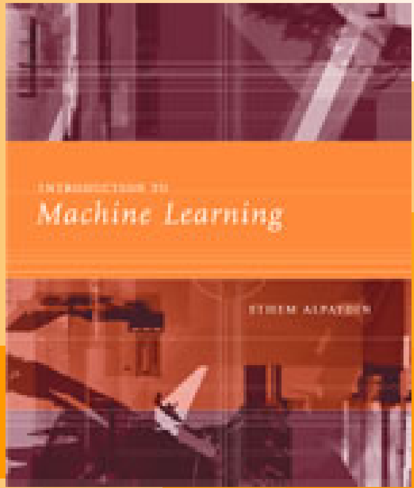


Lecture Slides for

INTRODUCTION TO

Machine Learning

ETHEM ALPAYDIN

alpaydin@boun.edu.tr
http://www.cmpe.boun.edu.tr/~ethem/i2ml

CHAPTER 4:

Parametric Methods

Parametric Estimation

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

  Assume a form for $p(x \mid \theta)$ and estimate θ, its sufficient statistics, using $\mathcal{X}$

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

Maximum Likelihood Estimation

- Likelihood of θ 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)

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

Examples: Bernoulli/Multinomial

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

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

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

  MLE: $p_o = \Sigma_t \, x^t / N$

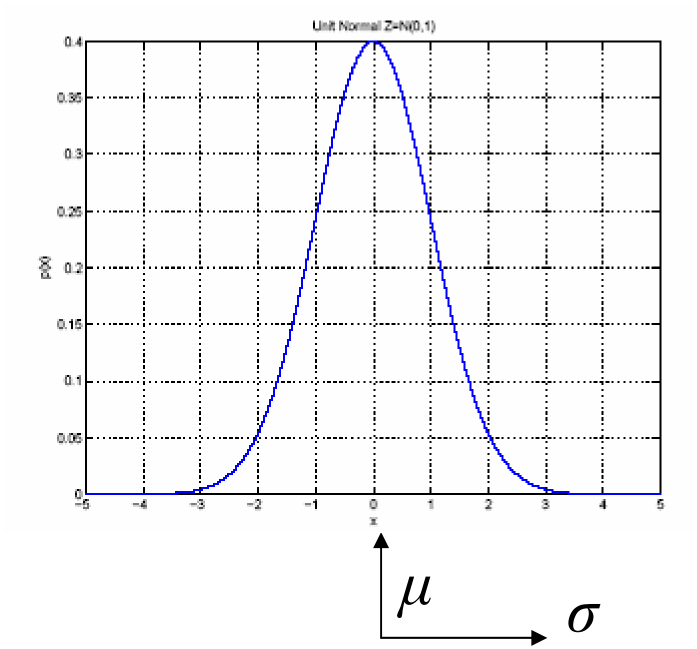
- Multinomial: K>2 states, x_i in {0,1}

  $P(x_1,x_2,...,x_K) = \Pi_i \, p_i^{x_i}$

  $$\mathcal{L}(p_1,p_2,...,p_K|\mathcal{X}) = \log \Pi_t \Pi_i \, p_i^{x_i^t}$$

  MLE: $p_i = \Sigma_t \, x_i^t / N$

Gaussian (Normal) Distribution



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

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

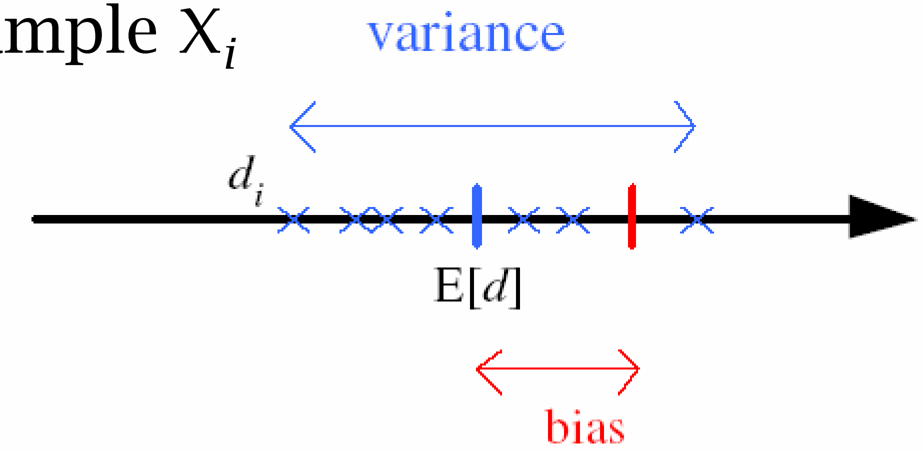
- MLE for μ and σ^2:

