UVA CS 4501: Machine Learning

Lecture 17b: Gaussian BC and Generative vs. Discriminative Classifier

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Course Content Plan ➔
Six major sections of this course

- ~~Regression (supervised)~~ — Y is a continuous
- Classification (supervised) — Y is a discrete
- Unsupervised models — NO Y
- Learning theory — About f()

- Graphical models — About interactions among X1,… Xp

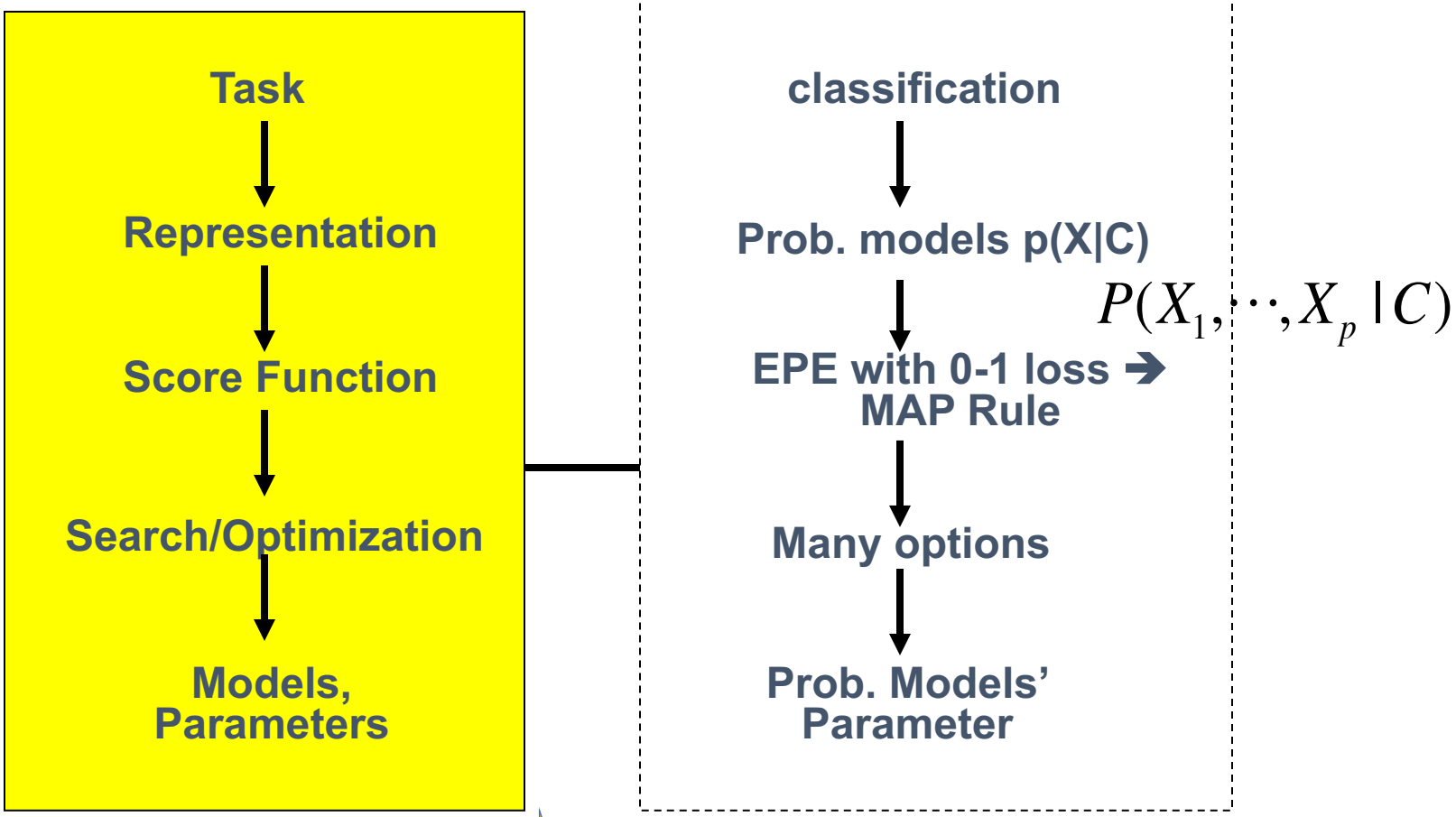
- Reinforcement Learning — Learn program to Interact with its environment

Today: More Generative Bayes Classifiers

- ✓ Generative Bayes Classifier
- ✓ Naïve Bayes Classifier
- ✓ Gaussian Bayes Classifiers
  - Gaussian distribution
  - Naïve Gaussian BC
  - Not-naïve Gaussian BC ➔ LDA, QDA
- ✓ Discriminative vs. Generative classifier

$$\underset{k}{\operatorname{argmax}}\, P(C\_k \mid X) = \underset{k}{\operatorname{argmax}}\, P(X,C) = \underset{k}{\operatorname{argmax}}\, P(X \mid C)P(C)$$

Generative Bayes Classifier



Bernoulli Naïve

$$p(W_i = true \mid c_k) = p_{i,k}$$

Gaussian Naive

$$\hat{P}(X_j \mid C = c_k) = \frac{1}{\sqrt{2\pi\sigma_{jk}}} \exp\left(-\frac{(X_j - \mu_{jk})^2}{2\sigma_{jk}^2}\right)$$

Multinomial

$$P(W_1 = n_1,\ldots,W_v = n_v \mid c_k) = \frac{N!}{n_{1k}!n_{2k}!..n_{vk}!}\theta_{1k}^{n_{1k}}\theta_{2k}^{n_{2k}}..\theta_{vk}^{n_{vk}}$$

Review: Continuous Random Variables

- Probability density function (pdf) instead of probability mass function (pmf)
  - For discrete RV: Probability mass function (pmf): $P(X = x_i)$

- A pdf (prob. Density func.) is any function $f(x)$ that describes the probability density in terms of the input variable x.

Review: Probability of Continuous RV

- Properties of pdf
  - $f(x) \geq 0, \forall x$
  - $\int_{-\infty}^{+\infty} f(x) = 1$ → $\sum_{i=1}^{k_i} P(X = x_i) = 1$

- Actual probability can be obtained by taking the integral of pdf
  - E.g. the probability of X being between 5 and 6 is

$$P(5 \leq X \leq 6) = \int_{5}^{6} f(x)dx$$

Review: Mean and Variance of RV

- Mean (Expectation):
  - Discrete RVs:

$$\mu = E(\mathrm{X})$$

$$E(\mathrm{X}) = \sum_{v_i} v_i \mathrm{P}(\mathrm{X} = v_i)$$

$$E(g(X)) = \sum_{v_i} g(v_i) P(X = v_i)$$

  - Continuous RVs:

