Point Estimation

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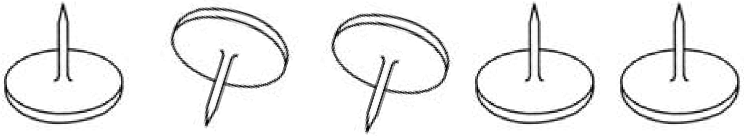
What you need to know

- Point estimation: (点估计)
  - **M**aximal **L**ikelihood **E**stimation (MLE)
  - Bayesian learning
  - **M**aximize **A** **P**osterior (MAP)
- Gaussian estimation
- Regression （回归）
  - Basis function = features
  - Optimizing sum squared error
  - Relationship between regression and Gaussians
- Bias-Variance trade-off

Your first consulting job

- An IT billionaire from Beijing asks you a question:
  - B: I have thumbtack, if I flip it, what’s the probability it will fall with the nail up?
  - Y: Please flip it a few times …



  - Y: The probability is 3/5
  - B: Why???
  - Y: Because…

Binomial Distribution

- $P(\text{Heads}) = \theta$, $P(\text{Tails}) = 1\text{-}\theta$ $\quad D = \{T, H, H, T, T\}$

$$P(D \mid \theta) = (1-\theta)\theta\theta(1-\theta)(1-\theta)$$

- Flips are i.i.d. (Independent Identically distributed)
  - Independent events
  - Identically distributed according to Binomial distribution
- Sequence D of α_H Heads and α_T Tails

$$P(D \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

Maximum Likelihood Estimation

- **Data**: Observed set D of α_H Heads and α_T Tails
- **Hypothesis**: Binomial distribution
- **Learning θ is an optimization problem**
  - What's the objective function?

$$D = \{T, H, H, T, T\}$$

- **MLE**: Choose θ that maximizes the probability of observed data:

$$\begin{aligned}\hat{\theta} &= \arg\max_{\theta} P(D \mid \theta) \\ &= \arg\max_{\theta} \ln P(D \mid \theta) = \ldots\end{aligned}$$

Maximum Likelihood Estimation (cont.)

$$\begin{aligned}
\hat{\theta} &= \arg\max_{\theta} P(D \mid \theta) \\
&= \arg\max_{\theta} \ln\left(\theta^{\alpha_H}(1-\theta)^{\alpha_T}\right) \\
&= \arg\max_{\theta} \left(\alpha_H \ln\theta + \alpha_T \ln(1-\theta)\right)
\end{aligned}$$

- Set derivative to zero:

$$\boxed{\frac{d}{d\theta} \ln P(D \mid \theta) = 0} \qquad \hat{\theta} = \frac{\alpha_H}{\alpha_H + \alpha_T} = \frac{2}{2+3}$$

How many flips do I need?

$$\hat{\theta} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

- B: I flipped 2 heads and 3 tails.
- Y: 1- θ = 3/5, I can prove it!
- B: What if I flipped 20 heads and 30 tails?
- Y: Same answer, I can prove it!
- B: What’s better?
- Y: Humm… The more the merrier???
- B: Is this why I am paying you the big bucks???

Simple bound (based on Höffding's inequality)

- For $N = \alpha_H + \alpha_T$ and $\hat{\theta} = \frac{\alpha_T}{\alpha_H + \alpha_T}$

http://omega.albany.edu:8008/machine-learning-dir/notes-dir/vc1/vc-l.html

- Let θ* be the true parameter, for any ε>0:

$$\boxed{P(|\hat{\theta} - \theta^*| \geq \varepsilon) \leq 2e^{-2N\varepsilon^2}} \leq \delta$$

$$N \geq \frac{1}{2\varepsilon^2}[\ln 2 - \ln \delta]$$

$$N \geq 270 \; ; (\varepsilon = 0.1, \delta = 0.01)$$

PAC Learning

- **PAC**: **Probably Approximate Correct**
- B: I want to know the thumbtack parameter θ, within ε = 0.1, with probability at least 1-δ = 0.99. How many flips?
- Y: 270, ☺

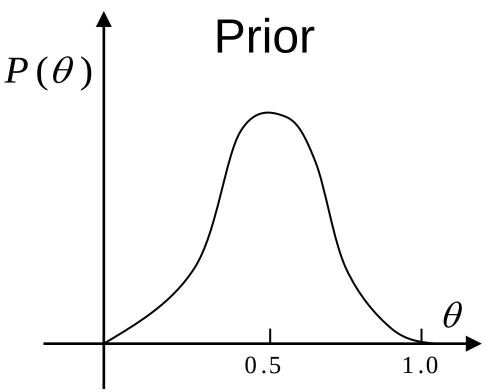
Prior: knowledge before experiments

- B: Wait, I know that the thumbtack is “close” to 50-50. What can you …?
- Y: I can learn it the Bayesian way…

- Rather than estimating a single θ, we obtain a distribution over possible values of θ

先验

Prior



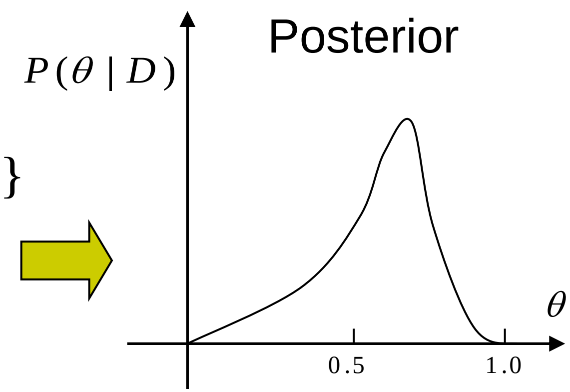
数据

Data

$$D = \{T, H, H, T, T\}$$

后验

Posterior



Bayesian Learning

- Bayes rule:

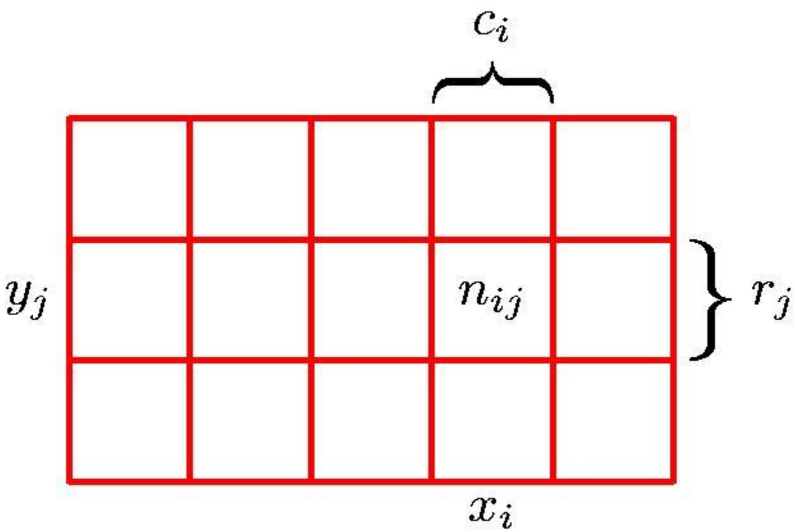
$$\underbrace{P(\theta \mid D)}_{\text{Posterior}} = \frac{\overbrace{P(\theta)}^{\text{Prior}}\,\overbrace{P(D \mid \theta)}^{\text{Likelihood}}}{\underbrace{P(D)}_{\text{Data distribution}}}$$

