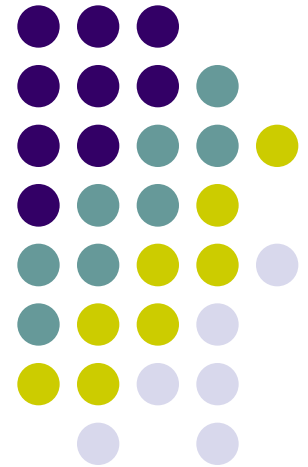
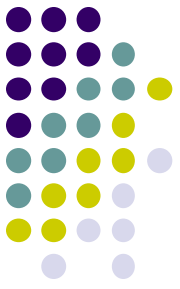


Point Estimation

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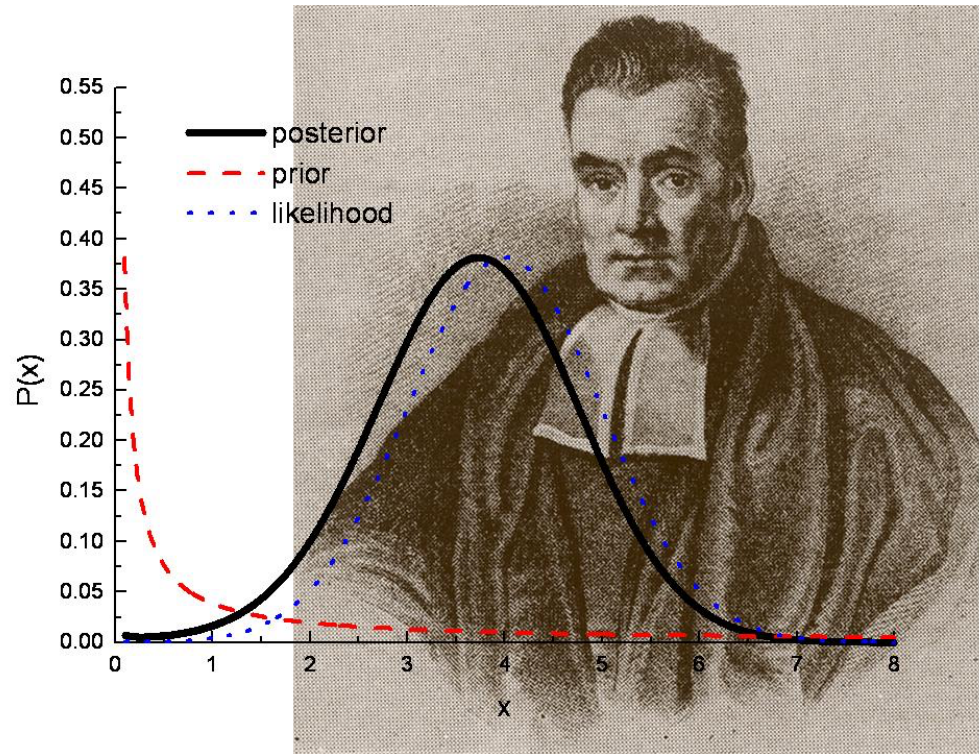
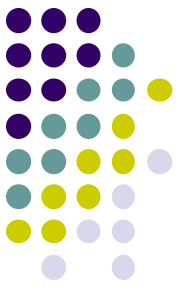
State Key Lab of CAD&CG, ZJU
2017-02-28





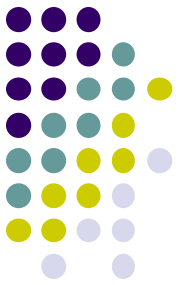
What you need to know

- Point estimation: (点估计)
 - Maximal Likelihood Estimation (MLE)
 - Bayesian learning
 - Maximize A Posterior (MAP)
- Gaussian estimation
- Regression (回归)
 - Basis function = features
 - Optimizing sum squared error
 - Relationship between regression and Gaussians
- Bias-Variance trade-off



点估计是非常重要的数据计算技术，是需要在入门阶段重点掌握的

Point estimation

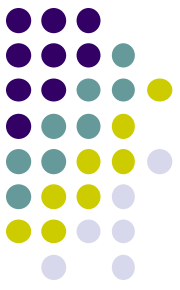


Your first consulting job

- 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...



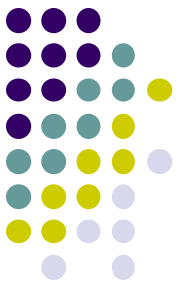
Binomial Distribution

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

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

- 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

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



Maximum Likelihood Estimation

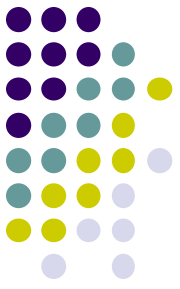
- **Data:** Observed set D of α_H Heads and α_T Tails
- **Hypothesis:** Binomial distribution
- **Learning θ is an optimization problem**
 - What's the objective function?

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

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

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

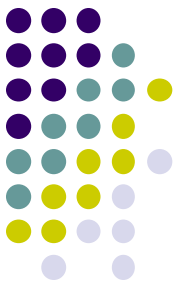
Maximum Likelihood Estimation (cont.)



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

- Set derivative to zero:

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

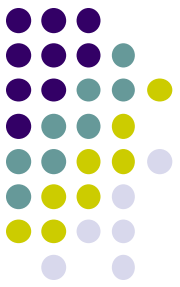


How many flips do I need?

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

- B: I flipped 2 heads and 3 tails.
- Y: $1 - \theta = 3/5$, 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 Höfding's inequality)



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

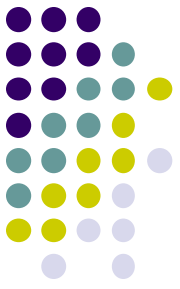
<http://omega.albany.edu:8008/machine-learning-dir/notes-dir/vc1/vc-l.html>

- Let θ^* be the true parameter, for any $\varepsilon > 0$:

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

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

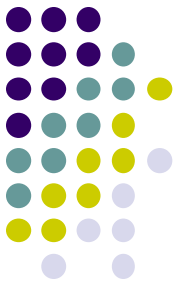
$$N \geq 270; (\varepsilon = 0.1, \delta = 0.01)$$



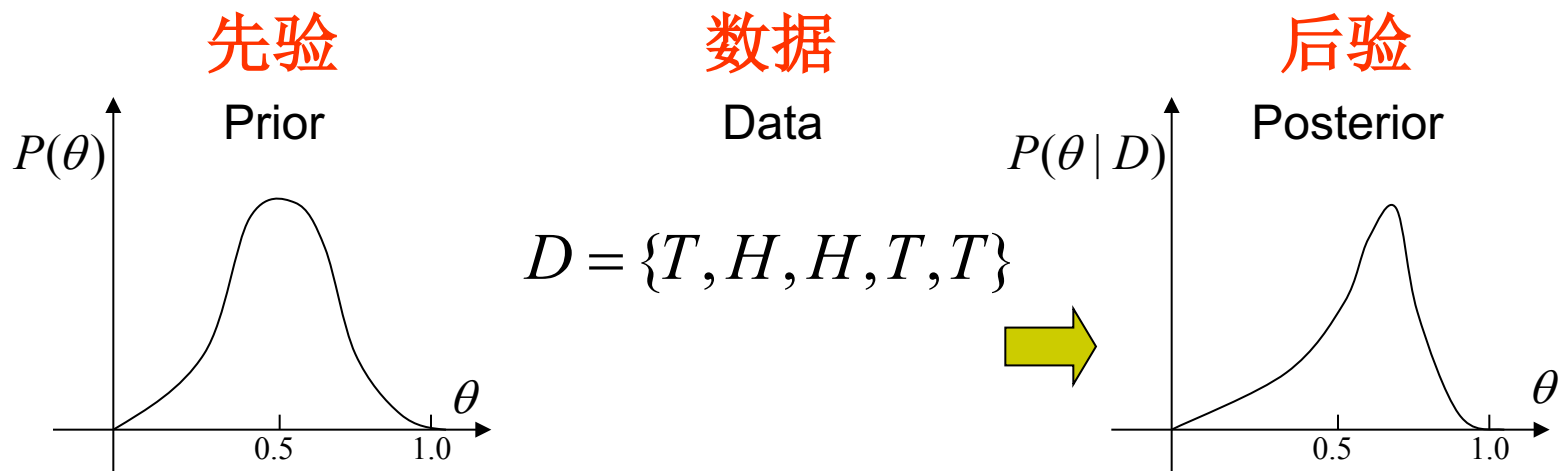
PAC Learning

- **PAC: Probably Approximate Correct**
- B: I want to know the thumbtack parameter θ , within $\varepsilon = 0.1$, with probability at least $1 - \delta = 0.99$. 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





