Filtering techniques for efficient inversion of two-dimensional NMR data

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Problem Description

- **NMR data model**: The distribution of amplitudes $F(T_1,T_2)$ of longitudinal and transversal relaxation times T_1, T_2 is related to the NMR data $S(t_1,t_2)$ by the first-kind Fredholm integral equation:

$$S(t_1,t_2)=\iint_0^\infty k_1(t_1,T_1)k_2(t_2,T_2)F(T_1,T_2)\,dT_1\,dT_2+e(t_1,t_2),\quad k_1(t_1,T_1)=1-2\exp(-t_1/T_1),\quad k_2(t_2,T_2)=\exp(-t_2/T_2) \tag{1}$$

where t_1 and t_2 are two independent evolution time variables and $e(t_1,t_2)$ is additive Gaussian noise

- **Reconstruction model**:

$$\min_{\mathrm{f}}\|(K_2\otimes K_1)\mathrm{f}-\mathrm{s}\|_2^2+\sum_{i=1}^{N}\lambda_i(\mathrm{Lf})_i^2\quad s.t.\ \ \mathrm{f}\geq 0 \tag{2}$$

- $\mathrm{s}\in\mathbb{R}^M$ vector ordering of $S\in\mathbb{R}^{M_1\times M_2}$ measured noisy signal
- $\mathrm{f}\in\mathbb{R}^N$ vector ordering of $F\in\mathbb{R}^{N_1\times N_2}$, unknown distribution
- $K_1\in\mathbb{R}^{M_1\times N_1}$, $K_2\in\mathbb{R}^{M_2\times N_2}$
- λ_i local spatially adapted regularization parameters
- $\mathrm{L}\in\mathbb{R}^{N\times N}$ discrete Laplacian operator
- $(\mathrm{Lf})_i$ i-th element Lf

Contribution

- **2DUPEN** is an *iterative algorithm* that computes the λ_i's by imposing that all the non-null products $\lambda_i(\mathrm{Lf})_i^2$ have the same constant value (UPEN principle [*Inv. Problems*, 33(1), 2016]) and an approximated distribution by solving a problem of the form (2) with the Newton Projection method
- 2DUPEN is able to achieve *high quality reconstructions* but requires a *high computational cost*
- The **Mean Windowing (MW)** and **Singular Value Decomposition (SVD)** filters can be used in order to reduce the computational cost of 2DUPEN when applied to *real* 2D NMR data
- The purpose of this work is to analyze the separate and combined effects of these filtering techniques on *synthetic 2D NMR data*.

Filtering techniques

The Mean Windowing-like filter

- Windowing the 2D IR-CPMG data reduces the points in the CPMG blocks: $\bar{\mathrm{s}}\in\mathbb{R}^{M_1\cdot\overline{M}_2}$ with $\overline{M}_2\ll M_2$
- Consider the *diagonal weighting matrix* $(\mathrm{B}\otimes\mathrm{I})$ where $\mathrm{B}\in\mathbb{R}^{\overline{M}_2\times\overline{M}_2}$ contains the numbers of points of each CPMG windowed block and $\mathrm{I}\in\mathbb{R}^{\overline{M}_1\times\overline{M}_1}$ is the identity matrix
- **Weighted least squares problem**:

$$\min_{\mathrm{f}\geq 0}\left\{\left\|(\widetilde{\mathrm{K}}_2\otimes\mathrm{K}_1)\mathrm{f}-\widetilde{\mathrm{s}}\right\|^2+\sum_{i=1}^{N}\lambda_i(\mathrm{Lf})_i^2\right\}$$

where $\widetilde{\mathrm{K}}_2=\mathrm{B}\overline{\mathrm{K}}_2$, $\overline{\mathrm{K}}_2\in\mathbb{R}^{\overline{M}_2\times N_2}$ and $\widetilde{\mathrm{s}}=(\mathrm{B}\otimes\mathrm{I})\bar{\mathrm{s}}$,

