

Lecture Slides for

INTRODUCTION TO

# Machine Learning

## 2nd Edition

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CHAPTER 4:

# Parametric Methods

# Parametric Estimation

- $\mathcal{X} = \{x^t\}_t$  where  $x^t \sim p(x)$

- Parametric estimation:

Assume a form for  $p(x | \theta)$  and estimate  $\theta$ , its sufficient statistics, using  $X$

e.g.,  $N(\mu, \sigma^2)$  where  $\theta = \{\mu, \sigma^2\}$

# Maximum Likelihood Estimation

- Likelihood of  $\theta$  given the sample  $\mathcal{X}$

$$l(\theta|\mathcal{X}) = p(\mathcal{X}|\theta) = \prod_t p(x^t|\theta)$$

- Log likelihood

$$\mathcal{L}(\theta|\mathcal{X}) = \log l(\theta|\mathcal{X}) = \sum_t \log p(x^t|\theta)$$

- Maximum likelihood estimator (MLE)

$$\theta^* = \operatorname{argmax}_{\theta} \mathcal{L}(\theta|\mathcal{X})$$

# Examples: Bernoulli/Multinomial

- Bernoulli: Two states, failure/success,  $x$  in  $\{0,1\}$

$$P(x) = p_o^x (1 - p_o)^{(1-x)}$$

$$\mathcal{L}(p_o|\mathcal{X}) = \log \prod_t p_o^{x^t} (1 - p_o)^{(1-x^t)}$$

$$\text{MLE: } p_o = \sum_t x^t / N$$

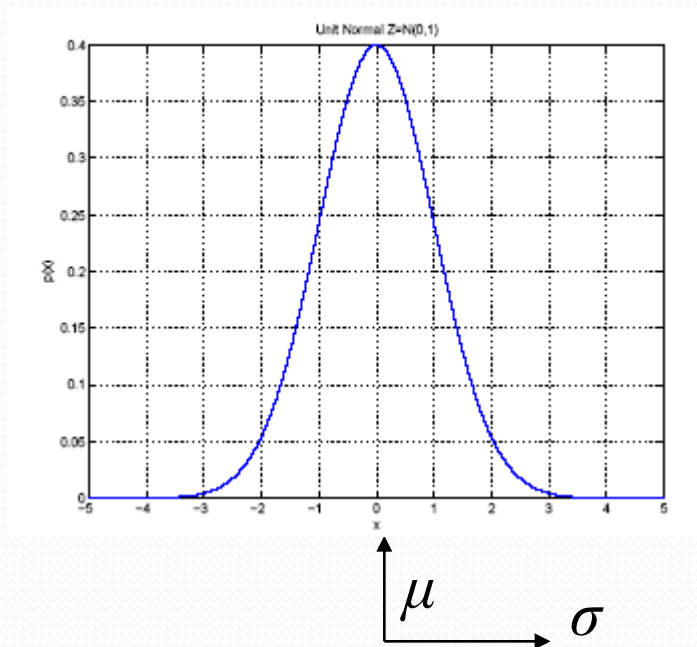
- Multinomial:  $K>2$  states,  $x_i$  in  $\{0,1\}$

$$P(x_1, x_2, \dots, x_K) = \prod_i p_i^{x_i}$$

$$\mathcal{L}(p_1, p_2, \dots, p_K|\mathcal{X}) = \log \prod_t \prod_i p_i^{x_i^t}$$

$$\text{MLE: } p_i = \sum_t x_i^t / N$$

# Gaussian (Normal) Distribution



- $p(x) = \mathcal{N}(\mu, \sigma^2)$

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$

- MLE for  $\mu$  and  $\sigma^2$ :

$$m = \frac{\sum_t x^t}{N}$$

$$s^2 = \frac{\sum_t (x^t - m)^2}{N}$$

# Bias and Variance

Unknown parameter  $\theta$

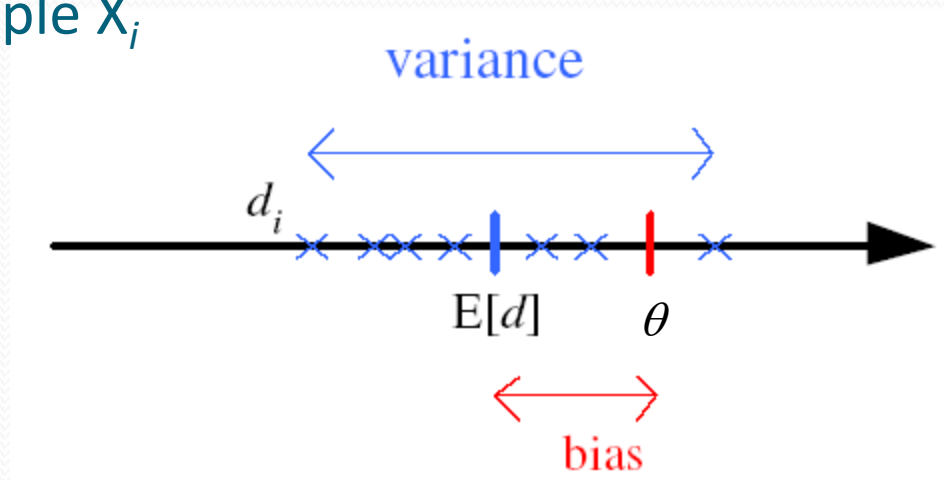
Estimator  $d_i = d(X_i)$  on sample  $X_i$

Bias:  $b_{\theta}(d) = E[d] - \theta$

Variance:  $E[(d - E[d])^2]$

Mean square error:

$$\begin{aligned} r(d, \theta) &= E[(d - \theta)^2] \\ &= (E[d] - \theta)^2 + E[(d - E[d])^2] \\ &= \text{Bias}^2 + \text{Variance} \end{aligned}$$



