

CFIT: A novel circle-fitting approach to spectral analysis

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Introduction

Spectral analysis of *in vivo* spectra is problematic due to low signal-to-noise ratio (SNR), overlapping peaks and intense artefacts. We present a new frequency-domain (FD) technique for MRS analysis, *CFIT*, wherein the circular trajectories that result when spectral peaks are projected onto the complex plane, are fitted with active circles. This eliminates the need for phasing spectra. The baseline is dealt with using active snakes. The stability and accuracy of *CFIT* is compared with standard time-domain (TD: AMARES) and FD (CSX) methods applied to 98 real human chest and heart ³¹P MRS data sets.

Theory

The complex time-domain MRS signal, $s(t)$, is modeled as the sum of exponentially damped sinusoids:

$$s(t) = \sum_{k=1}^K a_k e^{j\phi_k} e^{(-d_k - j2\pi f_k)t} + n(t) \quad (1)$$

where K = number of sinusoids in the signal, f_k = frequency of the k^{th} sinusoid of amplitude a_k , damping constant $d_k = 1/T^*_{2k}$ and phase ϕ_k ; $n(t)$ is random complex white Gaussian noise. In the FD, the spectrum, $S(f)$, is the sum of a series of Lorentzians:

$$S(f) = \sum_{k=1}^K \frac{a_k}{d_k} e^{j\phi_k} \left(\frac{1}{1 + (2\pi(f - f_k)/d_k)^2} + j \frac{2\pi(f - f_k)/d_k}{1 + (2\pi(f - f_k)/d_k)^2} \right) + N(f) \quad (2)$$

Eq. (2) describes a helix in the 3D space comprised of the complex plane and the chemical shift/frequency axis (Fig. 1). The bracketed terms are of the form, $x = 1/(1+t^2)$, $y = t/(1+t^2)$, or parametric equations of circles. Thus, in the complex plane, each peak is a circle with center at Re-Im coordinates $(a_k/2d_k, 0)$ and radius $a_k/2d_k$ for $\phi = 0$. The effect of a phase shift is simply to rotate the circle in the complex plane.

We model each peak as an active circle that adaptively deforms to best fit the measured spectrum while preserving a circular shape. An iterative gradient descent approach is used to minimize the energy of the fit error (complex difference between the actual spectrum and model), and exert compression/inflation forces on the circle that affect peak height and linewidth, and exert rotational forces that affect peak center frequency. The error forces are weighted with a bell function at the center frequency to reduce the effect of noise and to enable frequency-selective analysis. Baseline artefacts displace the circle end-points and are modeled by a free-form active contour or snake [1], which, while constrained by its elastic properties is adjusted to minimize the fit residuals in each iteration. Prior knowledge is included by assigning an energy penalty to each constraint.

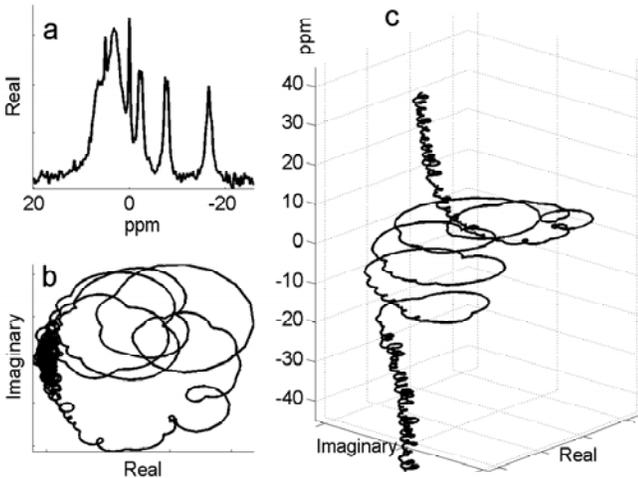


Fig. 1. (a) Real part of a ³¹P brain spectrum [2]. (b) Complex plot of the spectrum. (c) 3D trajectory of the spectrum showing the helical path.

Table: Mean RRMSE, minimum and maximum error relative to CSX for peak area estimates

Peak	Mean RRMSE [min / max](%)	
	AMARES	CFIT
β-ATP	30.6 [0.29 / 81]	25.4 [0.03 / 58]
α-ATP	69.8 [2.3 / 262]	58.9 [2.1 / 178]
γ-ATP	45.3 [1.7 / 93]	60.8 [0.67 / 254]
PCr	74.5 [2.4 / 477]	43.3 [0.04 / 93]

Experiment

98 *in vivo* 1.5T ³¹P spectra with SNR ≥ 5 were acquired in 5-7 min from the human chest and heart of normal subjects (30%) and heart patients (70%) using cardiac-gated 1D CSI with adiabatic excitation (TR ~ 1s; TE = 0.7 ms). The spectra were quantified using CFIT, AMARES [2], and with our current standard, CSX [3], with the same parameters (10 Hz filter, 8-fold zero-filling) and prior knowledge of the ATP multiplets for AMARES and CFIT. The ratio of γ-ATP/β-ATP, and the relative root mean square errors (RRMSE) were measured.

The number of fit failures involving one or more ATP or PCr peaks was 4/98 for CFIT, 29/98 for AMARES, and 8/98 for CSX. Excluding all (31) fit failures, CFIT exhibits the least error (RRMSE) in fitting ATP and PCr peak area (Table).

Conclusion

We have introduced a new FD spectral fitting technique, CFIT, and tested it on real *in vivo* cardiac ³¹P MRS data. CFIT exhibited the lowest failure rate on real data, performing with comparable accuracy to CSX our current standard, on peaks with SNR as low as ~5. It is therefore a suitable alternative to existing standards.

References

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- [2] L Vanhamme et al. J Magn Reson 129 (1997) 35-43.
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