Structured Sparsity in Numerical Optimisation

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by

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Contents

Mathematics

Numerical Optimisation

- $\mathcal{H}$ is a set
- $\Phi : \mathcal{H} \to \mathbb{R}$
- Find

$$x^* = \operatorname*{argmin}_{x \in \mathcal{H}} \Phi(x)$$

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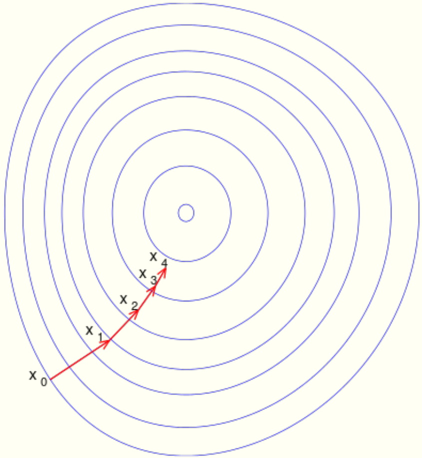
Our setting:

- $\mathcal{H} = \mathbb{R}^d$
- $\Phi(x) := f(x) + g(x)$
  - $f(x)$ is convex and has L-Lipschitz continuous gradient
  - $g(x)$ is convex and lower semi-continuous
- Find

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} f(x) + g(x)$$

Smooth case



Smooth case:

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} f(x).$$

Iteration:

$$x^+ = x - \gamma \nabla f(x)$$

with $\gamma = \frac{1}{L}$

Non-smooth case

Let $\{C_j\}_j$ sequence of cvx subsets of $\mathbb{R}^d$ with non-empty intersection,

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} \sum_j \iota_{C_j}(c)$$

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POCS: Projection Onto Convex Sets

$$x_{k+1} = \Pi_{C_1} \Pi_{C_2} \cdots \Pi_{C_N} x_k.$$

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POCS: Projection Onto Convex Sets

$$x_{k+1} = \Pi_{C_1} \Pi_{C_2} \cdots \Pi_{C_N} x_k.$$

Each projection is the solution of

$$\operatorname*{argmin}_{y \in \mathbb{R}^d} \frac{1}{2} \|x_k - y\|_2^2 + \iota_{C_j}(y).$$

Proximal operator

$\Gamma_0(\mathbb{R}^d) = \{g : \mathbb{R}^d \to \mathbb{R}$ l.s.c. and cvx with $\operatorname{dom}(g) \neq \emptyset\}$

Definition (Proximal Operator)

Let $g \in \Gamma_0(\mathbb{R}^d)$. For every $x \in \mathbb{R}^d$, the minimisation problem

$$\operatorname*{argmin}_{y \in \mathbb{R}^d} \frac{1}{2} \|x - y\|_2^2 + g(y)$$

admits a unique solution called $\operatorname{prox}_g(x)$.

Properties of prox

Separability:

$$g(x,y) = \varphi(x) + \psi(y) = \operatorname{prox}_{\varphi}(x) + \operatorname{prox}_{\psi}(y)$$

Firmly non-expansive:

$$\left\|\operatorname{prox}_g(x) - \operatorname{prox}_g(y)\right\|_2^2 \leq (x-y)^T\left(\operatorname{prox}_g(x) - \operatorname{prox}_g(y)\right)$$

Resolvent operator:

$$\operatorname{prox}_g(\cdot) = (I + \partial g)^{-1}(\cdot)$$

Moreau decomposition

Definition

The convex conjugate of $g : X \to \mathbb{R}$ is $g^* : X^* \to \mathbb{R}$

$$g^*(\xi) = \sup_{x \in X} \left\{ \langle \xi, x \rangle - g(x) \right\}.$$

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Moreau decomposition:

$$\begin{aligned} v &= \operatorname{prox}_g(v) + \operatorname{prox}_{g^*}(v) \\ v &= \Pi_L(v) + \Pi_{L^\perp}(v) \\ v &= \Pi_K(v) + \Pi_{K^\circ}(v) \end{aligned}$$

Proof.

