

# **Linear Inverse Problems (2/2)**

**Mathematical Foundations of Signal Processing** 

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# **Functional Linear Inverse Problems**

#### **Functional Inverse Problems**

In the previous lecture, we have constrained the signal *f* to be finite-dimensional:

$$f = \sum_{n=1}^{N} \alpha_n \psi_n = \Psi \boldsymbol{\alpha}, \qquad \boldsymbol{\alpha} = [\alpha_1, \dots, \alpha_N] \in \mathbb{R}^N,$$

for some suitable basis functions  $\{\psi_n, n=1,\ldots,N\}\subset \mathscr{L}^2(\mathbb{R}^d)$ . The idea was to reduce the number of degrees of freedom of the signal f to something manageable given the finite-dimensional data. While sensible, it is unclear if this discretisation step can be done canonically:

- How should we choose N?
- How should we choose the parametrising basis functions  $\{\psi_n, n=1,...,N\}$ ? (pixels, sines/cosines, radial basis functions, polynomials, splines...)

To answer these questions, we relax the finite-dimensional assumption and formulate the reconstruction problem directly in the continuous domain. We then characterise the form of the solutions and deduce canonical discretisation schemes.

<sup>&</sup>lt;sup>1</sup>Typically chosen as indicator functions of regular rectangular tiles of  $\mathbb{R}^d$  called pixels.

### **Functional Tikhonov Regularisation**

Consider the following functional penalised Tikhonov problem:<sup>2</sup>

$$\min_{f \in \mathcal{H}^k} F(\mathbf{y}, \Phi^* f) + \lambda \left\| D^k f \right\|_2^2, \tag{1}$$

where  $k \ge 0$ ,  $\lambda > 0$  and:

- $D^k$  denotes the k-th derivate operator on  $\mathbb{R}$ .
- $\mathcal{H}^k := \left\{ f \in \mathcal{L}^2(\mathbb{R}) : \left\| D^k f \right\|_2 < +\infty \right\}$  denotes the Hilbert space of functions with square-integrable k-th derivatives called Sobolev space.
- $\Phi^*: \mathcal{H}^k \to \mathbb{R}^L$  is the sampling operator associated with a linearly independent family of sampling functionals  $\{\varphi_1, \ldots, \varphi_L\} \subset \mathcal{H}^k$  and such that  $\mathcal{N}(\Phi^*) \cap \mathcal{N}(D^k) = \{0\}$ .
- $F: \mathbb{R}^L \times \mathbb{R}^L \to \mathbb{R}_+ \cup \{+\infty\}$  is a cost functional assumed proper convex, coercive and lwsc w.r.t. its second argument.

<sup>&</sup>lt;sup>2</sup>Note that the unknown signal  $f: \mathbb{R} \to \mathbb{R}$  in (1) is a function and not a discrete vector anymore.

### **Functional Representer Theorem**

#### Representer Theorem: (Functional Tikhonov) [1, Theorem 3]

Under the assumptions listed on Slide 5, the solution set of (1) is non empty, convex, compact. Moreover, any solution  $f^* \in \mathcal{V}$  can be written as:

$$f^{*}(x) = \sum_{i=1}^{L} \alpha_{i} (\rho_{k} * \varphi_{i})(x) + \sum_{j=0}^{k-1} \beta_{j} x^{j}, \qquad \forall x \in \mathbb{R},$$
 (2)

for some coefficients  $\alpha = [\alpha_1, \dots, \alpha_L] \in \mathbb{R}^L$ ,  $\beta = [\beta_0, \dots, \beta_{k-1}] \in \mathbb{R}^k$  such that

$$\sum_{i=1}^{L} \alpha_i \left\langle x^j, \varphi_i \right\rangle = \sum_{i=1}^{L} \alpha_i \int_{\mathbb{R}} \varphi_i(x) x^j dx = 0, \qquad \forall j = 0, \dots, k-1.$$
 (3)

and where

$$\rho_k(x) = \mathscr{F}^{-1}\left\{|\omega|^{-2k}\right\}(x) = \frac{|x|^{2k-1}}{2(-1)^k(2k-1)!}, \qquad x \in \mathbb{R}.$$
 (4)

Moreover if  $F(y, \cdot)$  is strictly convex, then the solution is unique.

#### **Canonical Discretisation**

We can re-write (2) as

$$f^{\star} = \Psi \boldsymbol{\alpha} + \Lambda \boldsymbol{\beta},$$

where  $\Psi: \mathbb{R}^L \to \mathscr{H}^k$  and  $\Lambda: \mathbb{R}^k \to \mathscr{H}^k$  are the synthesis operators associated to the family of functions  $\{\rho_k * \varphi_i, i=1,\ldots,L\}$  and  $\{x^j, j=0,\ldots,k-1\}$  respectively. We have then:

$$\Phi^* f^* = \Phi^* \Psi \alpha + \Phi^* \Lambda \beta = G\alpha + H\beta, \tag{5}$$

where  $G = \Phi^* \Psi \in \mathbb{R}^{L \times L}$  and  $H = \Phi^* \Lambda \in \mathbb{R}^{L \times k}$  are real matrices with entries given by:

$$G_{ij} := \langle \rho_k * \varphi_j, \varphi_i \rangle$$
,  $i, j = 1, ..., L$ , and  $H_{in} := \langle x^n, \varphi_i \rangle$   $i = 1, ..., L$ ,  $n = 0, ..., k-1$ .

We have moreover:

$$\|D^{k}f^{\star}\|_{2}^{2} = \left\langle D^{k}f^{\star}, D^{k}f^{\star} \right\rangle = \left\langle D^{k}\Psi\boldsymbol{\alpha} + \underbrace{D^{k}\Lambda\boldsymbol{\beta}}_{=0}, D^{k}\Psi\boldsymbol{\alpha} + \underbrace{D^{k}\Lambda\boldsymbol{\beta}}_{=0} \right\rangle = \left\langle D^{k*}D^{k}\Psi\boldsymbol{\alpha}, \Psi\boldsymbol{\alpha} \right\rangle$$

since  $\Lambda \beta = \sum_{j=0}^{k-1} \beta_j x^j$  is a polynomial of degree k-1 and hence  $D^k \Lambda \beta = 0$ .

