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# Solving singularity issues in the estimation of econometric models

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# Outline

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- Estimation of advanced discrete choice models
  - Singularity issues
  - Sources and drawbacks of singularity
- Structural singularity
- Singularity at the solution
  - Adaptation of optimization algorithms
  - Numerical results
- Conclusions and perspectives

# Recent advances in DCM

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- More Logit-like models in the GEV family
- Mixtures of Logit models
- Mixtures of GEV models
- Discrete mixtures of GEV models

⇒ Estimating those models (via maximum log-likelihood) becomes more and more problematic

# Difficulties in the estimation

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- **Objective function** becomes highly **nonlinear** and **non concave**
- **Computational cost** of evaluating the objective function and its derivatives can be significantly **high**
- **Constraints** imposed on parameters to **overcome overspecification** or to obtain meaningful values of parameters
- Identification issues  
⇒ **singularity** in the log-likelihood function
- Estimation requires **specific optimization algorithms**

# Sources of singularity

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- **Structural**
  - Identification issue for the parameters of the error terms
  - e.g. std. errors in heteroscedastic EC models
- **Contextual**
  - Identification issue for the parameters in the deterministic part
  - irrelevant attributes
  - data limitations

# Types of singularity

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We want to solve the **maximum log-likelihood estimation problem**

$$\max_{\beta \in \mathbb{R}^n} \bar{\mathcal{L}}(\beta)$$

- **Structural singularity**

$\Rightarrow \nabla^2 \bar{\mathcal{L}}(\beta)$  is singular  $\forall \beta \in \mathbb{R}^n$

- **Singularity at solution**

$\Rightarrow \nabla^2 \bar{\mathcal{L}}(\beta)$  is singular at  $\beta^* \in \mathbb{R}^n$  where  $\beta^*$  is the vector of estimated values of parameters

# Impacts of singularity

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- The **convergence** of the estimation process can be **much slower**
  - The **estimation time** can be **huge!**
  - **The variance-covariance matrix cannot be obtained**
    - Not possible to assess the quality of the calibrated model
  - Numerical difficulties can arise in the estimation
- ⇒ **Develop robust optimization algorithms**  
**able to solve efficiently singular problems**

# Dealing with singularity issues

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- Some of the algorithms implemented in the optimization package BIOGEME are already robust to face structural singularity issues
  - Focus our work on singularities issues at solution
    - Even if only  $\nabla^2 \bar{\mathcal{L}}(\beta^*)$  is singular, the convergence of the overall sequences of iterates  $\{\beta_k\}_{k \in \mathbb{N}}$  is significantly deteriorated
    - The associated optimization problem is ill-conditioned
- ⇒ Adapt existing optimization algorithms



# Adaptation of optimization algorithms

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- **Two main issues** have to be addressed
  - **Detection of a singularity** during the course of the optimization algorithm
  - Strategies to fix the singularity by adding constraints
- **No details about optimization algorithms themselves**
  - Description of the **identification process**
  - **Fixing the singularity by adding constraints to the problem**

# Problem formulation

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Defining  $x = \beta$  and  $f(x) = -\bar{\mathcal{L}}(\beta)$

$$\left\{ \begin{array}{l} \max \bar{\mathcal{L}}(\beta) \\ \beta \in \mathbb{R}^n \end{array} \right. \iff \left\{ \begin{array}{l} \min f(x) \\ x \in \mathbb{R}^n \end{array} \right.$$

- $\bar{\mathcal{L}}$  is the log-likelihood function
- $\beta$  is the vector of parameters to be estimated
- $f : \mathbb{R}^n \rightarrow \mathbb{R}$  twice continuously differentiable

# Problem formulation

Defining  $x = \beta$  and  $f(x) = -\bar{\mathcal{L}}(\beta)$

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- $\bar{\mathcal{L}}$  is the **log-likelihood function**
- $\beta$  is the vector of **parameters to be estimated**
- $f : \mathbb{R}^n \rightarrow \mathbb{R}$  twice continuously differentiable
- We assume that the **problem is singular at  $x^*$** , that is
  - $\nabla^2 f(x^*)$  is singular
  - $x^*$  is a **local minimum** of the problem

# Ideas of the algorithm

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- Identification of the singularity
  - Issue 1: must analyze  $\nabla^2 f(x^*)$ , without knowing  $x^*$
  - Issue 2: eigenstructure analysis is time consuming
- Fixing the singularity
  - Issue 1: how to correct the singularity?
  - Issue 2: how to adapt existing algorithms?

