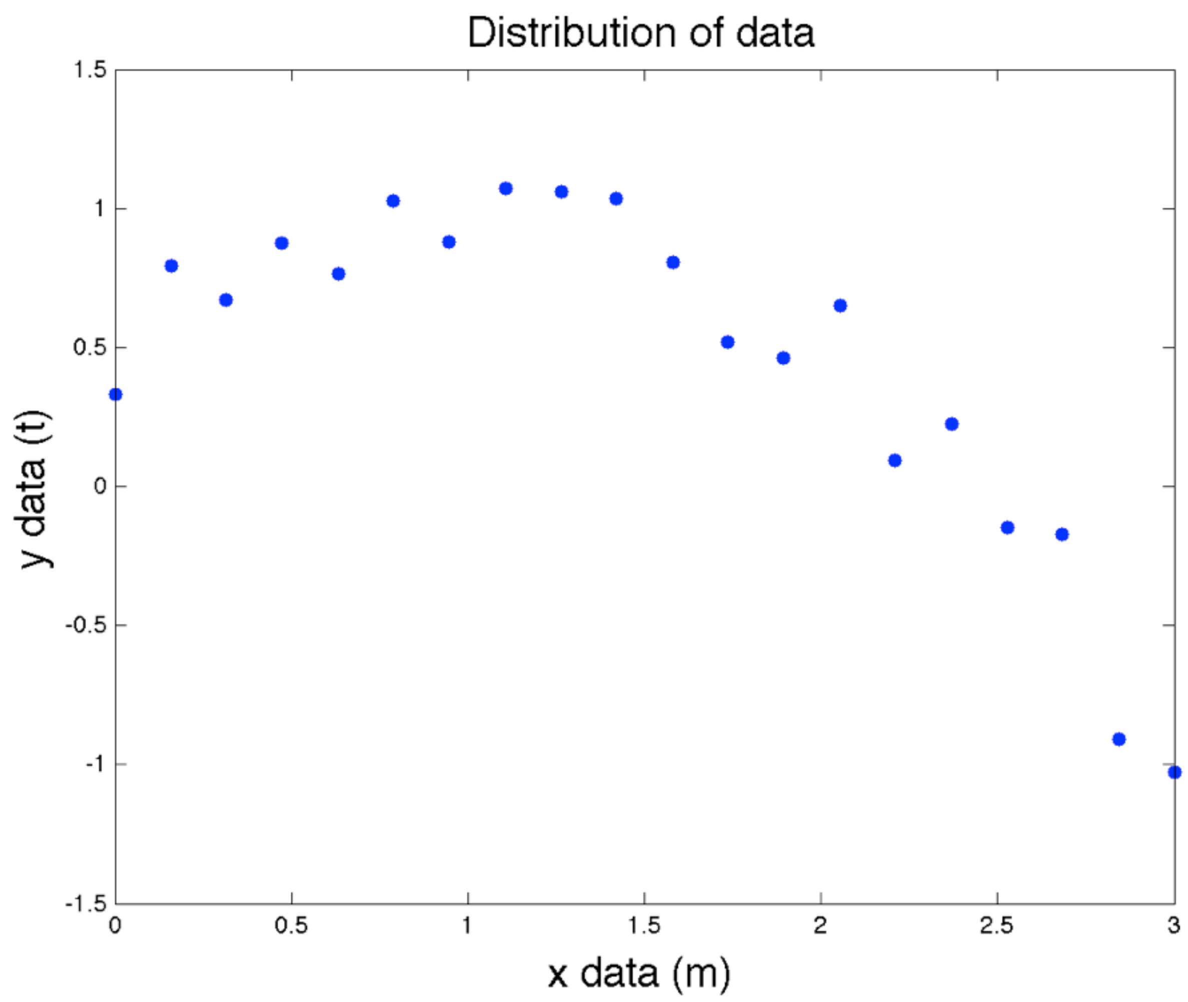
Curve fitting

Fitting parabolic and exponential curves

Linear least squares

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

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

Notice that the system is still *linear* in a,b, and c.