# **Canonical Discretisation (continued)**

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Additionally, we have from (4) and the convolution/multiplication theorem that:

$$D^{k*}D^k\Psi\pmb{\alpha} = \sum_{i=1}^L\alpha_i\mathcal{F}^{-1}\left\{-j\omega^kj\omega^k\hat{\rho}_k\hat{\varphi}_i\right\} = \sum_{i=1}^L\alpha_i\mathcal{F}^{-1}\left\{\frac{|\omega|^{2k}}{|\omega|^{2k}}\hat{\varphi}_i\right\} = \sum_{i=1}^L\alpha_i\varphi_i = \Phi\pmb{\alpha},$$

which yields:

$$\|D^{k}f^{\star}\|_{2}^{2} = \langle D^{k*}D^{k}\Psi\boldsymbol{\alpha}, \Psi\boldsymbol{\alpha} \rangle = \langle \Phi\boldsymbol{\alpha}, \Psi\boldsymbol{\alpha} \rangle = \langle \boldsymbol{\alpha}, \Phi^{*}\Psi\boldsymbol{\alpha} \rangle = \boldsymbol{\alpha}^{T}\boldsymbol{G}\boldsymbol{\alpha}.$$
 (6)

Finally, note that condition (3) translates into:

$$\sum_{i=1}^{L} \alpha_i \left\langle x^j, \varphi_i \right\rangle = 0, \qquad \forall j = 0, \dots, k-1, \quad \Leftrightarrow \quad \boldsymbol{\alpha}^T \boldsymbol{H} = \boldsymbol{0} \quad \Leftrightarrow \quad \boldsymbol{\alpha} \in \mathcal{R}(\boldsymbol{H})^{\perp} \subset \mathbb{R}^L.$$
 (7)

Plugging (5), (6) and (7) into (1) yields:

$$f^{\star} \in \mathop{\arg\min}_{f \in \mathcal{H}^k} F(\mathbf{y}, \Phi^* f) + \lambda \|D^k f\|_2^2 \quad \Leftrightarrow \quad (\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathop{\arg\min}_{\boldsymbol{\alpha} \in \mathcal{R}(\boldsymbol{H})^{\perp}, \boldsymbol{\beta} \in \mathbb{R}^k} F(\mathbf{y}, \boldsymbol{G}\boldsymbol{\alpha} + \boldsymbol{H}\boldsymbol{\beta}) + \lambda \boldsymbol{\alpha}^T \boldsymbol{G}\boldsymbol{\alpha}.$$

We have hence shown that the functional penalised Tikhonov problem (1) can be discretised canonically. Moreover this discretisation is lossless: the functional and discrete problems are both equivalent!

 $f(z_i) = \int_{\mathbb{R}} f(z) S(z-z_i) dx = \langle f, S(z-z_i) \rangle$ 

strot cux, rusc, proper

P2 (x-xi)

+ Bo + B1 x

Vardenmond = P2 (2; -x;)

 $\alpha^{\dagger}H = 0 = 0 \times (\frac{1}{2} \frac{2}{2}) = 0 H_{1} = (2^{\circ}, 8(-2) = 2)^{\circ}$ 

 $G_{ij} < P_2(--x_i), \delta(-x_j)$ 

JA2 { f: IR > IR , [ | (2) | dr <+= **Example: Ideal Sampling,** k = 2min  $\sum_{i=1}^{2} |y_i - \beta(x_i)|^2 + \lambda \|D^2 \beta\|_2^2$ 

# **Proximal Algorithms**

### **Proximal Operator**

#### **Definition: (Proximal Operator)**

Let  $f: \mathbb{R}^N \to \mathbb{R} \cup \{+\infty\}$  be a proper convex and lwsc functional. Then, the proximal operator  $\operatorname{prox}_f: \mathbb{R}^N \to \mathbb{R}^N$  of f is defined as

$$\mathbf{prox}_f(z) := \operatorname*{arg\,min}_{x \in \mathbf{JR}^{\mathbf{N}}} f(x) + \frac{1}{2} \|x - z\|_2^2, \quad \forall z \in \mathbb{R}^N.$$

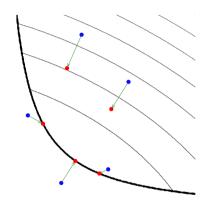
Since f proper convex and lwsc, it is easy to see that the objective functional defining the proximal operator is proper strictly convex, coercive, and lwsc, and hence  $\mathbf{prox}_f(z)$  exists and is unique for every  $z \in \mathbb{R}^N$ . The proximal operator is hence well defined. We will often encounter the proximal operator of the scaled function  $\tau f$ ,  $\tau > 0$ , which can be expressed as:

$$\mathbf{prox}_{\tau f}(z) := \underset{x \in \mathbf{PN}}{\operatorname{argmin}} f(x) + \frac{1}{2\tau} \|x - z\|_2^2, \quad \forall z \in \mathbb{R}^N.$$

We say that a function is proximable if its proximal operator admits a simple closed-form expression.

### Interpretation of Proximal Operator [2, Section 1.2]

- The thin black lines are level curves of f.
- The **bold** black line indicates the boundary of the domain of f.
- Evaluating prox<sub>rf</sub> at the blue points moves them to the corresponding red points.
- The three points in the domain of the function stay in the domain and move towards the minimum of the function (≈ descent step).
- The two points outside of the domain move to the boundary of the domain and towards the minimum of the function (≈ projection step).
- The parameter τ controls the amount of displacement towards the minimum.



### **Properties of Proximal Operators**

#### **Proposition: (Properties of Proximal Operators)**

1. **Separable Sum:** If  $f: \mathbb{R}^{N_1} \times \cdots \times \mathbb{R}^{N_n} \to \mathbb{R} \cup \{+\infty\}$  is defined as:  $f(x_1, \dots, x_n) = \sum_{i=1}^n f_i(x_i)$ ,  $\forall (x_1, \dots, x_n) \in \mathbb{R}^{N_1} \times \cdots \times \mathbb{R}^{N_n}$ , then the proximal operator of f is given by:

$$\mathbf{prox}_{\tau f} = \left[\mathbf{prox}_{\tau f_1}(x_1), \dots, \mathbf{prox}_{\tau f_n}(x_n)\right] \in \mathbb{R}^{N_1} \times \dots \times \mathbb{R}^{N_n}.$$

**2.** Precomposition: If  $f(x) = g(\alpha x + y)$ ,  $\alpha > 0$ ,  $y \in \mathbb{R}^N$ , then

$$\operatorname{prox}_{\tau f}(x) = \frac{1}{\alpha} \left( \operatorname{prox}_{\tau \alpha^2 g}(\alpha x + y) - y \right), \qquad \forall x \in \mathbb{R}^N.$$

3. Fixed Points & Minimisers:  $x^* \in \mathbb{R}^N$  minimises  $f: \mathbb{R}^N \to \mathbb{R} \cup \{+\infty\}$  iff  $\operatorname{prox}_f(x^*) = x^*$  [2, Section 2.3].

