

Chapter II.3

- 1. Hypothesis testing**
- 2. Linear regression**
 - 2.1. Regularizers**
 - 2.2. Model selection**
- 3. Logistic regression**
- 4. Summary**

Hypothesis testing

- Suppose we throw a coin n times and we want to estimate if the coin is fair, i.e. if $\Pr(\text{heads}) = \Pr(\text{tails})$.
- Let $X_1, X_2, \dots, X_n \sim \text{Bernoulli}(p)$ be the i.i.d. coin flips
 - Coin is fair $\Leftrightarrow p = 1/2$
- Let the **null hypothesis** H_0 be “coin is fair”.
- The **alternative hypothesis** H_1 is then “coin is not fair”
- Intuitively, if $|n^{-1} \sum_i X_i - 1/2|$ is large, we should reject the null hypothesis
- *But can we formalize this?*

Hypothesis testing terminology

- $\theta = \theta_0$ is called **simple hypothesis**
- $\theta > \theta_0$ or $\theta < \theta_0$ is called **composite hypothesis**
- $H_0: \theta = \theta_0$ vs. $H_1: \theta \neq \theta_0$ is called **two-sided test**
- $H_0: \theta \leq \theta_0$ vs. $H_1: \theta > \theta_0$ and $H_0: \theta \geq \theta_0$ vs. $H_1: \theta < \theta_0$ are called **one-sided tests**
- **Rejection region** R : if $X \in R$, reject H_0 o/w retain H_0
 - Typically $R = \{x : T(x) > c\}$ where T is a **test statistic** and c is a **critical value**

- **Error types:**

	Retain H_0	Reject H_0
H_0 true	✓	type I error
H_1 true	type II error	✓

The p -values

- The p -value is the *probability that **if H_0 holds**, we observe values at least as extreme as the test statistic*
 - It is *not* the probability that H_0 holds
 - If p -value is small enough, we can reject H_0
 - How small is small enough depends on application
- Typical p -value scale:

p -value	evidence
< 0.01	very strong evidence against H_0
$0.01\text{--}0.05$	strong evidence against H_0
$0.05\text{--}0.1$	weak evidence against H_0
> 0.1	little or no evidence against H_0

The Wald test

For two-sided test $H_0: \theta = \theta_0$ vs. $H_1: \theta \neq \theta_0$

Test statistic $W = \frac{\hat{\theta} - \theta_0}{\hat{se}}$, where $\hat{\theta}$ is the sample estimate and

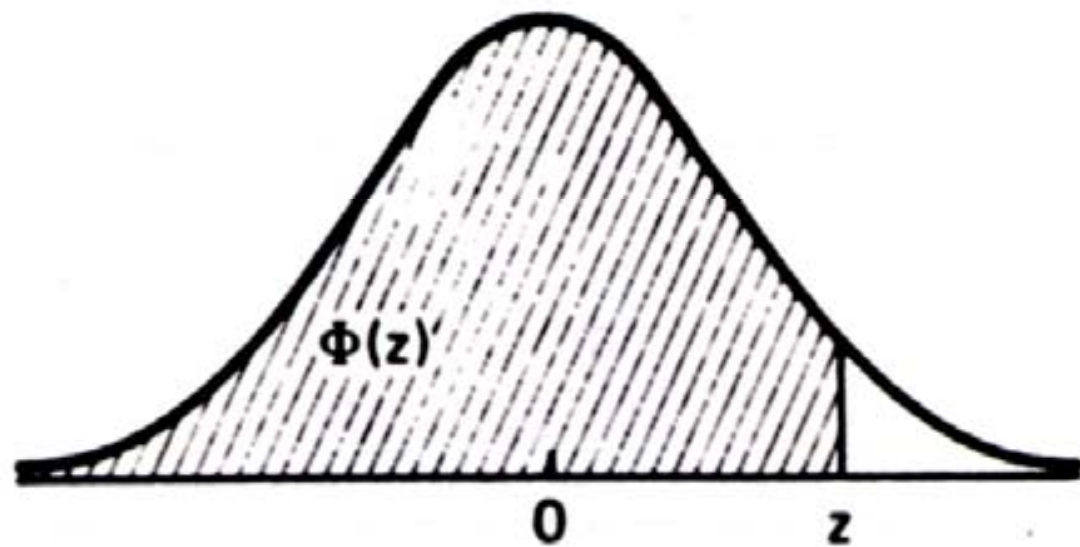
$\hat{se} = se(\hat{\theta}) = \sqrt{\text{Var}[\hat{\theta}]}$ is the standard error.

W converges in probability to $N(0,1)$.

If w is the observed value of Wald statistic, the p -value is $2\Phi(-|w|)$.

The coin-tossing example revisited

Using Wald test we can test if our coin is fair. Suppose the observed average is 0.6 with estimated standard error 0.049. The observed Wald statistic w is now $w = (0.6 - 0.5)/0.049 \approx 2.04$. Therefore the p -value is $2\Phi(-2.04) \approx 0.041$, and we have strong evidence to reject the null hypothesis.



The χ^2 distribution

Let X_1, X_2, \dots, X_n be i.i.d. $N(0,1)$ distributed random variables.

The random variable $\chi_n^2 = \sum_{i=1}^n X_i^2$
is χ^2 -distributed with n degrees of freedom.

$$f(x) = \frac{x^{(n/2)-1} e^{-x/2}}{2^{n/2} \Gamma(n/2)} \quad \text{for } x > 0$$

$$E[x] = n$$

$$\text{Var}[x] = 2n$$

Pearson's χ^2 test for multinomial data

If $X = (X_1, X_2, \dots, X_k)$ has Multinomial(n, \mathbf{p}) distribution, then MLE of \mathbf{p} is $(X_1/n, X_2/n, \dots, X_k/n)$. Let $\mathbf{p}_0 = (p_{01}, p_{02}, \dots, p_{0k})$ and we want to test $H_0: \mathbf{p} = \mathbf{p}_0$ vs. $H_1: \mathbf{p} \neq \mathbf{p}_0$.

Pearson's χ^2 statistic is

$$T = \sum_{j=1}^k \frac{(X_j - np_{0j})^2}{np_{0j}} = \sum_{j=1}^k \frac{(X_j - E_j)^2}{E_j}$$

where $E_j = E[X_j] = np_{0j}$ is the expected value of X_j under H_0 .

The p -value is $\Pr(\chi_{k-1}^2 > t)$ where t is the observed value of T .

Extending Pearson to non-multinomial

- Pearson's χ^2 can be used to test the fitness of sample to *any* distribution (goodness-of-fit test)
- Let X_1, X_2, \dots, X_n be the sample and $f(x; \theta)$ some probability distribution with parameters θ
- Divide the possible values of X_i s (under the null hypothesis) into k disjoint intervals and let O_j be the number of times we see value in interval I_j
- Compute the theoretical interval frequencies $p_j(\theta) = \int_{I_j} f(x; \theta) dx$
- Obtain estimates $\tilde{\theta}$ by maximizing

$$Q(\theta) = \prod_{j=1}^k p_j(\theta)^{O_j}$$

- Now the multinomial χ^2 test applies with $k-1-s$ degrees of freedom, where s is the number of parameters in θ

Extending Pearson to test of independence

- Pearson's χ^2 can also be used to test the independence of two variables
- Let X_1, X_2, \dots, X_n and Y_1, Y_2, \dots, Y_n be two samples
- Divide the outcomes into r (for X_i s) and c disjoint intervals and compute the frequencies
- Populate r -by- c table O with the frequencies (O_{lk} tells how many (X_i, Y_i) pairs have values from l th and k th interval, respectively)
- Assuming independency, the expected value for O_{lk} is

$$E_{lk} = \frac{\sum_{j=1}^c O_{lj} \sum_{i=1}^r O_{ik}}{\sum_{i=1}^r \sum_{j=1}^c O_{ij}}$$

- The value of the test statistic is $\chi^2 = \sum_{i=1}^r \sum_{j=1}^c \frac{(O_{ij} - E_{ij})^2}{E_{ij}}$
- There are $(r-1)(c-1)$ degrees of freedom

χ^2 distribution table

1.1.2.10. Obere 100 α -prozentige Werte χ^2_α der χ^2 -Verteilung (s. 5.2.3.)

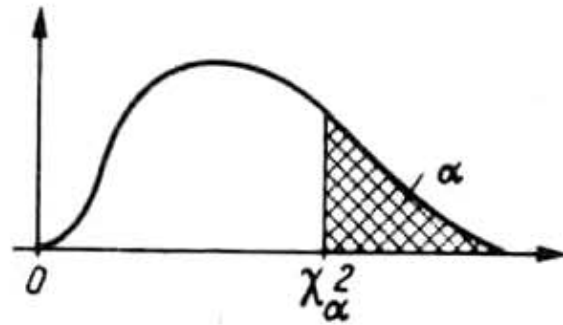


Abb. 1.4

Anzahl der Freiheitsgrade m	Wahrscheinlichkeit $p = \alpha$															
	0,99	0,98	0,95	0,90	0,80	0,70	0,50	0,30	0,20	0,10	0,05	0,02	0,01	0,005	0,002	0,001
1	0,00016	0,0006	0,0039	0,016	0,064	0,148	0,455	1,07	1,64	2,7	3,8	5,4	6,6	7,9	9,5	10,83
2	0,020	0,040	0,103	0,211	0,446	0,713	1,386	2,41	3,22	4,6	6,0	7,8	9,2	10,6	12,4	13,8
3	0,115	0,185	0,352	0,584	1,005	1,424	2,366	3,67	4,64	6,3	7,8	9,8	11,3	12,8	14,8	16,3
4	0,30	0,43	0,71	1,06	1,65	2,19	3,36	4,9	6,0	7,8	9,5	11,7	13,3	14,9	16,9	18,5
5	0,55	0,75	1,14	1,61	2,34	3,00	4,35	6,1	7,3	9,2	11,1	13,4	15,1	16,8	18,9	20,5
6	0,87	1,13	1,63	2,20	3,07	3,83	5,35	7,2	8,6	10,6	12,6	15,0	16,8	18,5	20,7	22,5
7	1,24	1,56	2,17	2,83	3,82	4,67	6,35	8,4	9,8	12,0	14,1	16,6	18,5	20,3	22,6	24,3
8	1,65	2,03	2,73	3,49	4,59	5,53	7,34	9,5	11,0	13,4	15,5	18,2	20,1	22,0	24,3	26,1
9	2,09	2,53	3,32	4,17	5,38	6,39	8,34	10,7	12,2	14,7	16,9	19,7	21,7	23,6	26,1	27,9
10	2,56	3,06	3,94	4,86	6,18	7,27	9,34	11,8	13,4	16,0	18,3	21,2	23,2	25,2	27,7	29,6
11	3,1	3,6	4,6	5,6	7,0	8,1	10,3	12,9	14,6	17,3	19,7	22,6	24,7	26,8	29,4	31,3
12	3,6	4,2	5,2	6,3	7,8	9,0	11,3	14,0	15,8	18,5	21,0	24,1	26,2	28,3	30,9	32,9
13	4,1	4,8	5,9	7,0	8,6	9,9	12,3	15,1	17,0	19,8	22,4	25,5	27,7	29,8	32,5	34,5
14	4,7	5,4	6,6	7,8	9,5	10,8	13,3	16,2	18,2	21,1	23,7	26,9	29,1	31,3	34,0	36,1
15	5,2	6,0	7,3	8,5	10,3	11,7	14,3	17,3	19,3	22,3	25,0	28,3	30,6	32,8	35,6	37,7
16	5,8	6,6	8,0	9,3	11,2	12,6	15,3	18,4	20,5	23,5	26,3	29,6	32,0	34,3	37,1	39,3
17	6,4	7,3	8,7	10,1	12,0	13,5	16,3	19,5	21,6	24,8	27,6	31,0	33,4	35,7	38,6	40,8
18	7,0	7,9	9,4	10,9	12,9	14,4	17,3	20,6	22,8	26,0	28,9	32,3	34,8	37,2	40,1	42,3
19	7,6	8,6	10,1	11,7	13,7	15,4	18,3	21,7	23,9	27,2	30,1	33,7	36,2	38,6	41,6	43,8
20	8,3	9,2	10,9	12,4	14,6	16,3	19,3	22,8	25,0	28,4	31,4	35,0	37,6	40,0	43,0	45,3
21	8,9	9,9	11,6	13,2	15,4	17,2	20,3	23,9	26,2	29,6	32,7	36,3	38,9	41,4	44,5	46,8
22	9,5	10,6	12,3	14,0	16,3	18,1	21,3	24,9	27,3	30,8	33,9	37,7	40,3	42,8	45,9	48,3
23	10,2	11,3	13,1	14,8	17,2	19,0	22,3	26,0	28,4	32,0	35,2	39,0	41,6	44,2	47,3	49,7
24	10,9	12,0	13,8	15,7	18,1	19,9	23,3	27,1	29,6	33,2	36,4	40,3	43,0	45,6	48,7	51,2
25	11,5	12,7	14,6	16,5	18,9	20,9	24,3	28,2	30,7	34,4	37,7	41,6	44,3	46,9	50,1	52,6
26	12,2	13,4	15,4	17,3	19,8	21,8	25,3	29,2	31,8	35,6	38,9	42,9	45,6	48,3	51,6	54,1
27	12,9	14,1	16,2	18,1	20,7	22,7	26,3	30,3	32,9	36,7	40,1	44,1	47,0	49,6	52,9	55,5
28	13,6	14,8	16,9	18,9	21,6	23,6	27,3	31,4	34,0	37,9	41,3	45,4	48,3	51,0	54,4	56,9

