Linear Regression

EECS 349

slides from Bryan Pardo, Mark Cartwright;
(also contains ideas and a few images from wikipedia and books by Alpaydin, Duda/Hart/ Stork, and Bishop.)

Outline

- Announcements
  - Homework #2 assigned Wednesday (due Wednesday)
- Linear regression

Regression Learning

There is a set of possible examples $X = \{\mathbf{x_1}, \ldots \mathbf{x_n}\}$

Each example is a **vector** of k **real valued attributes**

$$\mathbf{x}_i = < x_{i1}, \ldots, x_{ik} >$$

There is a target function that maps *X* onto some **real value** *Y*

$$f : X \rightarrow Y$$

The DATA is a set of tuples <example, response value>

$$\{< \mathbf{x}_1, y_1 >, \ldots < \mathbf{x_n}, y_n >\}$$

Find a hypothesis ***h*** such that...

$$\forall \mathbf{x}, h(\mathbf{x}) \approx f(\mathbf{x})$$

Why *Linear* Regression?

- Easily understood/interpretable
- Well-studied
- Computationally Efficient

Linear Regression Assumption

- Response is a linear function of input, plus Gaussian Noise

Observed response $$y = f(\mathbf{x}) + \varepsilon$$

Where $$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

Hypothesis Space

- Each hypothesis characterized by a weight vector **w**

$$h(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + \ldots w_k x_k$$

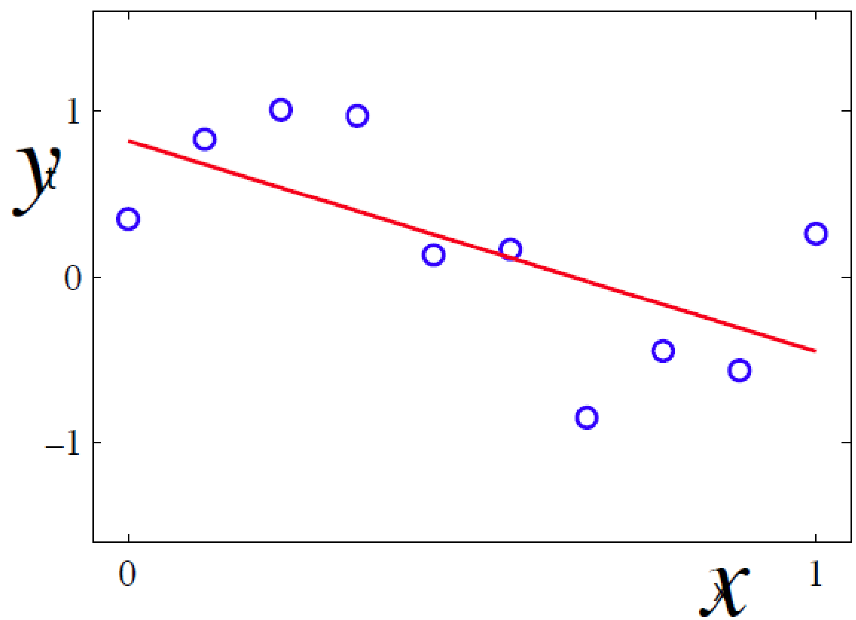
$$\mathbf{w} =< w_0, w_1, \ldots w_k >$$

- **Goal:** Find a good **w**
  - (One that minimizes some error criterion)

One-dimensional LR

- x has 1 attribute a (predictor variable)
- Hypothesis function is a line:

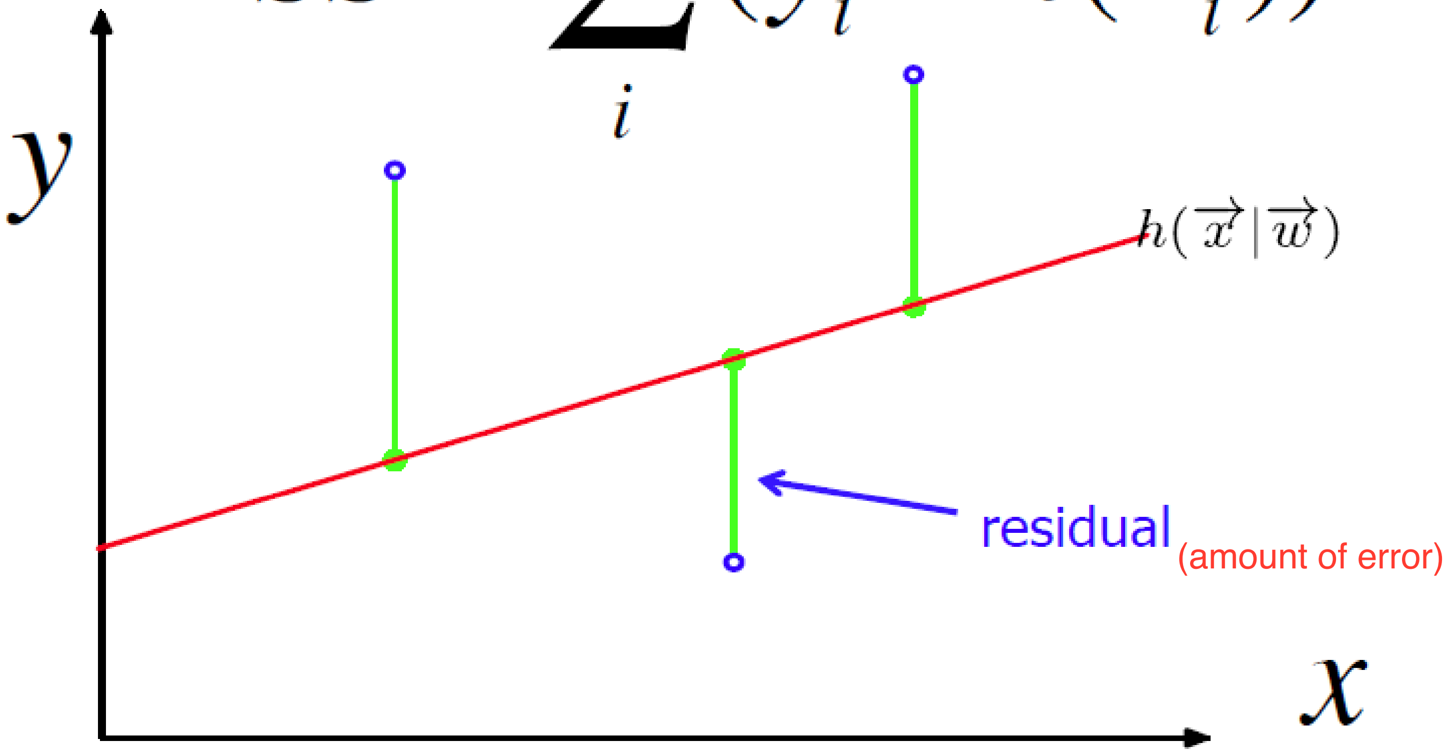
Example: $$\hat{y} = h(x) = w_0 + w_1 x$$



Minimize RSS (sum of squared residuals)

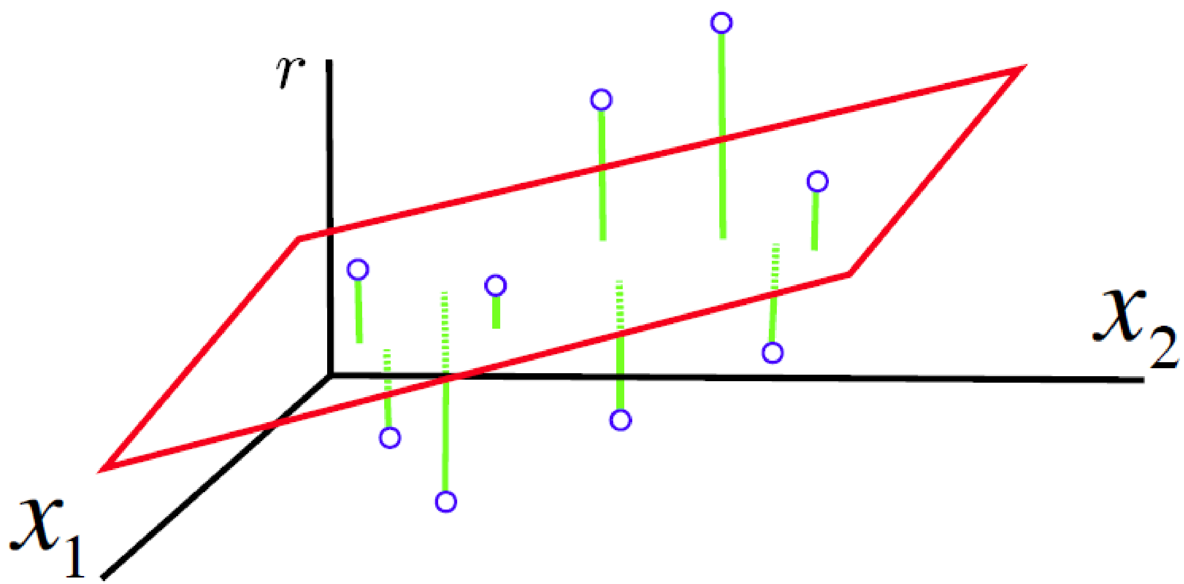
number of training examples

$$RSS = \sum_{i}^{n} (y_i - h(\mathbf{x}_i))^2$$



Multivariate Linear Regression

$$h(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + \ldots w_k x_k$$



Create a new 0 dimension with 1 and append it to the beginning of every example vector $\mathbf{x}_i$