$2 + 2 = 4 - 1 = 3$ quick mafhs. $\square$

Key property

A point $x^* \in \mathbb{R}^n$ is a minimiser of g
if and only if

$$\mathrm{prox}_g\left(x^*\right) = x^*$$

Greedy algorithm for non-smooth optimisation

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} g(x)$$

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Iteration:

$$x_{k+1} = \mathrm{prox}_g\left(x_k\right)$$

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If we don't know anything about the Lipschitz constant of prox_g

$$x_{k+1} = [(1-\alpha)I + \alpha \operatorname{prox}_g](x_k)$$

Cominetti et al., On the rate of convergence of Krasnoselskii-Mann iterations and their connection with sums of Bernoullis, 2014

Splitting algorithms

The problem

Let $f \in C^1(\mathbb{R}^d)$ and $g \in \Gamma_0\left(\mathbb{R}^d\right)$ two convex, proper and l.s.c. functions.

$$x^* = \operatorname*{argmin}_{y \in \mathbb{R}^d} f(y) + g(y).$$

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Idea

Gradient descent for the smooth part and proximal iteration for the non-smooth.

Forward-backward splitting

First order optimality condition

$$
\begin{aligned}
0 &\in \nabla f(x^*) + \partial g(x^*) \\
0 &\in \gamma \nabla f(x^*) + \gamma \partial g(x^*) \\
-\gamma \nabla f(x^*) &\in \gamma \partial g(x^*) \\
(I - \gamma \nabla f)(x^*) &\in (I + \gamma \partial g)(x^*) \\
(I + \gamma \partial g)^{-1} (I - \gamma \nabla f)(x^*) &= x^* \\
\operatorname{prox}_{\gamma g}(x^* - \gamma \nabla f(x^*)) &= x^*
\end{aligned}
$$

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$$

$$x_{k+1} = \operatorname{prox}_{\gamma g}(x_k - \gamma \nabla f(x_k))$$

FISTA

Fast Iterative Shrinkage Thresholding Algorithm (2009)

Objective:

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} \overbrace{f(x)}^{\text{s}} + \overbrace{g(x)}^{\text{ns}}$$

Algorithm ($t_0 = 1$):

$$x_k = \mathrm{prox}_{t_k g}\left(x_{k-1} - t_k \nabla f(x_{k-1})\right)$$

$$t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2}$$

$$y_{k+1} = x_k + \left(\frac{t_k - 1}{t_{k+1}}\right)(x_k - x_{k-1})$$

Rate of convergence:

$$\mathcal{O}\left(1/k^2\right)$$

Sum up...

- We are able to solve smooth + non smooth minimisation problems
- We need L-Lipschitz gradients for the smooth term
- We need to be able to compute prox of the non smooth term

Regularisation theory

Forward/Inverse problems

Forward:

- Input
  - Linear model $A : \mathbb{R}^d \to \mathbb{R}^n$
  - Set of weights $x \in \mathbb{R}^d$
  - Noise ε
- Output:
  - Data $y = Ax + \varepsilon$

Inverse:

- Input
  - Data $y \in \mathbb{R}^n$
  - Linear model $A : \mathbb{R}^d \to \mathbb{R}^n$
  - Desire to recover $x \in \mathbb{R}^d$
- Output:
  - Set of weights $x \in \mathbb{R}^d$

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  - Desire to recover $x \in \mathbb{R}^d$
- Output:
  - Set of weights $x \in \mathbb{R}^d$

NB: the noise is missing in the inverse problem

Inverse problem

$$x^* = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \underbrace{\frac{1}{2} \|Ax - y\|_2^2}_{\text{smooth}} + \underbrace{\lambda \Omega(x)}_{?}$$

with $\Omega : \mathbb{R}^d \to \mathbb{R}$ convex, proper and l.s.c.

Tikonov regularisation

$$x^* = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \frac{1}{2} \|Ax - y\|_2^2 + \lambda \|x\|_2^2$$

- Everything is smooth with L-Lipschitz gradient
- No need of proximal stuff

Smoothing splines

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} \frac{1}{2} \|f(x) - y\|_2^2 + \lambda \|\Delta x\|_2^2$$

- $\lambda \to 0$: interpolating spline
- $\lambda \to \infty$: linear least squares estimate

Sparse recovery

Goal: extract the **few relevant features** of x that let us reconstruct y.