Testing with implicit distribution

- Suppose we have found association rule “diapers” \Rightarrow “beer” with confidence 0.9
 - I.e. $E[\text{“}x \text{ buys beer”} \mid \text{“}x \text{ buys diapers”}] = 0.9$ in the sample
- Possible explanation: everybody buys beer
 - Result is not interesting
 - also “vegetables” \Rightarrow “beer” has high confidence, etc.
 - Null hypothesis: “Result is due to the fact that (almost) everybody buys beer”
- How can we test that?

Testing “diapers” \Rightarrow “beer”, part 1

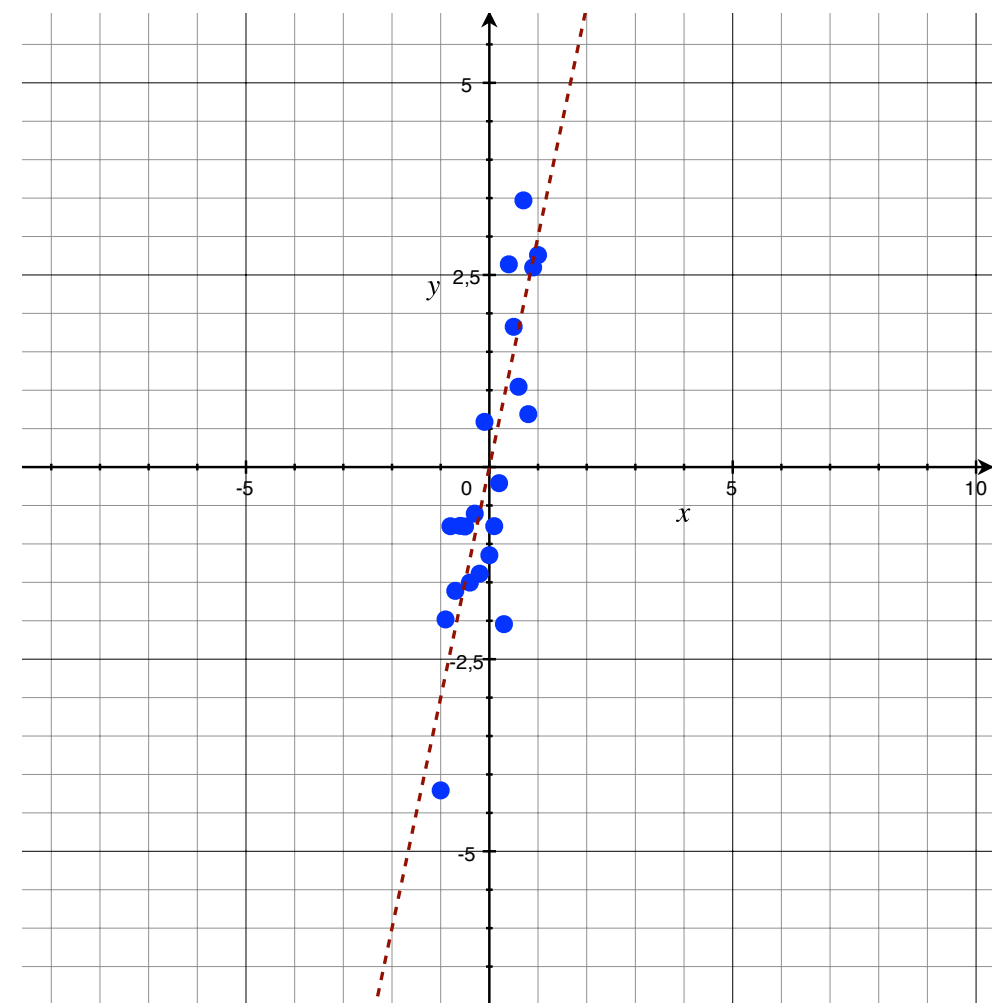
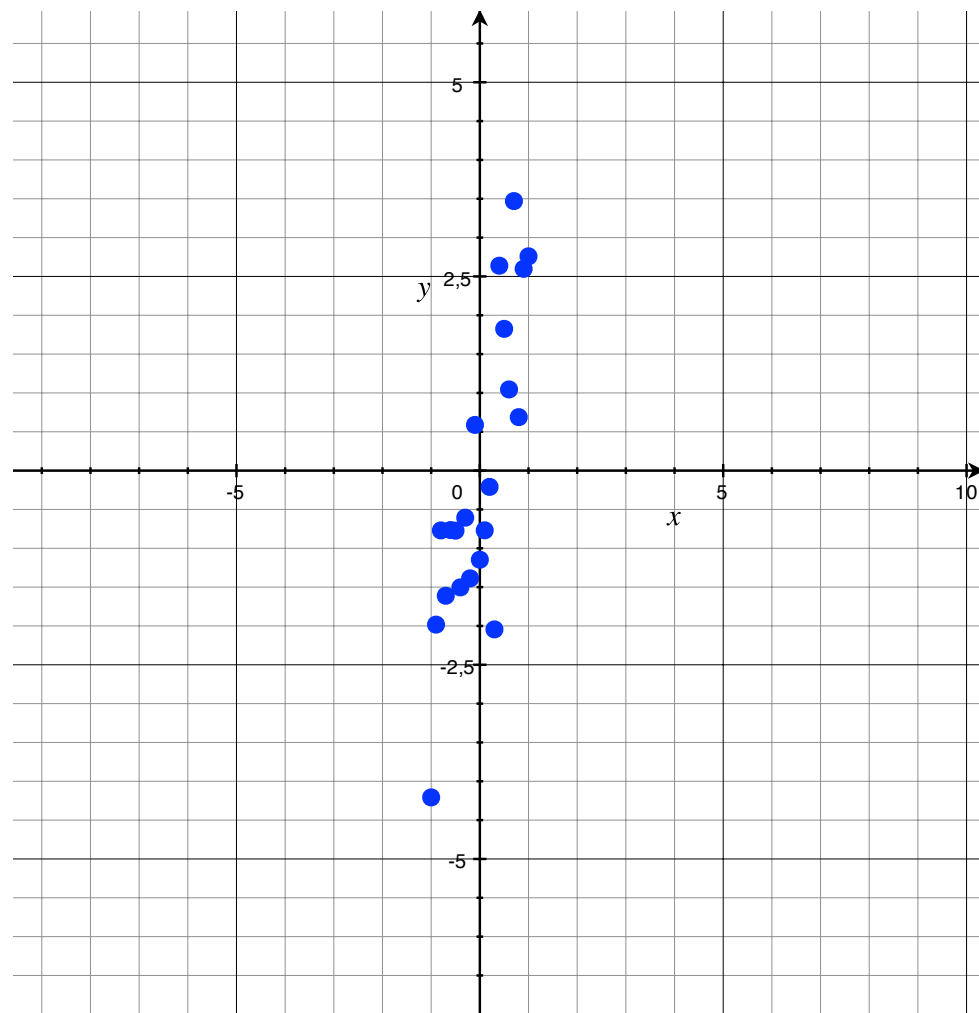
- The idea: generate data sets that have similar properties to the real data, but are random
 - See how good your result is in these random data sets
 - Let N be the number of data sets and M the number of times the result is at least as good in random data than it is in the real data
 - The empirical p -value is then $(M + 1)/(N + 1)$
- Independent random data:
 - Data is n -by- m (m items) binary matrix
 - Let \mathbf{c} be m -dimensional vector of column margins
 - Make random matrix (a_{ij}) by sampling $a_{ij} \sim \text{Bernoulli}(c_j)$

Testing “diapers” \Rightarrow “beer”, part 2

- Independent random samples have estimated column margins \mathbf{c}
- They do not take into account that some people buy many different things while others buy only few
 - Compute also row margins \mathbf{r}
- Let $\mathcal{M}(\mathbf{r}, \mathbf{c})$ be a family of 0/1 matrices with row margin \mathbf{r} and column margin \mathbf{c}
 - Sample u.a.r. from this family and test in that sample
- Problem: how to sample efficiently
 - In this case solution is known (so-called swap randomization)

Linear Regression

- Fit a line to a set of observation points



Intermission: basic linear algebra

A *linear combination* of n vectors \mathbf{v}_i is $\mathbf{w} = \sum_{i=1}^n \alpha_i \mathbf{v}_i$

A set of vectors $V = \{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n\}$ is *linearly independent* if no vector $\mathbf{v} \in V$ can be written as a linear combination of vectors of $V \setminus \{\mathbf{v}\}$. Otherwise V is *linearly dependent*.

The vector *inner product* of two vectors is $\langle \mathbf{v}, \mathbf{w} \rangle = \sum_{i=1}^n v_i w_i$

The vector *outer product* of n - and m -dimensional (row) vectors \mathbf{v} and \mathbf{w} is n -by- m matrix $\mathbf{v}^T \mathbf{w} = (a_{ij})$ where $a_{ij} = v_i w_j$.

Intermission: basic linear algebra

The product of n -by- k matrix A and k -by- m matrix B is the n -by- m matrix (c_{ij}) with $c_{ij} = \sum_{l=1}^k a_{il} b_{lj}$.

The column rank of matrix M is the number of linearly independent columns of M . The row rank is the number of linearly independent rows.

Fact. The row and column rank of n -by- m real matrix M are the same and called the *rank* of M . Hence $\text{rank}(M) \leq \min(n, m)$.