(Normalization constant)

- Or equivalently:

$$P(\theta \mid D) \propto P(\theta)P(D \mid \theta)$$

Probability Theory



- Sum Rule

$$p(X = x_i) = \frac{c_i}{N} = \frac{1}{N} \sum_{j=1}^{L} n_{ij}$$
$$= \sum_{j=1}^{L} p(X = x_i, Y = y_j)$$

Product Rule

$$\begin{aligned} p(X = x_i, Y = y_j) &= \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N} \\ &= p(Y = y_j | X = x_i) p(X = x_i) \end{aligned}$$

Probability concepts

- Random variables: x
- Probability (function): $P(X \leq x)$, $P(x)$
- Density (function): $f(x)$,
- Independency: $P(x, y)=P(x)P(y)$
- Feature quantities:
  - Mean, expectation $E(x) = \int x f(x)\, \mathrm{d}x$
  - Covariance
    - $\mathrm{cov}(x,y)=0$, uncorrelatedness / irrelevant (统计无关)
  - Higher order moments

The Rules of Probability

- Sum Rule $$p(X) = \sum_Y p(X, Y)$$
- Product Rule $$p(X, Y) = p(Y|X)p(X)$$

Bayes' Theorem

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

$$p(X) = \sum_{Y} p(X|Y)p(Y)$$

posterior $\propto$ likelihood $\times$ prior

Bayesian Learning in our case

- Likelihood function is simply Binomial:

$$P(D \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- What about prior?
  - Represent expert knowledge
  - Simple posterior form
- Conjugate priors: （共轭先验）
  - Closed-form representation of posterior
  - For Binomial, conjugate prior is Beta distribution

Beta prior distribution – P(θ)

- Prior: Beta distribution

$$\Gamma(x+1) = x\Gamma(x), \Gamma(1) = 1$$

$$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\theta \mid \beta_H, \beta_T) = \frac{\Gamma(\beta)}{\Gamma(\beta_H)\Gamma(\beta_T)}\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}$$

- Likelihood: Binomial distribution

$$P(D \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- Posterior:

$$\begin{aligned} P(\theta \mid D) &\propto P(\theta)P(D \mid \theta) \\ &\propto \theta^{\alpha_H}(1-\theta)^{\alpha_T}\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1} \\ &\sim Beta(\alpha_H + \beta_H, \alpha_T + \beta_T) \end{aligned}$$

Using Bayesian posterior

- Posterior distribution:

$$P(\theta \mid D) \sim Beta(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

- Bayesian inference:
  - No longer single parameter:

$$E[f(\theta)] \sim \int_0^1 f(\theta) P(\theta \mid D) d\theta$$

  - Integral, ☹

Expectation

- Random variable: θ
- Random function: $f(\theta)$
- Expectation:

$$E[f(\theta)] \sim \int_0^1 f(\theta) P(\theta \mid D) d\theta$$

MAP:
Maximum a posteriori approximation

$$P(\theta \mid D) \sim Beta(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta \mid D) d\theta$$

approximation

- MAP: use most likely parameter

$$\hat{\theta} = \arg\max_{\theta} P(\theta \mid D) \qquad E[f(\theta)] \approx f(\hat{\theta})$$

MAP for Beta distribution

$$P(\theta \mid D) \sim Beta(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

- MAP: use most likely parameter

$$\hat{\theta} = \arg\max_{\theta} P(\theta \mid D) = \frac{\alpha_T + \beta_T - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2}$$

- Beta prior equivalent to extra thumbtack flips
- As $N = \alpha_T + \alpha_H \rightarrow \infty$, prior is "forgotten"
- But, for small sample size, prior is important!

More …

- B: Can we handle more complex cases?
- Y: Yes, :-D

- Prior: a mixture of beta distribution
  - $P(\theta) \sim 0.4 Beta(20,1) + 0.4 Beta(1,20) + 0.2 Beta(2,2)$

Multinomial distribution

- B: Now if I give you a dice (骰子), then …
- Y: I can solve this problem in a similar way.
- Likelihood:

$$P(X = x^k \mid \boldsymbol{\theta}) = \theta_k, \; k = 1, 2, \ldots, r,$$

$$\boldsymbol{\theta} = \{\theta_1, \ldots, \theta_r\}, \; \theta_1 + \ldots + \theta_r = 1$$

$$D = \{X_1 = x_1, \ldots, X_N = x_N\} \Rightarrow \{N_1, \ldots, N_r\}$$

$$\boxed{P(D \mid \boldsymbol{\theta}) = \prod_{i=1}^{r} \theta_i^{N_i}}$$

Multinomial distribution

- Conjugate prior (Dirichlet distribution):

$$\boxed{P(\boldsymbol{\theta}) = \mathrm{Dir}(\boldsymbol{\theta} \mid \alpha_1, \ldots, \alpha_r) = \frac{\Gamma(\alpha)}{\prod_{k=1}^{r} \Gamma(\alpha_k)} \prod_{k=1}^{r} \theta_k^{\alpha_k - 1}, \quad \alpha = \sum_{k=1}^{r} \alpha_k}$$

- Solution:

$$\boxed{P(X_{N+1} = x^k \mid D) = \int \theta_k \mathrm{Dir}(\boldsymbol{\theta} \mid \alpha_1 + N_1, \ldots, \alpha_r + N_r) d\boldsymbol{\theta} = \frac{\alpha_k + N_k}{\alpha + N}}$$

- Important fact:

$$\boxed{P(D) = \frac{\Gamma(\alpha)}{\Gamma(\alpha + N)} \prod_{k=1}^{r} \frac{\Gamma(\alpha_k + N_k)}{\Gamma(\alpha_k)}}$$

Gaussian distribution

均值

Continuous random variable:

mean

$$P(x \mid \mu, \delta) \sim \frac{1}{\boxed{\delta}\sqrt{2\pi}} e^{-\frac{(x-\boxed{\mu})^2}{2\delta^2}}$$

variance

Normalize item

方差

Consider the difference between continuous and discrete variables?