$$E(\mathrm{X}) = \int_{-\infty}^{+\infty} x f(x) dx$$

$$E(g(X)) = \int_{-\infty}^{+\infty} g(x) f(x) dx$$

Adapt From Carols' prob tutorial

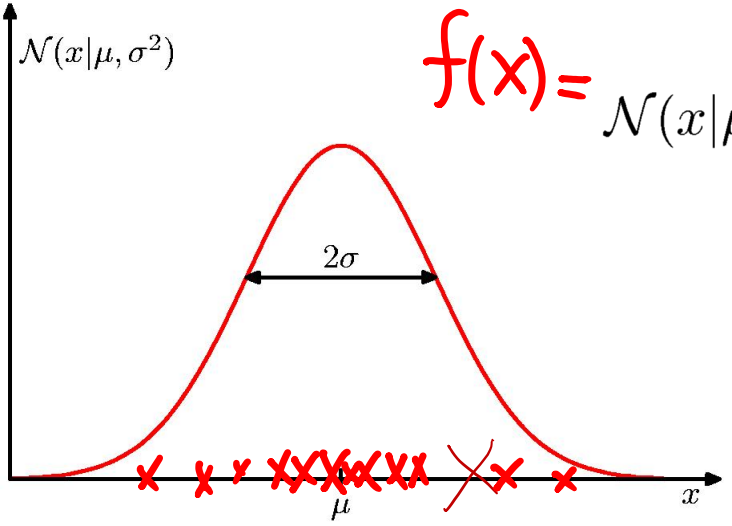
Review: Mean and Variance of RV

- Variance: $Var(X) = E((X - \mu)^2)$
  - Discrete RVs: $V(\mathrm{X}) = \sum_{v_i} (v_i - \mu)^2 \, \mathrm{P}(\mathrm{X} = v_i)$
  - Continuous RVs: $V(\mathrm{X}) = \int_{-\infty}^{+\infty} (x - \mu)^2 \, f(x) dx$
- Covariance:

$$Cov(X,Y) = E((X - \mu_x)(Y - \mu_y)) = E(XY) - \mu_x \mu_y$$

Adapt From Carols' prob tutorial

Single-Variate Gaussian Distribution



$$f(x) = \mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$

$$X \sim N(\mu,\sigma^2)$$

Courtesy: http://research.microsoft.com/~cmbishop/PRML/index.htm

Multivariate Normal (Gaussian) PDFs

The only widely used continuous joint PDF is the multivariate normal (or Gaussian):

$$f(\vec{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Where |*| represents determinant

Mean

Covariance Matrix

$f(x_1, x_2, \cdots, x_p)$

#para : $O(p + p^2)$

$\vec{\mu}_{p\times 1}$: mean vector

$\Sigma_{p\times p}$: covariance matrix

$$\begin{bmatrix} \sigma_1^2 & \cdots & \mathrm{cov}(X_i, X_j) \\ & \sigma_2^2 & \\ & & \ddots \\ & & & \sigma_p^2 \end{bmatrix} \uparrow j \quad \rightarrow i$$

Review: Discrete RV

$p(X_1 X_2 \cdots X_p)$

→ Nonnaive: 2^p

naive : p

Multivariate Normal (Gaussian) PDFs

The only widely used continuous joint PDF is the multivariate normal (or Gaussian):

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Where |*| represents determinant

Mean

Covariance Matrix

- Mean of normal PDF is at peak value. Contours of equal PDF form ellipses.

- The covariance matrix captures linear dependencies among the variables

Example: the Bivariate Normal distribution

$$f\left(x_1, x_2\right) = \frac{1}{\left(2\pi\right)\left|\Sigma\right|^{1/2}} \mathrm{e}^{-\frac{1}{2}\left(\vec{x}-\vec{\mu}\right)^T \Sigma^{-1}\left(\vec{x}-\vec{\mu}\right)}$$

with $\vec{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$ and

$$\underset{2\times 2}{\Sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix} = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

$[\sigma_{12} = \rho\sigma_1\sigma_2]$

$$\left|\Sigma\right| = \sigma_{11}\sigma_{22} - \sigma_{12}^2 = \sigma_1^2\sigma_2^2\left(1-\rho^2\right)$$

Example: the Bivariate Normal distribution

$$f\left(x_1, x_2\right) = \frac{1}{\left(2\pi\right)\left|\Sigma\right|^{1/2}} \mathrm{e}^{-\frac{1}{2}\left(\vec{x}-\vec{\mu}\right)^T \Sigma^{-1}\left(\vec{x}-\vec{\mu}\right)}$$

with $\vec{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$ 2x1 and

$$\underset{2\times 2}{\Sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix} = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

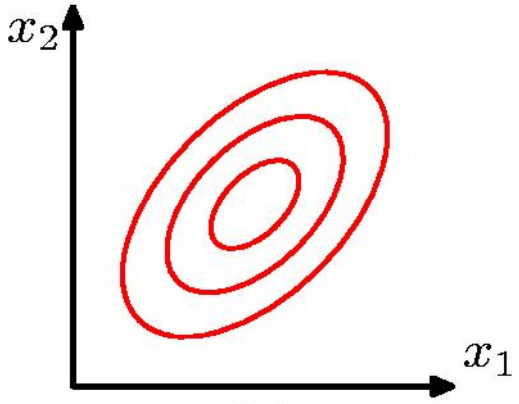
$V(X_1)$ $Cov(X_1, X_2)$ $V(X_2)$ 2 x 2

$$\left|\Sigma\right| = \sigma_{11}\sigma_{22} - \sigma_{12}^2 = \sigma_1^2\sigma_2^2\left(1-\rho^2\right)$$

