

User's guide

dPETSTEP kinetic model fitting GUI

This document shows the usage of the dPETSTEP GUI for kinetic model fitting, and explains the different inputs to the GUI.

The GUI can be run by typing in the MATLAB command prompt:

```
>> dPETSTEPgui_fit
```

This command opens the full window seen below. All fields have tool tips to guide you.

dPETSTEP kinetic model fitting

Dynamic PET data

Data
☒ From WS ☐ From file
 Name : (Bq/cc)

Fitting
☒ Voxel-wise ☐ ROI-based

ROI
☐ From WS ☐ From file
 Name :

Kinetic model

Model
☒ 1-Tissue ☐ FRTM ☐ SumExp
☐ 2-Tissue ☐ SRTM # exp:

Mid frame time points
☒ From WS ☐ From file
 Name : (sec)

Input / reference function

☒ Image-derived ☐ External

ROI
☒ From WS ☐ From file
 Name :

Read data
☐ From WS ☐ From file
 Name : (Bq/cc)

Fitting settings

Frame weight
Calculate
☒ Uniform ☐ 1/(df^2)
☐ 1/(L*df) ☐ L*exp(-lambda*t)
☐ 1/(C*L*df) ☐ L*exp(-lambda*t)/C
 Nuclide half-life: sec

Read data
☐ From WS ☐ From file
 Name :

Interpolation
☒ Linear ☐ Nearest ☐ PCHIP ☐ Spline
 Time step: sec

Solver
☒ trust-region-reflective
☐ levenberg-marquardt

Stopping criteria
☐ Max iterations:
☐ Func tolerance:
☐ Step tolerance:

CPUs
 Number of CPUs:

Parameter values

Rate constant unit: ☒ 1/sec ☐ 1/min

	Initial value	Lower bound	Upper bound
K1:	<input type="text"/>	<input type="text"/>	<input type="text"/>
k2:	<input type="text"/>	<input type="text"/>	<input type="text"/>
k3:	<input type="text"/>	<input type="text"/>	<input type="text"/>
k4:	<input type="text"/>	<input type="text"/>	<input type="text"/>
R1:	<input type="text"/>	<input type="text"/>	<input type="text"/>
BPnd:	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input checked="" type="checkbox"/> Va:	<input type="text"/>	<input type="text"/>	<input type="text"/>

Arbitrarily # of parameters:
 Initial:
 Lower:
 Upper:
 (Use comma separation "p1,p2,...,pN")

Output data names
☒ Parameter fits:
☐ Fit info:

Save Load Reset

Run

Created by Ida Häggström, 2017.08.07

1. Run test example

1.1 data_ex_dPETSTEP_modelFitting

This is for fitting a 4D PET image to a compartment model. Download the test example data found on Github at

https://github.com/CRossSchmidtlein/dPETSTEP/blob/master/example_modelFitting.

Load into Matlab the data in "data_ex_dPETSTEP_modelFitting.mat". Example settings can be found in "settings_dPETSTEPgui_modelFitting.xls", and loaded via the GUI. Resulting settings seen below:

dPETSTEP kinetic model fitting

Dynamic PET data

Data

☒ From WS ☐ From file

Name : image4D (Bq/cc)

Fitting

☐ Voxel-wise ☒ ROI-based

ROI

☒ From WS ☐ From file

Name : ROI_tumor

Kinetic model

Model

☐ 1-Tissue ☐ FRTM ☐ SumExp

☒ 2-Tissue ☐ SRTM #exp:

Mid frame time points

☒ From WS ☐ From file

Name : midFrame (sec)

Input / reference function

☐ Image-derived ☒ External

ROI

☒ From WS ☐ From file

Name : ROI_Cif

Read data

☒ From WS ☐ From file

Name : Cif (Bq/cc)

Fitting settings

Frame weight

Calculate

☒ Uniform ☐ 1/(df²)

☐ 1/(L*df) ☐ L*exp(-lambda*t)

☐ 1/(C*L*df) ☐ L*exp(-lambda*t)/C

Nuclide half-life: sec

Read data

☐ From WS ☐ From file

Name : weight

Interpolation

☒ Linear ☐ Nearest ☐ PCHIP ☐ Spline

Time step: 0.5 sec

Solver

☒ trust-region-reflective

☐ levenberg-marquardt

Stopping criteria

☒ Max iterations: 1000

☐ Func tolerance:

☐ Step tolerance:

CPUs

Number of CPUs: 1

Parameter values

Rate constant unit: ☐ 1/sec ☒ 1/min

	Initial value	Lower bound	Upper bound
K1:	0.01	0	10
k2:	0.01	0	10
k3:	0.01	0	10
k4:	0.01	0	10
R1:			
BPnd:			
<input checked="" type="checkbox"/> Va:	0.01	0	1

Arbitrary # of parameters:

Initial: 1,3,1e2,0.1

Lower: 0,0,0,1

Upper: 1,1,1,1

(Use comma separation "p1,p2,...,pN")

Output data names

☒ Parameter fits: pimFitted

☐ Fit info: fitInfo

Save Load Reset

Run

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2. GUI field explanations

Dynamic PET data

Dynamic PET data

Data

☒ From WS ☐ From file

Name : (Bq/cc)

Fitting

☒ Voxel-wise ☐ ROI-based

ROI

☒ From WS ☐ From file

Name :

Read dynamic (4D) PET uptake image matrix either from workspace (WS), or from *.mat-file. Enter the name (string) of the WS variable/file. The *.mat-file has to contain ONLY the dynamic image matrix, no other data.