# Bayes' Estimator

- Treat  $\theta$  as a random var with prior  $p(\theta)$
- Bayes' rule:  $p(\theta|\mathcal{X}) = p(\mathcal{X}|\theta) p(\theta) / p(\mathcal{X})$
- Full:  $p(x|\mathcal{X}) = \int p(x|\theta) p(\theta|\mathcal{X}) d\theta$
- Maximum a Posteriori (MAP):  $\theta_{\text{MAP}} = \operatorname{argmax}_{\theta} p(\theta|\mathcal{X})$
- Maximum Likelihood (ML):  $\theta_{\text{ML}} = \operatorname{argmax}_{\theta} p(\mathcal{X}|\theta)$
- Bayes':  $\theta_{\text{Bayes}'} = E[\theta|\mathcal{X}] = \int \theta p(\theta|\mathcal{X}) d\theta$



# Bayes' Estimator: Example

- $x^t \sim \mathcal{N}(\theta, \sigma_0^2)$  and  $\theta \sim \mathcal{N}(\mu, \sigma^2)$
- $\theta_{\text{ML}} = m$
- $\theta_{\text{MAP}} = \theta_{\text{Bayes'}} =$

$$E[\theta | \mathcal{X}] = \frac{N/\sigma_0^2}{N/\sigma_0^2 + 1/\sigma^2} m + \frac{1/\sigma^2}{N/\sigma_0^2 + 1/\sigma^2} \mu$$

# Parametric Classification

$$g_i(x) = p(x | C_i)P(C_i)$$

or

$$g_i(x) = \log p(x | C_i) + \log P(C_i)$$

$$p(x | C_i) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\frac{(x - \mu_i)^2}{2\sigma_i^2}\right]$$

$$g_i(x) = -\frac{1}{2}\log 2\pi - \log \sigma_i - \frac{(x - \mu_i)^2}{2\sigma_i^2} + \log P(C_i)$$

- Given the sample  $\mathcal{X} = \{x^t, r^t\}_{t=1}^N$

$$x \in \mathfrak{R} \quad r_i^t = \begin{cases} 1 & \text{if } x^t \in C_i \\ 0 & \text{if } x^t \in C_j, j \neq i \end{cases}$$

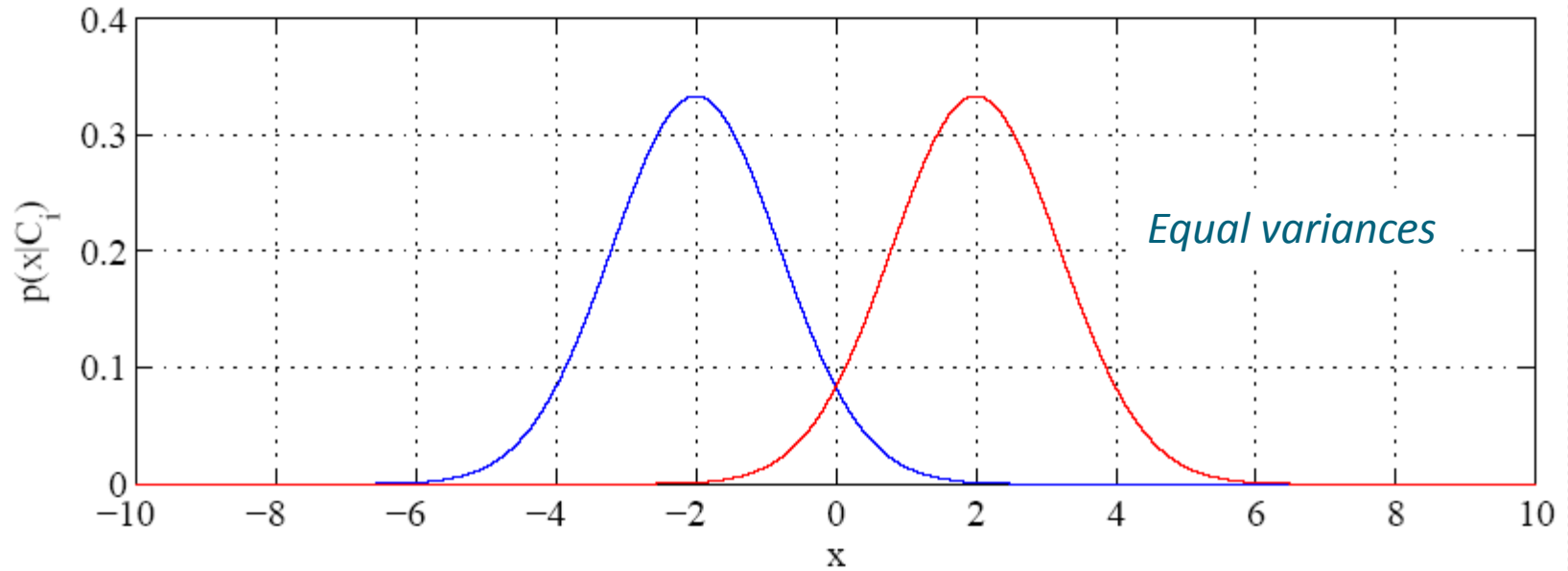
- ML estimates are

$$\hat{P}(C_i) = \frac{\sum_t r_i^t}{N} \quad m_i = \frac{\sum_t x^t r_i^t}{\sum_t r_i^t} \quad s_i^2 = \frac{\sum_t (x^t - m_i)^2 r_i^t}{\sum_t r_i^t}$$

