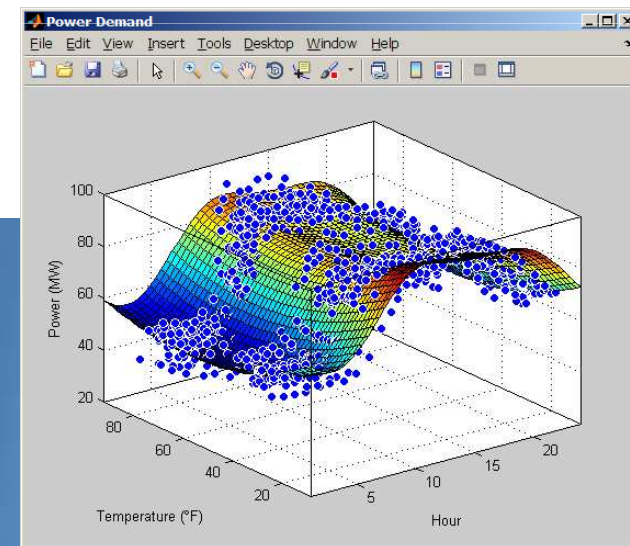


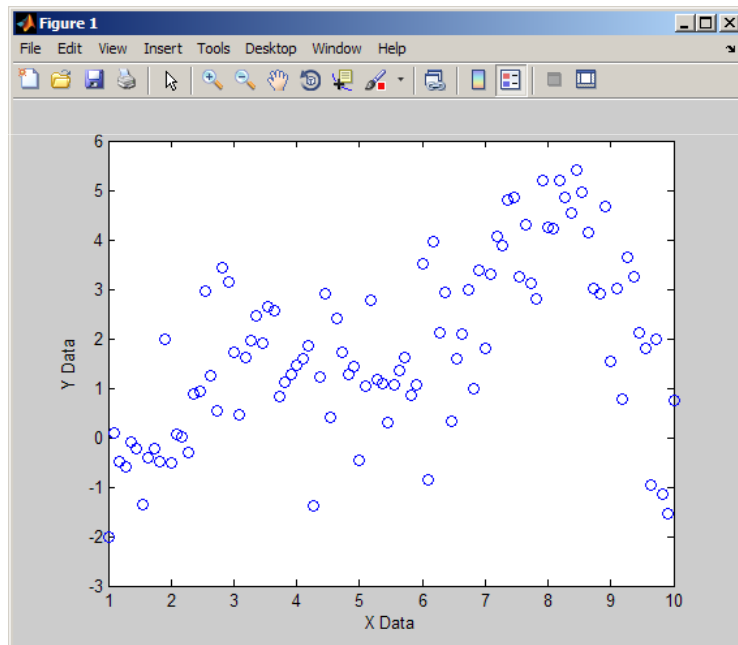
# New Surface Fitting and Global Optimization Capabilities for Solving Challenging Data Analysis Problems

