# Parametric Function Fitting

We consider fitting experimental data to a known function defined by several parameters. The particular scenario is the ubiquitous decaying sinusoidal function indicative of damped harmonic motion:

$$W(t) = A_0 + Ae^{-t/\tau} \sin\left[(\omega + \alpha t)\, t + \phi\right] \tag{1}$$

The unknown parameters are $A_0, A, \tau, \omega, \alpha, \phi$. The first term A_0 is some fixed offset, A is the zero-time sinusoidal amplitude, τ is a characteristic amplitude decay time, and the sinusoidal term includes a phase offset ϕ and a linearly-chirped frequency $\omega + \alpha t$. If $\alpha = 0$ we have a simple damped harmonic oscillator equation.

As a specific example, consider the scenario in the figure which describes how to measure the damped oscillation of an otherwise stationary fluid sphere. The spherical object is in the path of a collimated (uniform intensity) laser beam which is focused on a photodiode. The object scatters light out of the beam path (creates a shadow) so the intensity seen by the photodiode is a function of the cross sectional area of the sphere. The photodiode outputs a current proportional to the light intensity which can be determined by a voltage reading across a large resistor. The spherical object is initially driven into sinusoidal volume or shape oscillations which decay in amplitude due to natural viscous forces. The parameters τ, ω and α are important system quantities that tell us about fluid properties (viscosity, density, pressure, etc.) and interface properties (surface tension, impurities, etc.).
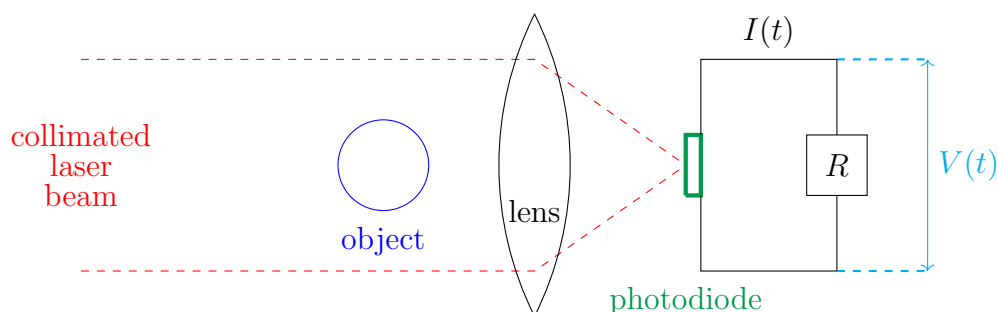
Typical data is as shown below, where the voltage is sampled at discrete times and contains some measurement noise.
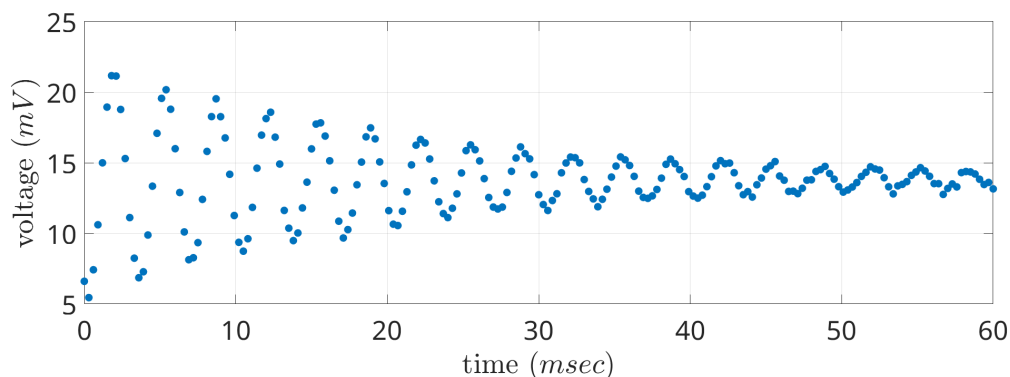
The goal is to determine the parameters which provide the best fit to the discrete data set $\{(t_k, V_k)\}_{k=1}^n$. That is, for any particular data point (t_k, V_k) we wish parameter choices for which

$$V_k \approx W(t_k) = A_0 + Ae^{-t_k/\tau} \sin\left[(\omega + \alpha t_k)\, t_k + \phi\right].$$

As an optimization problem, we want our parameter choices to be good for all data points. We can take a least squares approach and minimize the following objective:

$$f(A_0, A, \tau, \omega, \alpha, \phi) = \sum_{k=1}^n \left(W(t_k) - V_k\right)^2 \tag{2}$$

$$= \sum_{k=1}^n \left(A_0 + Ae^{-t_k/\tau} \sin\left[(\omega + \alpha t_k)\, t_k + \phi\right] - V_k\right)^2. \tag{3}$$

The gradient of the objective function is

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial A_0} \\ \frac{\partial f}{\partial A} \\ \frac{\partial f}{\partial \tau} \\ \frac{\partial f}{\partial \omega} \\ \frac{\partial f}{\partial \alpha} \\ \frac{\partial f}{\partial \phi} \end{bmatrix} = 2\sum_{k=1}^n \left(W(t_k) - V_k\right) \begin{bmatrix} \frac{\partial V(t_k)}{\partial A_0} \\ \frac{\partial V(t_k)}{\partial A} \\ \frac{\partial V(t_k)}{\partial \tau} \\ \frac{\partial V(t_k)}{\partial \omega} \\ \frac{\partial V(t_k)}{\partial \alpha} \\ \frac{\partial V(t_k)}{\partial \phi} \end{bmatrix} = 2\sum_{k=1}^n \left(W(t_k) - V_k\right) \begin{bmatrix} 1 \\ S_k \\ At_k\tau^{-2}S_k \\ At_kC_k \\ At_k^2C_k \\ AC_k \end{bmatrix}. \tag{4}$$

where $S_k = \exp(-t_k/\tau)\sin\left[(\omega + \alpha t_k)\, t_k + \phi\right]$ and $C_k = \exp(-t_k/\tau)\cos\left[(\omega + \alpha t_k)\, t_k + \phi\right]$.

An alternative way of expressing this gradient is

$$\nabla f = 2\nabla W(t)\left(W(t) - V\right), \tag{5}$$

where $W(t) \in \mathbb{R}^n$ is the vector of amplitudes predicted by the model, $V \in \mathbb{R}^n$ is the corresponding vector of data amplitudes, and $\nabla W(t) \in \mathbb{R}^{6\times n}$ is the matrix whose columns are the gradient vectors of the model evaluated at each time.

Complete the following tasks.

1. Obtain the data set from the course website.

2. Compose a function that returns the objective (f) and gradient (∇f) for a given set of input parameters $(A_0, A, \tau, \omega, \alpha, \phi)$ based on the given data ($\{t_k, V_k\}$).

3. Devise and employ a method for determining good initial values for the unknown parameters $(A_0, A, \tau, \omega, \alpha, \phi)$ based on the values given in the data set. In other words, try and automate selection of initial values that should work for any similar data set.

4. Compose general code for solving unconstrained problems in $\mathbb{R}^n$ by the method of gradient descent using appropriate line search concepts. Solve the data fitting problem using your code.

5. Compose general code for solving unconstrained problems in $\mathbb{R}^n$ by conjugate gradient using an update method of your choice. Solve the data fitting problem using your code.

6. Compose general code for solving unconstrained problems in $\mathbb{R}^n$ by the quasi-Newton method using a BFGS update. Solve the data fitting problem using your code.

7. Compare your solutions and explore relative efficiency and any other interesting features that you find.