MLE for Gaussian

- Prob. of i.i.d. samples $D = \{x_1, x_2, \ldots, x_N\}$

likelihood $$P(D \mid \mu, \sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}$$

- The magic of log (to log-likelihood)

$$\begin{aligned}\ln P(D \mid \mu, \sigma) &= \ln\left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}} \\ &= -N \ln(\sigma\sqrt{2\pi}) - \sum_{i=1}^{N} \frac{(x_i-\mu)^2}{2\sigma^2}\end{aligned}$$

MLE for mean of a Gaussian

$$\frac{\partial}{\partial \mu} \ln P(D \mid \mu, \sigma) = \frac{\partial}{\partial \mu} \ln \left(\frac{1}{\sigma \sqrt{2\pi}} \right)^{N} \prod_{i=1}^{N} e^{\frac{-(x_i - \mu)^2}{2\sigma^2}}$$

$$= \frac{\partial}{\partial \mu} - \sum_{i=1}^{N} \frac{(x_i - \mu)^2}{2\sigma^2}$$

$$= \sum_{i=1}^{N} \frac{(x_i - \mu)}{\sigma^2} = 0$$

$$\mu = \frac{1}{N} \sum_{i} x_i$$

MLE for variance of a Gaussian

$$\frac{\partial}{\partial\sigma}\ln P(D\mid\mu,\sigma) = \frac{\partial}{\partial\sigma}\ln\left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}$$

$$= \frac{\partial}{\partial\sigma}[-N\ln\sigma\sqrt{2\pi}] - \sum_{i=1}^{N}\frac{\partial}{\partial\sigma}[\frac{(x_i-\mu)^2}{2\sigma^2}]$$

$$= -\frac{N}{\sigma} + \sum_{i=1}^{N}\frac{(x-\mu)^2}{\sigma^3} = 0$$

$$\sigma^2 = \frac{1}{N}\sum_i (x_i-\mu)^2$$

Gaussian parameters learning

- MLE

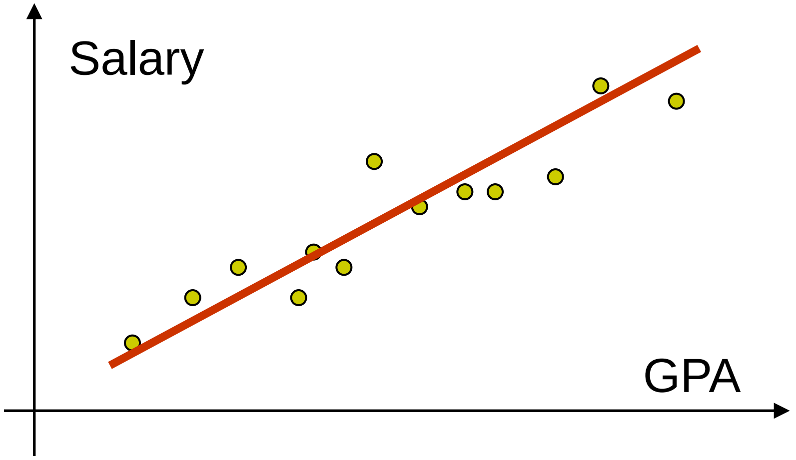
$$\hat{\mu} = \frac{1}{N} \sum_i x_i$$

$$\hat{\sigma}^2 = \frac{1}{N} \sum_i (x_i - \mu)^2$$

- Bayesian learning: prior?
- Conjugate priors:
  - Mean: Gaussian priors
  - Variance: Wishart Distribution

Prediction of continuous variable

- B: Wait, that's not what I meant!
- Y: Chill out, dude.
- B: I want to predict a continuous variable for continuous inputs: I want to predict salaries from GPA.
- Y: I can regress that…



The regression problem

- **Instances:** $< \mathbf{x}_i, t_i >$
- **Learn:** mapping from $\mathbf{x}$ to $t(\mathbf{x})$.
- **Hypothesis space:** $t(\mathbf{x}) \approx \hat{f}(x) = \sum_{i=1}^{k} w_i h_i$
  - Given, basis functions $H = \{h_1, \ldots, h_k\}$
  - Find coefficients $\mathbf{w} = \{w_1, \ldots, w_k\}$
- **Problem formulation:**

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_j [t(\mathbf{x}_j) - \sum_{i=1}^{k} w_i h_i(x)]^2$$

But, why sum squared error?

- Model:

$$P(t \mid \mathbf{x}, \mathbf{w}, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-[t - \sum_i w_i h_i(x)]^2}{2\sigma^2}}$$

- Learn **w** using MLE

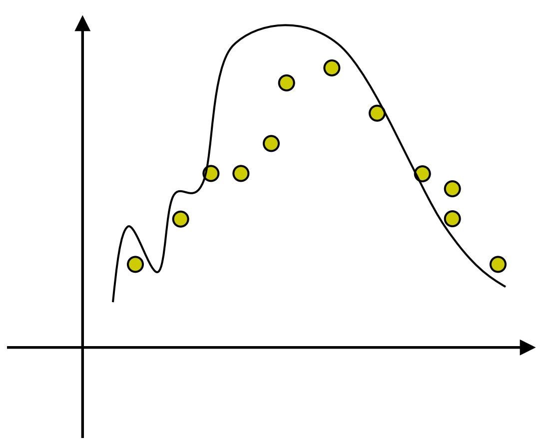
Maximizing log-likelihood

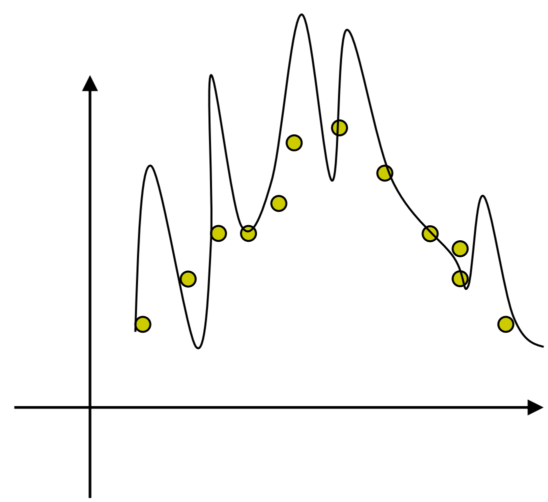
$$\ln P(D \mid \mathbf{w}, \sigma) = \ln \prod_j \left(\frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-[t_j - \sum_i w_i h_i(x_j)]^2}{2\sigma^2}} \right)$$

$$\Rightarrow \quad \min \sum_j \frac{-[t_j - \sum_i w_i h_i(x_j)]^2}{2\sigma^2}$$