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Idea

Penalise with the ℓ_0 ”norm” $\|x\|_0 = \sum x_j^0$

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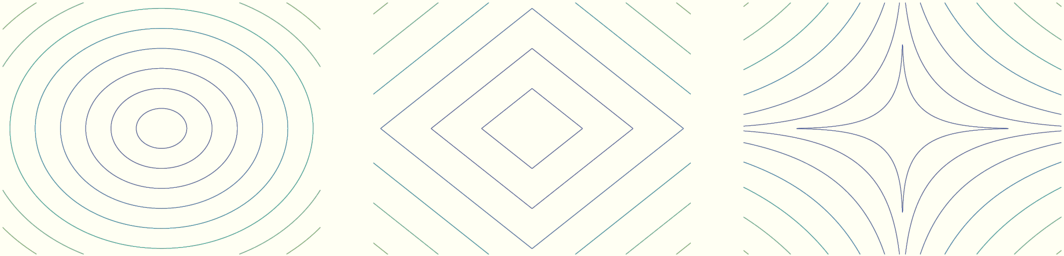
Problem

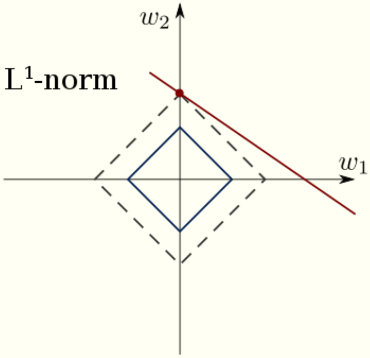
Combinatorial complexity

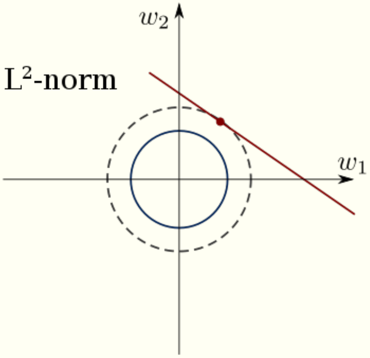
Shape of ℓ_p balls



ℓ_2 ℓ_1 $\ell_{0.4}$

Sparse recovery





Sparse recovery (Lasso)

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} \frac{1}{2} \|Ax - y\|_2^2 + \lambda \|x\|_1$$

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} \|x\|_1 \qquad \text{s.t. } \|Ax - y\|_2^2 \leq \varepsilon$$

prox of norms

Consider $g = \|\cdot\|$ and $\mathcal{B} = \{x : \|x\|_* \leq 1\}$, then

$$g^*(\xi) = \iota_{\mathcal{B}}(\xi)$$

By Moreau decomposition:

$$v = \operatorname{prox}_{\|\cdot\|}(v) + \Pi_{\mathcal{B}}(v)$$
$$\operatorname{prox}_{\|\cdot\|}(v) = v - \Pi_{\mathcal{B}}(v)$$

prox of norms

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By Moreau decomposition:

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$$\operatorname{prox}_{\|\cdot\|}(v) = v - \Pi_{\mathcal{B}}(v)$$

We have the proximal operator of norms!

Sparse recovery can be solved

Structured sparsity

Necessity to *exclude* blocks of x

- Non-Overlapping Group Lasso
- Overlapping Group Lasso
- Hierarchical Lasso

Non Overlapping Group Lasso

$$\Omega(x) = \|X_{\mathcal{G}}\|_1 = \sum_{g \in \mathcal{G}} w_g \left\|x_{|g}\right\|_2$$

Non Overlapping Group Lasso

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By separability of prox we have

$$\operatorname{prox}_{\Omega}(x) = \operatorname{prox}_{g_1}\left(\operatorname{prox}_{g_2}\left(\ldots \operatorname{prox}_{g_k}(x)\right)\right)$$

Overlapping Group Lasso

$$\Omega(x) = \sum_{g \in \mathcal{G}} w_g \left\| x_{|g} \right\|_2$$

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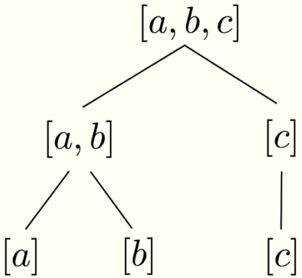
Much more complicated

