{\text{true}} \cdot d_{\text{estimated}}|),$$

(5.9)

where $d_{\text{true}}$ and $d_{\text{estimated}}$ are unitary vectors in the true fiber direction and the closest estimated direction. Note that indices $SR_\angle$, $n_+^\angle$ and $n_-^\angle$ represent mean values over all voxels of interest, whereas $\bar{\theta}$ is computed voxelwise and we study its statistical distribution to evaluate the general angular accuracy of each reconstruction.

5.2.7 Experimental setup

In the next section, we evaluate the quality of reconstructions using L2L0NW, both for numerical simulations and tests on real data. As shown in [87], L2L0 outperforms other state-of-the-art local methods that recover the FOD in the framework of spherical deconvolution. Consequently, we have chosen it as a benchmark to compare L2L0NW with respect to methods that perform voxel-by-voxel reconstruction of the fiber configuration. We had access to the original implementation to run L2L0 reconstructions.

We also compare the performance of L2L0NW, which jointly estimates the FOD and applies spatial regularization, with respect to applying first a nonlocal denoising procedure and subsequently perform local reconstruction. We have chosen an adaptation of the Linear Minimum Mean Squared Error (LMMSE) filter proposed in [88] to simultaneously filter all different gradient images. We use a publicly available implementation of the Joint
5.3. Results and discussion

Anisotropic LMMSE filter\(^3\) and subsequently apply L2L0 to reconstruct the FOD. We refer to this alternative as JAMMLSE+L2L0.

In addition, taking the advantage of the public results of the HARDI reconstruction Challenge 2012 \cite{96}, we can compare the performance of L2L0NW with a representative collection of state-of-the-art methods for simulations on phantom data. In particular, we are able to establish a comparison with other methods using different spatial regularization schemes – such as TV regularization mentioned above – with no need for an explicit implementation of these methods.

Our optimization code\(^4\) was implemented in MATLAB and run on a standard 2.4 GHz Intel Xeon processor. The non-optimized version of the code is able to reconstruct a whole brain volume of 106 × 106 × 51 voxels within approximately 4 hours.

5.3 Results and discussion

5.3.1 Phantom data

In this subsection we start comparing in detail the performance for L2L0NW relative to L2L0 and JAMMLSE+L2L0 for the phantom data set described in subsection 5.2.4. The performance of the three methods as a function of the undersampling rate in q-space is reported in Figure 5.4. We consider 5 different acquisitions schemes (30, 20, 15, 10 and 6 samples) and present results for two different noise levels, at SNR = 30 and SNR = 20. The plots demonstrate that L2L0NW outperforms L2L0 and JAMMLSE+L2L0 for all number of samples, in both noise conditions. L2L0NW exhibits an accurate reconstruction (SR\(\angle\) ≥ 85 and mean(\(\bar{\theta}\)) ≤ 6.5\(^{\circ}\)), robust to noise for different undersampling regimes, down to 15 samples. Denoising high-SNR data prior to reconstruction, as it is done in JAMMLSE+L2L0, seems not to improve the quality of the reconstructions. Indeed, at SNR = 30, 20 JAMMLSE+L2L0 exhibits slightly worse results than L2L0 (moderately lower SR\(\angle\) and \(\bar{\theta}\)). With high quality data (SNR = 30 and from 30 to 15 samples), the differences between the three methods are fairly mild. The superiority of L2L0NW compared to L2L0 and JAMMLSE+L2L0 appears clearer as we move to higher undersampling regimes and SNR = 20, specially in terms of the ability of identifying the correct number of fibers (higher SR\(\angle\)). The overall improvement in terms of the success rate is even more evident when we go down to 10 samples, where L2L0 and JAMMLSE+L2L0 exhibit a severe drop of the performance with SR\(\angle\) = 52 (L2L0) and SR\(\angle\) = 50 (JAMMLSE+L2L0) at SNR = 30 and SR\(\angle\) = 36 (L2L0) and SR\(\angle\) = 38 (JAMMLSE+L2L0) at SNR = 20, while SR\(\angle\) = 81 (SNR = 30) and SR\(\angle\) = 72 (SNR = 20) are obtained with L2L0NW. We notice a significant deterioration of the reconstructions with all methods when decreasing the number of samples down to 6.

A more detailed analysis in severe noise conditions (SNR = 10) is presented in Fig-

\(^3\)\url{http://www.nitrc.org/projects/jammlse_dwi/}

\(^4\)Code is available at \url{https://github.com/basp-group/co-dmri}. 
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Figure 5.5. The plots show an important difference between the performance achieved by L2L0, that solves the problem voxelwise, and L2L0NW and JAMMLSE+L2L0 that take into account the correlation between voxels and directions. At SNR=10, the denoising step in JAMMLSE+L2L0, specially indicated to correct the effect of the Rician noise at low SNR regimes [88], improves drastically the quality of the reconstructions. In particular, the overall (θ̂) performances differ significantly between L2L0 and JAMMLSE+L2L0, with an average enhancement of up to 5° in the mean (θ̂) in different undersampling regimes. While in terms of angular resolution both L2L0NW and JAMMLSE+L2L0 exhibit similar performance, L2L0NW shows a higher SR∠ down to 10 samples. In this noise setting, we analyze in detail the ability of correctly assessing the number of fibers through the false positives and negatives rates. Results show the effectiveness of the spatial regularization applied both in JAMMLSE+L2L0 and L2L0NW, specially in avoiding overestimated directions (extreme decrease of n⁺∠) even if the number of missed fibers (n−∠) is also significantly decreased.

Plots analogous to Figures 5.4 and 5.5 can be found in [96], where an exhaustive comparison of all methods participating in the HARDI reconstruction Challenge 2012 is presented. The performance of these algorithms is evaluated on the same phantom used in our simulations by computing the same quality metrics described in the present paper (SR∠, θ̂, n⁺ and n−). Figure 5.6 shows a comparison of the performance of L2L0NW run with 15 samples with the following eight representative methods participating in the Challenge**: (i) DTI_neigh, classical DTI method enhanced using contextual information [100]; (ii) L2-L1-DL, method using dictionary learning in the framework of ℓ2-ℓ1 reconstruction [20]; (iii - iv) L2-L1-TV and L2-L1-TGV, using the ℓ2-ℓ1 problem formulation and including spatial regularization schemes based on total variation and total generalized variation, respectively [86]; (v - vi) L2-L2 and NN-L2, based on ℓ2 norm priors [6, 25]; (vii) DOT, classical diffusion orientation transform [101]; (viii) DSI_L, classical DSI enhanced using Lucy-Richardson deconvolution [102]. For a more detailed explanation of each reconstruction method, you can refer to [96]. Direct quantitative comparisons with all these standard state-of-the-art algorithms is not straightforward from the results, since every method was tested using different sampling schemes (different number of samples and distribution of points). Yet, L2L0NW can be positioned in the overall picture. In Figure 5.6, participant methods are sorted by the number of samples used for the reconstruction, increasing from left to right. The actual number of samples is indicated on the plot for every method. In mild noise conditions (SNR = 30), L2L0NW is able to correctly assess the number of fibers in 85% of voxels (SR∠ = 85) using as few as 15 signal samples and this quality appears comparable to the best SR∠ scores obtained in the Challenge with methods using many more points (from 30 up to 257) to recover the fiber configuration. The superiority of L2L0NW appears to be even more significant when a more noisy setting is considered. At SNR = 10, L2L0NW using only 15 samples, shows the same quality of

