Reminders

- Sign up for GitHub
- Send me your username
- Ask questions on Piazza

Machine Learning

- Model algorithm
- Training algorithm
- Inference algorithm

Today

- Machine learning with ants data
  - polynomial model algorithm
  - least squares training algorithm
- Explore Cross-Validation (CV)
  - inference algorithm
  - pseudocode to R code
- Theory of bias-variance tradeoff

Basic full ML setup

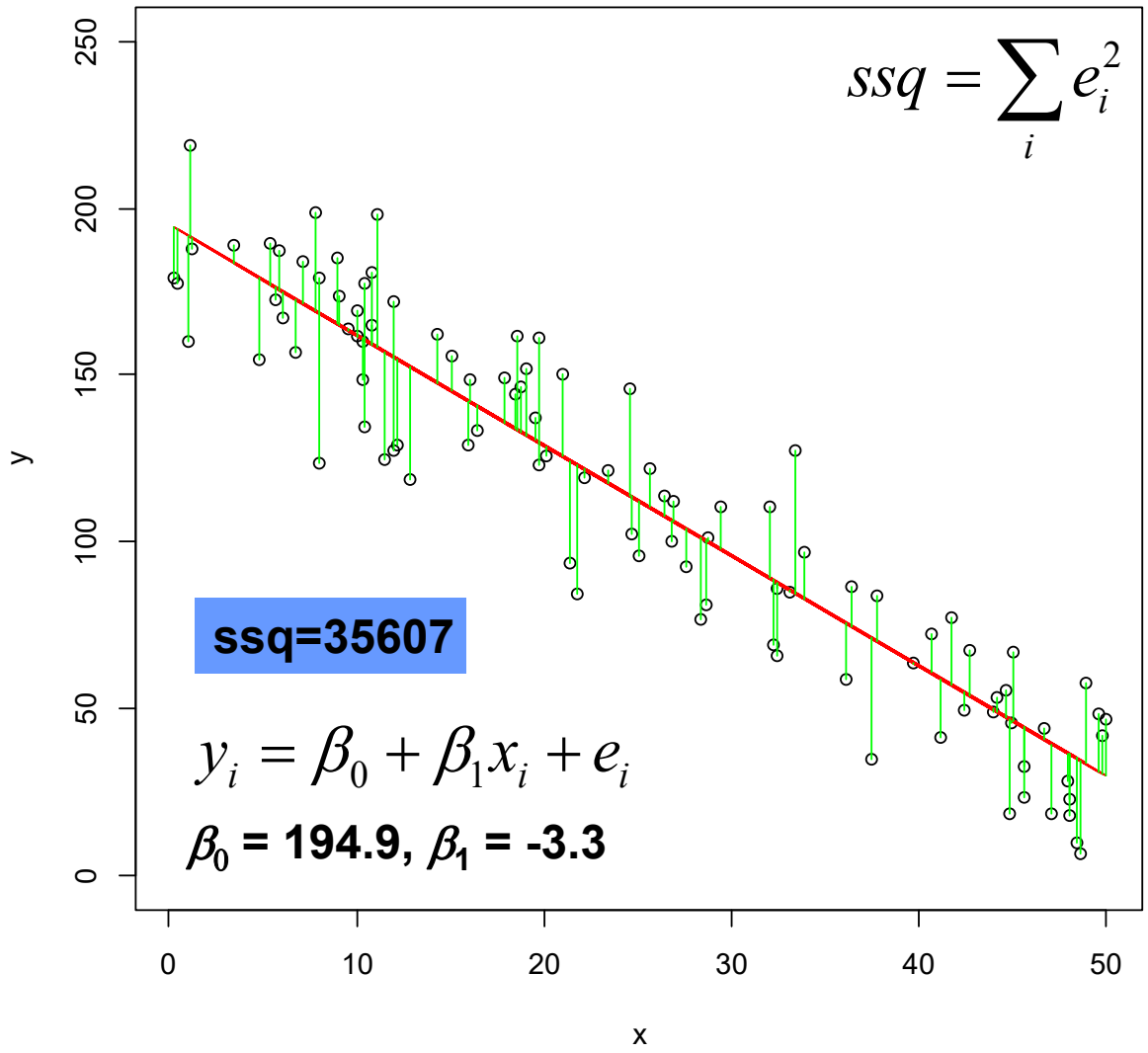
- Polynomial example, 3 algorithms:
  - model: flexible function $\hat{f}(x)$;
    polynomial linear model

    $$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \ ... + \beta_m x^m$$ m=order
  - training: optimize least squares objective function
  - minimize $SSQ = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ for training data
  - inference: tuning parameter (order of poly);
    k-fold cross validation → prediction error

