Machine Learning

Topic 4: Linear Regression Models

(contains ideas and a few images from wikipedia and books by Alpaydin, Duda/Hart/Stork, and Bishop. Updated Fall 2015)

Regression Learning Task

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 use a linear regression model?

- Easily understood
- Interpretable
- Well studied by statisticians
  - many variations and diagnostic measures
- Computationally efficient

Linear Regression Model

Assumption: The observed response (dependent) variable, r, is the true function, f(x), with additive Gaussian noise, ε, with a 0 mean.

noise

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

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

Assumption: The expected value of the response variable ***y*** is a linear combination of the k independent attributes/features)

The Hypothesis Space

Given the assumptions on the previous slide, our hypothesis space is the set of linear functions (hyperplanes)

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

(w_0 is the offset from the origin. You always need w_0)

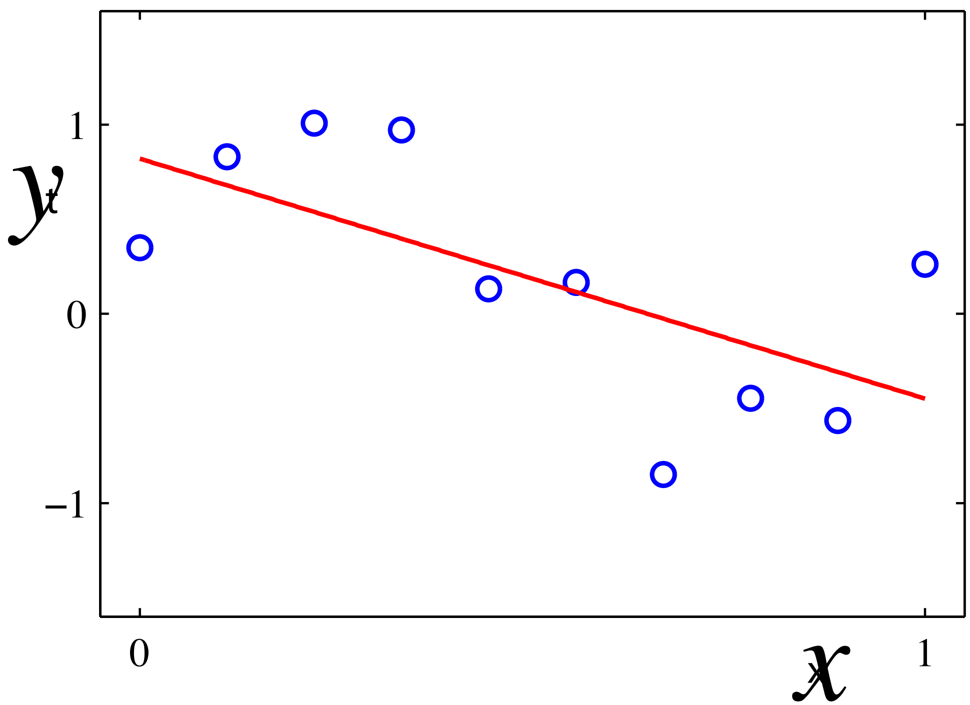
The goal is to learn a k+1 dimensional vector of weights that define a hyperplane minimizing an error criterion.

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

Simple Linear Regression

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

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



The Error Criterion

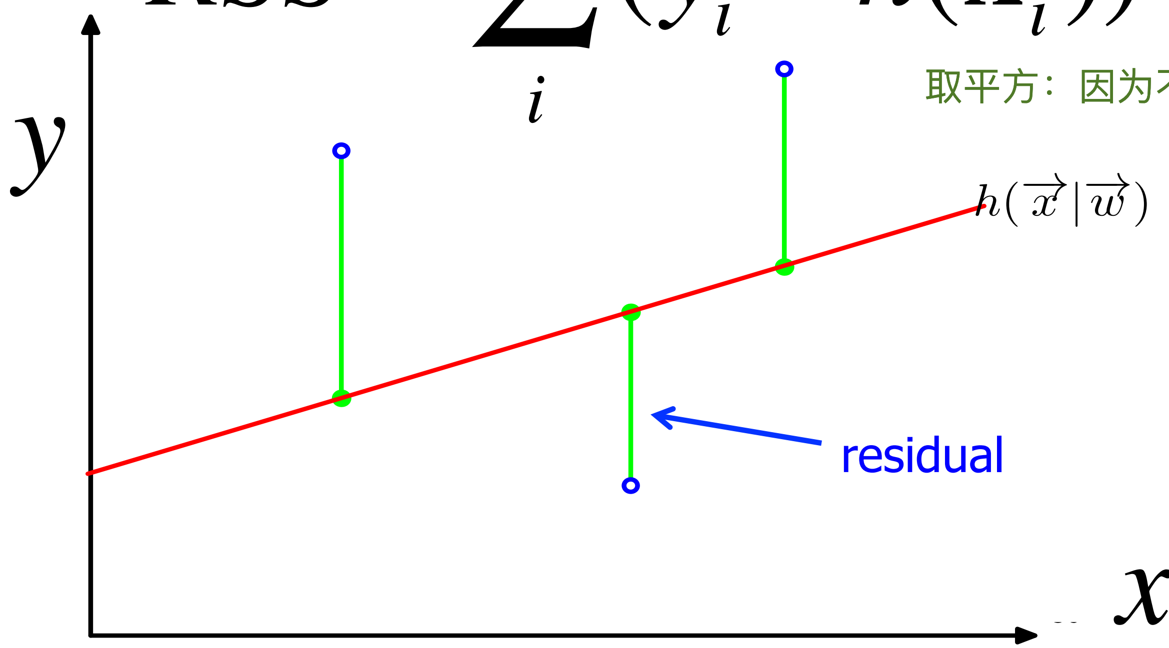
Typically estimate parameters by minimizing sum of squared residuals (RSS)...also known as the Sum of Squared Errors (SSE)