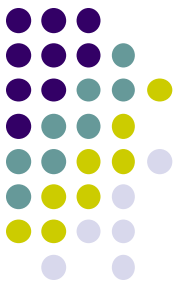
Bayesian Learning

- Bayes rule:

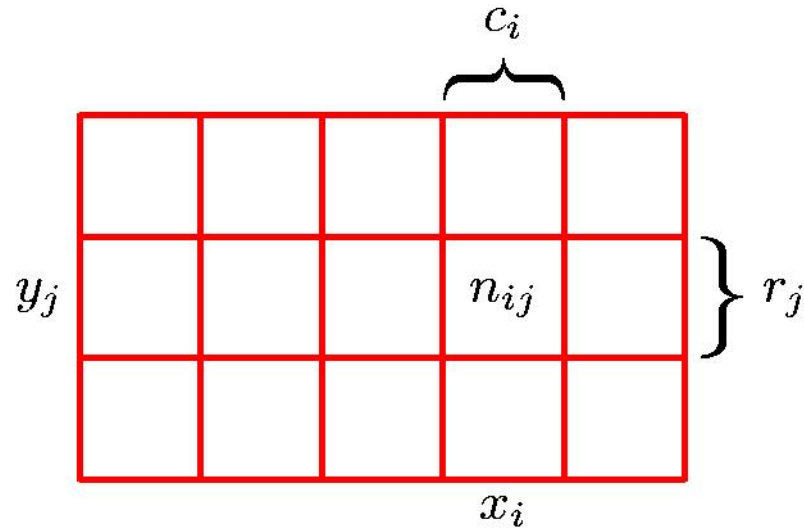
$$\text{Posterior} \rightarrow P(\theta | D) = \frac{\overset{\text{Prior}}{\downarrow} P(\theta) \overset{\text{Likelihood}}{\downarrow} P(D | \theta)}{P(D) \leftarrow \begin{array}{l} \text{Data distribution} \\ \text{evidence} \\ \text{(Normalization)} \end{array}}$$

- Or equivalently:

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



Probability Theory

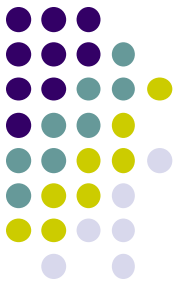


• Sum Rule

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

Product Rule

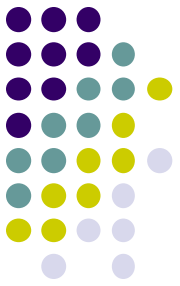
$$\begin{aligned} p(X = x_i, Y = y_j) &= \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N} \\ &= p(Y = y_j | X = x_i) p(X = x_i) \end{aligned}$$



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 $E(x) = \int x f(x) dx$
 - Covariance
 - $\text{cov}(x, y) = 0$, uncorrelatedness / irrelevant (统计无关)
 - Higher order moments

The Rules of Probability



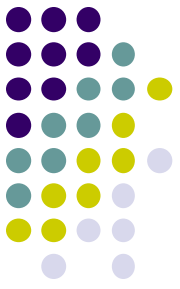
- Sum Rule

$$p(X) = \sum_Y p(X, Y)$$

- Product Rule

$$p(X, Y) = p(Y|X)p(X)$$

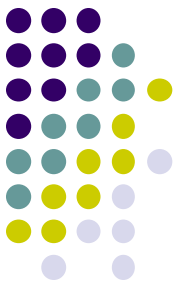
Bayes' Theorem



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

$$p(X) = \sum_Y p(X|Y)p(Y)$$

posterior \propto likelihood \times prior

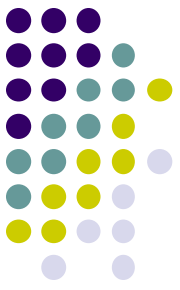


Bayesian Learning in our case

- Likelihood function is simply Binomial:

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

- 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 – $P(\theta)$

- Prior: Beta distribution

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

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

- Likelihood: Binomial distribution

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

- Posterior:

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



Using Bayesian posterior

- Posterior distribution:

$$P(\theta | D) \sim \text{Beta}(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

- Bayesian inference:

- No longer single parameter:

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

- Integral, ☹️



Expectation (数学期望)

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

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

MAP:

Maximum a posteriori approximation

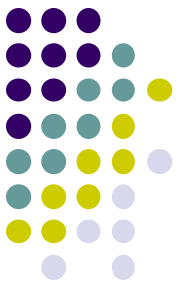


$$P(\theta | D) \sim \text{Beta}(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta | D) d\theta \leftarrow \text{approximation}$$

- MAP: use most likely parameter

$$\hat{\theta} = \arg \max_{\theta} P(\theta | D) \quad E[f(\theta)] \approx f(\hat{\theta}) \leftarrow$$



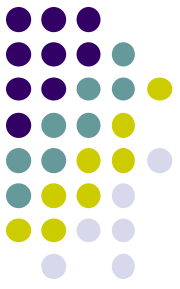
MAP for Beta distribution

$$P(\theta | D) \sim \text{Beta}(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

- MAP: use most likely parameter

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

- 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
 - $P(\theta) \sim 0.4\text{Beta}(20,1) + 0.4\text{Beta}(1,20) + 0.2\text{Beta}(2,2)$

Multinomial distribution



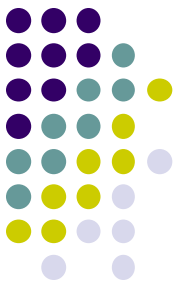
- B: Now if I give you a dice (骰子), then ...
- Y: I can solve this problem in a similar way.
- Likelihood:

$$P(X = x^k | \boldsymbol{\theta}) = \theta_k, \quad k = 1, 2, \dots, r,$$

$$\boldsymbol{\theta} = \{\theta_1, \dots, \theta_r\}, \quad \theta_1 + \dots + \theta_r = 1$$

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

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



Multinomial distribution

- Conjugate prior (Dirichlet distribution):

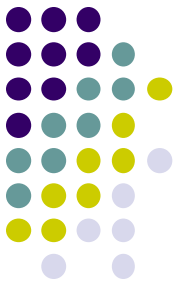
$$P(\boldsymbol{\theta}) = \text{Dir}(\boldsymbol{\theta} \mid \alpha_1, \dots, \alpha_r) = \frac{\Gamma(\alpha)}{\prod_{k=1}^r \Gamma(\alpha_k)} \prod_{k=1}^r \theta_k^{\alpha_k - 1}, \quad \alpha = \sum_{k=1}^r \alpha_k$$

- Solution:

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

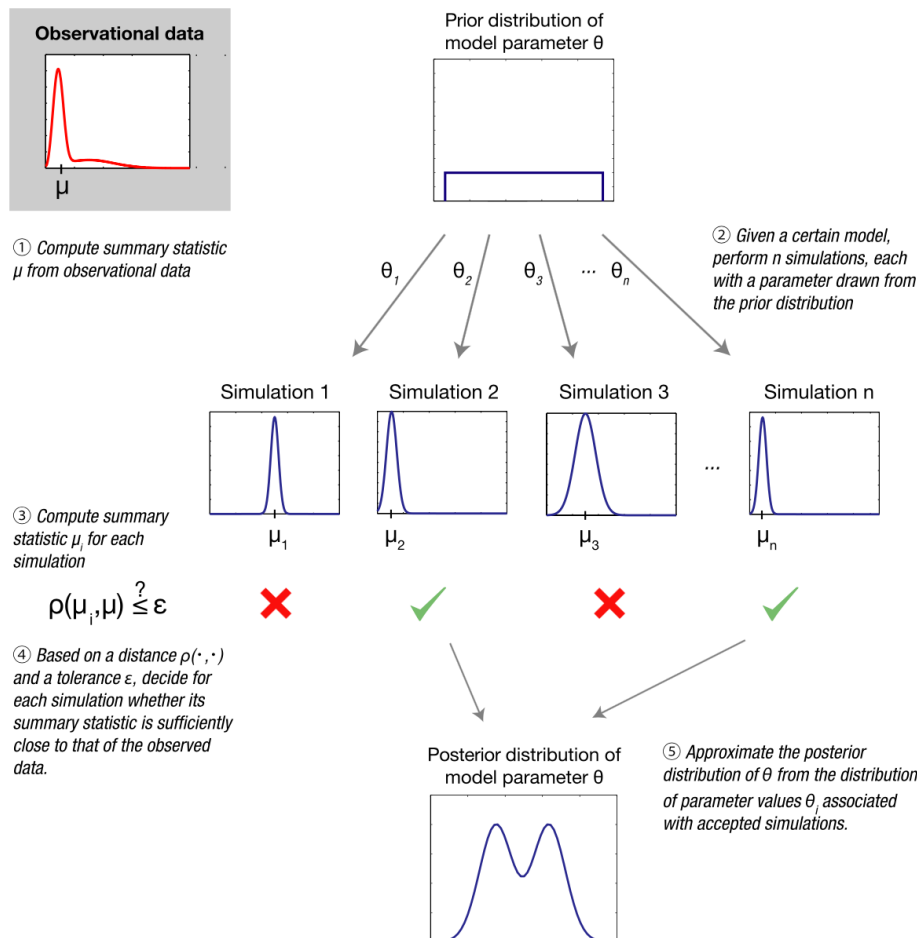
- Important fact:

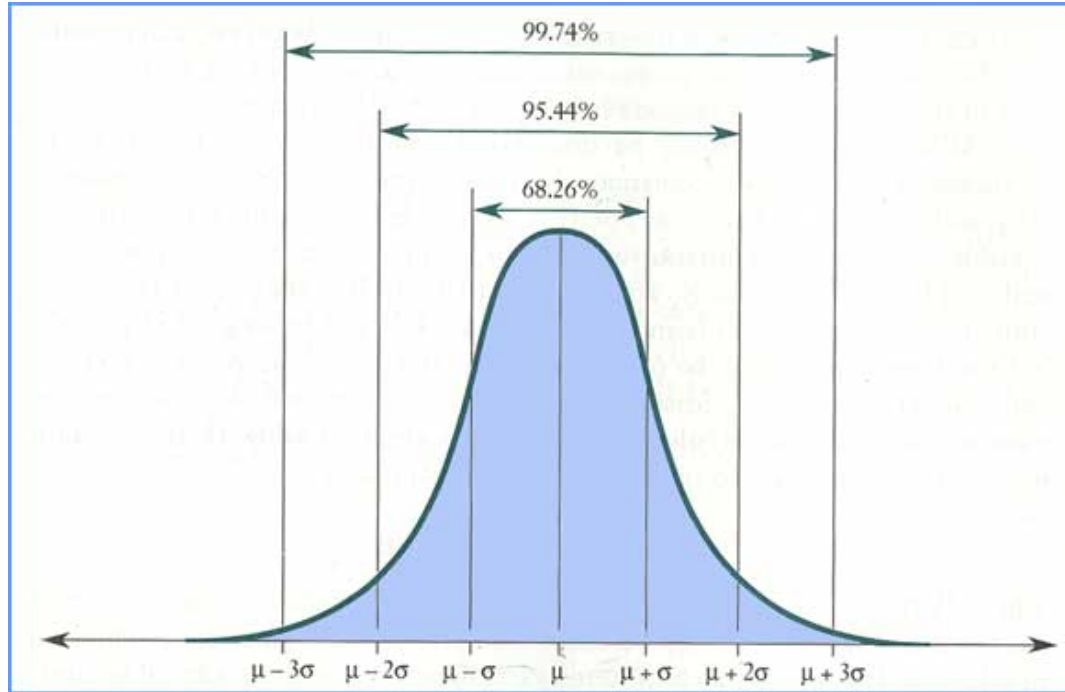
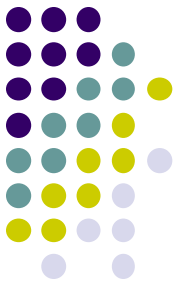
$$P(D) = \frac{\Gamma(\alpha)}{\Gamma(\alpha + N)} \prod_{k=1}^r \frac{\Gamma(\alpha_k + N_k)}{\Gamma(\alpha_k)}$$



Beyond MAP: Approximate Bayesian Computation

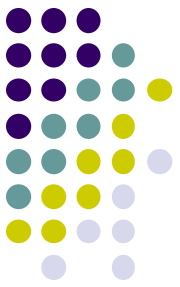
- Approximate Bayesian Computational methods [[ARXIV](#)]
- Approximate Bayesian Computation (ABC) in practice [[PDF](#)]





在数据处理中，高斯分布无处不在

Gaussian distribution



Gaussian distribution

均值

mean

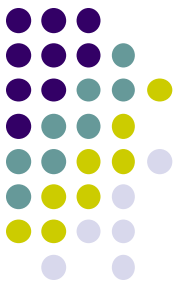
Continuous random variable:

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

variance Normalization

方差

Consider the difference between continuous and discrete variables?



MLE for Gaussian

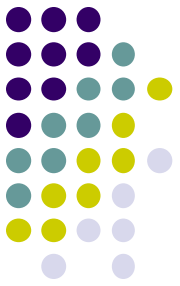
- Prob. of i.i.d. samples $D = \{x_1, x_2, \dots, x_N\}$

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

- The magic of log (to log-likelihood)

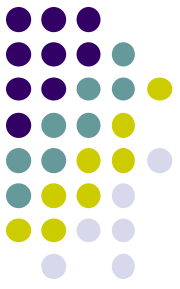
$$\begin{aligned} \ln P(D | \mu, \sigma) &= \ln \left(\frac{1}{\sigma \sqrt{2\pi}} \right)^N \prod_{i=1}^N e^{\frac{-(x_i - \mu)^2}{2\sigma^2}} \\ &= -N \ln(\sigma \sqrt{2\pi}) - \sum_{i=1}^N \frac{(x_i - \mu)^2}{2\sigma^2} \end{aligned}$$

MLE for mean of a Gaussian



$$\begin{aligned}\frac{\partial}{\partial \mu} \ln P(D | \mu, \sigma) &= \frac{\partial}{\partial \mu} \ln \left(\frac{1}{\sigma \sqrt{2\pi}} \right)^N \prod_{i=1}^N e^{-\frac{(x_i - \mu)^2}{2\sigma^2}} \\ &= \frac{\partial}{\partial \mu} - \sum_{i=1}^N \frac{(x_i - \mu)^2}{2\sigma^2} \\ &= \sum_{i=1}^N \frac{(x_i - \mu)}{\sigma^2} = 0\end{aligned}$$

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

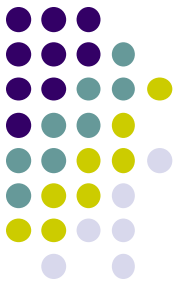


MLE for variance of a Gaussian

$$\begin{aligned}\frac{\partial}{\partial \sigma} \ln P(D | \mu, \sigma) &= \frac{\partial}{\partial \sigma} \ln \left(\frac{1}{\sigma \sqrt{2\pi}} \right)^N \prod_{i=1}^N e^{-\frac{(x_i - \mu)^2}{2\sigma^2}} \\ &= \frac{\partial}{\partial \sigma} [-N \ln \sigma \sqrt{2\pi}] - \sum_{i=1}^N \frac{\partial}{\partial \sigma} \left[\frac{(x_i - \mu)^2}{2\sigma^2} \right] \\ &= -\frac{N}{\sigma} + \sum_{i=1}^N \frac{(x_i - \mu)^2}{\sigma^3} = 0\end{aligned}$$

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

Gaussian parameters learning

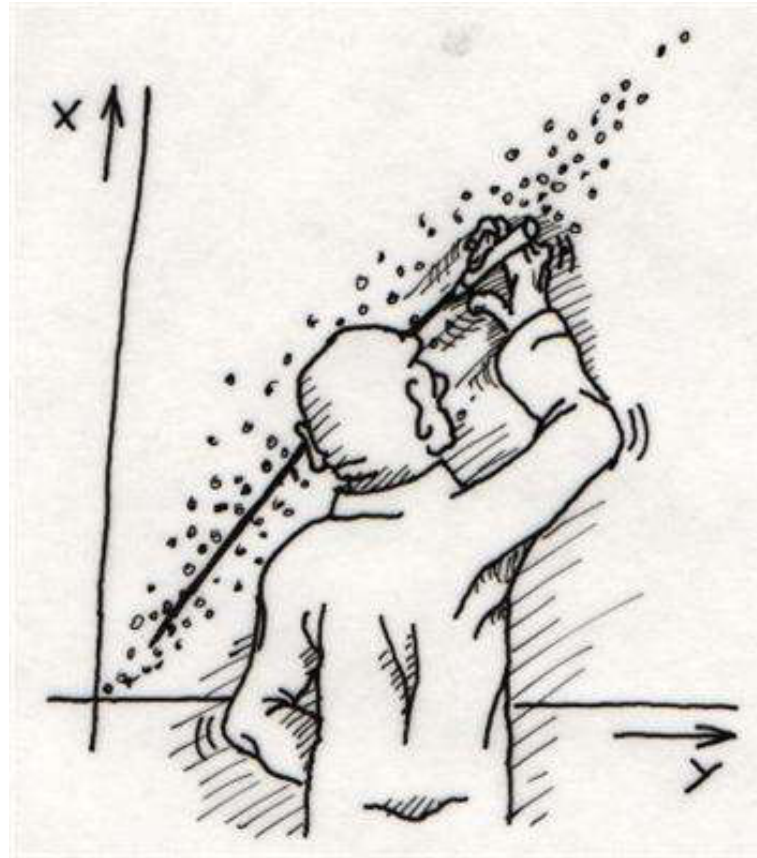
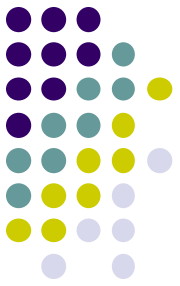


