FUNDAMENTALS OF MACHINE LEARNING

PARAMETRIC METHODS

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Introduction to Machine Learning

From Bayesian to Parametric Methods

In Chapter 3, we wrote posterior probability for class C_i

$$P(C_i|x) = \frac{p(x|C_i)P(C_i)}{p(x)} = \frac{p(x|C_i)P(C_i)}{\sum_{k=1}^{K} p(x|C_k)P(C_k)}$$

Using discriminant function

$$g_i(x) = p(x|C_i)P(C_i) \quad \text{or} \quad g_i(x) = \log p(x|C_i) + \log P(C_i)$$

We know how to get the prior $P(C_i)$,
but we have problem in getting $p(x|C_i)$

In parametric methods, we assume $p(x|C_i)$ follows some probability distributions, so we can use the probability density function of x to represent $p(x|C_i)$. The only question is how to "*estimate*" parameters of that distribution.

Outline

- Previously, we studied how to make optimal decision when uncertainty is modeled by probability (Bayes' rule)
- Focus of **SINGLE** dimension (or feature) first
- Now we learn how to *estimate these probabilities* from the training set
- **Parametric approach**
  - Classification
  - Regression
- Introduce bias/variance dilemma
- Introduce model selection methods

Parametric Estimation

- Assume samples are drawn from some distribution (e.g., Gaussian, Bernoulli,…etc)
- Once we know the parameters (e.g., mean, variance), we know the whole distribution
- **IID samples:** $\boldsymbol{X} = \{x^t\}_{t=1}^{N}$ where $x^t \sim p(x|\theta)$
- **Parametric estimation:**

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

  e.g., $N(\mu, \sigma^2)$ where $\theta = \{\mu, \sigma^2\}$
- Like to estimate the parameter θ **as likely as possible**

Maximum Likelihood Estimation

- **Likelihood** of θ given the sample X (due to iid)

$$l(\theta|X) \equiv p(X|\theta) = \prod_{t=1}^{N} p(x^t|\theta)$$

find θ which maximizes the likelihood function $l()$

Given example of flipping a coin N times to estimate p

- **Log likelihood** (sometimes to reduce computation)

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

- **Maximum likelihood estimator (MLE)**

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

Example: Bernoulli

- Bernoulli: Two states, failure/success, N iid x^t

$$P(x) = p^x(1-p)^{1-x} \qquad x \in \{0,1\}$$

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

$$= \sum_t x^t \log p + \left(N - \sum_t x^t\right) \log(1-p)$$

- To maximize $\mathcal{L}(p|\mathcal{X})$, take derivative with p and equate to 0
- MLE:

$$\hat{p} = \frac{\sum_t x^t}{N}$$

How?

Example: Bernoulli (derivation)

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

$$= \sum_t x^t \log p + \left(N - \sum_t x^t \right) \log(1-p)$$

$$\frac{d\mathcal{L}(p|X)}{dp} = \frac{1}{p} \sum_t x^t - \left(N - \sum_t x^t \right) \frac{1}{1-p} = 0$$

$$p \left(N - \sum_t x^t \right) = (1-p) \left(\sum_t x^t \right)$$

$$pN = \sum_t x^t$$

$$p = \frac{1}{N} \sum_t x^t$$

Explain how to get the MLE of Bernoulli parameter with N points

Application

In Chapter 3, we wrote posterior probability for class C_i

$$P(C_i|x) = \frac{p(x|C_i)P(C_i)}{p(x)} = \frac{p(x|C_i)P(C_i)}{\sum_{k=1}^{K} p(x|C_k)P(C_k)}$$

Using discriminant function

$$g_i(x) = p(x|C_i)P(C_i) \quad \text{or} \quad g_i(x) = \log p(x|C_i) + \log P(C_i)$$

$$g_i(x) = \log\left(\hat{p}^x(1-\hat{p})^{1-x}\right) + \log P(C_i)$$

Now we remove the limitation of Bayesian method

Application

Values	Class #
1	1
0	1
0	2
1	1
1	2
.....	
1	?

- *N* training data
- Value indicates whether the person is high risk (1) or low risk (0)
- Person can belong to class 1 or class 2

Example: Multinomial

- Outcome of the event is one of *K* mutually exclusive and exhaustive states (or classes) with p_i with $\sum_{i=1}^{K} p_i = 1.$
- Let $x_1, x_2, \ldots, x_K$ are the indicator variables
- x_i is *1* if the outcome is state (class) *i* and *0* otherwise
- We have $P(x_1, x_2, \ldots, x_K) = \prod_{i=1}^{K} p_i^{x_i}$
- *N* independent experiments:

$$\mathcal{X} = \{\boldsymbol{x}^t\}_{t=1}^{N}$$ **Note**: $\boldsymbol{x}^t$ *is a vector !!!*

$$x_i^t = \begin{cases} 1 & \text{if experiment } t \text{ chooses state } i \\ 0 & \text{otherwise} \end{cases} \qquad \text{with } \sum_i x_i^t = 1.$$

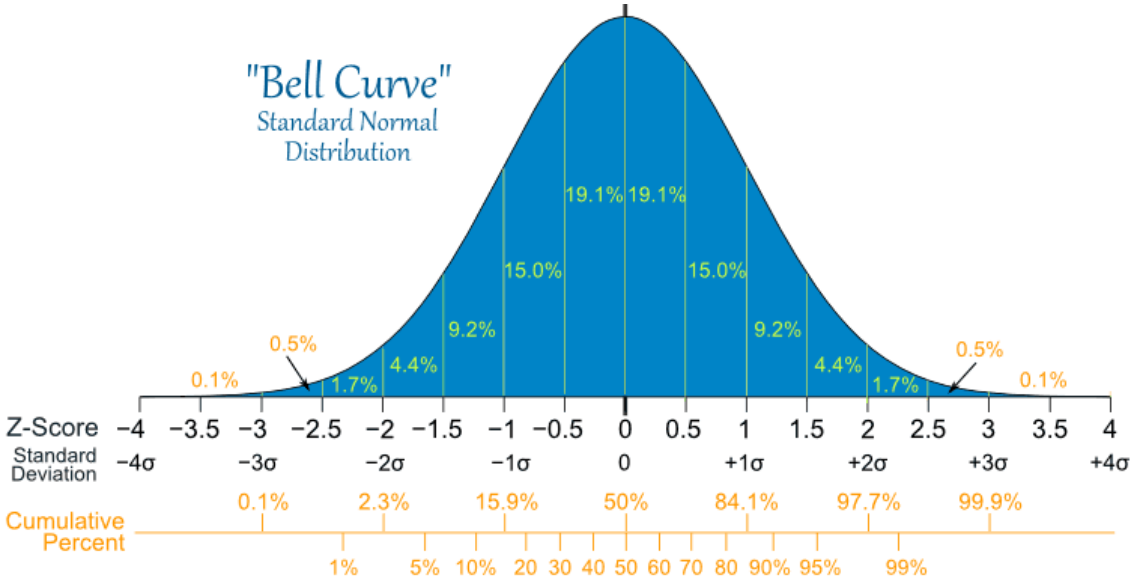
- **MLE:** $\hat{p}_i = \frac{\sum_t x_i^t}{N}$

Application

Values	Class #
1	1
0	1
0	2
2	1
2	2
.....	
2	?