Additional useful results can be found in [2, Section 2].

Proof (Point 1) 
$$n = 2$$

$$\frac{\beta(x,y)}{\beta(x,y)} = \frac{\beta_1(x)}{\beta(x)} + \frac{\beta_2(y)}{\beta(x)}$$

$$\frac{\beta(x,y)}{\beta(x)} = \frac{\beta_1(x)}{\beta(x)} + \frac{\beta_2(y)}{\beta(x)}$$

$$\frac{\beta(x,y)}{\beta(x)} = \frac{\beta_1(x)}{\beta(x)} + \frac{\beta_2(y)}{\beta(x)}$$

$$\operatorname{prox}_{z}(w,z) = \operatorname{argmin}_{(x,y) \in \mathbb{R}^{N_1} \times \mathbb{R}^{N_2}}$$

$$\begin{cases} (x,y) + \frac{1}{2z} \| (x,y) - (\omega,z) \|_{2}^{2} \end{cases}$$

= argmin 
$$f_1(z)$$

$$b_1(x) + b_2(y) + \frac{1}{2z} \left[ ||x - \omega||_2^2 + ||y - z||_2^2 \right]$$

= 
$$\left(\underset{\mathcal{Z}_{1}}{\text{argmin}}\right)_{1}\left(\mathcal{R}\right) + \frac{1}{2z}$$

$$f_{1}(z) + \frac{1}{2z} ||z - w||_{2}^{2}$$
, argmin  $f_{2}(y) + \frac{1}{2z} ||y - z||_{2}^{2}$   
 $f_{1}(z) + \frac{1}{2z} ||z - w||_{2}^{2}$ , argmin  $f_{2}(y) + \frac{1}{2z} ||y - z||_{2}^{2}$   
 $f_{2}(z)$ 

Proof (Point 2) 
$$\int_{0}^{x} (x)$$

$$f(x) = g(\alpha x + y) +$$

$$prox_{z}(z) = \underset{z \in \mathbb{R}^N}{\operatorname{argmin}} |f(z)| + \frac{1}{2z} ||z - z||_z^2$$

= argmin 
$$q(\alpha x + y) + \frac{1}{22} (|x-z||_2^2)$$

$$g(u) + \frac{1}{2z} || \frac{2z}{z} - \frac{1}{z^2} - \frac{1}{z^2} - \frac{1}{z} ||_2$$

argmin, 
$$g(u) + \frac{\alpha}{2(\alpha^2)} \| u - (\alpha z + y) \|_2^2$$

$$\frac{1}{\alpha} \left( prox_{z \propto 2g} (\alpha z + y) - y \right)$$

### **Examples of Simple Proximal Operators**

#### Examples of Simple Proximal Operators $(y \in \mathbb{R}^N)$ :

•  $f(x) = ||x - y||_2^2$ :

$$\operatorname{prox}_{\tau f}(x) = \frac{x - y}{1 + 2\tau} + y, \qquad x \in \mathbb{R}^N.$$

•  $f(x) = \iota_C(x - y)$  with  $C \subset \mathbb{R}^N$  convex:

$$\operatorname{prox}_{\tau f}(x) = P_C(x - y) + y, \qquad x \in \mathbb{R}^N,$$

where  $P_C$  is the projection operator onto the convex set C.

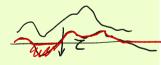
•  $f(x) = ||x - y||_1$ :

$$\operatorname{prox}_{\tau f}(x) = \operatorname{soft}_{\tau f}(x - y) + y, \qquad x \in \mathbb{R}^N,$$

where  $\mathbf{soft}_{\tau}(x) := \max\{|x| - \tau, 0\} \operatorname{sgn}(x)$ .

•  $f(\mathbf{x}) = D_{KL}(\mathbf{y}||\mathbf{x})$ :

$$\mathbf{prox}_{\tau f}(\mathbf{x}) = \frac{\mathbf{x} - \tau + \sqrt{(\mathbf{x} - \tau)^2 + 4\mathbf{y}\tau}}{2}, \qquad \mathbf{x} \in \mathbb{R}^N.$$



#### **Proximal Minimisation**

Consider the following problem:

$$\min_{\mathbf{x}\in\mathbb{R}^N}\mathcal{G}(\mathbf{x}),$$

where  $\mathscr{G}: \mathbb{R}^N \to \mathbb{R}$  is proper, lwsc and convex function with simple proximal operator. This optimisation problem can be solved by means of proximal minimisation:

#### Algorithm 1 Proximal Minimisation

- 1: **procedure** PROXMIN $(\tau, x_0)$
- 2: for all  $n \ge 1$  do
- 3:  $x_n = \mathbf{prox}_{\tau \mathscr{G}}(x_{n-1})$
- 4: **return**  $(x_n)_{n \in \mathbb{N}}$

If  $\mathcal{V} = \arg\min_{x \in \mathbb{R}^N} \mathscr{G}(x)$  is non empty, the sequence  $(x_n)_{n \in \mathbb{N}}$  converges to an element of  $\mathcal{V}$  for any  $\tau > 0$  [2, Section 4.1].