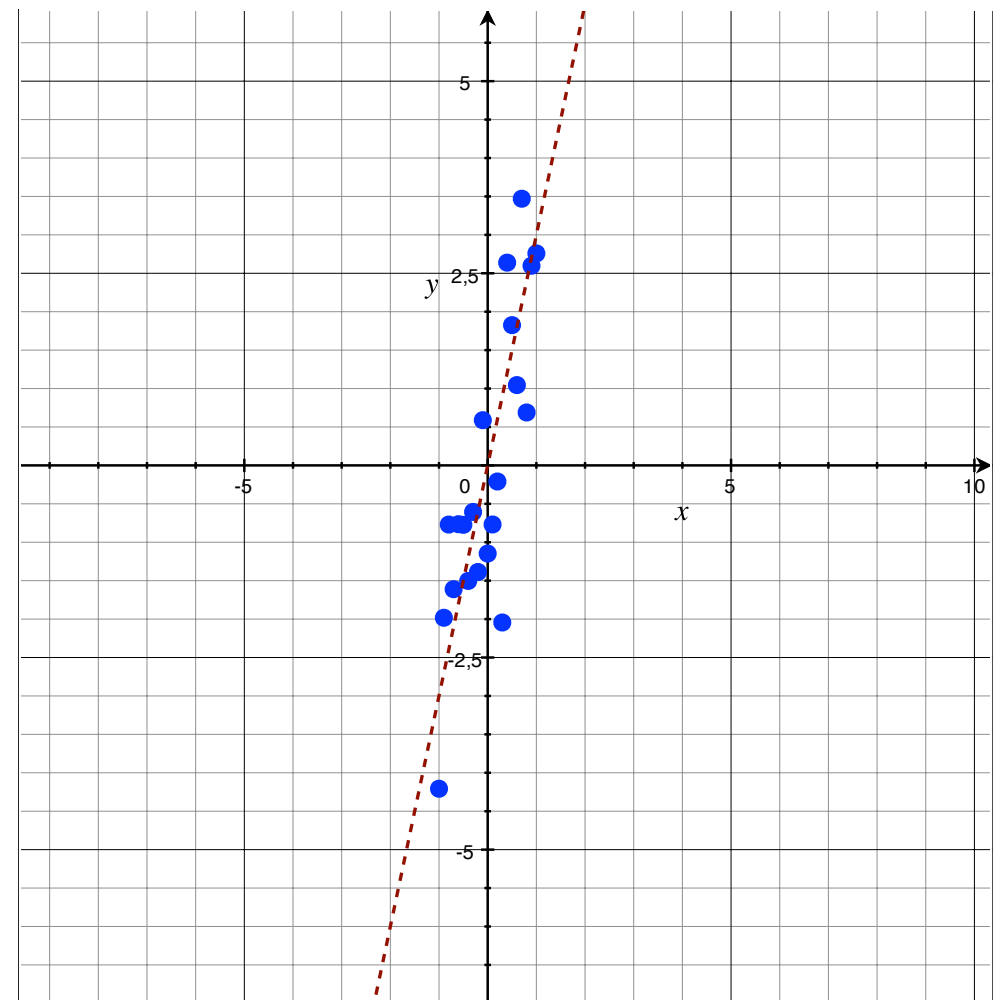
The *inverse* of an n -by- n square matrix A , if exists, is the unique n -by- n matrix B for which $AB = I$, where I is the n -by- n identity matrix. The inverse of A is denoted by A^{-1} .

An n -by- n matrix A is *invertible* (i.e. has inverse) iff $\text{rank}(A) = n$.

Single-variable case

- A simple case with one variable
 - vector \mathbf{y} is called the **response** variables (or *regressands*)
 - vector \mathbf{x} is called the **predictor** variables (or *regressors*)
 - constant β is called the **parameter**
 - random variable ε is called the **error**

$$\mathbf{y} = \beta \mathbf{x} + \varepsilon$$

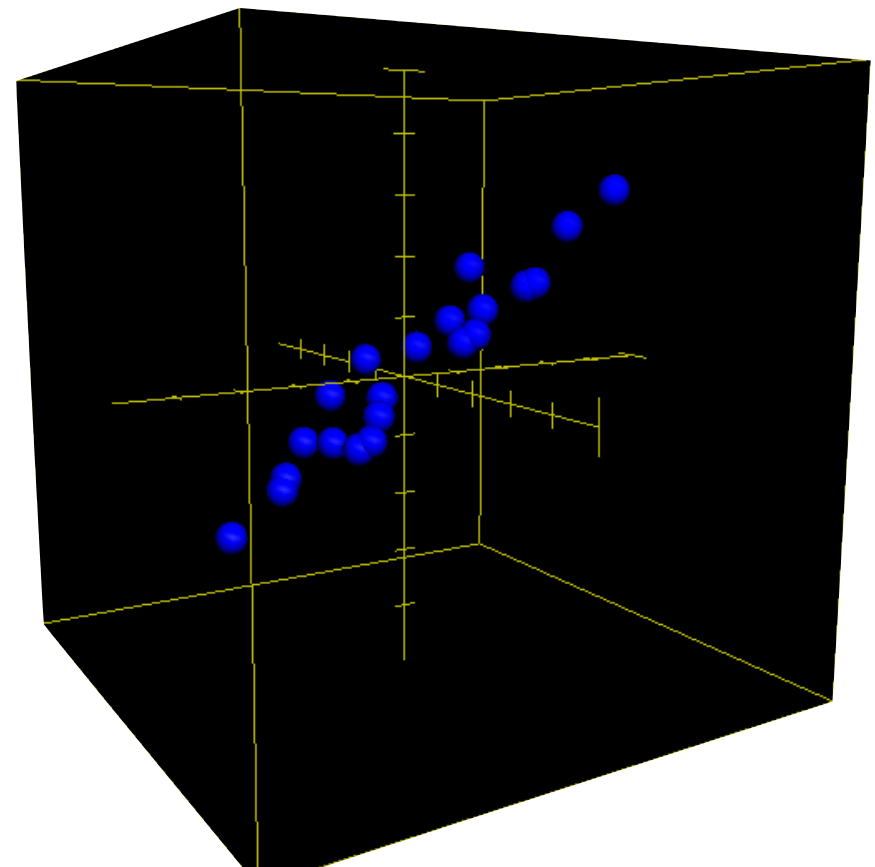


Multi-dimensional case

- The regressors are multi-dimensional
- Each regressor is a row of **design matrix** X
- Parameters form a vector β , and errors form a vector ε
 - n respond variables and errors, k parameters, X is n -by- k

$$y = X\beta + \varepsilon$$

$$y_i = \sum_{j=1}^k x_{ij} \beta_j + \varepsilon_i$$

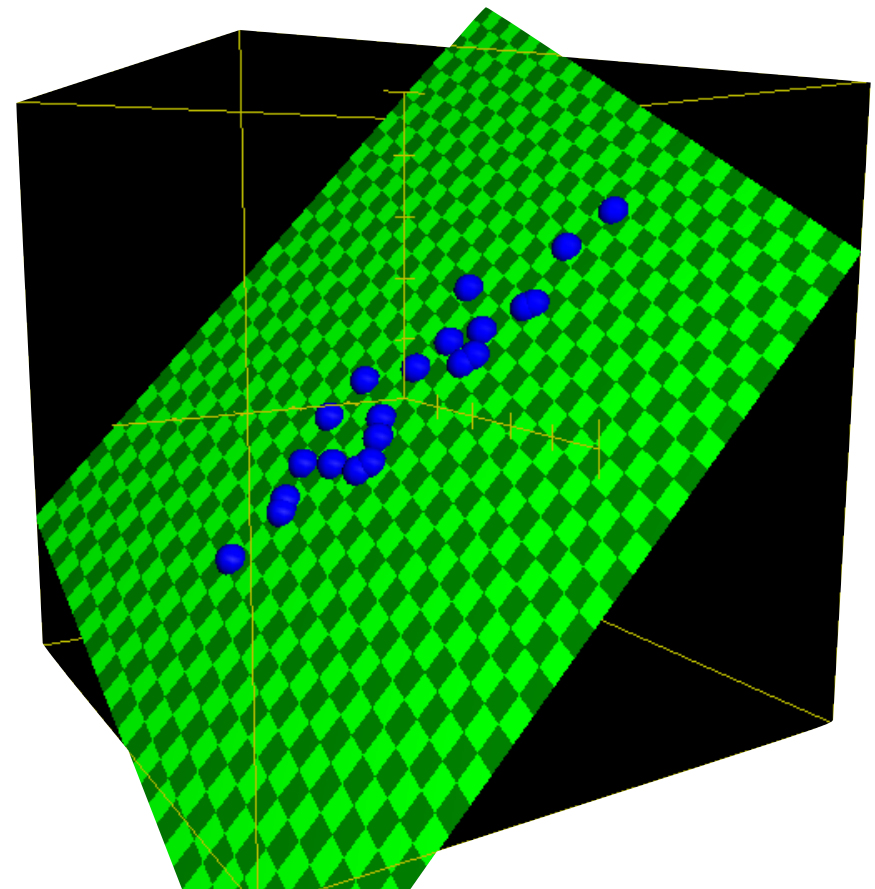


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Important assumptions

- The design matrix must have full column rank
 - $\text{rank}(X) \geq k$
 - $n \geq k$ is a necessary but not sufficient condition
 - “There has to be enough data per parameter”
- The i.i.d. errors ε_i are $\mathbf{N}(0, \sigma^2)$ distributed
 - With this assumption ordinary least squares matches maximum likelihood estimation
- The assumptions on errors can be weakened
 - Uncorrelated only conditional to regressors
 - Mean and variance only conditional to regressors

Ordinary least squares linear regression

Problem. Find $\boldsymbol{\beta}$ that minimize

$$\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 = \sum_{i=1}^n \left(y_i - \sum_{j=1}^k x_{ij} \beta_j \right)^2$$

Solution. Estimate $\boldsymbol{\beta}$ with

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

The fitted values of \mathbf{y} are

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$$

Some comments on OLS

- The matrix $X^\dagger = (X^T X)^{-1} X^T$ is the *Moore–Penrose pseudo-inverse* of X
 - The full column rank of X is required for $(X^T X)$ to be invertible (HW)
 - Alternatively, the full column rank guarantees unique solutions
- **Fact:** The Moore–Penrose pseudo-inverse is the least-squares solution to linear program $y = X\beta$
 - I.e. setting $\beta = X^\dagger y$ minimizes the squared error, as supposed
 - If X is invertible, $X^\dagger = X^{-1}$, as supposed (HW)

The intercept

- So far we have considered through-the-origin regression
 - The fitted line crosses the origin
- Usually we add an *intercept* β_0

$$y_i = \sum_{j=1}^k x_{ij} \beta_j + \beta_0 + \varepsilon_i$$

- To simplify notation, this is done by adding an extra column full of 1s to X

$$y_i = \sum_{j=0}^k x_{ij} \beta_j + \varepsilon_i \quad \text{where } x_{i0} = 1 \text{ for all } i$$

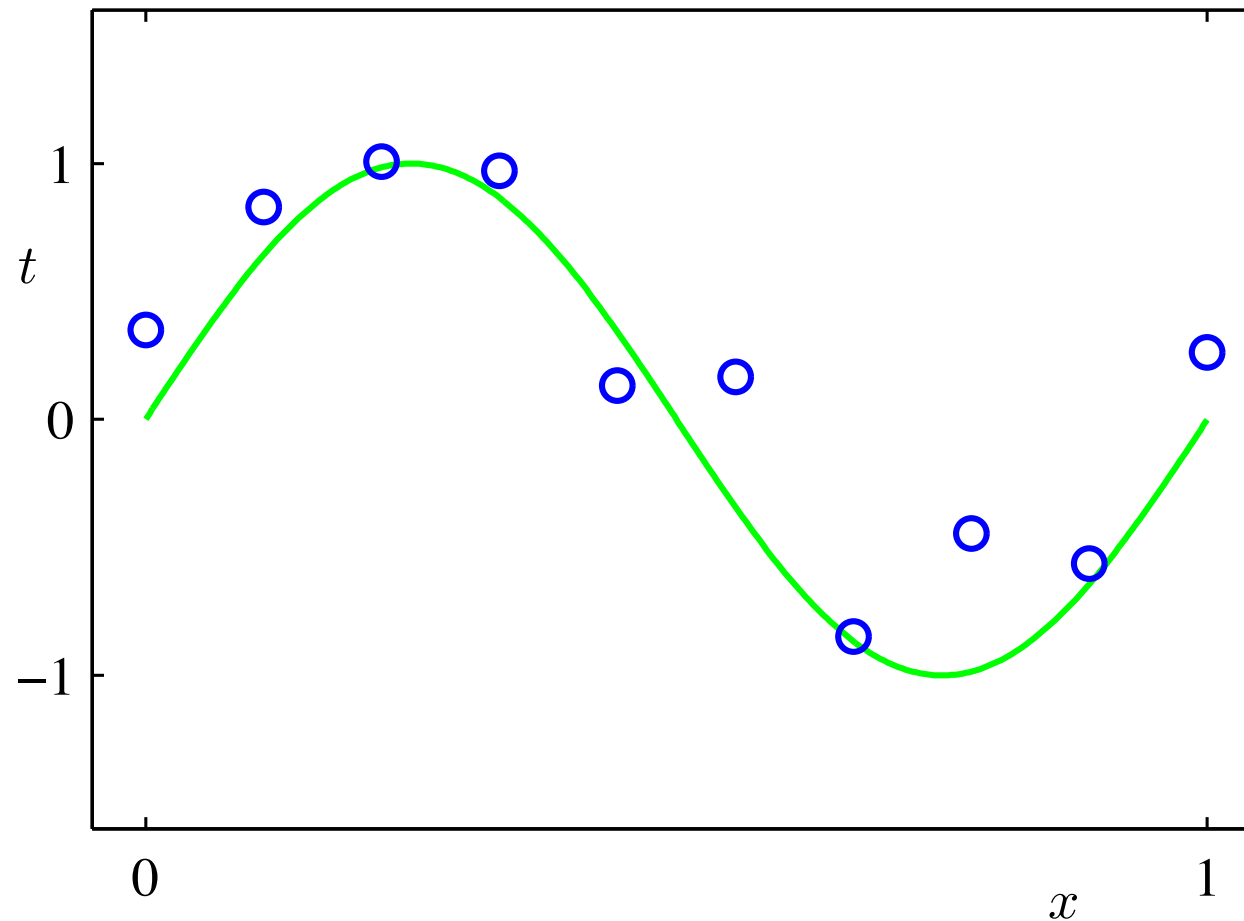
Non-linear regressors

- The all-linear model is very restrictive
- The regressors \mathbf{x} can be non-linear
 - But the response variables \mathbf{y} must be linear combination of regressors
 - An example: polynomial of degree M