This placeholder corresponds to the offset w_0

$$\mathbf{x}_i =< 1, x_{i,1}, x_{i,2} \ldots, x_{i,k} >$$

Format the data as a matrix of examples **x** and a vector of response values *y*...

One training example

$$\mathbf{X} = \begin{bmatrix} 1 & x_{1,1} & \ldots & x_{1,k} \\ 1 & x_{2,1} & \ldots & x_{2,k} \\ \ldots & \ldots & \ldots & \ldots \\ 1 & x_{n,k} & \ldots & x_{n,k} \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \ldots \\ y_n \end{bmatrix}$$

Closed-form solution

Our goal is to find the weights of a function….

$$h(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + \dots w_k x_k$$

…that minimizes the sum of squared residuals:

$$RSS = \sum_{i}^{n} (y_i - h(\mathbf{x}_i))^2$$

It turns out that there is a close-form solution to this problem!

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

$$
\begin{aligned}
RSS(\mathbf{w}) &= \sum\nolimits_{i=1}^{n} (y_i - h(\mathbf{x}_i))^2 \\
&= \sum\nolimits_{i=1}^{n} (y_i - w_0 - \sum\nolimits_{j=1}^{k} x_{ij} w_j)^2 \\
&= (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})
\end{aligned}
$$

$$RSS(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

$$\frac{\partial RSS}{\partial \mathbf{w}} = -2\mathbf{X}^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

$$0 = -2\mathbf{X}^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

$$0 = \mathbf{X}^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

$$0 = \mathbf{X}^T \mathbf{y} - \mathbf{X}^T \mathbf{X}\mathbf{w}$$

$$\mathbf{X}^T \mathbf{X}\mathbf{w} = \mathbf{X}^T \mathbf{y}$$

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

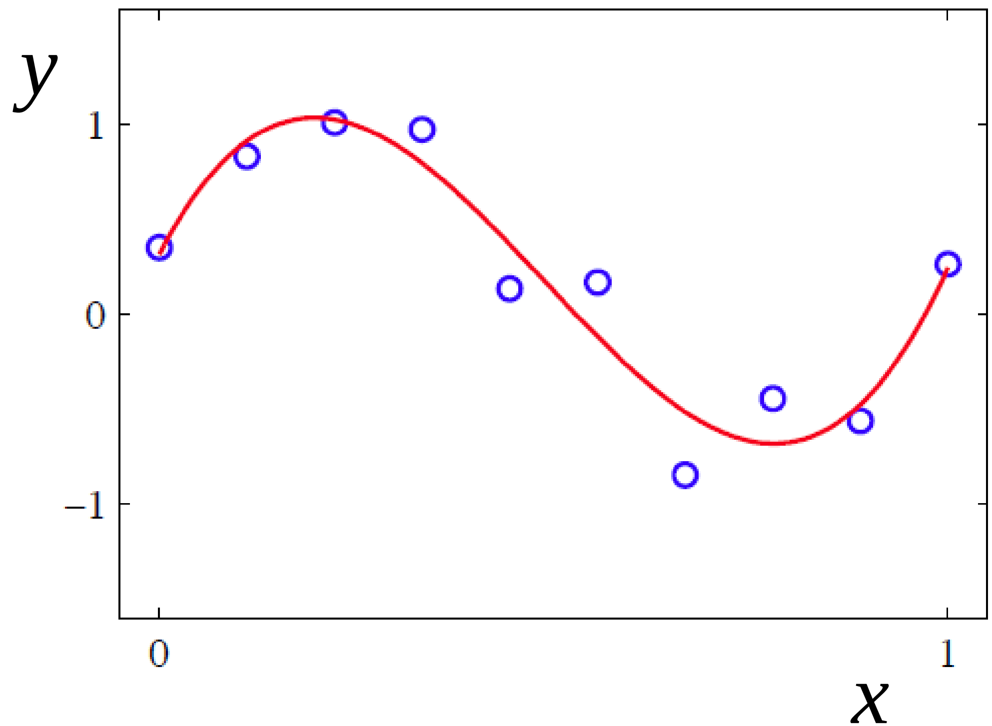
You're familiar with linear regression where the input has k dimensions.

