Primal-dual interior-point optimization for a regularized reconstruction of NMR relaxation time distributions

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Outline

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   - Principle
   - Problem statement
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   - Optimization framework
   - Main algorithm steps
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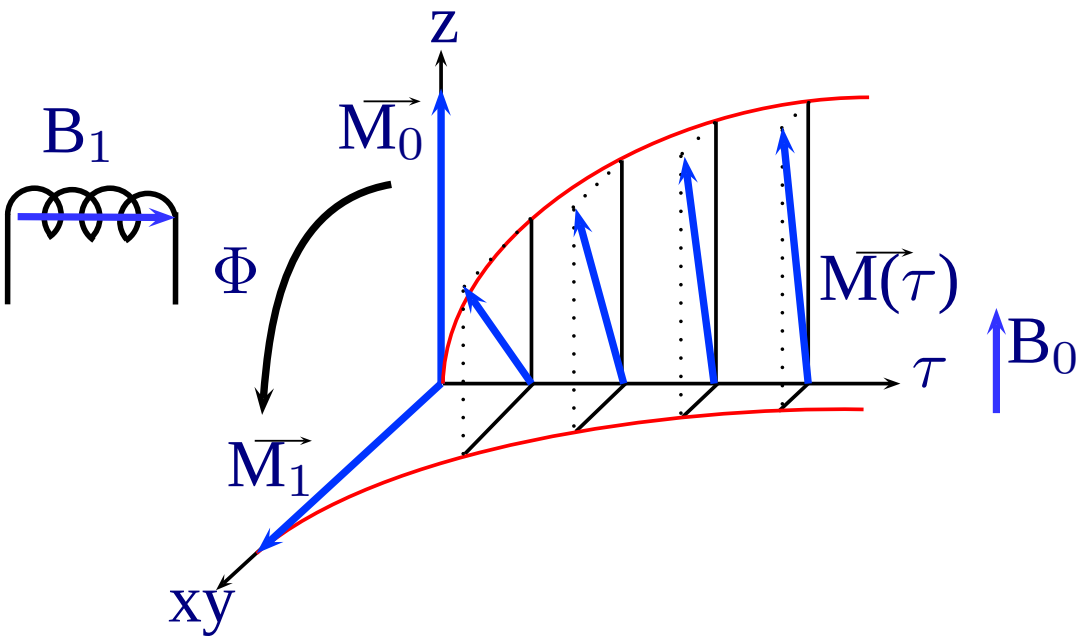
1. NMR Relaxation

How to identify the molecular structure of a material by observing its dynamics?