$$y_i = \sum_{d=0}^M x_i^d \beta_d + \varepsilon_i$$

Example: fitting $\sin(2\pi x)$

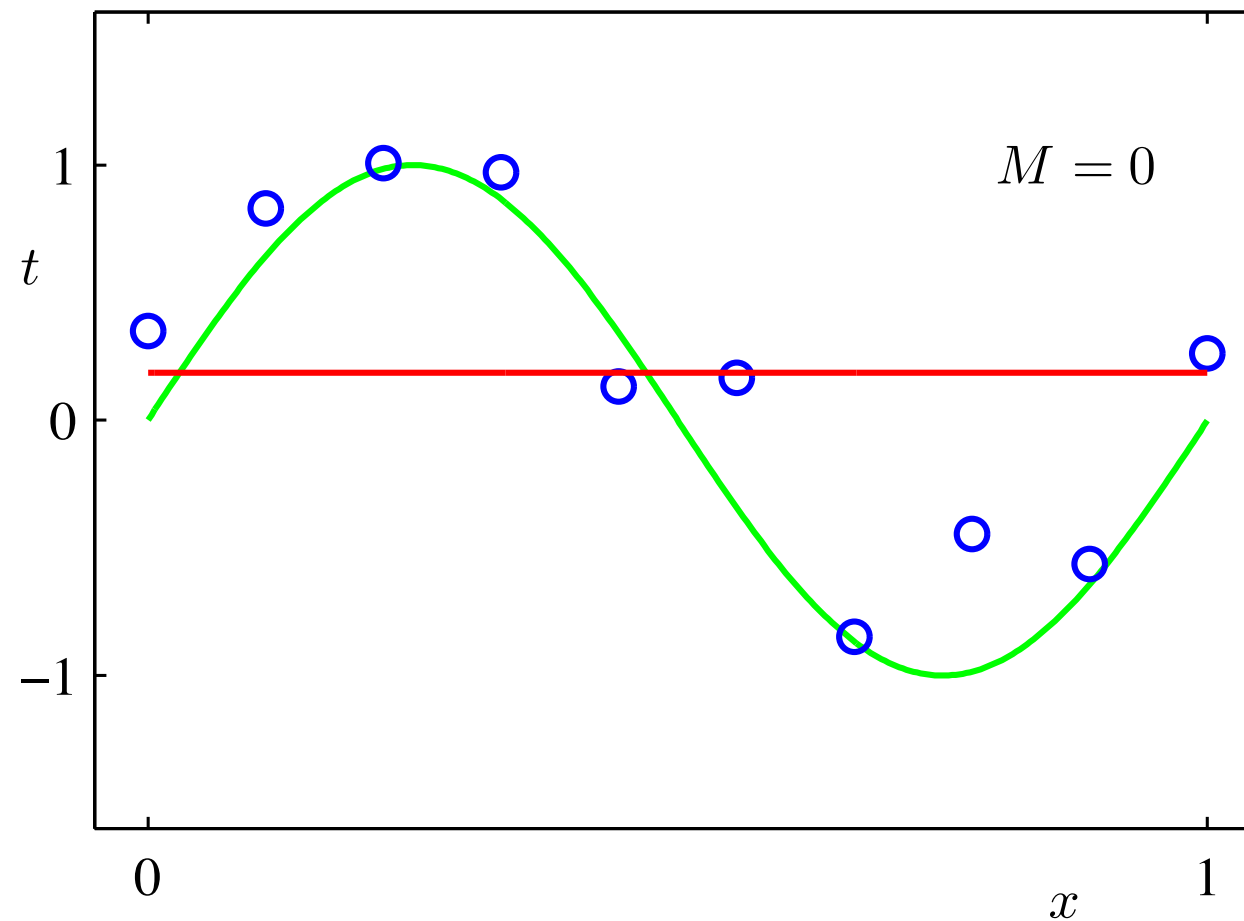
Example and images by Bishop (Chapter 1)



$N=10$ data points and $\sin(2\pi x)$

Example: fitting $\sin(2\pi x)$

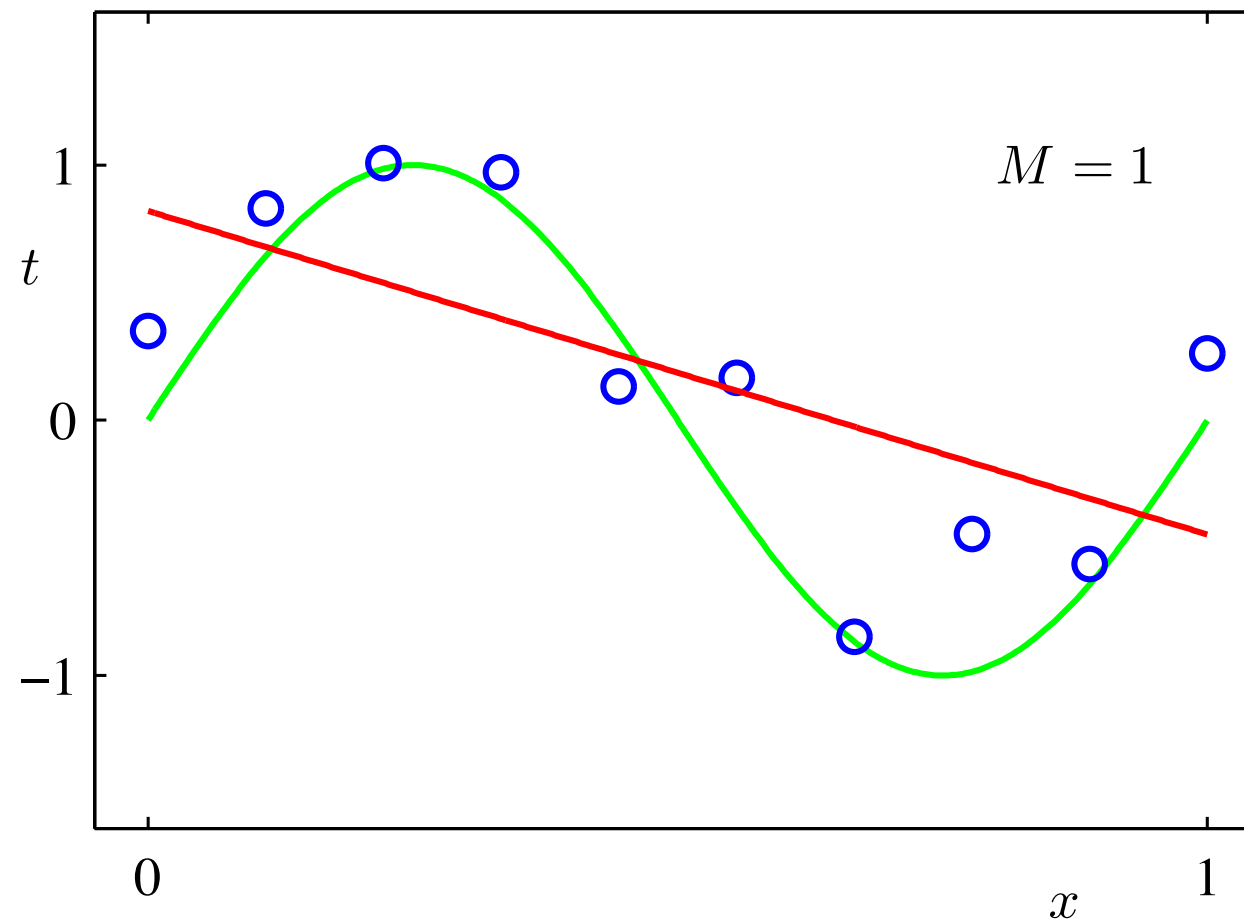
Example and images by Bishop (Chapter 1)



$$y = \beta_0$$

Example: fitting $\sin(2\pi x)$

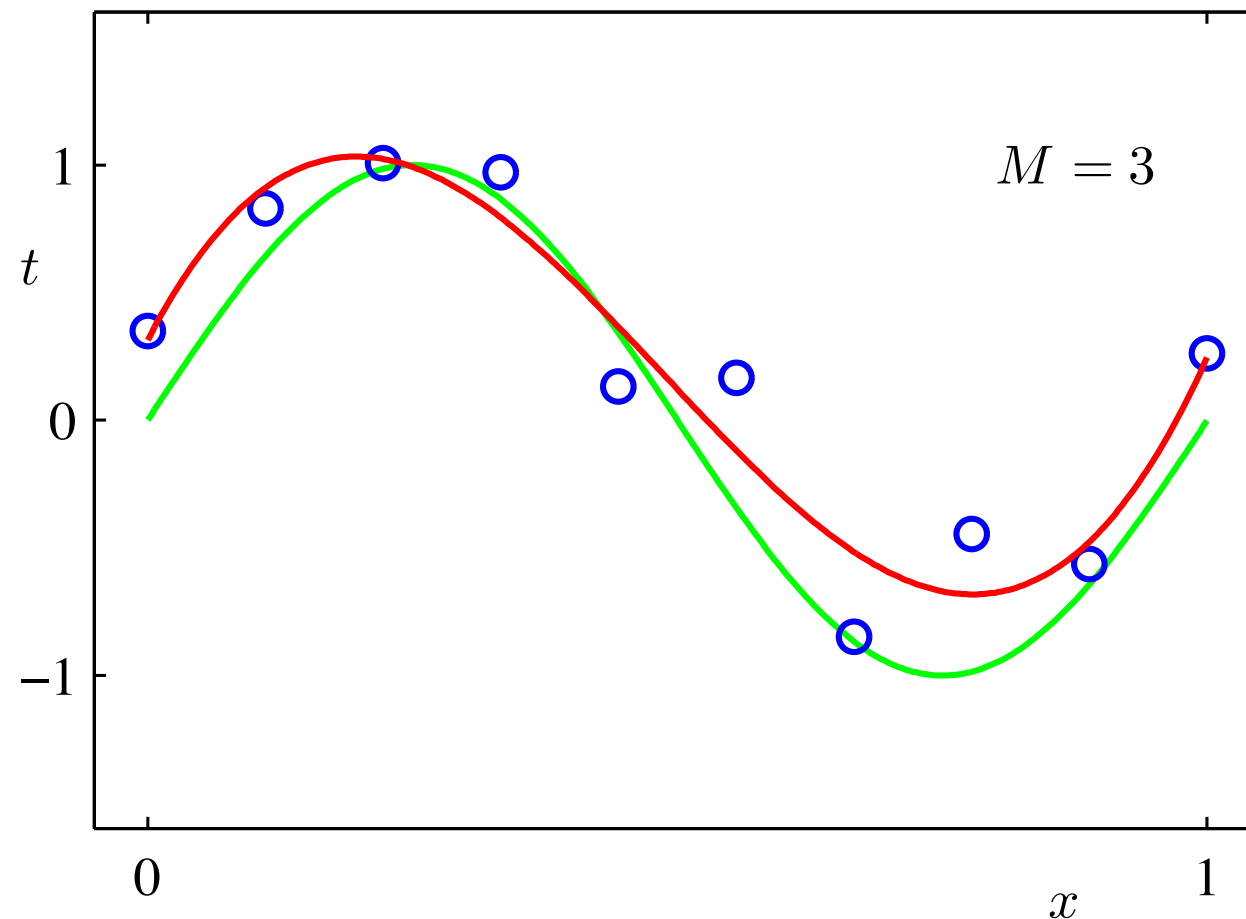
Example and images by Bishop (Chapter 1)