- MLE

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

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

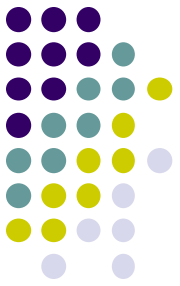
- Bayesian learning: prior?
- Conjugate priors:
 - Mean: Gaussian priors
 - Variance: Wishart Distribution



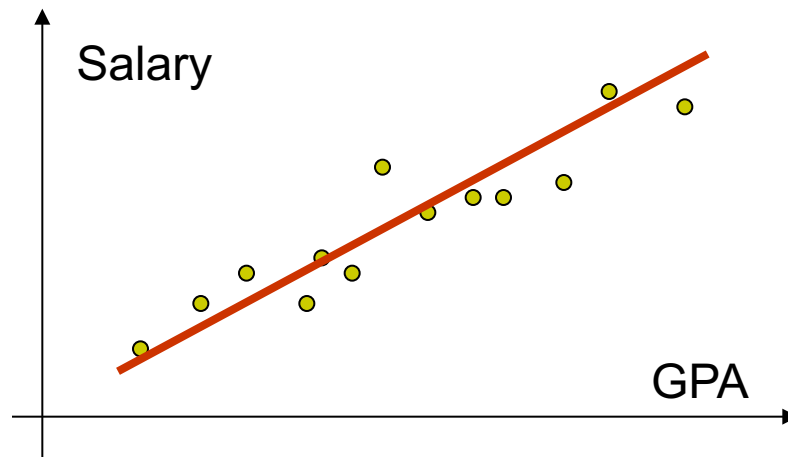
回归的思想，对于理解数据本身的特点与规律，是一种利器

Regression problems

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:** $\langle \mathbf{x}_i, t_i \rangle$
- **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 $H = \{h_1, \dots, h_k\}$
 - Find coefficients $\mathbf{w} = \{w_1, \dots, w_k\}$
- **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:

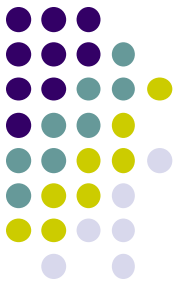
$$P(t \mid \mathbf{x}, \mathbf{w}, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{[t - \sum_i w_i h_i(x)]^2}{2\sigma^2}}$$

- Learn \mathbf{w} using MLE

Maximizing log-likelihood

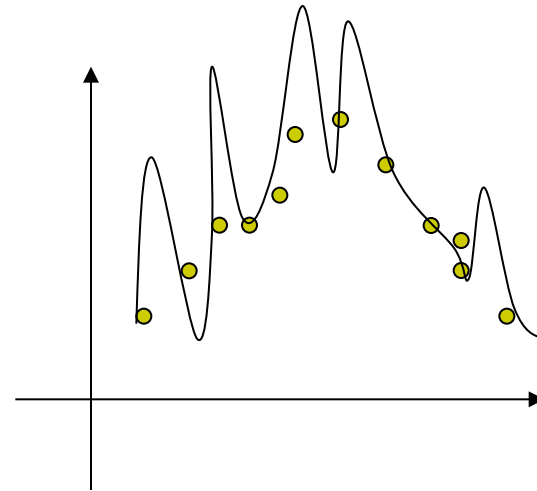
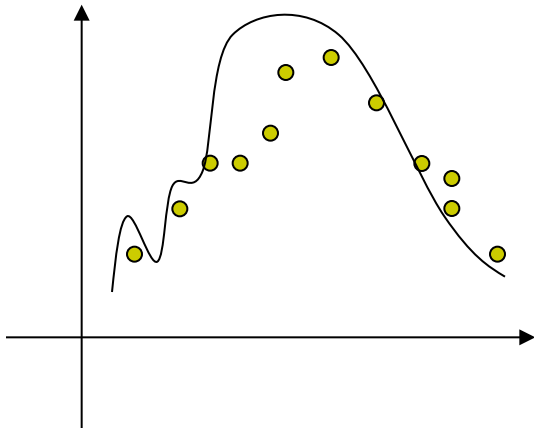


$$\ln P(D | \mathbf{w}, \sigma) = \ln \prod_j \left(\frac{1}{\sigma \sqrt{2\pi}} e^{\frac{-[t_j - \sum_i w_i h_i(x_j)]^2}{2\sigma^2}} \right)$$
$$\Rightarrow \min \sum_j \frac{-[t_j - \sum_i w_i h_i(x_j)]^2}{2\sigma^2}$$

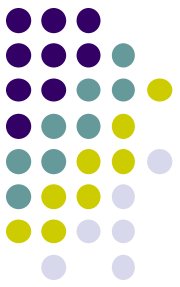


Bias-Variance Tradeoff

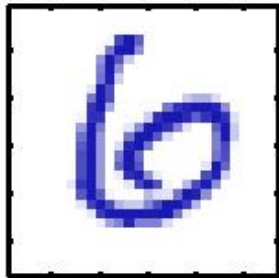
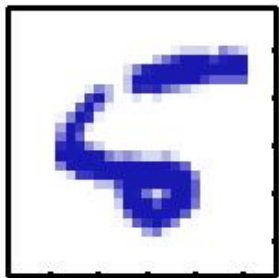
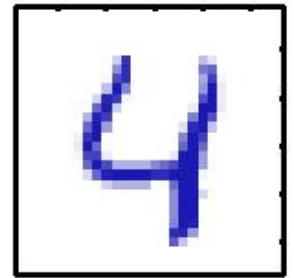
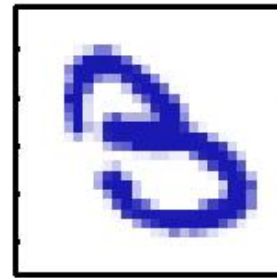
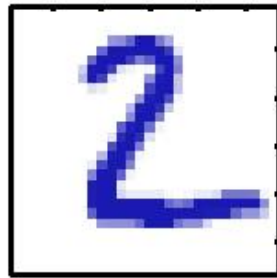
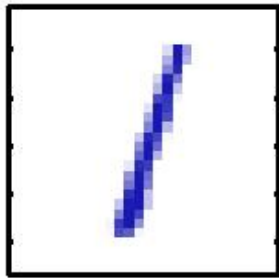
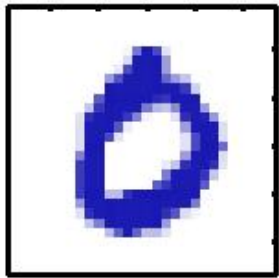
- Choice of hypothesis basis introduce learning bias:
 - More complex basis:
 - Less bias
 - More variance (over-fitting)