#### **Gradient Descent**

Consider the following problem:

$$\min_{\mathbf{x}\in\mathbb{R}^N}\mathcal{F}(\mathbf{x}),$$

where  $\mathscr{F}: \mathbb{R}^N \to \mathbb{R}$  is convex and differentiable, with  $\beta$ -Lipschitz continuous gradient:

$$\|\nabla \mathcal{F}(\mathbf{x}) - \nabla \mathcal{F}(\mathbf{x}')\|_{2} \le \beta \|\mathbf{x} - \mathbf{x}'\|_{2}, \qquad \forall (\mathbf{x}, \mathbf{x}') \in \mathbb{R}^{N} \times \in \mathbb{R}^{N},$$
(8)

for some Lipschitz constant  $\beta \in [0, +\infty[$ . This optimisation problem can be solved by means of gradient descent:

#### Algorithm 2 Gradient Descent

- 1: **procedure** GRADDESC $(\tau, x_0)$
- 2: for all  $n \ge 1$  do
- $\mathbf{x}_n = \mathbf{x}_{n-1} \tau \nabla \mathscr{F}(\mathbf{x}_{n-1})$
- 4: **return**  $(x_n)_{n \in \mathbb{N}}$

If  $\mathcal{V} = \arg\min_{\mathbf{x} \in \mathbb{R}^N} \mathscr{F}(\mathbf{x})$  is non empty, the sequence  $(\mathbf{x}_n)_{n \in \mathbb{N}}$  converges to an element of  $\mathcal{V}$  for any  $0 < \tau \le \frac{1}{B}$  [3, Section 2].

#### **Proximal Minimisation vs. Gradient Descent**

Consider the least-squares minimisation problem:

$$\min_{\boldsymbol{x}\in\mathbb{R}^N}\frac{1}{2}\|\boldsymbol{y}-\boldsymbol{G}\boldsymbol{x}\|_2^2,$$

with  $G \in \mathbb{R}^{L \times N}$ ,  $y \in \mathbb{R}^L$ . We can minimise the functional  $\mathscr{J}(x) = \frac{1}{2} \|y - Gx\|_2^2$  in two ways:

Via proximal minimisation since \( \mathcal{I} \) is proper convex, and lwsc. This yields the following iterations:

$$x_n = \mathbf{prox}_{\tau, \mathscr{J}}(x_{n-1}) \Leftrightarrow \left(\tau \mathbf{G}^T \mathbf{G} + \mathbf{I}\right) x_n = x_{n-1} + \mathbf{G}^T y, \qquad x_0 \in \mathbb{R}^N, n \ge 1.$$

We must solve a linear system of size  $N \times N$  at each iteration! Computationally expensive...

• Via gradient descent since  $\mathscr{J}$  is differentiable and its gradient  $\nabla \mathscr{J}(x) = G^T(Gx - y)$  is moreover  $\beta$ -Lipschitz continuous with Lipschitz constant  $\beta = \|G^TG\|_2$ . This yields the following iterations:

$$x_n = x_{n-1} + \tau G^T (y - Gx_{n-1}), \quad x_0 \in \mathbb{R}^N, n \ge 1.$$

The update equation only involves matrix/vector products with G and  $G^T$ . Much cheaper!

#### **Accelerated Proximal Gradient Descent**

Consider the following problem:

$$\min_{\mathbf{x}\in\mathbb{R}^N}\mathscr{F}(\mathbf{x})+\mathscr{G}(\mathbf{x}),$$

where  $\mathscr{F}: \mathbb{R}^N \to \mathbb{R}$  is as in Slide 18 and  $\mathscr{G}: \mathbb{R}^N \to \mathbb{R} \cup \{+\infty\}$  is as in Slide 17. This optimisation problem can be solved by means of Accelerated Proximal Gradient Descent (APGD):

#### Algorithm 3 Accelerated Proximal Gradient Descent (APGD)

- 1: **procedure** APGD $(\tau, \mathfrak{d}, x_0 = z_0)$
- 2: for all  $n \ge 1$  do
- 3:  $z_n = \mathbf{prox}_{\tau \mathscr{G}} (x_{n-1} \tau \nabla \mathscr{F}(x_{n-1}))$
- 4:  $x_n = z_n + \frac{n-1}{n+0}(z_n z_{n-1})$
- 5: **return**  $(x_n)_{n \in \mathbb{N}}$

The update equation at line 3 is the composition between a proximal step for  $\mathscr{G}$  and a gradient step for  $\mathscr{F}$ . Line 4 is an acceleration step.

### **Convergence of APGD**

For  $\delta > 2$  and  $0 < \tau \le \beta$ , APGD achieves the following (optimal) convergence rates:

$$\lim_{n \to \infty} n^2 \left| \mathcal{J}(\boldsymbol{x}^{\star}) - \mathcal{J}(\boldsymbol{x}_n) \right| = 0 \qquad \& \qquad \lim_{n \to \infty} n^2 \|\boldsymbol{x}_n - \boldsymbol{x}_{n-1}\|_{\mathcal{X}}^2 = 0,$$

for some minimiser  $x^* \in \operatorname{argmin}_{x \in \mathbb{R}^N} \{ \mathscr{J}(x) := \mathscr{F}(x) + \mathscr{G}(x) \}.$ 

In other words, both the objective functional and the APGD iterates  $\{x_n\}_{n\in\mathbb{N}}$  converge at a rate  $o(1/n^2)$ . Significant practical speedup can moreover be achieved for values of  $\delta$  in the range [50, 100] [4, 5].

<sup>3</sup>Assuming that the solution set is non empty.

### **Example: Fast Iterative Soft Thresholding Algorithm (FISTA)**

Consider the LASSO problem:

$$\min_{\mathbf{x} \in \mathbb{R}^N} \frac{1}{2} \|\mathbf{y} - \mathbf{G}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_1,$$

with  $G \in \mathbb{R}^{L \times N}$ ,  $y \in \mathbb{R}^L$ ,  $\lambda > 0$ . This problem can be solved via APGD with  $\mathscr{F}(x) = \frac{1}{2} \|y - Gx\|_2^2$  and  $\mathscr{G}(x) = \lambda \|x\|_1$ . We have:

$$\nabla \mathscr{F}(x) = G^T(Gx - y), \quad \operatorname{prox}_{\lambda \| \cdot \|_1}(x) = \operatorname{soft}_{\lambda}(x).$$

This yields the so-called Fast Iterative Soft Thresholding Algorithm (FISTA) [6]:

#### Algorithm 4 Fast Iterative Soft Thresholding Algorithm (FISTA)

- 1: **procedure** FISTA $(\tau, \mathfrak{d}, x_0 = z_0)$
- 2: for all  $n \ge 1$  do
- $z_n = \mathbf{soft}_{\tau \lambda} \left( x_{n-1} + \tau \mathbf{G}^T (\mathbf{y} \mathbf{G} x_{n-1}) \right)$
- 4:  $x_n = z_n + \frac{n-1}{n+0}(z_n z_{n-1})$
- 5: **return**  $(x_n)_{n \in \mathbb{N}}$

Convergence of FISTA is moreover guaranteed for  $\mathfrak{d} > 2$  and  $0 < \tau \le \beta^{-1} = \|G\|_2^{-2}$ .