http://hardi.epfl.ch/static/events/2012_ISBI

**For the sake of consistency, all methods are named following the same notation as in [96].
reconstruction, in terms of both $SR_\angle$ and $\bar{\theta}$, as DSI using an exhaustive cartesian sampling scheme of 257 points. NN-L2 stands as the only method presenting slightly better results in terms of $SR_\angle$, yet, using 48 samples. Only with 15 samples L2L0NW is able to attain comparable levels of performance, thus implying a speed-up factor of three. We pay special attention to the comparison with the rest of methods that promote any kind of spatial regularization. L2L0NW with 15 samples ($SR_\angle = 85$ and mean($\bar{\theta}$) = 6.4°) outperforms L2-L1-TV, the method imposing TV regularization ([96]; see also [86]), in terms of success rate ($SR_\angle = 75$) and present similar average angular error (mean($\bar{\theta}$) = 6°), stressing the fact that the latter uses a sampling scheme with the double number of points (30 samples). Overall, we point out that all participant methods imposing spatial regularization (L2-L1-TV, L2-L1-TGV) use a significant amount of measurements (from 30 to 64 points) to recover the fiber configuration. The anatomical structured sparsity prior that we impose allows us to yield the same quality in the reconstructions using higher undersampling regimes.
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Figure 5.5: Comparison of $SR$, $\bar{\theta}$, $n^{-}\angle$ and $n^{+}\angle$ between L2L0, JAMMLSE+L2L0 and L2L0$_{NW}$ approaches. Experiments are performed on the phantom dataset used in [96] for a fixed SNR = 10. On the top left, $SR$ represents the success rate. On the top right, the boxplot diagrams present the distribution of $\bar{\theta}$ with the same conventions as for Figure 5.4. On the bottom row, $n^{-}\angle$ and $n^{+}\angle$ represent the false negatives and positives rates. Figure published in [7].

5.3.2 Real Data

5.3.2.1 Quantitative comparison

In this subsection, we compare quantitatively the reconstructions obtained from undersampled real data (i.e. hardi$_{30}$, hardi$_{20}$ and hardi$_{10}$) to those with fully-sampled data (i.e. hardi$_{256}$), considering the latter as ground-truth, for L2L0, JAMMLSE+L2L0 and L2L0$_{NW}$. Results quoted next are in agreement with those obtained for numerical simulations on the phantom, confirming that L2L0$_{NW}$ actually outperforms L2L0 and JAMMLSE+L2L0. Bearing in mind that he actual SNR in the $b=0$ images is about 30, results for JAMMLSE+L2L0 and L2L0$_{NW}$ appear in line with conclusions driven from the HARDI Reconstruction Challenge 2012, where it was shown that spatial regularization appeared to be effective also in low noise regimes, while merely denoising the images did not [96].

The average mean angular error ($\bar{\theta}$) using 30 samples was $13.9^\circ \pm 11.4^\circ$ (mean ± standard deviation over WM voxels of the whole brain volume) for L2L0, $14.5^\circ \pm 10.8^\circ$ for JAMMLSE+L2L0 and $7.8^\circ \pm 9.1^\circ$ for L2L0$_{NW}$. Reconstructions using 20 samples had an average error of $15.7^\circ \pm 11.2^\circ$ for L2L0, $16.7^\circ \pm 11.8^\circ$ for JAMMLSE+L2L0 and $9.1^\circ \pm 9.6^\circ$ for L2L0$_{NW}$. When one goes down to 10 samples, reconstructions using L2L0 and JAMMLSE+L2L0 exhibit an angular error of $19.8^\circ \pm 11.2^\circ$ and $19.8^\circ \pm 12.0^\circ$, respectively,
Figure 5.6: Comparison of $SR_\angle$ and $\bar{\theta}$ between different reconstruction methods. Experiments are performed on the phantom dataset used in [96] for a fixed SNR = 30 (top row) and SNR = 10 (bottom row). On the left, $SR_\angle$ represents the success rate. For the sake of comparison, the number of samples used for the reconstruction is reported in parentheses next to the name of each method. On the right, the boxplot diagrams present the distribution of $\bar{\theta}$, with the edges of each box representing the 25th and 75th percentiles, the mean and median value appear as “square” and “circle” value and the outliers are plotted as red dots. Figure published in [7].

which is already higher than the resolution of the spherical discretization defined by our dictionary; while the angular error for $L2L0_{NW}$ is $13.6^\circ \pm 10.5^\circ$. Results for the success rate are as well consistent with the results obtained in simulations. As in numerical simulations, the benefits of imposing a spatial regularization directly on the fiber orientations are more remarkable when we go to higher subsampling regimes. The $SR_\angle$ was $31.1\% \pm 46.3\%$ for $L2L0$, $34.8\% \pm 47.6\%$ for $JAMMLSE+L2L0$ and $67.0\% \pm 47.0\%$ for $L2L0_{NW}$ with 30 samples; $27.9\% \pm 44.9\%$ for $L2L0$, $28.0\% \pm 45.0\%$ for $JAMMLSE+L2L0$ and $61.7\% \pm 48.6\%$ for $L2L0_{NW}$ at 20 samples. All methods present a degradation in the quality of their reconstructions when we go down to 10 samples, $SR_\angle$ decreasing to $16\% \pm 36.6\%$ for $L2L0$, $18.8\% \pm 39.0\%$ for $JAMMLSE+L2L0$ and $40.6\% \pm 49.1\%$ for $L2L0_{NW}$.

Figure 5.7 illustrate the numerical results for one representative slice of the brain volume. The angular accuracy of each reconstruction is presented by plotting the mean angular error $\bar{\theta}$ per voxel in Figure 5.7. A map of the number of false positives and false negatives per voxel is used to illustrate the ability of each method of correctly assessing the number of fibers in Figure 5.8. The images show the superiority of $L2L0_{NW}$ with respect
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Figure 5.7: Angular accuracy (map of $\bar{\theta}$ per voxel) in real data between L2L0, JAMMLSE+L2L0 and L2L0\textsubscript{NW} reconstructions with 30, 20 and 10 samples (\texttt{hardi30}, \texttt{hardi20}, \texttt{hardi10} datasets, respectively). Figure published in [7].

...to L2L0 and JAMMLSE+L2L0, specially in those voxels close to the boundaries with the grey matter and the cerebrospinal fluid.