$$h(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 + \ldots w_k x_k$$

We can use this same machinery to make polynomial regression from a one-dimensional input.....

$$h(x) = w_0 + w_1 x + w_2 x^2 + \ldots w_k x^k$$

$$h(x) = w_0 + w_1 z + w_2 z^2 + w_3 z^3$$



Parameter estimation (analytically minimizing sum of squared residuals):

One training example

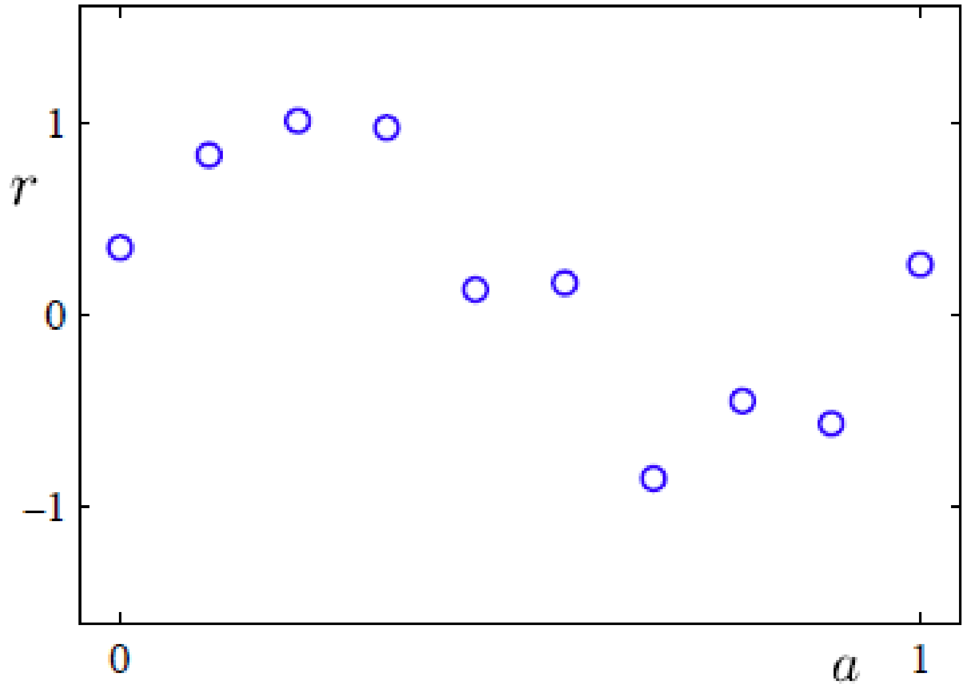
$$\mathbf{X} = \begin{bmatrix} \boxed{1 & z_1^1 & \dots & z_1^k} \\ 1 & z_2^1 & \dots & z_2^k \\ \dots & \dots & \dots & \dots \\ 1 & z_n^1 & \dots & z_n^k \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix}$$

(Note, there is only 1 attribute z for each training example.
Those superscripts are powers, since we're doing polynomial regression)

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Tuning Model Complexity: Example

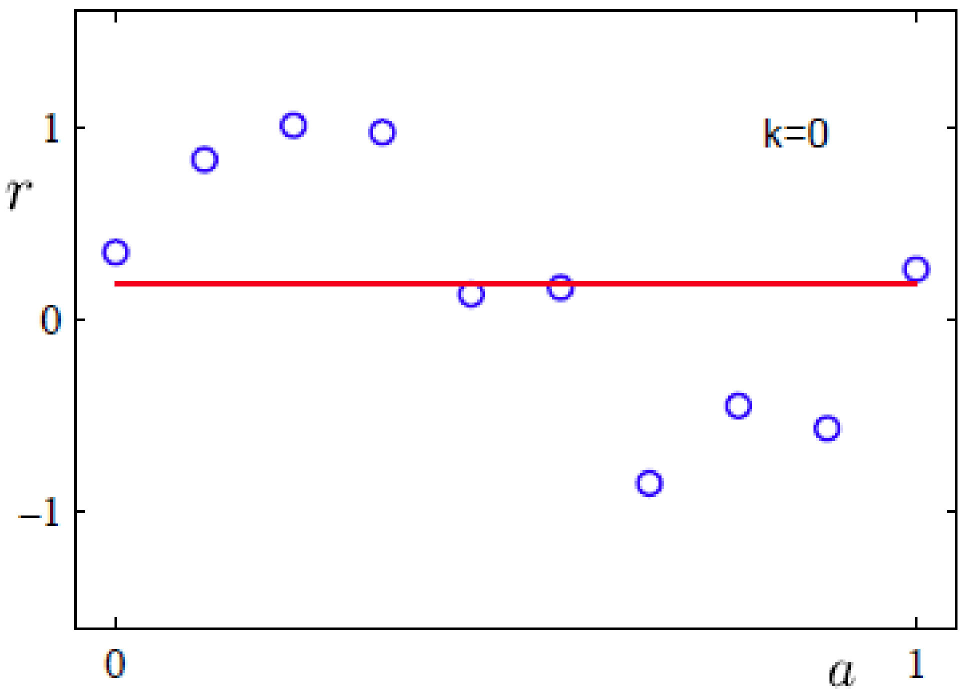
What is your hypothesis for $f(x)$?