Fitting a parabola

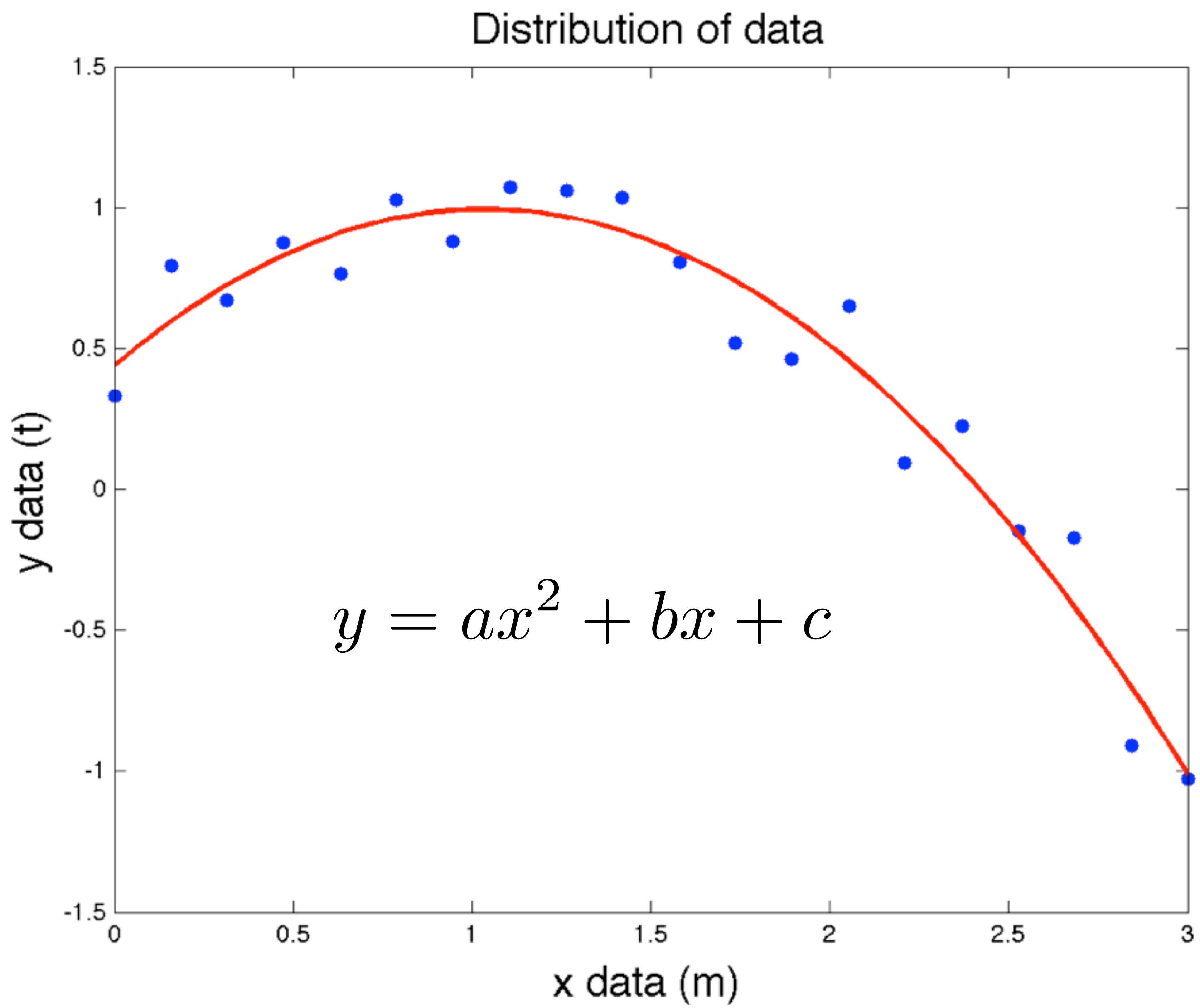
We can express this as a linear system in a, b, and c :

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

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

$$\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b}$$

Best fit parabola

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a =     -0.519047; b =      1.074011; c =      0.438339
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Fitting general polynomials