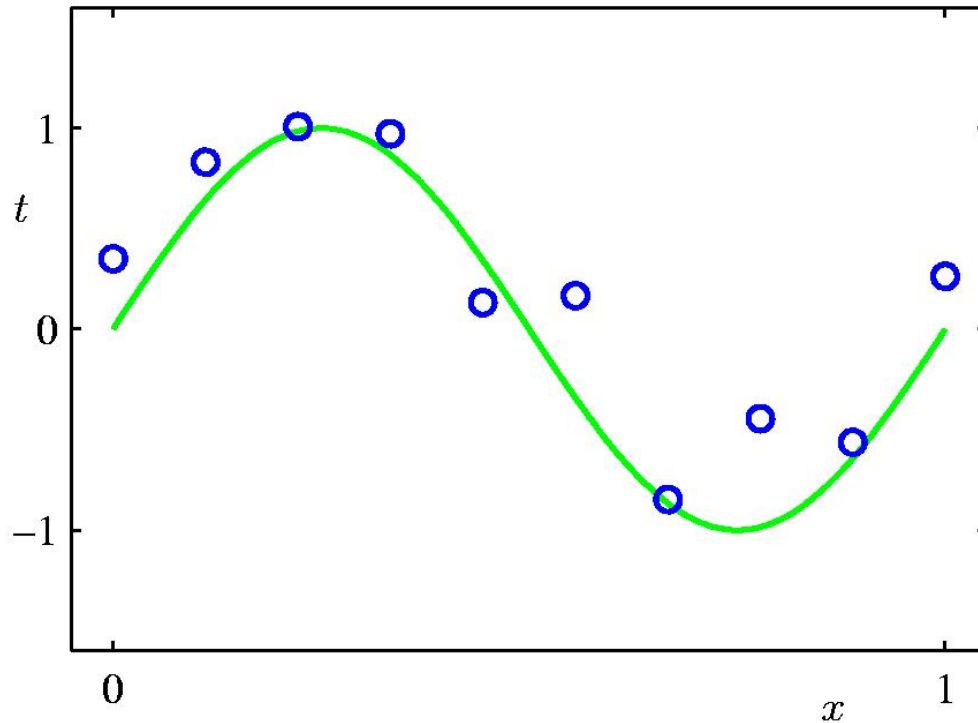
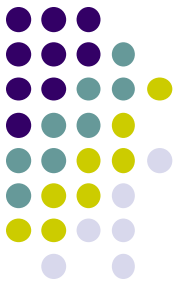
Example



Handwritten Digit Recognition

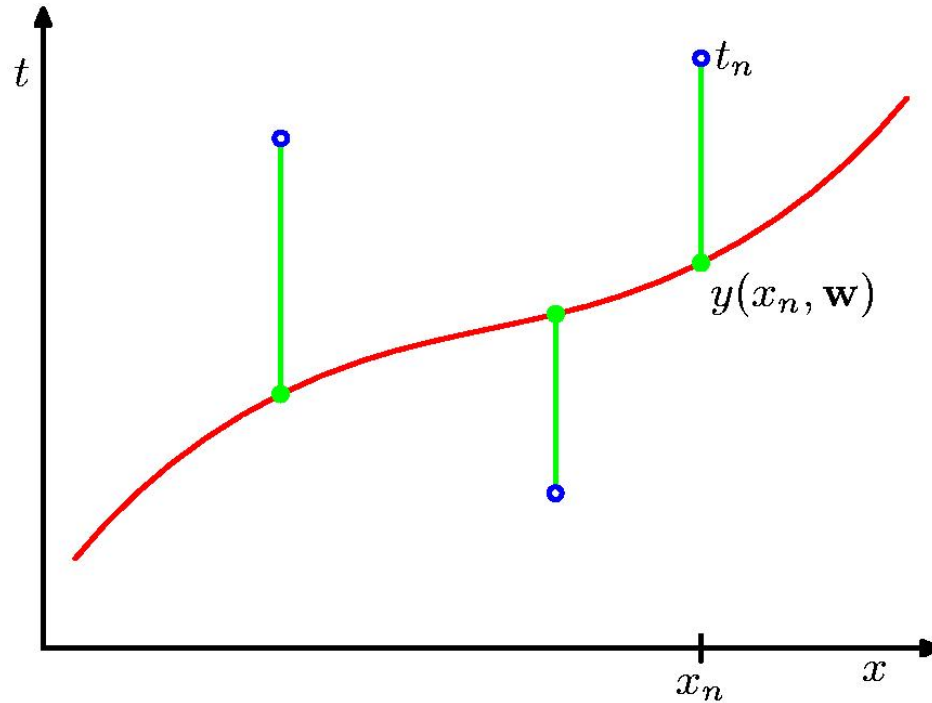
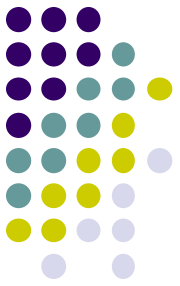


Polynomial Curve Fitting



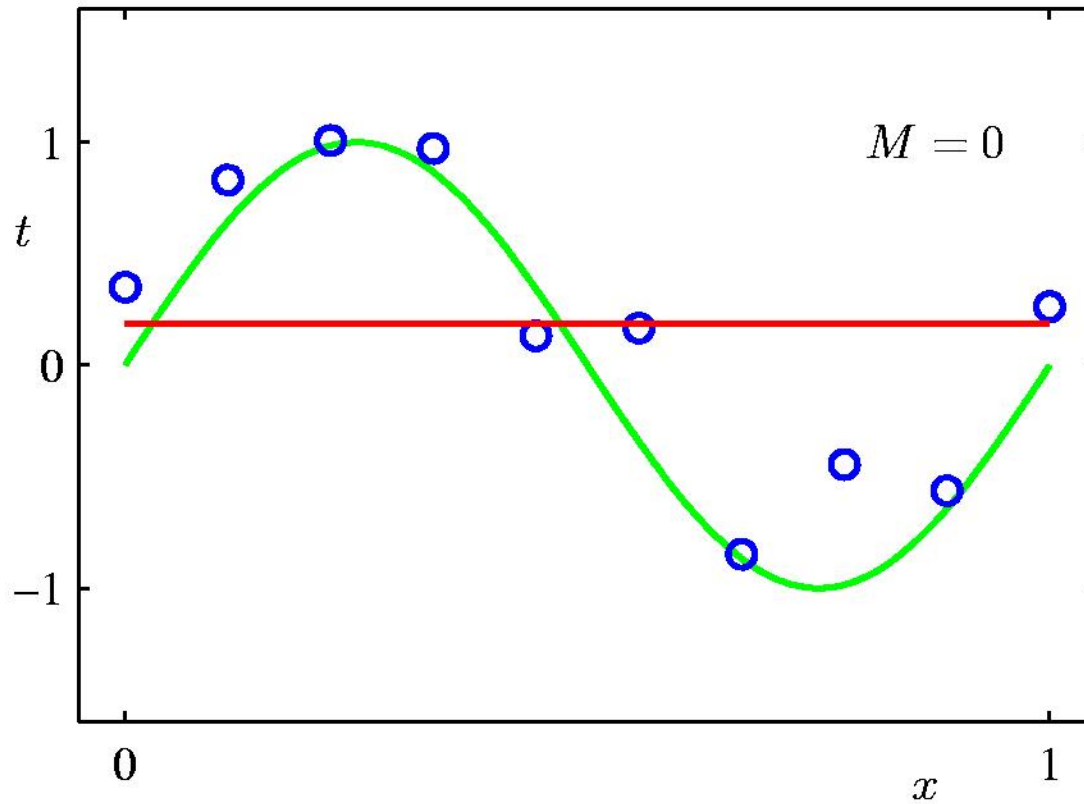
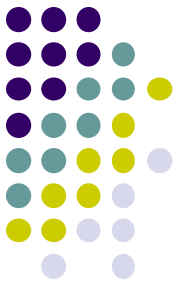
$$y(x, \mathbf{w}) = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M = \sum_{j=0}^M w_jx^j$$

Sum-of-Squares Error Function

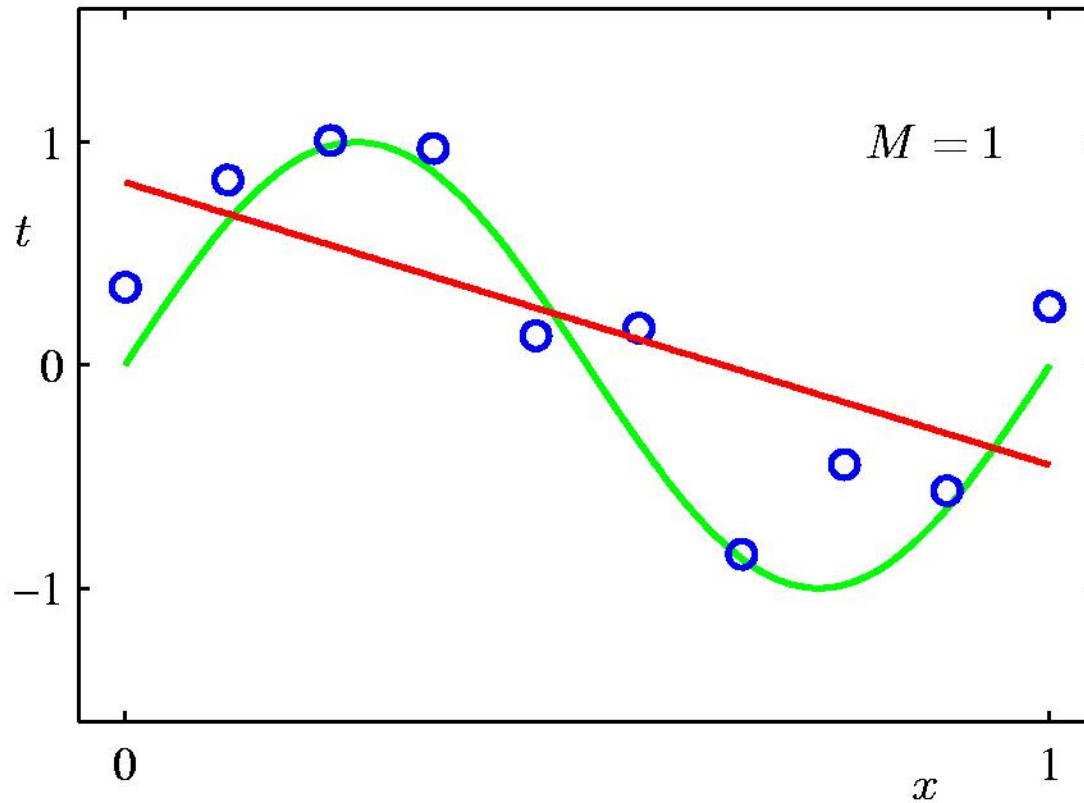
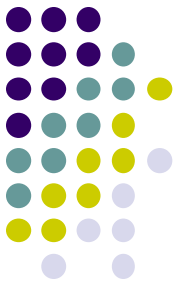