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

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

Bias and Variance

Unknown parameter θ
Estimator $d_i = d\,(\mathcal{X}_i)$ on sample X_i



Bias: $b_\theta(d) = E\,[d] - \theta$
Variance: $E\,[(d - E\,[d])^2]$

Mean square error:
$$r\,(d,\theta) = E\,[(d-\theta)^2]$$
$$= (E\,[d] - \theta)^2 + E\,[(d-E\,[d])^2]$$
$$= \text{Bias}^2 + \text{Variance}$$

Bayes' Estimator

- Treat θ 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): $\theta_{\mathrm{MAP}} = \mathrm{argmax}_\theta\, p(\theta|\mathcal{X})$
- Maximum Likelihood (ML): $\theta_{\mathrm{ML}} = \mathrm{argmax}_\theta\, p(\mathcal{X}|\theta)$
- Bayes': $\theta_{\mathrm{Bayes'}} = E[\theta|\mathcal{X}] = \int \theta\, p(\theta|\mathcal{X})\, d\theta$

Bayes' Estimator: Example

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

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

Parametric Classification

$$g_i(x) = p(x \mid C_i)P(C_i)$$

or equivalently

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

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

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

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

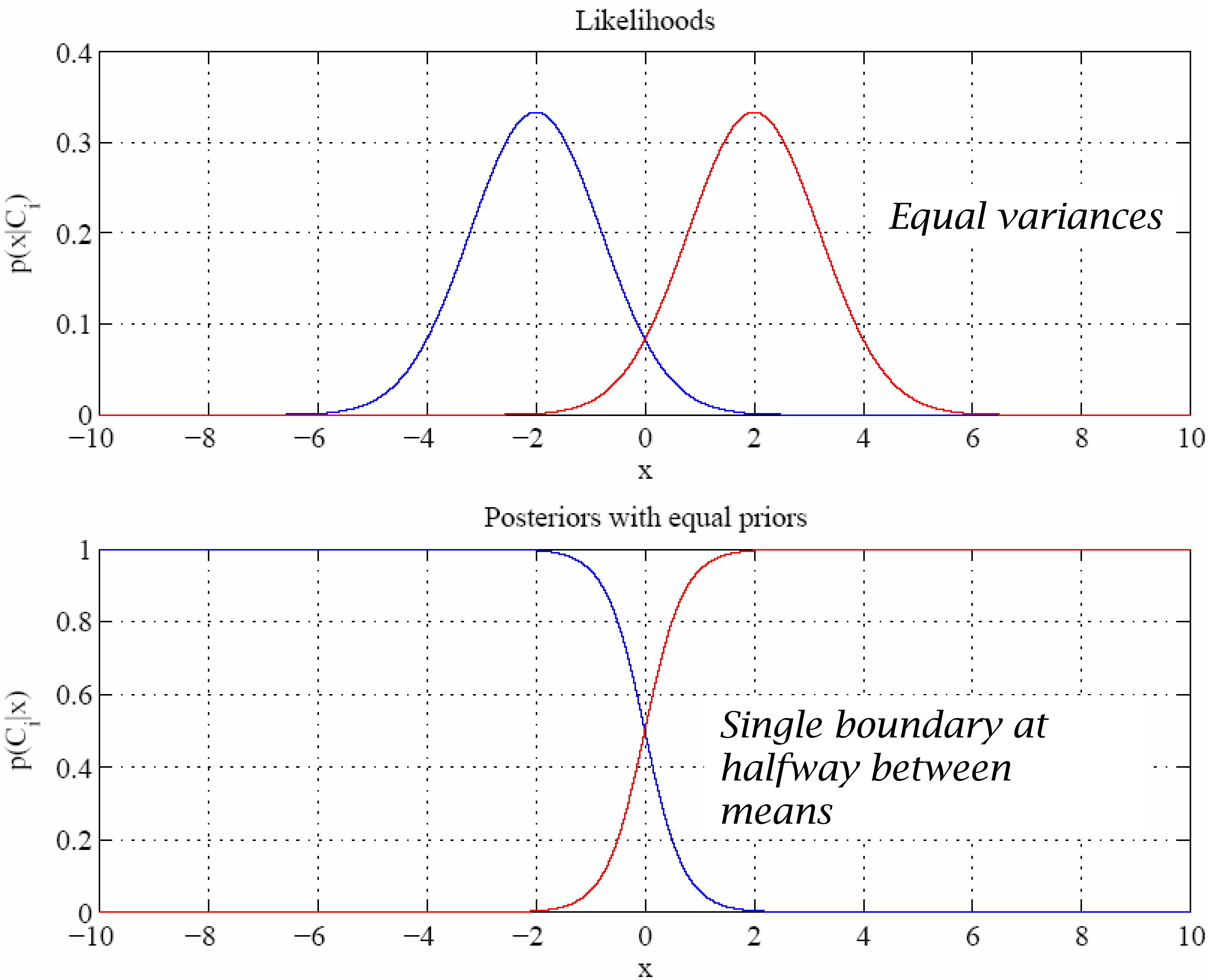
$$x \in \Re \qquad r_i^t = \begin{cases} 1 \text{ if } x^t \in C_i \\ 0 \text{ if } x^t \in C_j, j \neq i \end{cases}$$