Tuning Model Complexity: Example

What is your hypothesis for $f(x)$?

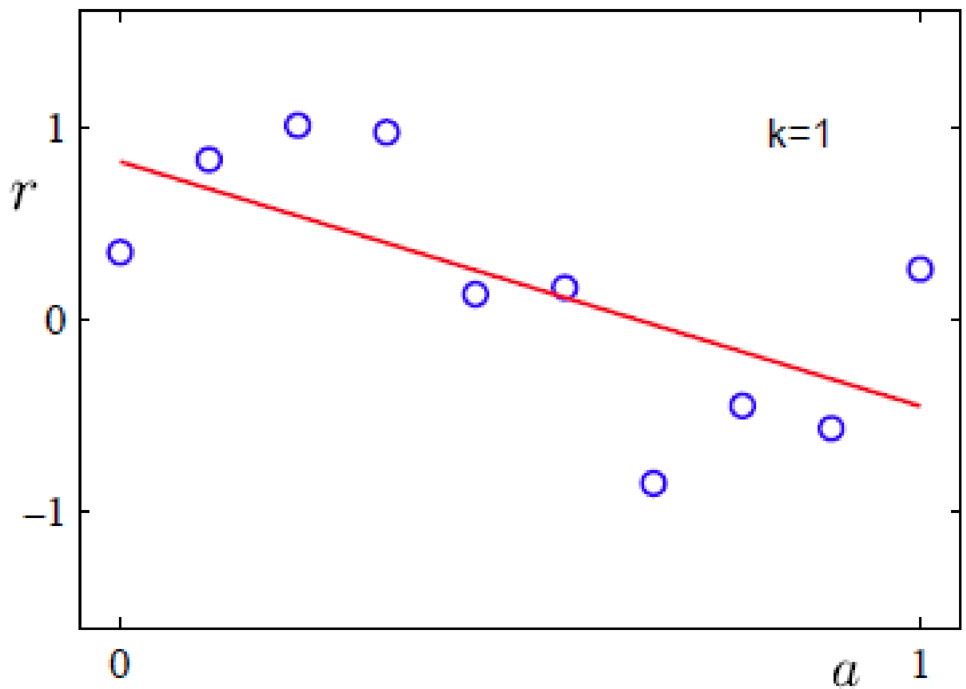
kth order polynomial regression



Tuning Model Complexity: Example

What is your hypothesis for $f(x)$?