- N training data
- Value indicates whether the person is high risk (1), low risk (0), or neutral (2)
- Person can belong to class 1 or class 2

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:

Log likelihood function

$$\mathcal{L}(\mu, \sigma | \mathcal{X}) = -\frac{N}{2}\log(2\pi) - N\log\sigma - \frac{\sum_t (x^t - \mu)^2}{2\sigma^2}$$

Show this in class

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

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

Gaussian (Normal) Distribution

Log likelihood function: $\mathcal{L}(\mu, \sigma|\mathcal{X}) = -\frac{N}{2}\log(2\pi) - N\log\sigma - \frac{\sum_t (x^t - \mu)^2}{2\sigma^2}$

$$\frac{d\mathcal{L}(\mu,\sigma|\mathcal{X})}{d\mu} = \frac{1}{2\sigma^2}(2)\sum_t (x^t - \mu) = 0$$

$$N\mu = \sum_t x^t$$

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

$$\frac{d\mathcal{L}(\mu,\sigma|\mathcal{X})}{d\sigma} = -\frac{N}{\sigma} + 2\frac{\sum_t (x^t - \mu)^2}{2\sigma^3} = 0$$

$$N\sigma^2 = \sum_t (x^t - \mu)^2$$

$$\sigma^2 = \frac{\sum_t (x^t - \mu)^2}{N}$$

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

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

Parametric Classification

In Chapter 3, we wrote posterior probability for class C_i

$$P(C_i|x) = \frac{p(x|C_i)P(C_i)}{p(x)} = \frac{p(x|C_i)P(C_i)}{\sum_{k=1}^{K} p(x|C_k)P(C_k)}$$

Using discriminant function

$$g_i(x) = p(x|C_i)P(C_i) \quad \text{or} \quad g_i(x) = \log p(x|C_i) + \log P(C_i)$$

If we can assume that $p(x|C_i)$ are Gaussian

$$p(x|C_i) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\frac{(x-\mu_i)^2}{2\sigma_i^2}\right] \qquad \sigma_1, \mu_i, P(C_i) = ?$$

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

Classification of K *cars*

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

$$x \in \Re \qquad \boldsymbol{r} \in \{0,1\}^K \text{ such that } \quad r_i^t = \begin{cases} 1 & \text{if } \boldsymbol{x}^t \in C_i \\ 0 & \text{if } \boldsymbol{x}^t \in C_k, k \neq i \end{cases}$$

- Want *posterior probability P(C$_i$|x), use Bayes Rule*
- **ML estimates** are

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

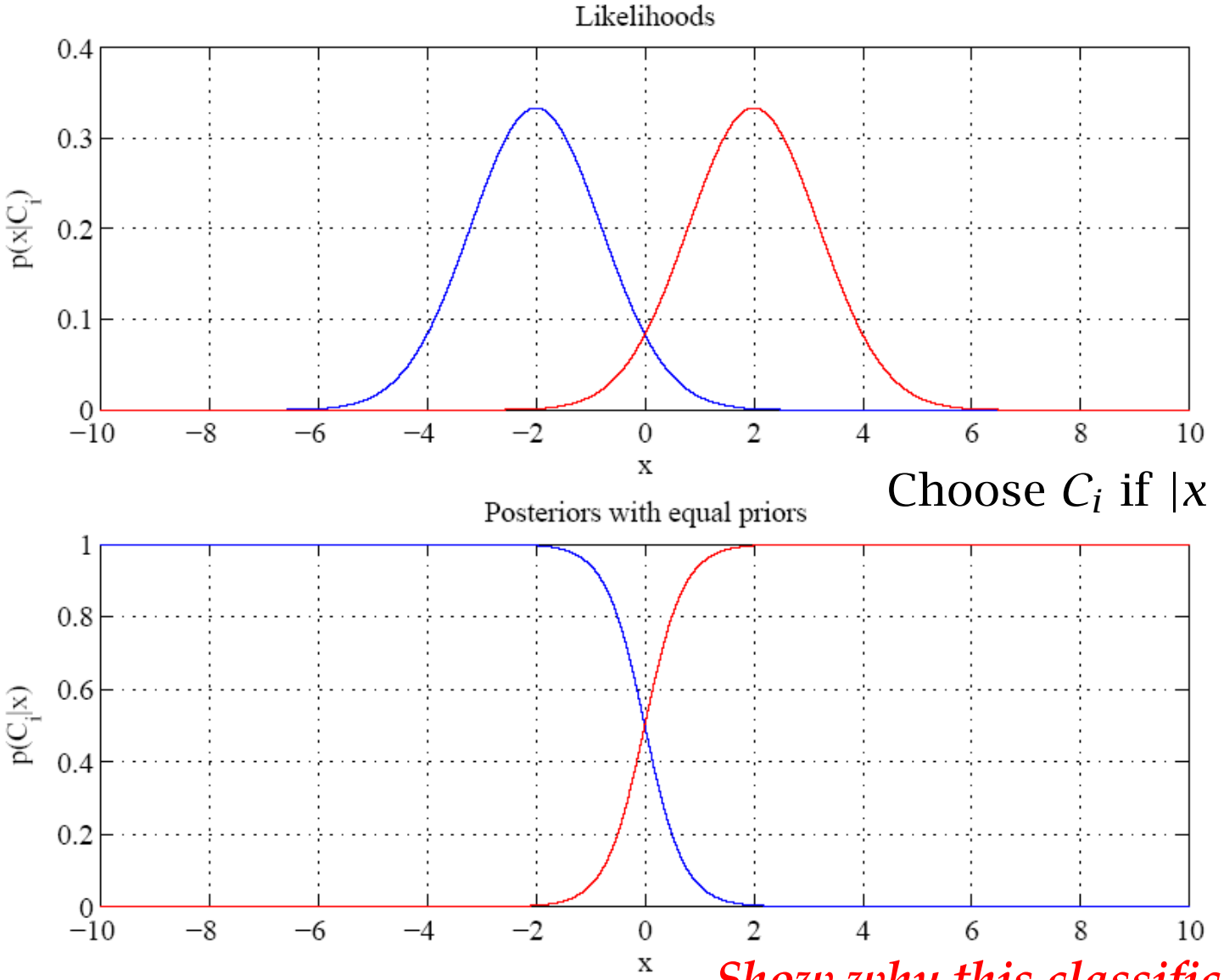
- Discriminant

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

- If prior probability and variances for **ALL CLASSES ARE THE SAME:** $g_i(x) = -(x - m_i)^2$

What is the physical meaning?

