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Time-Domain Quantitative Decomposition of MRS FID Signals: Hankel Singular Value Decomposition (HSVD) and the Fast Padé Transform (FPT) Methods

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ABSTRACT

Purpose: Accurate quantitative magnetic resonance spectroscopy (MRS) is critical for metabolic imaging, but conventional Fourier transform (FFT)-based analysis often fails under the extreme dynamic range encountered in hyperpolarized 13C MRS. The dominant substrate resonance compromises phase correction and peak fitting, making quantification of weak downstream metabolites unreliable. This study evaluates Hankel Singular Value Decomposition (HSVD) and the Fast Padé Transform (FPT) as physics-based, time-domain alternatives for robust MRS quantification.
Methods: Complex free induction decay (FID) signals were analyzed directly in the time domain using HSVD and FPT, without Fourier transformation, phase correction, or spectral peak fitting. Both methods model the FID as a sum of exponentially damped sinusoids to directly estimate resonance frequency, damping, amplitude, and phase. Quantitative metabolite peak areas were computed from the estimated signal parameters and compared with conventional FFT-based analysis.
Results: FFT-based spectra were dominated by the injected pyruvate resonance, leaving weak metabolites poorly phased and difficult to quantify. In contrast, HSVD and FPT directly separated low-amplitude metabolites from the FID, providing stable estimates of spectral parameters and reproducible peak areas. Both methods remained robust for truncated FID data, demonstrating resilience to reduced acquisition duration.
Conclusion: HSVD and Fast Padé Transform enable accurate, phase-independent quantification of MRS signals with extreme dynamic range. By eliminating global phase correction and empirical spectral fitting, these time-domain decomposition methods provide a robust framework for quantitative hyperpolarized 13C MRS with strong potential for metabolic imaging and clinical translation.

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INTRODUCTION

Magnetic resonance spectroscopy (MRS) is a powerful noninvasive technique for measuring tissue metabolism by analyzing the **Free Induction Decay (FID)** signal. Accurate decomposition of the FID into its individual spectral components is fundamental for quantitative metabolic analysis in neuroscience, cancer, cardiovascular disease, and numerous clinical and preclinical applications.
Conventional MRS processing follows the workflow:

Complex FID → Apodization → Zero Filling → FFT → Phase Correction → Peak Fitting → Metabolite Quantification

Although widely used, this frequency-domain approach depends on global phase correction and spectral peak fitting. These steps become increasingly unreliable for spectra containing overlapping resonances, low signal-to-noise ratio (SNR), non-Lorentzian peaks, or large dynamic ranges. Under these conditions, **global phase correction becomes mathematically ill-posed**, often leading to inaccurate quantification of weak metabolites.

Time-domain decomposition provides an alternative by modeling the FID directly as a sum of exponentially damped complex sinusoids. **Hankel Singular Value Decomposition (HSVD)** and the **Fast Padé Transform (FPT)** estimate the **frequency, damping factor, amplitude, and phase** of each resonance directly from the measured FID, eliminating the need for Fourier transformation, global phase correction, and empirical peak fitting.

METHODS AND MATERIALS

Hankel Singular Value Decomposition (HSVD)
The FID is modeled as:

$$s[n] = \sum_{k=1}^{K} c_k z_k^n$$

With $z_k = e^{(-d_k + i\omega_k)\Delta t}$

Step 1: Hankel Matrix Construction

$$H = \begin{bmatrix} s_0 & s_1 & \cdots & s_M \\ s_1 & s_2 & \cdots & s_{M+1} \\ \vdots & \vdots & \ddots & \vdots \\ s_L & s_{L+1} & \cdots & s_{N-1} \end{bmatrix}$$

Step 2: Singular Value Decomposition

$$H = U\Sigma V^H$$

Signal and noise subspaces are separated using the dominant singular values.
Step 3: Pole Extraction $U_1 Z = U_2$
Eigenvalues of Zyield: $z_k = e^{(-d_k + i\omega_k)\Delta t}$
Step 4: Amplitude Estimation
A Vandermonde matrix is constructed: $\Gamma c = s$
allowing estimation of: $c_k = A_k e^{i\phi_k}$
Thus, each metabolite is quantified directly by its Frequency, Damping, Amplitude and Phase without global phase correction.

