Supporting Information for Optimal Tikhonov Regularization for DEER Spectroscopy

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1. Bayesian inference

Fig. S1 shows Bayesian credible intervals (BCIs) for the $P(r)$s in Fig. 7 calculated according to the procedure introduced in [1]. Note that the 50th percentile BCI, which corresponds to the *maximum a posteriori* solution, is very close but not identical to the Tikhonov regularization solution in every case. This is due to the distribution of α values explored by the Bayesian MCMC method used to generate the estimate of the posterior PDF.

The question of optimal regularization parameter selection for Tikhonov regularization in DEER spectroscopy is independent of the Bayesian methodology introduced in [1]. The Bayesian approach is not yet fully realized, and may or may not require the use of the methods explored in the present study.

References

[1] Edwards T. H. and Stoll S. A Bayesian approach to quantifying uncertainty from experimental noise in DEER spectroscopy. *J. Magn. Reson.*, 270:87–97, 2016.

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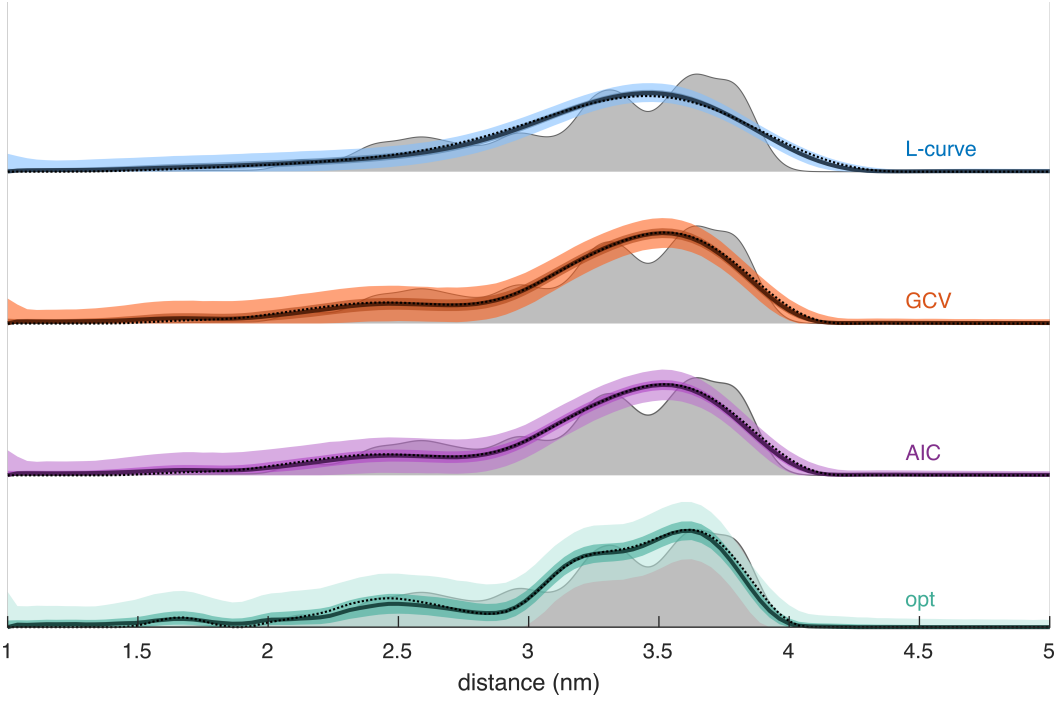

Figure 1: Bayesian credible intervals for the case shown in Fig. 7. In each plot, the model P(r) is shown in grey and the corresponding Tikhonov solution is in dotted black. The L_2 operator was used in each case.