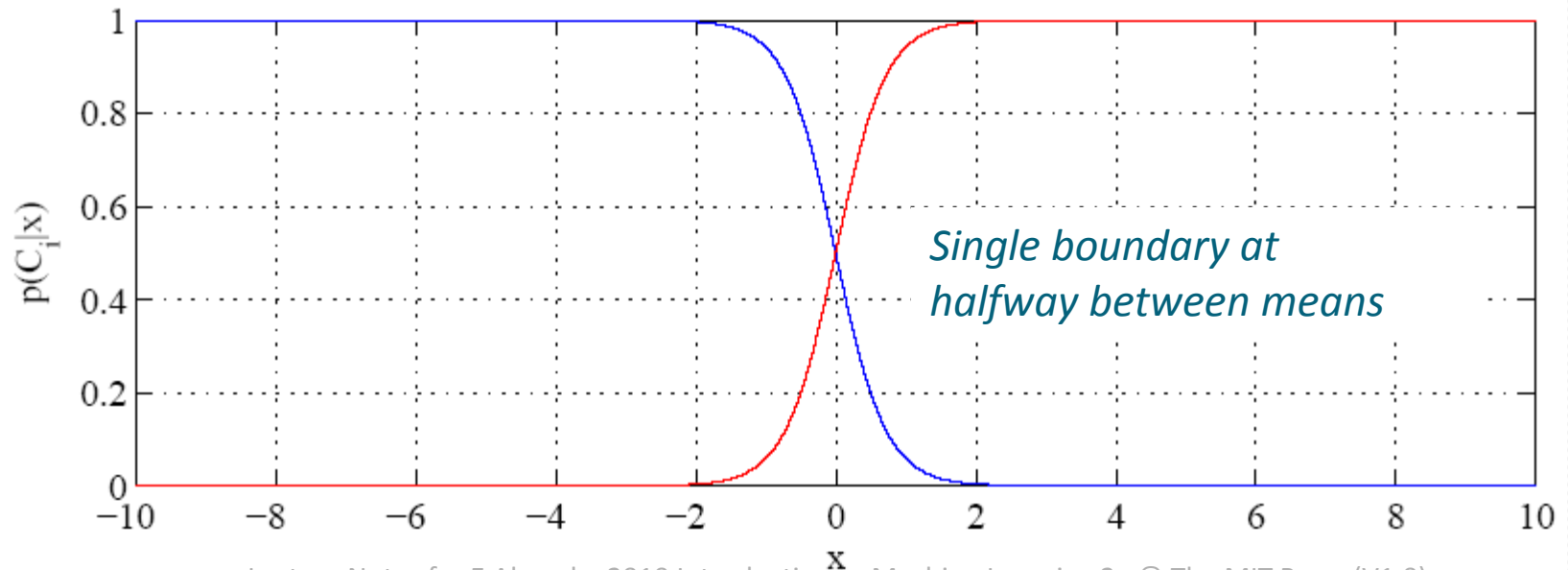
- Discriminant becomes

$$g_i(x) = -\frac{1}{2} \log 2\pi - \log s_i - \frac{(x - m_i)^2}{2s_i^2} + \log \hat{P}(C_i)$$