When prior ($P(C_i)$)and variance (s_i^2) are equal



$$g_i(x) = -(x - m_i)^2$$

Choose C_i if $|x - m_i| = \min_k |x - m_k|$

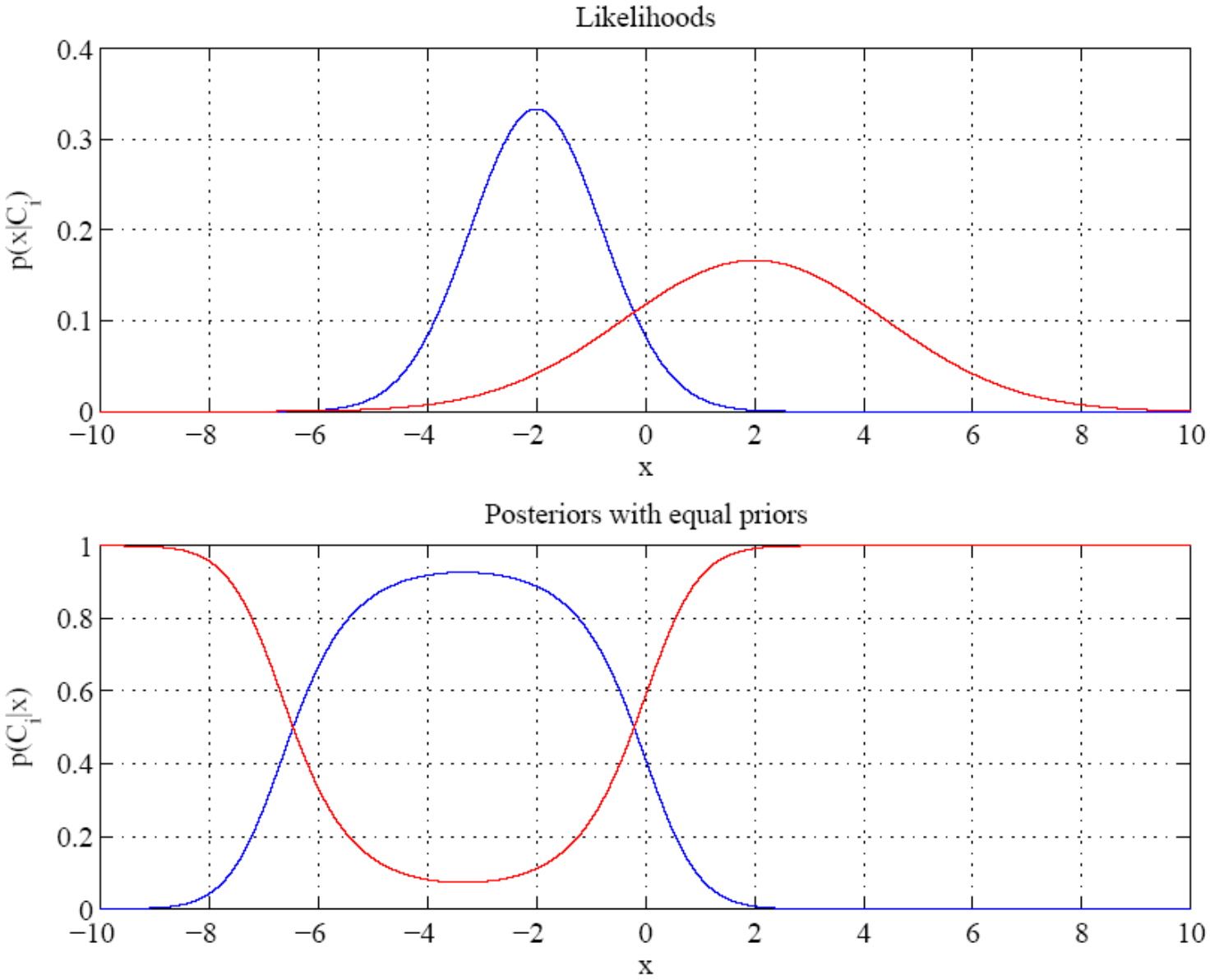
Single boundary at halfway between means, or when $g_1(x)=g_2(x)$

Show derivation

$$x = \frac{(m_1+m_2)}{2}$$

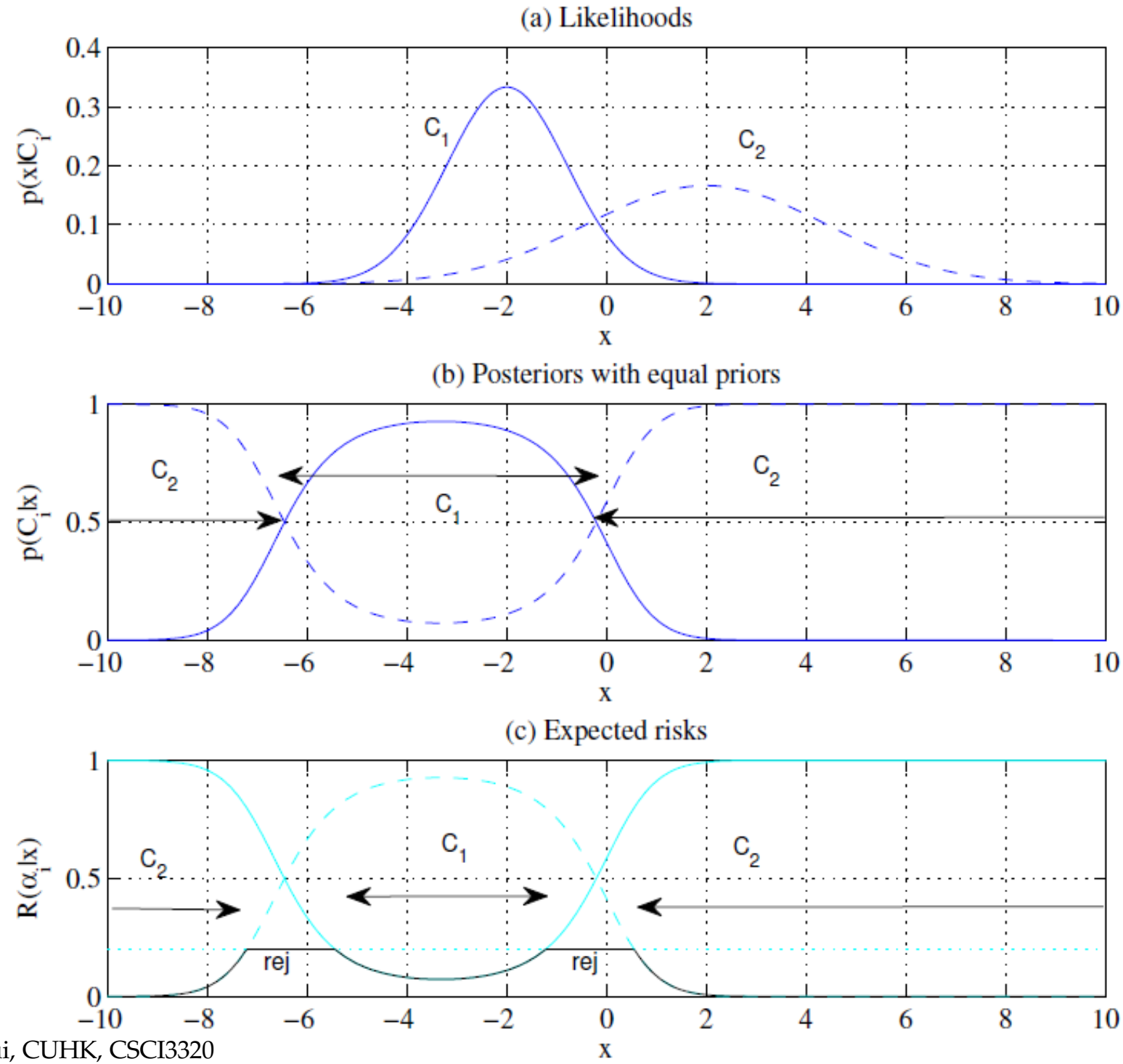
Show why this classification is intuitive

When variance (s_i^2) are different



Two boundaries.