# Ideas of the algorithm

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- Identification of the singularity
  - Solution 1: analyze  $\nabla^2 f(x_k)$  instead of  $\nabla^2 f(x^*)$
  - Solution 2: generalized inverse iteration
- Fixing the singularity
  - Solution 1: add curvature
  - Solution 2: trust-region framework is well designed for easy adaptations

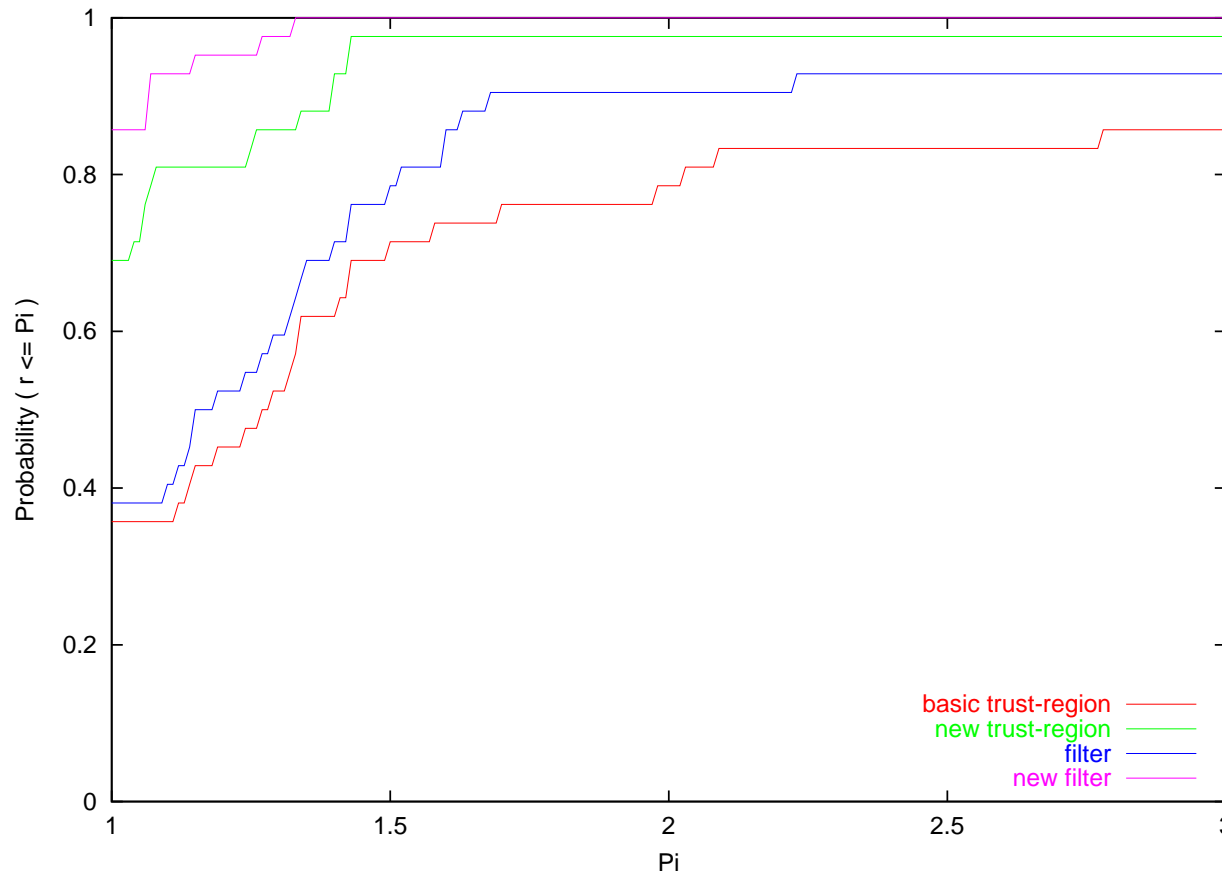
# Numerical tests

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- Around 75 test problems
  - All containing a singularity at solution
  - Dimension between 2 and 40
- 4 optimization algorithms
  - Basic trust-region algorithm (in BIOGEME)
  - Trust-region algorithm designed to handle singularity
  - Filter-trust-region algorithm
  - Filter-trust-region algorithm designed to handle singularity
- 2 measures of performance
  - Number of iterations
  - CPU time