**Giorgia Zucchelli**  
Application Engineer - MathWorks

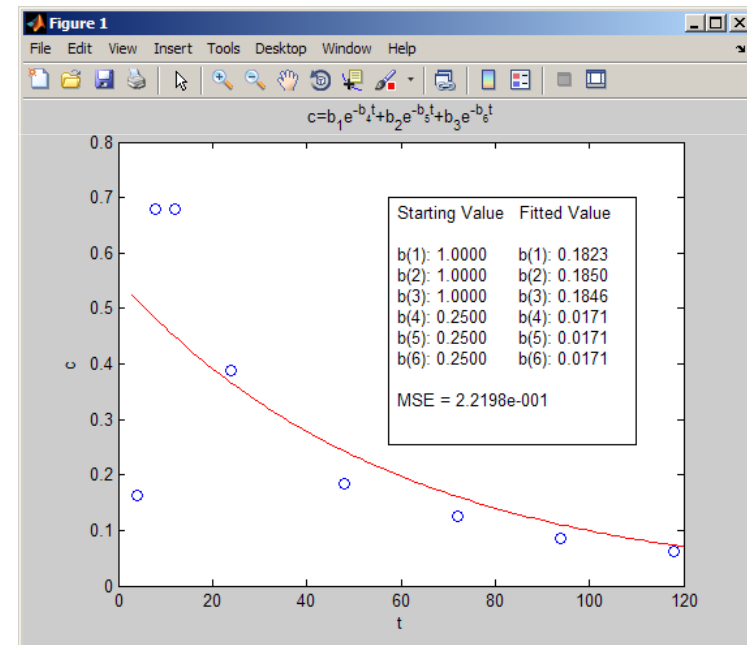


# Agenda

Two common challenges in creating an accurate curve fit:



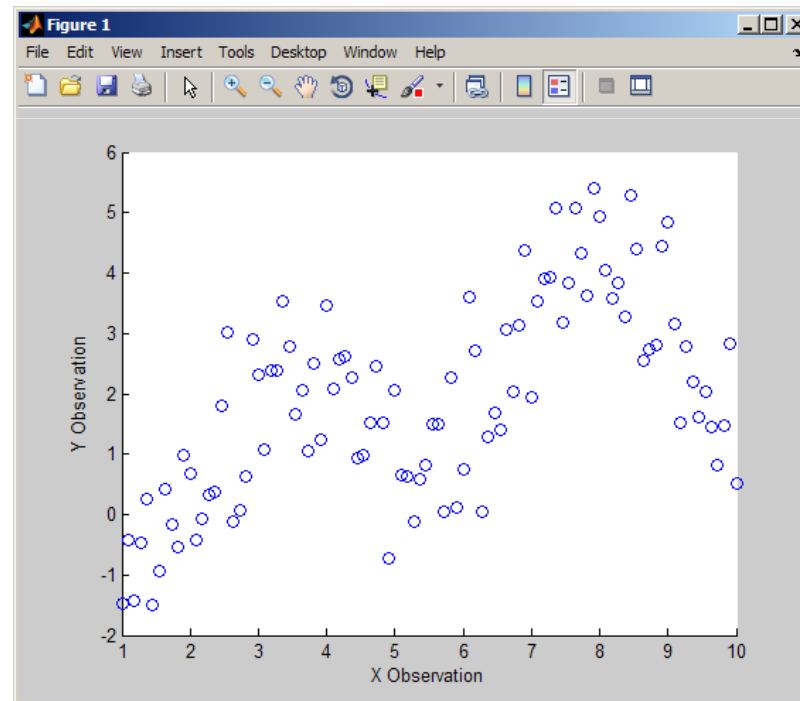
Can't describe the relationship  
between your variables



Can't specify good starting points  
for your solvers

# Challenge 1

## *Generating a Good Fit Without Domain Knowledge*



# Regression Techniques

- Require that the user specify a model
- Choice of model is based on domain knowledge