Homework !!!


(a) Likelihoods
p(x|C_i)
C_1
C_2
x
(b) Posteriors with equal priors
p(C_i|x)
C_2
C_1
C_2
x
(c) Expected risks
R(α_i|x)
C_2
C_1
C_2
rej
rej
x

More comment:

- If we have prior information about the means, we can use a Bayesian estimate of $p(x|C_i)$ with prior on μ_i. We will cover this in later chapter
- When x is continuous, don't assume it is Gaussian
- Use the data and test whether it is Gaussian
  - Via plotting to visually check (**remember QQ plot?**)
  - Use ***normality test*** in statistics
- Summary of current "***likelihood approach***" in classification
  - **Use data to estimate densities separately**
  - **Calculate posterior densities with Bayes' rules**
  - **Derive discriminant**

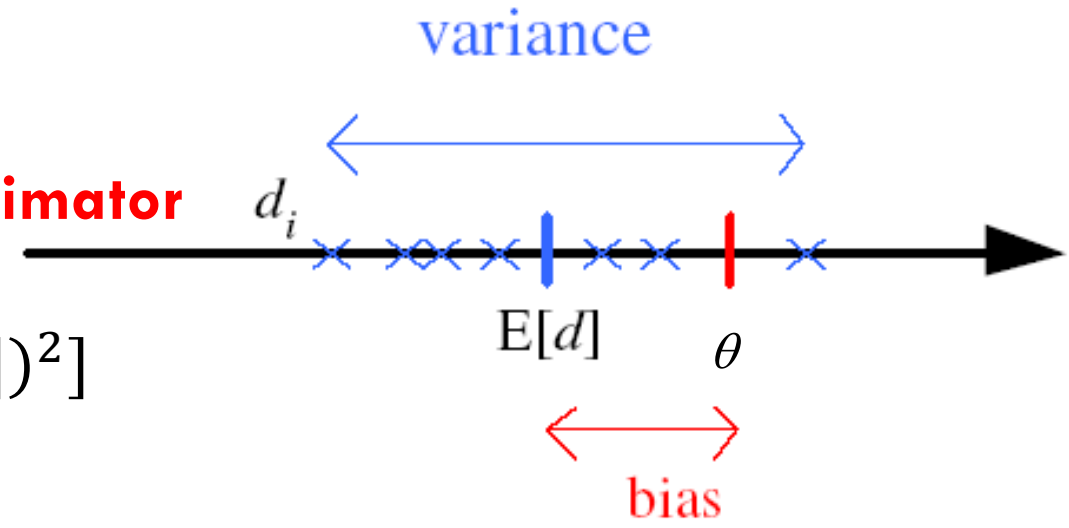
Evaluating an Estimator: Bias and Variance

Unknown parameter θ

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

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

when $b_{\theta(d)} = 0$, **unbiased estimator**



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

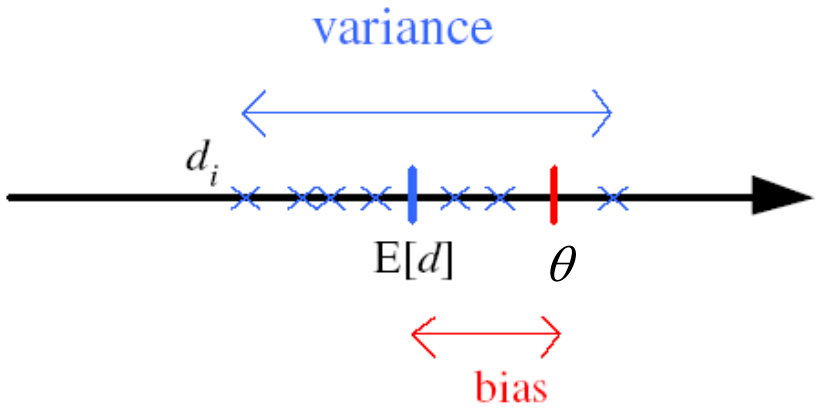
Mean square error:

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

Evaluating an Estimator: Bias and Variance

Mean square error:

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



$$\begin{aligned}
r(d,\theta) &= E\left[(d-\theta)^2\right] \\
&= E\left[(d-E[d]+E[d]-\theta)^2\right] \\
&= E\left[(d-E[d])^2 + (E[d]-\theta)^2 + 2(E[d]-\theta)(d-E[d])\right] \\
&= E\left[(d-E[d])^2\right] + E\left[(E[d]-\theta)^2\right] + 2E\left[(E[d]-\theta)(d-E[d])\right] \\
&= E\left[(d-E[d])^2\right] + (E[d]-\theta)^2 + 2(E[d]-\theta)E[d-E[d]] \\
&= \underbrace{E\left[(d-E[d])^2\right]}_{variance} + \underbrace{(E[d]-\theta)^2}_{bias^2}
\end{aligned}$$

$E[d-E[d]] = 0$

Explain physical meaning

Evaluating an Estimator: Unbiased Estimator

x^t drawn from some density with mean μ

sample average, m, is an unbiased estimator

$$E[m] = E\left[\frac{\sum_t x^t}{N}\right] = \frac{1}{N}\sum_t E[x^t] = \frac{N\mu}{N} = \mu$$ **meaning**

m is also a *consistent* estimator, that is, $\text{Var}(m) \to 0$ as $N \to \infty$.

$$\text{Var}(m) = \text{Var}\left(\frac{\sum_t x^t}{N}\right) = \frac{1}{N^2}\sum_t \text{Var}(x^t) = \frac{N\sigma^2}{N^2} = \frac{\sigma^2}{N}$$ **meaning**

Evaluating an Estimator: Unbiased Estimator

s^2, the MLE of σ^2:

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

show in class

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

Given that $\mathrm{Var}(X) = E[X^2] - E[X]^2$, we get $E[X^2] = \mathrm{Var}(X) + E[X]^2$,

show in class

$$E[(x^t)^2] = \sigma^2 + \mu^2 \text{ and } E[m^2] = \sigma^2/N + \mu^2$$

plugging these in, we get

$$E[s^2] = \frac{N(\sigma^2 + \mu^2) - N(\sigma^2/N + \mu^2)}{N} = \left(\frac{N-1}{N}\right)\sigma^2 \neq \sigma^2$$

s^2 is a biased estimator of σ^2

But an asymptotically unbiased estimator

Unbiased estimator: $(N/(N-1))s^2$

Bayes' Estimator (my notes)

- Sometimes, we know the possible value range of θ
- Treat θ as a random variable with prior $p(\theta)$
- Bayes' rule: $p(\theta|\mathcal{X}) = \dfrac{p(\mathcal{X}|\theta)p(\theta)}{p(\mathcal{X})}$
- To estimate density at x, we have

$$p(x|\mathcal{X}) = \int p(x|\theta')f(\theta')d\theta'$$

$$p(x|\mathcal{X}) = \sum_{\theta'} p(x|\theta')P(\theta')d\theta'$$

Bayes' Estimator (my note)