Overlapping Group Lasso

$$\Omega(x) = \sum_{g \in \mathcal{G}} w_g \left\| x_{|g} \right\|_2$$

Much more complicated but feasible

Hierarchical Sparsity



$$\mathrm{prox}_{\Omega}(x) = \mathrm{prox}_{g_1}\left(\mathrm{prox}_{g_2}\left(\ldots \mathrm{prox}_{g_k}(x)\right)\right)$$

Proximal of Hierarchical Sparsity

Let $(\mathcal{G}, \preceq)$ be ad ordered tree structure

1. Set $v = x$.
2. For $g \in \mathcal{G}$ following $\preceq$ do

$$v_{|g} \longleftarrow v_{|g} - \Pi_{\|\cdot\|_* \leq \omega_g} \left(v_{|g} \right) .$$

Non-Negativity constraint

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} \underbrace{f(x)}_{\text{s}} + \underbrace{g(x) + \iota_{\geq 0}(x)}_{\text{ns}}$$

Non-Negativity constraint

$$x^* = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \underbrace{f(x)}_{\text{s}} + \underbrace{g(x) + \iota_{\geq 0}(x)}_{\text{ns}}$$

Definition (Absolute norm)

A norm $\Omega : X \to \mathbb{R}$ is called *absolute* if $\forall u, v \in \mathbb{R}^N$ such that $|u_j| \leq |v_j|$ for all j implies $\Omega(u) \leq \Omega(v)$.

Theorem (Proximal operator of absolute norms)

Let $w \in \mathbb{R}^n$ and $\lambda > 0$. Consider an absolute norm Ω. We have

$$\underset{z \in \mathbb{R}^n}{\operatorname{argmin}} \left[\frac{1}{2} \| [w]_+ - z \|_2^2 + \lambda \Omega(z) \right] = \underset{z \in \mathbb{R}^n_+}{\operatorname{argmin}} \left[\frac{1}{2} \| w - z \|_2^2 + \lambda \Omega(z) \right].$$

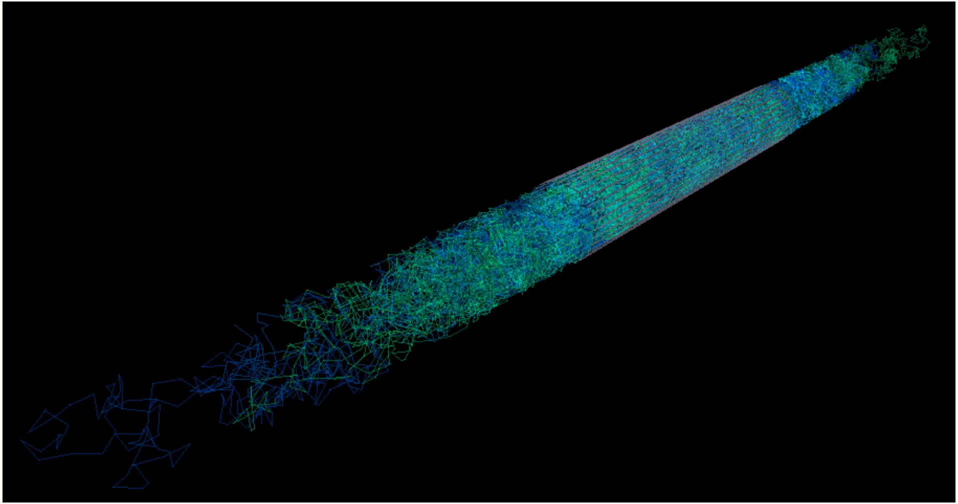
$$\operatorname{prox}_{\lambda\Omega}([w]_+) = \operatorname{prox}_{\lambda\Omega + \iota_{\geq 0}}(w)$$

Sum up...