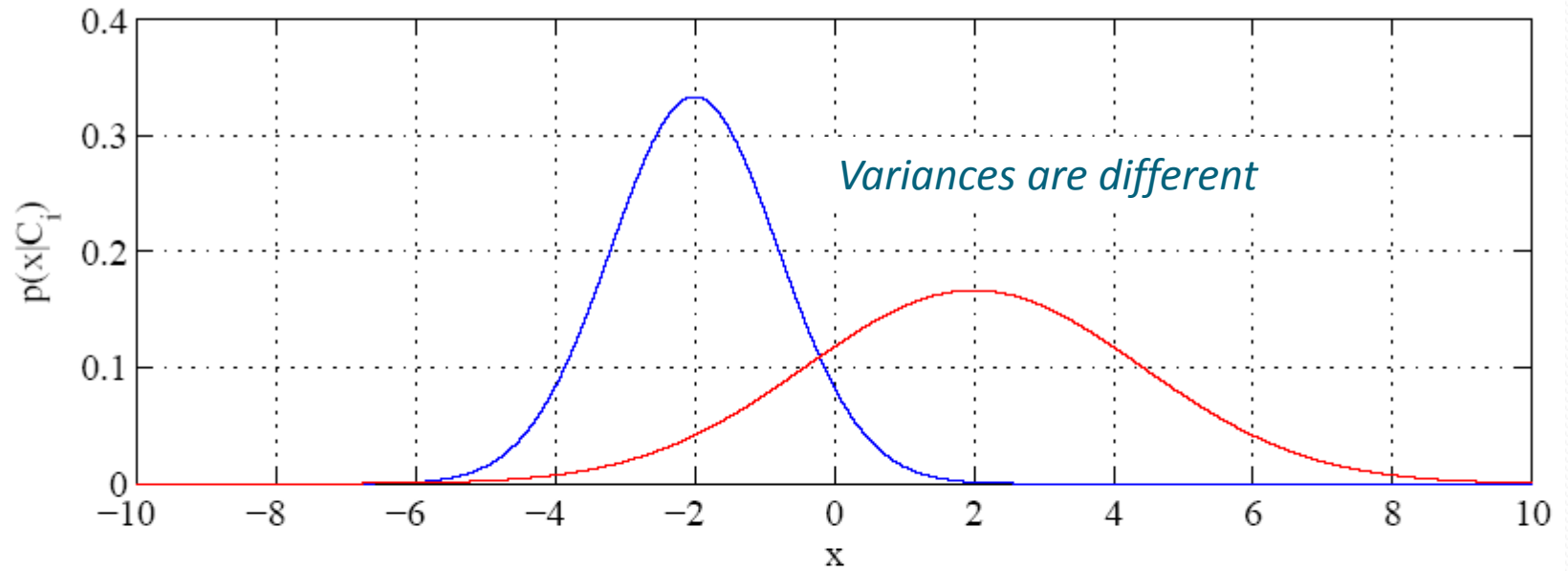
Likelihoods



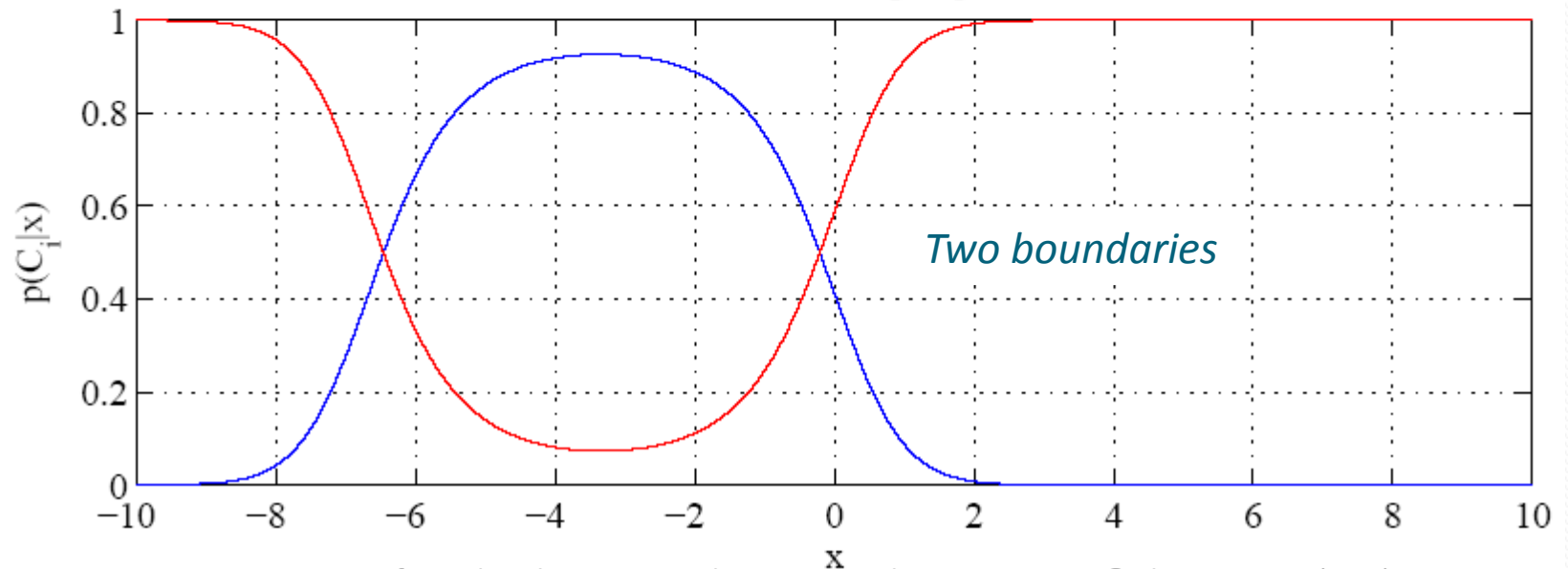
Posteriors with equal priors



### Likelihoods



### Posteriors with equal priors



# Regression

$$r = f(x) + \varepsilon$$

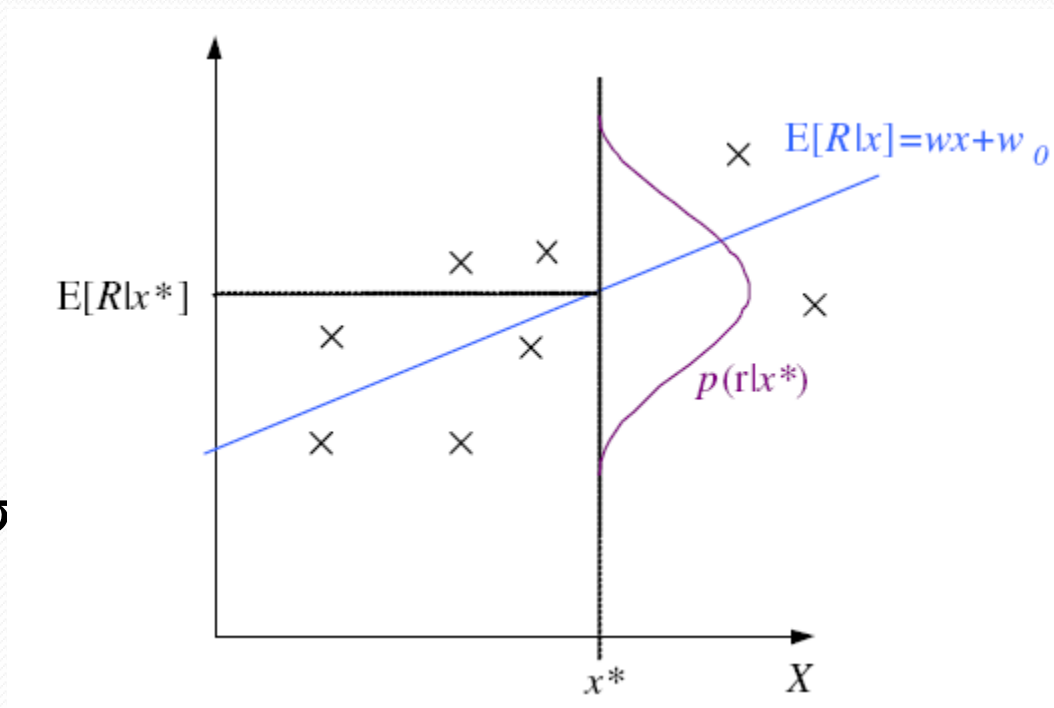
$$\text{estimator } g(x|\theta)$$

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

$$p(r|x) \sim \mathcal{N}(g(x|\theta), \sigma)$$

$$\mathcal{L}(\theta|\mathcal{X}) = \log \prod_{t=1}^N p(x^t, r^t)$$

$$= \log \prod_{t=1}^N p(r^t | x^t) + \log \prod_{t=1}^N p(x^t)$$



# Regression: From LogL to Error

$$\mathcal{L}(\theta | \mathcal{X}) = \log \prod_{t=1}^N \frac{1}{\sqrt{2\pi}\sigma} \exp \left[ -\frac{[r^t - g(x^t | \theta)]^2}{2\sigma^2} \right]$$