### **Lipschitzian, Proximable and Linear Composite Terms**

Consider the following problem:

$$\min_{\mathbf{x} \in \mathbb{R}^N} \mathscr{F}(\mathbf{x}) + \mathscr{G}(\mathbf{x}) + \mathscr{H}(\mathbf{K}\mathbf{x}). \tag{9}$$

with the following assumptions:

1.  $\mathscr{F}: \mathbb{R}^N \to \mathbb{R}$  is convex and differentiable, with  $\beta$ -Lipschitz continuous gradient:

$$\|\nabla \mathcal{F}(\mathbf{x}) - \nabla \mathcal{F}(\mathbf{x}')\|_{\mathscr{X}} \le \beta \|\mathbf{x} - \mathbf{x}'\|_{\mathscr{X}}, \quad \forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^N,$$

for some Lipschitz constant  $\beta \in [0, +\infty[$ .

- 2.  $\mathscr{G}: \mathbb{R}^N \to \mathbb{R} \cup \{+\infty\}$  and  $\mathscr{H}: \mathbb{R}^M \to \mathbb{R} \cup \{+\infty\}$  are two proper, lwsc and convex functions with simple proximal operators.
- 3.  $K: \mathbb{R}^N \to \mathbb{R}^M$  is a linear operator, with operator norm:  $\|K\|_2 = \sup_{x \in \mathbb{R}^N, \|x\|_2 = 1} \|Kx\|_2$ .
- **4.** The problem (9) is feasible –i.e. there exists at least one solution.

## **Variable Splitting**

Problem (9) cannot be solved via APGD:  $\mathscr{G}$  and  $\mathscr{H}$  have simple proximal operators, but the composite term  $\mathscr{G}(x) + \mathscr{H}(Kx)$  may not!<sup>4</sup>

To circumvent this issue, we perform variable splitting by re-writing (9) in consensus form:

$$\min_{\mathbf{x} \in \mathbb{R}^{N}, \mathbf{w} \in \mathbb{R}^{M}} \mathcal{F}(\mathbf{x}) + \mathcal{G}(\mathbf{x}) + \mathcal{H}(\mathbf{w}), \quad \text{s.t.} \quad \mathbf{w} = \mathbf{K}\mathbf{x}.$$
 (10)

The Lagrangian  $\mathcal{L}: \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^M \to \mathbb{R} \cup \{+\infty\}$  associated to this problem is given by:

$$\mathcal{L}(x, w, z) = \mathcal{F}(x) + \mathcal{G}(x) + \mathcal{H}(w) + z^{T}(Kx - w), \tag{11}$$

where the ancillary variable  $z \in \mathbb{R}^M$  is called a Lagrange multiplier. It is then possible to show that the saddle-point problem

$$\min_{\boldsymbol{x} \in \mathbb{R}^N, \boldsymbol{w} \in \mathbb{R}^M} \max_{\boldsymbol{z} \in \mathbb{R}^M} \mathcal{L}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{z})$$

is equivalent to (10). To this end, we introduce the notion of Fenchel conjugate of a function.

<sup>&</sup>lt;sup>4</sup>For example the TV proximal problem  $\operatorname{argmin}_{x \in \mathbb{R}^N} \|Kx\|_1 + \frac{1}{2\tau} \|x - z\|_2^2$  does not admit a simple closed-form expression.

### Fenchel Conjugate and Fenchel-Moreau Theorem

#### **Definition:** (Fenchel Conjugate/Biconjugate)

The Fenchel conjugate of a function  $f: \mathbb{R}^N \to \mathbb{R} \cup \{-\infty, +\infty\}$  is defined as:

$$f^*(z) := \sup_{x \in \mathbb{R}^N} \langle z, x \rangle - f(x), \quad \forall z \in \mathbb{R}^N.$$

The Fenchel biconjugate  $f^{**}: \mathbb{R}^N \to \mathbb{R} \cup \{-\infty, +\infty\}$  is the Fenchel conjugate of the Fenchel conjugate:

$$f^{**}(x) := \sup_{x \in \mathbb{R}^N} \langle x, z \rangle - f^*(z), \quad \forall x \in \mathbb{R}^N.$$

#### Theorem: (Fenchel-Moreau)

For f proper convex and lwsc we have  $f = f^{**}$ , i.e. f is equal to its Fenchel biconjugate.

## Saddle-Point Problem is Equivalent to (9)

Using the Fenchel-Moreau theorem applied to  ${\mathcal H}$  we get:

$$\min_{\boldsymbol{x} \in \mathbb{R}^{N}, \boldsymbol{w} \in \mathbb{R}^{M}} \left( \max_{\boldsymbol{z} \in \mathbb{R}^{M}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{z}) \right) = \min_{\boldsymbol{x} \in \mathbb{R}^{N}} \max_{\boldsymbol{z} \in \mathbb{R}^{M}} \mathcal{F}(\boldsymbol{x}) + \mathcal{G}(\boldsymbol{x}) + \left( \min_{\boldsymbol{w} \in \mathbb{R}^{M}} \mathcal{H}(\boldsymbol{w}) - \boldsymbol{z}^{T} \boldsymbol{w} \right) + \boldsymbol{z}^{T} \boldsymbol{K} \boldsymbol{x}$$

$$= \min_{\boldsymbol{x} \in \mathbb{R}^{N}} \max_{\boldsymbol{z} \in \mathbb{R}^{M}} \mathcal{F}(\boldsymbol{x}) + \mathcal{G}(\boldsymbol{x}) + \left( -\max_{\boldsymbol{w} \in \mathbb{R}^{M}} \boldsymbol{z}^{T} \boldsymbol{w} - \mathcal{H}(\boldsymbol{w}) \right) + \boldsymbol{z}^{T} \boldsymbol{K} \boldsymbol{x}$$

$$= \min_{\boldsymbol{x} \in \mathbb{R}^{N}} \mathcal{F}(\boldsymbol{x}) + \mathcal{G}(\boldsymbol{x}) + \max_{\boldsymbol{z} \in \mathbb{R}^{M}} \boldsymbol{z}^{T} \boldsymbol{K} \boldsymbol{x} - \mathcal{H}^{*}(\boldsymbol{z})$$

$$= \min_{\boldsymbol{x} \in \mathbb{R}^{N}} \mathcal{F}(\boldsymbol{x}) + \mathcal{G}(\boldsymbol{x}) + \mathcal{H}(\boldsymbol{K} \boldsymbol{x}).$$

