Reconstruction of DOSY NMR Signals

Lucas Saban

November 21, 2022

1 Introduction

The goal of this practical session is to gain hands-on experience with several optimization algorithms. The task will be to reconstruct a signal $\hat{x}$ from perturbed data y.

The program we seek to solve is :

$$\hat{x} = \arg\min_{x \in \mathbb{R}^N} \frac{1}{2}||Kx - y||^2 + \beta g(x) := F(x) \tag{1}$$

with $g \in \Gamma_0(\mathbb{R}^N)$, $\beta > 0$ and $K \in \mathbb{R}^{N \times N}$

2 Generation of synthetic data

From the original data, we generate a noisy and transformed signal according to step defined in the subject.

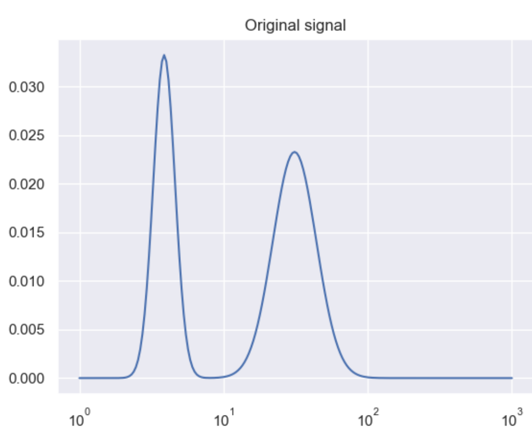

Figure 1: Original data

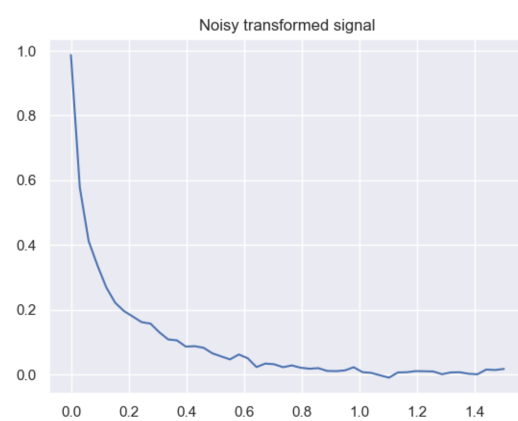

Figure 2: Synthetic data

3 Comparison of regularization strategies

In this report, we will test different penalization and implement the relevant optimization algorithms.

3.1 Smoothness prior

In this part, we take g such that $\forall x \in \mathbb{R}^N g(x) = ||Dx||^2$ with D the matrix of differences.

We can show that F is strictly convex. For any $x, z \in \mathbb{R}^N$ and $\lambda \in (0,1)$:

$$\begin{aligned} &\tfrac{1}{2}(||K(\lambda x + (1-\lambda)z) - y||^2 + \beta||D(\lambda x + (1-\lambda)z)||^2 \\ &\leq \tfrac{1}{2}\left(\lambda^2(||Kx - y||^2 + \beta||Dx||^2) + (1-\lambda)^2(||Kz - y||^2 + \beta||Dz||^2)\right) \\ &< \tfrac{1}{2}\left(\lambda(||Kx - y||^2 + \beta||Dx||^2) + (1-\lambda)(||Kz - y||^2 + \beta||Dz||^2)\right) \end{aligned} \tag{2}$$

Indeed, $\lambda^2 < \lambda$ on $(0,1)$ and as rank(D)= N and $y \neq O_M$, $||Kz - y||^2 + \beta||Dz||^2 > 0$. Hence, F is strictly convex, we have the guaranty that there exists one and only minimizer that we can get using first order condition.

$$\nabla F(x) = K^T(Kx - y) + \beta D^T Dx = 0$$

$$\implies \hat{x} = \underbrace{(K^T K + \beta D^T D)^{-1}}_{=\nabla^2 F \text{ and F strictly convex, thus invertible}} K^T y \tag{3}$$