5.3.2.2 Qualitative comparison

The reconstructions\footnote{The images have been created using the tool \texttt{mrview} of \textit{mrtrix}. This required the FOD from L2L0 and L2L0\textsubscript{NW} to be previously converted to spherical harmonics.} of the FOD obtained with L2L0 and L2L0\textsubscript{NW} for a significant slice of the brain in the corona radiata region are compared qualitatively in Figures 5.9 and 5.10. These plots show the robustness of each method to two different undersampling regimes, \texttt{hardi30} and \texttt{hardi10}. In the light of the quantitative results obtained for both phantom and real data and given the fact that qualitative differences between reconstructions using L2L0 and JAMMLSE+L2L0 are difficult to appreciate, we do not show qualitative results for JAMMLSE+L2L0. In all images, three meaningful regions with fiber bundle crossings have been highlighted. With 30 samples (Figure 5.9 corresponding to \texttt{hardi30}), the FODs reconstructed by L2L0\textsubscript{NW} present neater and sharper profiles with less presence of spurious peaks than the ones reconstructed by L2L0. In addition, the fiber orientation distribution field reconstructed by L2L0\textsubscript{NW} looks qualitatively smoother overall. As a consequence, fiber bundles are better defined through more clearly identified peaks. Plots in Figure 5.10 show reconstructions performed with only 4\% of the original data (10 samples). In these images – corresponding to reconstructions with highly undersampled data – the...
above-mentioned qualitative differences between the two methods are confirmed and even more easily noticeable. As discussed in section 3.1, these differences can have a significant impact when applying tractography methods on these fiber orientation fields.
5.4 Conclusion

In this chapter we have proposed a novel algorithm to recover the intra-voxel FOD simultaneously for all voxels. The method leverages a spatially structured sparsity prior
Figure 5.10: Qualitative comparison on HARDI human data. Reconstructions of the FODs in the corona radiata region are shown for $L_{2L0}$ (top) and $L_{2L0_{NW}}$ (bottom) for 10 samples superimposed to the FA map. Figure published in [7].

directly on the FOD, where the structure originates from the spatial coherence of the fiber orientation between neighbor voxels. We have made use of a reweighting scheme to enforce structured sparsity in the solution. We have shown through numerical simulations and tests on real data that this method outperforms a voxel-by-voxel reconstruction method
when assessing the correct number of fibers and the angular precision of their orientation. As shown in section 5.3, exploiting spatial information about the neighboring directions appears essential to ensure a stronger robustness to noise and ability to go to higher undersampling regimes, leading to accurate reconstructions with only 15 samples.

We also compare the performance of our proposed method with respect to applying first a nonlocal denoising procedure and subsequently perform local reconstruction. This comparison allows us to highlight the benefits of using a spatial regularization as in our approach as opposed to this decoupled strategy. As presented in simulations, our spatial prior on the FOD outperforms as well the empirical TV regularization of $q$-space images proposed by [86], being able to recover the fiber orientation distribution using fewer samples. Note that spatial regularization of the $q$-space images is actually complementary to our formulation and could be added as an additional prior to our method.

The regularization presented in this paper could as well be applied in a voxel-by-voxel configuration, redefining the weights in formulation (5.3) to account for the values of the FOD in a defined neighborhood. Preliminary investigations in this direction did not provide promising results. Fixing a single bound to estimate the number of fibers separately in every voxel of the brain appears to be too constraining. On the contrary, setting a bound on the total number of fibers of the whole volume and solving the problem for all voxels simultaneously leaves more freedom on the effective directions (number of nonzero coefficients) per voxel. Furthermore, future evolutions of this algorithm should enable undersampling in Fourier space ($k$-space) for each of the $q$-space images acquired. This combined $k - q$-space sampling approach, along the lines of work by [86], will potentially enable a significant additional acceleration, in which context a voxel-by-voxel approach is not an option. Regarding computing resources, the memory requirements of a reweighting scheme to solve each voxel independently but using neighborhood information to define the weights would not differ from $L2L0_{NW}$, bearing in mind that the main operator $\Phi$ remains exactly the same for both formulations (5.3) and (5.5). In any case, the computation time of $L2L0_{NW}$ is affordable for a single processor, as described in section 5.2.7.

In recent work [9], the authors present a general framework for Accelerated Microstructure Imaging via Convex Optimization (AMICO) to recover the microstructure configuration voxel-by-voxel in regions with one single fiber population. In the next chapter we consider the spatial coherence of the microstructural features of the fibers all over the brain with the aim of extending the AMICO framework to regions of the WM with multiple fiber populations and more complex configurations.

The work presented in this chapter has been published in [7, 8].
Chapter 6

Fast microstructure estimation in regions with multiple fibers

6.1 Introduction

Most microstructure imaging techniques recover the microstructure properties by modeling the signal decay in different tissue compartments, e.g. axons, glial cells and extraxonal space. These methods can infer not only the orientation of the main fiber population in a voxel, but also their microstructural properties, such as the apparent average diameter and density of the axons. For an exhaustive survey of the existing techniques in the field the reader can refer to chapter 4 and [75].

All the techniques mentioned in section 4.5 have demonstrated the practical possibility to estimate microstructural information from dMRI data and the estimated microstructural indices have been shown to agree very well with known anatomical patterns observed with histology [1, 82, 103]. However, they still suffer from severe limitations. On one hand, the nonlinear routines usually employed to fit these models are computationally very intensive and cause practical problems for their application in studies with several subjects. Secondly, they are only valid in regions with one single fiber population, making them inappropriate to characterize the microstructure of the majority of voxels in the brain. Furthermore, they still require acquisition times that make them difficult to implement in vivo in a clinical context.

Recently, Daducci et al. presented a flexible framework for Accelerated Microstructure Imaging via Convex Optimization (AMICO) [9] to reformulate these microstructure imaging techniques as linear systems that can be solved using convex optimization methods (see 4.5.1). The convex optimization framework enables to include prior information about the signal, such as positivity, as long as it is formulated as a convex constraint. Besides this flexibility, convex optimization methods are fast and many efficient numerical algorithms exist to solve them (see chapter 2). Despite the drastic improvement in speed, the current framework of AMICO replicates microstructure imaging techniques that so far are only valid in regions with one fiber population. Therefore, its use remains inadequate for many widespread regions of the brain with multiple fiber bundles. ActiveAx was recently extended to allow axon diameter mapping also in regions with crossing fibers [104] and
thus, overcome this limitation. Still, it requires about 1-hour scan and, thus, it is difficult to be routinely included in clinical studies.

In the first part of this chapter, we present a first preliminary extension of the AMICO framework to be able to recover microstructure parameters also in regions with multiple fiber populations using fast algorithms. Numerical simulations evidence the ability of our new approach to recover microstructure parameters in regions with crossing fibers.

In the second part of the chapter, we go one step further and propose a novel formulation that estimates the microstructure configuration and the fiber orientation simultaneously in all voxels as a global optimization problem, exploiting information from neighboring voxels that cannot be taken into account with existing techniques. Our preliminary results show the potential of our proposed method to enable robust reconstructions from a reduced number of diffusion measurements, thus leading to faster acquisitions, too.

### 6.2 AMICO\textsubscript{X}

#### 6.2.1 Materials and Methods

The reconstruction problem for microstructure features from diffusion data accounting for multiple fibers is presented here as an extension of AMICO [9]. In this preliminary work we focus on extending the formulation for the ActiveAx model [1] to enable axonal diameter mapping in case of multiple fiber populations within a voxel.