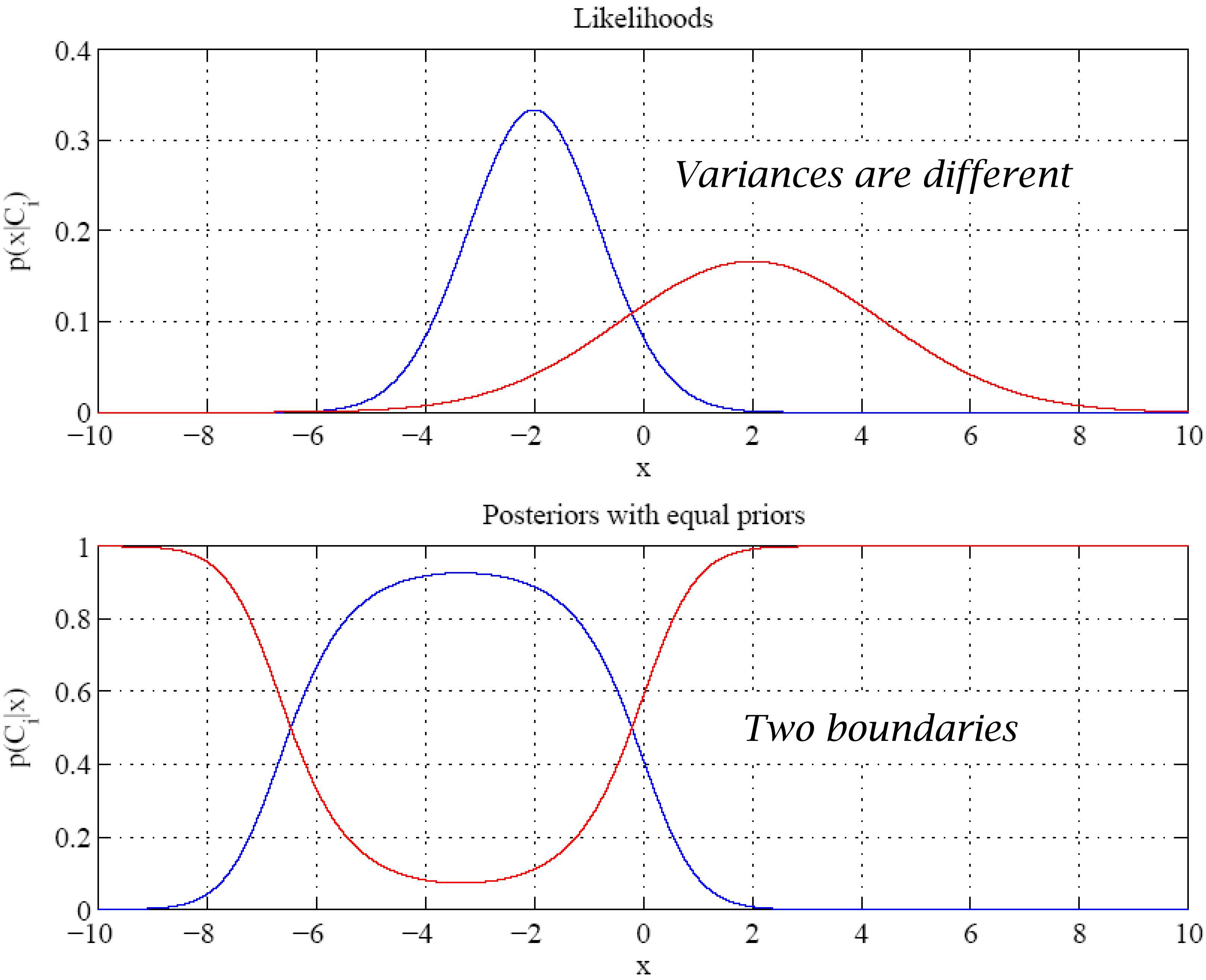
- ML estimates are

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

- 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
0.4
0.3
0.2
0.1
0
p(x|C_i)
−10
−8
−6
−4
−2
0
2
4
6
8
10
x
Equal variances
Posteriors with equal priors
1
0.8
0.6
0.4
0.2
0
p(C_i|x)
−10
−8
−6
−4
−2
0
2
4
6
8
10
x
Single boundary at halfway between means


Likelihoods
0.4
0.3
0.2
0.1
0
p(x|C_i)
−10
−8
−6
−4
−2
0
2
4
6
8
10
x
Variances are different
Posteriors with equal priors
1
0.8
0.6
0.4
0.2
0
p(C_i|x)
−10
−8
−6
−4
−2
0
2
4
6
8
10
x
Two boundaries