k^{th} order polynomial regression



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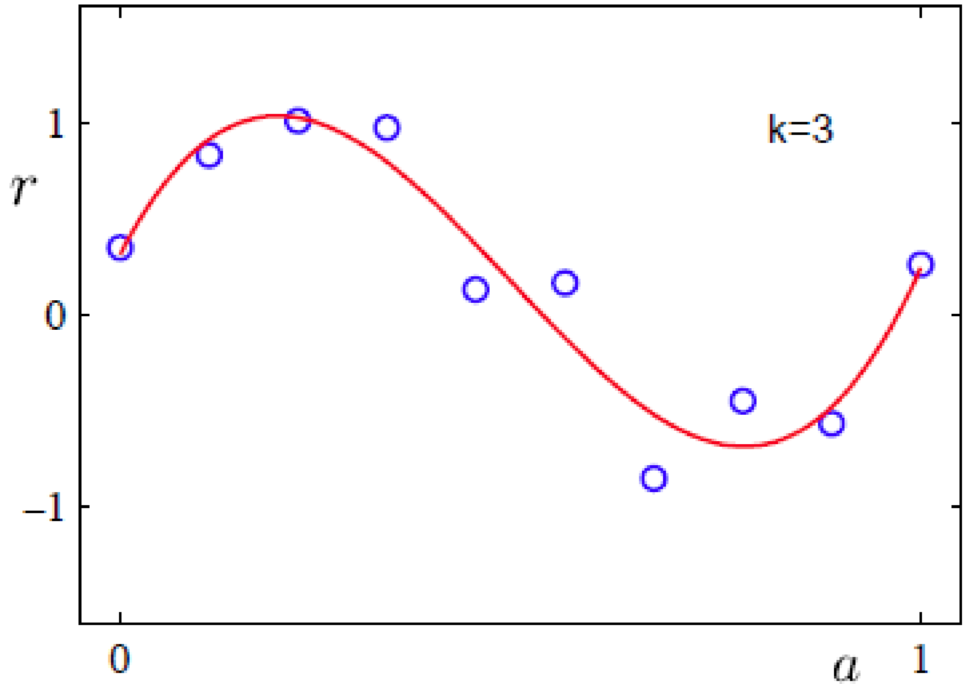

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What is your hypothesis for $f(x)$?

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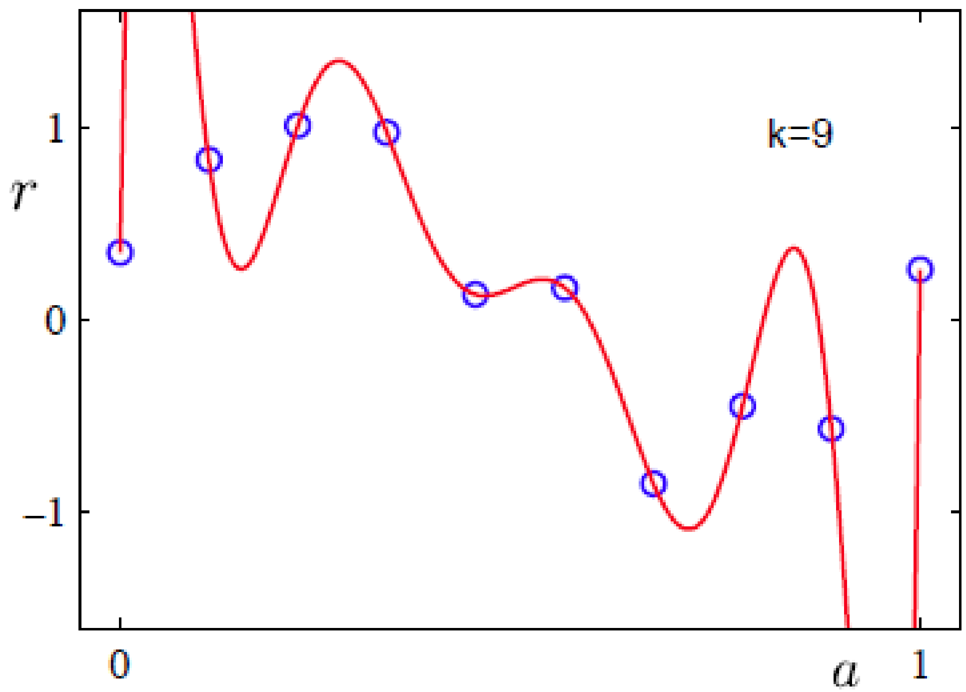
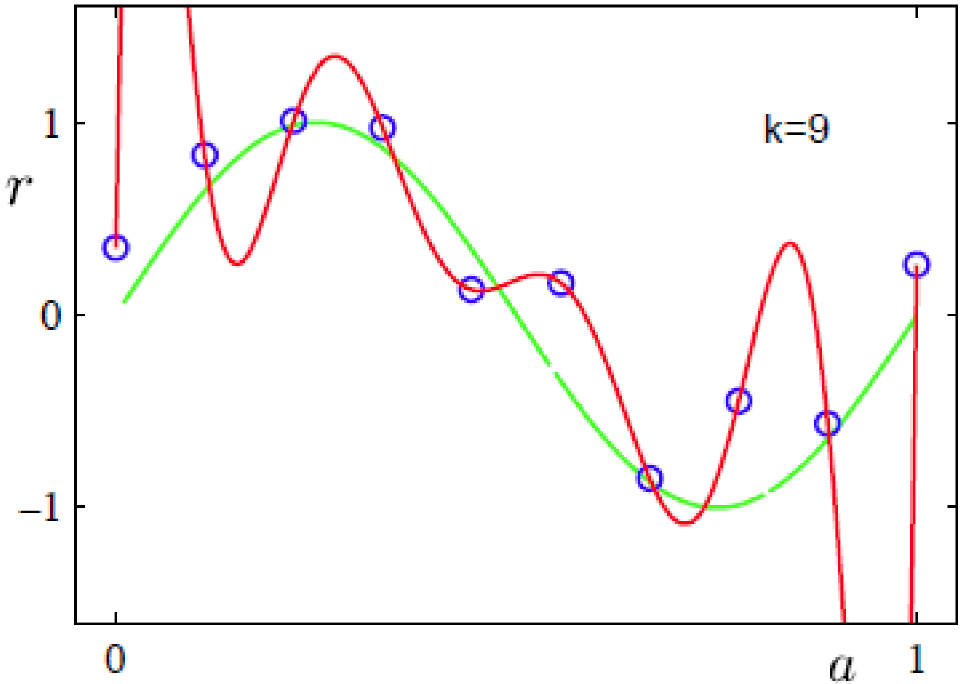


