

Pair Distributions by Tikhonov Regularization

- The determination of pair distance distributions by pulsed ESR using Tikhonov regularization

Regularization Program User Notes

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INTRODUCTION

This user manual is to provide a quick overall view of the program packages used for determining pair distance distributions from pulsed ESR experiments using Tikhonov regularization method [1]. Demo examples, which include a model study and a real experimental data, are enclosed in the package. All theoretical backgrounds regarding to the Tikhonov regularization, L-curve criterion for determining the optimal regularization parameter, and the equation of dipolar spectroscopy can be found in literature [1-4].

INSTALLATION

MATLAB version 6.5 or higher is required to perform the functions of the following program components. There are two program packages need to be downloaded to the search path of the MATLAB to perform Tikhonov Regularization. They are **1) Regularization Toolbox package**, which was created by Hansen's group[5] and is obtainable from the website: <http://www.imm.dtu.dk/~pch/> , and **2) PD_Tikhonov package**, which includes all necessary functions required to extract the pair distributions from pulsed ESR experiment and is obtainable from ACERT center upon request. The first package is very well documented with a manual and demonstrated with numerous examples. We strongly suggest people should get started from learning the first package.

DEMONSTRATION FOR USING THE PD_Tikhonov PACKAGE

There are two examples included in the package. One is a model test; the other is to demonstrate how to recover $P(r)$ from DQC experimental signal. The details about the model test can be found in the M-file, called **modeltest.m**. The procedure from generating a model distribution to using various subroutines in the Regularization Tool Package is clearly stated in this M-file. A real experimental data, named **ABC.dat**, is enclosed in the package. It is a DQC time domain signal obtained from a real experiment. Use the P-file (**PD_TKN.p**) to extract the distance distribution from this data file. All details about using **PD_TKN** are given in the following.

PD_TKN stands for Pair-Distributions by TiKhoNov regularization (PD_TKN). This is the main function of the PD_Tikhonov package. This function it to extract pair distribution

from the time evolution data of dipolar signal using Tikhonov regularization method. It requires the existence of the Regularization Toolbox in the search path of MATLAB. Three figures will come out after execution. They are 1) the L-curve plot, 2) the time evolution data of dipolar signal, and 3) the estimated pair distribution.

==> **PD_TKN(filnm , inparm);**

On Input:

filnm= 'filename.dat', the DQC time domain evolution signal whose baseline (assumed to be a triangular decay function) has been subtracted from the raw data.

NOTE: The .dat file must be a N by 2 matrix, where N represents the # of data points. The 1st column is time (t in unit of ns), and the 2nd column is the corresponding DQC signals V(t).

inparm=[**Deri, Rmin, Rmax**];

Deri = the L operator. (1: the identity derivative, 2: the second derivative).

R_min = the lower boundary for the estimated distribution. (in angstrom)

R_max = the upper boundary for the estimated distribution. (in angstrom).

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Example: Type the following command to extract Pr from ABC.dat.

PD_TKN('ABC.dat',[2 15 80]);

REFERENCE

- [1] Y.W. Chiang, P.P. Borbat, J.H. Freed, The Determination of Pair Distance Distributions by Pulsed ESR Using Tikhonov Regularization, *J Magn Reson* 172 (2005) 279-295.
- [2] P.C. Hansen, in P. Johnston (Ed.), *Computational Inverse Problems in Electrocardiology*. WIT Press, 2000, p. 119-142.
- [3] P.P. Borbat, J.H. Freed, in S.S. Eaton (Ed.), *Biological Magnetic Resonance*. Kluwer Academic Pub, 2001, p. 383-459.
- [4] A.N. Tikhonov: *Numerical methods for the solution of ill-posed problems*, Kluwer Academic Publishers, Dordrecht ; Boston, 1995.
- [5] P.C. Hansen, *Regularization tools Version 3.0 for Matlab 5.2*, Numer Algorithms 20 (1999) 195-196.