We can hence solve (9) by solving the saddle-point problem (also called primal-dual problem):

$$\min_{\boldsymbol{x} \in \mathbb{R}^N, \boldsymbol{w} \in \mathbb{R}^M} \max_{\boldsymbol{z} \in \mathbb{R}^M} \mathcal{L}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{z}) = \min_{\boldsymbol{x} \in \mathbb{R}^N} \max_{\boldsymbol{z} \in \mathbb{R}^M} \mathcal{F}(\boldsymbol{x}) + \mathcal{G}(\boldsymbol{x}) - \mathcal{H}^*(\boldsymbol{z}) + \boldsymbol{z}^T \boldsymbol{K} \boldsymbol{x}.$$

### **Primal-Dual Splitting Method**

The primal-dual problem

$$\min_{\mathbf{x} \in \mathbb{R}^{N}} \max_{\mathbf{z} \in \mathbb{R}^{M}} \mathcal{F}(\mathbf{x}) + \mathcal{G}(\mathbf{x}) - \mathcal{H}^{*}(\mathbf{z}) + \mathbf{z}^{T} \mathbf{K} \mathbf{x}$$
(12)

is much simpler to optimise:

- 1.  $\mathscr{F}: \mathbb{R}^N \to \mathbb{R}$  is convex and differentiable, with  $\beta$ -Lipschitz continuous gradient.
- 2.  $x \mapsto z^T K x$  and  $z \mapsto z^T K x$  are convex and differentiable functionals, with 0-Lipschitz continuous gradients.
- 3.  $\mathscr{G}: \mathbb{R}^N \to \mathbb{R} \cup \{+\infty\}$  and  $\mathscr{H}^*: \mathbb{R}^M \to \mathbb{R} \cup \{+\infty\}$  are two proper, lwsc and convex functions with simple proximal operators. Indeed, the proximal operator of the Fenchel conjugate  $\mathscr{H}^*$  is given by Moreau's identity:

$$\operatorname{prox}_{\sigma \mathcal{H}^*}(z) = z - \sigma \operatorname{prox}_{\mathcal{H}/\sigma}(z/\sigma), \qquad \forall z \in \mathbb{R}^M, \, \sigma > 0. \tag{13}$$

The primal-dual splitting method [7, Algorithm 3.1] can therefore be used to solve (12).

### **Primal-Dual Splitting Method**

#### Algorithm 5 Primal-Dual Splitting (PDS) Method

```
1: procedure PDS(\tau, \sigma, \rho, x_0, z_0)

2: for all n \ge 1 do

3: \tilde{x}_n = \mathbf{prox}_{\tau \mathscr{G}} (x_{n-1} - \tau \nabla \mathscr{F}(x_{n-1}) - \tau K^* z_{n-1})

4: \tilde{z}_n = \mathbf{prox}_{\sigma \mathscr{H}^*} (z_{n-1} + \sigma K[2\tilde{x}_n - x_{n-1}])

5: x_n = \rho \tilde{x}_n + (1 - \rho) x_{n-1}

6: z_n = \rho \tilde{z}_n + (1 - \rho) z_{n-1}

7: return \{(x_n, z_n)\}_{n \in \mathbb{N}}
```

### **Interpretation of PDS**

The algorithm performs alternating proximal gradient/ascent steps:

• Given an estimate  $z_{n-1}$ , Row 3 performs a proximal gradient descent with step size  $\tau > 0$  to minimise

$$\min_{\mathbf{x} \in \mathbb{R}^N} \mathcal{F}(\mathbf{x}) + \mathcal{G}(\mathbf{x}) - \mathcal{F}(\mathbf{x}) + \mathbf{z}_{n-1}^T \mathbf{K} \mathbf{x}$$

$$= \mathbf{z} \mathbf{x}$$

w.r.t. to the variable x (called primal variable).

• Row 4 uses the result of the proximal gradient descent step 3 and the previous primal estimate  $x_{n-1}$  and performs a proximal gradient ascent with step size  $\sigma > 0$  to maximise

$$\max_{\mathbf{z} \in \mathbb{R}^M} \mathbf{z}^T \mathbf{K} (2\tilde{\mathbf{x}}_n - \mathbf{x}_{n-1}) - \mathcal{H}^*(\mathbf{z})$$

w.r.t. to the variable z (called dual variable).

•  $\rho$  > 0 is a momentum term, used to combine the output of the gradient/ascent steps with previous estimates of the primal/dual variables.

# Convergence of PDS ( $\beta \neq 0$ )

#### Theorem: (Convergence of PDS, $\beta \neq 0$ ) [7, Theorem 3.1]

Consider problem (12) under the assumptions of Slide 23 and let  $\tau > 0$ ,  $\sigma > 0$  and  $\rho > 0$  be the *hyperparameters* of Algorithm 5. Suppose moreover that  $\beta > 0$  and that the following holds:

$$1. \ \frac{1}{\tau} - \sigma \|K\|_{2}^{2} \geq \frac{\beta}{2},$$

**2.** 
$$\rho \in ]0, \delta[$$
, where  $\delta := 2 - \frac{\beta}{2} \left( \frac{1}{\tau} - \sigma \| K \|_{2}^{2} \right)^{-1} \in [1, 2[$ .

Then, there exists a pair  $(x^*, z^*) \in \mathbb{R}^N \times \mathbb{R}^M s$  solution to (12), s.t. the primal and dual sequences of estimates  $(x_n)_{n \in \mathbb{N}}$  and  $(z_n)_{n \in \mathbb{N}}$  converge towards  $x^*$  and  $z^*$  respectively, i.e.

$$\lim_{n \to +\infty} \|x^* - x_n\|_2 = 0, \text{ and } \lim_{n \to +\infty} \|z^* - z_n\|_2 = 0.$$

## Convergence of PDS ( $\beta = 0$ )

#### Theorem: (Convergence of PDS, $\beta = 0$ ) [7, Theorem 3.1]

Consider problem (12) under the assumptions of Slide 23 and let  $\tau > 0$ ,  $\sigma > 0$  and  $\rho > 0$  be the *hyperparameters* of Algorithm 5. Suppose moreover that  $\beta = 0$  and that the following holds:

- $1. \ \tau\sigma \|K\|_{L^{2}(\mathbb{R}^{N})}^{2} \leq 1,$
- **2.**  $\rho \in [\epsilon, 2 \epsilon]$ , for some  $\epsilon > 0$ .

