Fitting parabolic and exponential curves
What if our data looks like this?

A linear equation may no longer be a good model of the underlying physical process that generated the data.
Parabolic model

A better fit might be

\[ y = ax^2 + bx + c \]

**Question:**
How do you know what is a good model?

**Answer:**
Depends on what you are trying to do. In many cases, you have an understanding of the physical processes that produced the data, and so you can develop a model based on the physical assumptions.
Fitting a parabola

Again, we are seeking model parameters. In this model, the unknown coefficients are $a$, $b$, and $c$.

$$y = ax^2 + bx + c$$

Just as in the linear case, we write down an expression for each data point, assuming that the data point “solves” the model:

Given data points $(x_i, y_i)$, we assume

$$y_i = ax_i^2 + bx_i + c, \quad i = 1, 2, \ldots, N$$

Notice that the system is still linear in $a$, $b$, and $c$. 
Fitting a parabola

We can express this as a linear system in $a$, $b$, and $c$:

$$
\begin{bmatrix}
    x_1^2 & x_1 & 1 \\
    x_2^2 & x_2 & 1 \\
    x_3^2 & x_3 & 1 \\
    \vdots & \vdots & \vdots \\
    x_N^2 & x_N & 1
\end{bmatrix}
\begin{bmatrix}
    a \\
    b \\
    c
\end{bmatrix}
=
\begin{bmatrix}
    y_1 \\
    y_2 \\
    y_3 \\
    \vdots \\
    y_N
\end{bmatrix}
$$

Again, the system does not have a solution in general. We can however, find a best fit solution, again using the normal equations.

$$\hat{x} = (A^T A)^{-1} A^T b$$
Best fit parabola

\[ y = ax^2 + bx + c \]

\[ a = -0.519047; \quad b = 1.074011; \quad c = 0.438339 \]
Fitting general polynomials

General polynomials can be fit using linear least squares.

\[ y = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a_0 \]

where it is assumed that the number of data points \( N \) is at least \( n + 1 \).

One must be careful, however, as the linear systems will become increasingly ill-conditioned as the \( n \) increases.
Many distributions of data may be better fit by an exponential curve. Can we still use linear least squares?
Fitting an exponential curve

An exponential model is:

\[ y = ae^{bx} \]

But the model is not linear in the parameters \( a \) and \( b \). How are we going to use linear least squares?

The trick is to take the natural logarithm of both sides to get:

\[ \ln(y) = \ln(a) + bx \]

The model is now linear in \( b \) and \( \ln(a) \).
Fitting an exponential curve

Again, we can set up a linear system:

\[
\begin{bmatrix}
  x_1 & 1 \\
  x_2 & 1 \\
  x_3 & 1 \\
  \vdots & \vdots \\
  x_N & 1 
\end{bmatrix}
\begin{bmatrix}
  b \\
  \tilde{a}
\end{bmatrix}
= \begin{bmatrix}
  \ln(y_1) \\
  \ln(y_2) \\
  \ln(y_3) \\
  \vdots \\
  \ln(y_N)
\end{bmatrix}, \quad \tilde{a} = \ln(a)
\]

We can then compute \( a = e^{\tilde{a}} \).
Fitting an exponential curve

\[ y = ae^{bx} \]

Coefficients: \( a = 1.944548; \ b = 0.509077 \)
The temperature dependence of the reaction rate coefficient of a chemical reaction is often modeled by the Arrhenius equation

\[ k = A \exp\left(-\frac{E_a}{RT}\right) \]

where \( k \) is the reaction rate, \( A \) is the preexponential factor, \( E_a \) is the activation energy, \( R \) is the universal gas constant, and \( T \) is the absolute temperature. Experimental data for a particular reaction yield the following results.

<table>
<thead>
<tr>
<th>( T(K) )</th>
<th>773</th>
<th>786</th>
<th>797</th>
<th>810</th>
<th>810</th>
<th>820</th>
<th>834</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k )</td>
<td>1.63</td>
<td>2.95</td>
<td>4.19</td>
<td>8.13</td>
<td>8.19</td>
<td>14.9</td>
<td>22.2</td>
</tr>
</tbody>
</table>

Use a least-squares fit of this data to obtain values for \( A \) and \( E_a \) for the reaction. Take \( R = 8314 \text{J/kg/K} \).