OPTIMIZATION OF A MAXIMUM ENTROPY CRITERION FOR 2D NUCLEAR MAGNETIC RESONANCE RECONSTRUCTION

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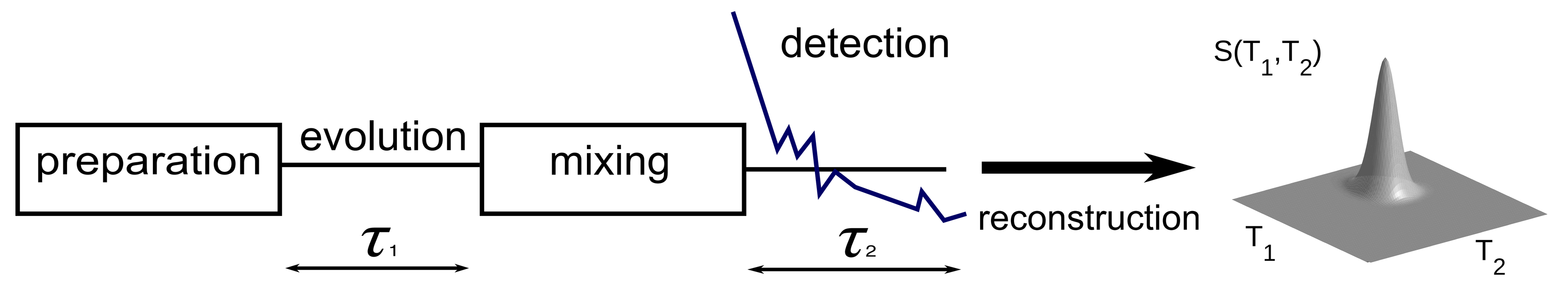
A T_1-T_2 spectrum is very useful in NMR spectroscopy since it reveals any coupling between T_1 and T_2 relaxations. The determination of such 2D spectrum is an ill-posed inverse problem. We propose an efficient iterative reconstruction method based on maximum entropy regularization.

PHYSICAL MODEL



$$Y(\tau_1,\tau_2) = \iint (1-\gamma e^{-\tau_1/T_1}) S(T_1,T_2) e^{-\tau_2/T_2}\, dT_1 dT_2 \;\xrightarrow{\text{discretization}}\; \begin{cases} Y = K_1 S K_2^t \\ y = Ks \end{cases}$$

with $K_1 \in \mathbb{R}^{m_1\times N_1}$, $K_2 \in \mathbb{R}^{m_2\times N_2}$, $Y \in \mathbb{R}^{m_1\times m_2}$, $S \in \mathbb{R}^{N_1\times N_2}$, $y = \text{vect}(Y)$, $s = \text{vect}(S)$ and $K = K_1 \otimes K_2$.

AIM Reconstruction of S given noisy measurements Y

DIFFICULTIES

- ⋆ POSITIVITY CONSTRAINT
- ⋆ HUGE MATRIX K
- ⋆ K_1, K_2 ILL-CONDITIONED

PROPOSAL Convergent iterative reconstruction method based on maximum entropy regularization and exploiting kernel separability

RECONSTRUCTION STRATEGY

MAXIMUM ENTROPY (ME) PENALIZATION

$$\min_{s\geqslant 0} L(s) = \tfrac{1}{2}\|y - Ks\|^2 + \lambda \sum_i s_i \log s_i$$

✓ Accounts for positivity ✓ Good results in 1D NMR [1]
✓ Well suited for distribution recovering