As in original AMICO, the reconstruction problem is decoupled into two simpler sub-problems. First, the number and orientation of the fiber populations $\mu_i \in \mathbb{S}^2$ in each voxel is estimated. This can be achieved using any of several reconstruction methods, such as the standard Constrained Spherical Deconvolution (CSD) method [73]. Secondly, the linear operator $\Phi$ to express ActiveAx as a linear system is built from different sub-matrices:

$$\Phi = [\Phi^r_1|\Phi^h_1|...|\Phi^r_M|\Phi^h_M|\Phi^i].$$

In equation (6.6), sub-matrices $\Phi^r_i \in \mathbb{R}^{m \times N_r}$ and $\Phi^h_i \in \mathbb{R}^{m \times N_h}$ model, respectively, the intra-axonal and extra-axonal contributions to the diffusion signal along the direction $\mu_i (i = 1, \ldots, M)$. $M$ stands for the total number of detected fiber populations in the voxel. Each atom in sub-matrices $\Phi^r_i$ models the diffusion signal corresponding to water molecules restricted within parallel cylinders of a specific diameter. Alternatively, the atoms in sub-matrices $\Phi^h_i$ describe the hindered space between the axons. $N_r$ and $N_h$ represent, respectively, the number of different axon radii and hindered environments considered to build the dictionary. Sub-matrix $\Phi^i \in \mathbb{R}^m$ has a single atom that models the isotropic contribution corresponding to the CSF (note that it is orientation-independent). The signal response matching both restricted and hindered water diffusion in a voxel is estimated using the same models and parameter set as in [9]. For further details, the reader can refer to the original manuscript and find a specific description of these models.
in [75].

The microstructure recovery problem is then solved as a Tikhonov-regularized least squares problem as follows:

\[
\min_{x \geq 0} \frac{1}{2} \| \Phi x - y \|_2^2 + \frac{1}{2} \lambda \| x \|_2^2,
\]

where \( \| \cdot \|_2 \) is the standard \( \ell_2 \) norm and the parameter \( \lambda \geq 0 \) controls the trade-off between data regularization terms. The microstructure indices of interest defined by Alexander et al. [1] can be estimated for each individual fiber population from the recovered coefficients \( x \) by partitioning them as \([x^r_1 | x^h_1 | \ldots | x^r_M | x^h_M | x^i]\), corresponding to the contributions of hindered, restricted and isotropic compartments from every fiber bundle. In every voxel, the intra-axonal volume fraction \( \nu' \) indicates the ratio between restricted and hindered compartments; and for each of the fiber populations \( i \) \((i = 1, \ldots, M)\), the mean axon diameter index \( a'_i \) is expressed as a weighted average of the coefficients corresponding to restricted water diffusion, \( x^r_i \):

\[
\nu' = \frac{\sum_{i=1}^M \sum_{j=1}^{N_r} x^r_{ij}}{\sum_{i=1}^M (\sum_{j=1}^{N_r} x^r_{ij} + \sum_{j=1}^{N_h} x^h_{ij})}
\]

\[
a'_i = \frac{\sum_{j=1}^{N_r} 2R_j x^r_{ij}}{\sum_{j=1}^{N_r} x^r_{ij}},
\]

where \( R_j, j \in \{1, \ldots, N_r\} \) indicates the radius of the cylinder corresponding to the \( j \)-th atom in \( \Phi^r_i \). \( x^r_{ij} \) (alternatively, \( x^h_{ij} \)) denotes the contribution corresponding to the \( j \)-th restricted (alternatively, hindered) atom oriented along direction \( \mu_i \). We underline the fact that \( a'_i \) denotes a \textit{weighted} mean axonal diameter and is not expected to correspond to the \textit{true} mean axonal diameter over the axonal diameter distribution corresponding to the \( i \)-th fiber bundle (see its precise definition in 4.5 or refer to [1]). However, by abuse of language, we often refer to \( a'_i \) as mean axonal diameter when discussing our results.

Hereafter, to make results easier to interpret for the reader, we refer to the original AMICO formulation [9] as AMICO\(_1\) and to its extended version for multiple fibers as AMICO\(_X\). In the next section, the performance of both formulations is compared through numerical simulations.

### 6.2.2 Experiments

To evaluate the effectiveness of AMICO\(_X\), we tested it on synthetic data generated using the Monte-Carlo diffusion simulator system available in Camino [105], with the imaging protocol corresponding to a gradient strength \( G_{\text{max}} = 140 \text{mT/m} \) with 270 measurements divided into 3 shells with \( b \)-values\( = \{1930, 3090, 13190\} \text{s/mm}^2 \), corresponding to \( G = \{140, 131, 140\} \text{mT/m} \), \( \delta = \{10.2, 7.6, 17.7\} \text{ ms} \), \( \Delta = \{16.7, 45.9, 35.8\} \text{ ms} \) and same
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\( TR/TE = 5000/60 \text{ms} \) for all images. In all experiments when building the linear operators, we considered \( N_r = 10 \) different axon radii in a range of 0.1 - 8.5 \( \mu \text{m} \), and \( N_h = 7 \) different hindered environments corresponding to intra-axonal volume fractions from 0.3 to 0.9. No partial volume with CSF was included in the simulations, thus we did not consider any isotropic compartment in our dictionary (\( \Phi^i = \emptyset \)). Since the goal of this study remains to evaluate the ability of AMICO\(_X\) to correctly retrieve the microstructure indices of interest, we have chosen the regularization parameter \( \lambda \) that gives the minimal average relative error when fitting the mean axonal index over a set of 5 different pair of WM substrates. As a result, \( \lambda \) was fixed to 0.25.

We first simulated raw voxels with two fiber populations crossing at different angles (from 30° to 90°). Each fiber population consisted of a distribution of different axon diameter, as done in [1], and several WM substrates were tested. For each configuration, different relative ratios of the two populations were evaluated. In each case, the mean and standard deviation of the estimated microstructural parameters was computed over 1000 repetitions, contaminating the signal with independent Rician noise realizations corresponding to SNR = 30, and compared them to the ground-truth. The estimation of the fiber orientations was performed using standard CSD [73] and the CSD peak estimation using the toolbox MRTrix\(^*\) with 90 measurements corresponding to the outer shell. For compactness, only results corresponding to relative volume fractions \( f_{r_1} = \{0.5, 0.5\} \) and fiber population with 2 different radii – gamma distributions with parameters \((3.27, 4.9 \cdot 10^{-7})\) and \((4.82, 2.6 \cdot 10^{-7})\), respectively – corresponding to average axon diameters about 5.6 and 3.6 micrometers are reported here. Results on the other substrates are consistent.

6.2.3 Results and discussion

To show evidence of the need to consider more than one fiber population in the model, we fitted AMICO\(_1\) in the experimental settings described above to assess the impact of using this single-fiber model in regions with more than one fiber population. In these experiments, the atoms of the dictionary were oriented in the direction estimated with DTI, as in the original formulation [9]. The estimated microstructure indices (mean axon diameter and intra-cellular volume fraction) are compared with the ground-truth in Figure 6.1. AMICO\(_1\) assumes that the fibers inside the voxel follow only one direction. Results show that making such an assumption in voxels that actually contain more than one fiber leads to erroneous estimation of microstructural properties. Mean axonal diameter appears overestimated whereas the intra-axonal volume fraction is underestimated; and the absolute error increases with the crossing angle of the ground-truth fibers. As expected, in the AMICO framework, the importance of correctly estimating the number of fiber bundles in order to choose a correct model appears to be crucial.