1.1 Principle



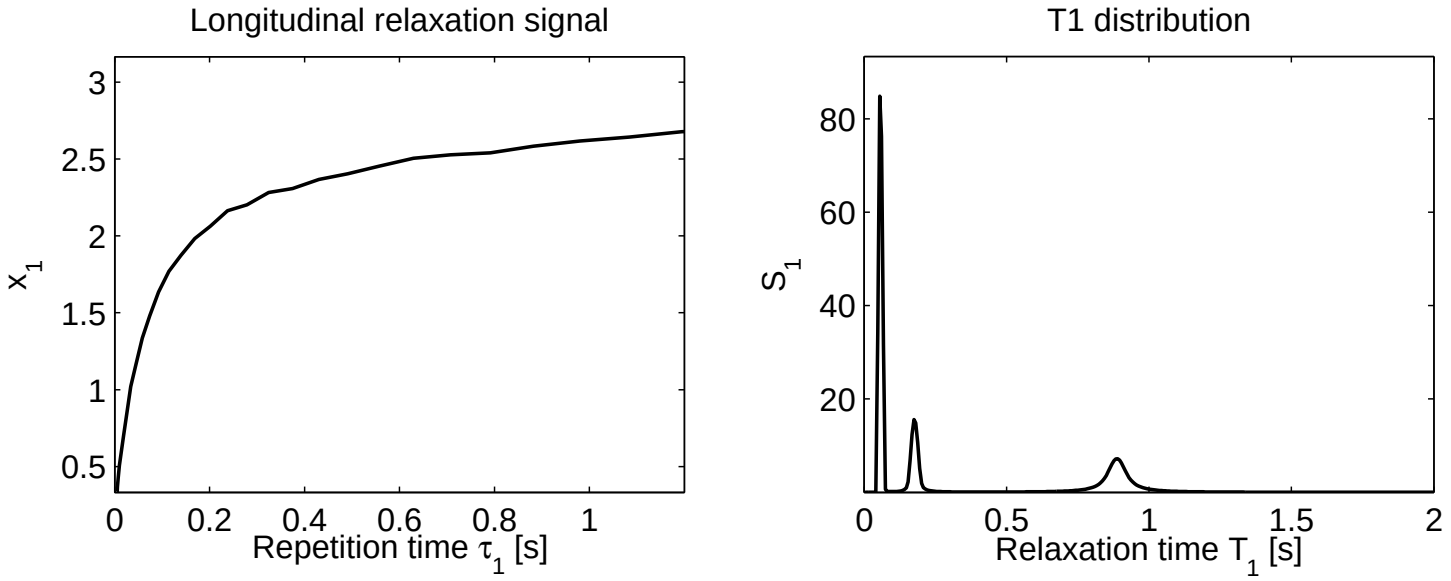
- Static field $B_0 \Rightarrow$ nuclear spin alignment (z axis)
- Short magnetic pulse $B_1 \Rightarrow$ flip angle Φ
- Relaxation: return to the equilibrium state
  1. Longitudinal dynamics (z axis)
     $\Rightarrow T_1$ relaxation: $x_1(\tau_1) = M_{\mathrm{z}}(\tau_1)$
  2. Transverse dynamics (xy plane)
     $\Rightarrow T_2$ relaxation: $x_2(\tau_1) = M_{\mathrm{xz}}(\tau_1)$

1) One-dimensionnal analysis

✓ Find T1 or T2 relaxation time constants distribution

$$x_i(\tau_i) = \int k_i(\tau_i, T_i)\, S(T_i)\, dT_i \longrightarrow \boldsymbol{y} = \boldsymbol{K}\boldsymbol{s} + \boldsymbol{e}$$

with $k_1(\tau_1) = 1-(1-\cos\Phi)e^{-\tau_1/T_1}$ in T_1 relaxation and $k_2(\tau_2) = e^{-\tau_2/T_2}$ for T_2 relaxation



⟶ Numerical inversion of a Laplace transfrom

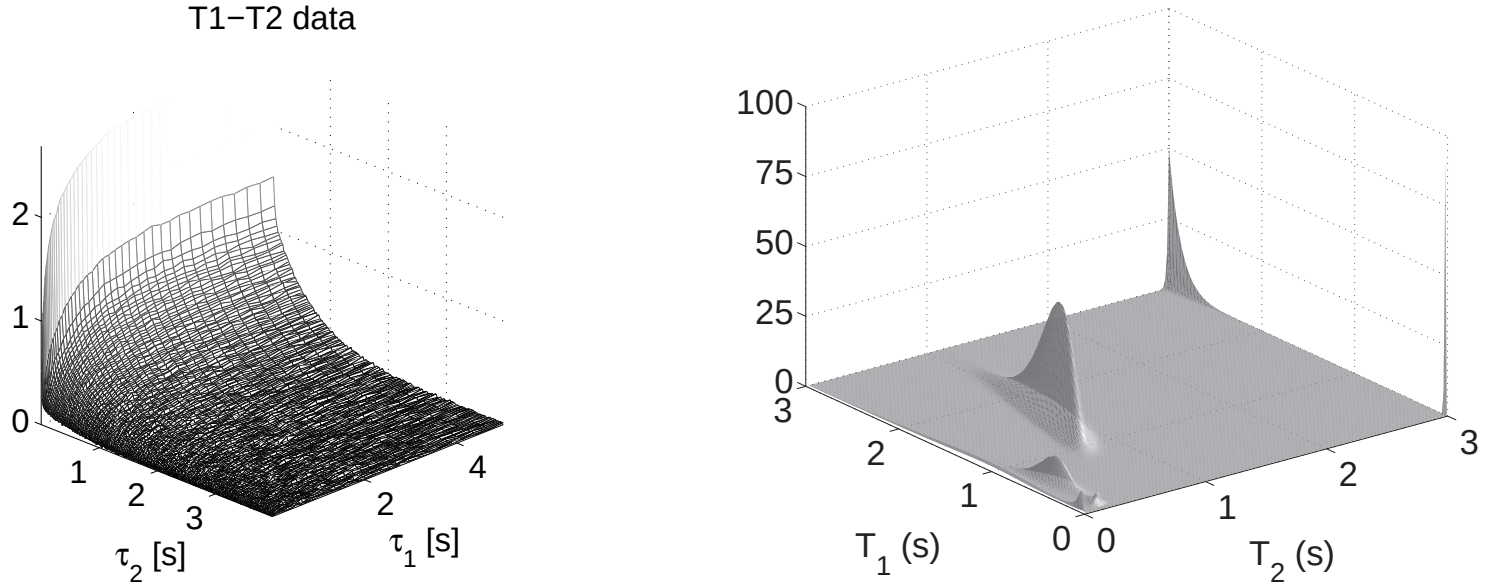
2) Two-dimensional analysis [English 1991]

