Simple harmonic oscillator based estimation and reconstruction for one-dimensional q-space MR

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INTRODUCTION:

The *q*-space spectroscopy/imaging method provides important insights into tissue microstructure by enabling the calculation of ensemble average diffusion propagators through a Fourier transform. Descriptors of the diffusion propagators such as its moments and return-to-origin probability may be indicators of tissue microstructure which could be sensitive to changes due to aging, development and disease. Moreover, the non-monotonic dependence of the *q*-space signal on the wave number, *q*, [1] may provide a direct means to determine cell sizes. Estimations of the derived quantities and reconstruction of the propagators can be significantly improved if the signal decay can be expressed parametrically. For this purpose, biexponential fitting [2] and cumulant expansion techniques have been applied to *q*-space data. However, biexponential functions are monotonic by design, and as such, they can not model diffraction-like features. The cumulant expansion method is bound to fail as well, because the signal minima are typically beyond the radius of convergence [3] for such expansions. In this work, we propose to express the MR signal in terms of the eigenfunctions of the simple harmonic oscillator Hamiltonian, which form a complete orthogonal basis for the space of square integrable functions.

METHOD:

The *q*-space MR signal, *S(q)* can be written as

$$S(q) = S_0 \sum_{n=0}^{N-1} a_n \, \Phi_n(q,u)\,, \text{ where } \quad \Phi_n(q,u) = i^n (2^n n!)^{-1/2} \, e^{-2\pi^2 q^2 u^2} H_n(2\pi u q)\,,$$

where $H_n(x)$ is the *n*-th order Hermite polynomial, and *u* is a characteristic length. Note that this basis has the desired Gaussian behavior in the small-*q* regime. Therefore, an estimate of *u* can be determined from the first few points of the *S(q)* profile. Furthermore, this construction ensures that when a_n are real, the real and imaginary parts of the signal are even and odd, respectively, which in turn assures that the probabilities will be real. The estimation of the coefficients, a_n, can be performed by expressing the problem as a linear system **S=Qa**, where **Q** is the (number-of-*q*-values x N) design matrix of Φ values, and then constructing the pseudoinverse of the design matrix using singular value decomposition.

One of the most interesting characteristics of the basis used is that the Fourier transform of an eigenfunction Φ_n can be expressed in terms of itself. This property makes it possible to immediately reconstruct the average propagator using the same basis and the same coefficients a_n,:

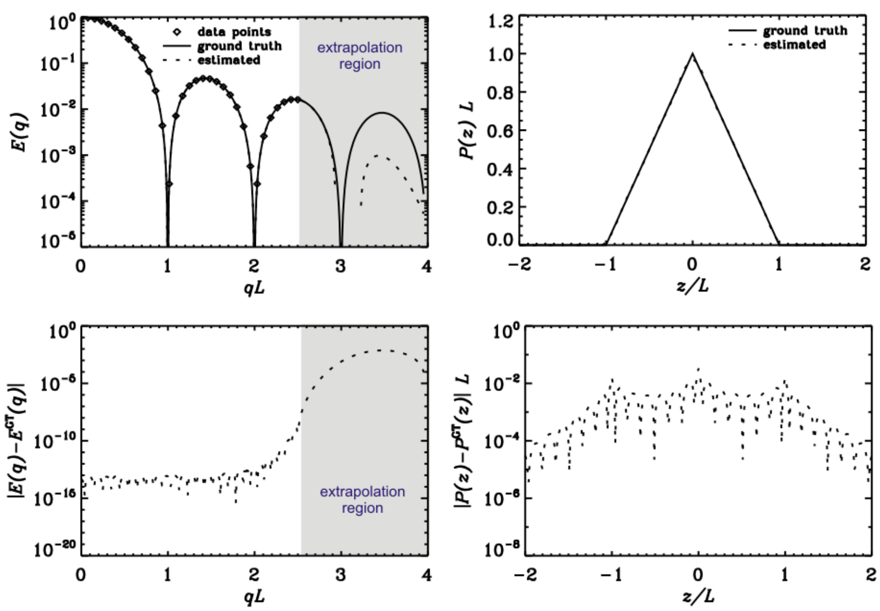
$$P(x) = \sum_{n=0}^{N-1} \frac{(-i)^n}{\sqrt{2\pi u}} a_n \, \Phi_n(x, (2\pi u)^{-1})\,.$$

Having an analytical form of the signal and the probabilities, scalars such as the return-to-origin probability and the moments of the distribution can be computed rapidly. The return-to-origin probability is given simply by setting *x*=0 in the above expression. The evaluation of the moments is more difficult. After some algebra, the *m*-th order moment was found to be given by

$$\langle x^m \rangle = u^m \sum_{k=0,2,\ldots}^{N-1} \frac{(k+m-1)!!}{k!} \sum_{l=0,2,\ldots}^{N-k-1} (-1)^{l/2} \frac{\sqrt{2^{k-l}(k+l)!}}{(l/2)!} a_{k+l}$$

where *m* is even. For odd-order moments, the index *k* takes odd values, i.e., *k*=1,3,5… .

RESULTS:



The proposed scheme was used to estimate the signal intensity and the associated average propagator parametrically. As an example, we demonstrate the results obtained from modeling the long diffusion time pulsed-field-gradient signal from a rectangular pore where the separation between the two sides of the pore is *L*. The signal decay is an oscillatory function whose average propagator is a triangular function. The estimations were performed using only 33 data points reaching a *qL* value of 2.5. A total of 28 terms were kept in the series. The estimated signal intensity was indistinguishable from the ground truth (GT) signal in the approximation region as shown on the top left panel, whereas reasonable performance was also observed in the extrapolation region. The reconstructed propagator was barely distinguishable from the estimated probabilities despite its challenging non-smooth form.

The return-to-origin probability and the even-order moments were computed as described above. The percentage deviations from analytically evaluated (exact) values were: 3.3 in return-to-origin probability, 1.7×10^{-6} in $\langle x^0\rangle$, 5.1×10^{-5} in $\langle x^2\rangle$, 6.7×10^{-4} in $\langle x^4\rangle$, 6.7×10^{-3} in $\langle x^6\rangle$ and 5.4×10^{-2} in $\langle x^8\rangle$. These per cent deviations suggest that the estimated form of *E*(*q*) can be used to accurately estimate the derivatives of *E*(*q*) as well.

DISCUSSION & CONCLUSION:

The proposed basis has several desirable properties that suit problems of q-space signal and average propagator estimation: The basis naturally implies a Gaussian (monoexponential) signal decay at low *q*-values. Unlike biexponential fitting and cumulant expansion methods, it is linear. Moreover, estimation is fast, accurate and automatically provides a simple way to estimate the Fourier transform, i.e., the average propagator and several scalar indices from the estimated series coefficients. Finally, the one dimensional simple harmonic oscillator based estimation technique is able to accurately handle challenging signal decays and average propagators.

References:

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