number of training examples

通过使RSS最小来选参数

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

取平方：因为不取会被距离正负抵消



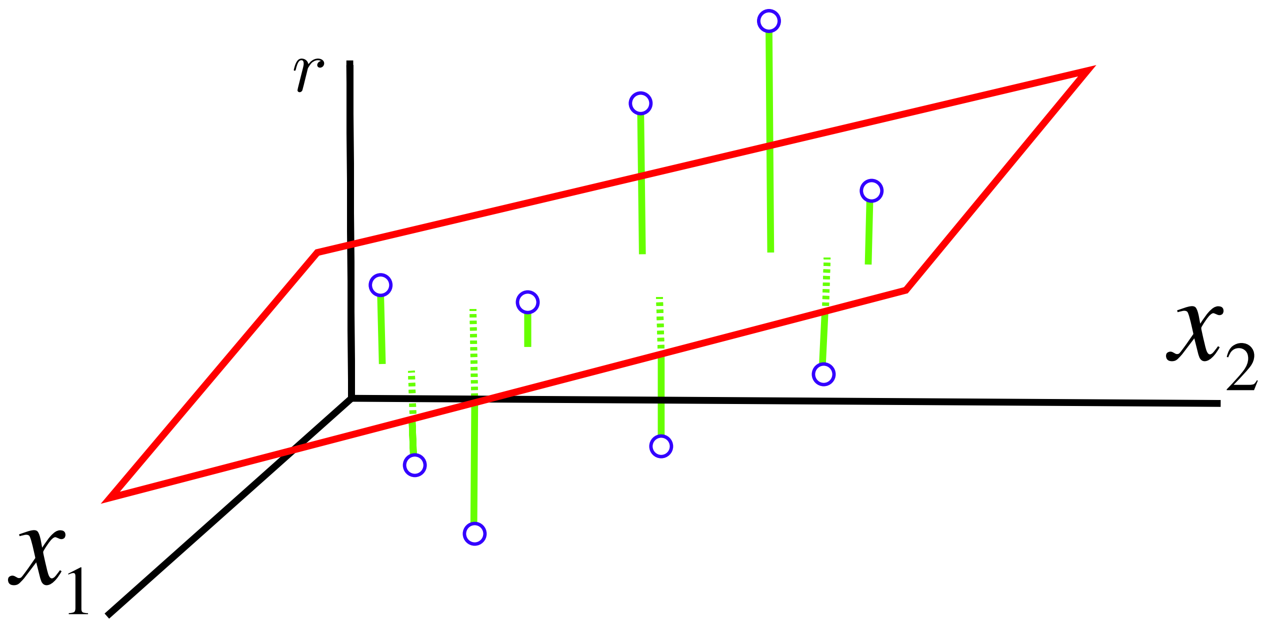
Multiple (Multivariate*) Linear Regression

- Many attributes $x_1, \ldots x_k$
- h(**x**) function is a hyperplane

*NOTE: In statistical literature, multivariate linear regression is regression with multiple outputs, and the case of multiple input variables is simply "multiple linear regression"

超平面

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



Formatting the data

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

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

There is a closed-form solution!

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

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

…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!

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

Just plug your training data into the above formula and the best hyperplane comes out!

RSS in vector/matrix notation

$$RSS(\mathbf{w}) = \sum_{i=1}^{n} (y_i - h(\mathbf{x}_i))^2$$

$$= \sum_{i=1}^{n} (y_i - w_0 - \sum_{j=1}^{k} x_{ij} w_j)^2$$

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

Deriving the formula to find w

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

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

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

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

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

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

1. X有重复的column则不可
2. 可以加入random noise to X,
3. 或者做 dimensionality reduction 消去重复columns

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

多项式

Making polynomial regression

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.....

矩阵X还是和之前一样都是1打头

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

Making polynomial regression

Given a scalar example z. We can make a k+1 dimensional example x

X的一个具体值

$$\mathbf{x} = \left\langle z^0, z^1, z^2, \ldots, z^k \right\rangle$$

The *i*th element of x is the power z^i

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

Making polynomial regression

Since $x_k \equiv z^k$ we can interpret the output of the regression as a polynomial function of z

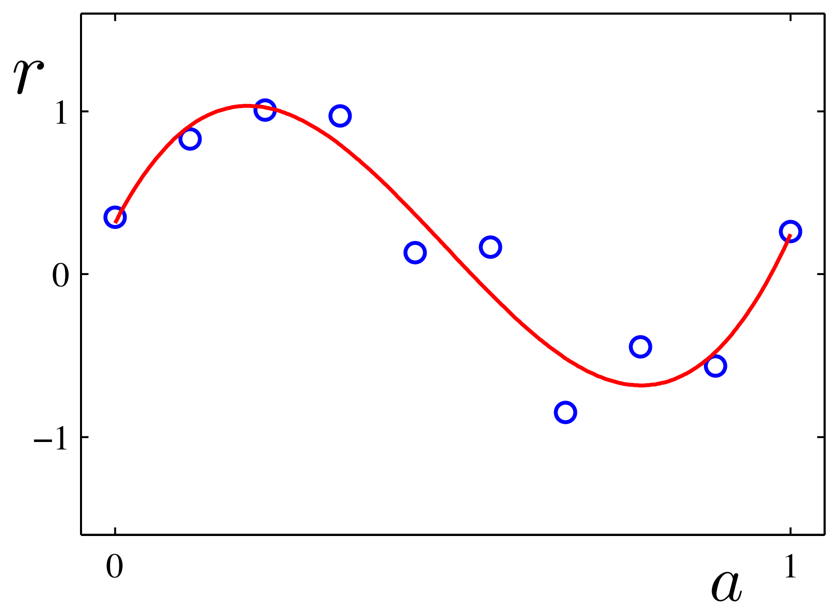
$$h(x) = w_0 + w_1 x_1 + w_2 x_2 + \ldots w_k x_k$$
$$= w_0 + w_1 z + w_2 z^2 + \ldots w_k z^k$$

Polynomial Regression

- Model the relationship between the response variable and the attributes/predictor variables as a k-th-order polynomial. While this can model non-linear functions, it is still linear with respect to the coefficients.

系数

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



Polynomial Regression

Parameter estimation (analytically minimizing sum of squared residuals):

One training example

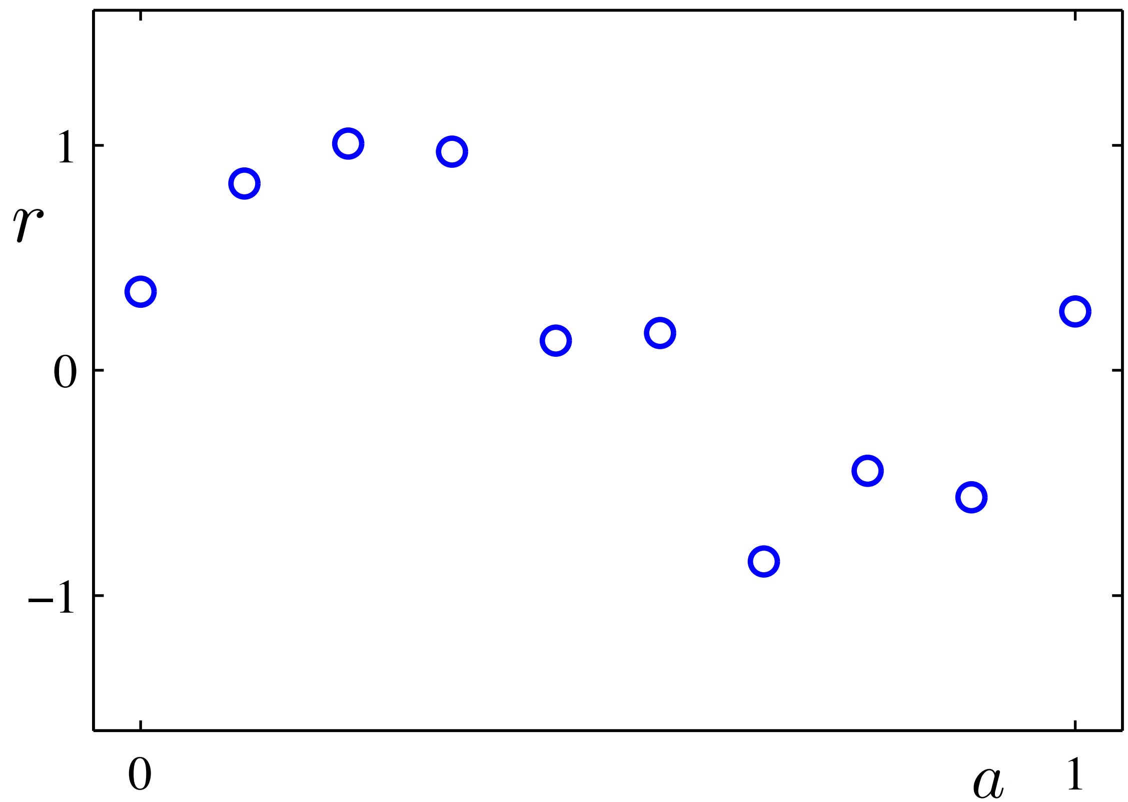
$$\mathbf{X} = \begin{bmatrix} 1 & z_1^1 & \dots & z_1^k \\ 1 & z_2^1 & \dots & z_2^k \\ \dots & \dots & \dots & \dots \\ 1 & z_n^1 & \dots & z_n^k \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix}$$