$$= -N \log \sqrt{2\pi}\sigma - \frac{1}{2\sigma^2} \sum_{t=1}^N [r^t - g(x^t | \theta)]^2$$

$$E(\theta | \mathcal{X}) = \frac{1}{2} \sum_{t=1}^N [r^t - g(x^t | \theta)]^2$$

# Linear Regression

$$g(x^t | w_1, w_0) = w_1 x^t + w_0$$

$$\sum_t r^t = N w_0 + w_1 \sum_t x^t$$

$$\sum_t r^t x^t = w_0 \sum_t x^t + w_1 \sum_t (x^t)^2$$

$$\mathbf{A} = \begin{bmatrix} N & \sum_t x^t \\ \sum_t x^t & \sum_t (x^t)^2 \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} \sum_t r^t \\ \sum_t r^t x^t \end{bmatrix}$$

$$\mathbf{w} = \mathbf{A}^{-1} \mathbf{y}$$



# Polynomial Regression

$$g(x^t | w_k, \dots, w_2, w_1, w_0) = w_k (x^t)^k + \dots + w_2 (x^t)^2 + w_1 x^t + w_0$$

$$\mathbf{D} = \begin{bmatrix} 1 & x^1 & (x^1)^2 & \dots & (x^1)^k \\ 1 & x^2 & (x^2)^2 & \dots & (x^2)^k \\ \vdots & & & & \\ 1 & x^N & (x^N)^2 & \dots & (x^N)^k \end{bmatrix} \quad \mathbf{r} = \begin{bmatrix} r^1 \\ r^2 \\ \vdots \\ r^N \end{bmatrix}$$

$$\mathbf{w} = (\mathbf{D}^T \mathbf{D})^{-1} \mathbf{D}^T \mathbf{r}$$

# Other Error Measures

- Square Error:  $E(\theta | \mathcal{X}) = \frac{1}{2} \sum_{t=1}^N [r^t - g(x^t | \theta)]^2$
- Relative Square Error:  $E(\theta | \mathcal{X}) = \frac{\sum_{t=1}^N [r^t - g(x^t | \theta)]^2}{\sum_{t=1}^N [r^t - \bar{r}]^2}$
- Absolute Error:  $E(\theta | \mathcal{X}) = \sum_t |r^t - g(x^t | \theta)|$
- $\epsilon$ -sensitive Error:  $E(\theta | \mathcal{X}) = \sum_t 1(|r^t - g(x^t | \theta)| > \epsilon) (|r^t - g(x^t | \vartheta)| - \epsilon)$

# Bias and Variance

$$E[(r - g(x))^2 | x] = \underbrace{E[(r - E[r | x])^2 | x]}_{\text{noise}} + \underbrace{(E[r | x] - g(x))^2}_{\text{squared error}}$$

$$E_x[(E[r | x] - g(x))^2] = \underbrace{(E[r | x] - E_x[g(x)])^2}_{\text{bias}} + \underbrace{E_x[(g(x) - E_x[g(x)])^2]}_{\text{variance}}$$

# Estimating Bias and Variance

- $M$  samples  $X_i = \{x_i^t, r_i^t\}$ ,  $i=1, \dots, M$   
are used to fit  $g_i(x)$ ,  $i=1, \dots, M$

