### Reminders

- Take charge of your GitHub repo
- git clone ...

# Machine Learning

- Supervised learning
  - labeled response data
  - compare prediction to labeled ("known") response
  - this semester
- Unsupervised learning
  - unlabeled response data, discover patterns
  - aka traditional topic: "multivariate analysis"
  - clustering, ordination etc

## Machine Learning algorithms

- Model algorithm
- Training algorithm
- Inference algorithm

# Today

- Machine learning with ants data
  - polynomial model algorithm
  - least squares training algorithm
  - cross validation inference algorithm
- R code

# Machine learning workflow

#### Overall algorithm:

- 1. Create model algorithm(s) for  $\hat{f}(x)$
- 2. Use a training algorithm to find parameter values of  $\hat{f}(x)$
- 3. Use an inference algorithm to measure prediction error and compare predictive skill among models (model families, tuning parameters, *x* sets, etc).

### Basic full ML setup

#### 3 algorithms:

- model: flexible function  $\hat{f}(x)$ ; e.g. polynomial linear model

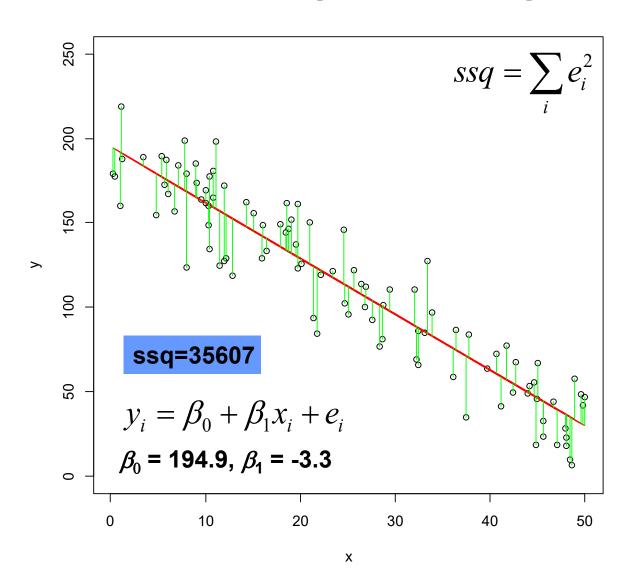
$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + ... + \beta_m x^m$$
 m=order

- training: optimize objective function e.g. least squares
- minimize  $SSQ = \sum_{i=1}^{n} (y_i \hat{y}_i)^2$  for training data
- inference: measure error by cross validation;
  tuning parameter (order of poly)

### Code

- 02\_2\_ants\_cv\_polynomial.R
- 02\_2\_ants\_cv\_polynomial.py

### Least squares optimization



General algorithmic idea:

Vary model parameters until we find the parameter values that minimize the distance of the model from the data

# Optimization algorithms

### Strategies

- Systematically try all combinations of parameters Grid search algorithms
- 2. Narrowing in: keep changing parameters in the direction that leads to lower SSQ Descent algorithms
- 3. Try random values for parameter combinations Monte Carlo algorithms
- 4. Solve for parameters using math Analytical or numerical algorithms

#### Linear regression in R uses strategy 4

Im(y ~ x) solves a system of linear equations using linear algebra

Mathematical theory shows what to do (QR decomposition)

Numerical algorithm is needed to do it (householder algorithm)

Fast, specialized, guaranteed to find the minimum SSQ. Only works for SSQ: limited to ordinary linear regression.