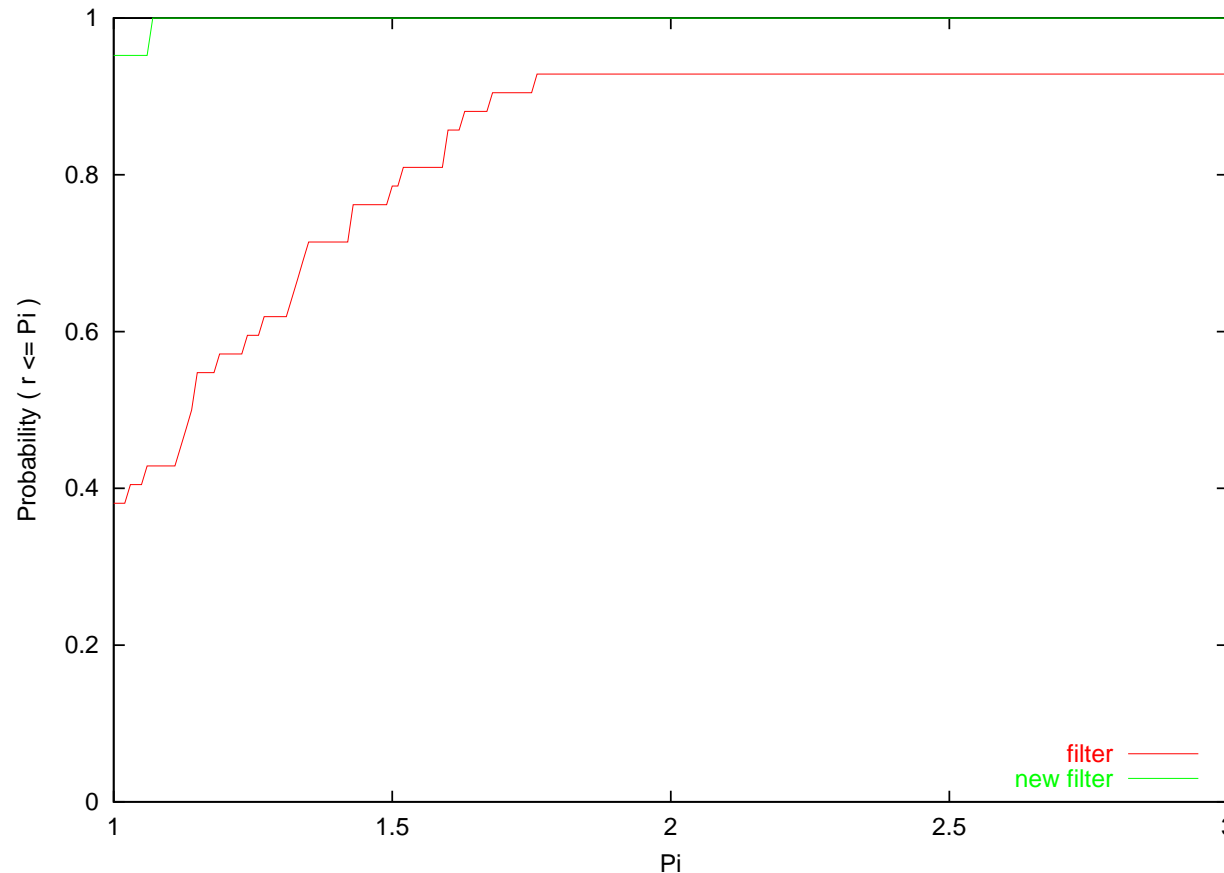
# Performance profile 1

- All algorithms
- Number of iterations