Tuning Model Complexity: Example

What is your hypothesis for $f(x)$?

how do we choose the # of k?
cross validation

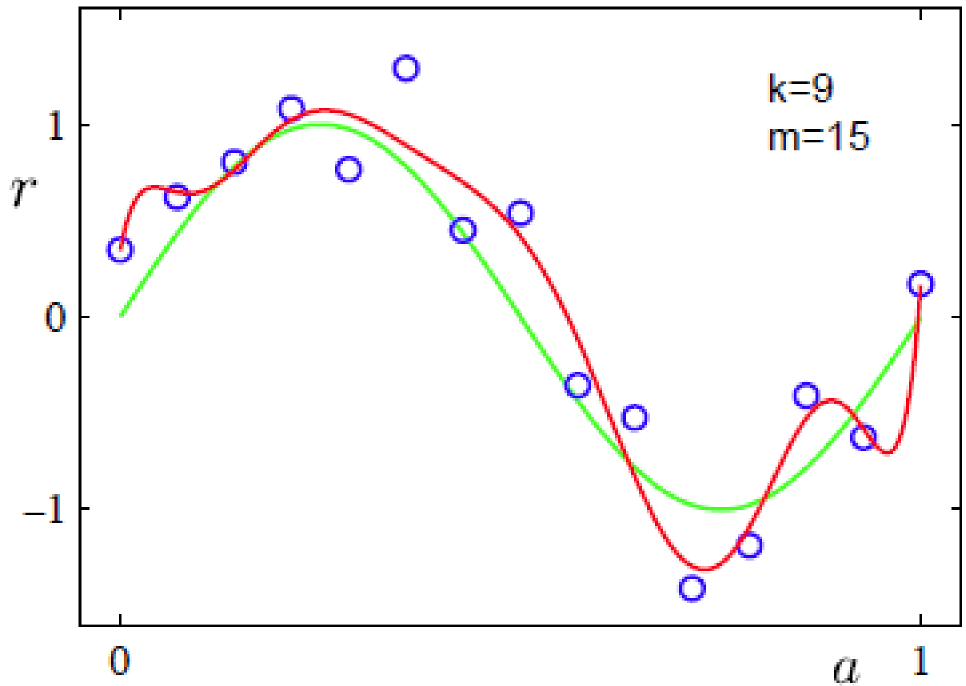
k^{th} order polynomial regression



Tuning Model Complexity: Example

What happens if we fit to more data?