Bi-Variate Gaussian (normal) PDF

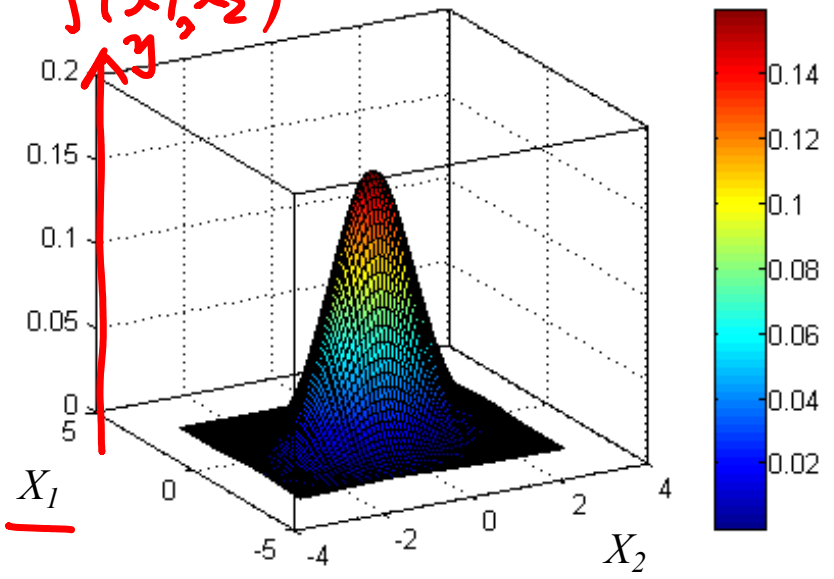
$f(x_1, x_2)$

Contour Plot



y = PDF $f(x_1, x_2)$

Surface Plot



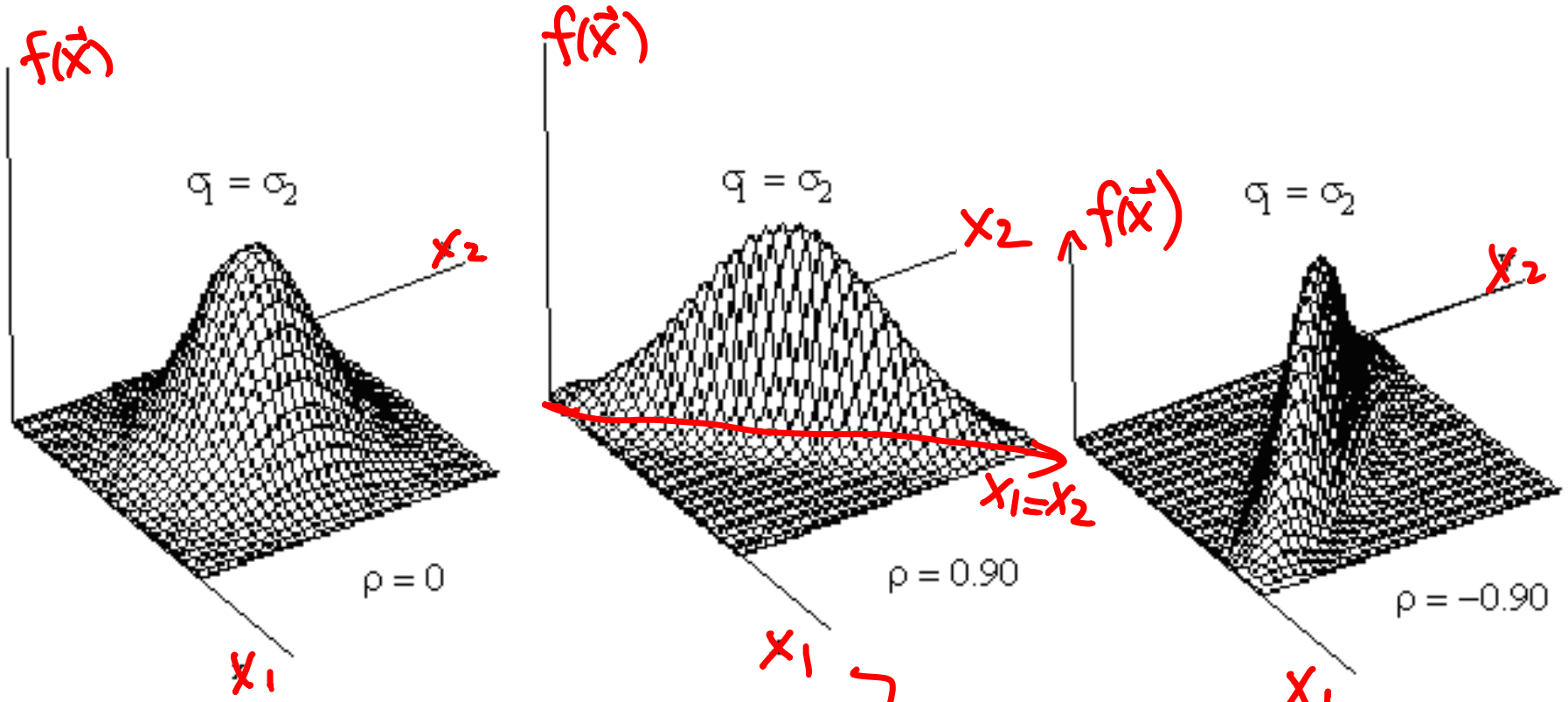
$\vec{\mu} = \begin{bmatrix} \mu_{X_1} \\ \mu_{X_2} \end{bmatrix}$

- Mean of a normal PDF is at peak value. Contours of equal PDF form ellipses.

- The covariance matrix captures linear dependencies among the variables

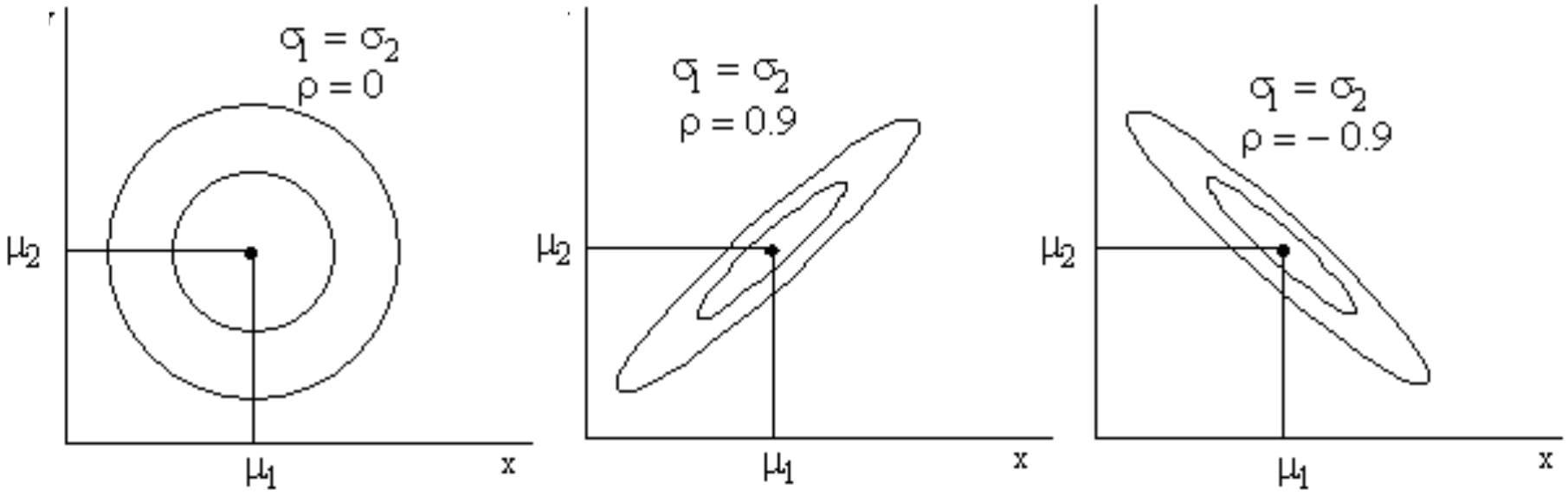
Courtesy: http://research.microsoft.com/~cmbishop/PRML/index.htm