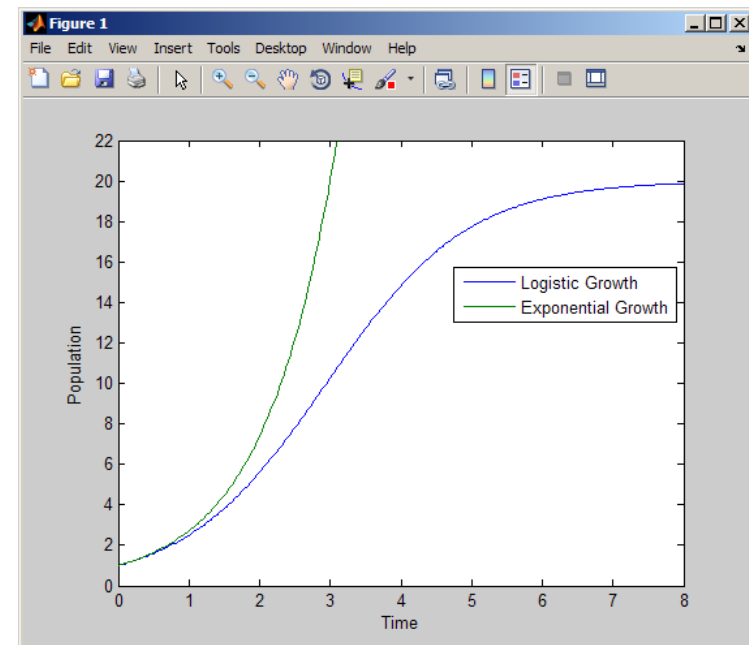
## *Example - population models*

Logistic Growth

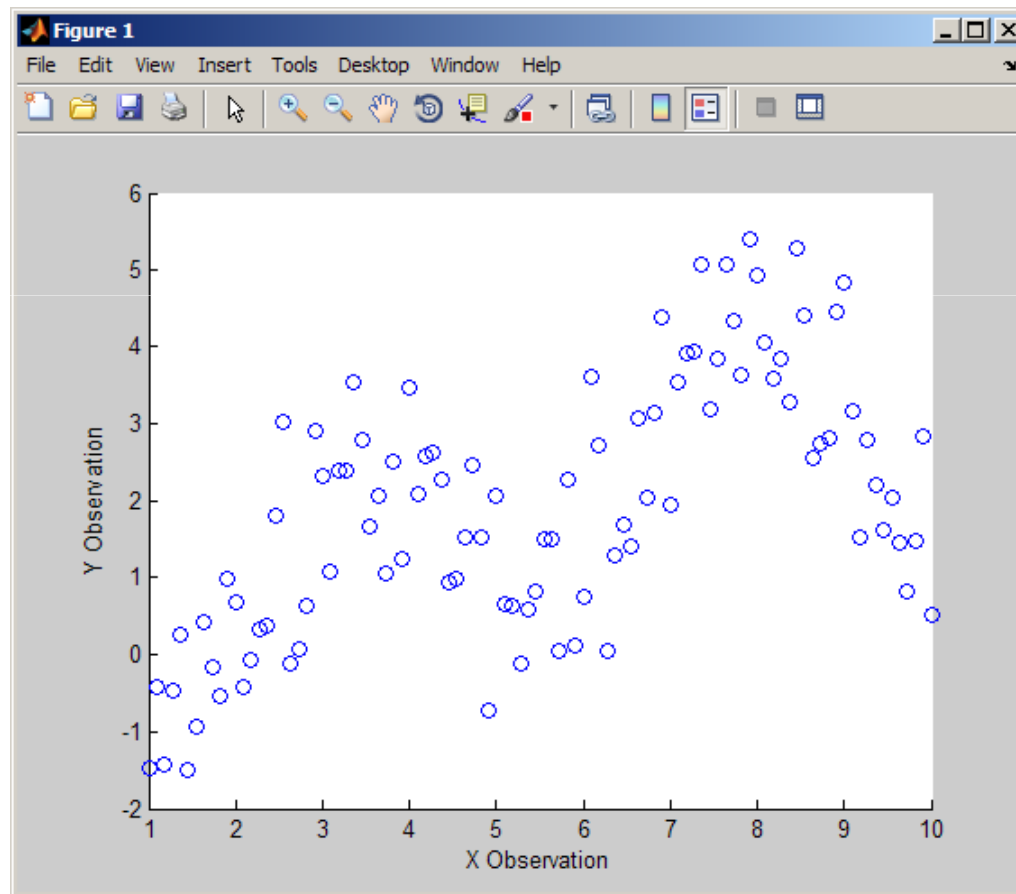
$$N_t = \frac{N_0 \times K}{N_0 + (K - N_0) \times \exp(-r_0 \times t)}$$