- **Maximum a Posteriori (MAP):** $\theta_{MAP} = \arg\max_{\theta} p(\theta|\mathcal{X})$

Thus, we have $p(x|\mathcal{X}) \quad = \quad p(x|\theta_{MAP})$

- If no prior values of θ, prior density $p(\theta)$ is flat, MAP estimate is equivalent to maximum likelihood estimate
- **Maximum Likelihood (ML):** $\theta_{ML} = \arg\max_{\theta} p(\mathcal{X}|\theta)$
- **Bayes' estimator** (or expected value of the posterior probability):

$$E[\theta|\mathcal{X}] = \int \theta p(\theta|\mathcal{X}) d\theta$$

Bayes' Estimator: Example

$x^t \sim \mathcal{N}(\theta, \sigma^2)$ and $\theta \sim \mathcal{N}(\mu_0, \sigma_0^2)$, μ_0, σ_0^2, and σ^2 are known

$$p(\mathcal{X}|\theta) = \frac{1}{(2\pi)^{N/2}\sigma^N} \exp\left[-\frac{\sum_t (x^t - \theta)^2}{2\sigma^2}\right]$$

$$p(\theta) = \frac{1}{\sqrt{2\pi}\sigma_0} \exp\left[-\frac{(\theta - \mu_0)^2}{2\sigma_0^2}\right]$$

reduce the posterior density to a single pt

It can be shown that $p(\theta|\mathcal{X})$ is normal with

$$E[\theta|\mathcal{X}] = \frac{N/\sigma^2}{N/\sigma^2 + 1/\sigma_0^2} m + \frac{1/\sigma_0^2}{N/\sigma^2 + 1/\sigma_0^2} \mu_0$$

Thus the Bayes' estimator is a weighted average of the prior mean μ_0 and the sample mean m, with weights being inversely proportional to their variances. As the sample size N increases, the Bayes' estimator gets closer to the sample average, using more the information provided by the sample. When σ_0^2 is small, that is, when we have little prior uncertainty regarding the correct value of θ, or when N is small, our prior guess μ_0 has a higher effect.

Example of Bayes' Estimator

Let $(X_1, X_2, ..., X_n)$ be the random sample of a Bernoulli R.V. X with

$$P(x) = p^x(1-p)^{1-x} \qquad x = 0, 1.$$

p is unknown but it is uniformly distributed on $(0, 1)$, or

$$f(p) = 1 \qquad 0 < p < 1.$$

The posterior pdf of p is: $f(p|x_1, ..., x_n) = \dfrac{f(x_1, ..., x_n, p)}{P(x_1, .., x_n)}$

$$\begin{aligned} f(x_1, ..., x_n, p) &= f(x_1, ..., x_n|p)f(p) \\ &= p^{\sum_{i=1}^n x_i}(1-p)^{n-\sum_{i=1}^n x_i} = p^m(1-p)^{n-m} \times 1 \end{aligned}$$

where $m = \sum_{i=1}^n x_i$

Example of Bayes' Estimator

$$P(x_1, .., x_n) \quad = \quad \int_0^1 f(x_1, ..., x_n, p)dp = \int_0^1 p^m(1-p)^{n-m}dp$$

From calculus, we have: $\int_0^1 p^m(1-p)^k dp = \frac{m!k!}{(m+k+1)!}$

So: $f(p|x_1, ..., x_n) = \frac{f(x_1,..,x_n,p)}{P(x_1,..,x_n)} = \frac{(n+1)!p^m(1-p)^{n-m}}{m!(n-m)!}$

Example of Bayes' Estimator

Bayes' estimator $E[p|\mathcal{X}]$:

$$\begin{aligned} E[p|\mathcal{X}] &= \int_0^1 p f(p|x_1,..,x_n)dp \\ &= \frac{(n+1)!}{m!(n-m)!}\int_0^1 p^{(m+1)}(1-p)^{n-m}dp \\ &= \frac{(n+1)!}{m!(n-m)!}\frac{(m+1)!(n-m)!}{(n+2)!} = \frac{m+1}{n+2} \\ &= \frac{1}{n+2}\left(\sum_{i=1}^{n} x_i + 1\right) \end{aligned}$$

Bayes' estimator p_B is $\frac{1}{n+2}\left(\sum_{i=1}^{n} x_i + 1\right)$

Regression

r: dependent variable
x: independent variable

unknown function *f()*

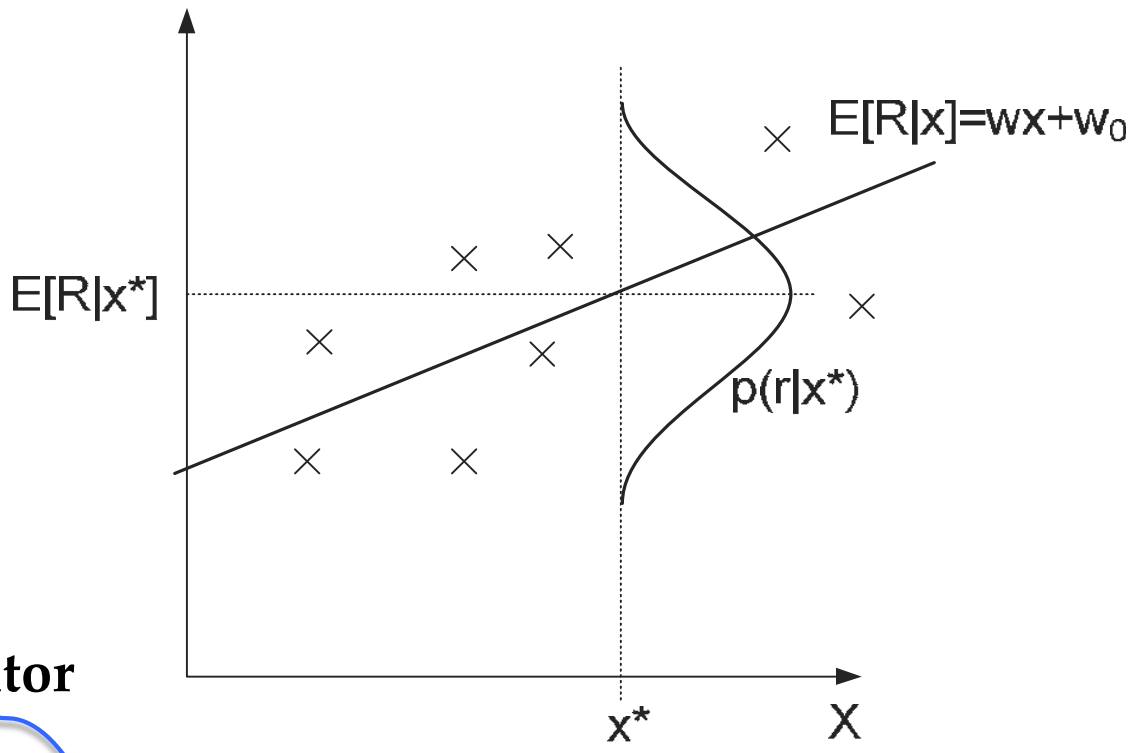
noise

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

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

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

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



log maximum likelihood estimator

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

can be ignored

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

Regression: From LogL to Error

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

First term is not a function of θ, maximize the above term is equivalent to **minimize** the following error expression (E) :