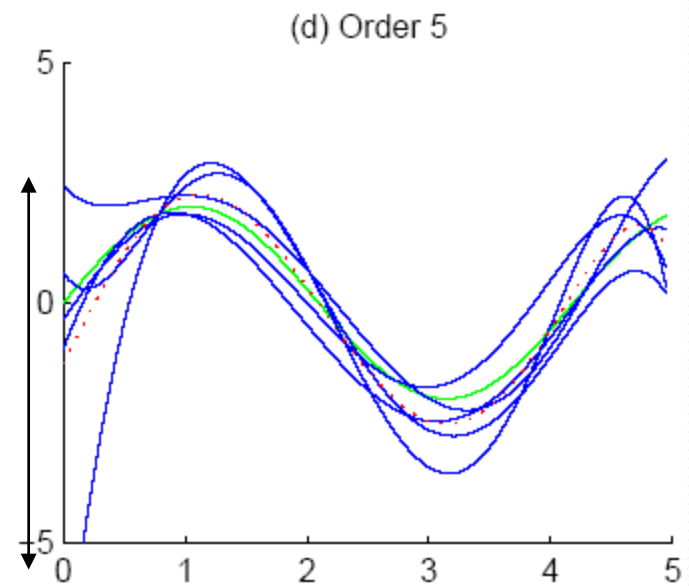
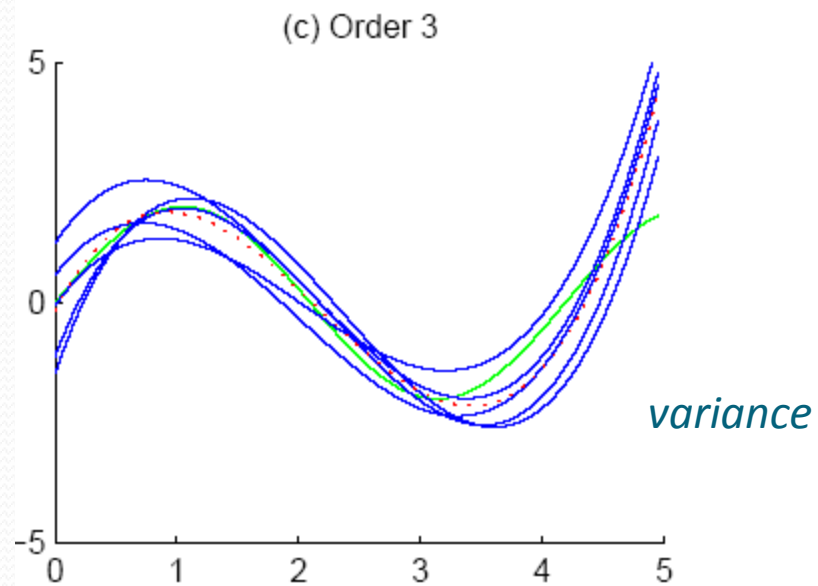
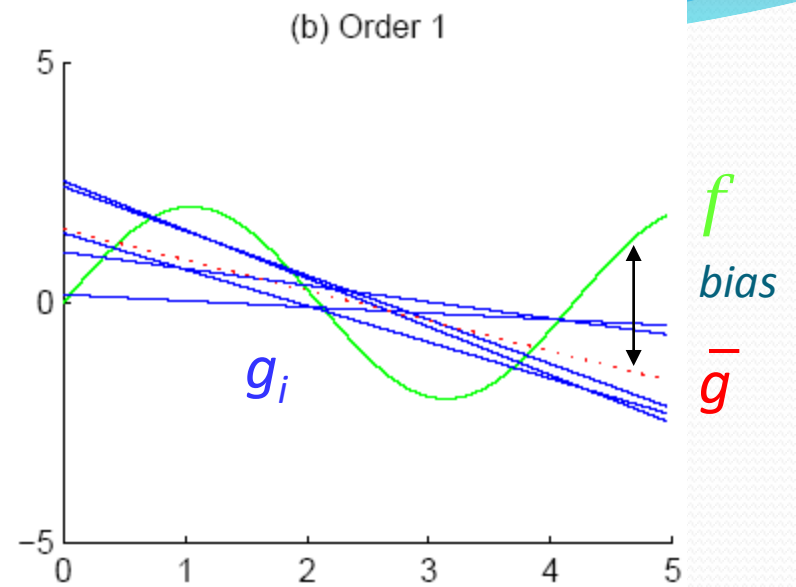
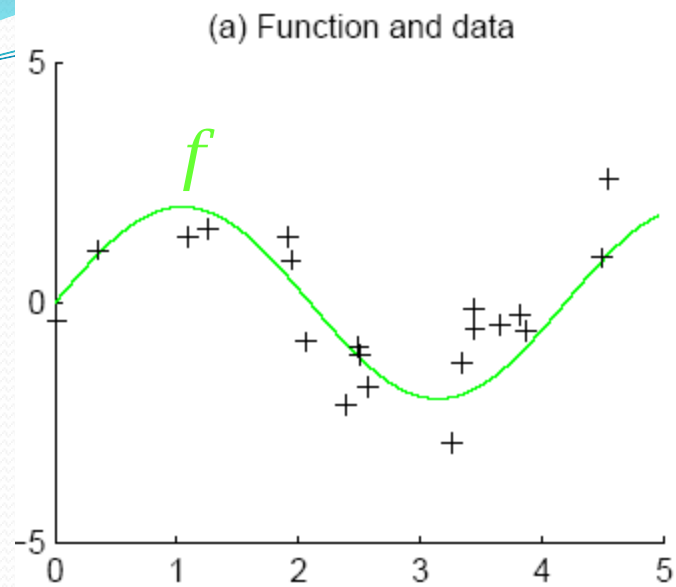
$$\text{Bias}^2(g) = \frac{1}{N} \sum_t [\bar{g}(x^t) - f(x^t)]^2$$

$$\text{Variance}(g) = \frac{1}{NM} \sum_t \sum_i [g_i(x^t) - \bar{g}(x^t)]^2$$

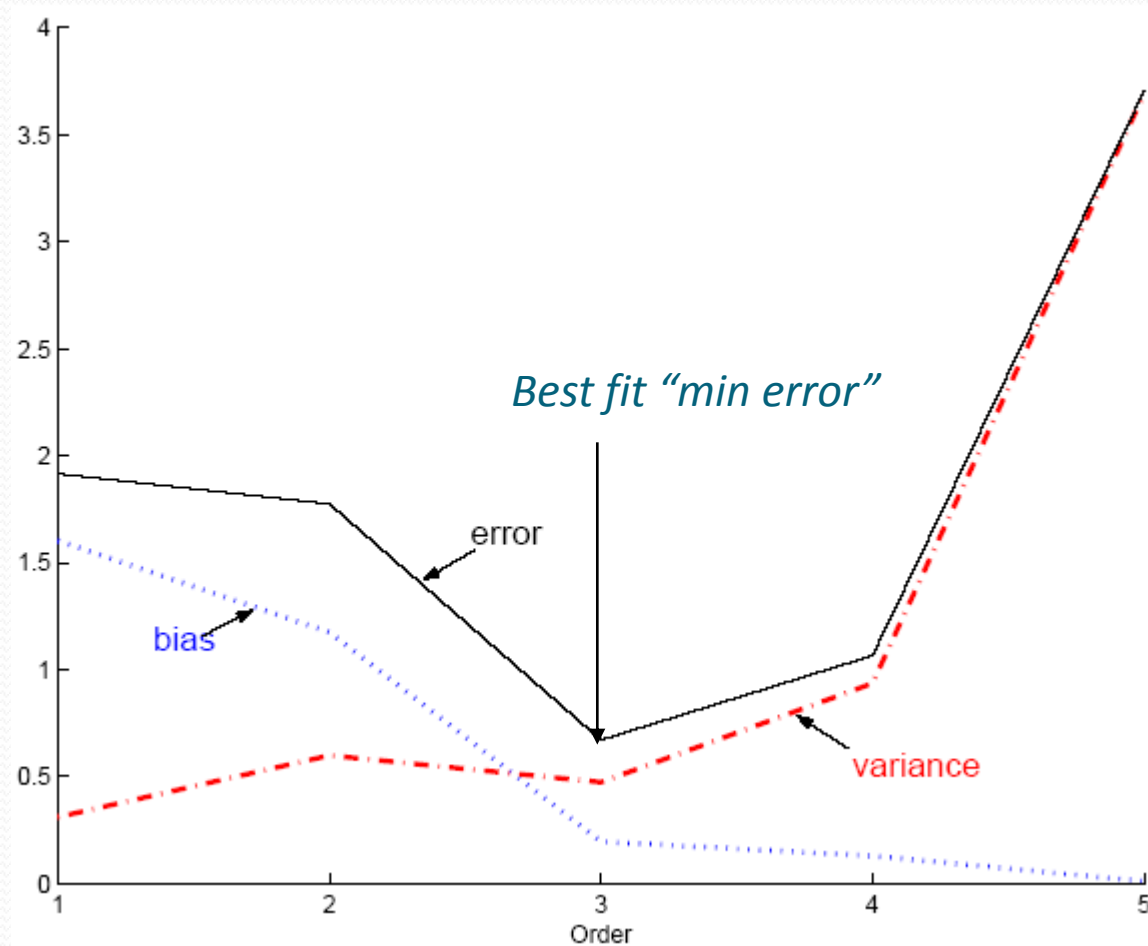
$$\bar{g}(x) = \frac{1}{M} \sum_i g_i(x)$$