Exponential Growth

$$N_t = N_0 \times e^{(r \times t)}$$

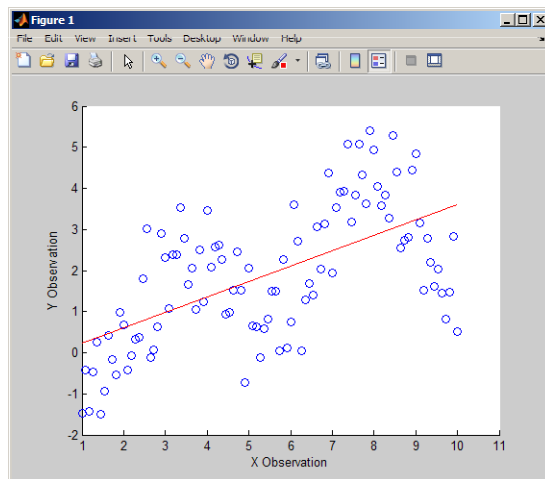


# What if you don't know what type of model to use?

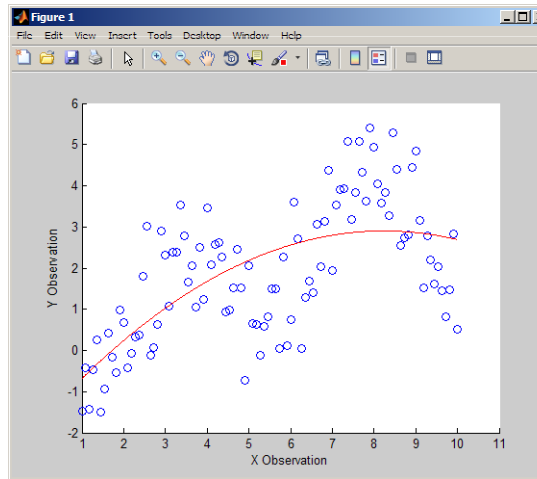


# What if you don't know what type of model to use?