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

θ that minimize this function is the ***least square estimates***

Example: Linear Regression

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

Using the error function in previous slide, taking derivatives for two unknowns, we have:

$$\begin{aligned} \sum_t r^t &= N w_0 + w_1 \sum_t x^t \\ \sum_t r^t x^t &= w_0 \sum_t x_t + w_1 \sum_t (x^t)^2 \end{aligned}$$

vector-matrix form as $\mathbf{A}\boldsymbol{w} = \boldsymbol{y}$

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

2 x 2 matrix *2 x 1 vector* *2 x 1 vector*

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

Example: Polynomial Regression of order k

$$g(x^t|w_k,\ldots,w_2,w_1,w_0) = w_k(x^t)^k + \cdots + w_2(x^t)^2 + w_1x^t + w_0$$

Taking (*k+1*) derivatives of *E*, we have (*k+1*) equations :

$\mathbf{A}\bar{\boldsymbol{w}} = \boldsymbol{y}$ where

$$\mathbf{A} = \begin{bmatrix} N & \sum_t x^t & \sum_t (x^t)^2 & \cdots & \sum_t (x^t)^k \\ \sum_t x^t & \sum_t (x^t)^2 & \sum_t (x^t)^3 & \cdots & \sum_t (x^t)^{k+1} \\ \vdots & & & & \\ \sum_t (x^t)^k & \sum_t (x^t)^{k+1} & \sum_t (x^t)^{k+2} & \cdots & \sum_t (x^t)^{2k} \end{bmatrix}$$

$$\boldsymbol{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_k \end{bmatrix}, \quad \boldsymbol{y} = \begin{bmatrix} \sum_t r^t \\ \sum_t r^t x^t \\ \sum_t r^t (x^t)^2 \\ \vdots \\ \sum_t r^t (x^t)^k \end{bmatrix}$$

Example: Polynomial Regression of order k

We can write $\mathbf{A} = \mathbf{D}^T\mathbf{D}$ and $\boldsymbol{y} = \mathbf{D}^T\boldsymbol{r}$ where

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

solve for the parameters as

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

Other Error Measures

- **Square Error:**

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

- **Relative Square Error:** $E(\theta|\mathcal{X}) = \frac{\sum_{t=1}^{N}\left[\boldsymbol{r}^t - g(\boldsymbol{x}^t|\theta)\right]^2}{\sum_{t=1}^{N}(\boldsymbol{r}^t - \bar{\boldsymbol{r}})^2}$

- **Absolute Error:** $E(\theta|\mathcal{X}) = \sum_{t=1}^{N}|\boldsymbol{r}^t - g(\boldsymbol{x}^t|\theta)|$

- **ε-sensitive Error:**

$$E(\theta|\mathcal{X}) = \sum_{t=1}^{N} 1\left(|\boldsymbol{r}^t - g(\boldsymbol{x}^t|\theta)| > \epsilon\right)\left(|\boldsymbol{r}^t - g(\boldsymbol{x}^t|\theta)| - \epsilon\right)$$

Bias and Variance

The expected square error at the point x is:

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

variance *bias²*

The expected value (average over samples X, all of size N and drawn from the same joint density $p(r,x)$ is):

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

Illustrating Bias and Variance

- M samples $X_i = \{x_i^t, r_i^t\}, i = 1, \ldots, M$ of known function $f()$ with added noise. Use each data sets to fit estimator $g_i(x)$, $i = 1,\ldots,M$
- $E[g(x)]$ is estimated by average over M of $g_i()$

$$\bar{g}(x) = \frac{1}{M}\sum_{i=1}^{M} g_i(x)$$

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

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

Bias/Variance Dilemma (or tradeoff)

- If $g_i(x) = 2$: It has no variance and high bias
- If $g_i(x) = \sum_t \frac{r_i^t}{N}$: It has *lower bias, higher variance*
- As we increase complexity,

  bias decreases (a better fit to data) and

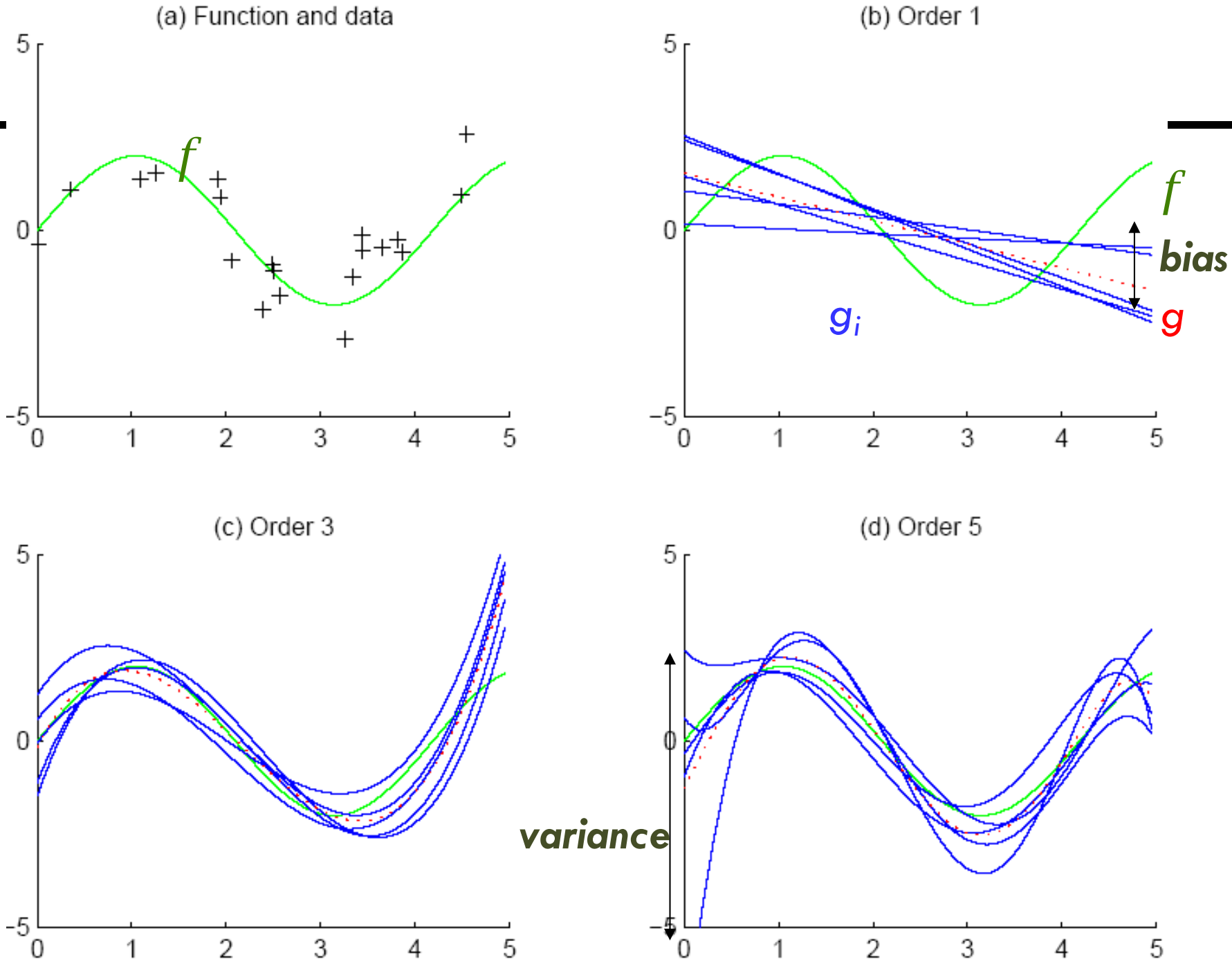
  variance increases (fit varies more with data)
- Bias/Variance dilemma: (Geman et al., 1992)