(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

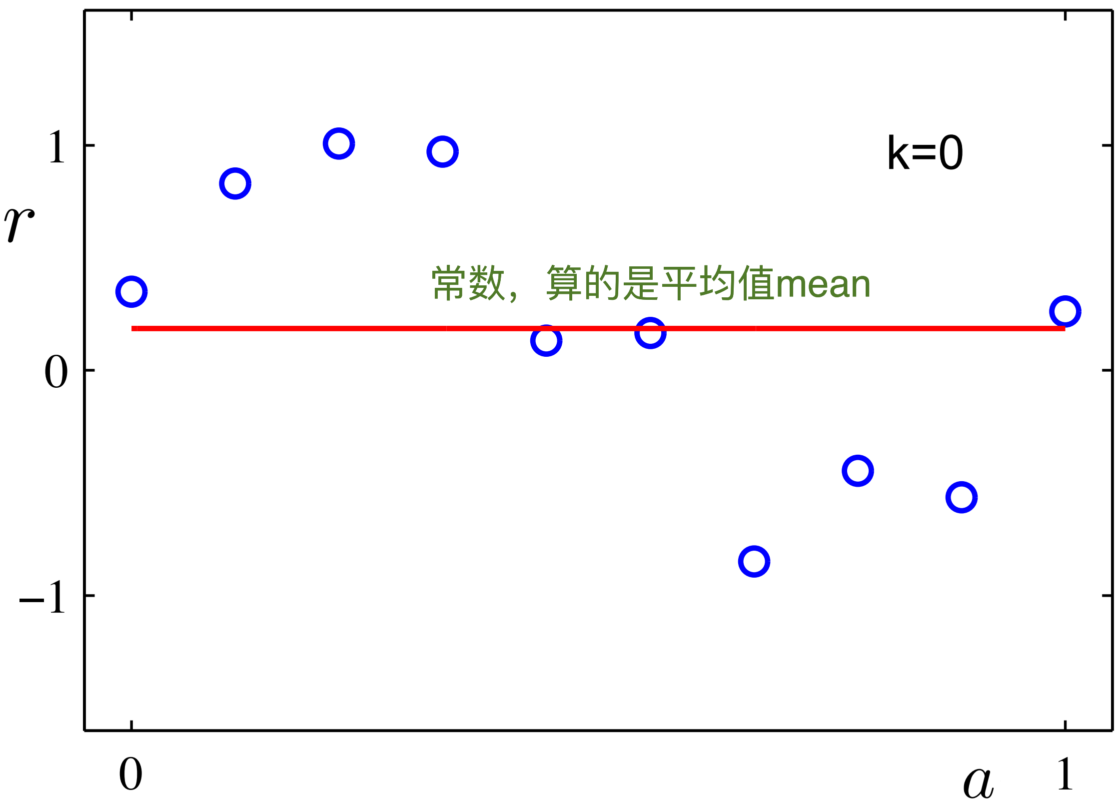
What is your hypothesis for $f(x)$?