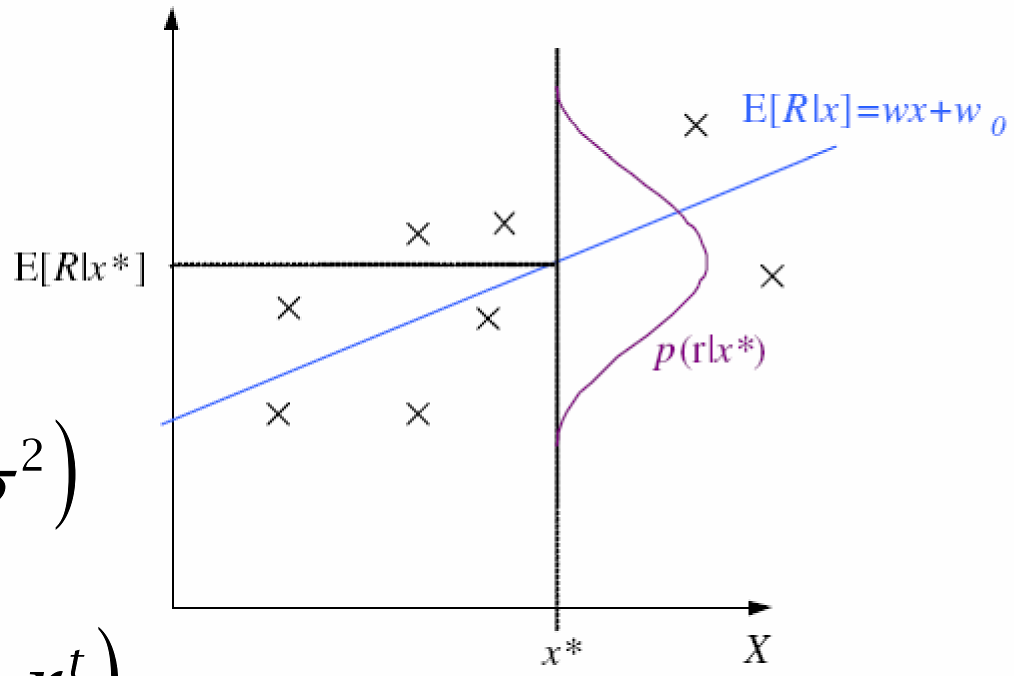
Regression

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

$$\text{estimator}: g(x \mid \theta)$$

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

$$p(r \mid x) \sim \mathcal{N}(g(x \mid \theta), \sigma^2)$$



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

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

Regression: From LogL to Error

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

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

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

Linear Regression

$$g\left(x^t \mid w_1, w_0\right) = w_1 x^t + w_0$$

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

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

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

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

Polynomial Regression

$$g\left(x^t \mid w_k,\ldots,w_2,w_1,w_0\right) = w_k\left(x^t\right)^k + \cdots + w_2\left(x^t\right)^2 + w_1 x^t + w_0$$

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

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

Other Error Measures

- Square Error: $E(\theta \mid \mathcal{X}) = \frac{1}{2}\sum_{t=1}^{N}\left[r^t - g(x^t \mid \theta)\right]^2$
- Relative Square Error: $E(\theta \mid \mathcal{X}) = \frac{\sum_{t=1}^{N}\left[r^t - g(x^t \mid \theta)\right]^2}{\sum_{t=1}^{N}\left[r^t - \overline{r}\right]^2}$
- Absolute Error: $E(\theta|\mathcal{X}) = \sum_t |r^t - g(x^t|\theta)|$
- ε-sensitive Error:

$$E(\theta|\mathcal{X}) = \sum_t 1(|r^t - g(x^t|\theta)| > \varepsilon)\ (|r^t - g(x^t|\theta)| - \varepsilon)$$

Bias and Variance

$$E\left[(r-g(x))^2 \mid x\right] = E\left[(r-E[r \mid x])^2 \mid x\right] + (E[r \mid x] - g(x))^2$$

noise *squared error*

$$E_X\left[(E[r \mid x] - g(x))^2 \mid x\right] = (E[r \mid x] - E_X[g(x)])^2 + E_X\left[(g(x) - E_X[g(x)])^2\right]$$

bias *variance*

Estimating Bias and Variance

- M samples $\mathcal{X}_i=\{x^t_i, r^t_i\}$, $i=1,...,M$ are used to fit $g_i(x)$, $i=1,...,M$