Illustration

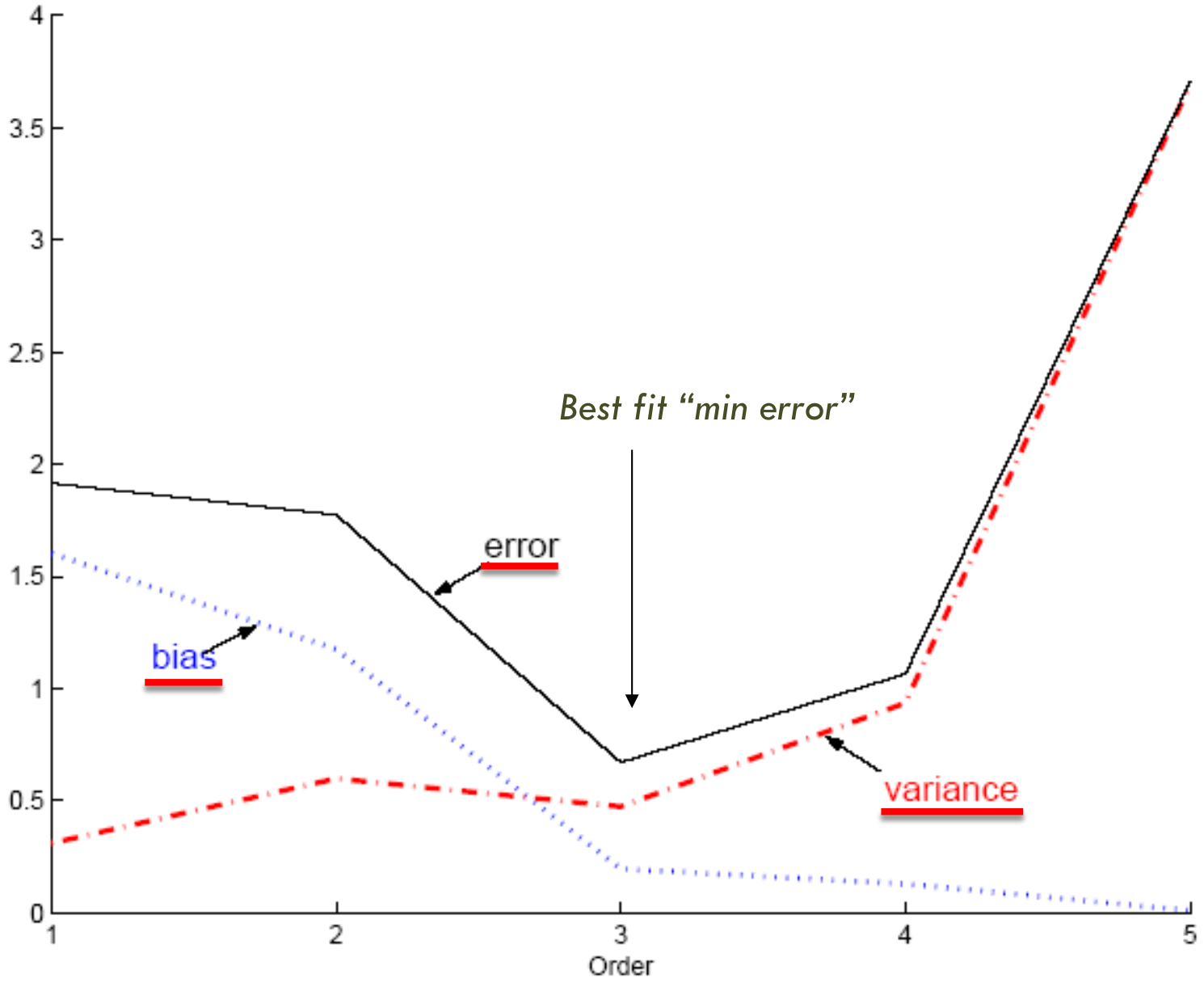
$$r = f(x) + \varepsilon$$

- **Function**: $f(x) = 2\sin(1.5x)$
- **Noise:** $(\mathcal{N}(0,1))$
- **Samples:** *M=5 samples are taken, each contains N=20 points*
- **Five polynomial fit:**

  $g_i(x)$, *i=1,…,5 of order 1, 3, and 5*


(a) Function and data
f
(b) Order 1
f
bias
g
g_i
(c) Order 3
(d) Order 5
variance

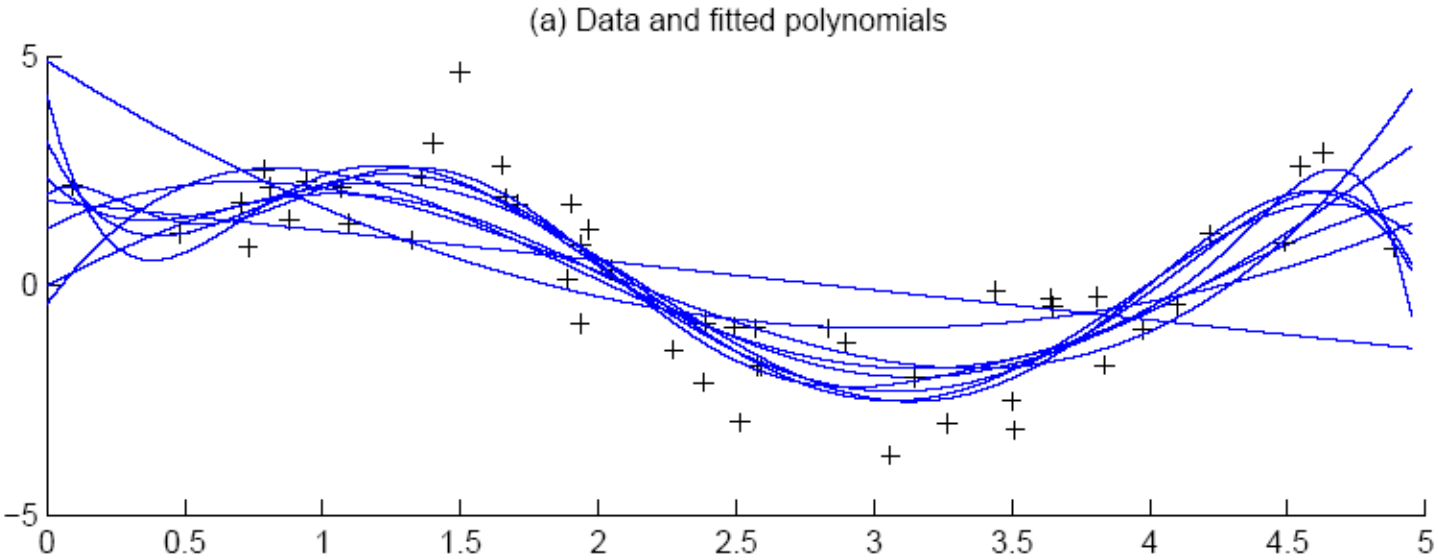
Polynomial Regression (*M=100*)