✓ Apply two successive magnetic pulses with a predefined time spacing τ_1

$$x(\tau_1, \tau_2) = \int \int k_1(\tau_1, T_1) S(T_1, T_2) k_2(\tau_2, T_2)\, dT_1\, dT_2$$

$$\boldsymbol{Y} = \boldsymbol{K}_1 \boldsymbol{S} \boldsymbol{K}_2^{\mathsf{T}} + \boldsymbol{E} \Longleftrightarrow \boldsymbol{y} = (\boldsymbol{K}_1 \otimes \boldsymbol{K}_2)\boldsymbol{s} + \boldsymbol{e}$$

✓ Find the joint distribution $S(T_1, T_2)$ of the relaxation time constants



1.2 Relaxation time estimation ... problem statement

- Ill-conditioned matrices $\boldsymbol{K}_1, \boldsymbol{K}_2$. The singular values of $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ decay exponentially

  $\lhd$ *Direct inversion yields unstable results*

- Large-size problem in the case of T1-T2 analysis

  ⊛ **Typical setup**

  1. $m_1 = 50$ repetition time values τ_1
  2. $m_2 = 5000$ echo time instants τ_2
  3. $N_1 = N_2 = 300$ values of T_1 and T_2

  $\lhd$ *Matrix* $\boldsymbol{K} := \boldsymbol{K}_1 \otimes \boldsymbol{K}_2$ *of size* $m_1 m_2 \times N_1 N_2$ *contains over* 10^{10} *elements !!*

1.3 Relaxation time estimation ... regularization framework

- The relaxation time distribution is a solution of

$$\min_{\boldsymbol{s}\in\mathbb{R}^{N+}} \left(F(\boldsymbol{s}) = \frac{1}{2}\|\boldsymbol{K}\boldsymbol{s} - \boldsymbol{y}\|_2^2 + \beta R(\boldsymbol{s}) \right)$$

  where $R(\boldsymbol{s})$ is a *convex and differentiable* regularization criterion

  $\longrightarrow$ Solve a *non-negativity constrained* optimization problem

  $\longrightarrow$ Avoid the storing of matrix $\boldsymbol{K}$ in the 2D case

- Previous works

  1. Data compression and Tikhonov regularization [Venkataramanan, 2002]
  2. Maximum entropy and truncated Newton algorithm [Chouzenoux, 2010]