Figure 6.2 compares the microstructure parameters estimated from AMICO\(_X\) with the

\(^*\)http://www.nitrc.org/projects/mrtrix/
ground-truth as a function of the crossing angles between the two fiber populations. The intra-cellular volume fraction can be estimated very accurately for all crossing angles (slightly over-estimated by about 4%). The mean axonal diameter of the two fiber populations can be as well estimated pretty robustly (both slightly under-estimated) for all crossing angles. However, when the two orientations are too close ($\approx 30^\circ$), the errors as well as the standard deviations of the estimates with respect to the ground-truth increase. These results are in line with (and slightly improve) those previously reported in [104]. The higher instability shown at $30^\circ$ can be well related to the performance of CSD in the peak-detection step. While the average angular error committed over the 1000 repetitions in crossings from $90^\circ$ to $40^\circ$ is less than $2^\circ$, CSD often identifies spurious peaks as true fiber directions for angles crossing at $30^\circ$, leading to a more unstable behavior and higher average angular error.

Figure 6.3 illustrates the impact of the angular inaccuracy of the orientation of the fiber populations $\mu_i$ on the estimation of the microstructure indices. In a substrate with two fibers crossing at a fixed angle of $60^\circ$, one of the directions used to build the dictionary was deviated from $1^\circ$ to $10^\circ$ from the actual orientation of the fiber. The intra-cellular volume fraction can be estimated accurately for all angular deviations, up to $10^\circ$. The estimation of the mean axonal diameter degrades progressively, yet absolute errors are smaller than $1\mu m$ for angular deviations up to $7^\circ$. These results are in-line with the angular accuracy of AMICO$_1$ [9].

Lastly, the proposed model was tested also in a voxel with 3 non-coplanar fiber populations, as a proof of concept that evidences its generalization to multiple fiber crossings. In this experiment, the crossing angle between two of the fibers was fixed to $90^\circ$ and the angle between the third one and the others varying between $30^\circ$ and $90^\circ$. Only results corresponding to a crossing of two populations with an average axon diameters about 5.6 and one of about 3.6 micrometers are reported. Again, results with different substrates...
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Crossing angles (degrees) Crossing angles (degrees)

Figure 6.2: Performance of AMICO\textsubscript{X} on 2-fiber synthetic substrates as a function of the crossing angle between the fibers. Plots show the mean and standard deviation of the estimated mean axonal diameter (left) and intra-axonal volume fraction (right) for the two different fiber populations. Dashed lines represent the ground-truth values for the two populations.

Angular shift (degrees) Angular shift (degrees)

Figure 6.3: Robustness to inaccuracies in the estimation of $\mu_2$. Plots show the estimated mean axonal diameter (left) and intra-axonal volume fraction (right) as a function of the angular deviation of the estimated direction $\mu_2$ with respect to the actual orientation of fiber population 2. Dashed lines represent the ground-truth values for the two populations.

are consistent. Figure 6.4 compares the estimated microstructure features with the ground truth as a function of the crossing angles between the 3 estimated populations.

The non-optimized version of the code, implemented in MATLAB and run on a standard 2.70GHz Intel Core i7-3740QM processor, is able to fit the model in approximately 3.7ms/voxel. Therefore, AMICO\textsubscript{X} still enables a drastic reduction of the computation time to solve the microstructure imaging problem as well in regions with multiple fiber populations compared to other nonlinear routines, such as ActiveAx, which take $\approx 20s$/voxel to fit its model [9].

So far, we have extended the original AMICO framework, that enables fast axonal diameter mapping with ActiveAx [1], to include crossing fiber populations within a voxel. Our results show through numerical simulations that AMICO\textsubscript{X} is indeed able to robustly
Figure 6.4: Performance of AMICO on 3-fiber synthetic substrates as a function of the crossing angle between the fiber population 1 and 2. The crossing angle between populations 1 and 3 is fixed to 90°. Plots show the mean and standard deviation of the estimated mean axonal diameter (left) and intra-axonal volume fraction (right) for the three different fiber populations. Dashed lines represent the ground-truth values for the three populations.

estimate the microstructure parameters, provided the number and orientation of the fiber populations in a voxel is correctly estimated (up to ≈ 7° of angular accuracy). We have as well shown how, thanks to the fast convex optimization methods, AMICO enables a reduction of the computation time by orders of magnitude with respect to other microstructure imaging techniques also in voxels with complex fiber configurations. The extended data model of AMICO can be fitted fast and accurately in all voxels of the brain, as in [104], thanks to the generalization of the original formulation to environments with multiple fibers.

In the next section, a reformulation of the AMICO framework is proposed to enable microstructure reconstructions from a reduced number of measurements, thus leading to faster acquisitions.

6.3 AMICO

6.3.1 Materials and Methods

With the goal of enabling reconstructions in a highly-undersampled regime and thus speeding-up the acquisition time, we decide to impose a stronger regularization prior to exploit the smoothness of the fiber characteristics throughout the brain. To do so, we reformulate the microstructure recovery problem for the whole field of voxels simultaneously and therefore, we can take advantage of the neighbor information that cannot be taken into account when considering the problem independently in each voxel. Inspired by AMICO for ActiveAx to cope with multiple fiber populations and adapting the weighting scheme described in chapter 5 to exploit neighboring information, axon diameter mapping is presented here as a sequence of weighted linear problems as follows:
\[
\min_{X \in \mathbb{R}^{N_c \times N}} \|\Phi X - Y\|_2^2 + \lambda \|X\|_{W,1}. \tag{6.5}
\]

In (6.5), matrix \(Y \in \mathbb{R}^{m \times N}\) contains the \(m\) diffusion measurements from all \(N\) voxels of the image. The dictionary:

\[
\Phi = [\Phi_1 | \ldots | \Phi_n] = [\Phi^r_1 | \Phi^h_1 | \ldots | \Phi^r_n | \Phi^h_n] \tag{6.6}
\]

is a concatenation of sub-dictionaries \(\Phi_i\), built as in section 6.2.1, each modeling the intra- and extra-axonal contributions to the dMRI signal along direction \(\mu_i\), and \(\{\mu_1, \ldots, \mu_n\}\) is the set of discrete orientations uniformly distributed on the half-sphere used in the reconstruction.

Each recovered coefficient is associated to a restricted (or hindered) compartment with axonal diameter (or perpendicular diffusivity) \(m\), oriented in direction \(d\) for voxel \(v\), and therefore can be indexed using a triple index \(dvm\). Throughout this section we refer to each coefficient as an element of a three dimensional tensor \(X\); however, formally we organize them in matrix form – \(X \in \mathbb{R}^{N_c \times N}\), with \(N_c = n \cdot (N_r + N_h)\) – so that we can easily express the linear convolution as a matrix product, see Figure 6.5. These coefficients allow us to recover, for every voxel:

(i) The orientation of the fiber bundles.

(ii) The microstructure indices defined in [1], which are estimated in every voxel and for each individual fiber population from the recovered coefficients \(X\), as described in formulations (6.3) and (6.4).

We highlight that, unlike the original AMICO framework, this new formulation enables the simultaneous estimation of the number of fiber populations present in the voxel, their orientation(s) and their microstructure characteristics.