Then, there exists a pair  $(x^*, z^*) \in \mathbb{R}^N \times \mathbb{R}^M s$  solution to (12), s.t. the primal and dual sequences of estimates  $(x_n)_{n \in \mathbb{N}}$  and  $(z_n)_{n \in \mathbb{N}}$  converge towards  $x^*$  and  $z^*$  respectively, i.e.

$$\lim_{n \to +\infty} \|x^* - x_n\|_2 = 0$$
, and  $\lim_{n \to +\infty} \|z^* - z_n\|_2 = 0$ .

## **Choosing the Step Sizes**

In practice, the convergence speed of Algorithm 5 is improved by choosing  $\sigma$  and  $\tau$  as large as possible and relatively well-balanced –so that both the primal and dual variables converge at the same pace. In practice, it is hence recommended to choose perfectly balanced parameters  $\sigma = \tau$  saturating the inequalities 1 and 1. For  $\beta > 0$  this yields:

$$\frac{1}{\tau} - \tau \| \mathbf{K} \|_2^2 = \frac{\beta}{2} \iff -2\tau^2 \| \mathbf{K} \|_2^2 - \beta \tau + 2 = 0,$$

which admits one positive root

$$\tau = \sigma = \frac{1}{\|\mathbf{K}\|_{2}^{2}} \left( -\frac{\beta}{4} + \sqrt{\frac{\beta^{2}}{16}} + \|\mathbf{K}\|_{2}^{2} \right).$$
 (14)

For  $\beta = 0$ , this yields

$$\tau = \sigma = \|\boldsymbol{K}\|_2^{-1}.\tag{15}$$

### Computing the Lipschitz Constant $\beta$

Sometimes, computing the Lipschitz constant  $\beta$  of  $\mathscr{F}$  can be difficult. In which case, it can be beneficial to overestimate it slightly using properties of sums/compositions of Lipschitz continuous functions:

- Let  $\mathscr{F} = \mathscr{F}_1 \circ \mathscr{F}_2$  where  $\mathscr{F}_1, \mathscr{F}_2$  are Lipschitz continuous functions with Lipschitz constants  $\gamma_1, \gamma_2$  respectively. Then  $\mathscr{F}$  is Lipschitz continuous with Lipschitz constant  $\beta \leq \gamma_1 \gamma_2$ .
- Let  $\mathscr{F}=\mathscr{F}_1+\mathscr{F}_2$  where  $\mathscr{H}_1,\mathscr{F}_2$  are Lipschitz continuous functions with Lipschitz constants  $\gamma_1,\gamma_2$  respectively. Then  $\mathscr{F}$  is Lipschitz continuous with Lipschitz constant  $\beta \leq \gamma_1+\gamma_2$ .

#### **Example:**

Assume that  $\mathscr{F}(x) = \mathscr{E}(Gx) + \lambda \|Dx\|^2$  where  $\mathscr{E}$  is differentiable with  $\gamma$ -Lipschitz continuous gradient ( $\gamma$  known). Then,

$$\nabla \mathscr{F}(\mathbf{x}) = \mathbf{G}^T \nabla \mathscr{E}(\mathbf{G}\mathbf{x}) + 2\lambda \mathbf{D}^T \mathbf{D}\mathbf{x}, \qquad \forall \mathbf{x} \in \mathbb{R}^N.$$

We have moreover

$$\|\nabla \mathscr{F}(\mathbf{x}) - \nabla \mathscr{F}(\mathbf{x}')\| \le \left(\gamma \|\mathbf{G}\|^2 + 2\lambda \|\mathbf{D}\|^2\right) \|\mathbf{x} - \mathbf{x}'\|, \quad \forall (\mathbf{x}, \mathbf{x}') \in \mathbb{R}^N \times \mathbb{R}^N,$$

and hence  $\nabla \mathscr{F}$  is  $\beta$ -Lipschitz continuous, with  $\beta \leq \gamma \|\mathbf{G}\|^2 + 2\lambda \|\mathbf{D}\|^2$ .

### **Computing Operator Norms**

Computing the operator norm  $\|K\|_2$  of the linear operator  $K: \mathbb{R}^N \to \mathbb{R}^M$  amounts to finding its largest singular value. Performing this computation via a full SVD is wasteful and expensive: the full spectrum is computed when only the leading singular value is needed.

Instead, it is recommended to use the routine  $scipy.linalg.svds()^5$  which is capable of computing only the leading (or more generally k leading) singular values.

This routine is moreover matrix-free: the operator K needs not be stored as an array, but can be an instance of the abstract class <code>scipy.sparse.linalg.LinearOperator</code> with methods <code>matvec()</code> and <code>rmatvec()</code> for matrix/vector products Kx and  $K^Tx$  respectively. This is particularly useful when N and M are very large (e.g. in computational imaging) and K cannot be stored in memory as a Numpy array.

<sup>5</sup>Or its companion routines scipy.linalg.eigs(), scipy.linalg.eigsh() for square/Hermitian matrices respectively

# **Example of a Matrix-Free Linear Operator**

```
def matvec(self, x: np.ndarray) -> np.ndarray:
    return x[self.mask]
```

def rmatvec(self, y: np.ndarray) -> np.ndarray:
 x = np.zeros(shape=self.in\_size, dtype=self.dtype)
 x[self.mask] = y
 return x