$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{y(x_n, \mathbf{w}) - t_n\}^2$$

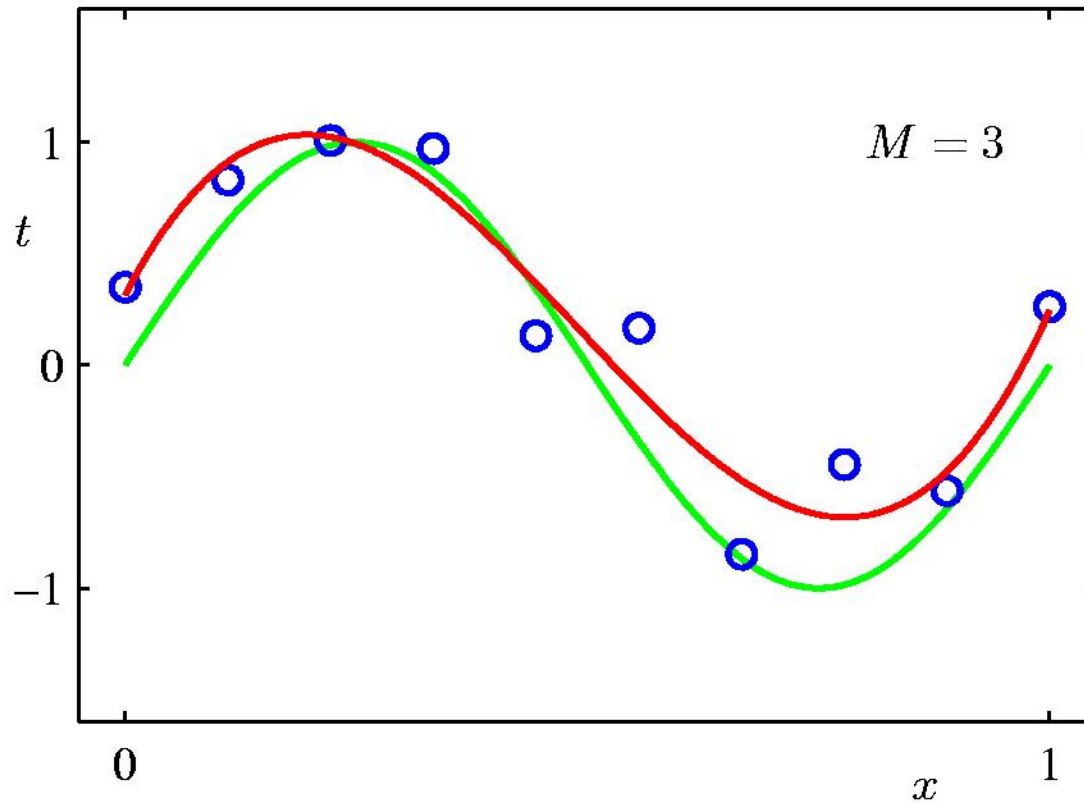
0th Order Polynomial



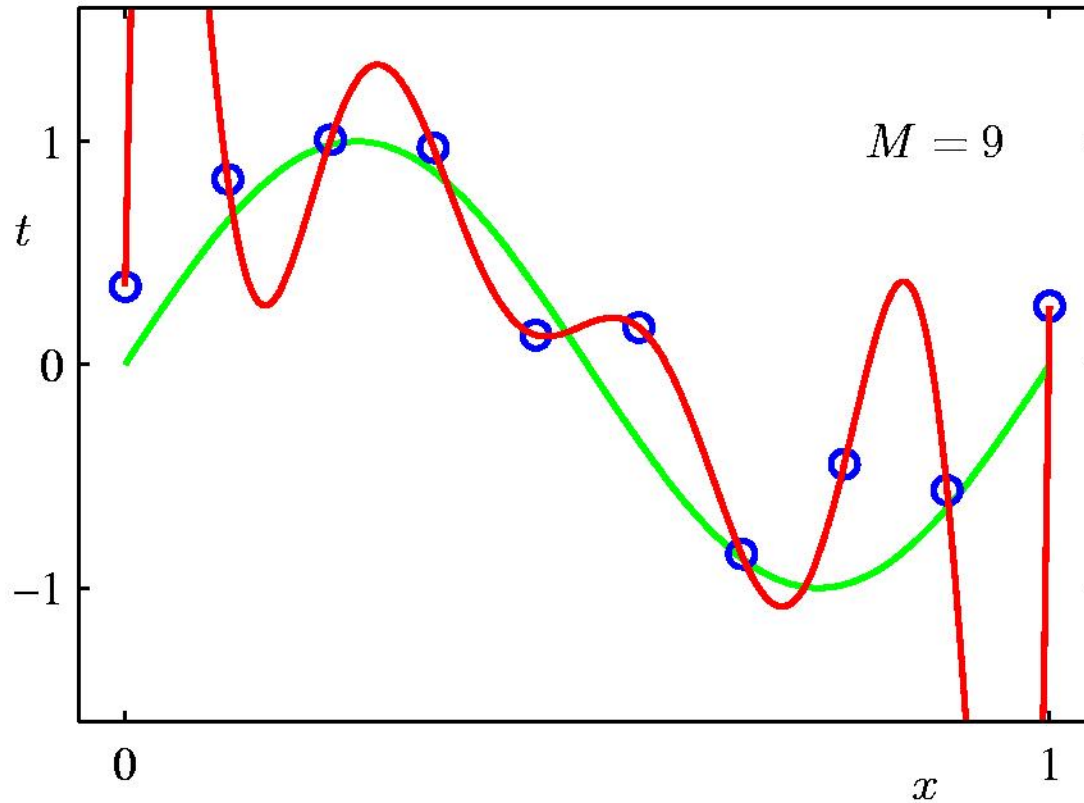
1st Order Polynomial



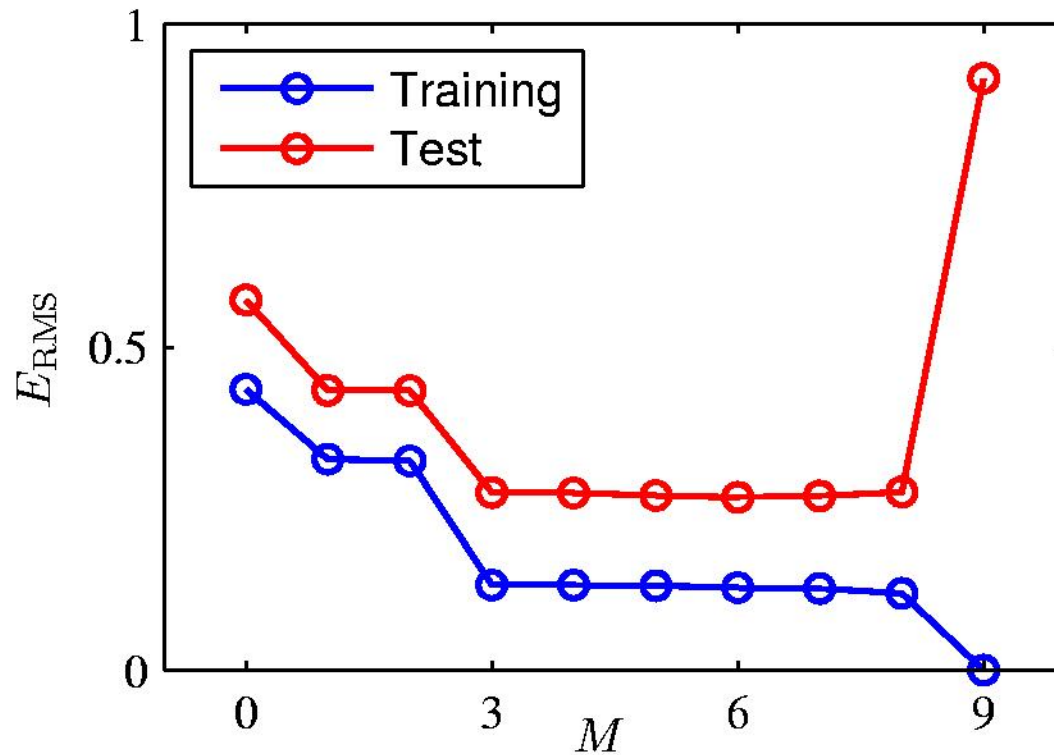
3rd Order Polynomial



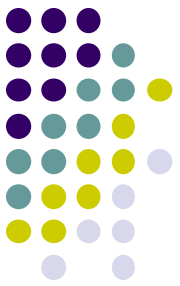
9th Order Polynomial