# Performance profile 2

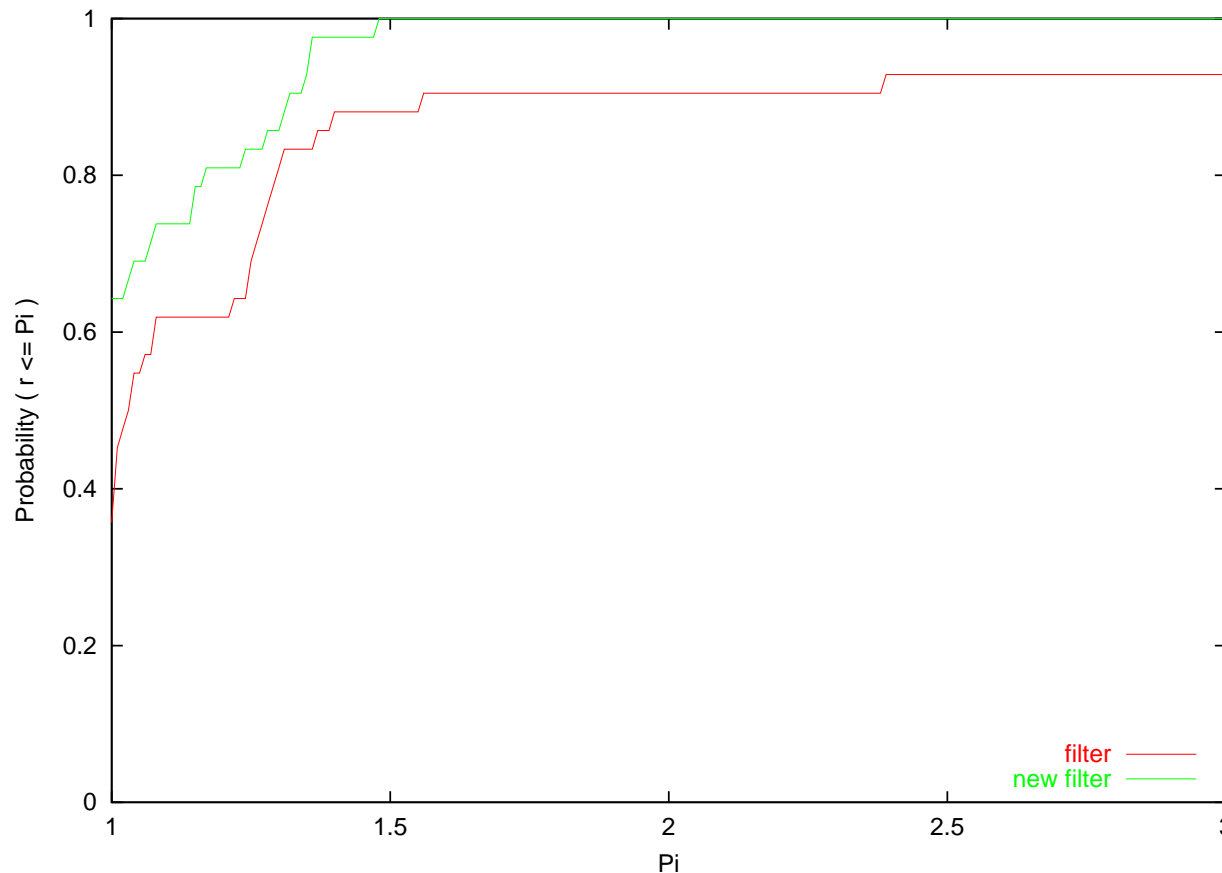
- Two filter-trust-region variants
- Number of iterations