In (6.5), we minimize a global data term and a sparsity constraint that simultaneously promotes spatial coherence of the solution, like in formulation (5.5). In this case, the sparsity stems from the small number of fiber directions of interest. Indeed, among the considered set of \(n\) discrete directions we expect only a few of them to have non-negligible values. \(\|\cdot\|_{W,1}\) stands for the weighted \(\ell_1\)-norm which, by properly designing \(W\), induces spatially structured sparsity in the solution following the principle introduced in chapter 5 (see equation (5.6) and explanation below). In this case, the weights \(W\) allow us to exploit neighborhood information and promote coherence in the so-called “spatial-angular-microstructure” (SAM) space. Since each restricted atom is associated to a specific diameter, we define its microstructural neighborhood \(N(m)\) as the two atoms with the closest bigger and smaller associated diameter. Figure 6.6 shows a visual representation of \(N(m)\), analogous to \(N(d)\) and \(N(v)\) defined in chapter 5. Similarly, for each hindered
atom associated to a specific perpendicular diffusivity, its neighborhood is defined as the two atoms with the closest larger and smaller diffusivity.

The weights regularize the coefficients in the microstructure dimension depending on their spatial position and orientation, and promote anatomical coherence among them according to the underlying fiber structure. Formally, they are defined adding the microstructural dimension to equation (5.7), as follows:
Chapter 6. Fast microstructure estimation in regions with multiple fibers

\[ W_{dvm}^{(t+1)} = \left[ \tau^{(t)} + \frac{1}{N(v)} \sum_{d'v'm' \in N(dvm)} |X_{d'v'm'}^{(t)}| \right]^{-1}. \]  

(6.7)

In (6.7), the weights \( W \) are expressed in tensor form to make use of the triple indexing. However, we formally organize them in matrix form \( W \) so that \( \|X\|_{W,1} \) is well defined.

The whole reweighting scheme imposes a structured sparsity of the solution, encouraging that neighbor voxels present the same or close – neighbor – directions and microstructure. Indeed, these weights promote that in every voxel, the directions and the microstructure features are coherent with their environment.

The role and updating strategy for parameter \( \tau \) in (6.7), as well as the main steps of the reweighting scheme are the same as described in chapter 5.

6.3.2 Experiments

To evaluate the effectiveness of AMICO\textsubscript{SAM}, we tested it on synthetic data generated using the Monte-Carlo diffusion simulator system available in Camino [105], with the same imaging protocol detailed in section 6.2.2. In order to assess the robustness to data undersampling, we simulated different datasets using a decreasing number of measurements, from 270 (fully-sampled) to 54 (as typical HARDI protocols). The microstructural indices estimated with AMICO\textsubscript{SAM} were compared to the original voxelwise fitting, AMICO\textsubscript{X}, and results are reported as averages over 10 Rician noise realizations (SNR=30).

Since the goal of this study is mainly to investigate the behavior of AMICO\textsubscript{SAM} in highly undersampled regimes, in all experiments, we tuned \( \lambda \) empirically to get the minimum average absolute error of the estimated parameters over several WM substrates.

We present results on two different kind of simulated substrates. We first show simulations considering only the signal decay due to water diffusion in the intra-axonal compartments. We simulated a field of 10 \( \times \) 10 raw voxels corresponding to two fiber populations, consisting of cylinders with different radii distributions – as in [1] – crossing at given angles (30° – 90°). As in the previous section, we performed the following tests with different WM substrates but, for compactness, we report only results corresponding to populations with mean axonal diameter 2.9 and 5.2\( \mu \)m. Results on other substrates were consistent.

Secondly, to account for a more realistic situation, we simulated the signal corresponding to a field of 10 \( \times \) 10 raw voxels with two fiber populations crossing, including this time the contribution due to water diffusing outside the axons.

In all simulations, when building the linear operators, we considered \( n = 50 \) directions uniformly distributed on the half sphere and \( N_r = 7 \) different axon radii in a range of 1 - 7 \( \mu \)m. In simulations where the extra-axonal compartment is not taken into account, we considered \( N_h = 0 \), otherwise \( N_h = 7 \) corresponding to volume fractions from 0.3 to 0.9.
6.3.3 Results and Discussion

Simulations without extra-axonal compartment

Figures 6.7 and 6.8 show the reconstructions for the two methods corresponding to 270 and 54 samples, respectively. The estimated microstructure indices (mean axonal diameter and population ratio) are shown as a function of the crossing angle between the fibers; dashed lines correspond to the ground truth values. In a fully-sampled context (Figure 6.7), there are no significant differences between the quality of the two reconstructions other than an increasing variability in the estimation with AMICOX compared to AMICOSAM, mainly when fibers get closer (30°). However, in a highly undersampled regime (Figure 6.8), AMICOSAM continues to estimate accurately and precisely the population relative ratio whereas AMICOX shows difficulties when the fibers are too close (≤ 45°). Regarding the estimation of the mean axonal diameter with 54 samples, AMICOX shows very unstable reconstructions and does not reliably assess the true values. On the other hand, AMICOSAM is able to disentangle the two fiber populations and shows more accurate estimations at all crossing angles, even if we can observe a lower precision (higher std) in the estimates with respect to the reconstructions with a fully-sampled dataset.

Simulations including extra-axonal compartment

Figures 6.9 and 6.10 show the microstructure estimates for two WM substrates with mean axonal diameters 5.6 and 2.8 μm and an intra-axonal volume fraction of 0.75. These reconstructions appear in general more unstable than those considering only the intra-axonal compartment (Figures 6.7 and 6.8). We have observed that in some cases the algorithm “confuses” the restricted atoms associated to the highest diameters and hindered atoms, leading to an increasing general variability in the microstructure estimates.

In a fully-sampled context (Figure 6.9), there are no significant differences in the quality of the volume fraction and population relative ratio estimates between the two methods, even if we can observe a higher variability in the intra-axonal volume fraction estimated with AMICOSAM. However, regarding the mean axonal diameters, AMICOX estimates them accurately for both fiber populations, whereas AMICOSAM consistently underestimates the highest mean axonal diameter by about 10%. We suspect the higher variability that AMICOSAM shows in the estimation of the intra-axonal volume fraction compared to AMICOX is linked to this underestimation of the mean axonal diameter, pointing to a confusion between some restricted/hindered atoms that we referred to in the former paragraph.

In a highly-undersampled regime (Figure 6.10), AMICOX shows a very unstable reconstruction of the mean axonal diameters for both populations and an increasing degradation of the population relative ratio estimates as the two fibers get closer. On the other hand, the mean axonal diameters, relative population ratio and intra-axonal volume fraction recovered with AMICOSAM are consistent for all crossing angles and coherent with the es-
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Figure 6.7: Detailed comparison of the mean axonal diameter index and population relative ratio estimated with AMICO$_X$ (left) and AMICO$_{SAM}$ (right), as a function of the crossing angle between the fiber populations. Results correspond to the fully-sampled protocol with 270 measurements, considering only the water diffusion inside the axons.

Estimations using 270 samples, even if we observe an increased variability (higher standard deviation). Considering that AMICO$_X$ is a 2-step procedure, a deeper analysis to better understand the origin of the instability of its highly-undersampled reconstructions should be carried out. Indeed, we should evaluate the angular errors committed when assessing the main fiber orientations and their impact on the estimation of the microstructure indices. Anyway, the inability of disentangling the 2 fiber populations at 75° suggests that the main source of error comes from the minimization problem itself, and not from the angular error.