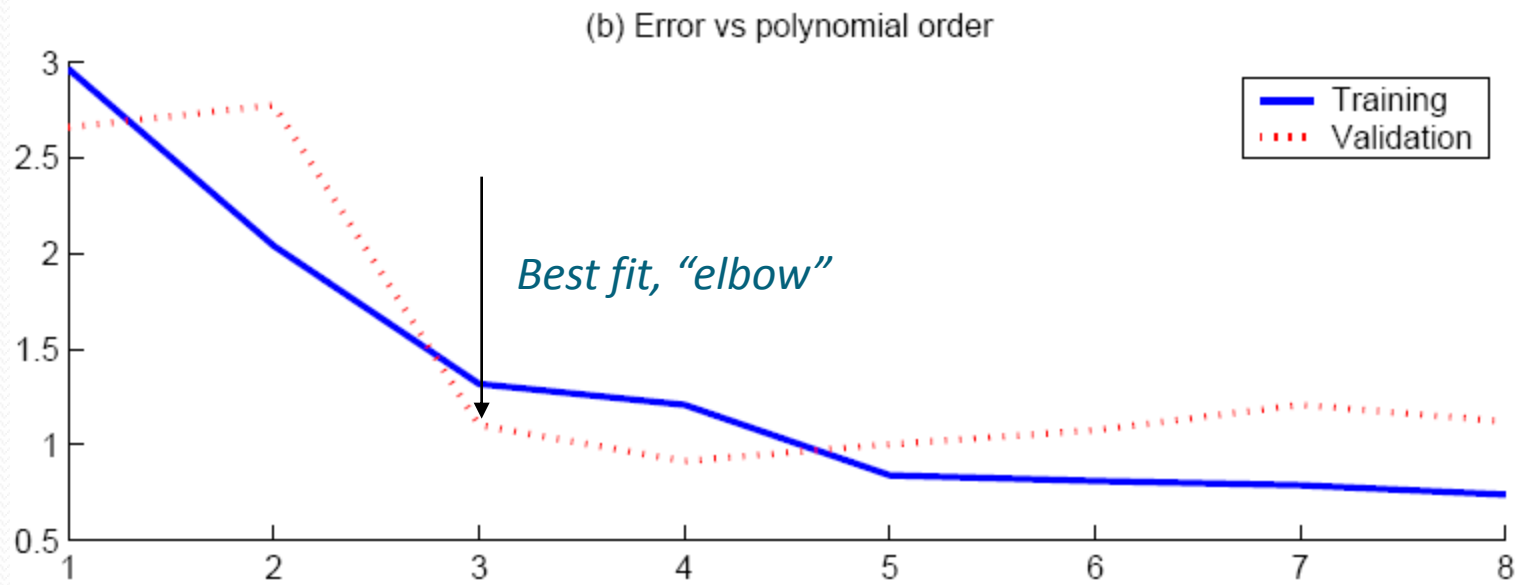
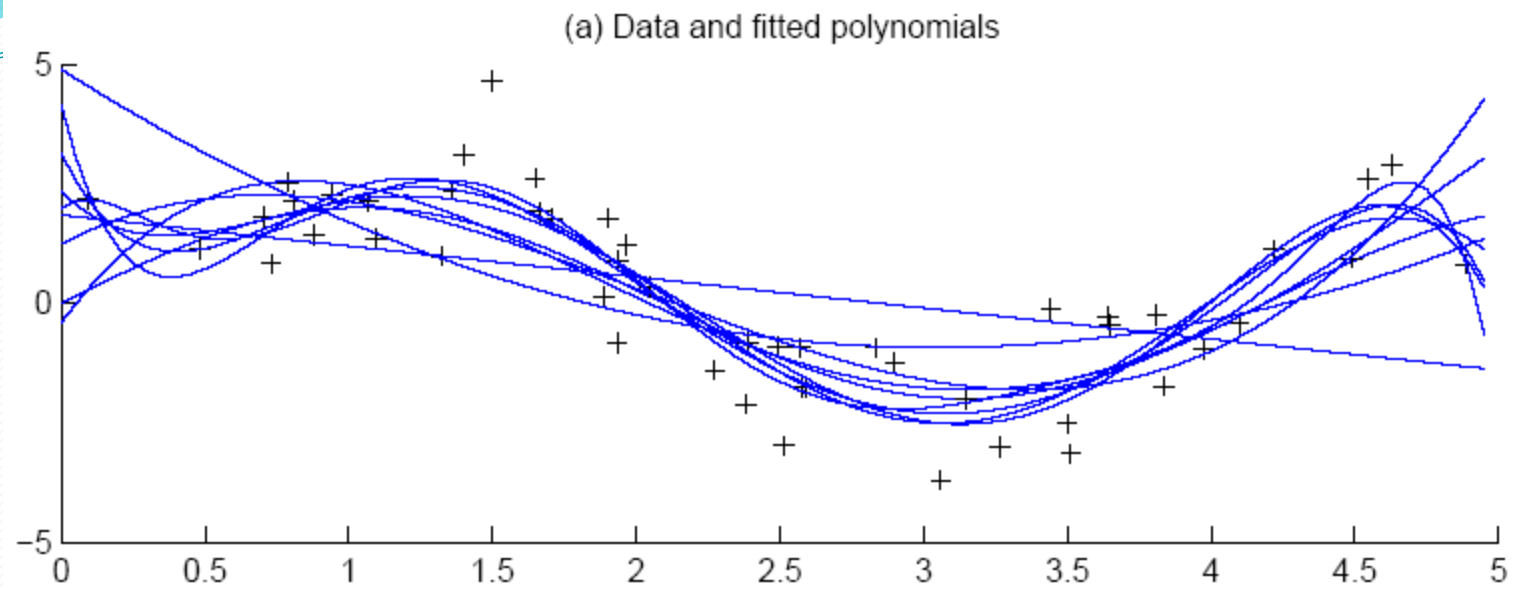
# Bias/Variance Dilemma