Code

- 02_2_ants_cv_polynomial.R

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

1. 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

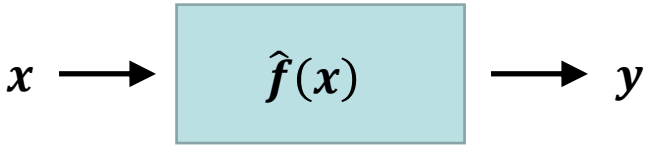
lm(y ~ x) solves a system of linear equations using linear algebra

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**.

Prediction



Goal: find function $\hat{f}$ that has good predictive performance

Accurate on new observations of y

(out-of-sample accuracy)

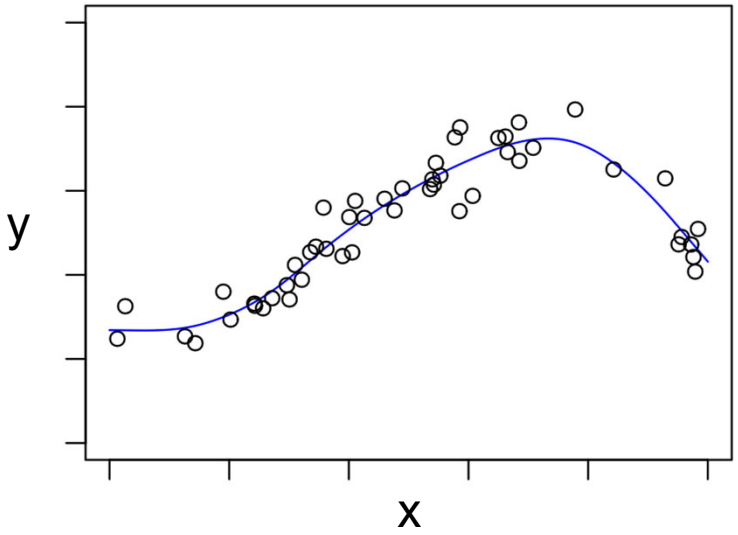
Tuning parameters

- Order of polynomial
- Different values of tuning parameters give different models
- Use CV inference algorithm to choose model with best predictive performance

