

DEER analysis report on dataset 220603_KAq195.15_DEER_208032_66pc_p i

**DEERNet Spinach SVN Rev 5662 and DeerLab
0.9.1 Tikhonov regularization**

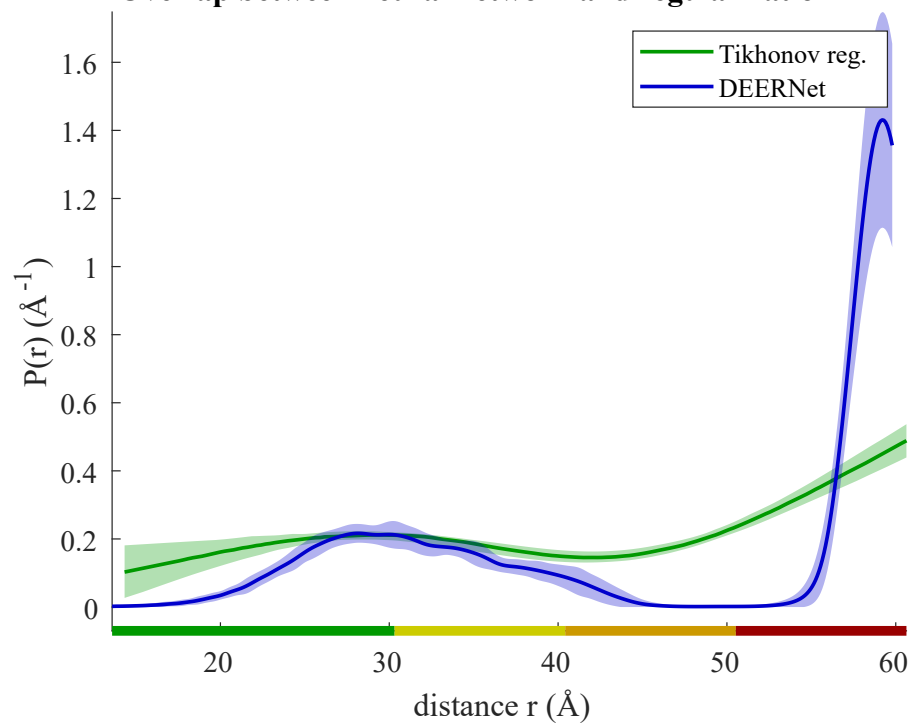
ComparativeDEERAnalyzer version 2.0

see: S. G. Worswick et al., DOI: 10.1126/sciadv.aat5218, L. Fabregas Ibanez et al., DOI: 10.5194/
mr-1-209-2020

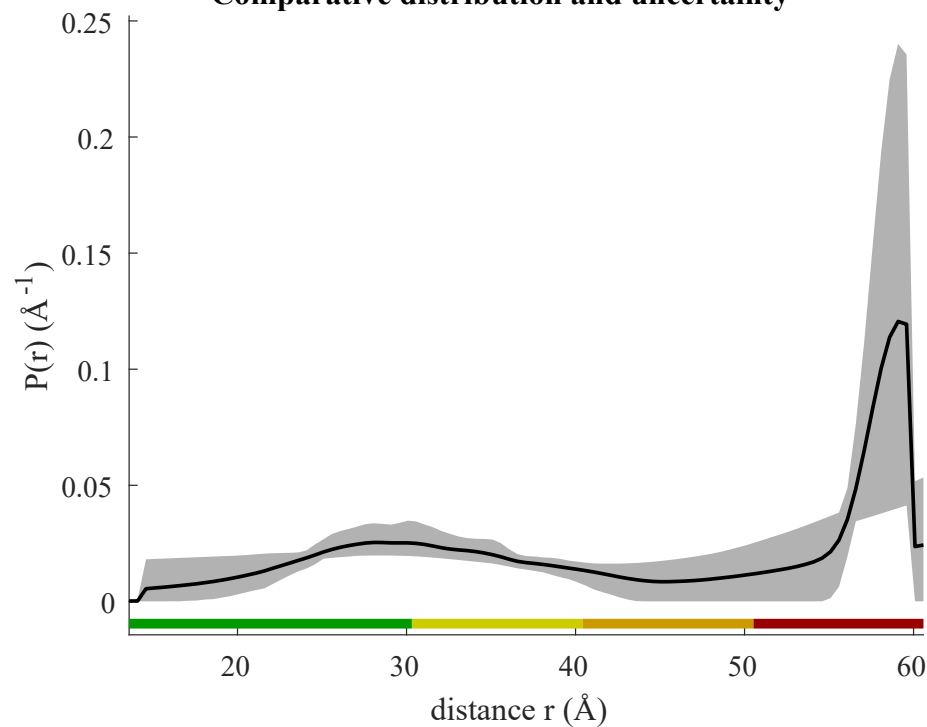
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1. Distance distributions