# **Example 1: TV-Penalised Basis Pursuit**

$$\frac{\min_{x \in \mathbb{R}^{N}} \frac{1}{2} \|y - Gx\|_{2}^{2} + \lambda \|Dx\|_{1}}{x^{2}(x)} = \frac{1}{2} \|y - Gx\|_{2}^{2} + \lambda \|Dx\|_{1}$$

$$\frac{1}{2} \|y - Gx\|_{2}^{2} , \quad \nabla \mathcal{P}(x) = G^{T}(Gx - Y) \qquad \beta = \|G^{T}G\|_{2} = \|G\|_{2}^{2}$$

$$\frac{1}{2} \|y - Gx\|_{2}^{2} , \quad \nabla \mathcal{P}(x) = G^{T}(Gx - Y) \qquad \beta = \|G^{T}G\|_{2} = \|G\|_{2}^{2}$$

$$\frac{1}{2} \|y - Gx\|_{2}^{2} + \lambda \|Dx\|_{1}$$

$$\frac{1}{2} \|y - Gx\|_{2}^{2} + \lambda \|Gx\|_{2}$$

$$\frac{1}{2} \|y - Gx\|_{2}^{2}$$

**Example 1: TV-Penalised Basis Pursuit** 

$$Z = 0 = \frac{1}{\|D\|_{2}^{2}} \left( -\frac{\|G\|_{2}^{2}}{4} + \sqrt{\frac{\|G\|_{2}^{4}}{16} + \|D\|_{2}^{2}} \right)$$

$$\mathcal{R}(x) = 0$$

$$Z = 0 = \frac{1}{\|D\|_{2}^{2}} \left( -\frac{\|G\|_{2}^{2}}{4} + \sqrt{\frac{\|G\|_{2}^{4}}{16}} + \right)$$

 $\begin{array}{lll}
\mathcal{G}(x) = 0 \\
\mathcal{G}(x) = \frac{1}{2} \| y - Gx \|_{2}^{2} & \rightarrow & \text{prox}_{2g}(z) = \text{argmin} \frac{1}{2} \| y - Gx \|_{2}^{2} + \frac{1}{2} z^{2} \\
\mathcal{E}(x) = 0 \\
\mathcal{E}(x) = \frac{1}{2} \| y - Gx \|_{2}^{2} & \rightarrow & \text{prox}_{2g}(z) = \text{argmin} \frac{1}{2} \| y - Gx \|_{2}^{2} + \frac{1}{2} z^{2} \\
\mathcal{E}(x) = 0 \\
\mathcal{E}(x) = 0$ 

Example 2: Tikhonov-Penalised Least Absolute Deviation
$$\text{Tr}(x) = C \qquad \min_{x \in \mathbb{R}^N} \|y - Gx\|_1 + \frac{\lambda}{2} \|Dx\|_2^2 \qquad \text{Tr}(x) = C$$

$$\mathcal{P}(x) = \frac{1}{2} || D \times ||_{2}^{2} \rightarrow \nabla \mathcal{P}(x) = \lambda D^{T}D \times \rightarrow \beta = \lambda || D ||_{2}^{2}$$

$$M(z) = 11y-z11+1+z \in \mathbb{R}^{L}$$
,  $K = G \in \mathbb{R}^{L\times N}$   
 $Prox_{zh}(z) = soft_{z}(z-y)+y$ ,  $Prox_{zh}(z) = Moreon_{zh}(z)$ 

PDS 
$$\begin{cases} (x_0, z_0) \in (\mathbb{R}^N \times \mathbb{R}^L) \\ \widehat{z}_n = z_{n-1} - z_n D^T D \times - z_n G^T z_{n-1} \\ \widehat{z}_n = \text{prox}_{\text{orgs}} (z_{n-1} + \sigma G(2z_n - z_{n-1})) \end{cases}$$
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# Example 2: Tikhonov-Penalised Least Absolute Deviation

$$B = \lambda \frac{\|D\|_{2}^{2}}{5}$$

$$S = Z = \frac{1}{\|K\|_{2}^{2}} \left( -\frac{3}{4} + \sqrt{\frac{8^{2}}{16} + \|K\|_{2}^{2}} \right)$$

$$= \frac{1}{\|6\|_{2}^{2}} \left( -\frac{\lambda \|D\|_{2}^{2}}{4} + \sqrt{\frac{\lambda^{2} \|D\|_{2}^{4}}{16} + \|6\|_{2}^{2}} \right)^{36}$$

$$\min_{\mathbf{x} \in \mathbb{R}^N} D_{KL}(\mathbf{y} || \mathbf{G} \mathbf{x}) + \lambda || \mathbf{D} \mathbf{x} ||_1$$

TH 
$$(z, u)$$
: 
$$\begin{cases} \mathbb{R}^{L} \times \mathbb{R}^{2N} \\ (z, u) \mapsto D_{KL}(y||z) + \lambda \|u\|_{1} \end{cases}$$

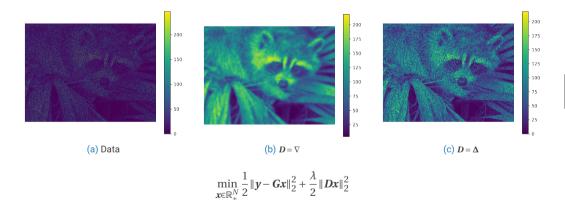
$$K: \begin{cases} \mathbb{R}^N & \longrightarrow \mathbb{R}^L \times \mathbb{R}^{2N} \\ \mathcal{Z} & \longmapsto (G \times , D \times) \end{cases}$$

Example 3: KL-Divergence + TV 
$$\mathcal{A}(z,u) = D_{KL}(y||z) + \lambda ||u||_{A}$$

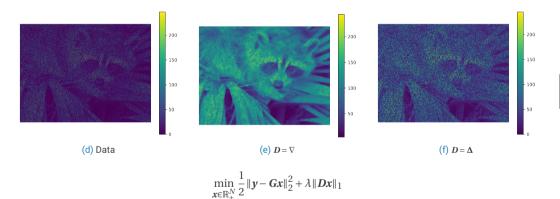
$$Prox_{zH}(z,u) = \left(Prox_{zD_{KL}}(z)\right) Prox_{zH}(u)$$

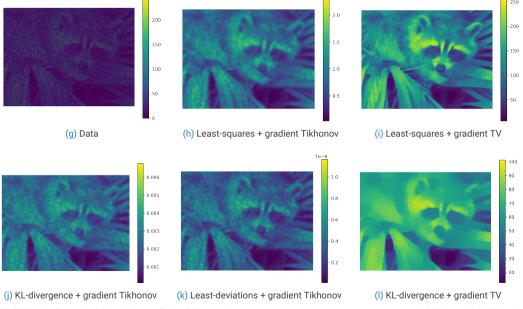
$$Prox_{zH}(z,u) = \left(Prox_{zD_{KL}}(z)\right) Prox_{zH}(u)$$

# **Effect of Regularisation Operator (Tikhonov)**



# **Effect of Regularisation Operator (TV)**





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