Nonlinear Optimization of a Chemical Reaction Model

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Introduction

Chemical reaction systems are often modeled using nonlinear differential equations. Estimating reaction parameters from experimental data is a central task in chemical engineering, process optimization, and kinetic modeling.

This project asks:

How can we estimate the reaction rate constant of a first-order reaction using nonlinear least squares?

We construct a simple reaction model, generate synthetic data, and use numerical optimization to recover the underlying kinetic parameter. This demonstrates nonlinear model fitting, sensitivity analysis, and scientific interpretation.

Methods

Reaction Model

We consider a first-order irreversible reaction:

$$A \to B$$

with concentration dynamics:

$$\frac{dA}{dt} = -kA$$

The analytical solution is:

$$A(t) = A_0 e^{-kt}$$

but we solve the ODE numerically to maintain generality.

Synthetic Data

We simulate concentration measurements over 10 time units using a true rate constant $k_{\text{true}} = 0.35$. Gaussian noise is added to mimic experimental uncertainty.

These data serve as the target for parameter estimation.

Parameter Estimation

We estimate k by minimizing the sum of squared residuals:

$$\min_k \sum_{i=1}^{n} \left(A_{\text{model}}(t_i; k) - A_{\text{obs}}(t_i)\right)^2$$

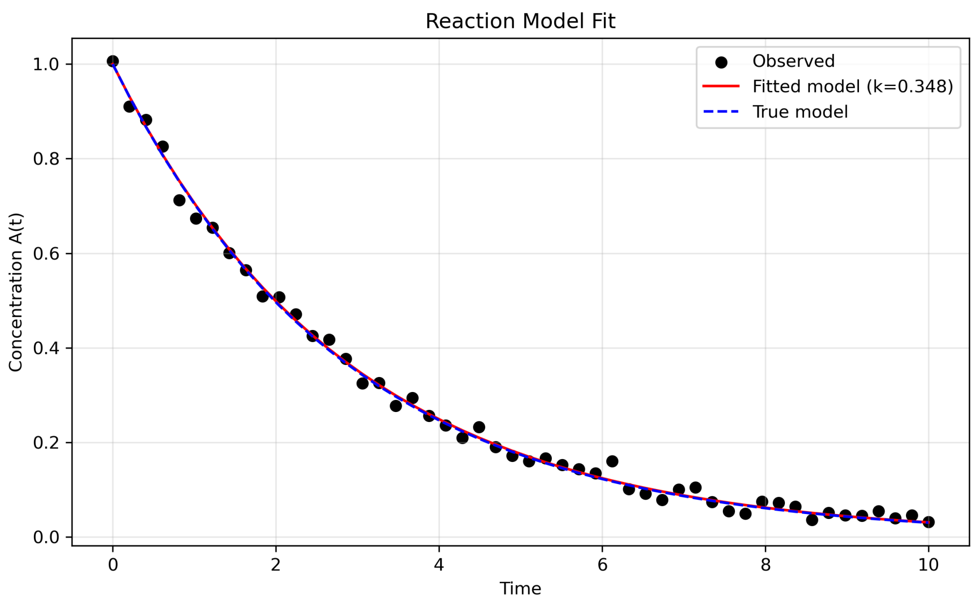
This is a nonlinear least-squares problem solved using SciPy's `least_squares` algorithm.

Sensitivity Analysis

To assess robustness, we vary k around the estimated value and compute the mean squared error. This reveals how sharply the model fit depends on the reaction rate.

Results

Model Fit

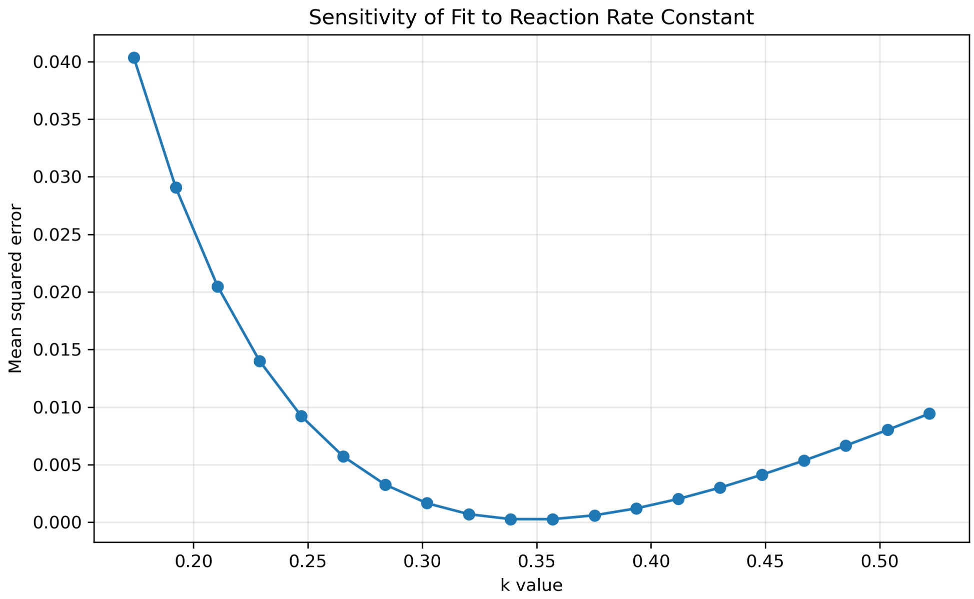


The fitted model closely matches the observed data:

- The estimated rate constant is near the true value.
- The fitted curve lies between the noisy observations and the true underlying trajectory.
- Deviations reflect measurement noise rather than model error.

This demonstrates successful parameter recovery.

Sensitivity Curve



The sensitivity curve shows:

- A clear minimum at the estimated k.
- Rapid increase in error as k moves away from the optimum.
- Strong identifiability of the reaction rate parameter.

This confirms that the optimization landscape is well-behaved for this model.

Discussion

This project illustrates key concepts in nonlinear optimization:

- **Model-based parameter estimation** using differential equations.
- **Nonlinear least squares** as a flexible and powerful fitting method.
- **Sensitivity analysis** to assess parameter robustness.

From an applied mathematics perspective, this demonstrates your ability to:

- translate physical systems into ODEs,
- implement numerical solvers,
- formulate and solve nonlinear optimization problems,
- interpret results scientifically.

These skills are directly relevant to chemical engineering, process optimization, and computational modeling roles.

Conclusion

By fitting a first-order reaction model to synthetic data, we successfully estimated the reaction rate constant using nonlinear optimization. The combination of ODE modeling, least-squares fitting, and sensitivity analysis provides a rigorous and interpretable framework for kinetic parameter estimation.

This project completes the numerical optimization series and further strengthens your portfolio with a mathematically rich, scientifically grounded example of nonlinear modeling.