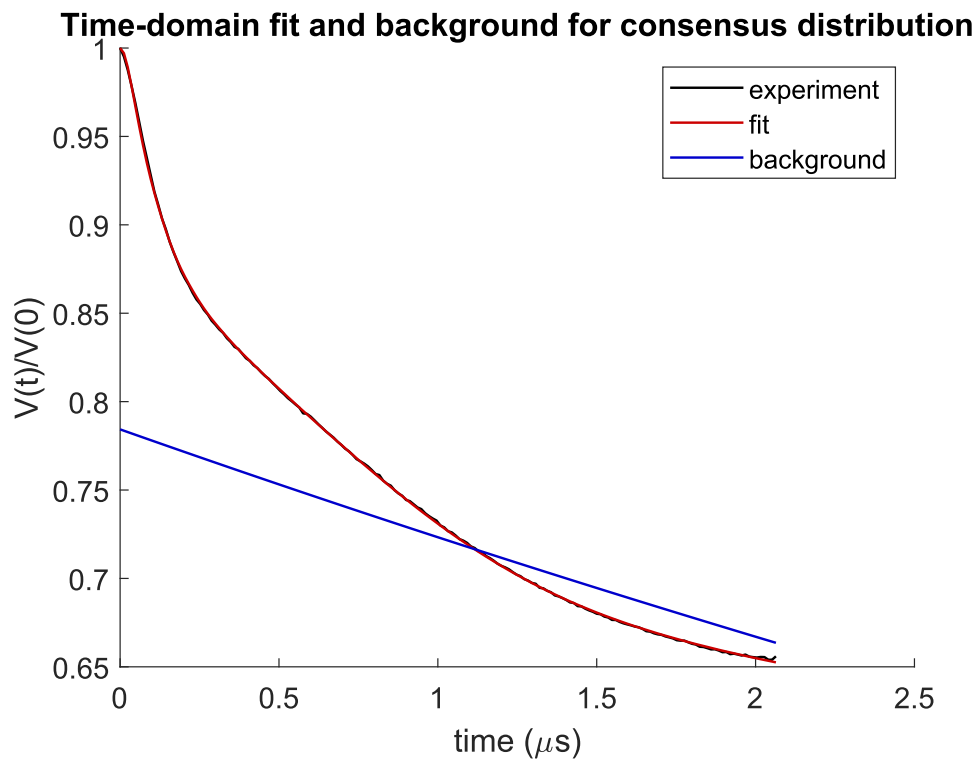
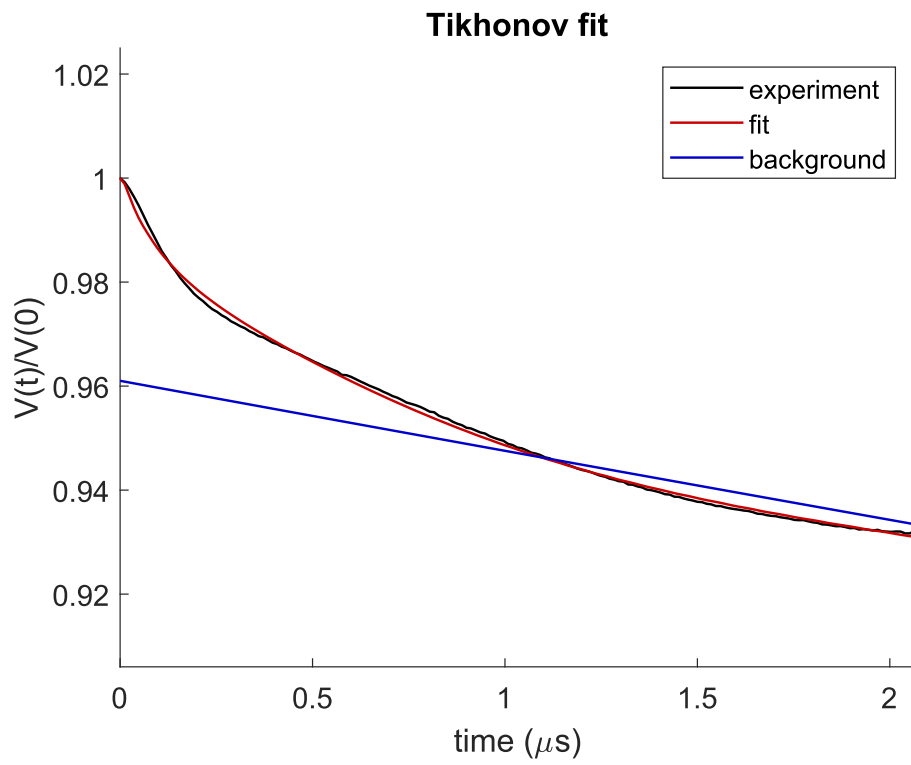
Overlap between neural network and regularization



Comparative distribution and uncertainty



2. Fits of time-domain data



3. Experimental and processing parameters

DEERNet background not provided, as it was considered unreliable.

Ghost suppression for a 7-spin system was applied.

Modulation depth: 0.216

Signal-to-noise ratio: 131.9 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00060

From Tikhonov fit: 0.00334

Zero time: 290 ns

Maximum time: 2064 ns

Time increment: 12 ns

Phase: -4.2 degree

Ensemble of 32 neural networks

Background separation by DeerLab bilevel optimization

Background dimension: 3

Regularization parameter by best overlap with neural network solution

Regularization parameter used: 5.70

Reg. par. initial estimate by lr: 0.13

Overlap between DEERNet and regularization solutions: 0.594

Predicted overlap of consensus solution with ground truth: 0.48...0.66

Mean distance: 43.6 Å

Single Gaussian provided different mean distance. Distribution may be incomplete.

Distance standard deviation: 14.2 Å

Full data set in Matlab format: C:\Users\Katrin\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_Mary_220518\KAq195\220603_KAq195.15_DEER_208032_66pc_pi_comparative_DEER_analysis.mat

Distance distributions in text format: C:\Users\Katrin\Documents\OneDrive - University of St

3. Experimental and processing parameters

Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_Mary_220518\KAq195\220603_KAq195.15_DEER_208032_66pc_pi_consensus_DEER_distribution.csv

Fit and background in text format: C:\Users\Katrin\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_Mary_220518\KAq195\220603_KAq195.15_DEER_208032_66pc_pi_consensus_DEER_fit.csv

Metadata: C:\Users\Katrin\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_Mary_220518\KAq195\220603_KAq195.15_DEER_208032_66pc_pi_comparative_DEER_meta_data.csv