Bias-Variance Tradeoff

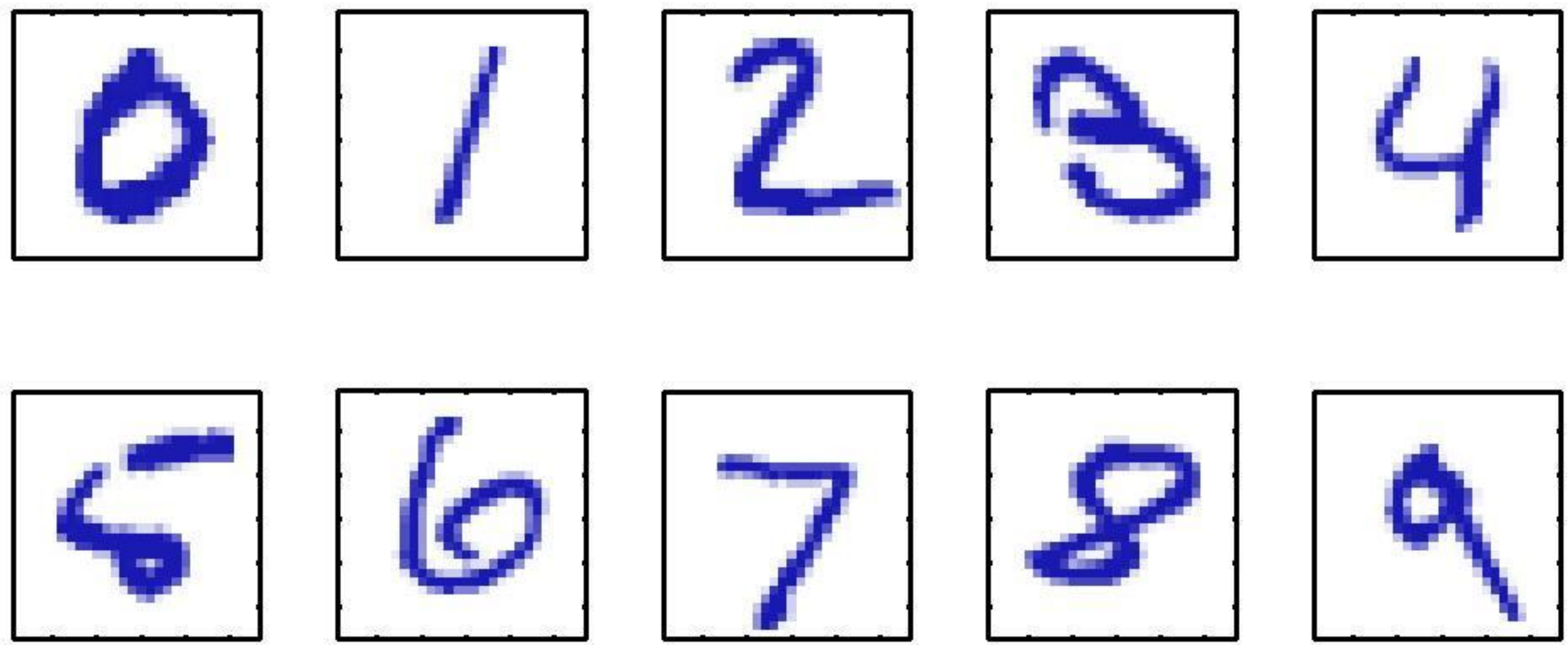
- Choice of hypothesis basis introduce learning bias:
  - More complex basis:
    - Less bias
    - More variance (over-fitting)



