

A classical benchmark problem for nonlinear regression algorithms is to determine the reaction coefficients for the thermal isomerization of  $\alpha$ -pinene. The model takes the form of a set of five, coupled linear differential equation:

$$\begin{aligned}\dot{x}_1 &= -(\theta_1 + \theta_2)x_1 \\ \dot{x}_2 &= \theta_1x_1 \\ \dot{x}_3 &= \theta_2x_1 - (\theta_3 + \theta_4)x_3 + \theta_5x_5 \\ \dot{x}_4 &= \theta_3x_3 \\ \dot{x}_5 &= \theta_4x_3 - \theta_5x_5\end{aligned}$$

- a. Write the model equations in the form  $\dot{\mathbf{x}} = A(\theta)\mathbf{x}$  where the matrix  $A(\theta) \in \mathbb{R}^{5 \times 5}$  depends on the parameters  $\theta$  and is independent of  $\mathbf{x}$ .

- b. The formal solution to the this differential equation is  $\mathbf{x}(t) = e^{A(\theta)t}\mathbf{x}(0)$  where  $e^{A(\theta)t} \in \mathbb{R}^{5 \times 5}$  refers to the *matrix exponential function*. The exponential of a matrix is defined in terms of a power series in analogy to a scalar exponential,

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!},$$

and nearly all numerical linear algebra libraries have efficient implementations of this function. Find a function in your environment that implements the matrix exponential and write a routine that takes three arguments:  $t \in \mathbb{R}^n$ ,  $\mathbf{x}(0) \in \mathbb{R}^5$  and  $\theta \in \mathbb{R}^5$ . It should return a 5 by  $n$  matrix whose  $i^{th}$  column correspond to  $\mathbf{x}(t_i) = e^{A(\theta)t_i}\mathbf{x}(0)$ .

- c. The files *iad\_x.txt*, *iad\_t.txt*, *iad\_x0.txt* contain data, time points, and initial conditions respectively for this model. Formulate and solve a learning problem from this data using the function you wrote in part b. Report the numerical values for your parameters estimates and plot the curves  $\hat{\mathbf{x}}(t)$  for your learned model.