The 4D data matrix [nx,ny,nz,nt] should be in units (Bq/cc).

Fit each voxel of the 4D image to get parametric image, or fit only single ROI time-activity curve.

For ROI-based fitting, enter the name (string) of the WS variable/*.mat file. The data file has to contain ONLY the ROI mask matrix, no other data.

The ROI is a mask matrix [nx,ny,nz] of only values 0 and 1.

Kinetic model

Kinetic model

Model

☒ 1-Tissue ☐ FRTM ☐ SumExp

☐ 2-Tissue ☐ SRTM # exp:

Mid frame time points

☒ From WS ☐ From file

Name : (sec)

Choose which kinetic model to fit to. For general sum of exponentials model (SumExp), also specify number of exponentials (integer number).

Read mid frame time points either from workspace (WS), or from *.mat, *.txt, or *.xls file. Enter the name (string) of the WS variable/file. The data file has to contain ONLY the mid frame vector, no other data.

The mid frame point data [nt,1] should be in unit (sec).

Input/reference function

Input / reference function

☒ Image-derived ☐ External

ROI

☒ From WS ☐ From file

Name :

Read data

☒ From WS ☐ From file

Name : (Bq/cc)

Choose image-derived (from ROI) input/reference function, or an external one. Used as arterial input function for kinetic models 1-tissue, 2-tissue and sum of exponentials, and as reference function for FRTM and SRTM.

For image-derived input/reference function, enter the name (string) of the ROI mask WS variable/*.mat file. The data file has to contain ONLY the ROI mask matrix, no other data.

The ROI is a mask matrix [nx,ny,nz] of only values 0 and 1.

For external input/reference function, enter the name (string) of the WS variable/*.mat, *.txt or *.xls file. The data file has to contain ONLY the input/ref function vector, no other data.

The input/ref function vector [nt,1] should be in units (Bq/cc).

Fitting settings

Fitting settings

Frame weight

Calculate

☒ Uniform ☐ $1/(df^2)$
☐ $1/(L*df)$ ☐ $L*\exp(-\lambda*t)$
☐ $1/(C*L*df)$ ☐ $L*\exp(-\lambda*t)/C$

Nuclide halflife: sec

Read data

☐ From WS ☐ From file

Name:

Interpolation

☒ Linear ☐ Nearest ☐ PCHIP ☐ Spline

Time step: sec

Solver

☒ trust-region-reflective
☐ levenberg-marquardt

Stopping criteria

☐ Max iterations:
☐ Func tolerance:
☐ Step tolerance:

CPUs

Number of CPUs:

Choose if you want to calculate or read external frame weight vector for the fit.

If calculating the weights, chose uniform (no) weighting, or calculated from 1 of four models. Lambda = decay factor, L = frame length, df = $\lambda*L/(\exp(-\lambda*t1)-\exp(-\lambda*t2))$, C = activity.

For some models the halflife of the nuclide is also needed. It should be a number in unit (sec).

If reading external weight data, enter the name (string) of the weight vector WS variable/*.mat, *.txt or *.xls file. The data file has to contain ONLY the weight vector, no other data.

The frame weight is a vector [nt,1], and unitless.

If uneven time sampling, the data will be interpolated to even sampling (for convolution) during fitting. Choose interpolation method, and time step for the interpolation.

The time step is a number in units (sec).

The fitting is done by nonlinear-least-squares. Chose what type of solver algorithm the optimization should use during fitting.

If you want to set stopping criteria other than the default values. Each input should be a number. If not checked, MATLAB will use default values: max iterations=400, function tolerance=1e-6, step tolerance=1e-6.

Specify the number of CPUs to use. Only relevant if doing voxel-wise fitting. Value should be an integer number.

Parameter values

Set unit of parameter initial values, upper and lower bounds. Only relevant for parameters K1, k2, k3, k4, and sum of exponentials parameters.

Set initial values of the parameters relevant to your chosen kinetic model. If using the trust-region-reflective algorithm, also set lower and upper bounds of the parameter estimates.

You can choose to include the blood fraction (Va) in the fitting or not by checking the Va box.

All parameter values should be numbers. K1 in unit (cc/g/sec) or (cc/g/min), k2, k3 and k4 in (1/sec) or (1/min), R1 and BPnd are unitless, and Va in (cc/g).

If chosen kinetic model is an arbitrary sum of exponentials, you specify initial values, lower and upper bounds here.

The number of values specified should be 2*number of exp. You can still add the blood fraction by checking the Va box above.

The inputs should be numbers, and values should be comma separated, like "0.1,0.01,0.01,0.01" (w/o quotation marks).

Output data names

Choose what data you want as output from the fit, and set the name (string) of that data. Will end up in your WS after run.

You can get the parameter fits (parametric image matrix for voxel-wise fit, vector for ROI fit), and the fitting information.

The fitted parameters will be (depending on kinetic model) K1 in unit (cc/g/sec) or (cc/g/min), k2, k3 and k4 in (1/sec) or (1/min), R1 and BPnd unitless, and Va in (ml/g). The fitting information is a structure with resnorm, residual, exitflag, output, lambda, and jacobian. Note that for voxel-wise fitting, there will be one of each structure field per voxel, leading to a potentially very large data structure.

Buttons

Load settings from chosen *.xls-file.

Reset all settings.

Executes the fitting main program.

Save all current settings to *.csv-file.