Iterative descent algorithm

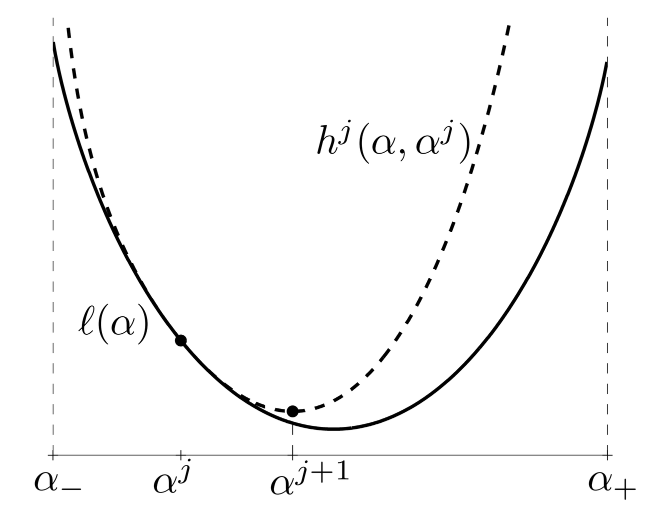
At each iteration k, $k = 1, \ldots, K$,
1. Compute a descent direction d_k
2. Determine the stepsize α_k according to a linesearch strategy aimed at minimizing $\ell(\alpha) = L(s_k + \alpha d_k)$.
3. Update $s_{k+1} = s_k + \alpha_k d_k$.

- d_k results from conjugate gradient (CG) or truncated Newton algorithm
- Entropy is a *barrier* function for the positive orthant
  - ➩ $\dot\ell(\alpha)$ **unbounded** for α cancelling a component of $s_k + \alpha d_k$
  - ➩ $\nabla^2 L$ **ill-conditioned** near the boundary of the domain
- K is large and rank-deficient.

Proposed approach

① Specific linesearch strategy for barrier function
② Convergence acceleration with a new preconditioner
③ Computational cost reduction by exploiting kernel separability

MAJORIZE-MINIMIZE LINESEARCH STRATEGY



$h^j(.,\alpha^j)$ **tangent majorant** for ℓ at α^j i.e.,

$$\begin{cases} h(\alpha,\alpha^j) \geqslant \ell(\alpha) \\ h(\alpha^j,\alpha^j) = \ell(\alpha^j) \end{cases}$$

Majorize Minimize recurrence
$\alpha^{j+1} = \arg\min_\alpha h^j(\alpha,\alpha^j)$, $j \leqslant J$
with $h^j(\alpha,\alpha^j) = p_0 + p_1\alpha + p_2\alpha^2 - p_3\log(\alpha - \alpha_\pm)$.

➩ **Ensures theoretical convergence of the descent algorithm [2]**

LOW RANK PRECONDITIONER

Preconditioner P_k approximates the inverse Hessian using truncated SVDs of K_n at rank v ($\tilde U_n^t \tilde\Sigma_n \tilde V_n$), and the matrix inversion lemma:

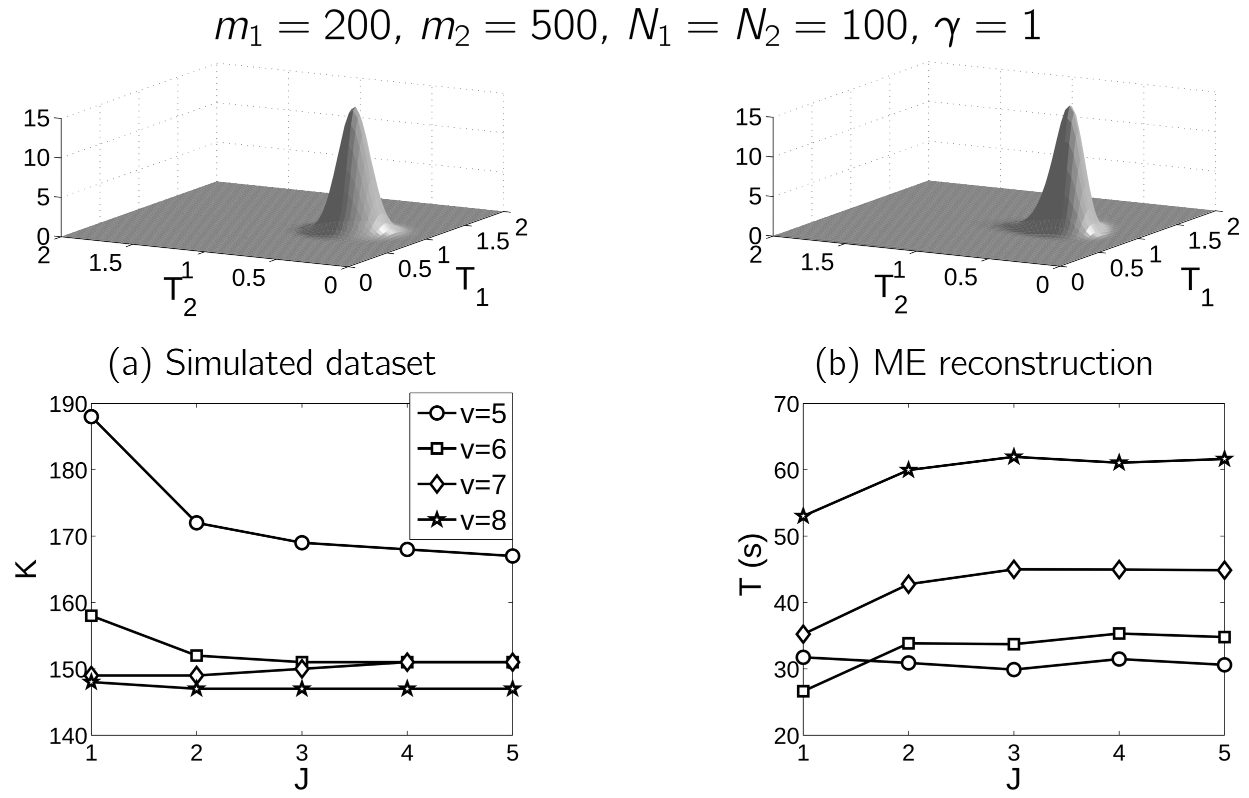
$$P_k = \left[\tilde V \tilde\Sigma^2 \tilde V^t + \lambda\,\text{diag}(s_k)^{-1}\right]^{-1} = A_k - A_k\tilde V(\tilde\Sigma^{-2} + \tilde V^t A_k \tilde V)^{-1}\tilde V^t A_k$$

with $A_k = \lambda^{-1}\text{diag}(s_k)$ and $\begin{cases} \tilde V = \tilde V_1 \otimes \tilde V_2 \\ \tilde\Sigma = \tilde\Sigma_1 \otimes \tilde\Sigma_2 \end{cases}$.

EXPERIMENTAL RESULTS

SYNTHETIC EXAMPLE (40 dB)