Fast Padé Transform (FPT)
Rational Approximation
The Z-transform of the FID is represented as:

$$S(z) = \frac{P(z)}{Q(z)}$$

Pole Estimation
Roots of:

$$Q(z_k) = 0$$

produce the resonance poles.
Residue Estimation

$$c_k = \frac{P(z_k)}{Q'(z_k)}$$

Physical Parameters

$$d_k = -\frac{\ln |\, z_k \,|}{\Delta t}$$

$$\omega_k = \frac{\arg(z_k)}{\Delta t}$$

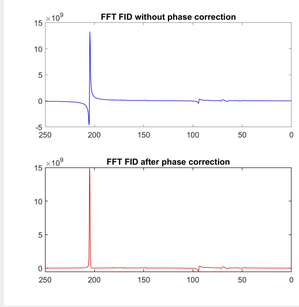
$$A_k = |\, c_k \,|$$

$$\phi_k = \arg(c_k)$$

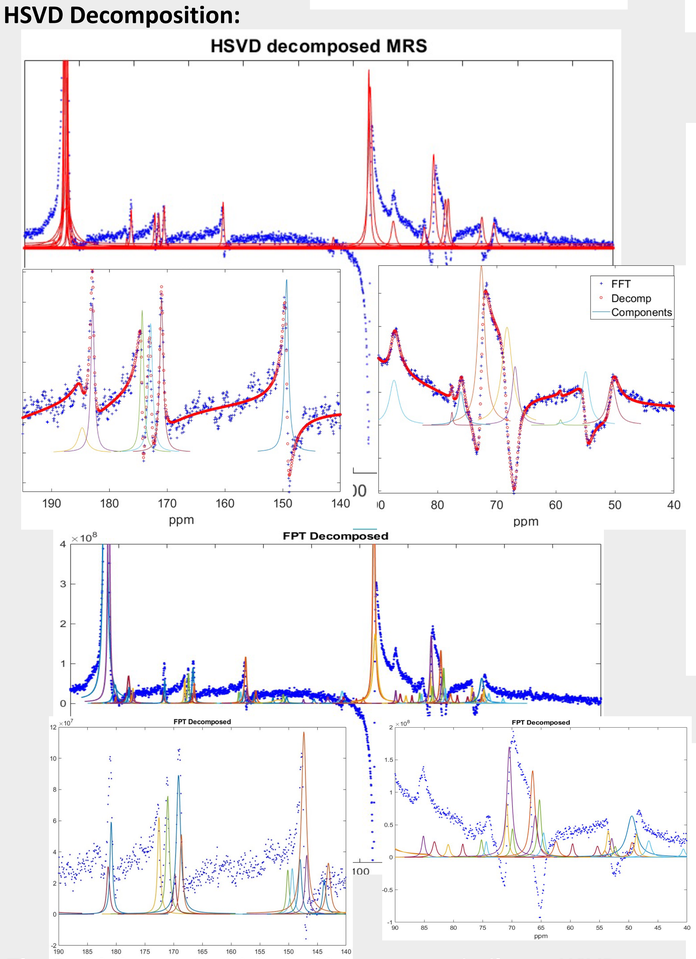
FPT therefore produces the same physical quantities as HSVD but with substantially lower computational cost.

RESULTS

Conventional FFT Analysis:
Dominant [2-^{13}C]pyruvate peak successfully phased. Weak metabolites remain poorly phased. Reliable peak fitting is difficult or impossible. Quantitative analysis becomes unreliable.



HSVD Decomposition:



The Padé decomposition results are very similar to HSVD.

DISCUSSION

Both HSVD and Fast Padé Transform treat MRS quantification as an inverse parameter estimation problem rather than a Fourier transform problem.
Instead of estimating metabolite concentrations from transformed spectra, these methods directly recover the underlying physical parameters governing the FID.

Major advantages include:
- Phase-independent quantification
- High spectral resolution
- Intrinsic noise suppression
- Robust handling of overlapping resonances
- Direct estimation of relaxation and linewidth parameters
- Flexible representation of non-Lorentzian peaks through pole clustering

These advantages are particularly important for hyperpolarized $[2-^{13}C]$pyruvate MRS, where the dominant substrate resonance creates severe challenges for conventional FFT-based analysis.

The proposed methods were also successfully applied to other MRS FIDs, including in vivo hyperpolarized [1-^{13}C]pyruvate and conventional ^{1}H PRESS MRS. These datasets generally exhibited even more robust decomposition because the individual spectral components had relatively higher signal intensities and less extreme dynamic range than hyperpolarized [2-^{13}C]pyruvate MRS.

CONCLUSIONS

- HSVD and Fast Padé Transform provide robust time-domain decomposition of MRS FID signals.
- Both methods directly estimate frequency, damping, amplitude, and phase without phase correction.
- Weak metabolites obscured by dominant substrate signals can be accurately quantified.
- Time-domain decomposition eliminates the need for empirical peak fitting.
- FPT achieves performance comparable to HSVD with reduced computational complexity.
- These approaches provide a powerful framework for quantitative metabolic imaging and future translational MRS applications.

REFERENCES

1. G.L. MILLHAUSER, et al, Rapid SVD for Time-Domain Analysis of MR Signals by Use of the Lanczos Algorithm, JMR 82,150(1989)
2. M.F. Callaghan et al, Pade´ Methods for Reconstruction and Feature Extraction in MRI, MRM 54:1490–1502(2005)