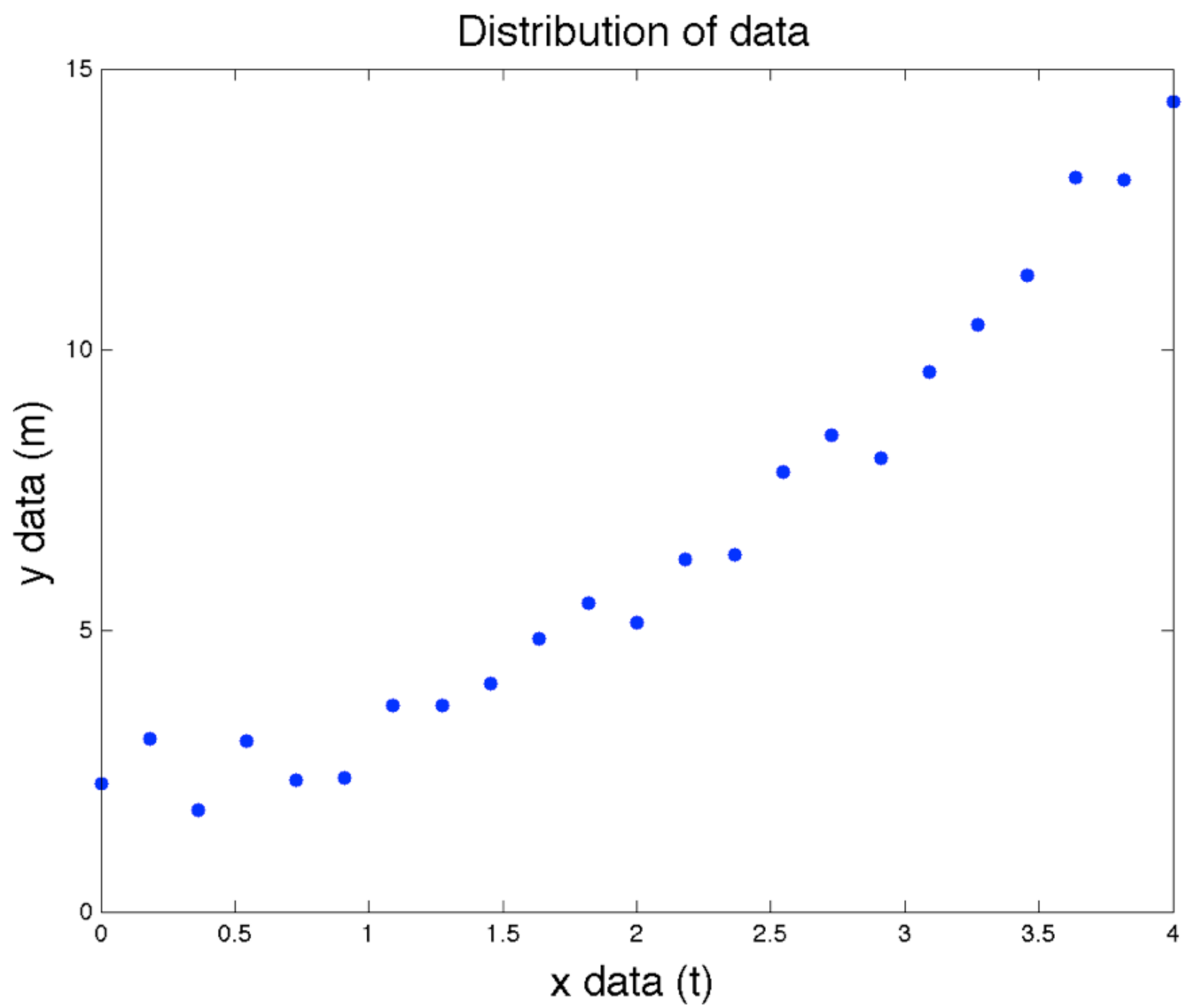
General polynomials can be fit using linear least squares.

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

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.

Fitting an exponential curve



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 $\ln(a)$.