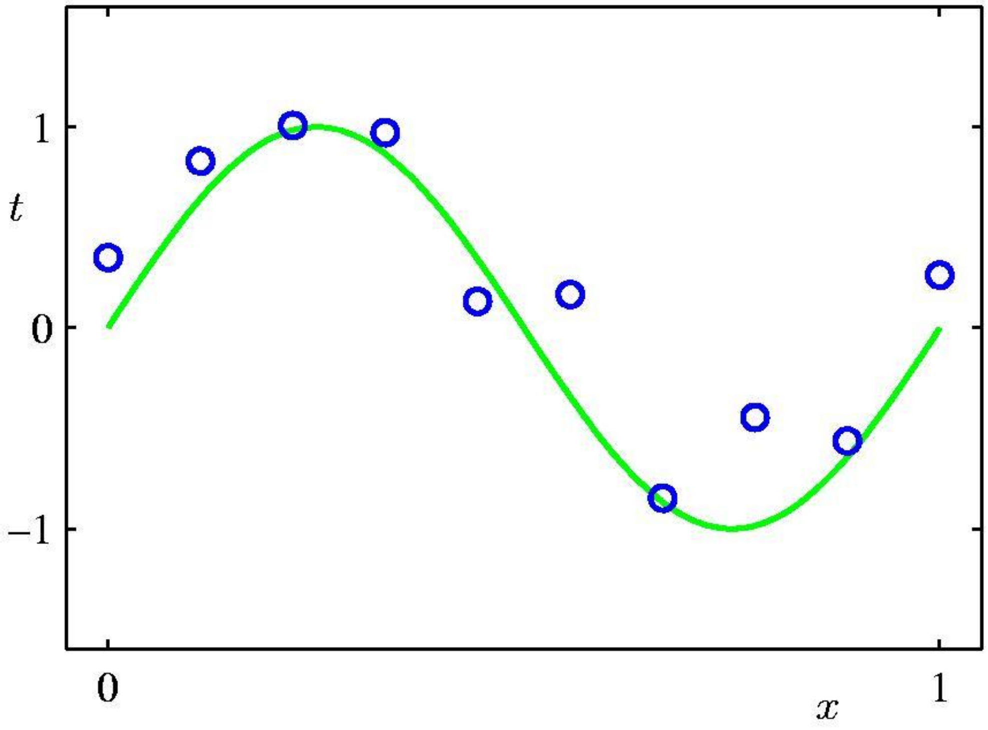


Example

Handwritten Digit Recognition

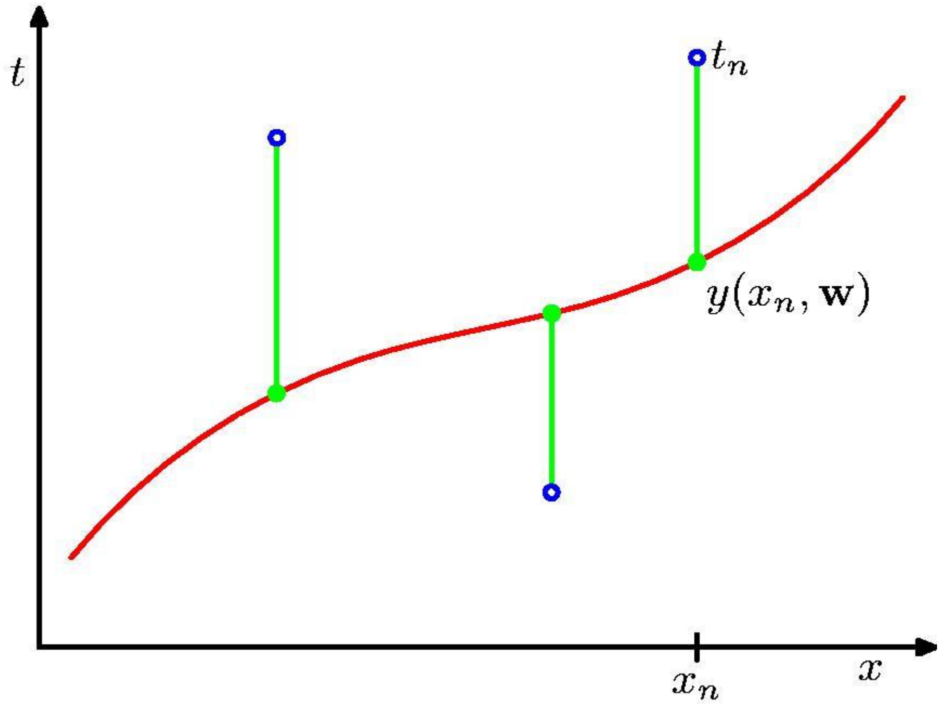


Polynomial Curve Fitting



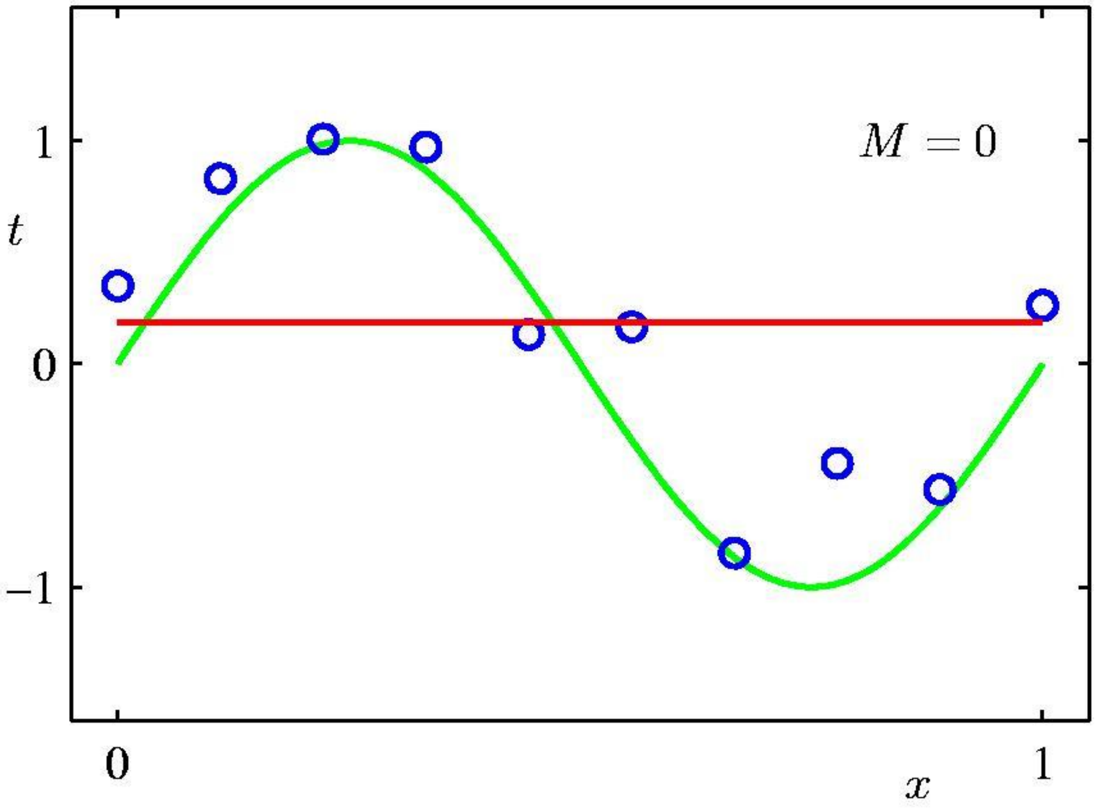
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Sum-of-Squares Error Function