Surface Plots of the bivariate Normal distribution

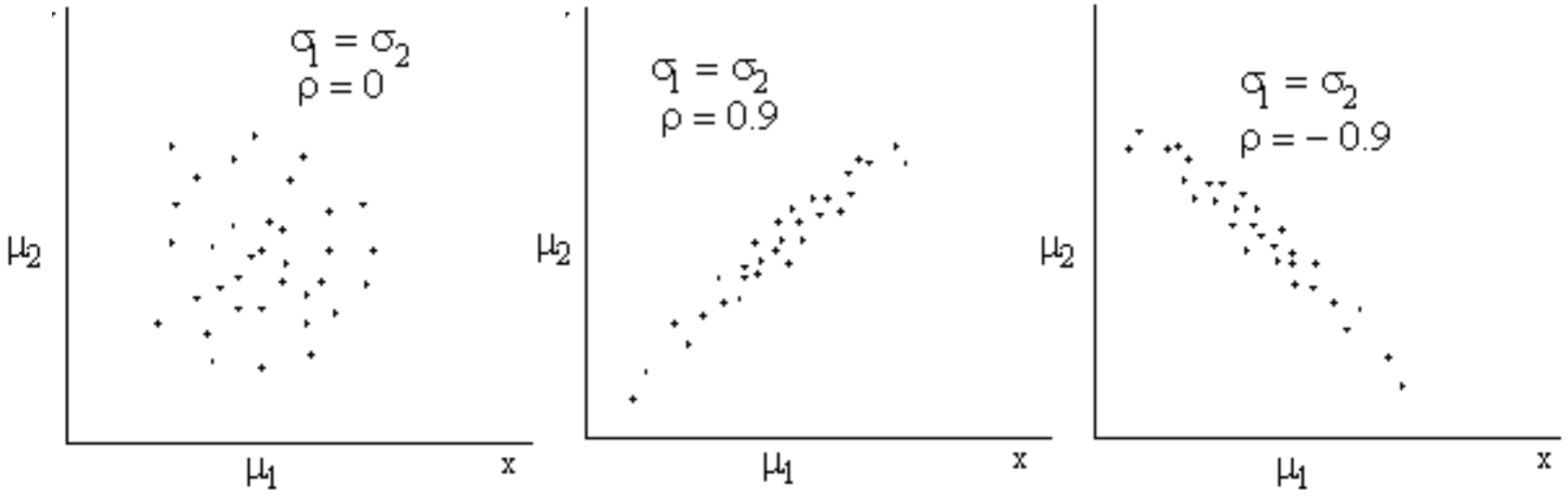


$$\Sigma = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

Contour Plots of the bivariate Normal distribution

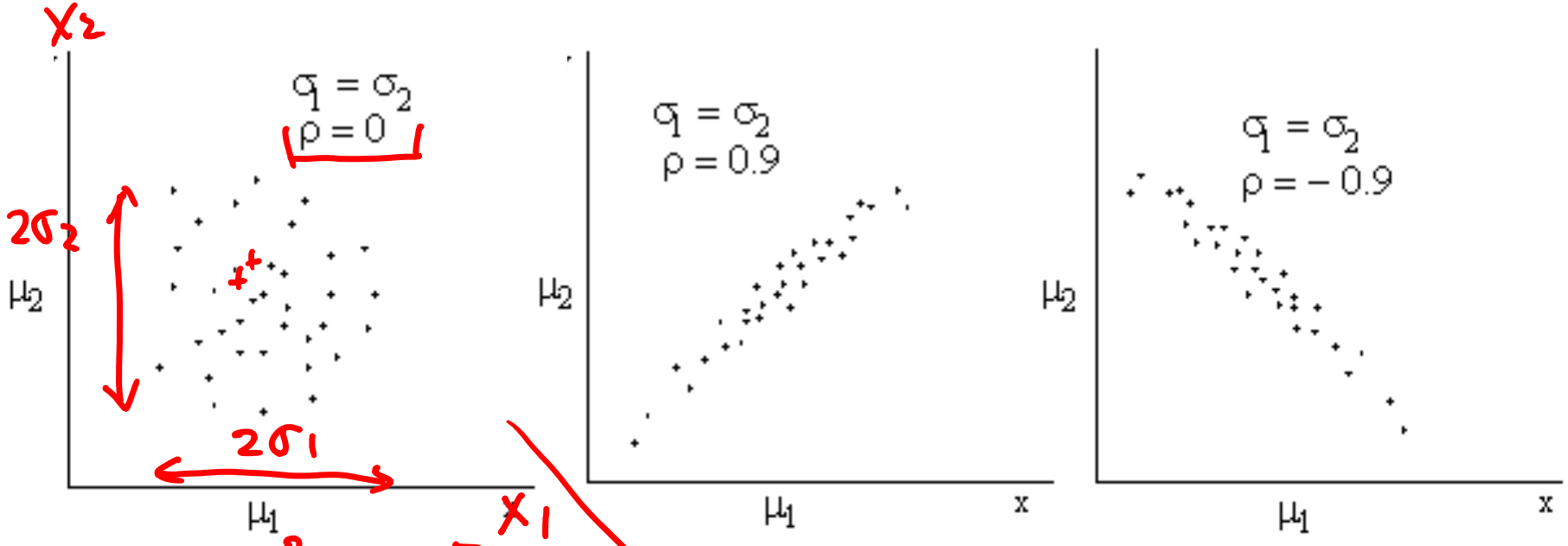


Scatter Plots of samples from the three bivariate Normal distributions



$N(\vec{\mu}, \Sigma)$

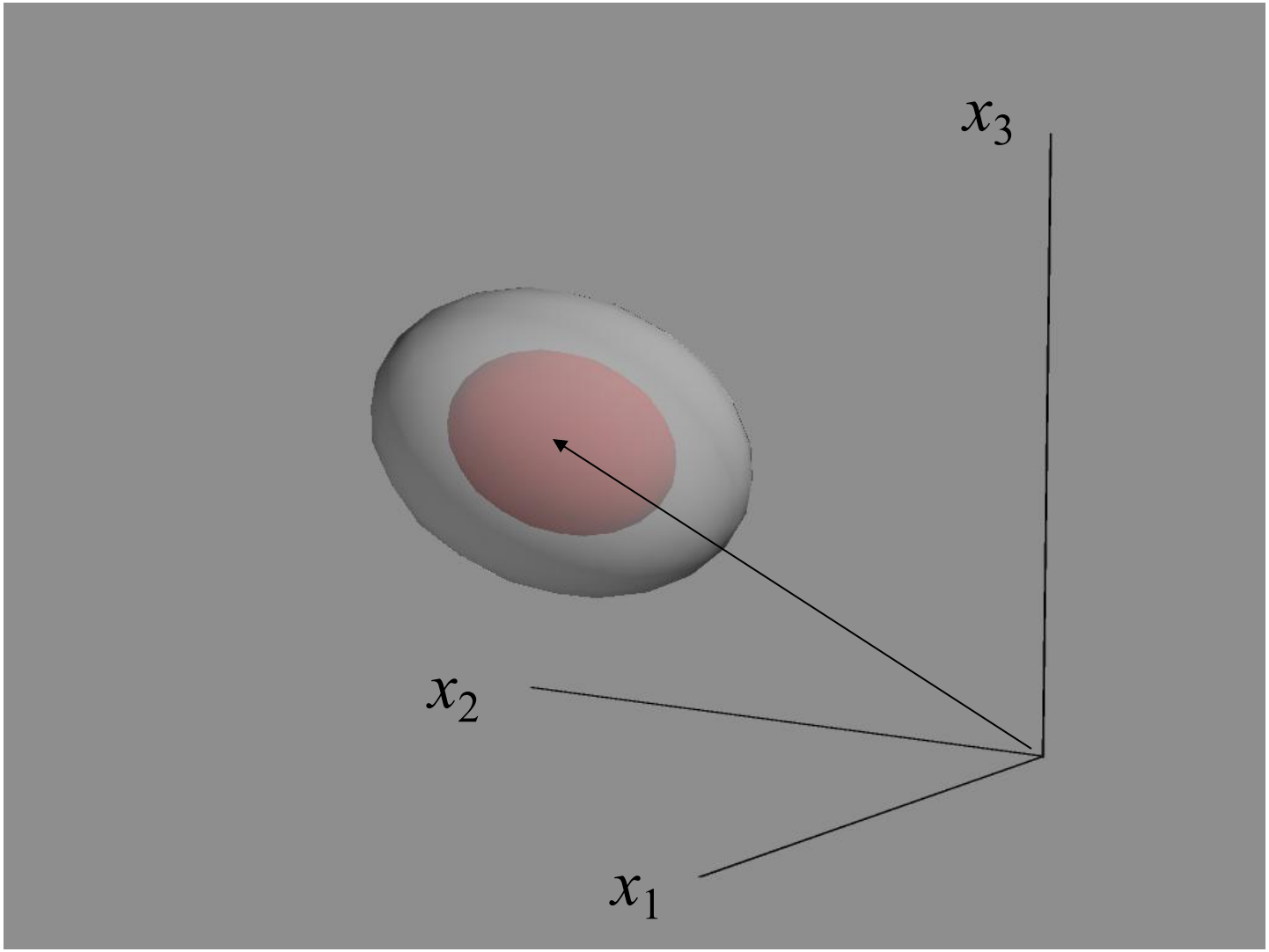
Scatter Plots of samples from the three bivariate Normal distributions



