ECP
LSD
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Reconstruction of DOSY NMR signals - Part II

1 Maximum entropy regularization

In the context of DOSY NMR data processing, a standard strategy for restoring the target signal is to define it as the solution of the so-called maximum entropy problem :

$$\widehat{x} = \underset{x \in \mathbb{R}^N}{\operatorname{argmin}} \ \frac{1}{2}\|Kx - y\|^2 + \beta \ \mathrm{ent}(x), \tag{1}$$

where

$$(\forall x \in \mathbb{R}^N) \quad \mathrm{ent}(x) = \sum_{n=1}^{N} \varphi(x^{(n)}), \tag{2}$$

with

$$(\forall u \in \mathbb{R}) \quad \varphi(u) = \begin{cases} u \log u & \text{if } u > 0, \\ 0 & \text{if } u = 0 \\ +\infty & \text{elsewhere.} \end{cases} \tag{3}$$

1. Is ent convex ? proper ? lower-semicontinuous ? differentiable ?
2. Has the optimization problem a solution ? Is it unique ?
3. Give the expression of the proximity operator of ent at some $x \in \mathbb{R}^N$. (Hint : Use the Lambert W-function).
4. Propose a forward-backward and a Douglas-Rachford algorithm to solve problem (1).
5. Implement them both and evaluate their performances for $\beta = 10^{-2}$.
6. What is the best choice for parameter β in terms of reconstruction error between the estimated object and the ground truth ?
7. Compare the maximum entropy regularization with the ones proposed in the previous part in terms of reconstruction quality.
8. In practice, adjusting the parameter β may be difficult, while one has often informations about the level of noise corrupting the data. A more practical formulation may therefore be obtained by solving the following optimization problem :

$$\underset{x \in \mathbb{R}^N}{\operatorname{minimize}} \ \mathrm{ent}(x) \quad \text{subject to} \quad \|Kx - y\|^2 \leq \eta M \sigma^2, \tag{4}$$

with $\eta > 0$. Propose an algorithm providing a numerical solution to this problem and implement it.