$$y = \beta_1 x + \beta_0$$

Example: fitting $\sin(2\pi x)$

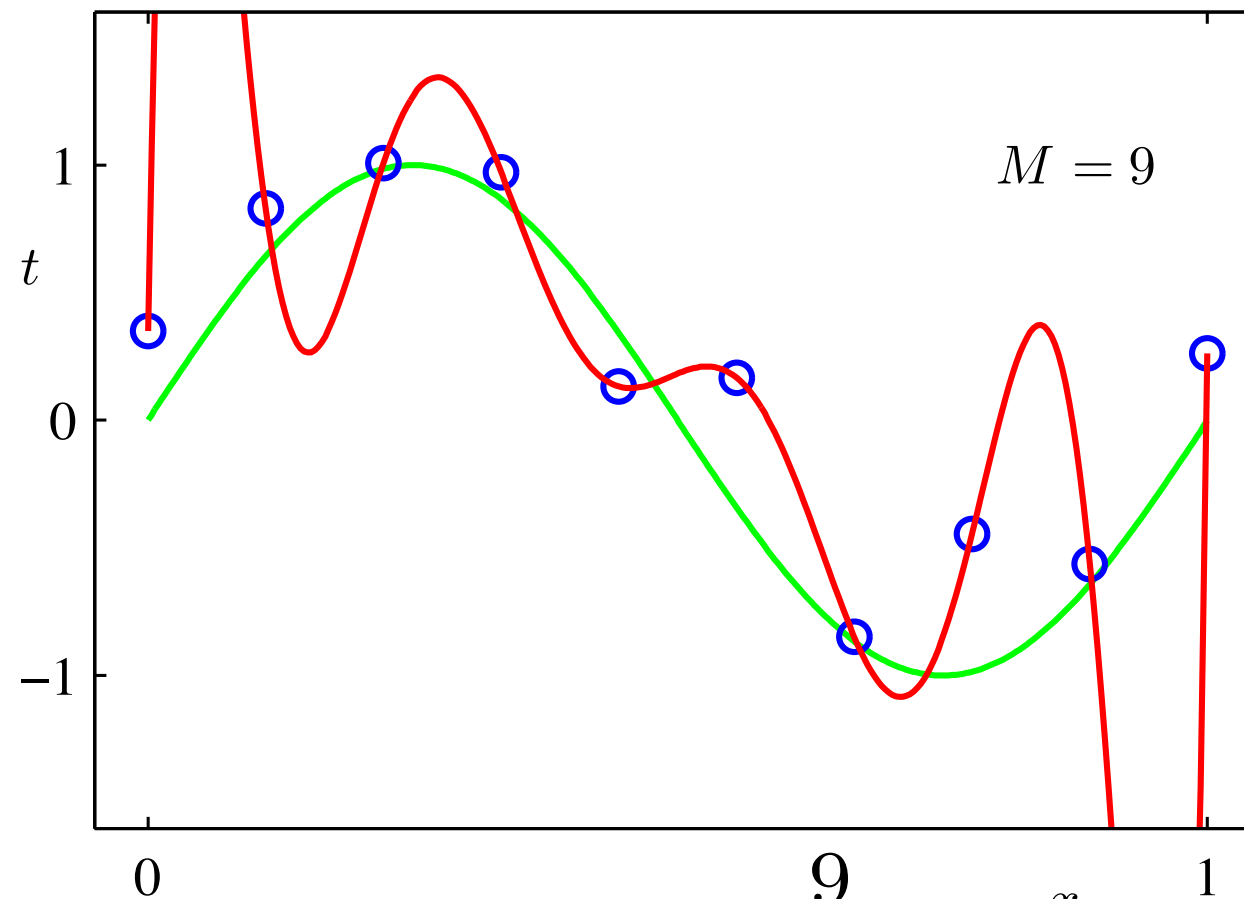
Example and images by Bishop (Chapter 1)



$$y = \beta_3 x^3 + \beta_2 x^2 + \beta_1 x + \beta_0$$

Example: fitting $\sin(2\pi x)$

Example and images by Bishop (Chapter 1)



$$y = \sum_{d=0}^9 \beta_d x^d$$

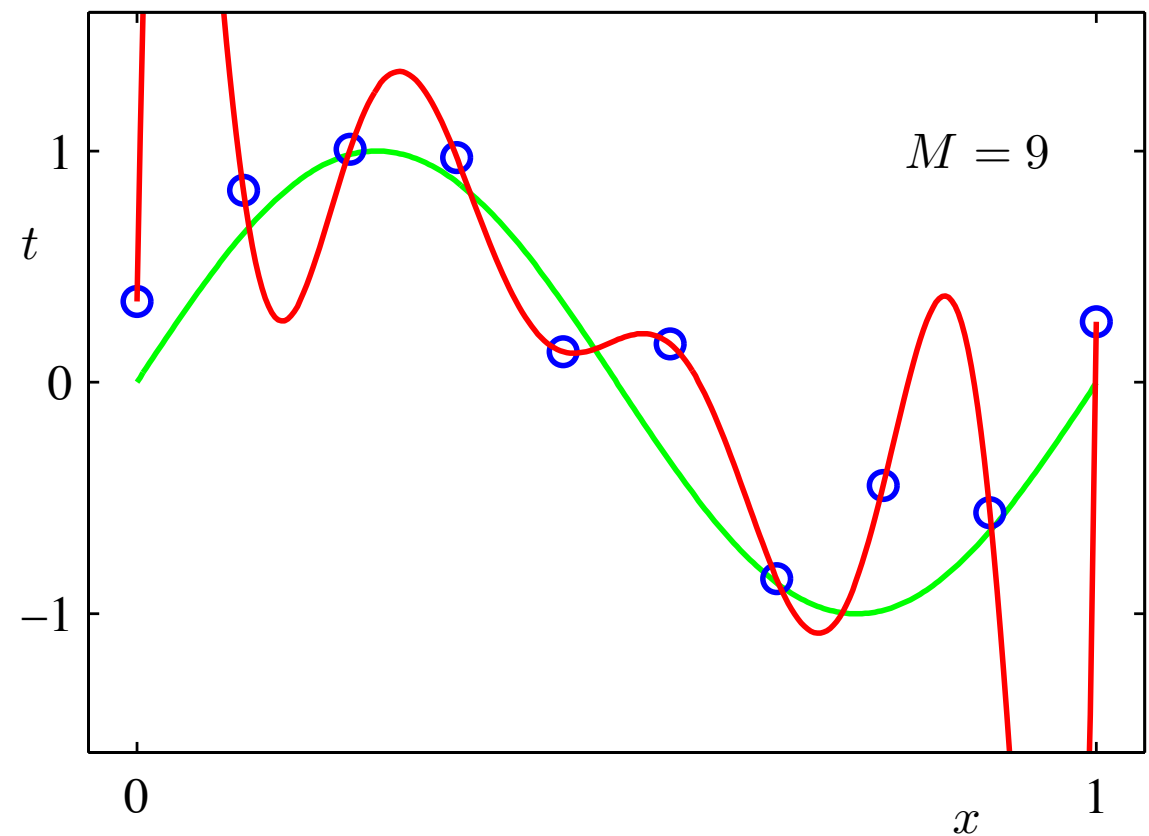
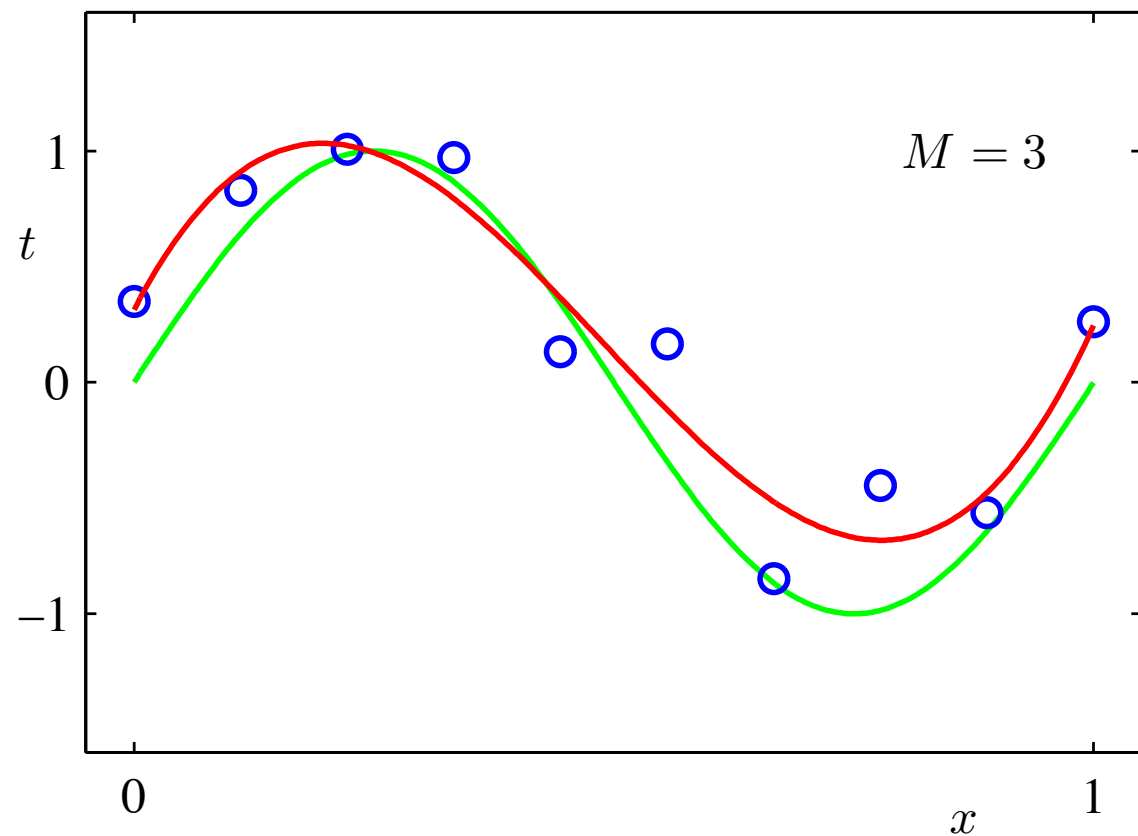
Non-linear regressors (cont'd)

- In general we have $k+1$ **basis functions** $\varphi_j(x)$
 - φ_0 is constant ($\varphi_0(x) = 1$) for the intercept
 - In the previous example, $\varphi_j(x) = x^j$
 - Other basis functions are possible
- The design matrix X is replaced with Φ :

$$\Phi = \begin{pmatrix} \varphi_0(x_1) & \varphi_1(x_1) & \cdots & \varphi_k(x_1) \\ \varphi_0(x_2) & \varphi_1(x_2) & \cdots & \varphi_k(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_0(x_n) & \varphi_1(x_n) & \cdots & \varphi_k(x_n) \end{pmatrix}$$

