Challenges in Reconstructing the Propagator via a Cumulant Expansion of the One-Dimensional q-space MR Signal

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INTRODUCTION:

Generalized Diffusion Tensor Imaging (GDTI) [1] is one of the few methods that estimate the ensemble average diffusion propagator from the diffusion weighted signal. It has a statistical approach and views the signal, which under the *q*-space formalism is the Fourier transform of the propagator, as the characteristic function of the propagator. Instead of taking the inverse Fourier transform of the signal, GDTI estimates the cumulants of the propagator from the signal (characteristic function) and then approximates the propagator using the Gram-Charlier Type-A series, which is a series approximation of a probability density function based on its cumulants. However, it is well known that the Gram-Charlier series has a poor convergence, especially since only a truncated series is considered (order-4 in [1]). The Edgeworth series, which is a reordering of the terms from the Gram-Charlier series, is known to perform better since it is a true asymptotic expansion [2]. GDTI has never been validated numerically. We propose, here, to compare the Gram-Charlier and the Edgeworth series in 1D on known diffusion propagators, where the propagator, the signal and the cumulants have analytical forms. We also compare with cumulants estimated from the signal. Our experiments strongly suggest that for analytical cumulants the Edgeworth series improves on the Gram-Charlier series, and estimating the cumulants from the signal is numerically a sensitive and important problem.

METHODS:

The Gram-Charlier series attempts to estimate a probability density function in terms of a Gaussian probability and all its infinite derivatives. However there are criteria for which the entire series converges [2]. In practice though, the infinite series is never available and only a truncated series can be computed. The Edgeworth series rearranges the terms of the Gram-Charlier series so that the truncated series becomes an asymptotic expansion of the density function to be estimated [2].

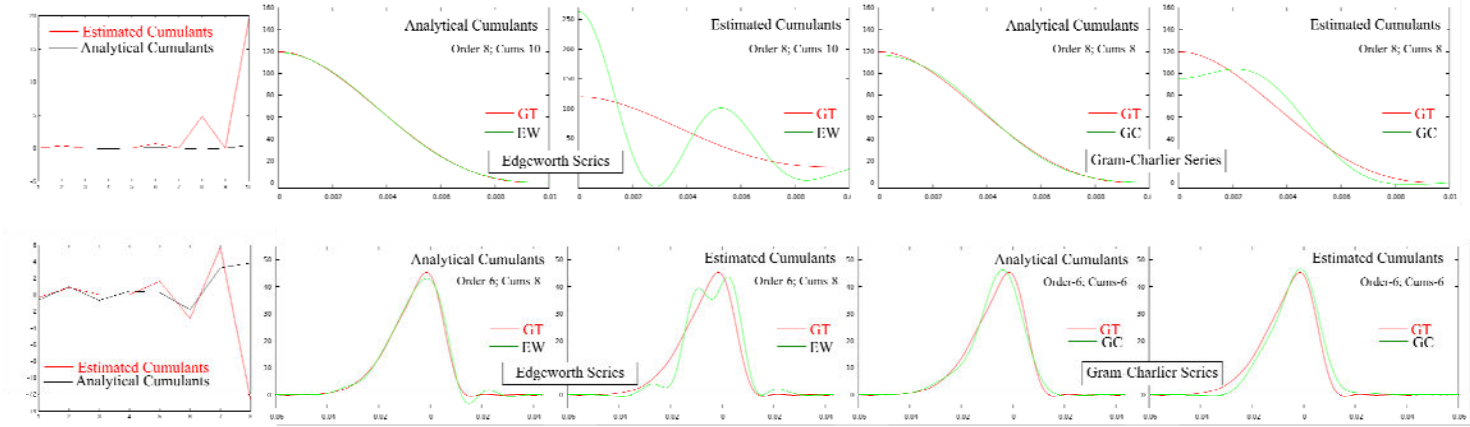
Here we consider two diffusion scenarios, both of which have closed-forms for the signal and the cumulants. We compare the Gram-Charlier and the Edgeworth series of equal order from the analytically known cumulants. These are also compared to the Gram-Charlier and the Edgeworth series arising from cumulants estimated from a sampled set of the signal, to simulate GDTI. (a) The first scenario considered is diffusion within a spherical pore of radius 5 microns. The closed-forms of the signal and the propagator can be found in [4], and the cumulants are computed by analytically expanding the logarithm of the signal around the origin. This is a symmetric propagator, therefore both the signal and the propagator are real. (b) The second scenario is the simulation of a voxel of dimension 12 microns located adjacent to a single infinite plate with diffusion coefficient $1\text{x}10^{-3}\text{mm}^2/\text{s}$ and a diffusion time of 100ms. The signal has a closed form in [5], and the propagator is obtained by a numerical Fourier transform. The cumulants are again obtained by taking a Taylor expansion of the signal around the origin. This is an asymmetric propagator, therefore the signal is complex.

We estimate the cumulants up to order N from the truncated definition of the cumulants $\exp\left(\sum_{n=1}^{N}\kappa_n\frac{(iq)^n}{n!}\right)=\int_{-\infty}^{\infty}\exp(iqr)P(r)dr$. This can be linearized and solved for $\{\kappa_n\}$ using either a pseudo-inverse or an SVD (Singular Value Decomposition) [1]. We consider the noiseless signal.

The Edgeworth series of order n requires $n+2$ cumulants, whereas the Gram-Charlier series of order n requires n. For (a) we estimate 10 cumulants and therefore compute the Edgeworth series up to order 8. To compare for the same order we also compute the Gram-Charlier series up to order 8. In (b) we estimate 8 cumulants, and therefore compute the Edgeworth and Gram-Charlier series up to order 6. Increasing the order of the Gram-Charlier series doesn't necessarily improve on the estimation since it's not an asymptotic expansion [2].

RESULTS:

The first row of figures corresponds to case (a), and the second row to case (b). In the first column are compared the estimated cumulants to the analytical cumulants, where in the graph we plot a dimensionless quantity by normalizing the cumulants appropriately. The next two columns show the Edgeworth series, and the last two columns the Gram-Charlier series. The ground truth (GT) propagator is drawn in red, and the series-estimated propagator is drawn in green. It is clear that for analytical cumulants the Edgeworth series performs better than the Gram-Charlier series. However, as the estimated cumulants differ from the analytical cumulants (column-1), we see their effects on both the Edgeworth and the Gram-Charlier series.



DISCUSSION & CONCLUSION:

We compared the Edgeworth series, which is an asymptotic expansion of a density function, with the Gram-Charlier series on two known diffusion scenarios with closed-forms in 1D. In one case we considered a symmetric propagator, and in the second an asymmetric. When the cumulants are known the Edgeworth series, as expected, improves on the Gram-Charlier series of the same order. However, when the cumulants have to be estimated from the signal, and are only approximate values of the true cumulants, both the series are strongly affected. The Edgeworth series which is theoretically an asymptotic expansion also diverges greatly. Therefore estimating the cumulants from the signal plays an important role in the outcome of the series approximation of the propagator.

References: [1] Liu et al, Israel J Chem 43, 145–154, 2003; [2] Cramer, H. Mathematical Methods of Statistics. (PMS-9), Princeton University Press, 1999; [3] Blinnikov, S., Moessner, R., Astron. Astrophys. Suppl. Ser 130, 193–205, 1997; [4] Özarslan et al, Magn Reson Imaging 27, 834–844, 2009; [5] Özarslan et al, Biophysical J, 94(7), 2809–2818, 2008