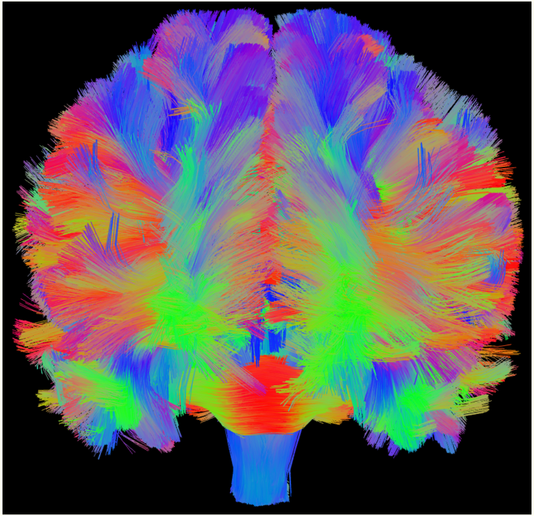
- We can recover sparse variables/signals/codes/...
- Intrinsic structures can be exploited
- Proximal methods are the correct tools for sparse reconstruction
- Non-Negativity constraint can be embedded almost for free

Brain Imaging

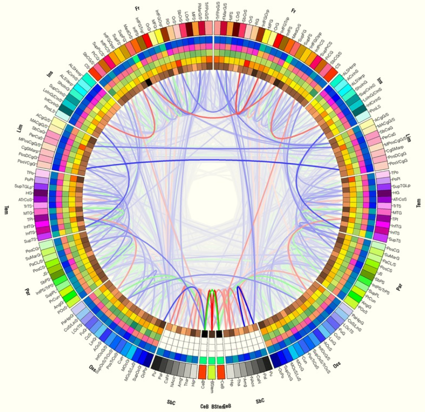
Diffusion MRI

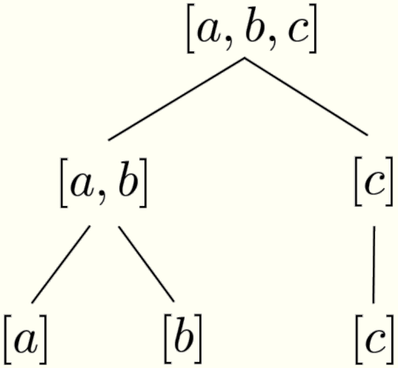


Tractography



Brain hierarchy





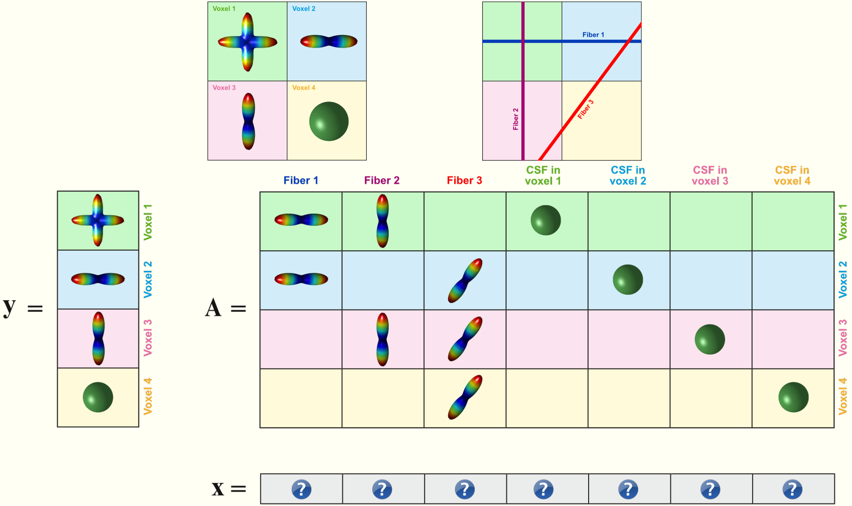
The problem: false positives

The challenge of mapping the human connectome based on diffusion tractography

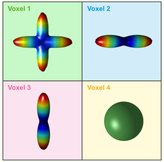
Maier-Hein et al., 2017 (Nature)

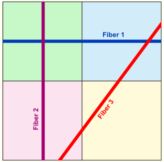
- 96 distinct tractography pipelines
- *“most algorithms routinely extracted many false positive bundles”*
- *“Tractography identifies more invalid than valid bundles”*
- **“Tractography is fundamentally ill-posed”**