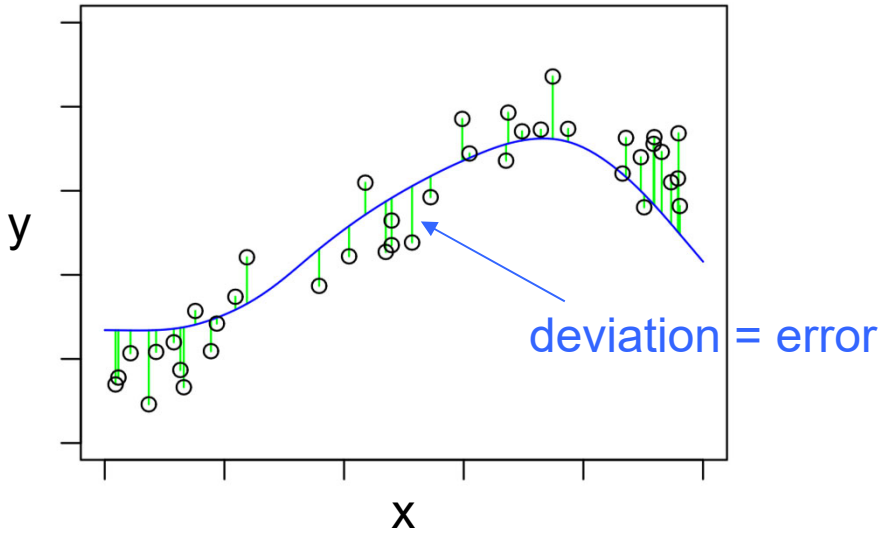
Inference algorithm

Basic idea: out-of-sample validation

Fit model to training dataset



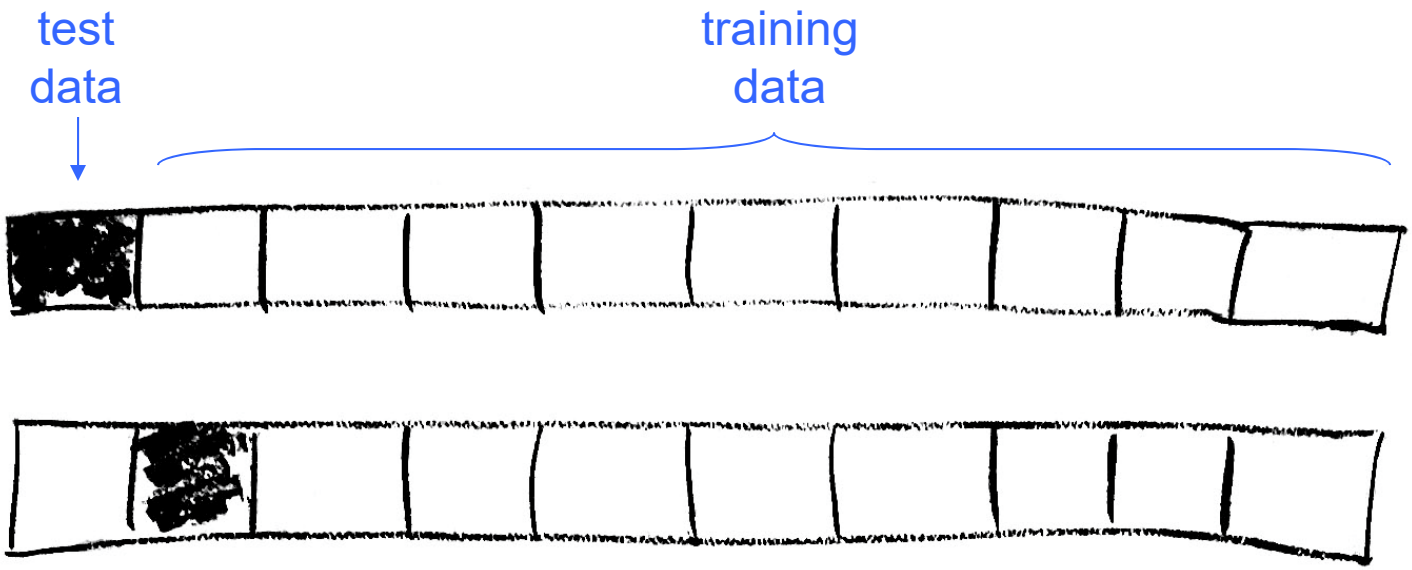
Test model on validation dataset



e.g. mean square error (MSE)

k-fold cross validation (CV)

Divide dataset into k parts (preferably randomly)