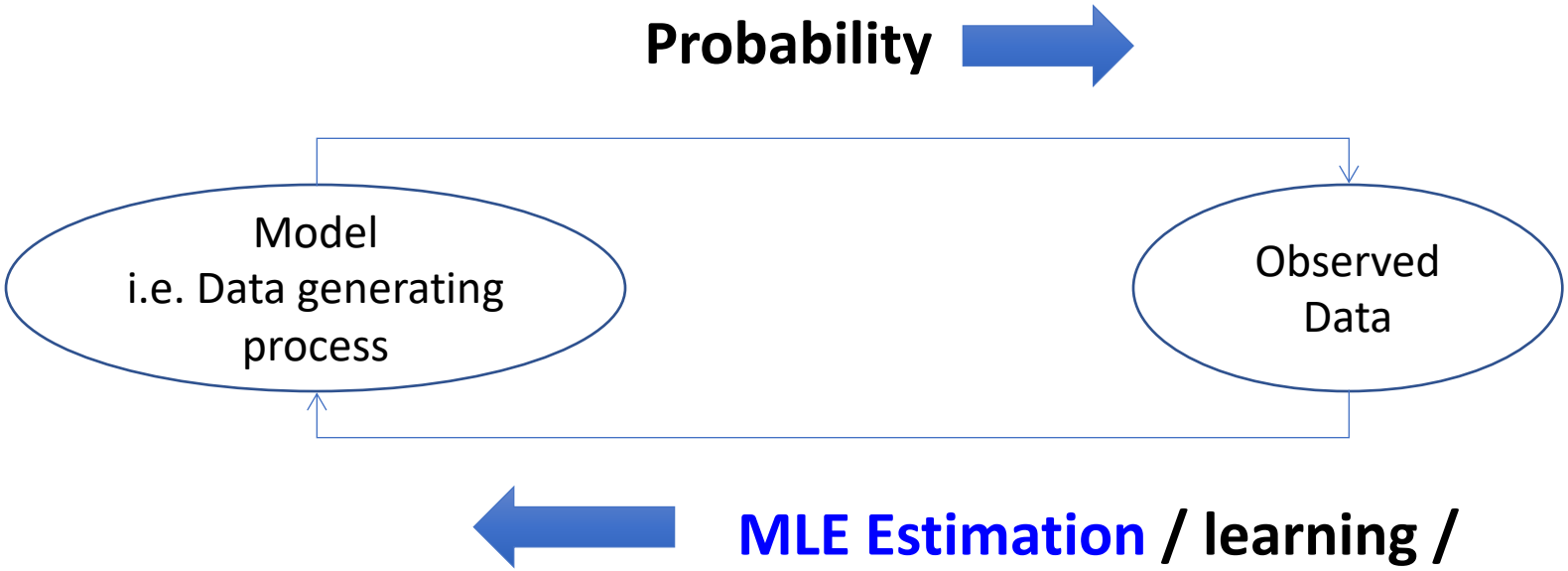
When $\Sigma = \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix} \Rightarrow f(x_1, x_2) = f(x_1) f(x_2)$ $\Rightarrow$ data $\{\mu_1, \ldots, \mu_p$ $\sigma_1, \ldots, \sigma_p$ $O(2p)$

Trivariate Normal distribution (Countour plot

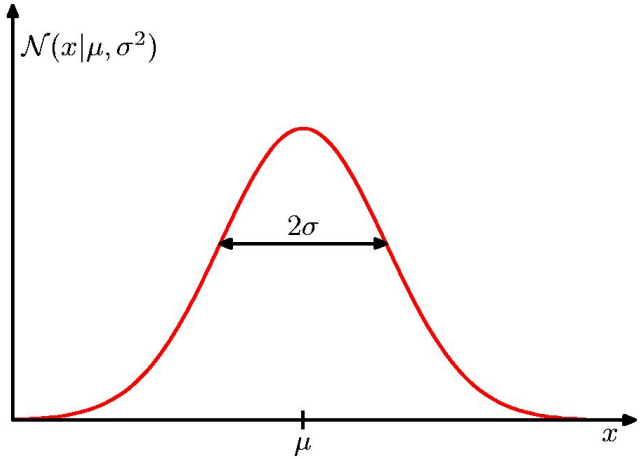
When
x_1
x_2
x_3



The Big Picture



How to Estimate 1D Gaussian: MLE



• In the 1D Gaussian case, we simply set the mean and the variance to the sample mean and the sample variance:

$$\bar{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\overline{\sigma^2} = \frac{1}{n}\sum_{i=1}^{n} \left(x_i - \overline{\mu}\right)^2$$

How to Estimate p-D Gaussian: MLE

$\in \{1, 2, \cdots, p\}$

$$< X_1, X_2 \cdots, X_p > \sim N\left(\vec{\mu}, \Sigma\right)$$

How to Estimate p-D Gaussian: MLE

$$< X_1, X_2 \cdots, X_p > \sim N\left(\vec{\mu}, \Sigma\right)$$

$$\vec{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_p \end{bmatrix}_{p \times 1} \qquad \mu_i = \frac{1}{n} \sum_{j=1}^{N} X_j^{(i)}$$

$i \in \{1, 2, \cdots, p\}$: i-th feature

$j \in \{1, 2, \cdots, N\}$: j-th sample

$$\underset{p \times p}{\Sigma} = \begin{bmatrix} Var(X_1) & \cdots & Cov(X_i, X_j) & \cdots \\ & \ddots & & \\ & & & Var(X_p) \end{bmatrix}$$