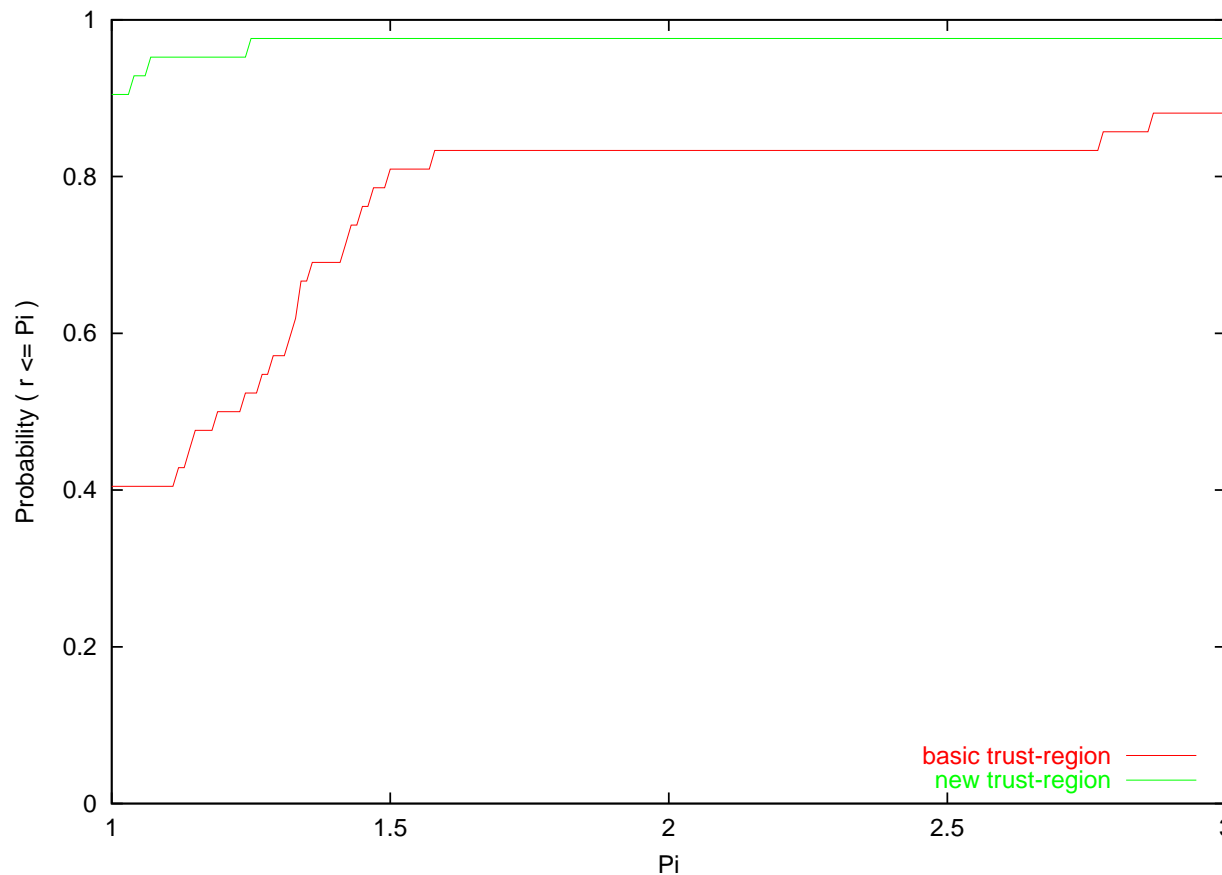
# Performance profile 3

- Two filter-trust-region variants
- CPU time



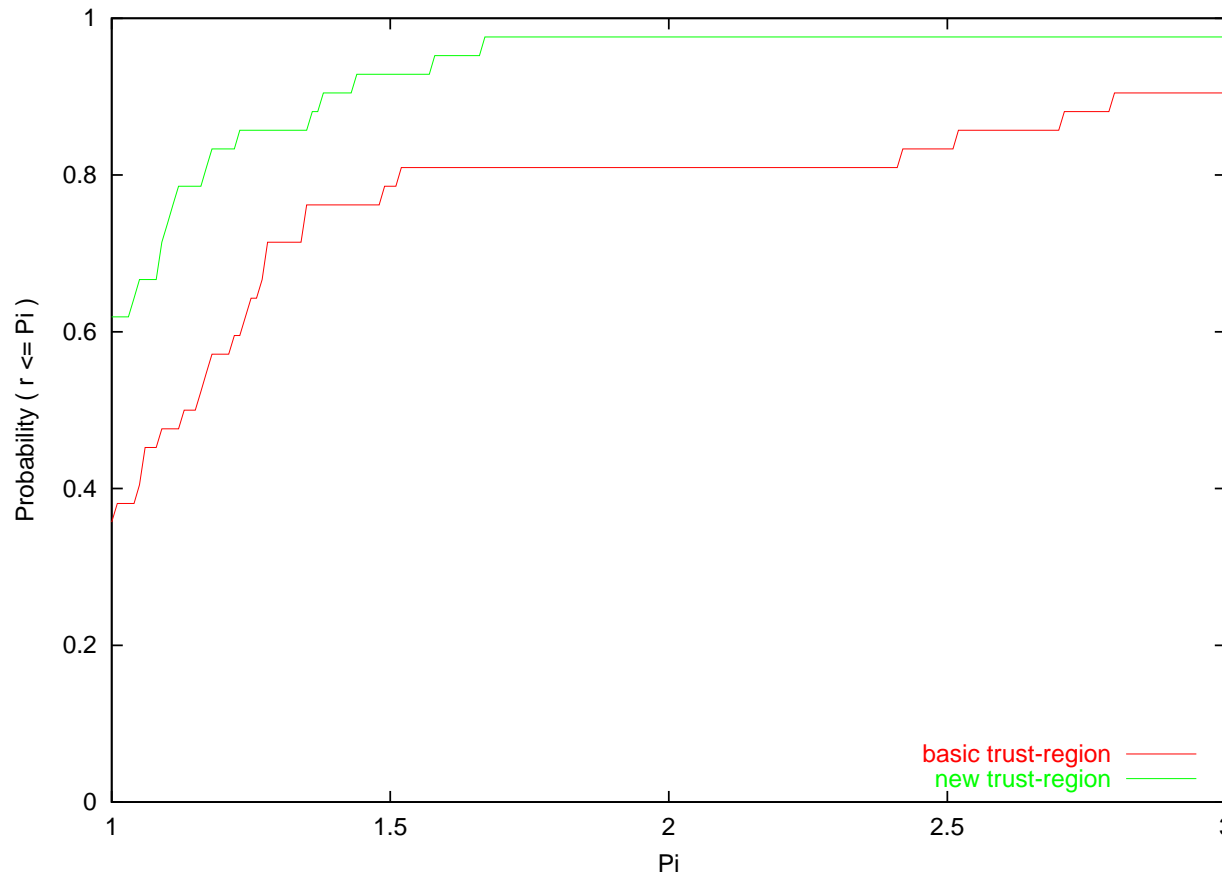
# Performance profile 4

- Two trust-region variants
- Number of iterations



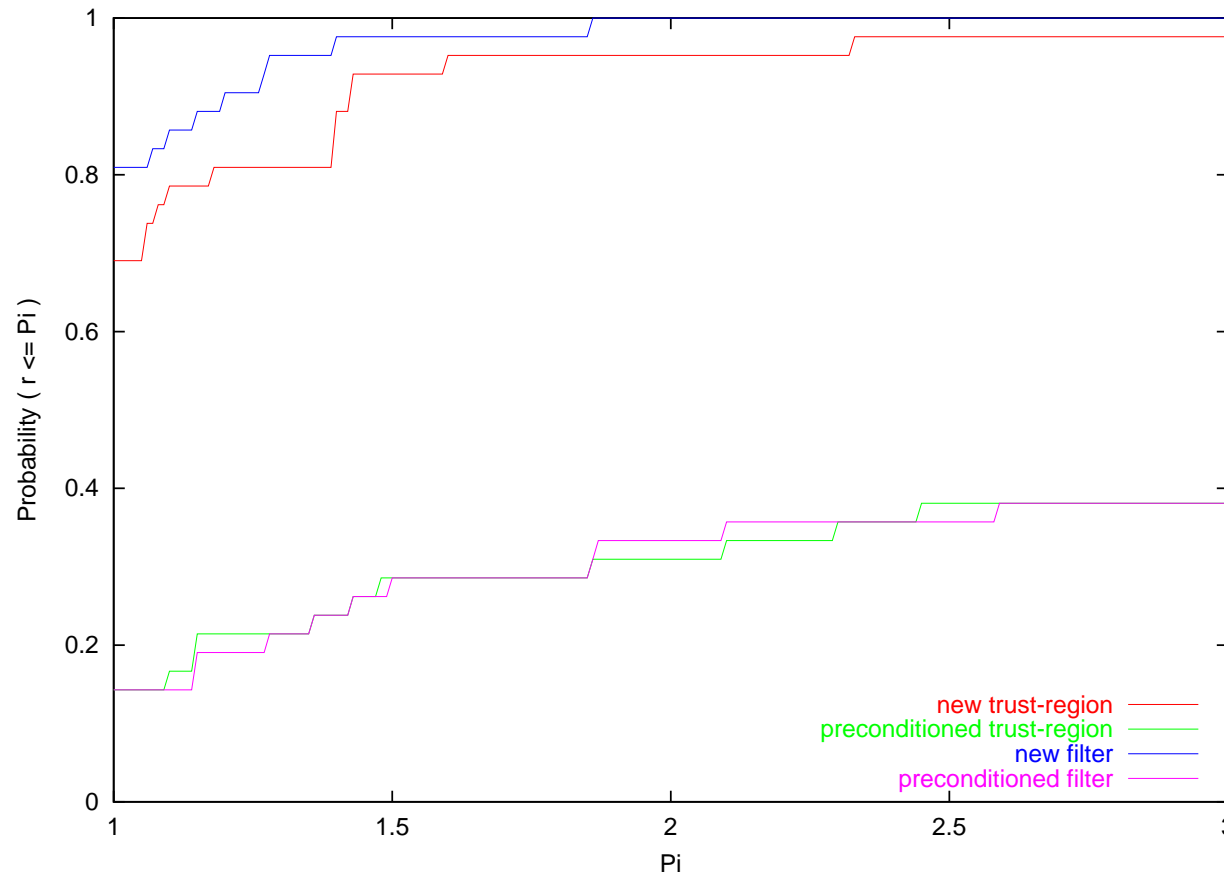
# Performance profile 5

- Two trust-region variants
- CPU time



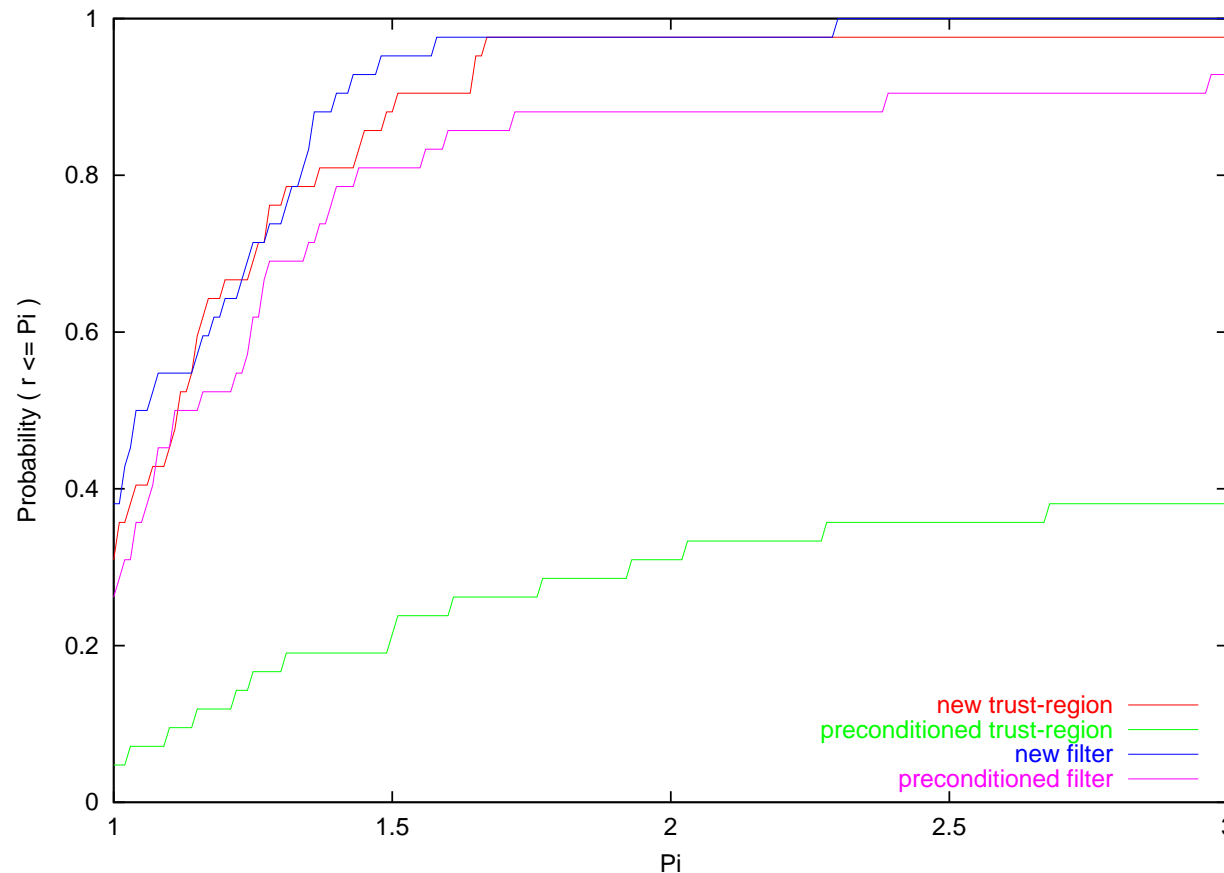
# Test against preconditioning 1

- New variants vs preconditioned version of algorithms
- Number of iterations



# Test against preconditioning 2

- New variants vs preconditioned version of algorithms
- CPU time



# Conclusions

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- Issues of **singularity often arise in the estimation of DCM**
- Adaptation of optimization algorithms to deal with a type of singularity
- Numerical **results are very good**
  - Significant improvement in term of number of iterations
  - Computational **overhead highly compensated by the better efficiency**
  - Significant **gain expected in the estimation time of advanced DCM** (Simulated Maximum Likelihood)

# Perspectives

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- Singularity issues
  - Perform tests on real DCM involving singularities at the solution
  - Generalization of both theoretical and algorithmic ideas to singular constrained nonlinear optimization
- Non-concavity issues
  - Nonlinear global optimization
  - Adapt optimization algorithms in order to be able to identify the global maximum of the optimization problem
  - A global maximum makes much more sense

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**Thank you for your  
attention !**