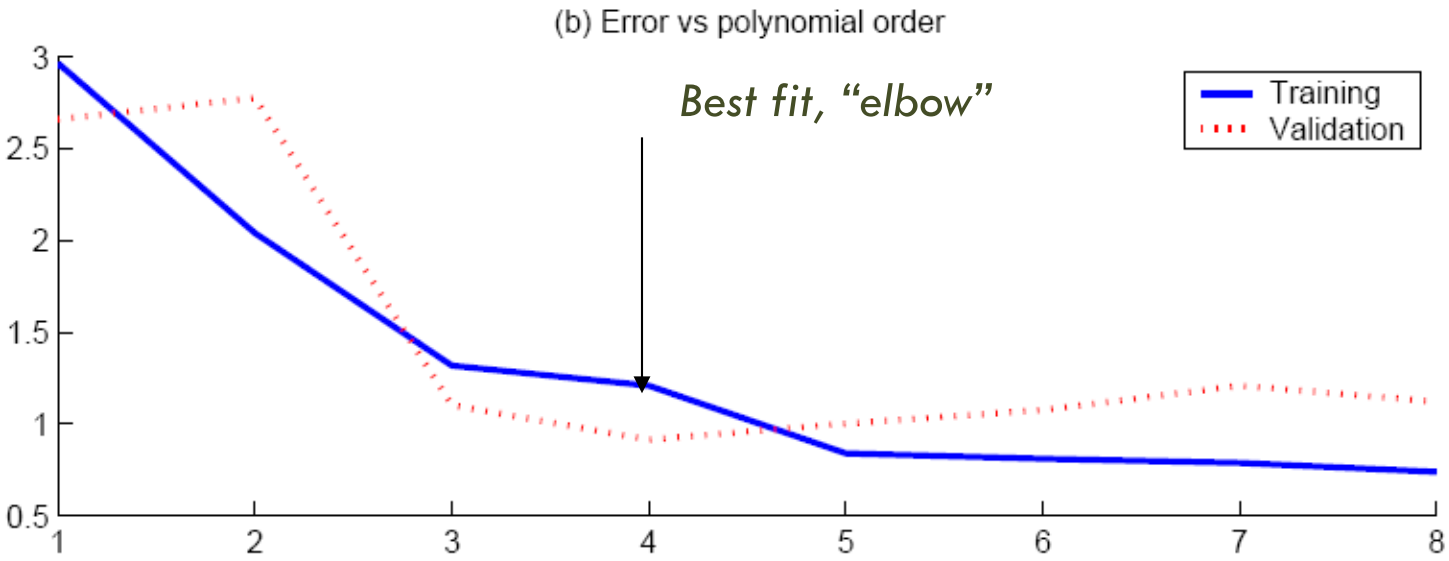


Underfitting vs. Overfitting

- High bias implies "*underfintting*"
- High variance implies "*overfitting*"
- Tradeoff via *cross-validation*

M=50


(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
Best fit, "elbow"
Training
Validation
3
2.5
2
1.5
1
0.5
1
2
3
4
5
6
7
8

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)**

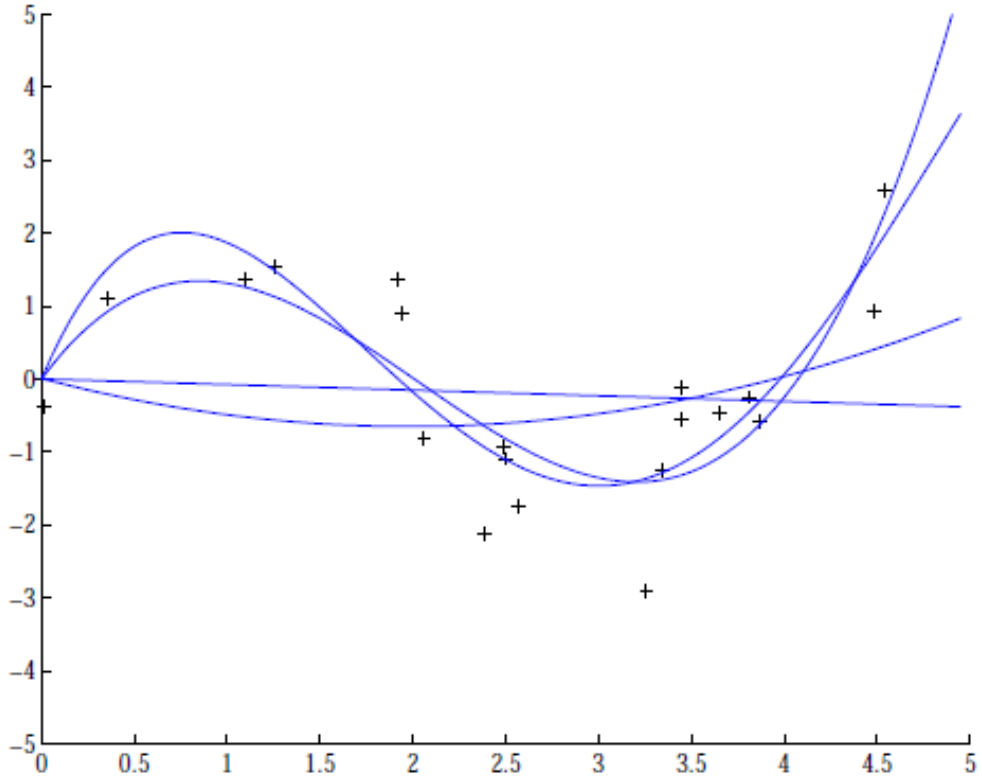
Bayesian Model Selection

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

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

- 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]

Regularization (L2): $E = \sum_t [r^t - g(x^t|\boldsymbol{w})]^2 + \lambda \sum_i w_i^2$

Conclusion

- Simple Bayesian (or Bayes' rule) has some shortcomings, in particular, when $\boldsymbol{x}$ is not in the database/training data. So we have problem getting the likelihood (or evidence)
- In parametric methods, we assume $\boldsymbol{x}$ follows some probability distribution. So if we can have an "accurate" estimate of the parameters of the distribution, we can use the probability density for the point $\boldsymbol{x}$, this can overcome the problem in the Bayesian method.
- We discuss how to obtain the MLE for parameters in Bernoulli, multinomial, Gaussian probability distribution
- We discuss how to do regression using parametric method
- We discuss Unbiased estimation
- We discuss mean square *error* $= bias^2 +$ *variance*
- We discuss their tradeoffs.