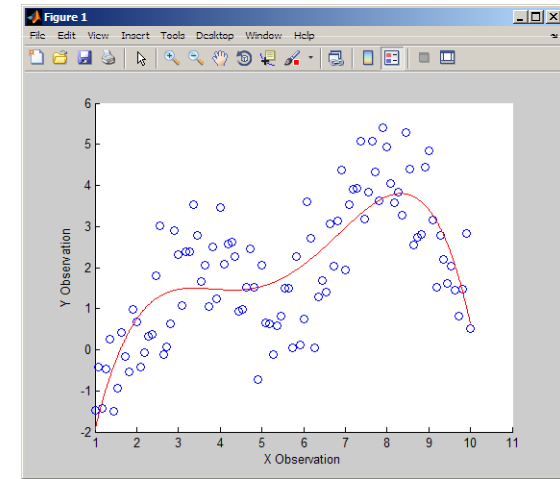
Line



Quadratic



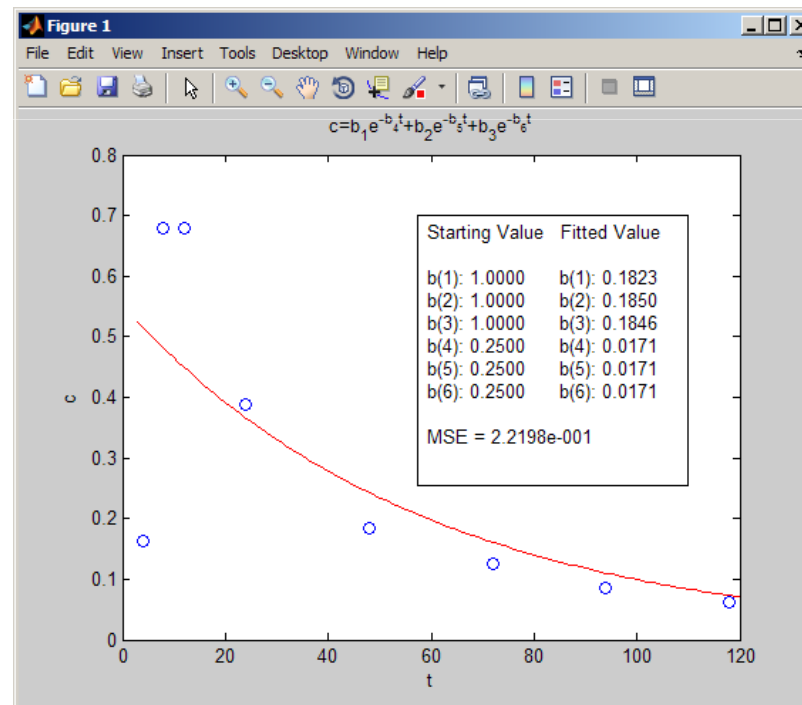
Rational



# Demo 1

# Challenge 2

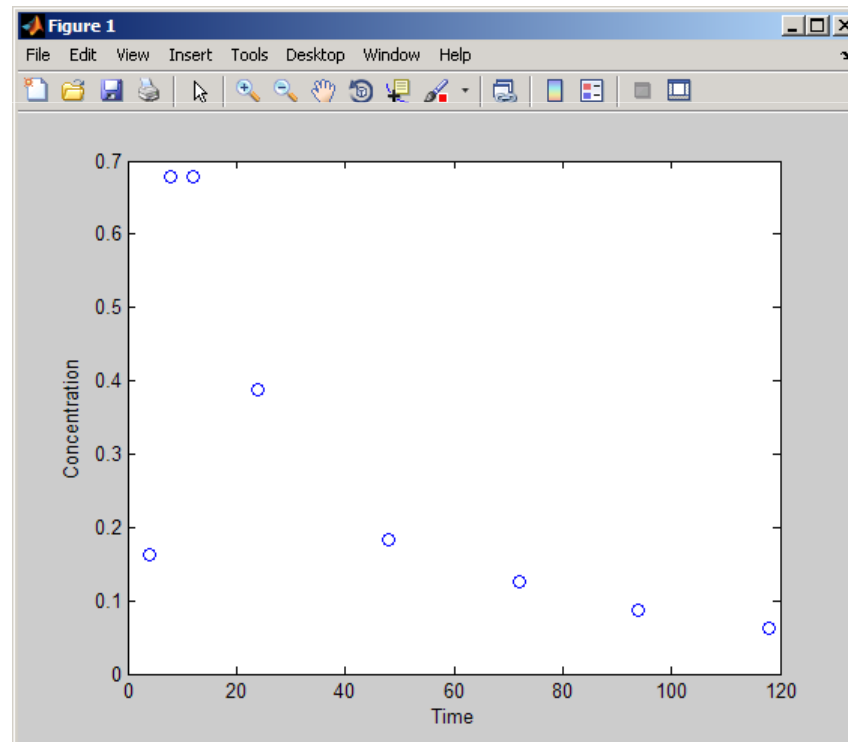
## *Pitfalls Using Nonlinear Regression*