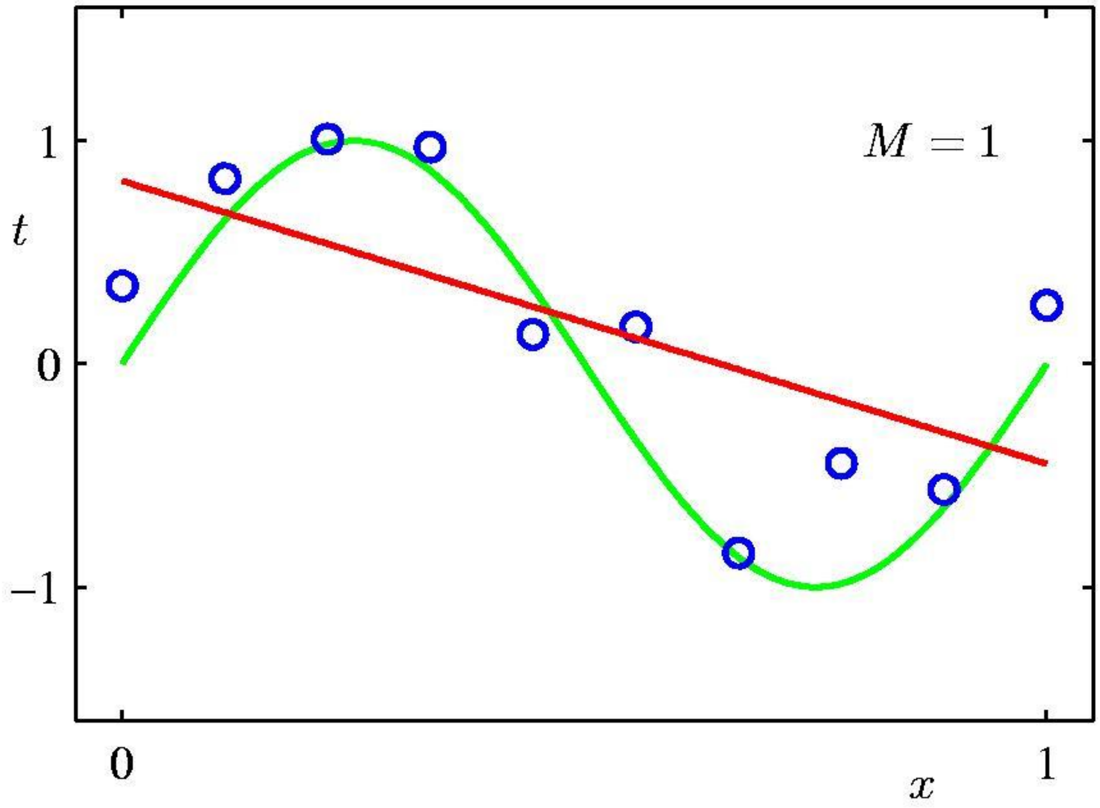


$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

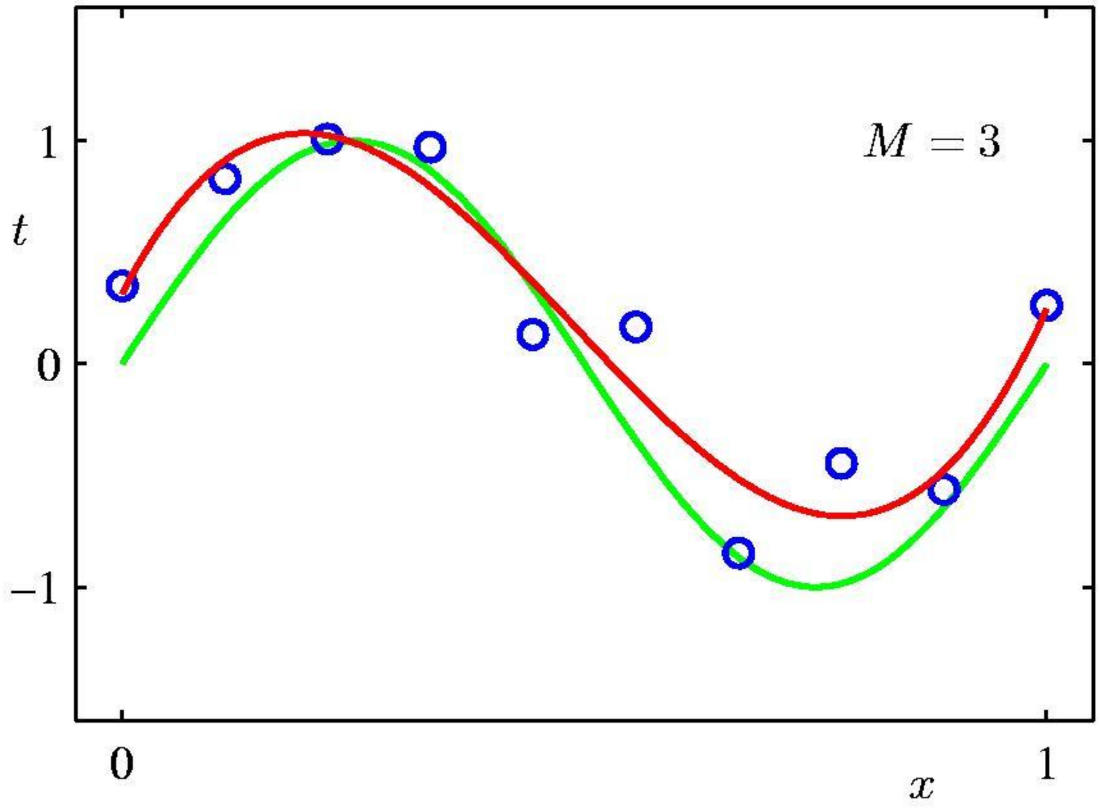
0^{th} Order Polynomial



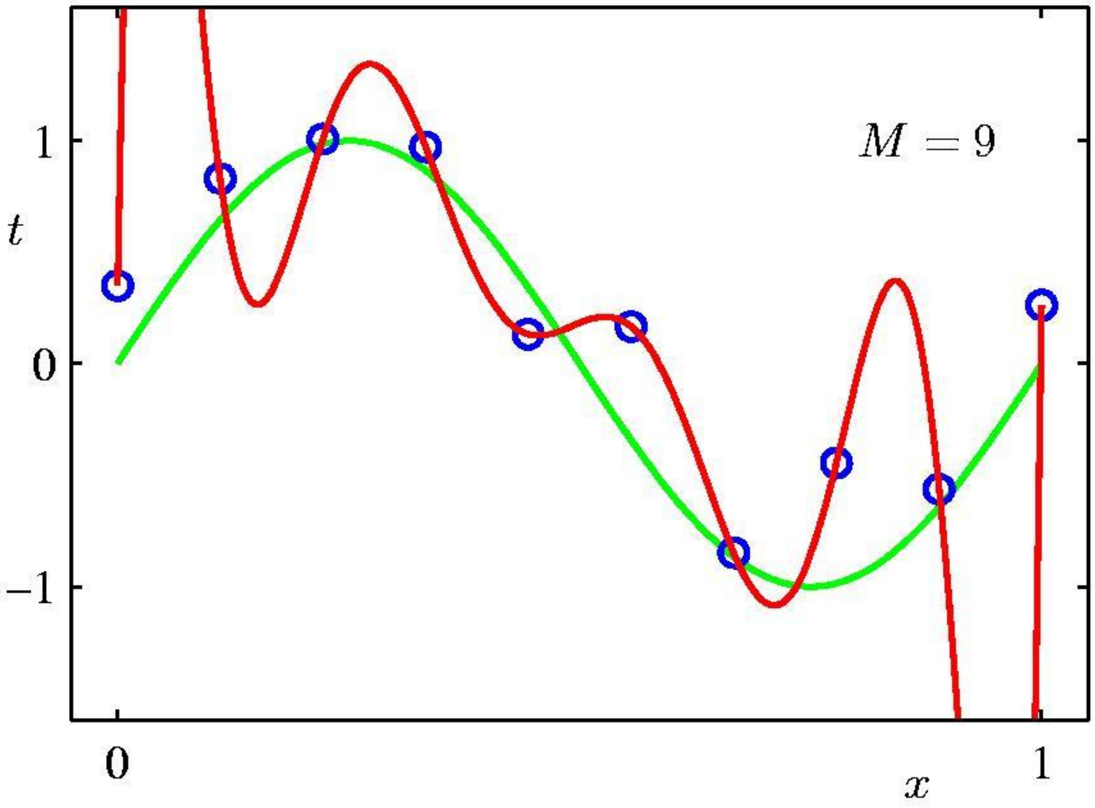
1st Order Polynomial