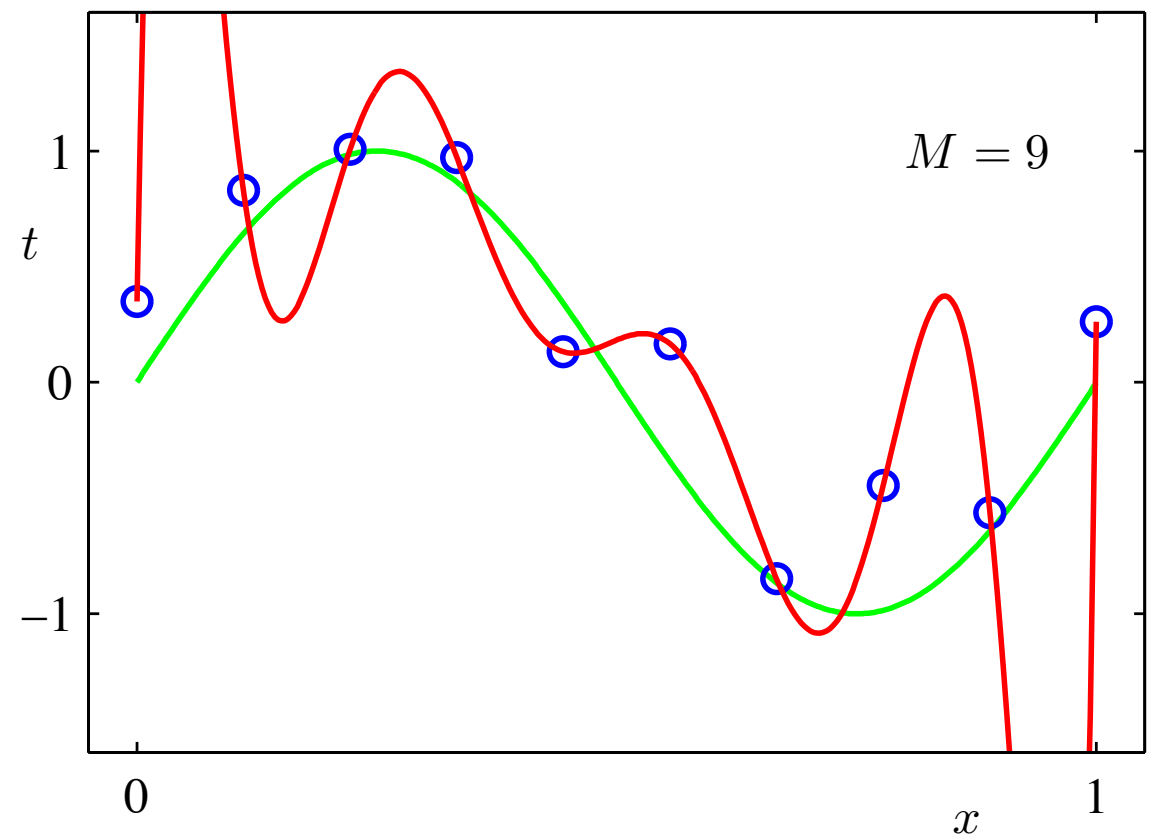
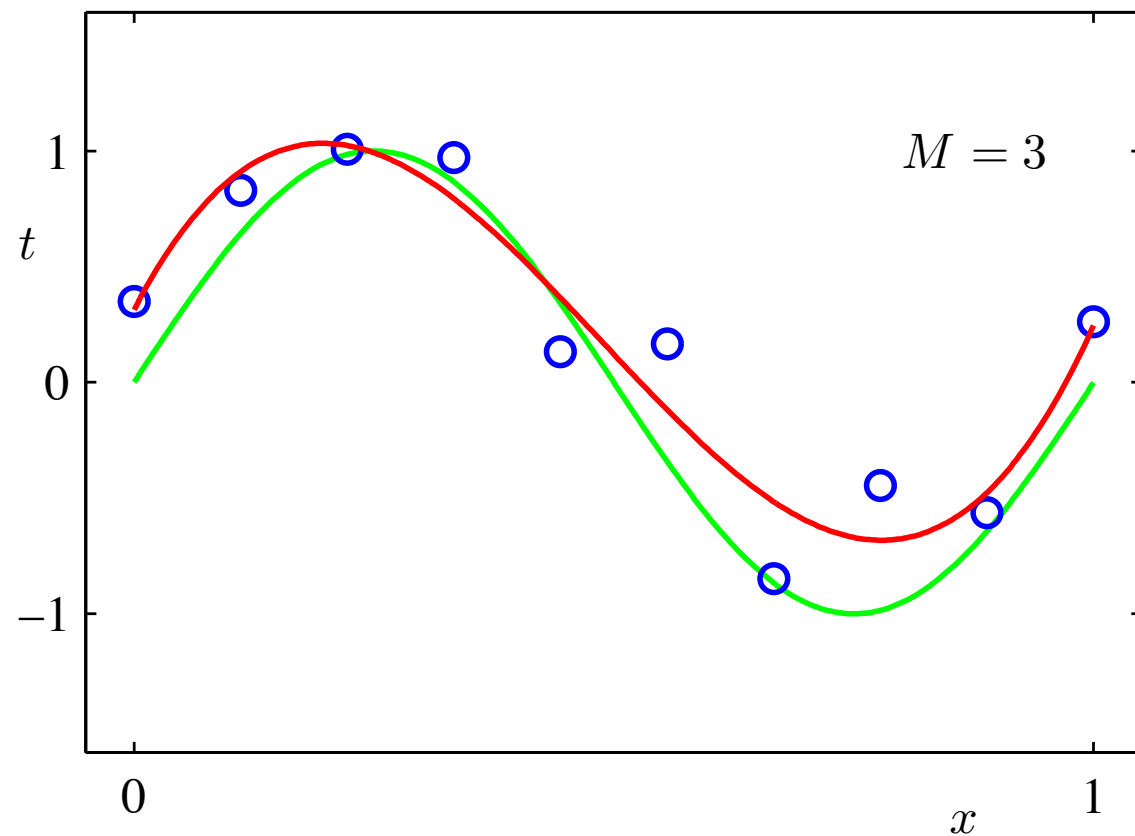
Regularization

- Which of the two models fit the data better?



Regularization

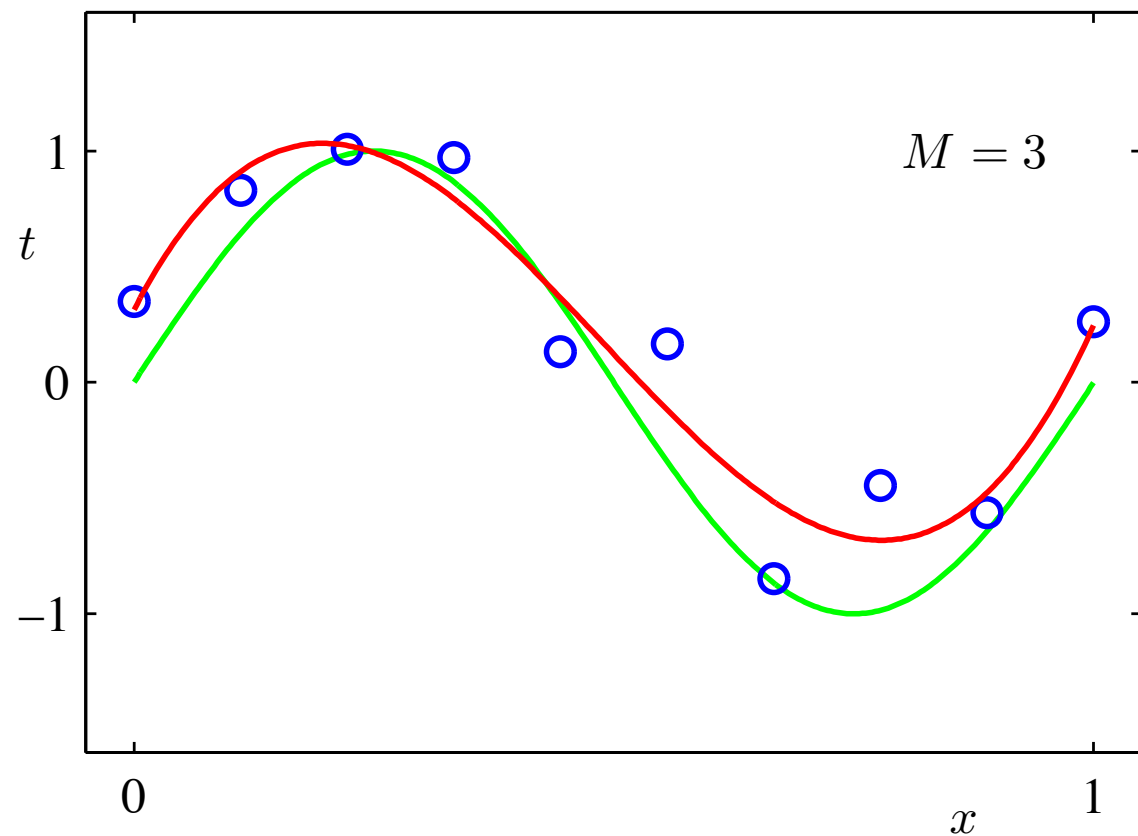
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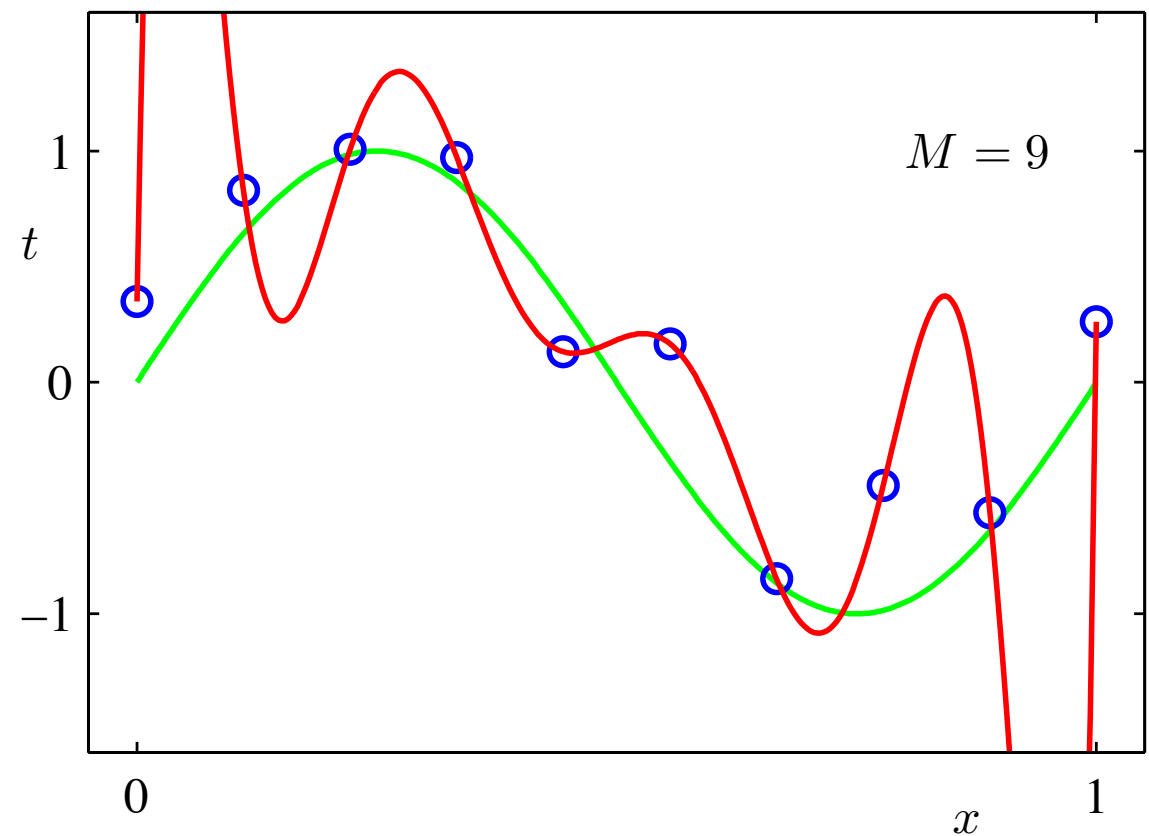
This looks better