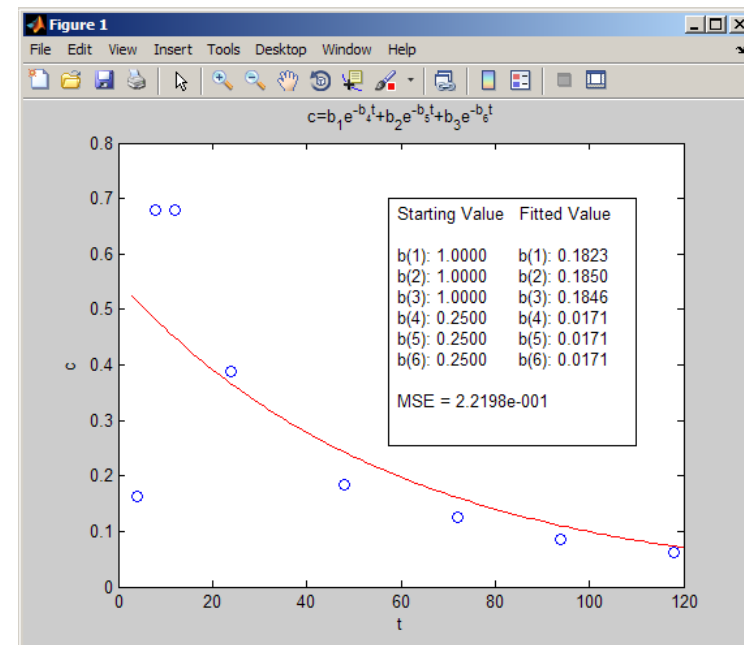
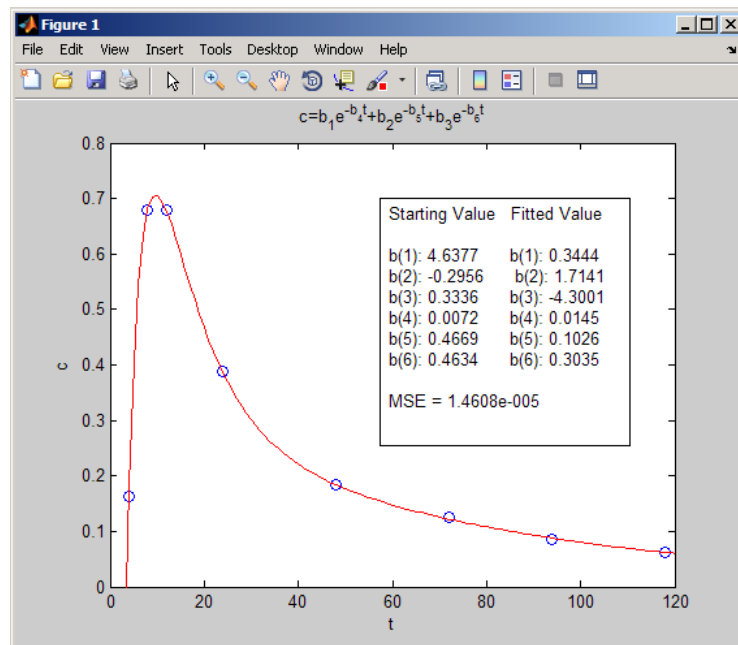
# Nonlinear Regression Example

$$\text{Concentration} = \beta_1 e^{-\beta_4 T} + \beta_2 e^{-\beta_5 T} + \beta_5 e^{-\beta_6 T}$$