- Example:  $g_i(x)=2$  has no variance and high bias  
 $g_i(x)=\sum_t r_i^t/N$  has lower bias with variance
- As we increase complexity,  
    bias decreases (a better fit to data) and  
    variance increases (fit varies more with data)
- Bias/Variance dilemma: (Geman et al., 1992)



# Polynomial Regression







# Model Selection

- **Cross-validation:** Measure generalization accuracy by testing on data unused during training
- **Regularization:** Penalize complex models  
 $E' = \text{error on data} + \lambda \text{ model complexity}$   
Akaike's information criterion (AIC), Bayesian information criterion (BIC)
- **Minimum description length (MDL):** Kolmogorov complexity, shortest description of data
- **Structural risk minimization (SRM)**

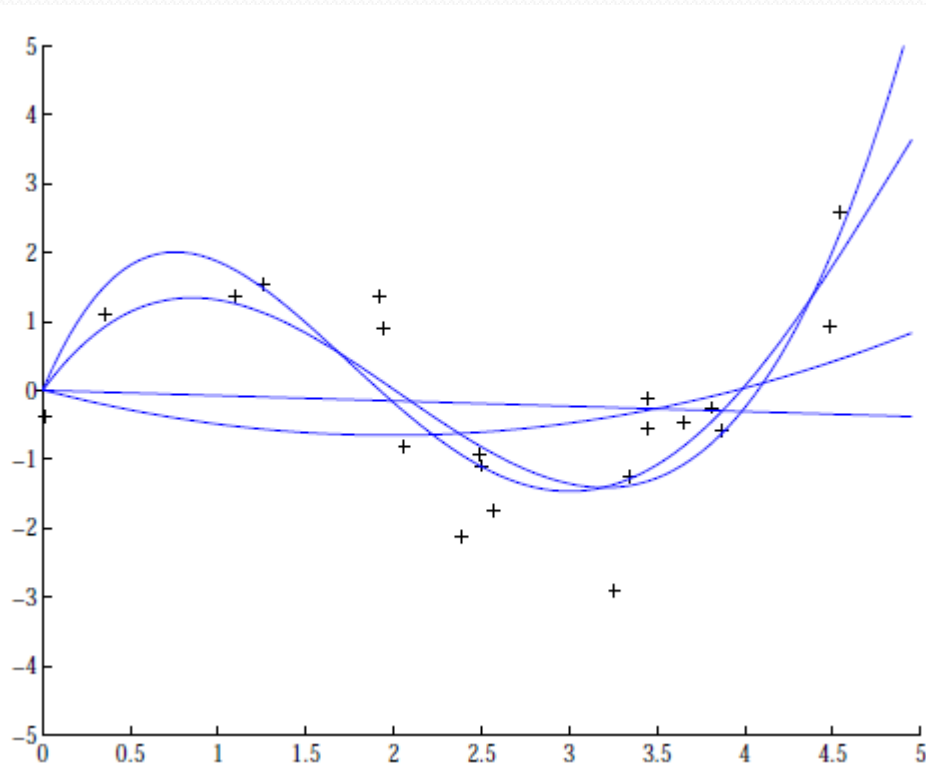
# Bayesian Model Selection

- Prior on models,  $p(\text{model})$

$$p(\text{model} | \text{data}) = \frac{p(\text{data} | \text{model}) p(\text{model})}{p(\text{data})}$$

- Regularization, when prior favors simpler models
- Bayes, MAP of the posterior,  $p(\text{model} | \text{data})$
- Average over a number of models with high posterior (voting, ensembles: Chapter 17)

# Regression example



Coefficients increase in magnitude as order increases:

1: [-0.0769, 0.0016]

2: [0.1682, -0.6657, 0.0080]

3: [0.4238, -2.5778, 3.4675, -0.0002]

4: [-0.1093, 1.4356, -5.5007, 6.0454, -0.0019]

$$\text{regularization: } E(\mathbf{w} \mid \mathcal{X}) = \frac{1}{2} \sum_{t=1}^N [r^t - g(x^t \mid \mathbf{w})]^2 + \lambda \sum_i w_i^2$$