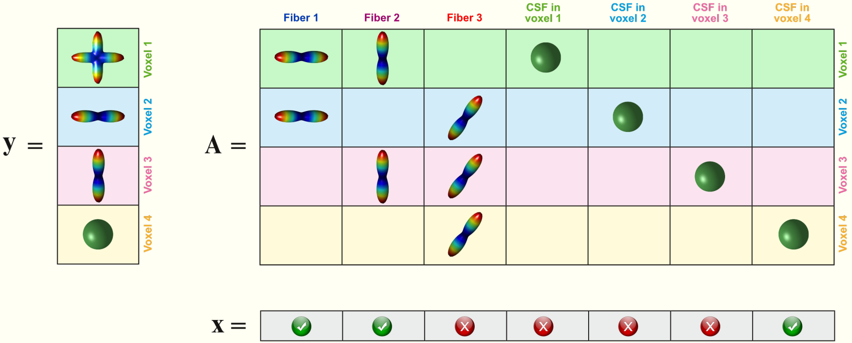
Forward model: COMMIT



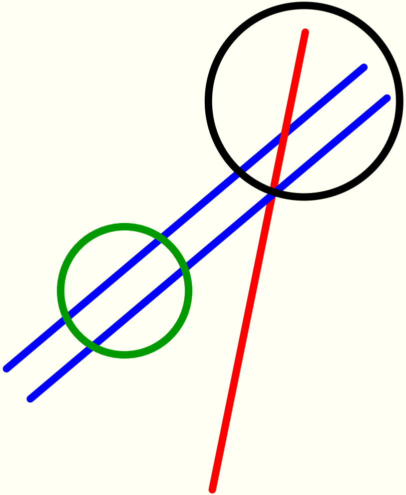
Forward model: COMMIT

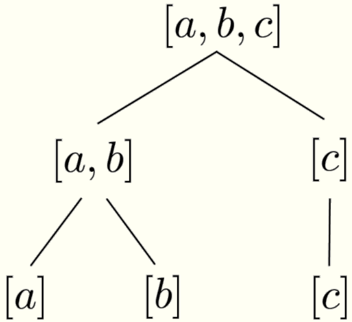






Hierarchical pattern





$$\mathcal{G} = \Big(\big[[a], [b], [a,b], [c], [a,b,c] \big], \preceq \Big)$$

NB:

$$[a] \preceq [a,b] \preceq [c] \qquad [a,b,c] \not\preceq [c]$$

False positives detection

- Build the dictionary/matrix A
- Fit the acquired dMRI signal
- Force hierarchical sparsity

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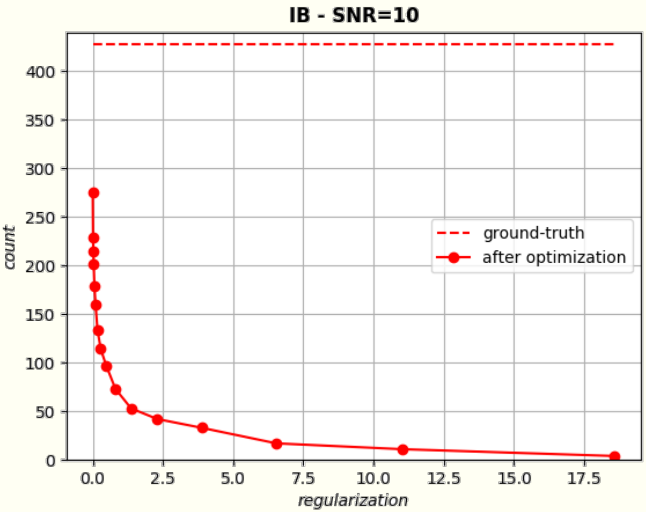
- **Impose non-negativity of x**

False positives detection

- Build the dictionary/matrix A
- Fit the acquired dMRI signal
- Force hierarchical sparsity
- **Impose non-negativity of x**

$$x^* = \operatorname*{argmin}_{x \in \mathbb{R}^d} \frac{1}{2} \|Ax - y\|_2^2 + \lambda \sum_{g \in \mathcal{G}} w_g \left\| x_{|g} \right\|_2 + \iota_{\geq 0}(x)$$

Results


IB - SNR=10
count
regularization
400
350
300
250
200
150
100
50
0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
ground-truth
after optimization

Sum up...

- Brain connections are organised with an hierarchical pattern
- False positives can be detected with structured sparsity
- The solution can be obtained via proximal splitting methods

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Grazie per l'attenzione