Tuning Model Complexity: Example

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

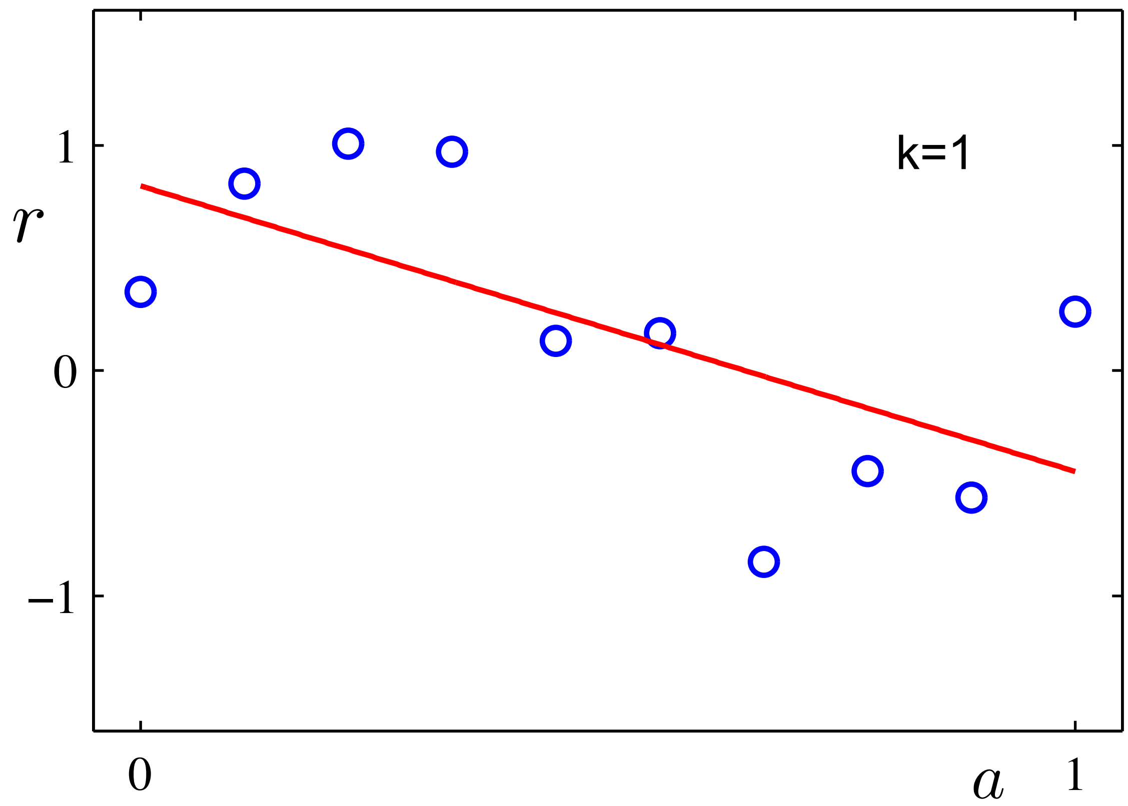
kth order polynomial regression



Tuning Model Complexity: Example

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

k^{th} order polynomial regression



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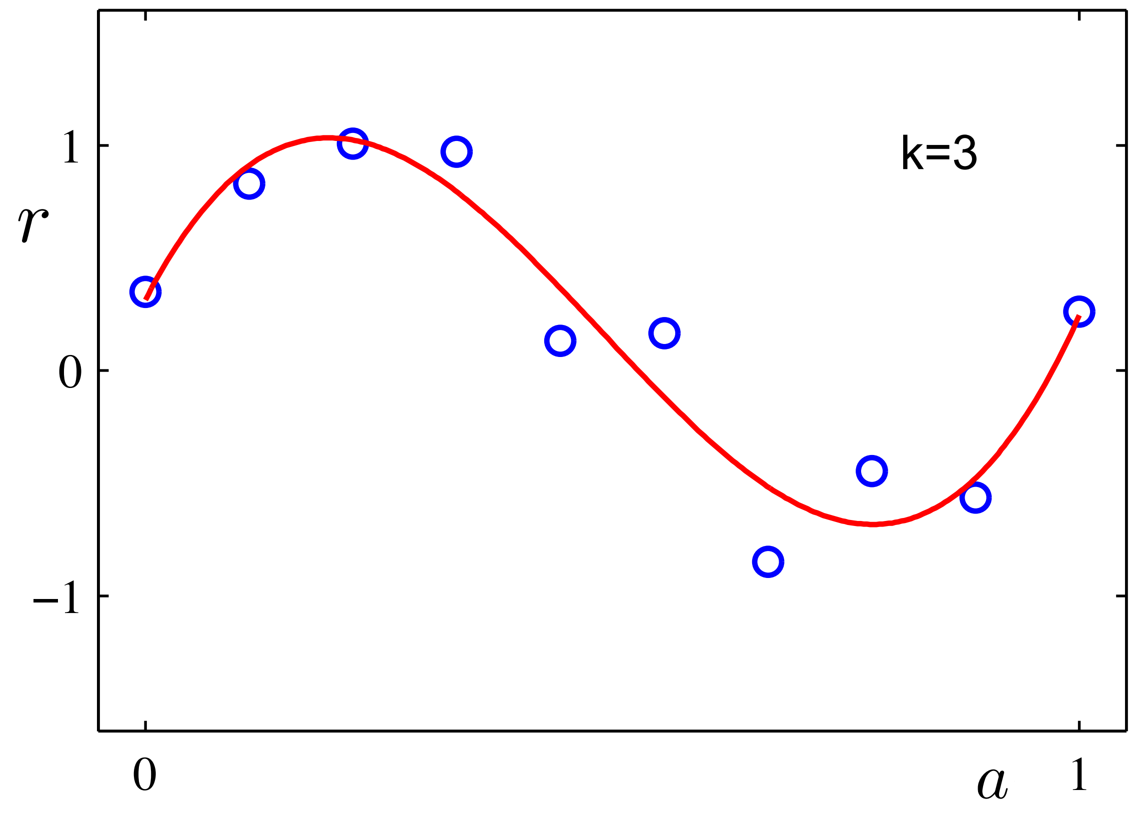

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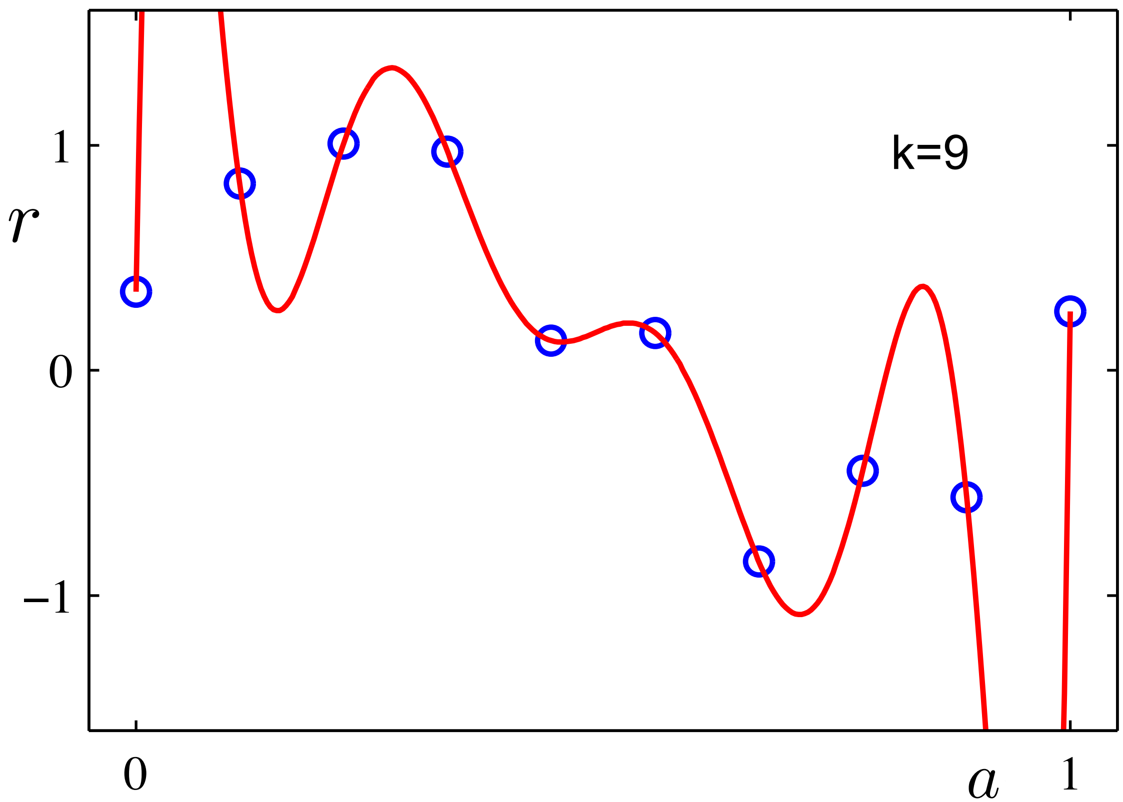
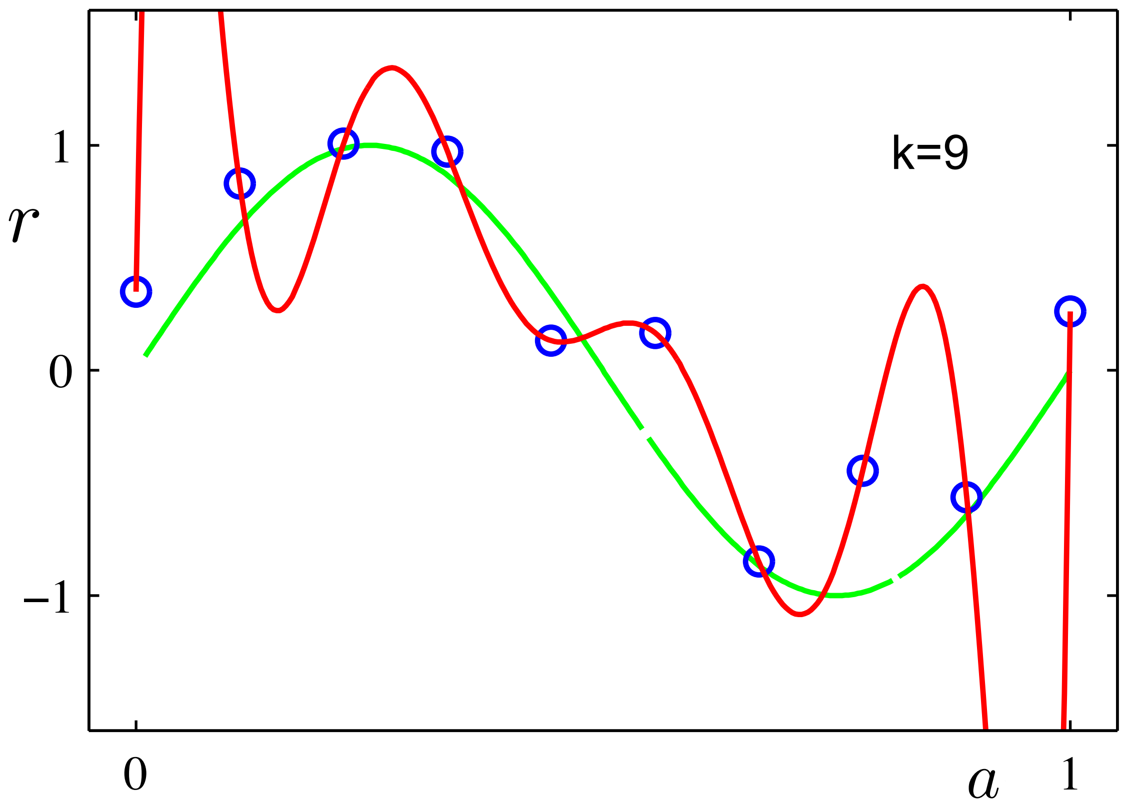