- Our proposal

  Adopt and adapt an *inexact primal-dual interior-point method*

2. Primal-dual interior point optimization

2.1 Problem formulation

$$\underbrace{\min_{\boldsymbol{s}} F(\boldsymbol{s}) \text{ s.t. } \boldsymbol{s} \succeq \mathbf{0}}_{\text{Primal problem}} \quad \text{and} \quad \underbrace{\max_{\boldsymbol{\lambda}} g(\boldsymbol{\lambda}) \text{ s.t. } \boldsymbol{\lambda} \succeq \mathbf{0}}_{\text{Dual problem}}$$

where $g(\boldsymbol{\lambda})$ is the *Lagrange dual* function: $g(\boldsymbol{\lambda}) = \inf_{\boldsymbol{s} \succeq \mathbf{0}} (L(\boldsymbol{s}) := F(\boldsymbol{s}) - \boldsymbol{\lambda}^{\mathsf{T}} \boldsymbol{s})$

1) Optimality conditions (Karush Kuhn Tucker)

$$\text{(C1) } \nabla F(\boldsymbol{s}) - \boldsymbol{\lambda} = \mathbf{0}, \quad \text{(C2) } \boldsymbol{\Lambda s} = \mathbf{0}, \quad \text{(C3) } \boldsymbol{s} \succeq \mathbf{0}, \quad \text{(C4) } \boldsymbol{\lambda} \succeq \mathbf{0}$$

But in practice, take:

$$\text{(C2) } \boldsymbol{\Lambda s} = \boldsymbol{\mu}_k$$

with $\mu_k > 0$ a perturbation parameter such that $\lim_{k \to \infty} \mu_k = 0$.

2) Interior point-algorithm ... four steps [Armand, 2000]

① Calculate the *primal and dual directions* $(\boldsymbol{d}_k^s\ ,\ \boldsymbol{d}_k^\lambda)$

A Newton step on (C1) and (C2) gives:

$$\begin{bmatrix} \nabla^2 F(\boldsymbol{s}_k) & -\boldsymbol{I} \\ \boldsymbol{\Lambda}_k \boldsymbol{I} & \mathrm{Diag}(\boldsymbol{s}_k) \end{bmatrix} \begin{bmatrix} \boldsymbol{d}_k^s \\ \boldsymbol{d}_k^\lambda \end{bmatrix} = \begin{bmatrix} \boldsymbol{\lambda}_k - \nabla F(\boldsymbol{s}_k) \\ \boldsymbol{\mu}_k - \boldsymbol{\Lambda}_k \boldsymbol{s}_k \end{bmatrix}$$

$\lhd$ *System of large size ... infeasible in 2D NMR !*

② Find a step-size α_k by a *backtracking linesearch* and Armijo's condition on:

$$F_\mu(\boldsymbol{s}, \boldsymbol{\lambda}) = F(\boldsymbol{s}) + \boldsymbol{\lambda}^\intercal \boldsymbol{s} - \mu_k \sum_{n=1}^{N} \log(\lambda_n s_n^2)$$

③ Update primal and dual variables: $\left(\boldsymbol{s}_{k+1} = \boldsymbol{s}_k + \alpha_k \boldsymbol{d}_k^s, \boldsymbol{\lambda}_{k+1} = \boldsymbol{\lambda}_k + \alpha_k \boldsymbol{d}_k^\lambda\right)$

④ Decrease the perturbation parameter value: $\mu_{k+1} = \theta \dfrac{\boldsymbol{\lambda}_{k+1}^\intercal \boldsymbol{s}_{k+1}}{N}$, with $\theta \in]0, 1)$.

3) Primal and dual direction calculation

A variable substitution gives: $\boldsymbol{d}_k^{\lambda} = \mathrm{Diag}(\boldsymbol{s}_k)^{-1}\left[\boldsymbol{\mu}_k - \boldsymbol{\Lambda}_k\boldsymbol{s}_k - \boldsymbol{\Lambda}_k\boldsymbol{d}_k^{s}\right]$, and

$$\left[\nabla^2 F(\boldsymbol{s}_k) + \mathrm{Diag}(\boldsymbol{s}_k)^{-1}\boldsymbol{\Lambda}_k\right]\boldsymbol{d}_k^{s} = -\nabla F(\boldsymbol{s}_k) + \mathrm{Diag}(\boldsymbol{s}_k)^{-1}\boldsymbol{\mu}_k$$

where $\nabla^2 F(\boldsymbol{s}_k) = (\boldsymbol{K}_1^{\intercal}\boldsymbol{K}_1) \otimes (\boldsymbol{K}_2^{\intercal}\boldsymbol{K}_2) + \nabla^2 R(\boldsymbol{s}_k)$