... repeat with each test subset

k-fold CV inference algorithm

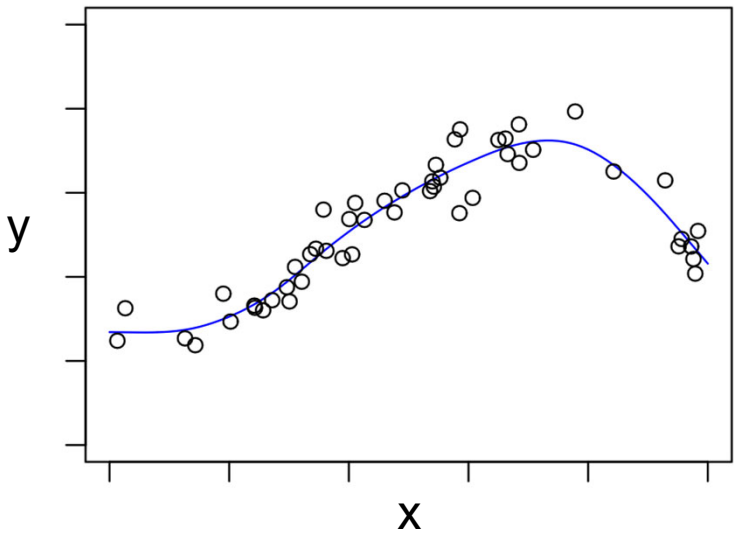
Algorithm

divide dataset into k parts i = 1...k
for each i
    test dataset = part i
    training dataset = remaining data
    find f using training dataset
    use f to predict for test dataset
    e_i = prediction error
CV_error = mean(e)