Overall, we highlight that even if AMICO$_{SAM}$ consistently underestimates the highest mean axonal diameter, it is able to correctly disentangle the two fiber populations for all crossing angles also in a highly-undersampled regime and that the three microstructure features are robustly estimated as we undersample.

6.3.4 Limitations and future work

In this section we have presented AMICO$_{SAM}$, that provides a flexible framework to solve both the fiber orientation and the microstructure recovery problems simultaneously.
6.3. AMICO SAM

Figure 6.8: Detailed comparison of the mean axonal diameter index and population relative ratio estimated with AMICO\textsubscript{x} (left) and AMICO\textsubscript{SAM} (right), as a function of the crossing angle between the fiber populations. Results correspond to an undersampled protocol with 54 measurements (≈ 20% of the fully-sampled protocol), considering only the water diffusion inside the axons.

while applying a regularization in three spaces: spatial, angular and microstructural. The preliminary work that we have presented so far shows robust reconstructions from a reduced number of diffusion measurements, opening the door to fast acquisitions for diffusion microstructure imagine. However it still shows many limitations that need to be overcome and appear as the target for our future work.

Study different sampling schemes/sequences

In this work, we have simulated data assuming PGSE sequences with the same sampling protocol used in [1], that corresponds to 3 shells with a maximum gradient strength \( G_{max} = 140\text{mT/m} \). Different sequences (other than PGSE) and sampling protocols need to be investigated. Indeed, problem (6.5) is ill-posed since operator \( \Phi \) is extremely ill-conditioned. One of the strategies to improve the conditioning of our linear operator \( \Phi \) would be to decrease the correlation between its columns by designing a different sampling protocol. We are confident that this would help the algorithm in correctly distinguishing between atoms corresponding to intra- and extra-axonal compartments.
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Figure 6.9: Detailed comparison of the mean axonal diameter index and population relative ratio estimated with AMICO\(_x\) (left) and AMICO\(_\text{SAM}\) (right), as a function of the crossing angle between the fiber populations. Results correspond to the fully-sampled protocol with 270 measurements.

Study the design of the dictionary

Intrinsic parameters of the algorithm, such as the chosen number of directions on the half-sphere \(n\) or the number and the range of the intra- and extra-axonal compartments have a direct impact on the complexity of the dictionary. In close relation with the previous point, the design of the dictionary should be optimized so that the linear inverse problem to be solved is the least ill-posed as possible.
Figure 6.10: Detailed comparison of the mean axonal diameter index and population relative ratio estimated with AMICO\textsubscript{x} (left) and AMICO\textsubscript{SAM} (right), as a function of the crossing angle between the fiber populations. Results correspond to an undersampled protocol with 54 measurements, corresponding to \(\approx 20\%\) of the fully-sampled protocol.

**Study different q-space undersampling strategies**

AMICO\textsubscript{SAM} appears as an extension of the AMICO framework to enable microstructure reconstructions from a reduced number of measurements, thus leading to faster acquisitions. To undersample our fully-sampled dataset, so far we have uniformly reduced the number of points in every shell, i.e. our undersampled datasets contain the same number of data points in every shell and they are located along the same orientations. Different undersampling strategies should be investigated. As pointed out in [106], a careful design is central in the success of multi-shell acquisition and reconstruction techniques. In their
work, the authors provide a general method to design multi-shell acquisition with uniform angular coverage that should be studied in the framework of our problem.

**Study different regularization strategies**

As mentioned in section 6.3.1, the weights regularize the coefficients and thus, the proposed reweighting scheme imposes smoothness through structured sparsity of the solution. Thanks to the flexibility of convex optimization, different prior information can be easily imposed through a different definition of the weights and its effect can therefore be investigated. For instance, we could make only the intra-axonal compartments be dependent on the surrounding voxels and not the extra-axonal ones, or vice versa.

An alternative regularization function, a weighted mixed $\ell_{2,1}$ norm\(^1\) to promote *group sparsity* in the solution was also considered. Preliminary results justify a deeper investigation in that direction. Moreover, the reformulation of the unconstrained problem into a constrained one would avoid tuning the regularization parameter $\lambda$, provided a good approximation of the overall bound on the level of the noise could be estimated.

**Further validation**

Synthetic data obtained from a Monte-Carlo diffusion simulator offers a good starting validation strategy, commonly used by the community \cite{1, 9}. However, a validation of AMICO\(_{\text{SAM}}\) on more complex phantoms to test its ability to correctly assess the number and orientation of the fiber populations, as well as their microstructure features in a more challenging context appears as the next natural step. Furthermore, other validation strategies both on *ex-vivo* and *in-vivo* data should be designed and obviously follow.

**6.4 Conclusion**

In this chapter, we have first presented AMICO\(_X\), a convex framework for microstructure imaging that enables fast microstructure feature mapping in regions with multiple fiber populations. In the second part, we have applied the idea of spatial regularization through structured sparsity described in chapter 5 to the microstructure recovery problem. As a result, we propose a new formulation that estimates simultaneously the orientation and the microstructure of the fiber bundles. AMICO\(_{\text{SAM}}\) exploits neighboring information to impose a strong regularization in the so-called “spatial-angular-microstructure” (SAM) space. Consequently, it enables robust reconstructions from a low number of measurements, thus leading to faster acquisitions.

Preliminary results on synthetic data show that AMICO\(_{\text{SAM}}\) has the potential to disentangle different fiber populations and to correctly assess both intra-axonal volume fraction

\(\text{For an arbitrary matrix } X \in \mathbb{R}^{m \times n} \text{ its } \ell_{2,1} \text{ norm is defined as } ||X||_{2,1} = \sum_{i=1}^{m} \sqrt{\sum_{j=1}^{n} X_{ij}^2}.\)
and relative population ratio with as few as $\approx 50$ measurements (as typical HARDI protocols). It is plausible to think that the powerful regularization prior in the SAM space can as well guarantee a strong robustness to noise. AMICO$_{\text{SAM}}$ should be tested under different noise conditions to confirm this hypothesis. Also, further validation on real data is still needed.

We highlight that AMICO$_{\text{SAM}}$ provides a versatile and flexible model-independent framework for microstructure imaging. In this chapter we have presented results on AMICO$_{\text{SAM}}$ for ActiveAx [1], but, as the original AMICO [9], it can potentially be applied to any other microstructure imaging modality. Moreover, the weights can be easily redefined to impose smoothness priors according to the context of study.

The fact that AMICO$_{\text{SAM}}$ simultaneously estimates the fiber orientations and their microstructure features, brings this algorithm specially close to the field of microstructure informed tractography [107, 108], that combines microstructure information and tractography. Future work should consider merging the principles behind AMICO$_{\text{SAM}}$ with algorithms such as COMMIT [107].