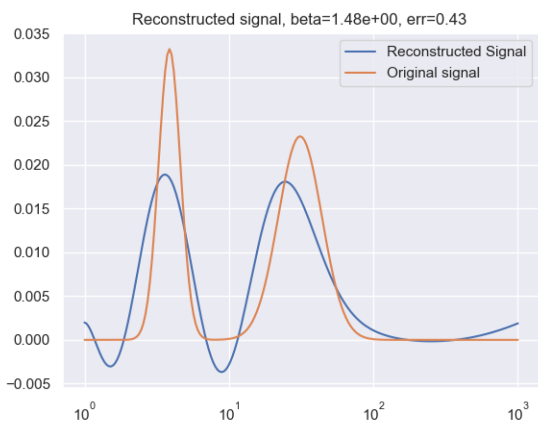

Figure 3: Reconstructed signal with smoothness regularization

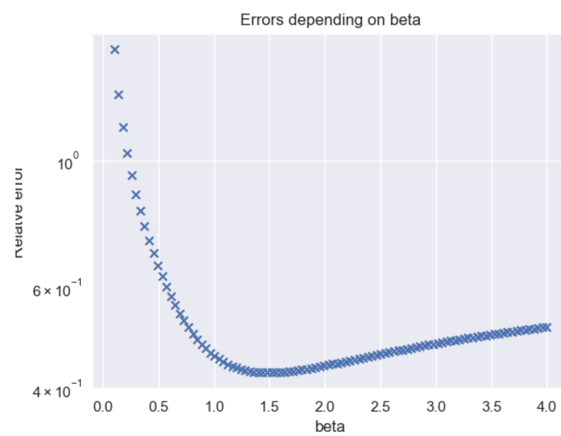

Figure 4: Final error = f(β)

As we can see, the reconstructed signal takes negative values. The error of beta shows a clear minima.

3.2 Smoothness prior + Constraints

Here, we take $g : x \in \mathbb{R}^d \longrightarrow \iota_C(x)$. C is equal to the segment $[x_{min}, x_{max}]$. As F is continuous over the compact C, we know that the set of minimizers is non-empty. Furthermore, as C is convex and F strictly convex, the problem is strictly convex, which assures us that there is at most one minizer.

For this situation, the projected gradient algorithm is the most relevant.

The projection on C is, for any $x \in \mathbb{R}^d$:

$$P_C(x) := \begin{cases} x & \text{if } x \in [x_{min}, x_{max}] \\ x_{max} & \text{if } x \geq x_{max} \\ x_{min} & \text{if } x \leq x_{min} \end{cases}$$

We can define the algorithm as follows,

1. Initialize x_0
2. for $k \geq 1$
    - Compute $g_k = \nabla F(x_{k-1})$
    - $x_k = x_{k-1} + \lambda(P_C(x_{k-1} - \gamma g_k) - x_{k-1})$

The conditions are $\lambda \in [O, \frac{2}{\nu}]$ and $\gamma \in [0, 2 - \nu\lambda/2]$ where $\nu = ||\nabla^2 F|| = ||K^T K + \beta D^T D|| > 0$

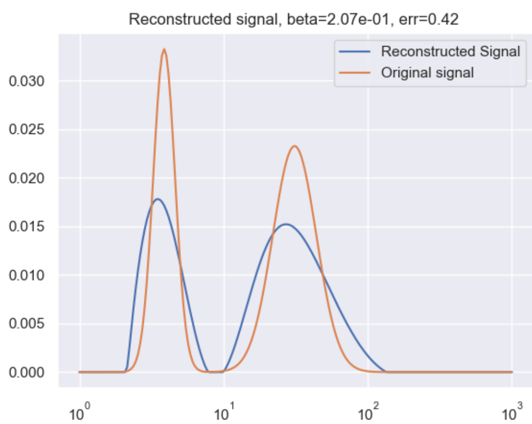

Figure 5: Reconstructed signal for l2-smoothness penalization and projection

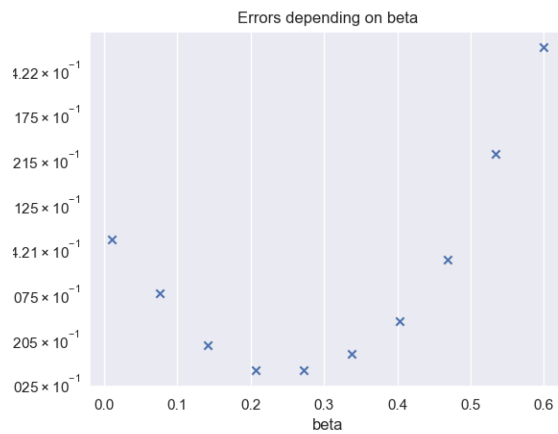

Figure 6: Final error = f(β)

Forcing bounded image space for the reconstructed signal helps having positive values. Nonetheless, the signal seems to have difficulties reaching the highest values of the original signal.