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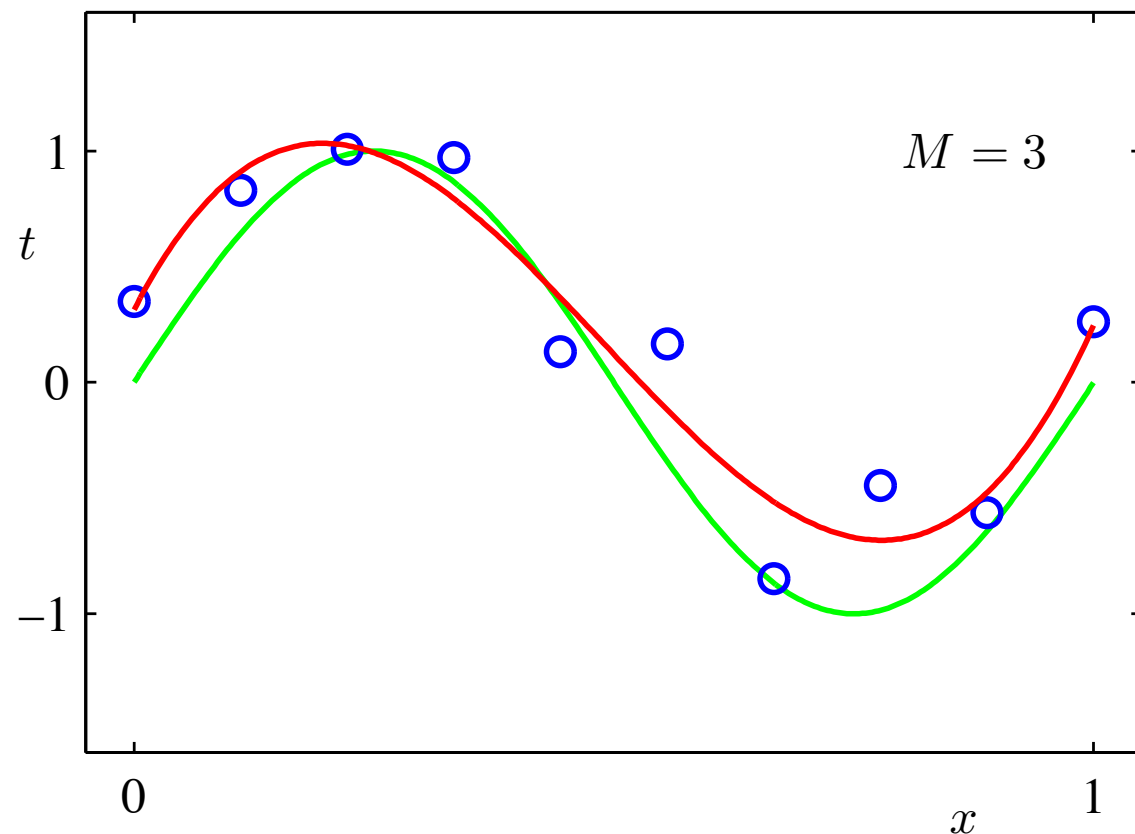
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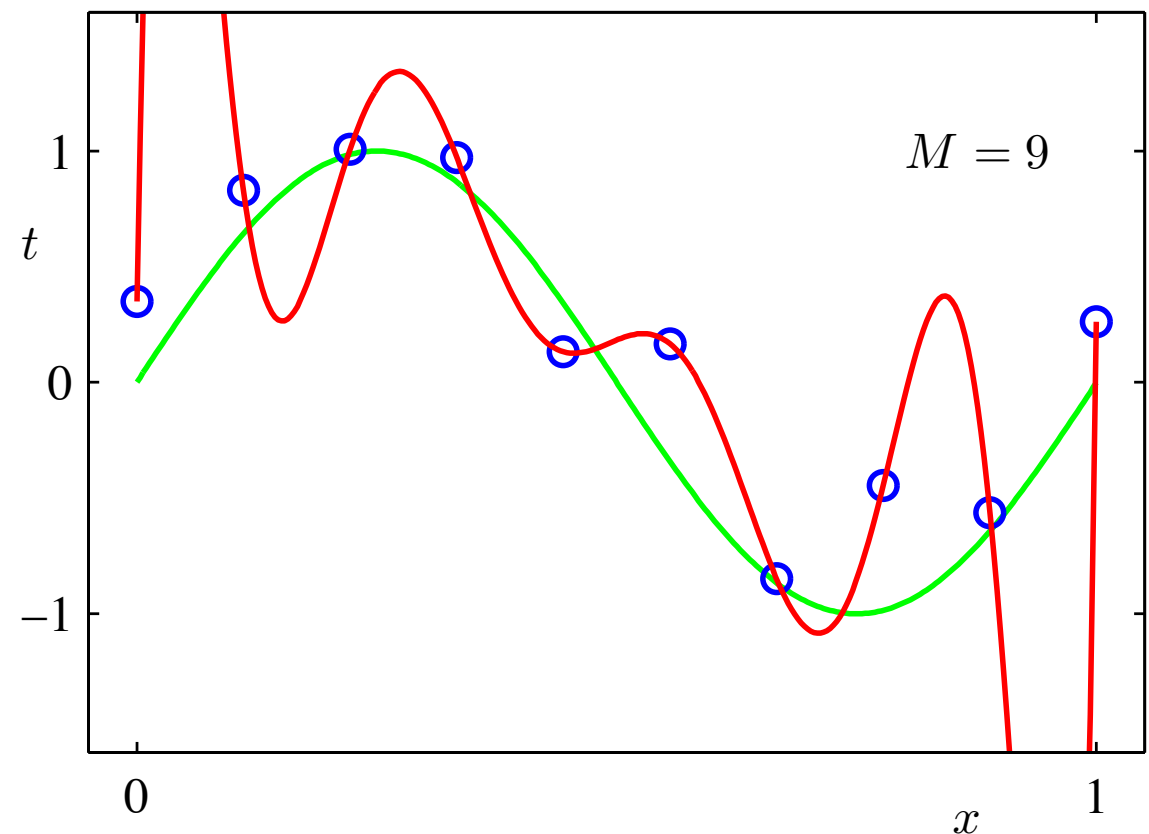
This has no error

Regularization

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This looks better



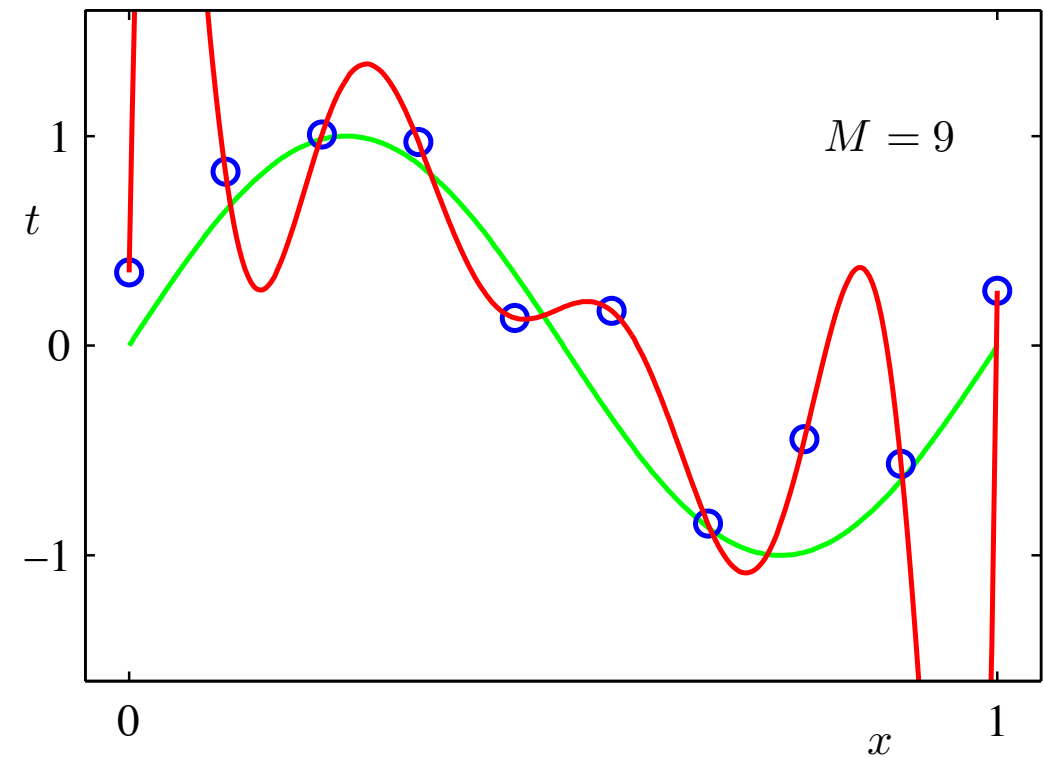
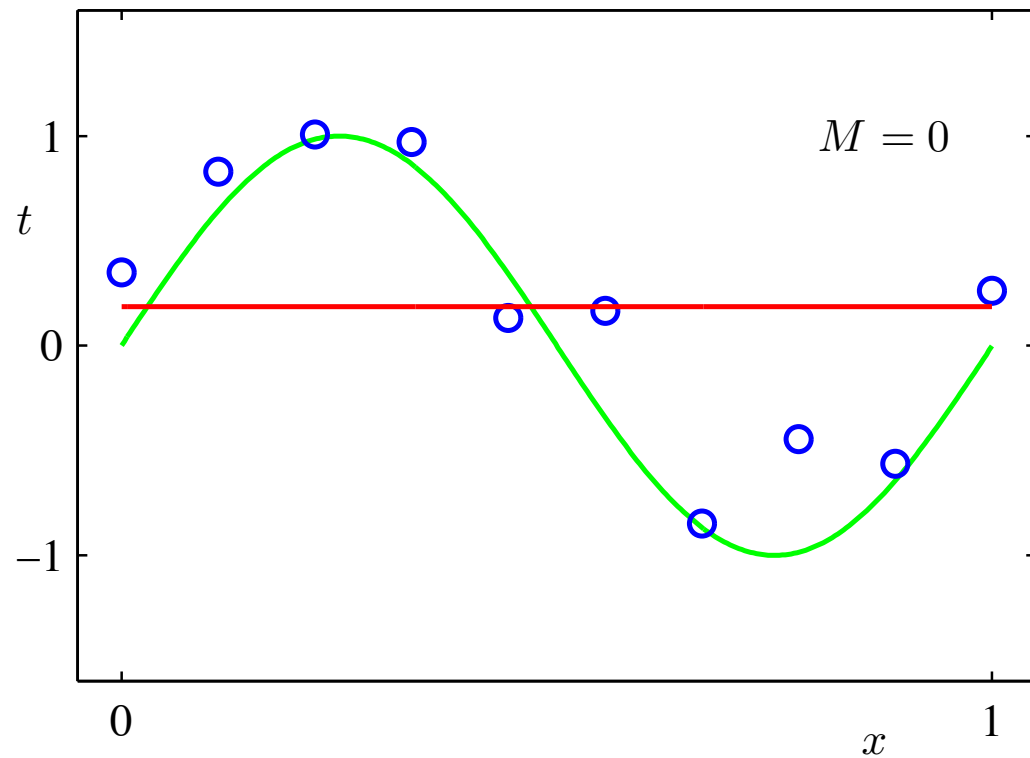
This has no error

- Can we formalize why we think left is better?

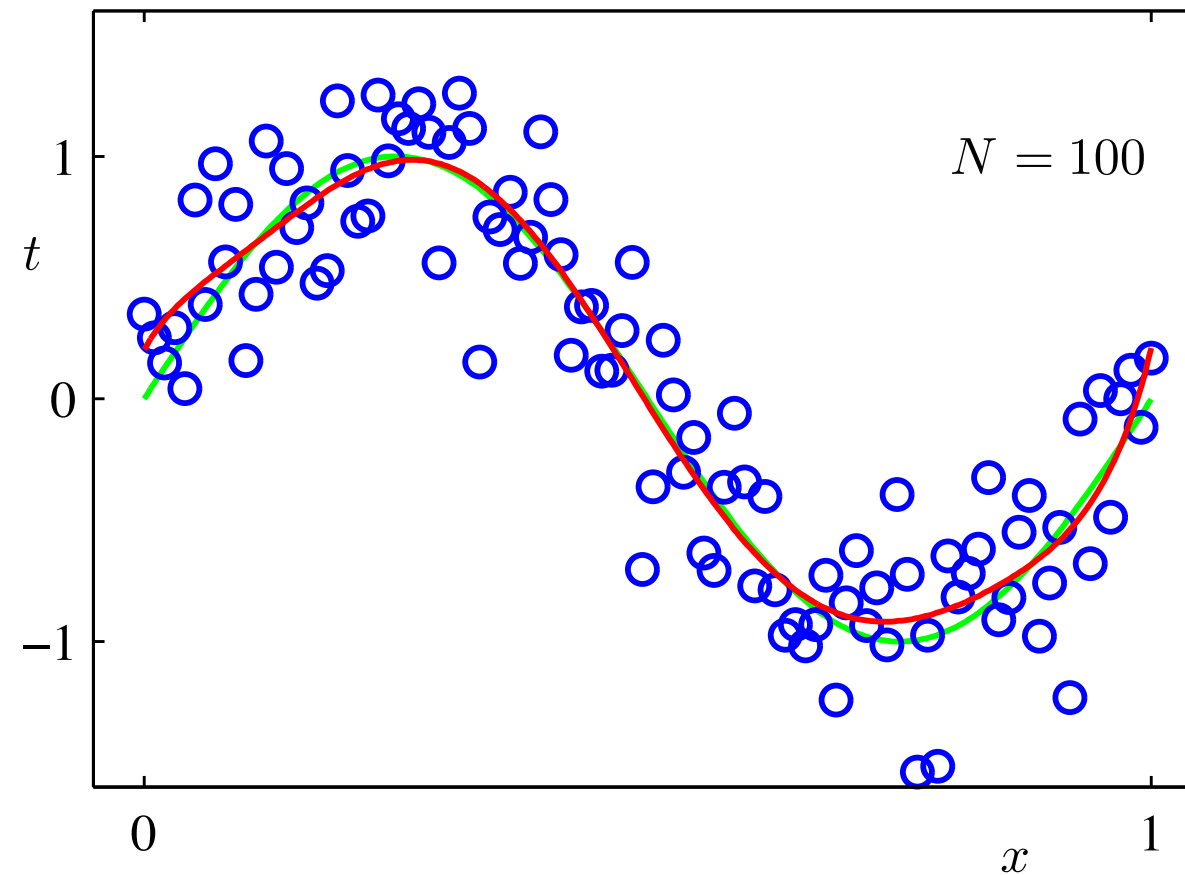
Two roles of regression

- We can approach regression either as
 - descriptive method explaining the data
 - predictive method allowing us to make predictions of future data
- For predicting, we need to combat against **under-fitting** and **over-fitting**
 - Under-fit model gives poor predictions because it doesn't model the process well
 - Over-fit model gives poor predictions because it models also the error