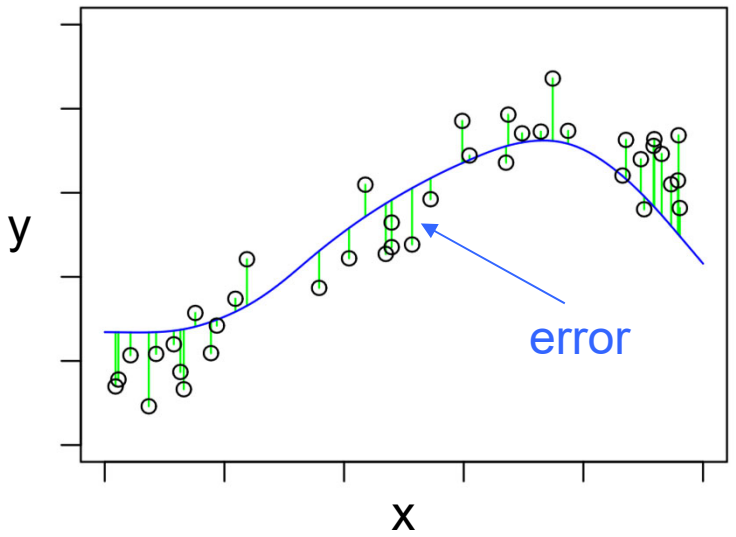
Typical values for k: 5, 10, n

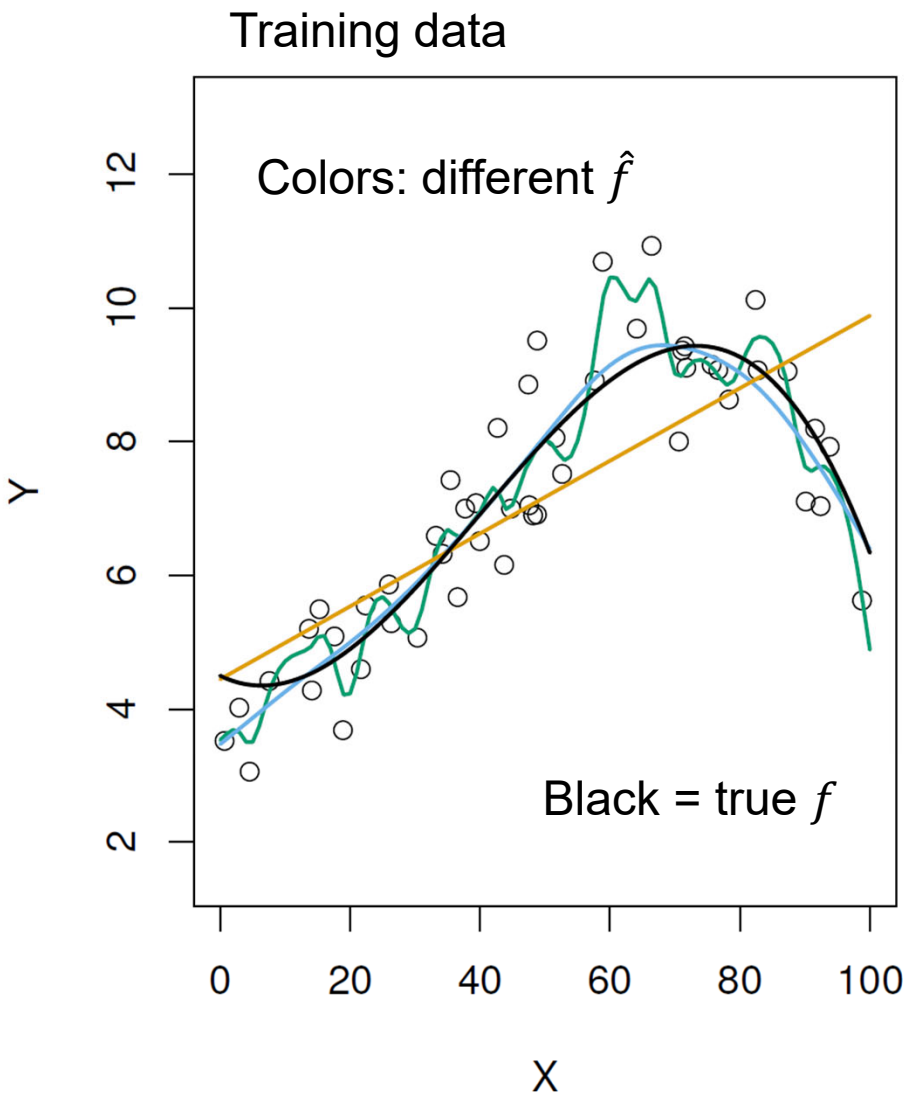
Bias-variance tradeoff

$\hat{f}$ fitted on training data

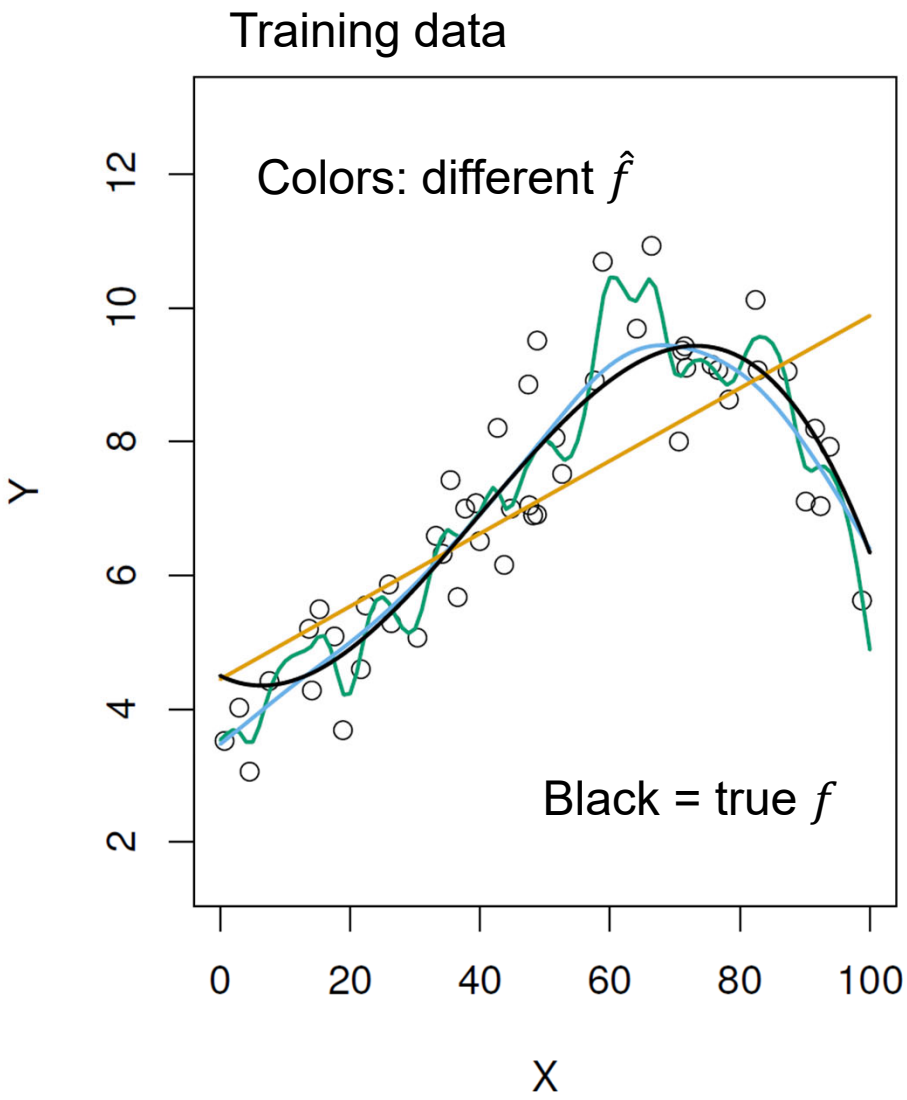


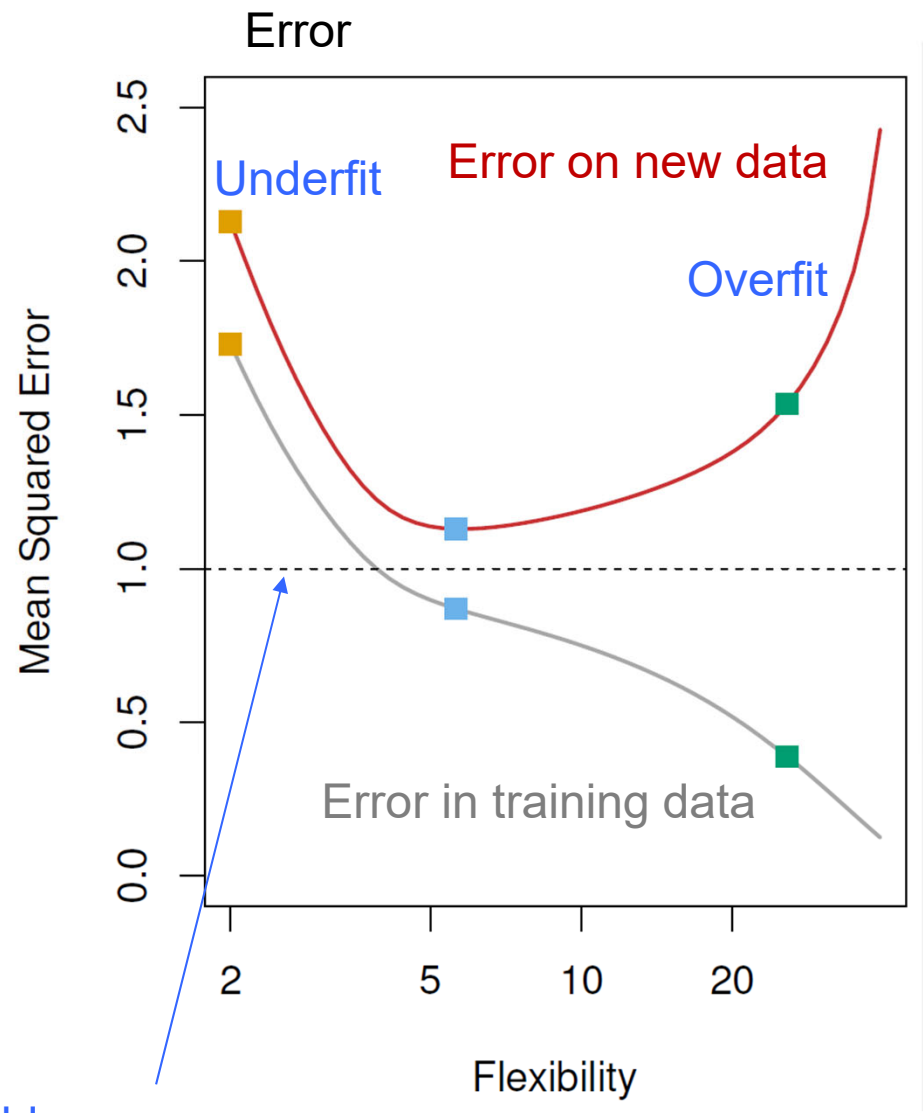
$\hat{f}$ predicting new data





Amount of "wiggliness" in $\hat{f}$





Goal: balance underfit and overfit

Bias-variance tradeoff

$$\text{Total error} = \text{Var}\left(\hat{f}\right) + \text{Bias}\left(\hat{f}\right)^2 + \text{Var}(\epsilon)$$