Tuning Model Complexity: Example

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

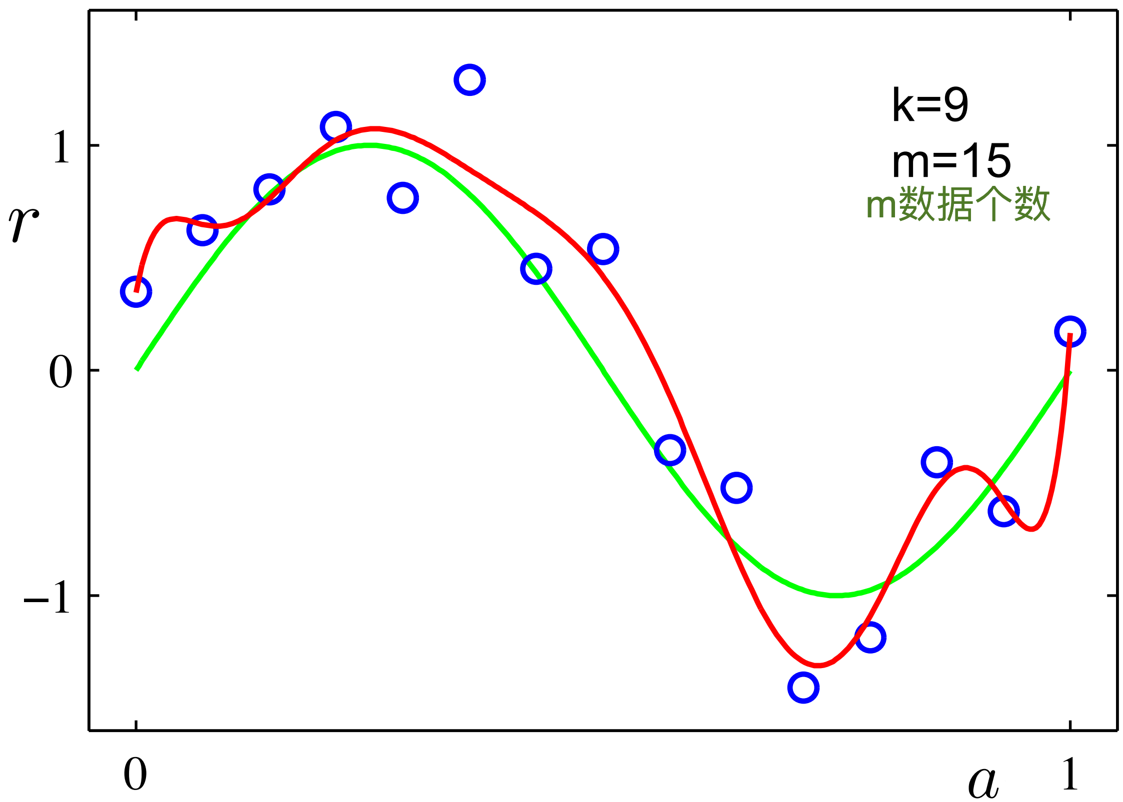
kth order polynomial regression



Tuning Model Complexity: Example

What happens if we fit to more data?