The Singular Value Filter filter

- SVD of $K_1=U_1\Sigma_1V_1^T$ and $K_2=U_2\Sigma_2V_2^T$ where U_i,V_i, are orthogonal matrices and Σ_i are the diagonal matrices of the singular values $(i=1,2)$
- $\|(\mathrm{K}_2\otimes\mathrm{K}_1)\mathrm{f}-\mathrm{s}\|^2=\|(\Sigma_2\mathrm{V}_2^T\otimes\Sigma_1\mathrm{V}_1^T)\mathrm{f}-(\mathrm{U}_2^T\otimes\mathrm{U}_1^T)\mathrm{s}\|^2$
- ρ_i $(i=1,2)$ is the number of singular values of Σ_i greater than the threshold τ
- **SVD compressed problem**:

$$\min_{\mathrm{f}\geq 0}\left\{\|(\hat{\mathrm{K}}_1\otimes\hat{\mathrm{K}}_2)\mathrm{f}-\hat{\mathrm{s}}\|^2+\sum_{i=1}^{N}\lambda_i(\mathrm{Lf})_i^2\right\}$$

where: $\hat{\mathrm{K}}_1=\hat{\Sigma}_1\hat{\mathrm{V}}_1^T$, $\hat{\mathrm{K}}_2=\hat{\Sigma}_2\hat{\mathrm{V}}_2^T$, $\hat{\mathrm{s}}=(\hat{\mathrm{U}}_2^T\otimes\hat{\mathrm{U}}_1^T)\mathrm{s}$, $\hat{\Sigma}_i$ has the first ρ_i diagonal elements of Σ_i and $\hat{U}_i,\hat{V}_i$ are made by the first ρ_i columns of U_i,V_i

Algorithm

Filtered 2DUPEN methods

- $2\mathrm{DUPENm}_1$: SVD filter without MW data reduction
- $2\mathrm{DUPENm}_2$: SVD filter, MW data reduction without weighting matrix $(\mathrm{B}\otimes\mathrm{I})$
- $2\mathrm{DUPENm}_3$: MW data reduction, weighting matrix $(\mathrm{B}\otimes\mathrm{I})$ without SVD
- Improved 2DUPEN: SVD filter, MW data reduction, weighting matrix $(\mathrm{B}\otimes\mathrm{I})$

Notation

- p_μ,c_μ are the local slope and curvature values of the 2D distribution
- I_i are the indices subset related to the neighborhood of the distribution point i
- β_0,β_p,β_c are parameters depending on the nature of the measured data

Data preprocessing

- Compute $\widetilde{\mathrm{K}}_2=\mathrm{B}\overline{\mathrm{K}}_2$
- Compute $\widetilde{\mathrm{s}}=(\mathrm{B}\otimes\mathrm{I})\bar{\mathrm{s}}$
- Compute the TSVD of K_1 and $\widetilde{\mathrm{K}}_2$ and set $\hat{\mathrm{K}}_1=\hat{\Sigma}_1\hat{\mathrm{V}}_1^T$, $\hat{\mathrm{K}}_2=\hat{\Sigma}_2\hat{\mathrm{V}}_2^T$
- Compute $\hat{\mathrm{s}}=(\hat{\mathrm{U}}_2^T\otimes\hat{\mathrm{U}}_1)\widetilde{\mathrm{s}}$

Improved 2DUPEN (I2DUPEN) Algorithm

Set $k=0$ and compute an over smoothed solution $\mathrm{f}^{(k)}$ of the problem

$$\min_{\mathrm{f}\geq 0}\|(\hat{\mathrm{K}}_2\otimes\hat{\mathrm{K}}_1)\mathrm{f}-\hat{\mathrm{s}}\|_2^2$$

by applying a few iterations of the Gradient Projection method

`repeat`

1. Compute $\lambda_i^{(k)}$, $i=1,\dots,N$

$$\lambda_i^{(k)}=\frac{\|(\hat{\mathrm{K}}_2\otimes\hat{\mathrm{K}}_1)\mathrm{f}^{(k)}-\hat{\mathrm{s}}\|^2}{N\left(\beta_0+\beta_p\max_{\mu\in I_i}(p_\mu^{(k)})^2+\beta_c\max_{\mu\in I_i}(c_\mu^{(k)})^2\right)}$$