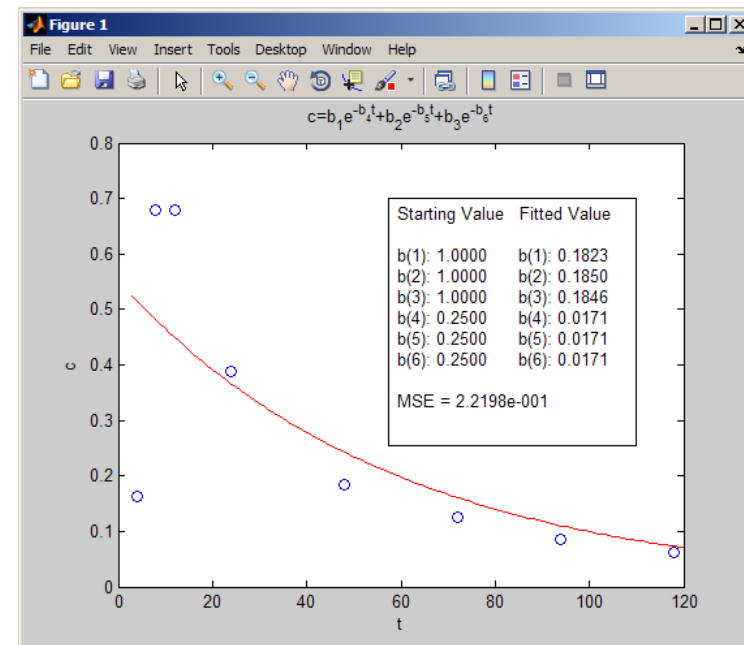
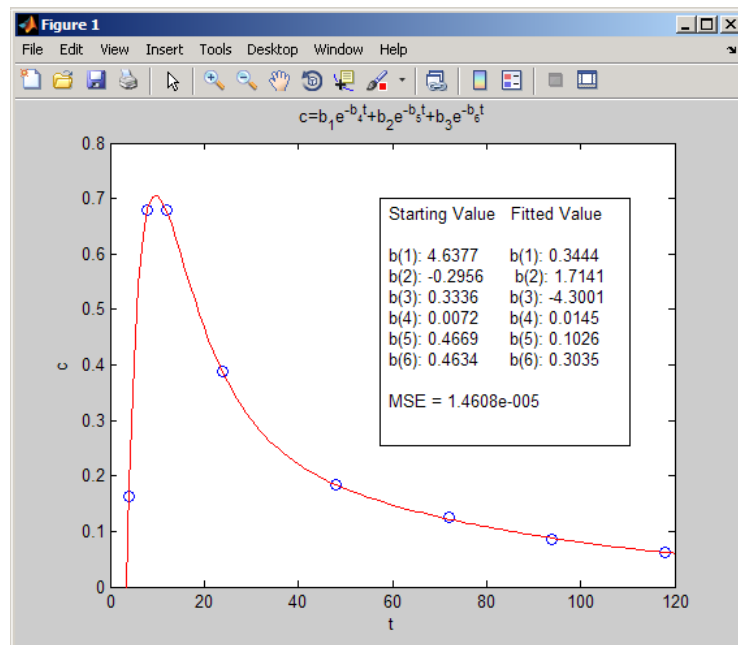
# Nonlinear Regression Example

$$\text{Concentration} = \beta_1 e^{-\beta_4 T} + \beta_2 e^{-\beta_5 T} + \beta_5 e^{-\beta_6 T}$$



# Practical Implications: *What does a bad $R^2$ mean?*

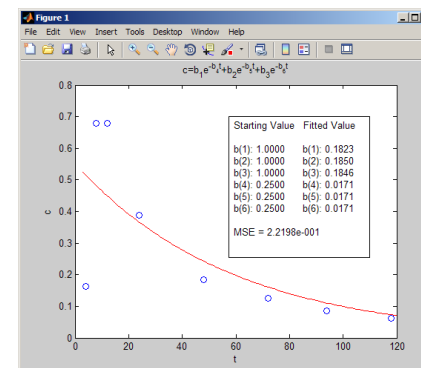
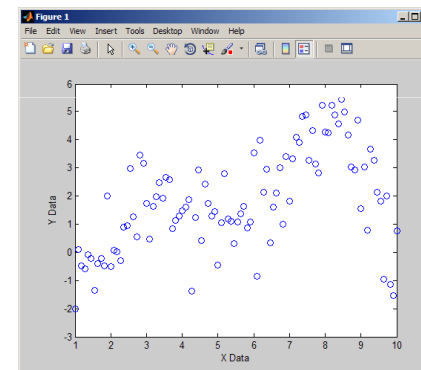
- Bad model specification?
- Poor set of starting conditions?



# Demo 2

# Summary

- Examined two common curve fitting challenges
  - Can't describe the relationship between your variables
  - Can't specify good starting points for your solvers



# Summary

- Showed how MathWorks products can be used to solve these problems
  - Nonparametric fitting
    - LOWESS: Curve Fitting Toolbox
    - Cross Validation: Statistics Toolbox
  - Use `MultiStart` to identify good starting conditions
    - Global Optimization Toolbox