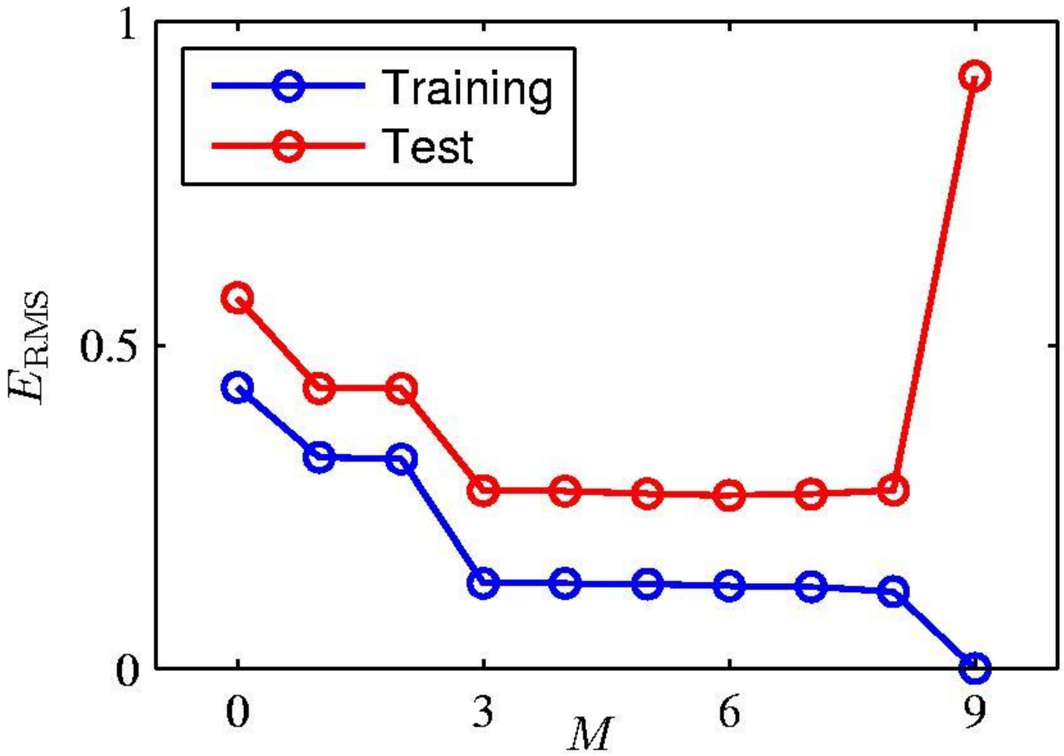
3rd Order Polynomial



9^{th} Order Polynomial



Over-fitting



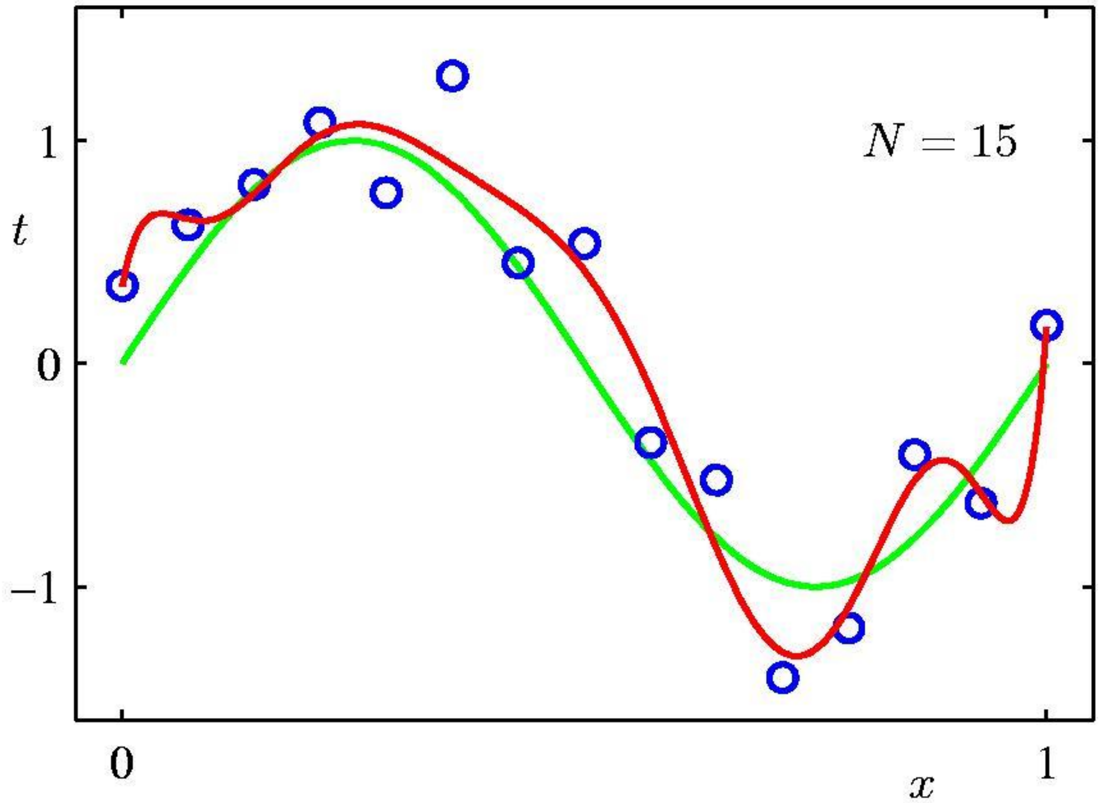
Root-Mean-Square (RMS) Error: $E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$