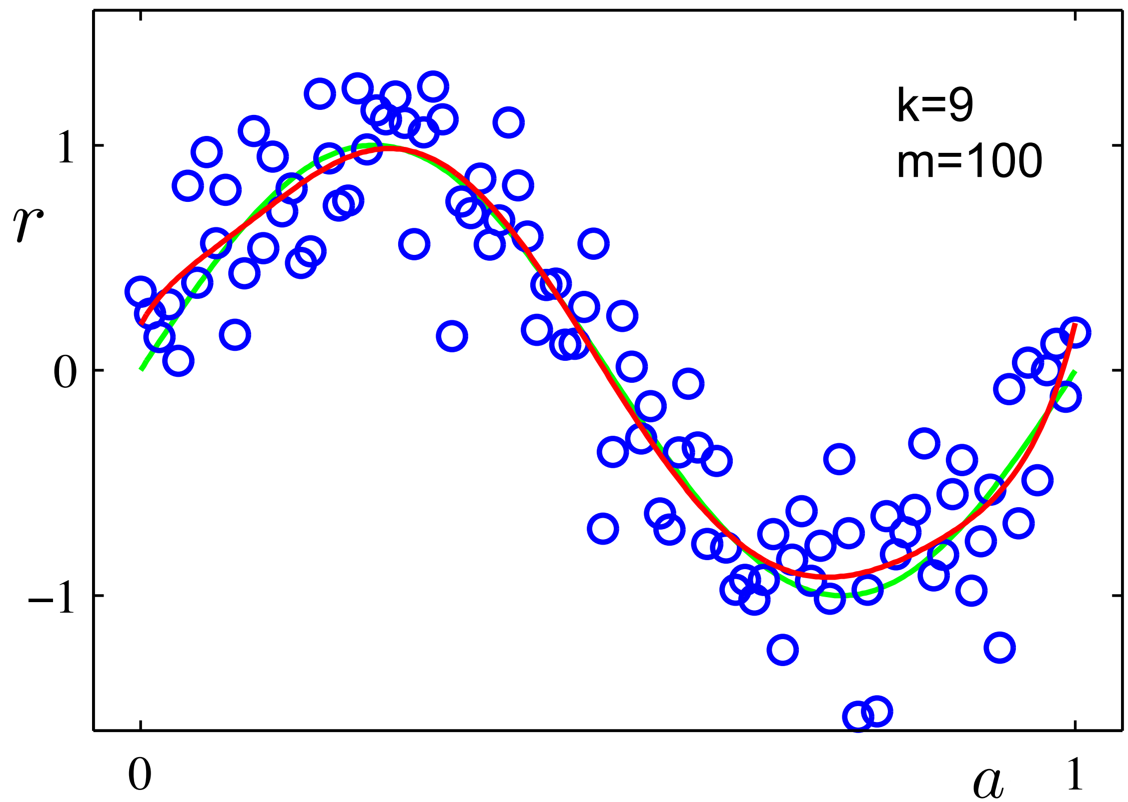
k^{th} order polynomial regression



Tuning Model Complexity: Example

What happens if we fit to more data?

k^{th} order polynomial regression



偏差 和 方差

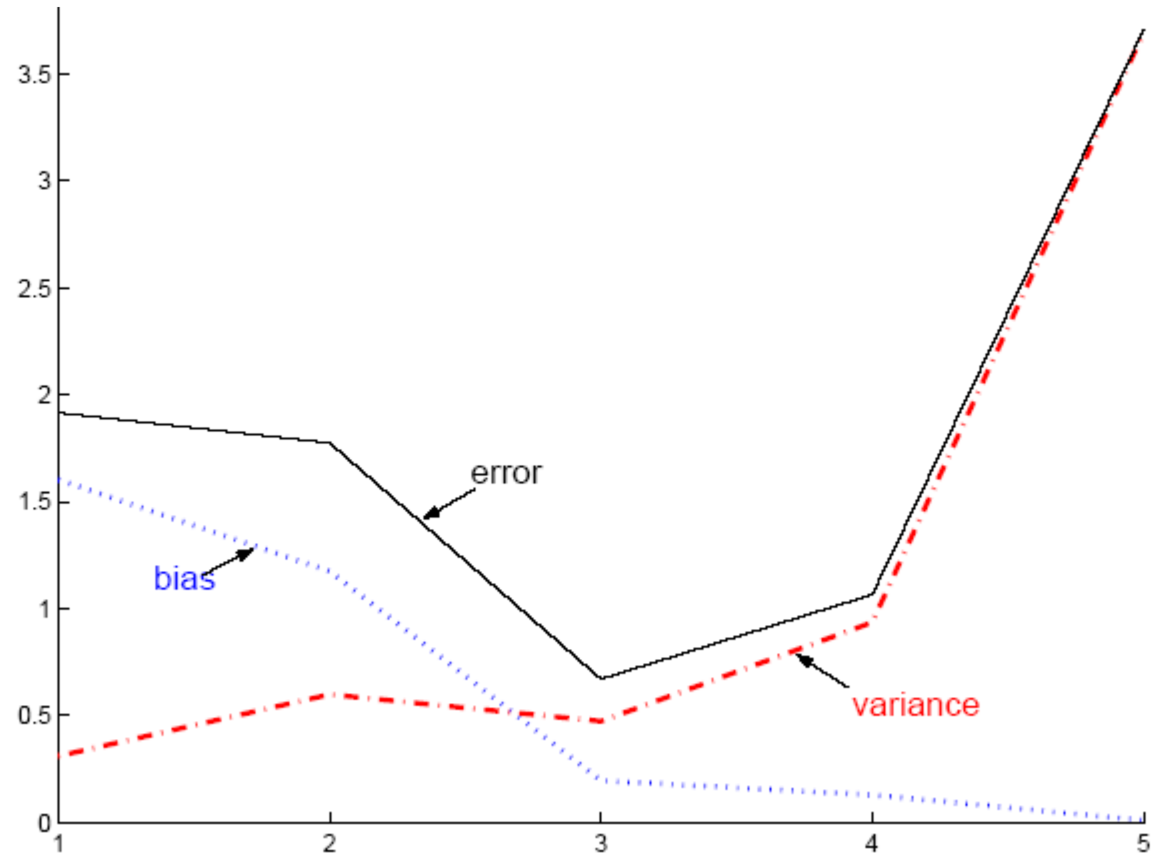
Bias and Variance of an Estimator

- 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

随着复杂度增加，bias减小（fit的更好），方差增大（估计值随着数据的变化越剧烈）

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

Bias and Variance of Hypothesis Fn

- Bias:

  忽视数据的变化，看h(x)是多么错误

  Measures how much *h(x)* is wrong disregarding the effect of varying samples (This the statistical bias of an estimator. This is NOT the same as inductive bias, which is the set of assumptions that your learner is making)

- Variance:

  h(x)值是如何随着数据不同而变化的

  Measures how much *h(x)* fluctuate around the expected value as the sample varies.

NOTE: These concepts are general machine learning concepts, not specific to linear regression.