**Generalization to multiple correlated sparse signal recovery**

Before concluding, we would like to highlight that our proposed formulation to promote spatial regularization through a structured sparsity prior can actually be applied in a more generic framework for *multiple correlated sparse signal recovery*. In sections 5.2 and 6.3.1, spatially-correlated vectors are concatenated to build matrix $X$. Formulations (5.5) and (6.5) can actually be generalized to recover multiple sparse signals correlated through a smoothness prior on the variation of the signal support in the inter-signal dimension. Indeed, considering the concatenation of $n_D$ correlated sparse signals into a tensor $X \in \mathbb{R}^{n_1 \times \ldots \times n_D}$ and a linear operator $\Phi$ that models a measurement process on them, equation (5.5) can be rewritten as:

$$\min_{X \in \mathbb{R}^{n_1 \times \ldots \times n_D}} \|\Phi(X) - y\|_2^2 \text{ s.t. } \|X\|_{W,1} \leq K, \quad (6.8)$$

with $\| \cdot \|_{W,1}$ denoting a weighted-$\ell_1$ norm of a generic tensor defined as:

$$\|X\|_{W,1} = \sum_{i_1,\ldots,i_D} W_{i_1\ldots i_D} |X_{i_1\ldots i_D}|. \quad (6.9)$$

The definition of the weights and neighborhoods will enable the embedding of the smoothness prior in the signal support through the structure on the sparsity and must, of course, be adapted to the application. Our method stands in contrast to other joint sparsity models [109, 110] that assume a common support of the correlated signals. Social sparsity models [111, 112] also leverage the concept of neighborhoods to promote sparsity. However, our proposed algorithms are essentially inspired from the reweighting scheme.
proposed by Candes et al. [24] to approach $\ell_0$ minimization through the convex minimization of a weighted $\ell_1$ norm. Our contributions lie in enforcing a \textit{structured version} of the $\ell_0$ norm of the solution at convergence and thus, the weights should continue to represent the inverse value of the associated entry at the previous iteration, to converge to an $\ell_0$ norm.

Part of the work presented in this chapter has been published in [8, 10, 11, 12, 13].
In this thesis, we have studied sparse Fourier sensing problems in the fields of optical interferometry and diffusion MRI. In both applications, we face ill-posed (with less available measurements than the dimension of the signal) and highly nonlinear problems. Our strategy to solve these originally nonlinear problems resorts to reformulating them as linear inverse problems that can be solved using convex optimization methods. Inspired by the compressed sensing framework, we propose novel priors to leverage the sparse structure (i.e. low dimensionality) of the solution.

All nice properties of the convex optimization framework prove to be the cornerstone of our contributions:

- **From the formulation point of view**, convex optimization constitutes an extremely adaptable framework that enables the straightforward inclusion of prior information about the signal, as long as it is formulated as a convex constraint. In this thesis we have immensely taken advantage of this characteristic to design the proposed novel algorithms. In the application for optical interferometry, we regularize the linearized inverse problem through a nuclear norm relaxation of a low rank constraint, easily imposing also positive-semidefiniteness, reality, positivity and optionally sparsity constraints. In diffusion MRI, we resort to a reweighted scheme and design a flexible weighting system that enforces structured sparsity and promotes spatial regularization in the solution simultaneously. Thanks to this flexibility, we design powerful regularization priors that guarantee a strong robustness to noise and the ability to go to higher undersampling regimes. In diffusion MRI, where the measuring process is considerably time consuming, this ability of solving the problem with few data points appears crucial for the technique to be clinically feasible.

- **From the reconstruction point of view**, convex problems converge to a global minimum and do not depend on the initialization. These two properties are key to our contribution in the field of optical interferometry, where state-of-the-art methods generally perform local optimization, highly dependent on both the initial image and the path followed by the method. Moreover, convex problems can conveniently be solved using fast proximal splitting methods. The increase of speed with respect to other nonlinear routines represents also a contribution in the
field of microstructure imaging.

We note that our original formulation presented in Part I can be seen as a generalization of the Phase Lift approach for the phase retrieval problem [2]. Indeed, we lift the ambient dimension of the problem to formulate a tensor completion problem from a set of linear measurements on the tensor. We have therefore proposed a novel linear alternative to deal with bispectrum (nonlinear) measurements that can be useful to other fields facing bispectral analysis.

We would also like to highlight that the method presented in Part II of this thesis to promote spatial regularization through a structured sparsity prior can actually be applied in a more generic framework for multiple correlated sparse signal recovery. A generalization of our formulation can account for multidimensional signals and correlations of different nature - such as temporal - between them. The definition of the neighborhoods as well as the weights should be adapted to the application.

7.1 Perspectives

7.1.1 Optical Interferometry

Among our two proposed methods to solve the imaging problem in the field of optical interferometry, the AM approach has been further studied and developed in [63], including sparsity priors and presenting convergence guarantees. On the other hand, our proposed linear and convex approach NM ensures desirable properties of convergence and independence on the initialization and we are convinced it is worth a deeper study. The main challenge associated to the practical implementation of this approach lies in the increase of the ambient dimension, as the price to pay for the linearization. Indeed, the linear approaches NM and NM-RW turn out to be extremely demanding from the computational point of view. Therefore, in our opinion, all efforts should be focused on studying software and hardware optimization to solve the problem for higher dimension images, e.g. using graphics processing units [61]. Additionally, recent approaches for radio interferometry [60] justify the investigation of different kind of sparsity priors, thanks to the versatility of convex optimization. Finally, our theoretical results should be confirmed on real data and be explicitly compared to other state-of-the-art methods. Bringing our theoretical results closer to reality would enhance our contribution that remains a unique approach to formulate the challenging problem of image reconstruction in optical interferometry as a tensor completion problem.
7.1. Perspectives

7.1.2 diffusion MRI

Unified framework with fiber tracking

Results of the HARDI reconstruction challenge (ISBI 2013) [113], in which we participated, already gave evidence that local reconstruction methods and global tractography cannot be treated separately any more. In our opinion, intra-voxel dMRI and global tractography should be unified in a single framework, intending to (i) reconstruct the fiber configuration (orientation and microstructure) in each voxel and (ii) solve the fiber-tracking across the whole brain, simultaneously. Work in this direction should consider merging our approach with COMMIT [107], that provides a Convex Optimization Model for Microstructure Informed Tractography.

Combined $k$-space and $q$-space undersampling

Further evolutions of our method for fiber reconstruction (either orientation or microstructure) should consider undersampling in Fourier space ($k$-space) for each of the $q$-space images acquired, along the lines of work in [86]. Indeed, the assumption that our function of interest is sparse in fiber space enables $q$-space undersampling, as we have shown. As soon as the problem is formulated globally (i.e., solved for all voxels simultaneously instead of voxelwise), as we do, the sparsity of the signal can also be considered in voxel space; thus leading to combined $q$-space and $k$-space undersampling and potentially resulting into a significant additional acceleration.

In a setting where the acquisition can be accelerated either by undersampling in $q$-space (probing the signal with less diffusion vectors) and/or in $k$-space (probing the signal in less voxels), the optimal acceleration scheme in terms of acquisition speed (number of measurements) and reconstruction quality should be studied. Recent work [114, 115] initiated this line of investigation for fiber orientation recovery; analogous work for microstructure estimation should follow.

Implementation on real MR scanners

In close relationship with our previous point, implementation on real MR scanners of sampling sequences optimized for our proposed formulation should follow. Collecting real data and confirming our numerical results would represent the ultimate validation of the ability of our novel formulation to perform fiber reconstruction in all regions of the brain in a clinical context.


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List of Publications

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