Example of under- and over-fitting



More data allows complex models



Polynomial of degree 9 fitted to $N = 100$ data points

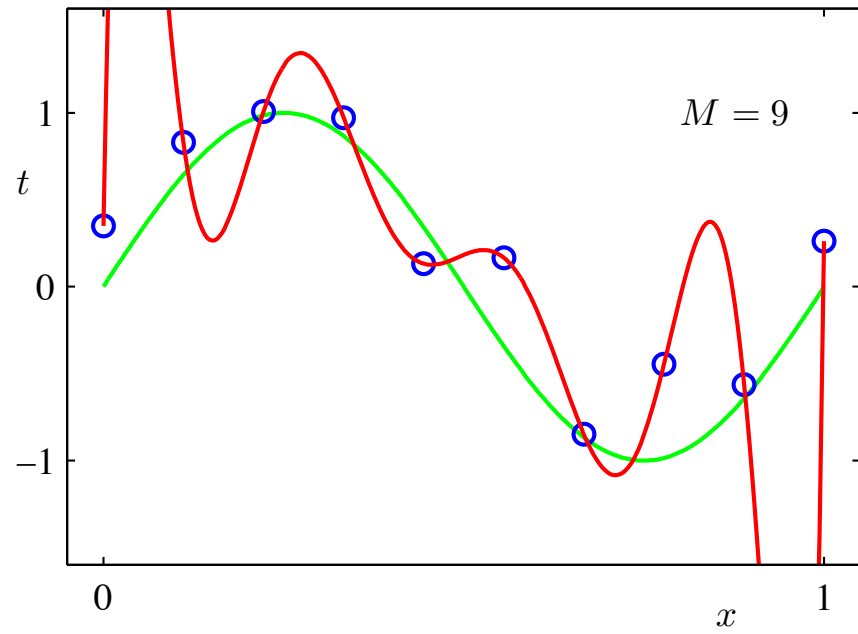
Regularizers

- Selecting the model based on data size does not sound good
- A **regularizer** penalizes on too complex models

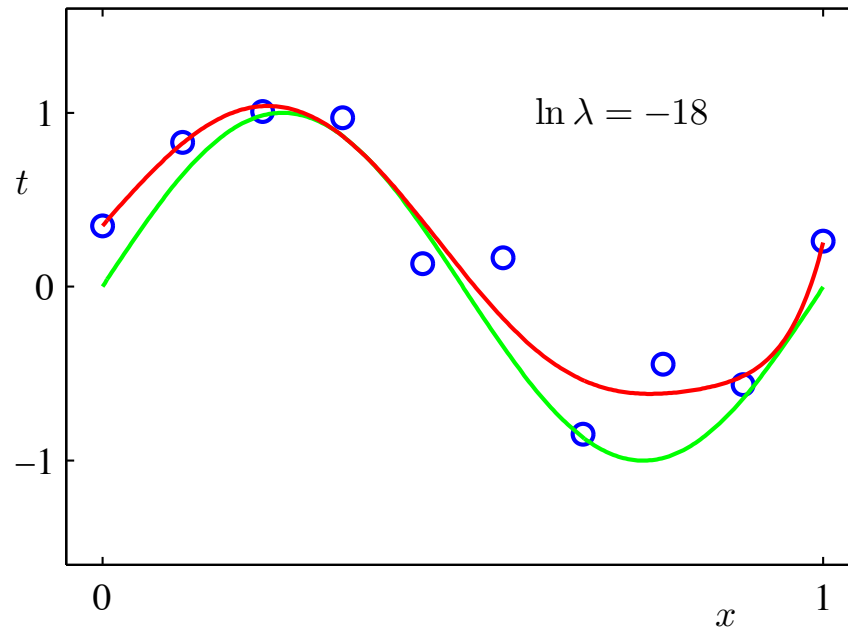
$$\begin{aligned} & \| \mathbf{y} - \Phi \boldsymbol{\beta} \|^2 + \lambda \left\| (\beta_j)_{j=1}^k \right\|^2 \\ &= \sum_{i=1}^n \left(y_i - \sum_{j=0}^k \varphi_j(x_i) \beta_j \right)^2 + \lambda \sum_{j=1}^k \beta_j^2 \end{aligned}$$

- Variable λ is called *regularization parameter*
- Intercept is not included in regularization

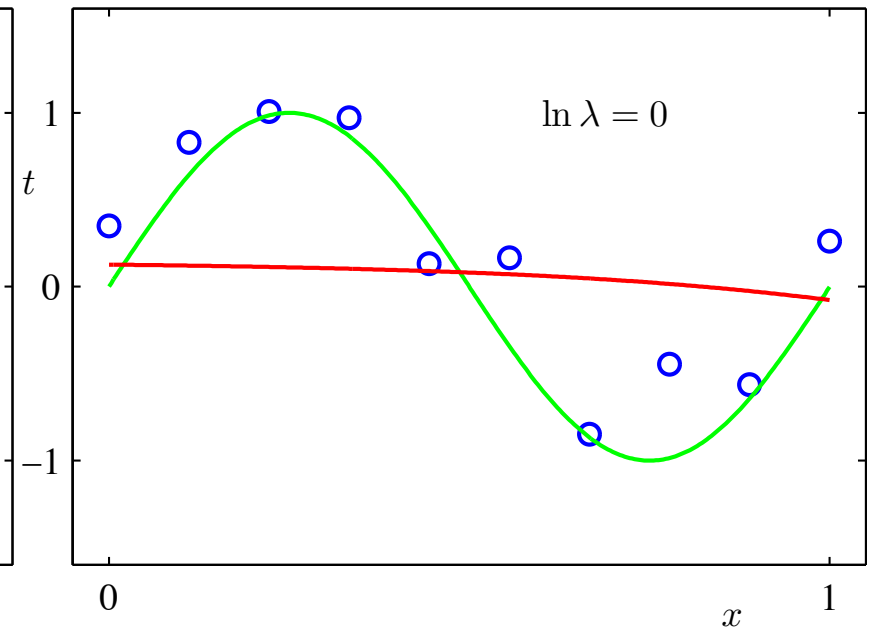
An example



$$\lambda = 0$$



$$\lambda = e^{-18}$$



$$\lambda = 1$$

More on regularizers

- In statistics, regularizers are called *shrinkage methods*
- Regression with quadratic regularizer is also known as *ridge regression*
- Quadratic (L^2) regularizer keeps the loss function quadratic
- The sum-of-absolute-values regularizer $\lambda \sum |\beta_i|$ is known as *lasso* or L^1 regularizer
 - With sufficiently large λ this forces some β_i s to 0

Model selection

- **How do we select λ ?**
- The goal is prediction, so test which λ predicts best
 - Divide data to training data and test data
 - E.g. y_i and x_i for $i = 1..n-1$ are training data and y_n and x_n are test data
 - Learn β s with training data
 - Measure the error with training and test data
 - Repeat with other values of λ and select the one with least over-all error

S -fold cross validation

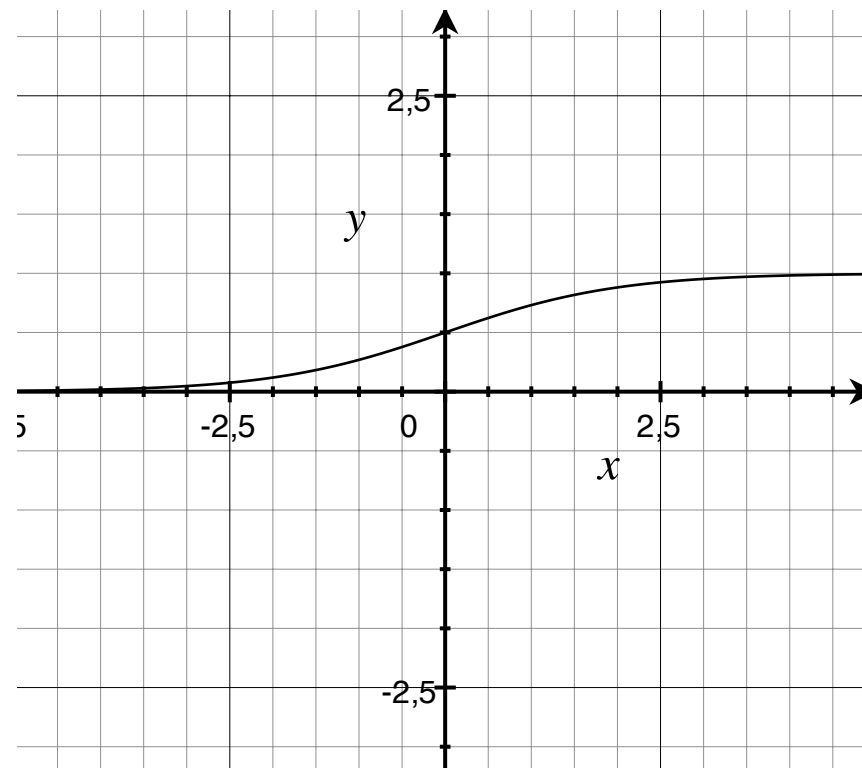
- Divide data to S subsets
- Use $S-1$ of these subsets as training data and the last subset as test data
- Repeat S times with different subset being the test data
- Average errors over different runs and select the best

Logistic Regression

- Actually classification
- Response variables $y_i \in \{0,1\}$
- Name comes from the *logistic function*

$$f(x) = \frac{e^x}{1 + e^x} = \frac{1}{1 + e^{-x}}$$

- The logistic function maps values from $(-\infty, \infty)$ to $(0,1)$



Logistic regression

Given k -dimensional regressors X_i , we estimate y_i as

$$\hat{y}_i = \frac{e^{\beta_0 + \sum_{j=1}^k \beta_j x_{ij}}}{1 + e^{\beta_0 + \sum_{j=1}^k \beta_j x_{ij}}}$$

or, equivalently

$$\text{logit}(\hat{y}_i) = \beta_0 + \sum_{j=1}^k \beta_j x_{ij}$$

where

$$\text{logit}(x) = \ln \left(\frac{x}{1 - x} \right)$$

Notes on logistic regression

- No analytic solution to β
- Finding β needs to use numerical methods
 - Fast method called Iterative Re-Weighted Least Squares is often used
- Logistic function is also known as *sigmoid function*
- Similar to linear regression, we can apply fixed non-linear basis functions ϕ to \mathbf{X}
- Other classification methods will be discussed later in the course

Summary of Chapter 2.3

- Hypothesis testing can be used to test if sample has certain properties
 - same mean, same parameters, goodness-of-fit, etc.
- Linear regression fits linear function of regressors to response variables
- We can combat over-fitting using regularizers
 - Regularizer parameter needs to be selected
- Logistic regression takes the logistic function of linear combination of regressors to classify response variables