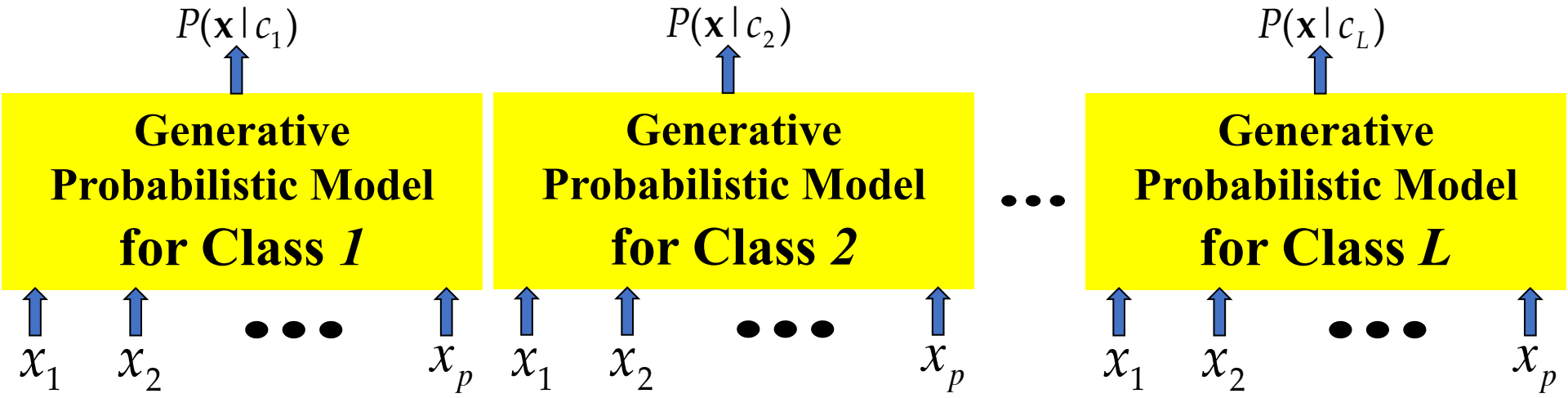
i j

$O(p + p^2)$

Review: Generative BC

$$c^* = argmax \;\; P(C = c_i | \mathbf{X} = \mathbf{x})$$
$$\propto P(\mathbf{X} = \mathbf{x} | C = c_i) P(C = c_i)$$
$$for \; i = 1,2,\cdots, L$$

$$P(\mathbf{X}|C),$$
$$C = c_1, \cdots, c_L, \mathbf{X} = (X_1, \cdots, X_p)$$



$$\mathbf{x} = (x_1, x_2, \cdots, x_p)$$

Adapt from Prof. Ke Chen NB slides

Review: Generative BC

$$c^* = argmax \;\; P(C = c_i | \mathbf{X} = \mathbf{x}) \propto P(\mathbf{X} = \mathbf{x} | C = c_i) P(C = c_i) \quad for \; i = 1,2,\cdots, L$$

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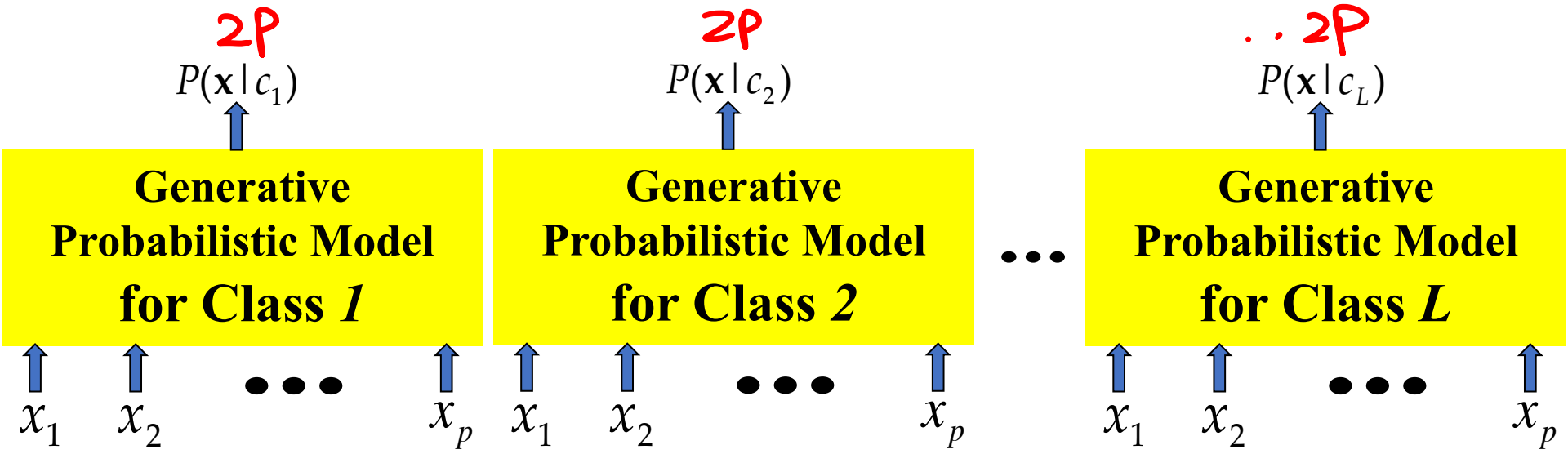

$$\mathbf{x} = (x_1, x_2, \cdots, x_p)$$

Adapt from Prof. Ke Chen NB slides

Review: Naïve Bayes Classifier

$$\underset{C}{\operatorname{argmax}}\, P(C \mid X) = \underset{C}{\operatorname{argmax}}\, P(X, C) = \underset{C}{\operatorname{argmax}}\, P(X \mid C)P(C)$$

Naïve Bayes Classifier

$$P(X_1, X_2, \cdots, X_p | C) = P(X_1|C)P(X_2|C) \cdots P(X_p|C)$$

Today: More Generative Bayes Classifiers

- ✓ Generative Bayes Classifier
- ✓ Naïve Bayes Classifier
- ✓ Gaussian Bayes Classifiers
  - Gaussian distribution
  - Naïve Gaussian BC
  - Not-naïve Gaussian BC ➔ LDA, QDA
- ✓ Discriminative vs. Generative

Gaussian Naïve Bayes Classifier

$$\underset{C}{\operatorname{argmax}} P(C \mid X) = \underset{C}{\operatorname{argmax}} P(X, C) = \underset{C}{\operatorname{argmax}} P(X \mid C) P(C)$$

Naïve Bayes Classifier

$$P(X_1, X_2, \cdots, X_p \mid C) = P(X_1 \mid C) P(X_2 \mid C) \cdots P(X_p \mid C)$$

$$\hat{P}(X_j \mid C = c_i) = \frac{1}{\sqrt{2\pi}\sigma_{ji}} \exp\left(-\frac{(X_j - \mu_{ji})^2}{2\sigma_{ji}^2} \right)$$

μ_{ji} : mean (avearage) of attribute values X_j of examples for which $C = c_i$

σ_{ji} : standard deviation of attribute values X_j of examples for which $C = c_i$

Gaussian Naïve Bayes Classifier

- Continuous-valued Input Attributes
  - Conditional probability modeled with the normal distribution

$$\hat{P}(X_j \mid C = c_i) = \frac{1}{\sqrt{2\pi}\sigma_{ji}} \exp\left(-\frac{(X_j - \mu_{ji})^2}{2\sigma_{ji}^2}\right)$$