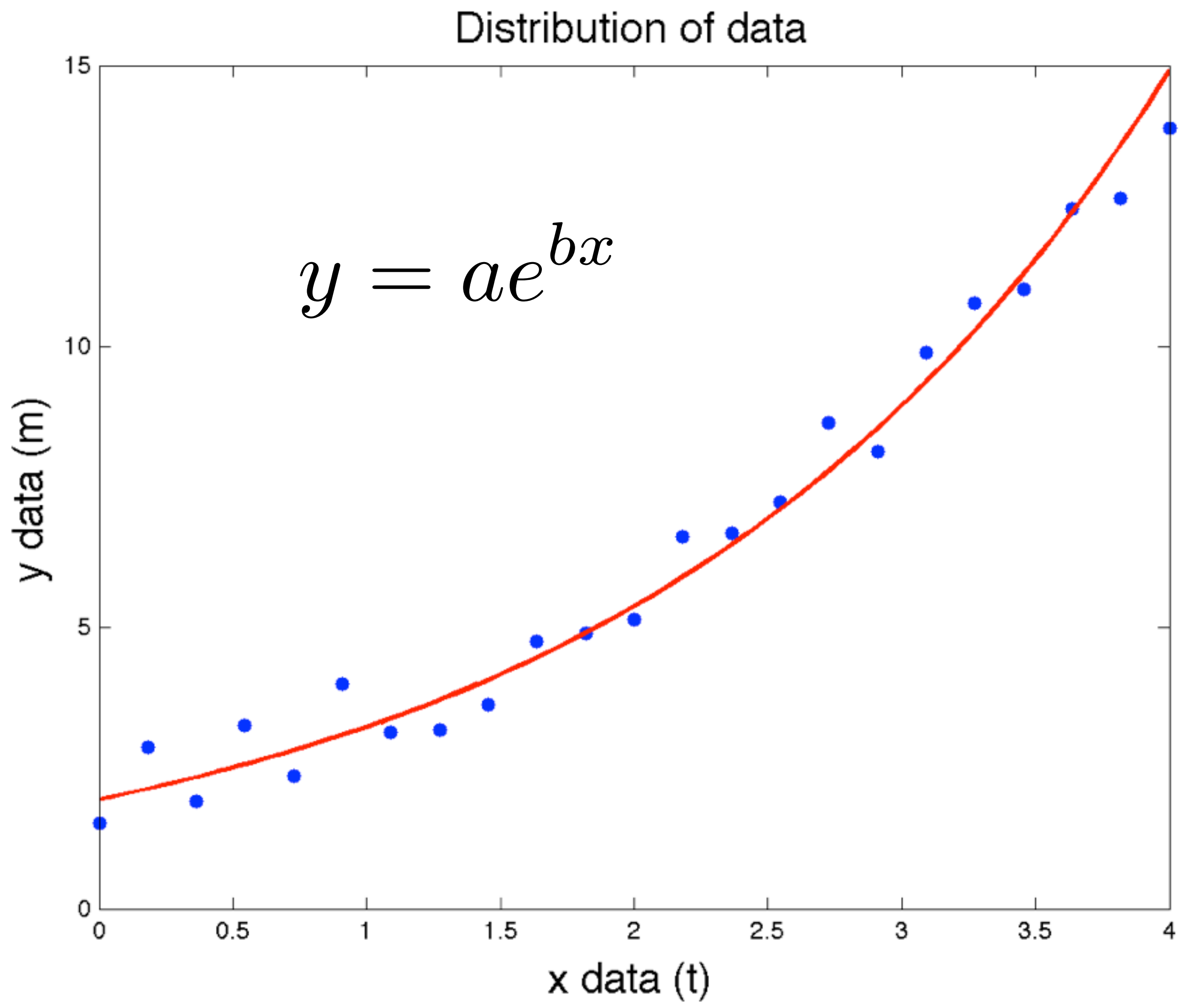
Fitting an exponential curve

Again, we can set up a *linear* system :

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{bmatrix} \begin{bmatrix} b \\ \widetilde{a} \end{bmatrix} = \begin{bmatrix} \ln(y_1) \\ \ln(y_2) \\ \ln(y_3) \\ \vdots \\ \ln(y_N) \end{bmatrix}, \qquad \widetilde{a} = \ln(a)$$

We can then compute $a = e^{\widetilde{a}}$.

Fitting an exponential curve

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Coefficients : a =      1.944548; b =      0.509077
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Example

The temperature dependence of the reaction rate coefficient of a chemical reaction is often modeled by the Arrhenius equation

$$k = A\exp(-E_a/RT)$$

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.

$T(K)$	773	786	797	810	810	820	834
k	1.63	2.95	4.19	8.13	8.19	14.9	22.2

Use a least-squares fit of this data to obtain values for A and E_a for the reaction. Take $R = 8314J/kg/K$.

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