系数

Coefficient of Determination

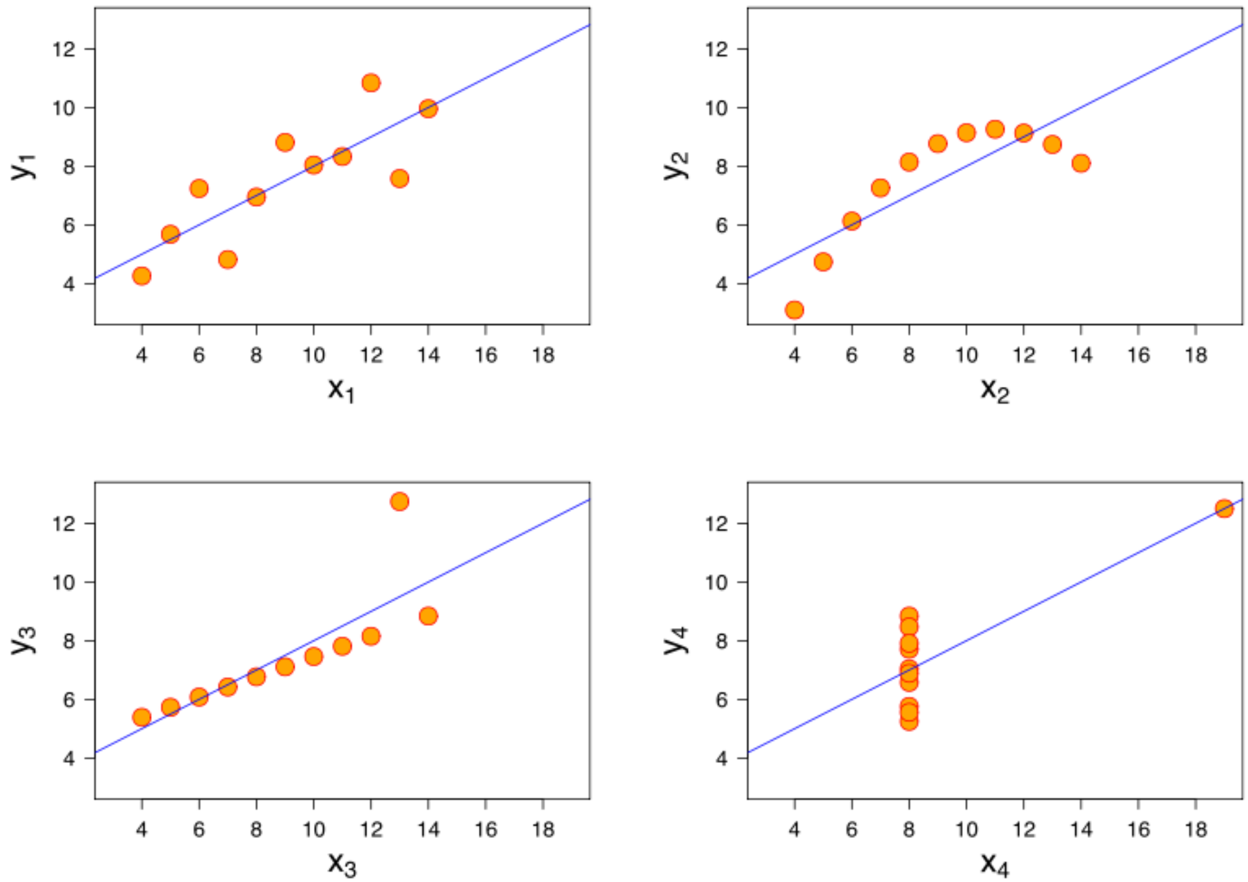
- the **coefficient of determination**, or ***R*²** indicates how well data points fit a line or curve. We'd like R^2 to be close to 1

$$R^2 = 1 - E_{RSE}$$

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

where $\overline{y}$ is the sample mean

Don't just rely on numbers, visualize!



For all 4 sets: same mean and variance for x, same mean and variance (almost) for y, and same regression line and correlation between x and y (and therefore same R-squared).

Summary of Linear Regression Models

- Easily understood
- Interpretable
- Well studied by statisticians
- Computationally efficient
- Can handle non-linear situations if formulated properly

权衡(兼顾？)

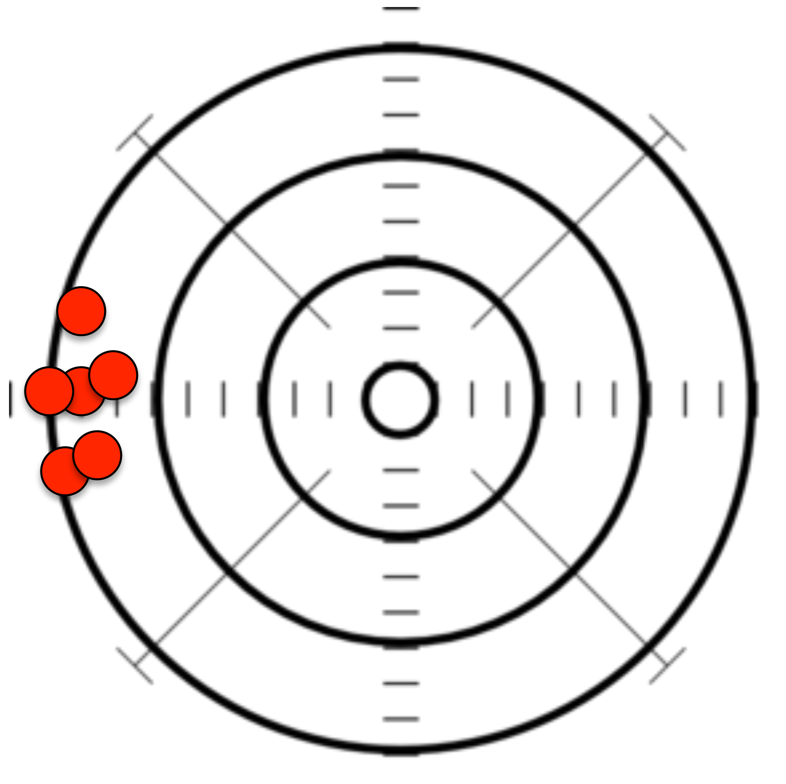
- Bias/variance tradeoff (occurs in all machine learning)
- Visualize!!
- GLMs

Appendix

(Stuff I couldn't cover in class)