◁ *Still remains a huge system in 2D relaxation*

◁ *Approximate resolution using a preconditioned conjugate gradient algorithm*

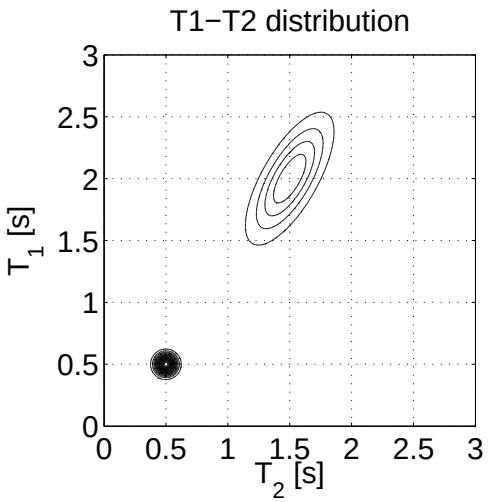
1. Perform TSVDs of $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ to construct an efficient preconditioner,
2. Calculate with a low complexity *Hessian-vector* and *Preconditioner-vector* products,
3. See the paper for the stopping criteria.

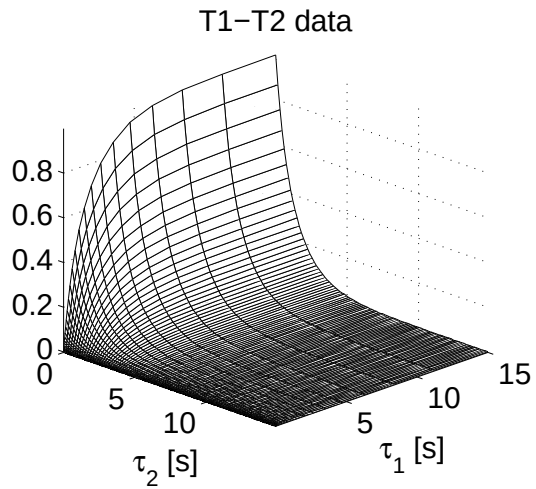
◁ *The convergence proof is established when $\boldsymbol{d}_k^{s}$ is obtained by an approximate resolution.*

3. Illustration

3.1 Synthetic data

- Mixture of two Gaussian distributions,
- ($m_1 = 50$, m_2=5000) values of (τ_1, τ_2),
- A flip angle $\Phi = 90^\circ$ in the T1-T2 model,
- Additive Gaussian noise with SNR=20 dB.



