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Notation

In general, boldface capital characters denote matrices and boldface lower case characters denote vectors.

$\mathbf{A}$ $((M\text{-}S)\times 3)$	The matrix with concentration profiles obtained from a GEP
$\mathbf{A}^{(j)}$ $((M\text{-}S)\times 3)$	The matrix $\mathbf{A}$ after the jth iteration
$\tilde{\mathbf{A}}$ $((M\text{-}S)\times 3)$	The new matrix $\mathbf{A}$ obtained by an initial estimate for k_1 and k_2
$\tilde{\tilde{\mathbf{A}}}$ $((M\text{-}S)\times 2)$	The first two columns of matrix $\tilde{\mathbf{A}}$
$\mathbf{a}_i$	The ith column of matrix $\mathbf{A}$
$\mathbf{a}_i^{(j)}$	The ith column of matrix $\mathbf{A}$ after the jth iteration
$\mathbf{B}$ $((N+1)\times 3)$	The matrix with combined spectra obtained from a GEP
$\mathbf{C}$ (2×3)	The matrix with scaling factors obtained from a GEP
$C_{U,0}$	The initial concentration of species U
$C_{U,i}$	The concentration of species U at time point i; $C_{W,i}$ and $C_{Y,i}$ for W and Y, respectively
$\mathbf{D}$ $(N\times K)$	Matrix with pure spectra
$\mathbf{E}$ $(M\times N)$	Matrix with spectral residuals
$\underline{\mathbf{E}}^*$ $((M\text{-}S)\times(N+1)\times 2)$	Three-way array with spectral residuals
$\mathbf{F}$ $(M\times K)$	Matrix with concentration profiles
G	The step size parameter
K	Number of reacting absorbing species
k_a, k_b	Second order reaction rate constants
k_1, k_2	(Pseudo-) first order reaction rate constants
k	Equals $\frac{k_1}{(k_2 - k_1)}$
$\bar{\hat{k}}_1$, $\bar{\hat{k}}_2$	Mean estimated k_1 and k_2 calculated over the individual estimates
M	Number of time points
N	Number of wavelengths
S	The time shift parameter
t_i	The time at point i
$\mathbf{X}$ $(M\times N)$	Matrix with spectra during a certain time course
$\mathbf{X}^*$ $(M\times(N+1))$	The augmented datamatrix
$\mathbf{X}^*_1$ $((M\text{-}S)\times(N+1))$	Datamatrix 1 formed by splitting $\mathbf{X}^*$

$\mathbf{X}^*_2$ $((M\text{-}S)\times(N+1))$	Datamatrix 2 formed by splitting $\mathbf{X}^*$
$\underline{\mathbf{X}}^*$ $((M\text{-}S)\times(N+1)\times 2)$	Three-way array formed by stacking $\mathbf{X}^*_1$ and $\mathbf{X}^*_2$
$\tilde{\mathbf{X}}^*$ $((M\text{-}S)\times(2N+2))$	Matrix obtained by matricizing $\underline{\mathbf{X}}^*$
$\dot{\mathbf{X}}^*$ $((M\text{-}S)\times 2N)$	Matrix obtained by removing the two columns of constants from $\tilde{\mathbf{X}}^*$
$\mathbf{X}^T$	Transpose of $\mathbf{X}$
$\mathbf{X}^{-1}$	Inverse of $\mathbf{X}$
$\hat{\mathbf{X}}$	Estimate of $\mathbf{X}$