Amount $\hat{f}$ would change if fitted on different data

Average deviation of $\hat{f}$ from true f

Irreducible error

Bias-variance tradeoff

$$\text{Total error} = \text{Var}\left(\hat{f}\right) + \text{Bias}\left(\hat{f}\right)^2 + \text{Var}(\epsilon)$$

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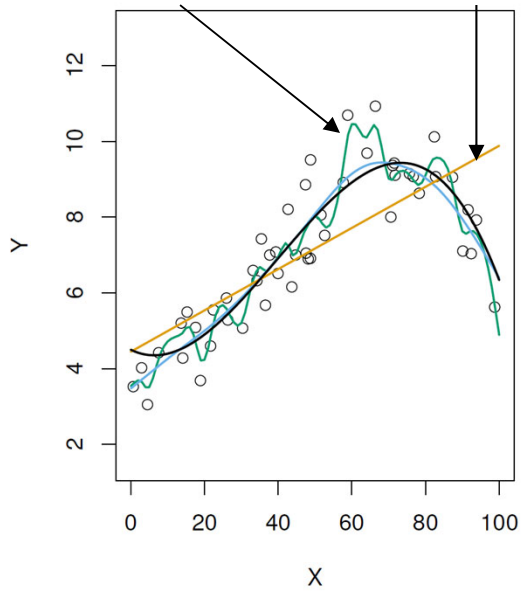
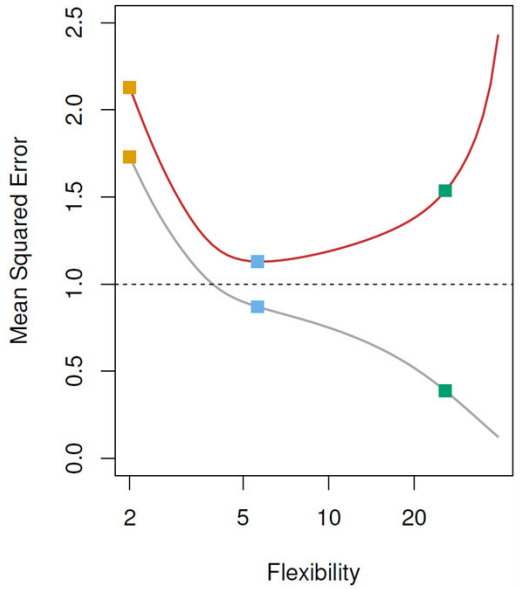
Average deviation of $\hat{f}$ from true f

Irreducible error

High variance

High bias





Bias-variance tradeoff

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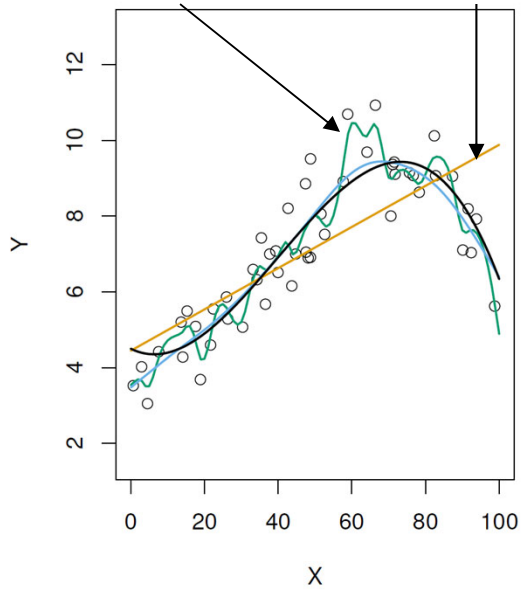
Average deviation of $\hat{f}$ from true f

Irreducible error

High variance

High bias



High bias

High variance

Sweet spot:
low variance
low bias