Polynomial Coefficients

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

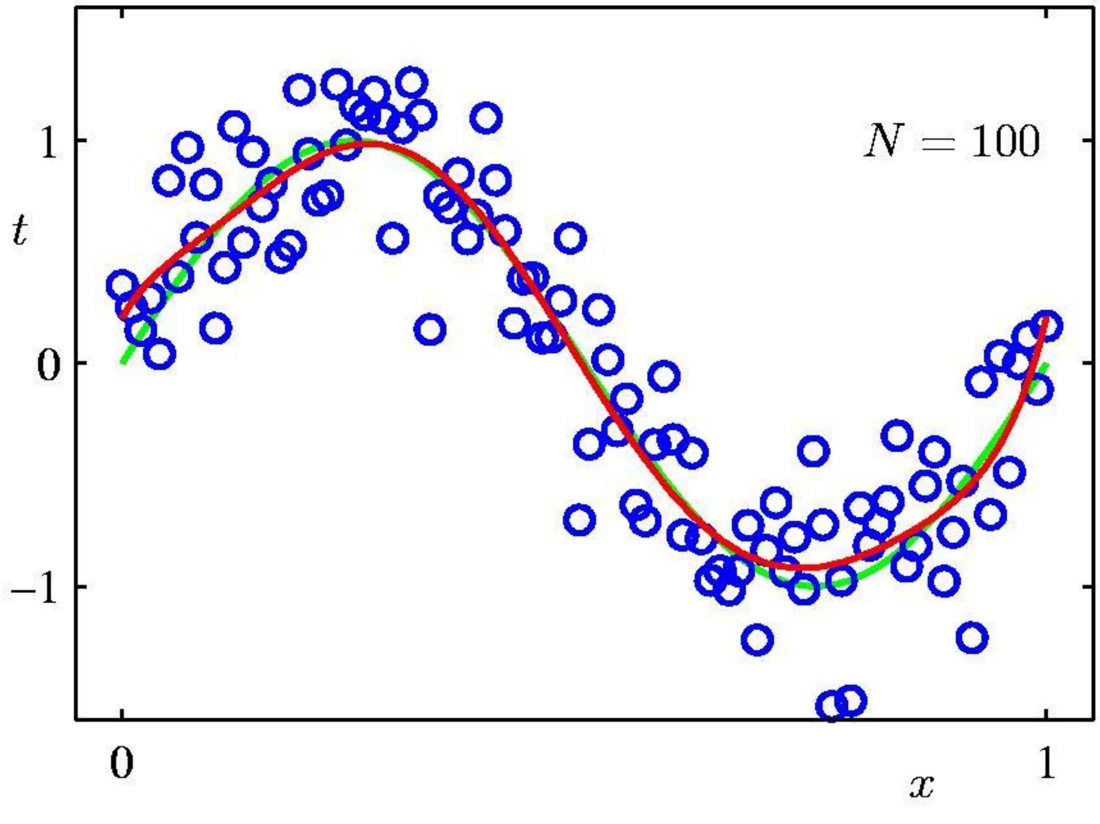
Data Set Size: $N = 15$

9th Order Polynomial



Data Set Size: $N = 100$

9th Order Polynomial

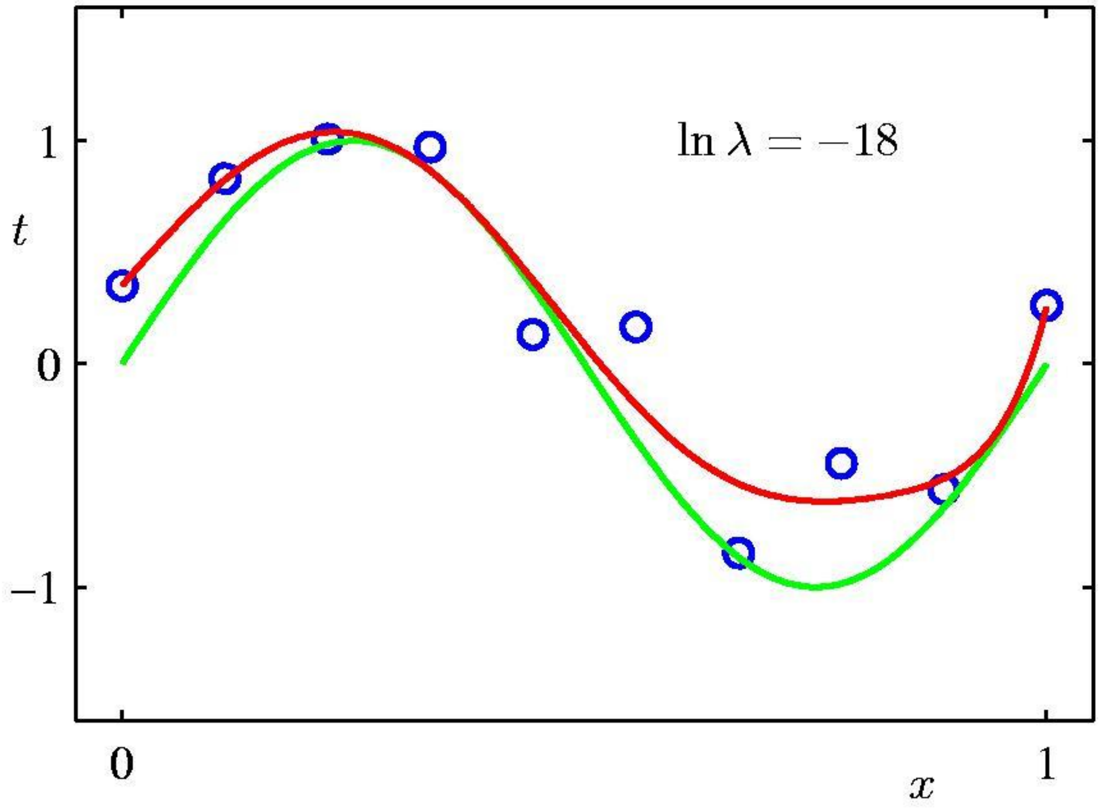


Regularization

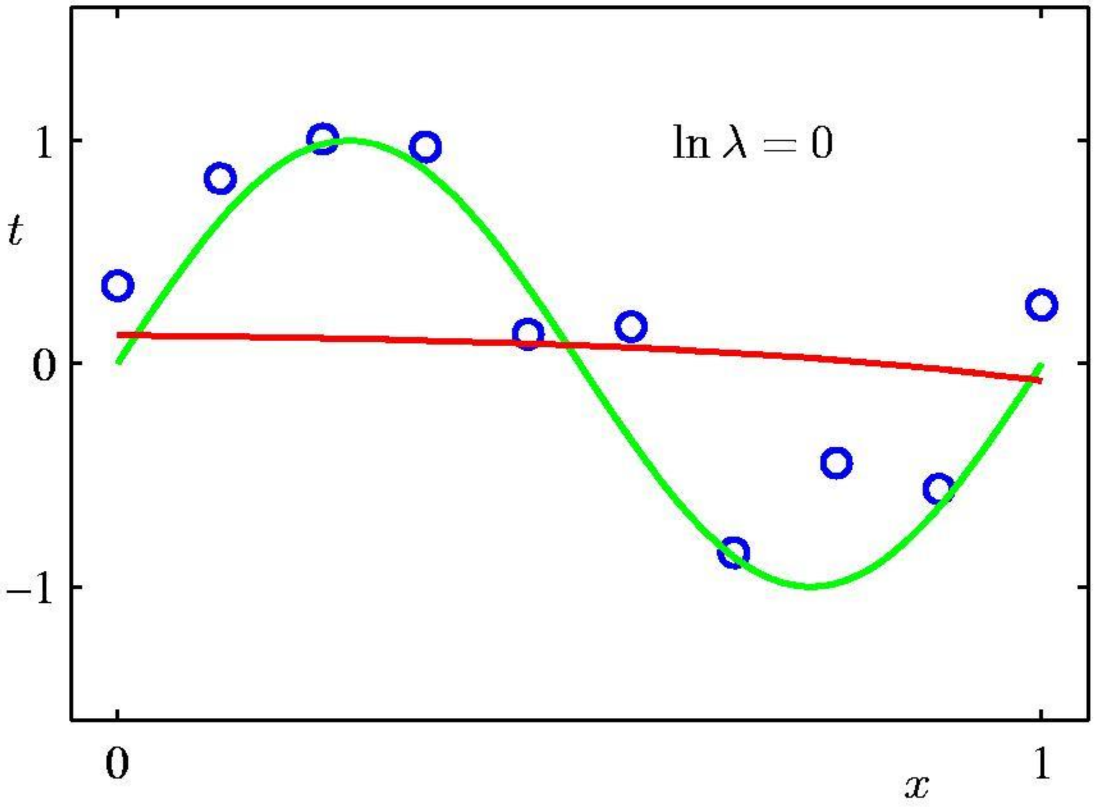
- Penalize large coefficient values

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

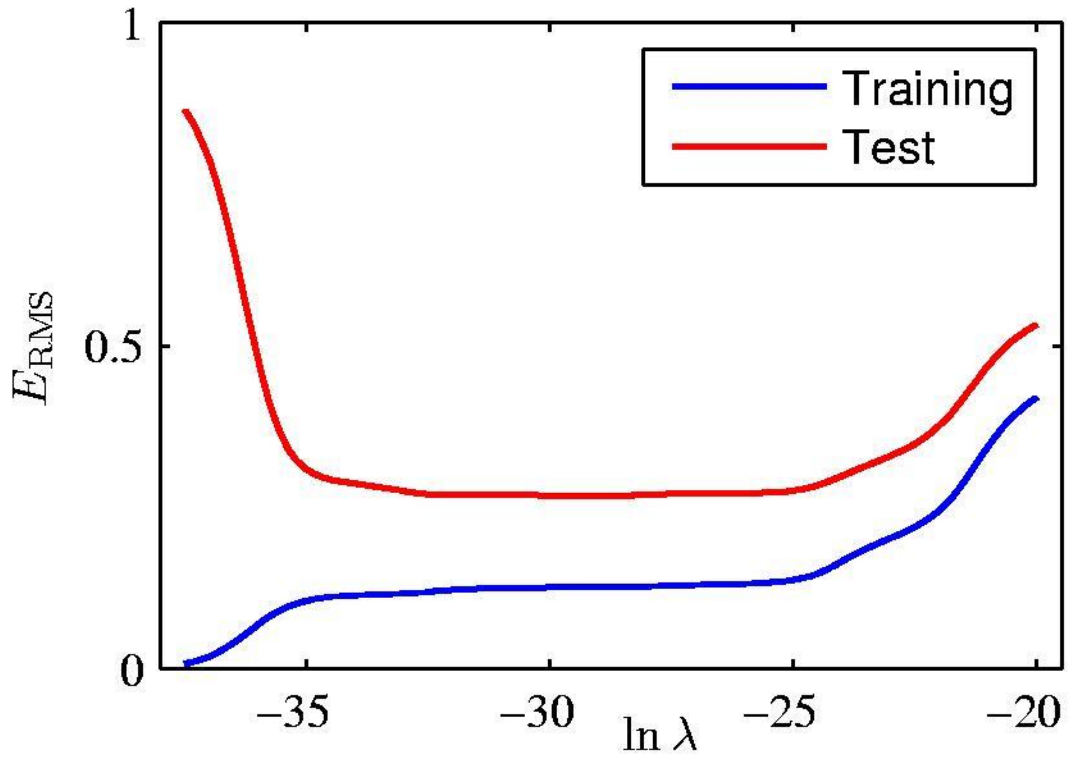
Regularization: $\ln \lambda = -18$



Regularization: $\ln \lambda = 0$



Regularization: E_{RMS} vs. $\ln\lambda$



What you need to know

- Point estimation:
  - Maximal Likelihood Estimation
  - Bayesian learning
  - Maximal a Posterior
- Gaussian estimation
- Regression
  - Basis function = features
  - Optimizing sum squared error
  - Relationship between regression and Gaussians
- Bias-Variance trade-off

Homework

- Python programming
  - 1-D regression

- Finish the “Gaussian parameters learning”
  - Please use google, ^_*

The End

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