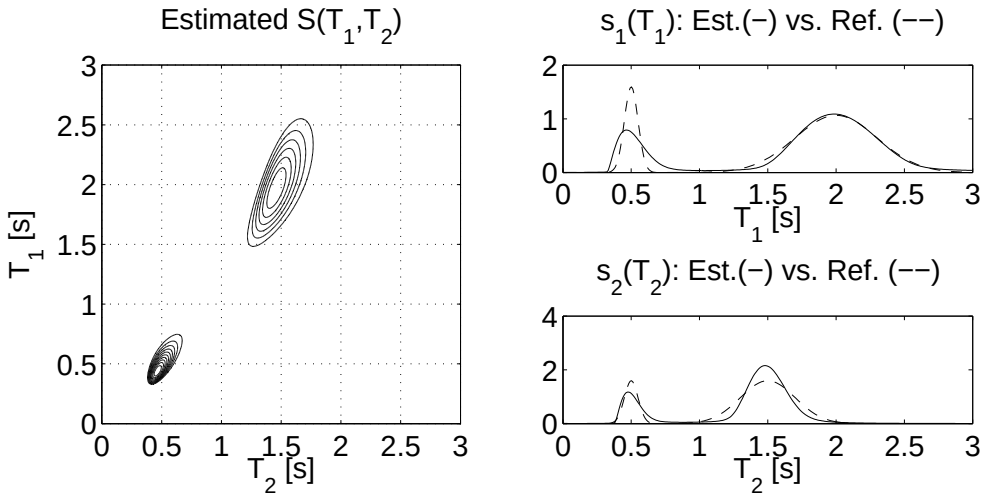


⊛ Reconstruction

1. $(N_1 = 300,\ N_2 = 300)$ with uniform spacing

2. Use a Tikhonov regularization criterion $R(\boldsymbol{s}) = \|\boldsymbol{s}\|_2^2$

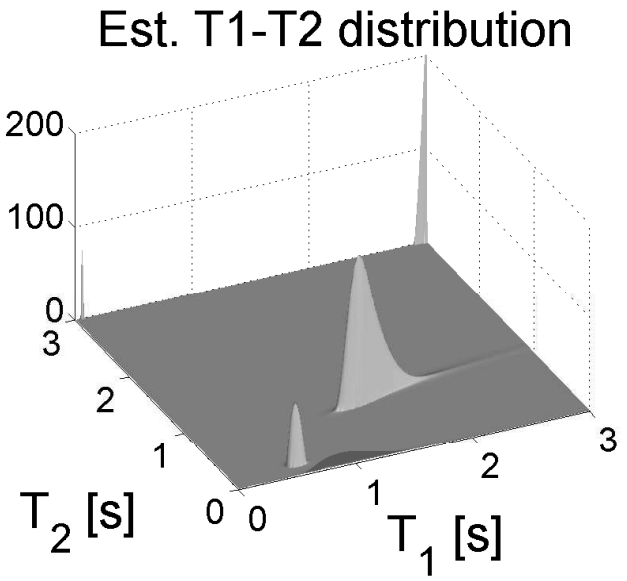
3. Set the regularization parameter $\beta = 100$ (unsupervised tuning [Chouzenoux, 2010])

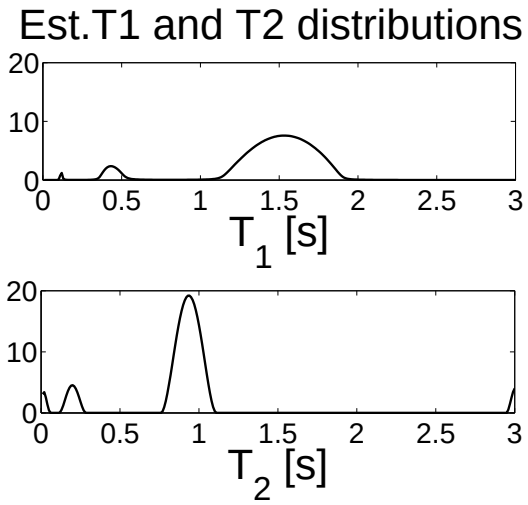


4. Computation time: (20 it., $1s$) in 1D and (36 it., 55 s) for 2D reconstruction.

3.2 Real data: Analysis of an organic matter (apple)

- Measurements: $(m_1 = 50, m_2 = 10000)$
- Reconstruction for $N_1 = N_2 = 300$
- The flip angle is set to $\Phi = 85^o$
- T1-T2 Computation time: 260 s for 61 iterations.
- T1 (resp. T2) computation time: 0.3 s for 21 iterations (resp. 9 s for 35 iterations).





Summary

⊛ **Main contributions**

- Address the inverse problem of 2D NMR relaxation times estimation
- Propose an efficient optimization algorithm for a *differentiable convex* regularization
- Exploit de forward model structure to reduce the computational complexity.

⊛ **Future investigations**

1. Estimate the flip angle
2. Gaussian noise assumption is not valid on the nuclear spin module
3. Compare with alternative constrained optimization methods.

References

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