Over-fitting



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

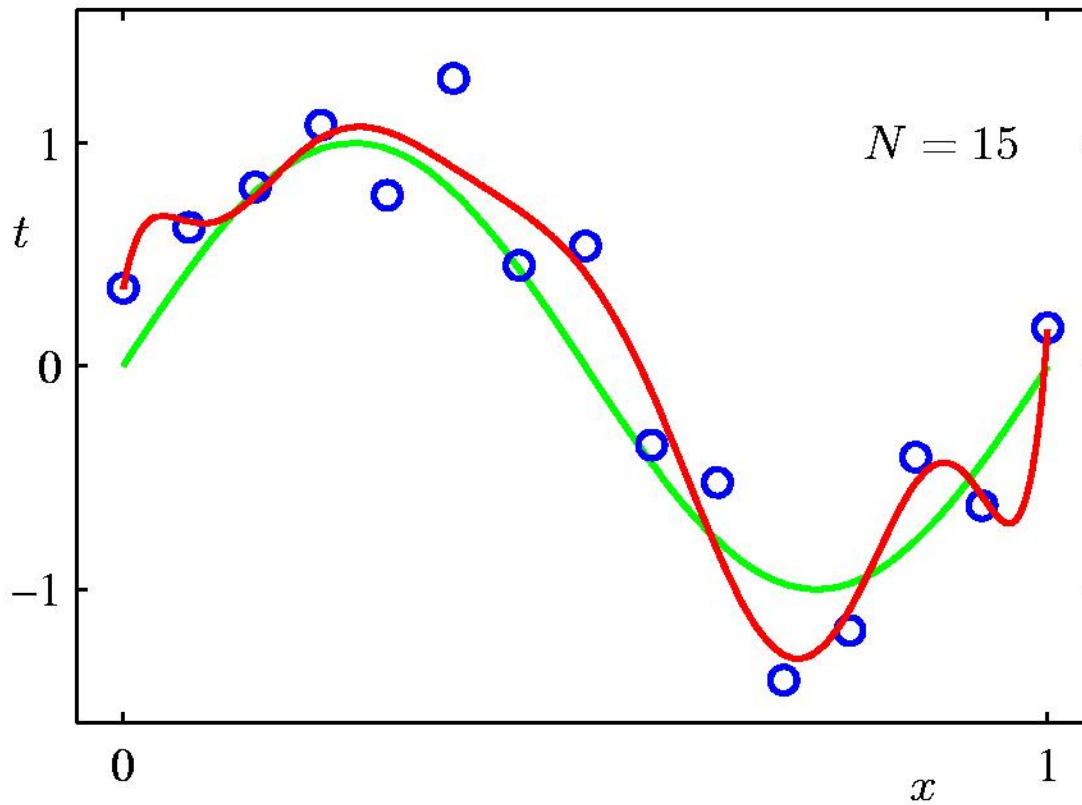
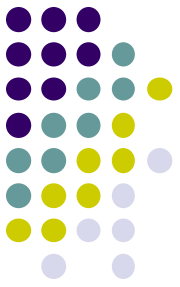


Polynomial Coefficients

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

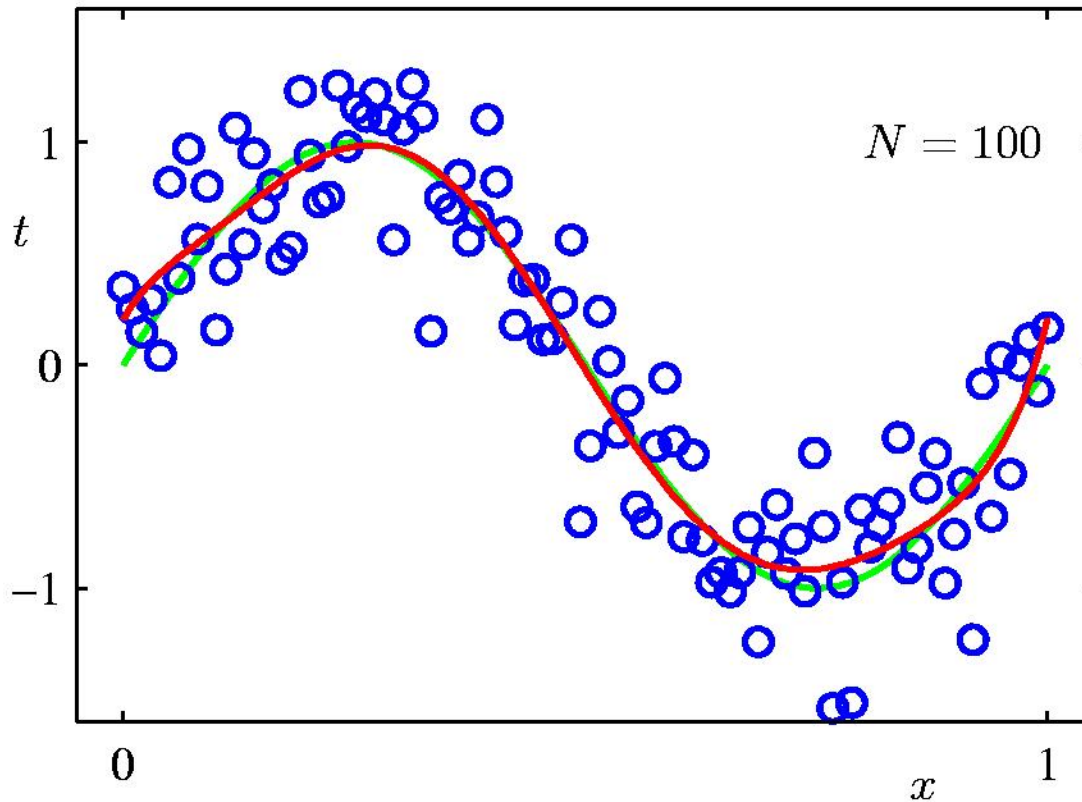
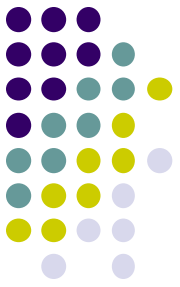
Data Set Size: $N = 15$