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

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

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

Bias/Variance Dilemma

- Example: $g_i(x)=2$ has no variance and high bias

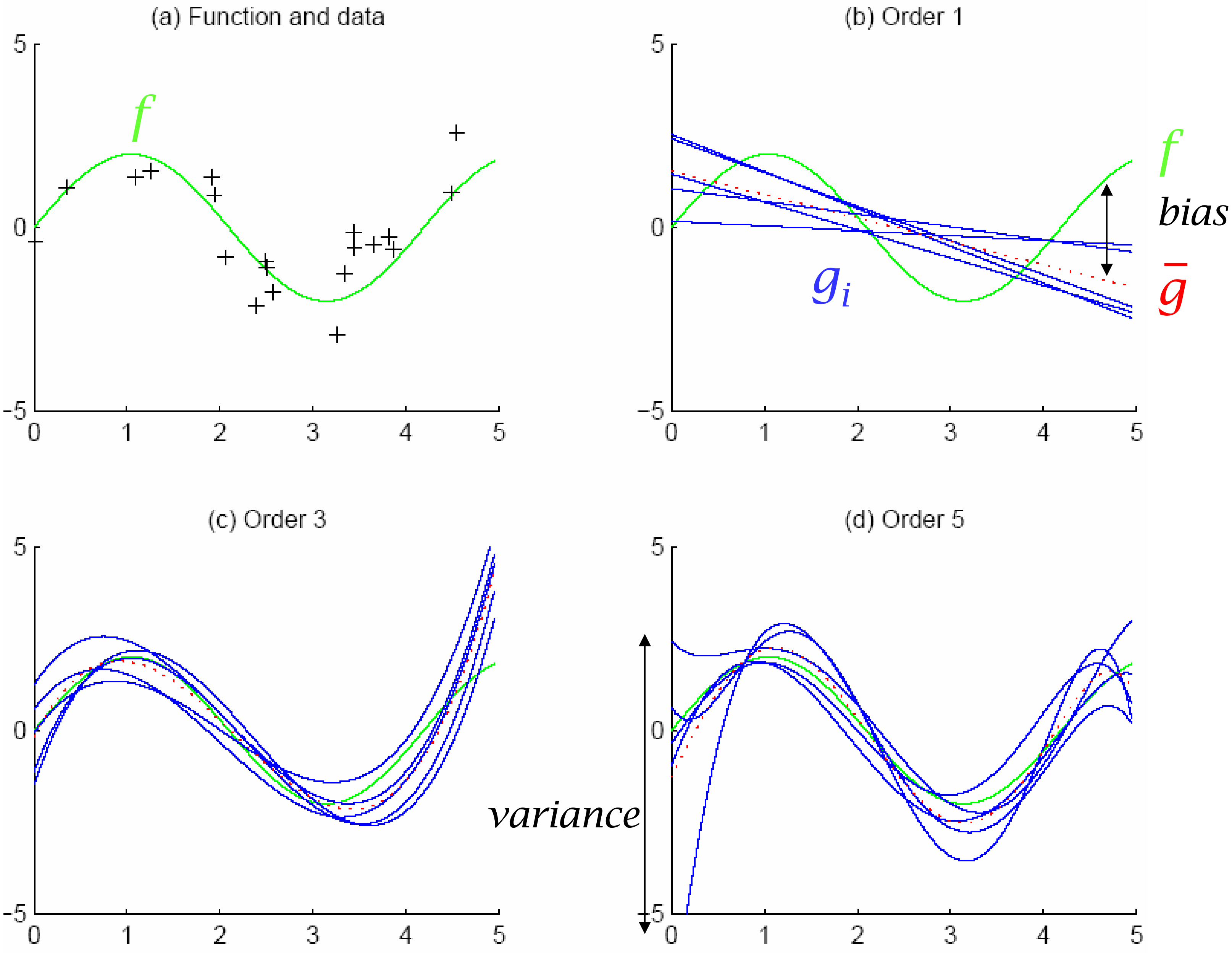
  $g_i(x)=\sum_t r^t_i/N$ has lower bias with variance