3.3 Sparsity Prior

This time $g = || \cdot ||_1$. F is coercive is always greater than $\gamma|| \cdot ||_1$ As F can be separated in $F = F_1 + F_2$ with $F_2 = \gamma g$, we have that ∇F_1 is $\nu - Lipschitz$ with $\nu \in (0, ||K^T K||]$. $prox_{\gamma\beta||\cdot||_1}$ is available in the usual proximal tables. Therefore we can use the forward-backward algorithm.

We will use it as follows :

1. Initialize x_0
2. for $k \geq 1$
    - Compute $y_k = x_k - \gamma K^T(Kx_k - y)$
    - $x_{k+1} = x_k + \lambda(prox_{\gamma\beta||\cdot||_1}(y_k) - x_k)$

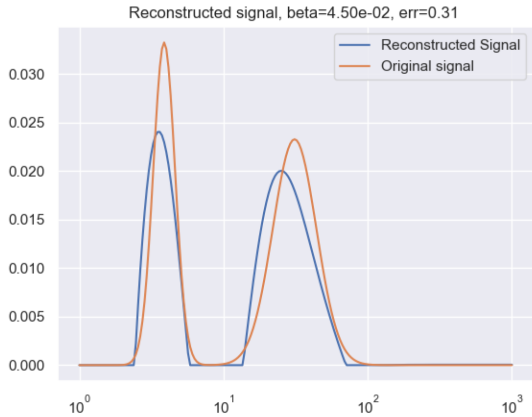

Figure 7: Reconstructed signal with sparsity prior

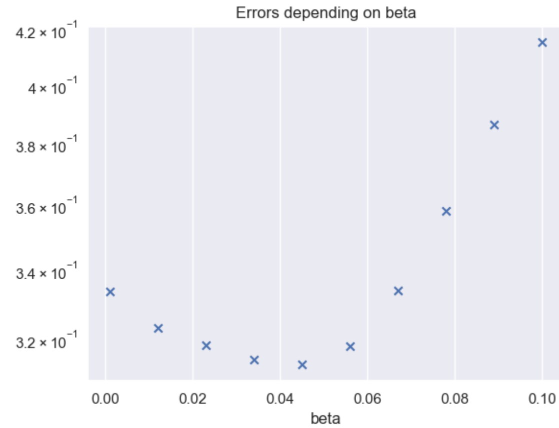

Figure 8: Final error = f(β)

Compared to the sparse priors, we get higher maximal values. The errors on beta shows a clear minima.

3.4 Entropy regularization

First, we will show that $F \in \Gamma_0(\mathbb{R}^)$:

- $\mathbb{R}^N \ni x \longrightarrow \sum_{i=1}^N \phi(x_i)$ with the entropy function on $\mathbb{R}$. Therefore it is separable and as ϕ is proper, so is F.
- ϕ is continuous on $\mathbb{R}_+^*$ and tends by the right to 0. As it is fixed to ∞ when x is negative, ϕ is lower semi-continuous. Thus, F too.
- On $\mathbb{R}_+^*$, ϕ'' is the inverse function, thus strictly convex. For the other cases, we will use that $f convex \iff \forall x, y f(y) \geq f(x) + f'(x)(y - x)$
  - The cases where one or both x, y are equal to 0, trivially verify the inequality.
  - if both are negative then by using the definition of convexity, we would end up comparing infinite quantities. We would have equality and therefore convexity.
  - if only one them is negative and if the other is equal to zero, we would also have infinite members in each side of the equation as $\phi'(0) = -\infty$.
  - Finally, if one of them is negative and the other positive, the inequality obviously holds as the left term is ∞ and the right one is bounded.

Hence, $F \in \Gamma_0(\mathbb{R}^)$ by double positive summation (sum on coordinate of x, then with $||K \cdot -y||^2$)

As ϕ is coercive and as $||K \cdot -y||^2$ is positive, F is coercive also by double positive summation. Therefore F as at least one minimizer.

By the strict convexity of F, we also know that this minimizer is unique.