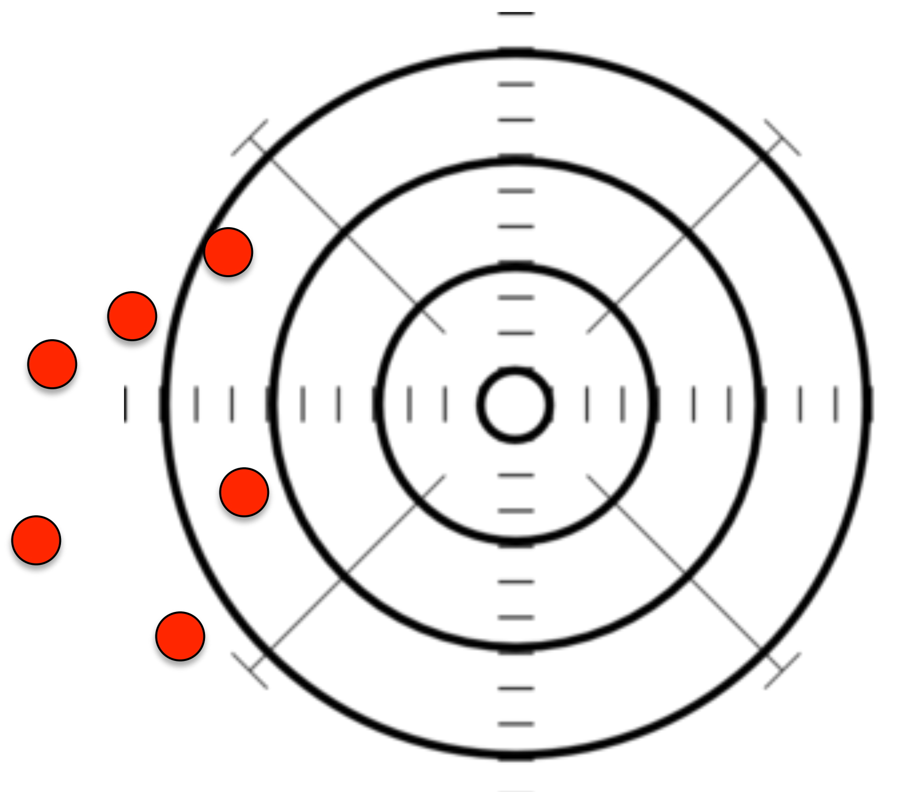
Bias and Variance

high bias, low variance



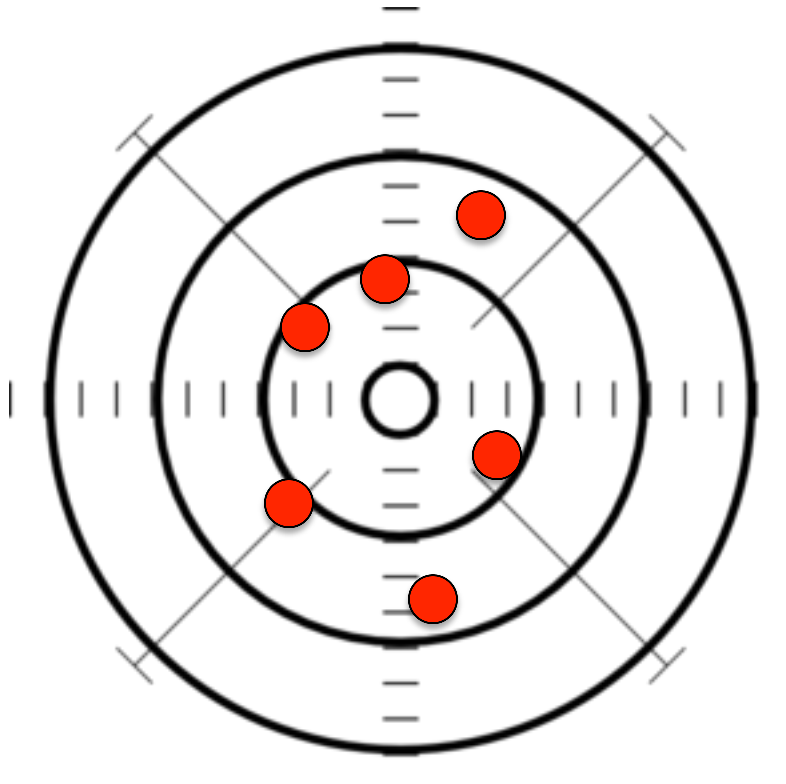
Bias and Variance

high bias, high variance



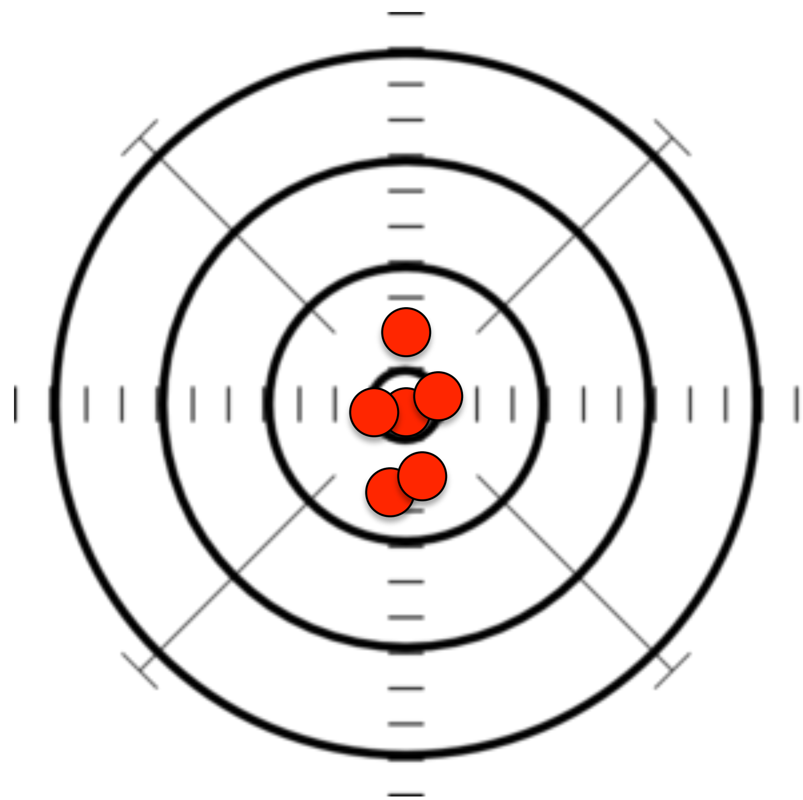
Bias and Variance

low bias, high variance



Bias and Variance

low bias, low variance



Bias and Variance

- Bias:

  Measures how much *h(x)* is wrong disregarding the effect of varying samples

  high bias → underfitting

- Variance:

  Measures how much *h(x)* fluctuate around the expected value as the sample varies.

  high variance → overfitting

There's a trade-off between bias and variance

权衡

high variance

Ways to Avoid Overfitting

- Simpler model
  - E.g. fewer parameters
- Regularization
  - penalize for complexity in objective function
- Fewer features
- Dimensionality reduction of features (e.g. PCA)
- More data…

Model Selection

例如10折交叉验证(10-fold cross validation)，将数据集分成十份，轮流将其中9份做训练1份做验证，10次的结果的均值作为对算法精度的估计，一般还需要进行多次10折交叉验证求均值，例如：10次10折交叉验证，以求更精确一点。

通过一边训练一边使用未用的数据测试来衡量generalization的精确度

- **Cross-validation**: Measure generalization accuracy by testing on data unused during training

- **Regularization**: Penalize complex models
  E′=error on data + λ model complexity
  Akaike's information criterion (AIC), Bayesian information criterion (BIC)

- **Minimum description length (MDL)**: Kolmogorov complexity, shortest description of data

- **Structural risk minimization (SRM)**

Generalized Linear Models

- Models shown have assumed that the response variable follows a Gaussian distribution around the mean 展示的model已经假设response variable服从围绕平均值的高斯分布

可以generalized to生成任何指数族分布的response variable

- Can be generalized to response variables that take on *any* exponential family distribution (Generalized Linear Models - GLMs)