$m_1 = 200$, $m_2 = 500$, $N_1 = N_2 = 100$, $\gamma = 1$

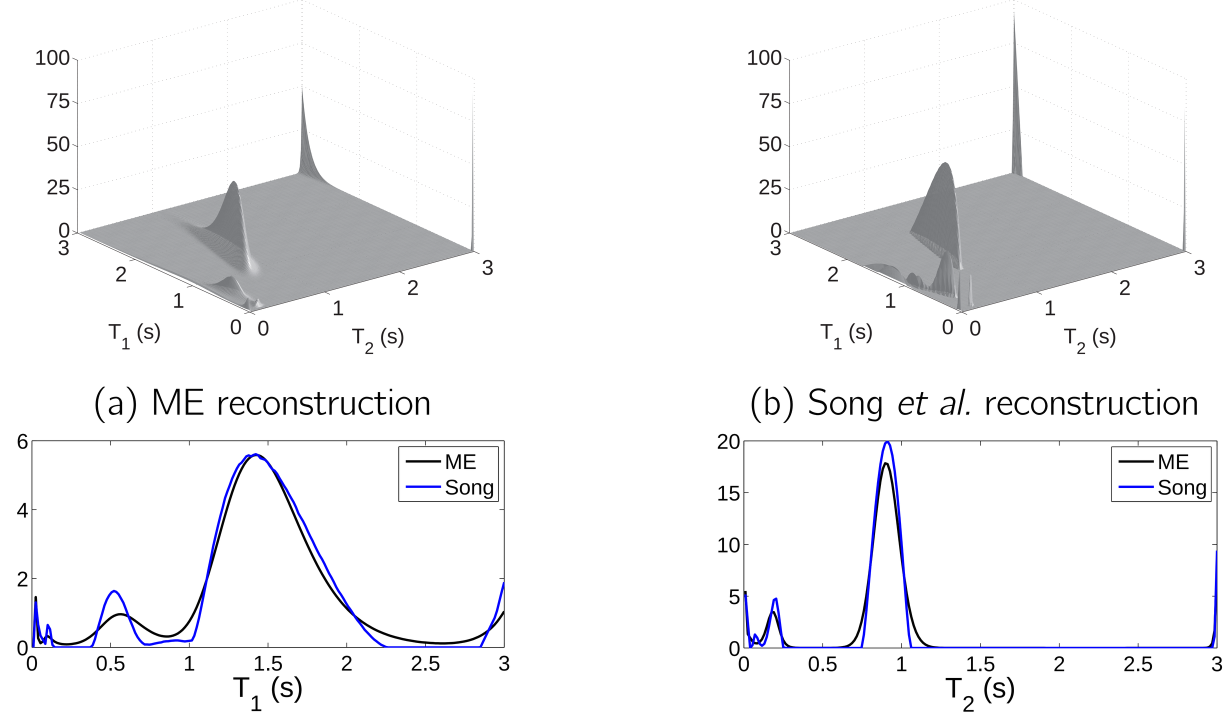


(a) Simulated dataset (b) ME reconstruction
(c) Number of iterations (d) Computational time

PCG direction	$d_k = -P_k g_k + \beta_k d_{k-1}$
Stopping criterion	$\|\nabla L(s_k)\|_\infty < 10^{-8}(1 + \|L(s_k)\|)$
MM subiterations in linesearch	$J \nearrow$ implies $K \searrow$ but time $\nearrow$
Truncation rank in preconditioner	$v \nearrow$ implies $K \searrow$ but time $\nearrow$

REAL DATA PROCESSING (APPLE)

$m_1 = 50$, $m_2 = 10000$, $N_1 = N_2 = 300$, $\gamma = 0.92$



(a) ME reconstruction (b) Song *et al.* reconstruction
(c) T_1 spectra (d) T_2 spectra

- Comparison with Song *et al.* strategy [3]
  Principle: Tikhonov regularization, KKT conditions, data compression
- Similar data fits (82%) but different spectra shapes (false peaks?)
- Correlation between T_1 and T_2 ⇒ Advantage of 2D spectroscopy

CONCLUSION

- Theoretically convergent algorithm
- Reasonable computational cost and memory requirement
- Does not require data compression

In prospect:

- ➢ Theoretical analysis of 2D spectra obtained from real data
- ➢ Deeper comparison with Song *et al.* algorithm
- ➢ Other optimization algorithms: Truncated Newton, Subspace
- ➢ Strategy for setting the regularization parameter λ

References

[1] F. Mariette, J. P. Guillement, C. Tellier, and P. Marchal, "Continuous relaxation time distribution decomposition by MEM," *Signal Treat. and Signal Anal. in NMR*, pp. 218–234, 1996.

[2] E. Chouzenoux, S. Moussaoui, and J. Idier, "A majorize-minimize line search algorithm for barrier functions," submitted to Comput. Optim. and Appli., November 2009.

[3] L. Venkataramanan, Y. Q. Song, and M. D. Hürlimann, "Solving Fredholm integrals of the first kind with tensor product structure in 2 and 2.5 dimensions," *IEEE Trans. Signal Processing*, vol. 50, no. 5, pp. 1017–1026, 2002.