3.4.1 Forward Backward Algorithm

In this setup, with a not-everywhere differentiable penalization, the forward backward algorithm is relevant. We can compute $prox_{\gamma\beta ent}$ by separability.

$$x \longrightarrow prox_{\gamma\beta\phi}(x) = \arg\min_{y\in\mathbb{R}} \frac{1}{2}||y-x||^2 - \gamma\beta\phi(y)$$

Equivalently, as the member to minimize is ∞ for negative values, it is equivalent to minimize for non negative values. Furthermore, it is convex, differentiable and coercive. Therefore we can use the first order condition for optimality : $(y-x)+\gamma\beta ln(x)+\gamma\beta = 0$

Hence $prox_{\gamma\beta\phi}(x) = y^* = \gamma\beta W(\exp(\frac{x}{\gamma\beta} - 1 - \ln(\gamma\beta))$ where W is the inverse function of $x \longrightarrow x\exp^x$

The Forward- Backward algorithm would then be :

1. Initialize x_0
2. for $k \geq 1$
   - Compute $y_k = x_k - \gamma K^T(Kx_k - y)$
   - $x_{k+1} = x_k + \lambda(prox_{\gamma\beta ent}(y_k) - x_k)$

With $\gamma \in (0, \frac{2}{\nu})$ and $\lambda \in (0, 2 - \frac{\nu\gamma}{2})$

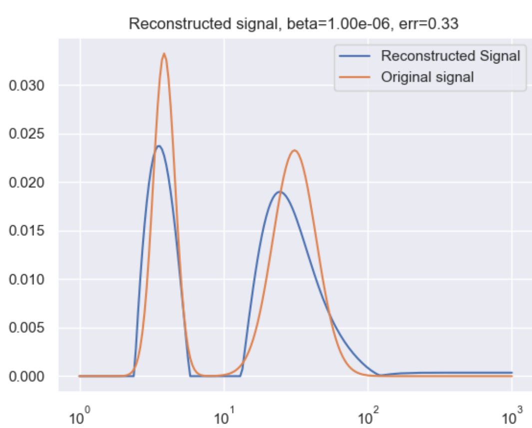

Figure 9: Reconstructed signal for entropy regularization with Forward-Backward algorithm

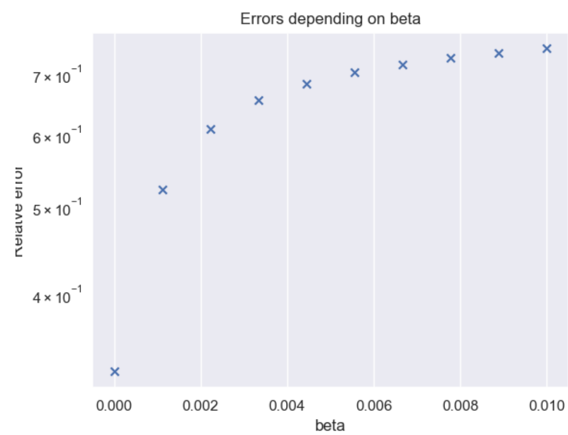

Figure 10: Final error = f(β)

The errors on betas seem to be strictly decreasing which prevent us to find the optimal beta. Our hypothesis is that we would need to explore very small betas to find a minima because of the value of gamma.

3.4.2 Douglas-Rashford Algorithm

Furthermore, to implement the Douglas-Rashford algorithm, we will also need $prox_{\frac{\gamma}{2}||K\cdot-y||^2}$. By using the proximal tables we have $prox_{\frac{\gamma}{2}||K\cdot-y||^2}(x) = (\gamma K^TK + Id)^{-1}(\gamma K^Ty + x)$

1. Initialize x_0

2. for $k \geq 1$

   - Compute $y_k = prox_{\gamma\beta ent}(x_k)$
   - $z_k = prox_{\frac{\gamma}{2}||K\cdot - y||^2}(2y_k. - x_k)$
   - $x_{k+1} = x_k + \lambda(z_k - y_k)$