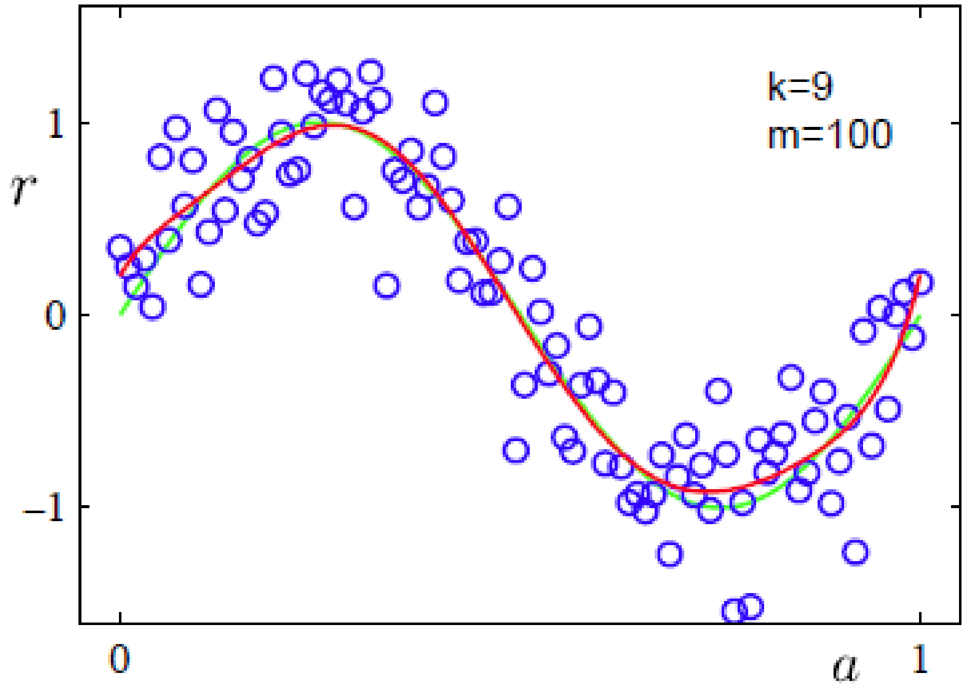
k^{th} order polynomial regression



Tuning Model Complexity: Example

What happens if we fit to more data?

k^{th} order polynomial regression



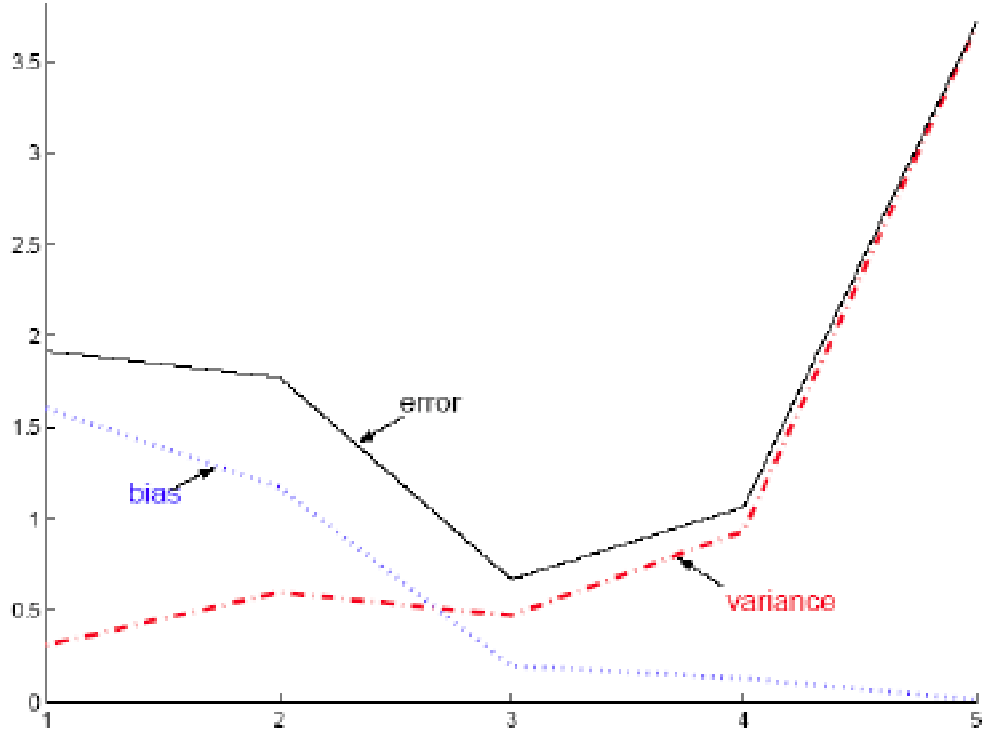
Bias and Variance of an Estimator

- Let X be a sample from a population specified by a true parameter θ
- Let d=d(X) be an estimator for θ

$$\mathbb{E}[(d-\theta)^2] = \mathbb{E}[(d-\mathbb{E}[d])^2] + (\mathbb{E}[d]-\theta)^2$$

mean square error *variance* *bias²*

Bias and Variance



Order of a polynomial fit to some data

As we **increase complexity**, **bias decreases** (a better fit to data) and **variance increases** (fit varies more with data)

Reading

- Chapter 3 from Elements of Statistical Learning
  - https://web.stanford.edu/~hastie/ElemStatLearn/