- As we increase complexity,

  bias decreases (a better fit to data) and

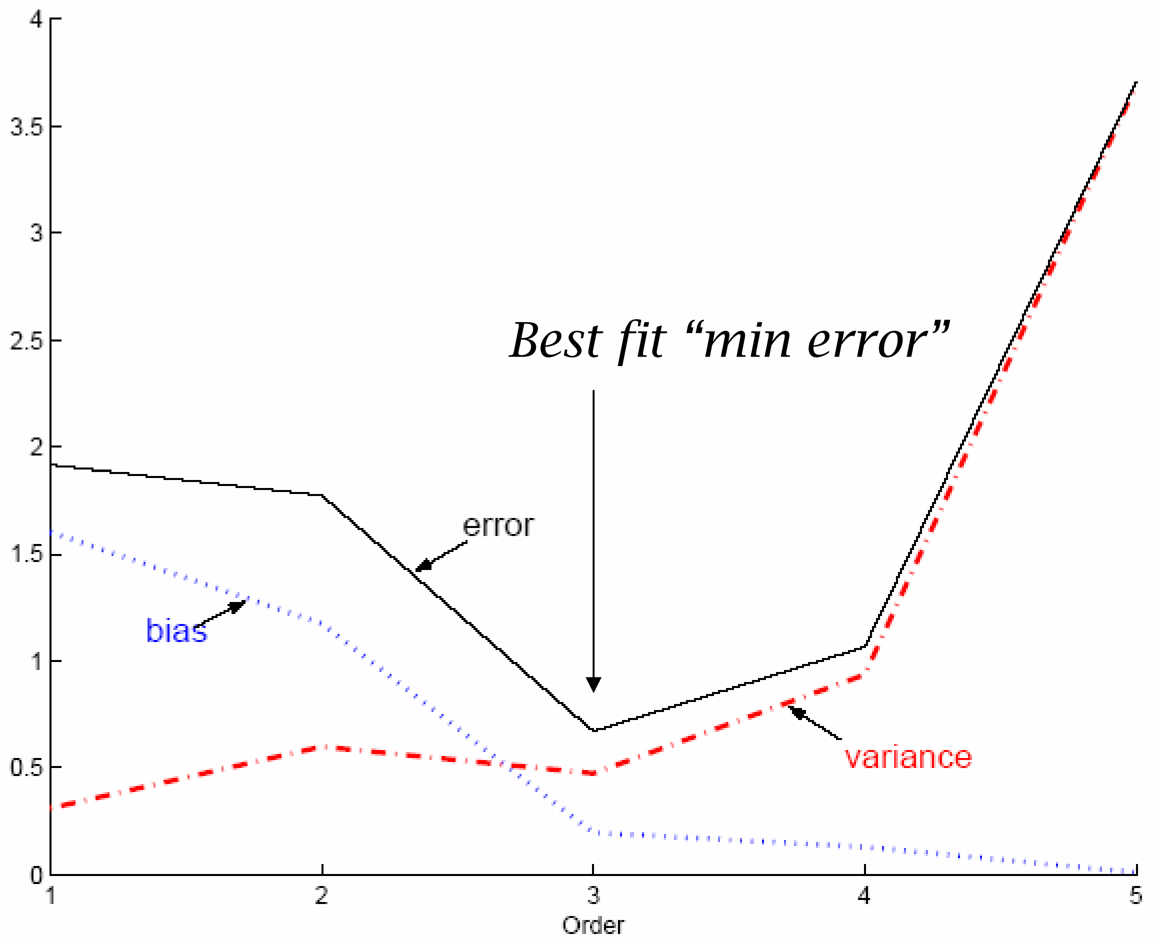
