

An Inverse Problem of a Pharmacokinetics Model : Documentation

main.m

input :

output : y_star.mat : target data for the later references
 S_pk.mat : scaling matrix for x-variables for the later references
 X.mat : matrix X found by solving the inverse problem
 Y.mat : matrix Y corresponding to the matrix X above

parameters : num_iter : number of iterations for the inverse problem solver
 num_samp : number of x vectors in matrix X (number of “virtual population”)
 y_star : target data (clinically measured data from Slatter et al.)

initiaDistribution.m

input : num_samp : number of points in the initial distribution
output : X0_normalized : normalized initial distribution
 S_pk : scaling matrix for x-variables (x_not_normalized=(S_pk* X_normalized))

parameters : x_typical : the “center” of the initial distribution (x values obtained from literatures)
 range_ratio_pharmaco_para : “width” of the initial distribution for the pharmacokinetics parameters
 range_ratio_physio_para : “width” of the initial distribution for the physiological parameters
 range_ratio_adm_para : “width” of the initial distribution for the administration parameters

PBPK_model.m (includes el, RHS)

input : x_in : a not normalized x vector
output : y_out : s solution of the forward problem obtained via solving ODEs (excretion profile)

Please refer to aoki_hayami_konagaya_inverse_pharmakokinetics.pdf pages 3-6 for the details.

twiceLSmethod.m

input : f : non-linear function
 X0 : normalized initial distribution
 num_iter : number of iterations
 y_star : target data (clinically measured excretion profile)
 S_pk : scaling matrix

output: A : Linear approximation matrix
 X : solutions of the inverse problem
 Y : Y values associated with the solutions

Please refer to [aoki_hayami_konagaya_inverse_pharmakokinetics.pdf](#) pages 12-13 for the details.