9th Order Polynomial

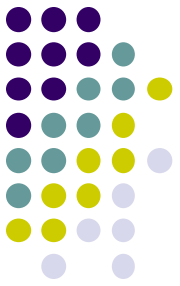


Data Set Size: $N = 100$

9th Order Polynomial



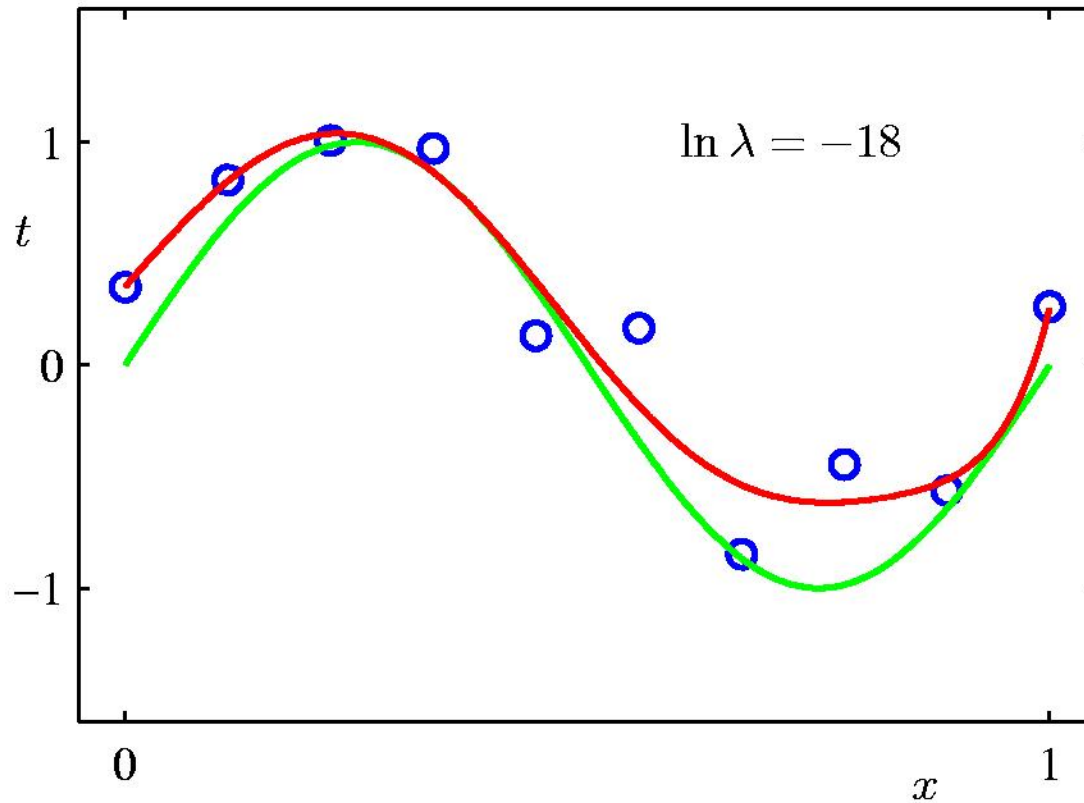
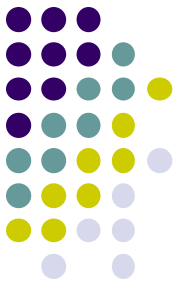
Regularization



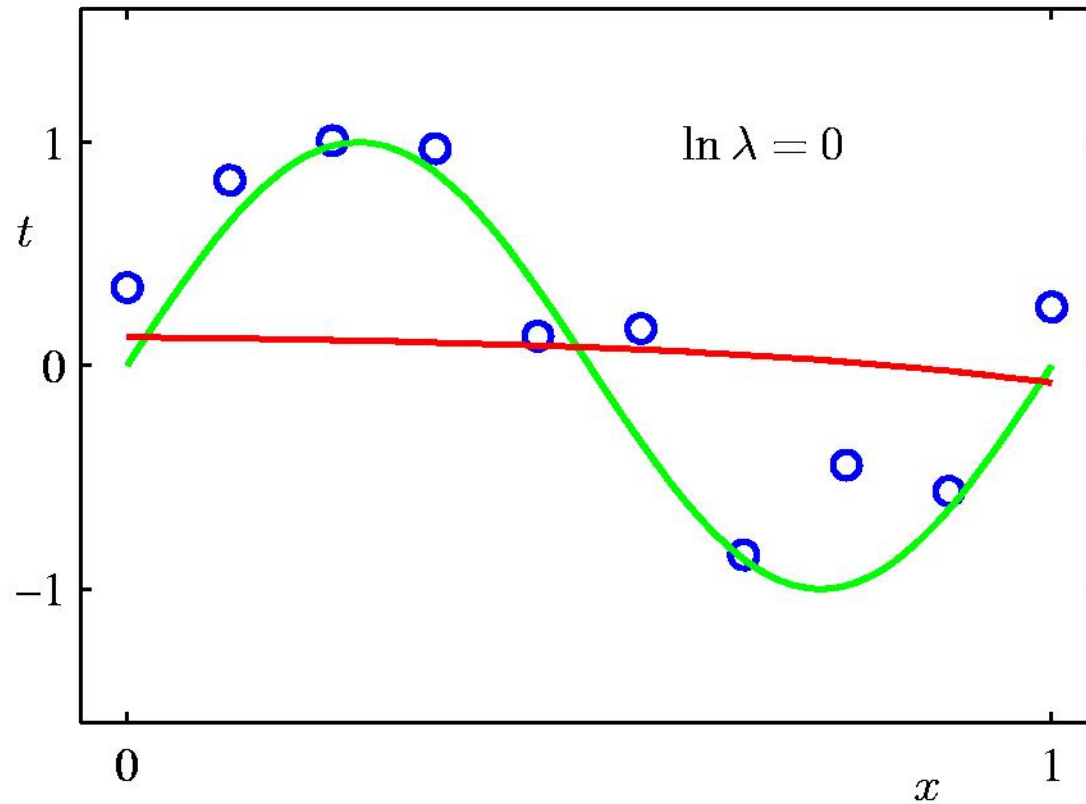
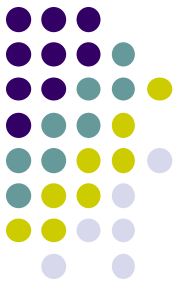
- Penalize large coefficient values

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

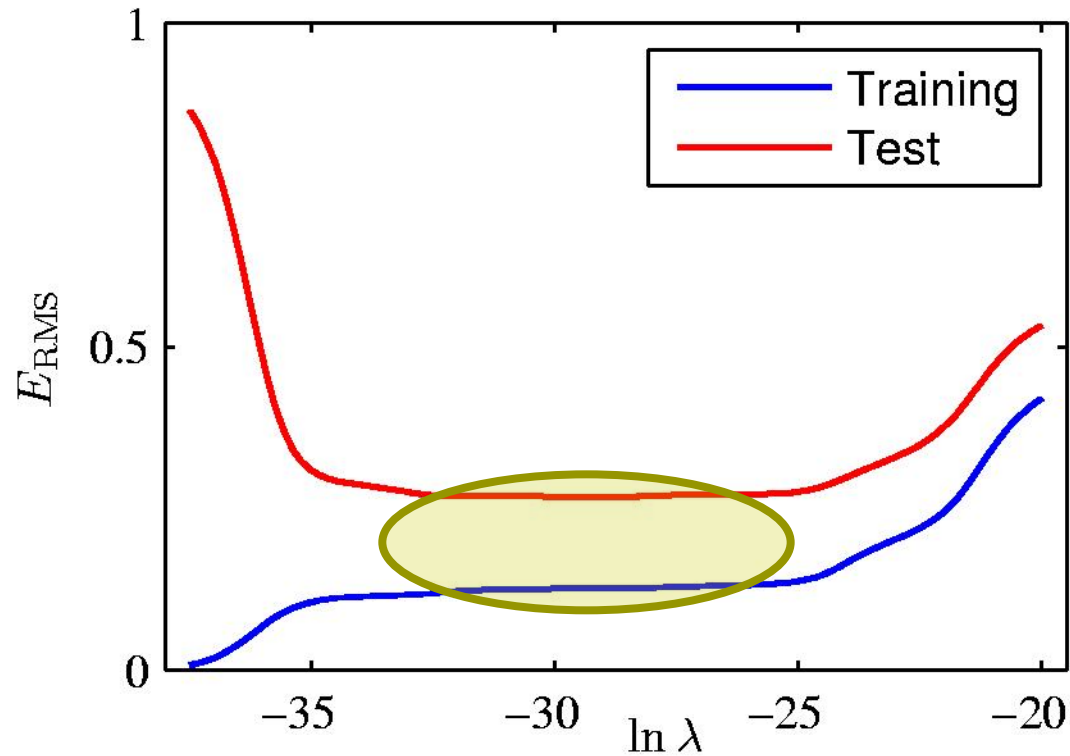
Regularization: $\ln \lambda = -18$

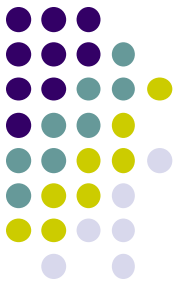


Regularization: $\ln \lambda = 0$



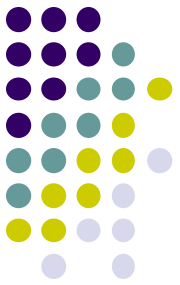
Regularization: E_{RMS} vs. $\ln \lambda$





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



Homework01

- Python programming
 - 1-D regression
 - Learn TensorFlow
- Finish the “Gaussian parameters learning”
 - Please use google, \wedge_*

The End

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