  variance increases (fit varies more with data)

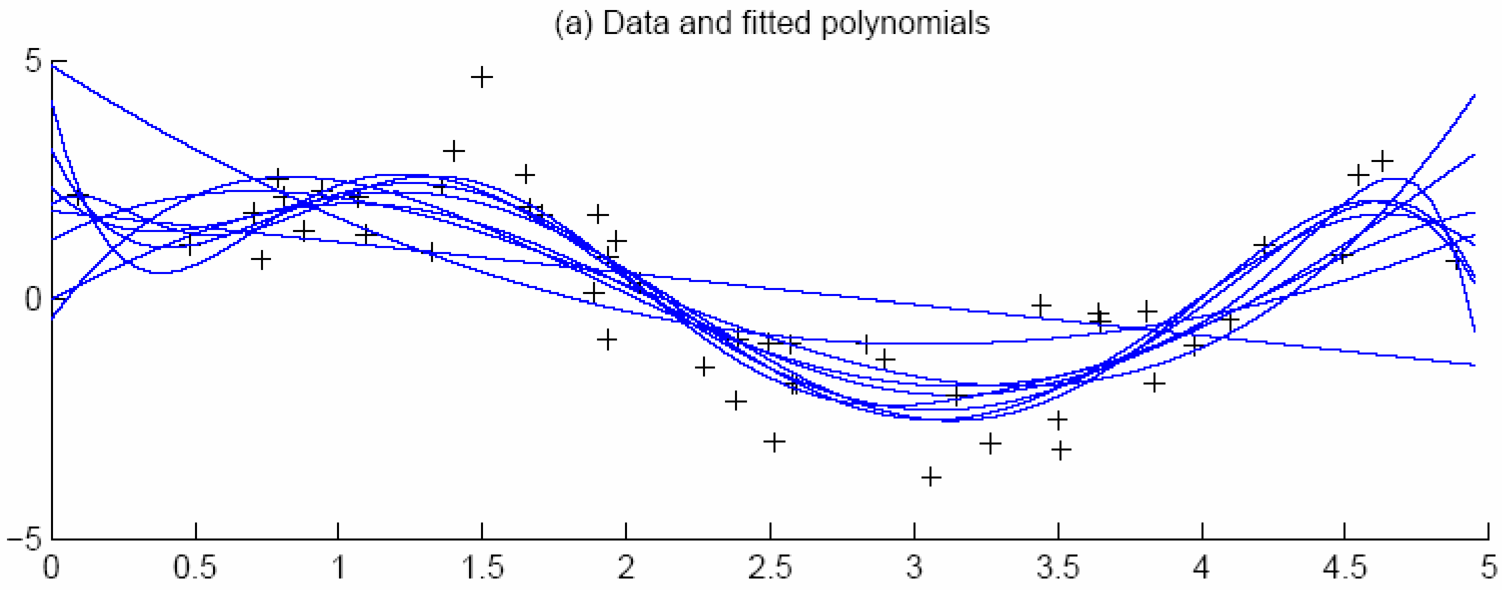
- Bias/Variance dilemma: (Geman et al., 1992)