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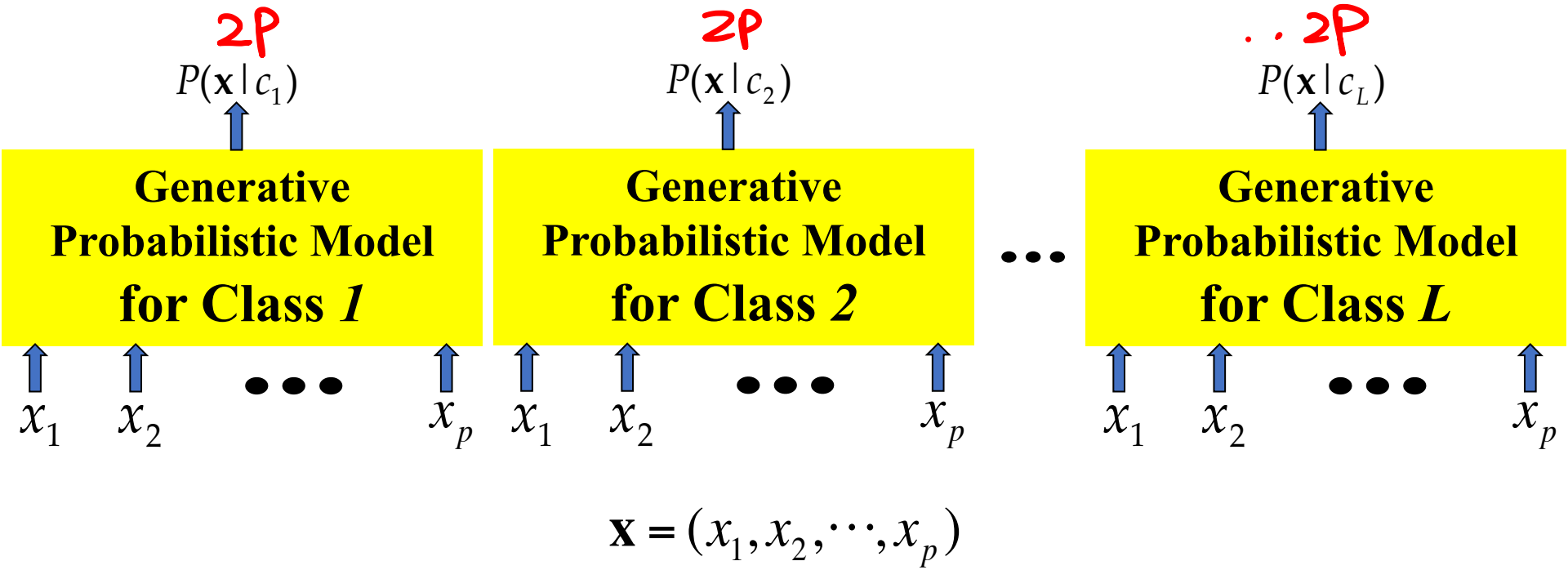
  - Learning Phase: for $\mathbf{X} = (X_1, \cdots, X_p)$, $C = c_1, \cdots, c_L$
    Output: L different p-normal distributions and $P(C = c_i)$ $i = 1, \cdots, L$

Review: Generative BC

$$c^* = argmax \;\; P(C = c_i | \mathbf{X} = \mathbf{x}) \propto P(\mathbf{X} = \mathbf{x} | C = c_i) P(C = c_i) \quad for \; i = 1,2,\cdots,L$$

$$P(\mathbf{X}|C),$$
$$C = c_1,\cdots,c_L, \mathbf{X} = (X_1,\cdots,X_p)$$



$$\mathbf{x} = (x_1, x_2, \cdots, x_p)$$

Adapt from Prof. Ke Chen NB slides

Gaussian Naïve Bayes Classifier

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$$\underset{C}{\operatorname{argmax}} P(C \mid X) = \underset{C}{\operatorname{argmax}} P(X, C) = \underset{C}{\operatorname{argmax}} P(X \mid C) P(C)$$

Naïve Bayes Classifier

$$P(X_1, X_2, \cdots, X_p \mid C) = P(X_1 \mid C) P(X_2 \mid C) \cdots P(X_p \mid C)$$

O (L × 2P + L)

$$\hat{P}(X_j \mid C = c_i) = \frac{1}{\sqrt{2\pi}\sigma_{ji}} \exp\left(-\frac{(X_j - \mu_{ji})^2}{2\sigma_{ji}^2} \right)$$

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    Output: L different p-normal distributions and $P(C = c_i)$ $i = 1, \cdots, L$

  - Test Phase: for $\mathbf{X}' = (X_1', \cdots, X_p')$
    - Calculate conditional probabilities with all the normal distributions
    - Apply the MAP rule to make a decision

$$\underset{i}{\operatorname{argmax}}\ P(C=i)\,P(X_1 \mid i) \cdots P(X_p \mid i)$$

when $\Sigma = \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix} \Rightarrow f(x_1, x_2) = f(x_1) f(x_2)$ $\Rightarrow$ data $\{\mu_1, \cdots, \mu_p, \sigma_1, \cdots, \sigma_p$ $O(2p)$

Naïve

$$P(X_1, X_2, \cdots, X_p \mid C = c_j) = P(X_1 \mid C) P(X_2 \mid C) \cdots P(X_p \mid C)$$

$$= \prod_i \frac{1}{\sqrt{2\pi}\sigma_{ji}} \exp\left(-\frac{(X_j - \mu_{ji})^2}{2\sigma_{ji}^2} \right)$$

Diagonal Matrix

$$\Sigma\_c_k = \Lambda\_c_k$$

Each class' covariance matrix is diagonal

When $\Sigma = \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix} \Rightarrow f(x_1, x_2) = f(x_1) f(x_2)$ data $\Rightarrow \{\mu_1, \cdots, \mu_p, \sigma_1, \cdots, \sigma_p$ $O(2p)$

Total #para $\Rightarrow L \times (p + pf$

Naïve

$$P(X_1, X_2, \cdots, X_p \mid C = c_j) = P(X_1 \mid C) P(X_2 \mid C) \cdots P(X_p \mid C)$$

$$= \prod_i \frac{1}{\sqrt{2\pi}\sigma_{ji}} \exp\left(-\frac{(X_j - \mu_{ji})^2}{2\sigma_{ji}^2} \right)$$

$\Sigma | C_i = \begin{bmatrix} \sigma_{1i} & & 0 \\ & \sigma_{2i} & \\ 0 & & \sigma_{pi} \end{bmatrix}$

Diagonal Matrix $\Sigma\_c_k = \Lambda\_c_k$

Each class' covariance matrix is diagonal

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- ✓ Generative Bayes Classifier
- ✓ Naïve Bayes Classifier
- ✓ Gaussian Bayes Classifiers
  - Gaussian distribution
  - Naïve Gaussian BC
  - Not-naïve Gaussian BC ➔ LDA, QDA
    - LDA: Linear Discriminant Analysis
    - QDA: Quadratic Discriminant Analysis
- ✓ Discriminative vs. Generative

Not Naïve Gaussian means ?

Not Naïve

$$P(X_1, X_2, \cdots, X_p \mid C) =$$

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Naïve

$$P(X_1, X_2, \cdots, X_p \mid C = c_j) = P(X_1 \mid C) P(X_2 \mid C) \cdots P(X_p \mid C)$$

$$= \prod_i \frac{1}{\sqrt{2\pi}\sigma_{ji}} \exp\left(-\frac{(X_j - \mu_{ji})^2}{2\sigma_{ji}^2}\right)$$

Diagonal Matrix

$$\Sigma\_c_k = \Lambda\_c_k$$

Each class' covariance matrix is diagonal

Not Naïve Gaussian means ?