2. Compute $\mathrm{f}^{(k+1)}$ by solving

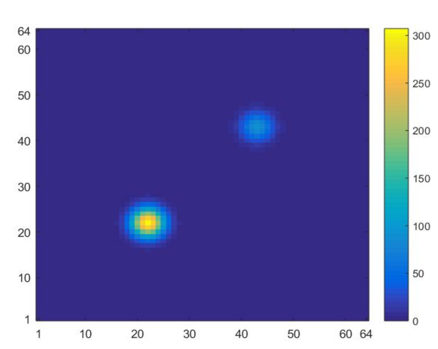
$$\min_{\mathrm{f}\geq 0}\|(\hat{\mathrm{K}}_2\otimes\hat{\mathrm{K}}_1)\mathrm{f}-\hat{\mathrm{s}}\|^2+\sum_{i=1}^{N}\lambda_i^{(k)}(\mathrm{Lf})_i^2$$

using the Newton Projection method

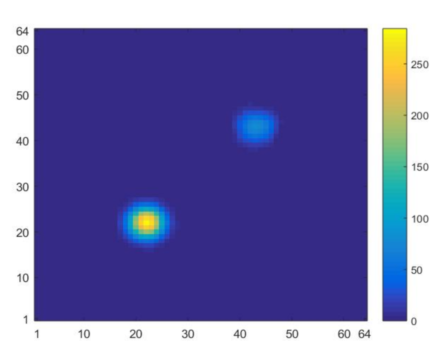
`until` $\|\mathrm{f}^{(k+1)}-\mathrm{f}^{(k)}\|\leq tol\ \|\mathrm{f}^{(k)}\|$

Tests on Synthetic NMR relaxation data

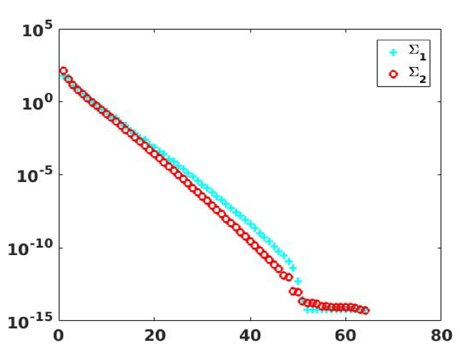
- Synthetic data: $M_1=128$, $M_2=2048$, $\overline{M}_2=118$, $N_1=N_2=64$
- Gaussian random noise added with variance 10^{-2}.
- 2DUPEN parameters: $\beta_0=10^{-6}$, $\beta_p=\beta_c=1$, $tol=0.001$.



exact



I2DUPEN



SVD

	$2\mathrm{DUPENm}_1$			$2\mathrm{DUPENm}_2$			I2DUPEN		
τ	ρ_1,ρ_2	Err	Time(s)	ρ_1,ρ_2	Err	Time(s)	ρ_1,ρ_2	Err	Time(s)
0	64 64	2.749e-02	1352.93	64 64	3.717e-02	2444.87	64 64	7.402e-02	925.04
10^{-6}	32 29	2.620e-02	1455.08	32 28	3.768e-02	1598.35	32 29	5.571e-02	884.07
10^{-4}	24 22	2.731e-02	1252.22	24 21	3.827e-02	1362.99	24 22	6.124e-02	840.35
10^{-3}	20 18	2.841e-02	907.54	20 17	3.878e-02	1409.33	20 18	5.655e-02	915.50
10^{-2}	16 15	3.245e-02	839.48	16 14	3.914e-02	1295.50	16 15	5.833e-02	826.31
10^{-1}	12 11	4.459e-02	738.53	12 10	5.214e-02	778.53	12 11	6.706e-02	720.71

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