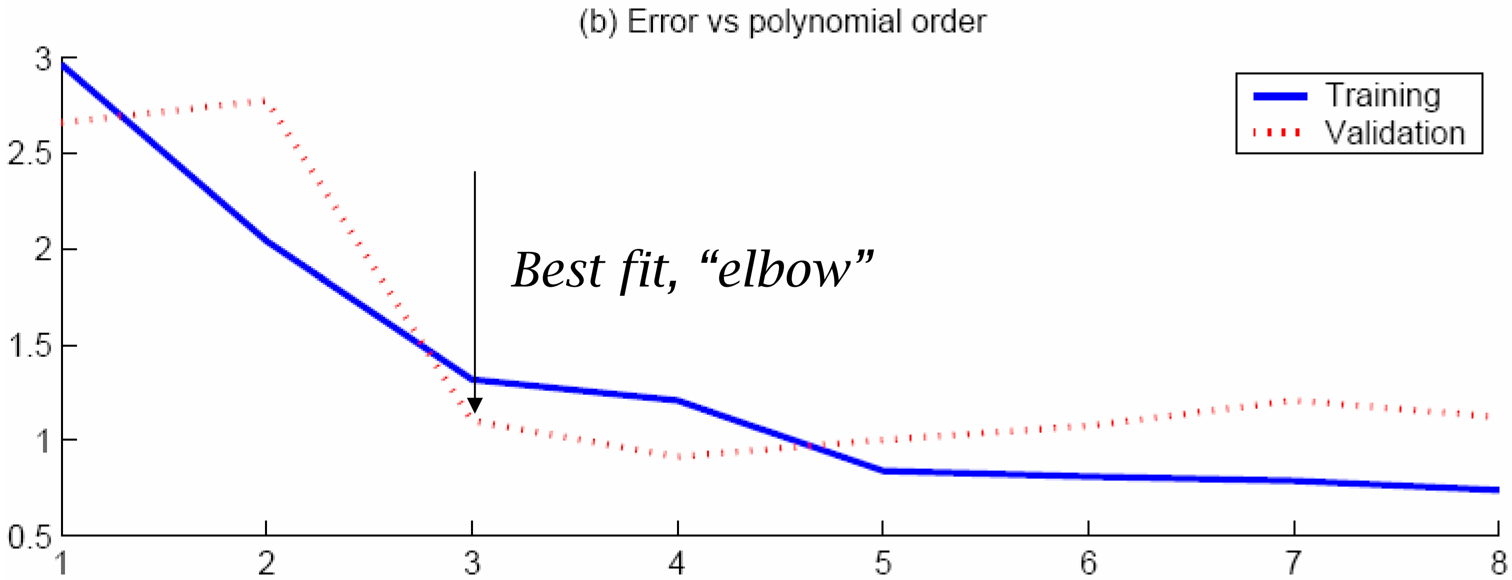

(a) Function and data
f
(b) Order 1
f
bias
g_i
$\bar{g}$
(c) Order 3
variance
(d) Order 5

22

Polynomial Regression




(a) Data and fitted polynomials
5
0
−5
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5


(b) Error vs polynomial order
3
2.5
2
1.5
1
0.5
1
2
3
4
5
6
7
8
Training
Validation
Best fit, “elbow”

Model Selection

- 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)

Bayesian Model Selection

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

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

- 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 15)