Here, we only need γ to be positive and $\lambda \in (0, 2)$

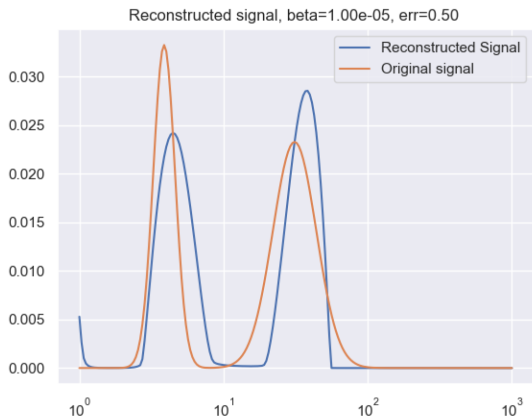

Figure 11: Reconstructed signal with Douglas-Rashford algorithm

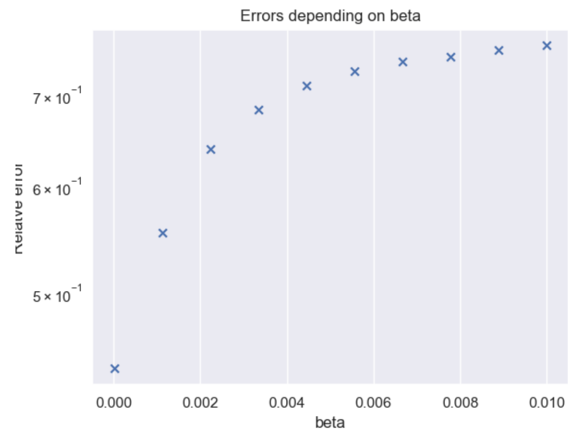

Figure 12: Final error = f(β)

The error seems to be stricly decreasing in β. It is likely that $prox_{\gamma\beta ent}$ takes high values, which prevents us to find an appropriate β.

4 Conclusion

We can see in Figure 13 that the best reconstructed signal seems to be obtained for the entropy regularization.

The sparse penalization induces steep variations. The projected gradient seems to fail reaching the top of the curves.

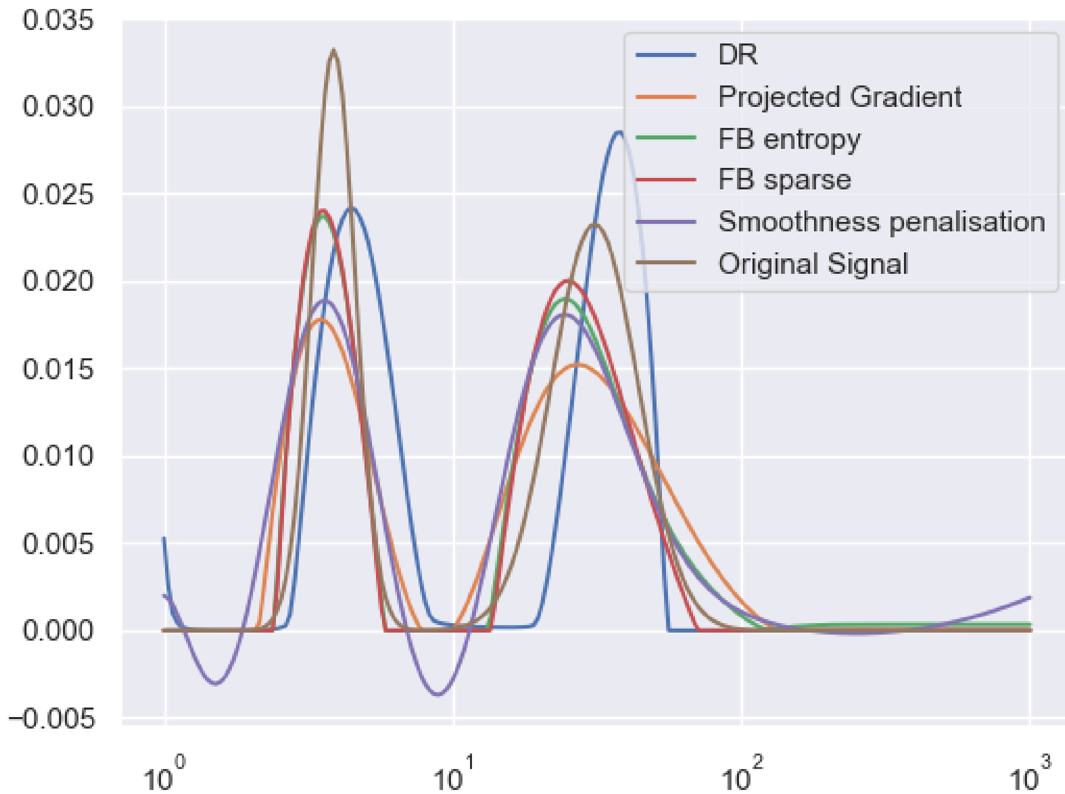

Figure 13: All reconstructed signals