$P = 28 \times 28 \sim 10^3$, $L \sim 10 \Rightarrow 10^7$

$\vec{\Sigma}_c$, $\vec{\mu}_c \Rightarrow O(LP + LP^2)$

Not Naïve

$$P(X_1, X_2, \cdots, X_p \mid C) =$$

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) = \frac{1}{(2\pi)^{P/2}} \frac{1}{|\boldsymbol{\Sigma}_c|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

$\Rightarrow O(2PL)$

Naïve

$$P(X_1, X_2, \cdots, X_p \mid C = c_j) = P(X_1 \mid C)P(X_2 \mid C)\cdots P(X_p \mid C)$$

$$= \prod_i \frac{1}{\sqrt{2\pi}\sigma_{ji}} \exp\left(-\frac{(X_j - \mu_{ji})^2}{2\sigma_{ji}^2}\right)$$

Diagonal Matrix

$$\Sigma\_c_k = \Lambda\_c_k$$

Each class' covariance matrix is diagonal

Not Naïve Gaussian means ?

Not Naïve

$$P(X_1, X_2, \cdots, X_p \mid C) =$$

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Total # para $\Rightarrow L \times \{p + p \times p\}$ (M/C, Σ/C)

Naïve

$$P(X_1, X_2, \cdots, X_p \mid C = c_j) = P(X_1 \mid C) P(X_2 \mid C) \cdots P(X_p \mid C)$$

$$= \prod_i \frac{1}{\sqrt{2\pi}\sigma_{ji}} \exp\left(-\frac{(X_j - \mu_{ji})^2}{2\sigma_{ji}^2}\right)$$

Total # para $\Rightarrow L \times (p + p)$

$\Sigma | C_i = \begin{bmatrix} \sigma_{1i} & & \\ & \sigma_{2i} & \\ & & \sigma_{pi} \end{bmatrix}$

Diagonal Matrix

$$\Sigma\_c_k = \Lambda\_c_k$$

Each class' covariance matrix is diagonal

Not-naïve Gaussian BC

- LDA: Linear Discriminant Analysis
- QDA: Quadratic Discriminant Analysis

$\Sigma_1 = \cdots = \Sigma_L = \Sigma$

$\Sigma \Rightarrow p^2$, $p \sim 100$, $L \sim 10$

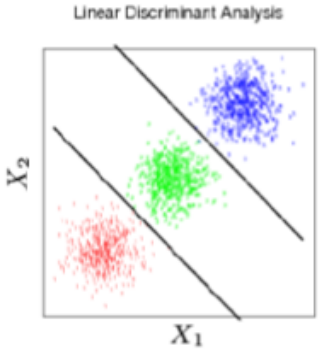
$O(n) < 10k$ (10^4) $\not\Rightarrow$ $O(Lp^2 + Lp) \sim 10^5$

LDA $\Longrightarrow$ $O(p^2 + Lp)$

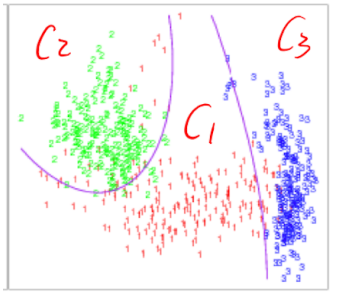
$\vec{\mu}_c$

Not-naïve Gaussian BC

- LDA: Linear Discriminant Analysis



- QDA: Quadratic Discriminant Analysis



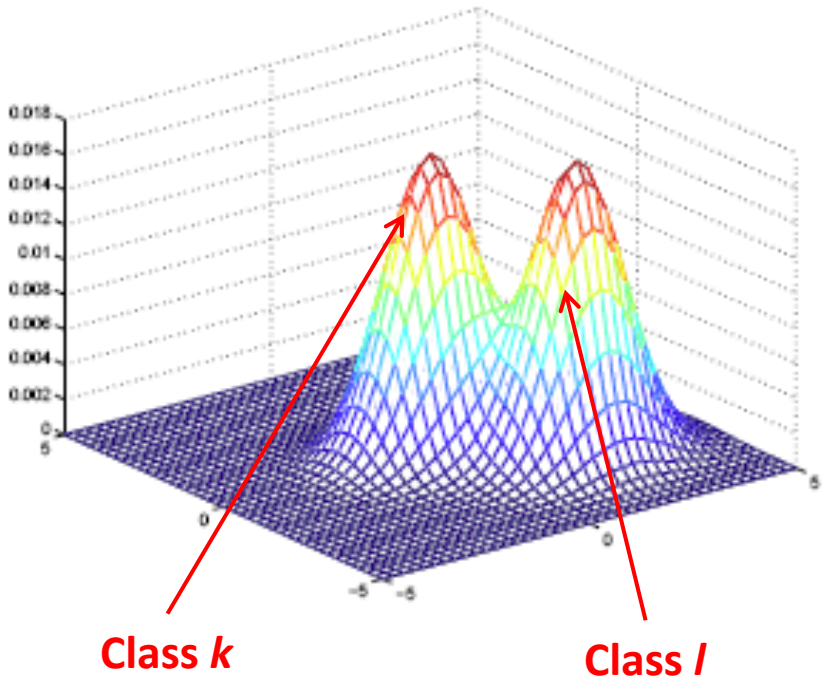
(1) covariance matrix are the same across classes

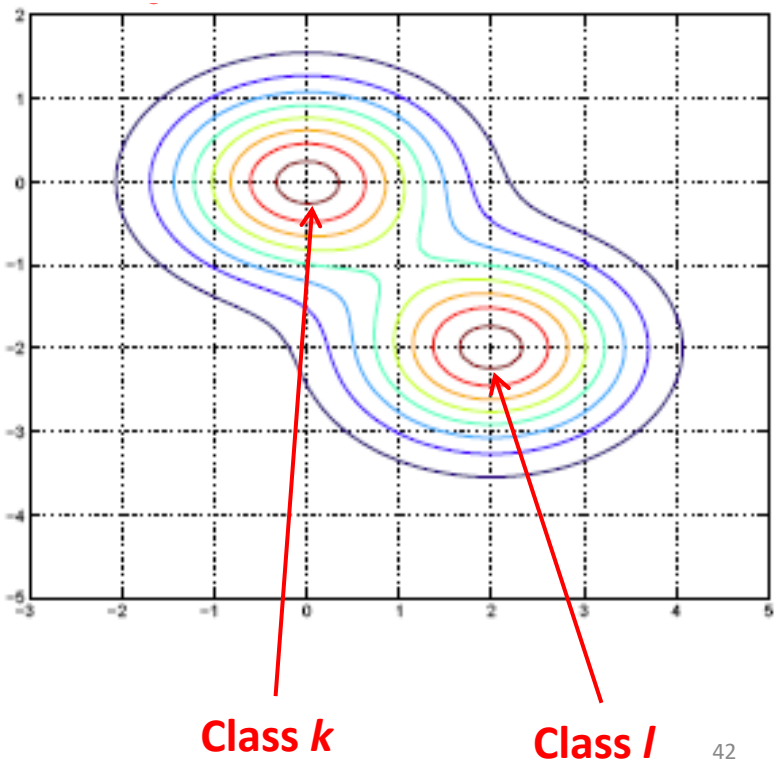
➔ LDA (Linear Discriminant Analysis)

Linear Discriminant Analysis : $\Sigma_k = \Sigma, \ \forall k$ (pxp)

Each class' covariance matrix is the same

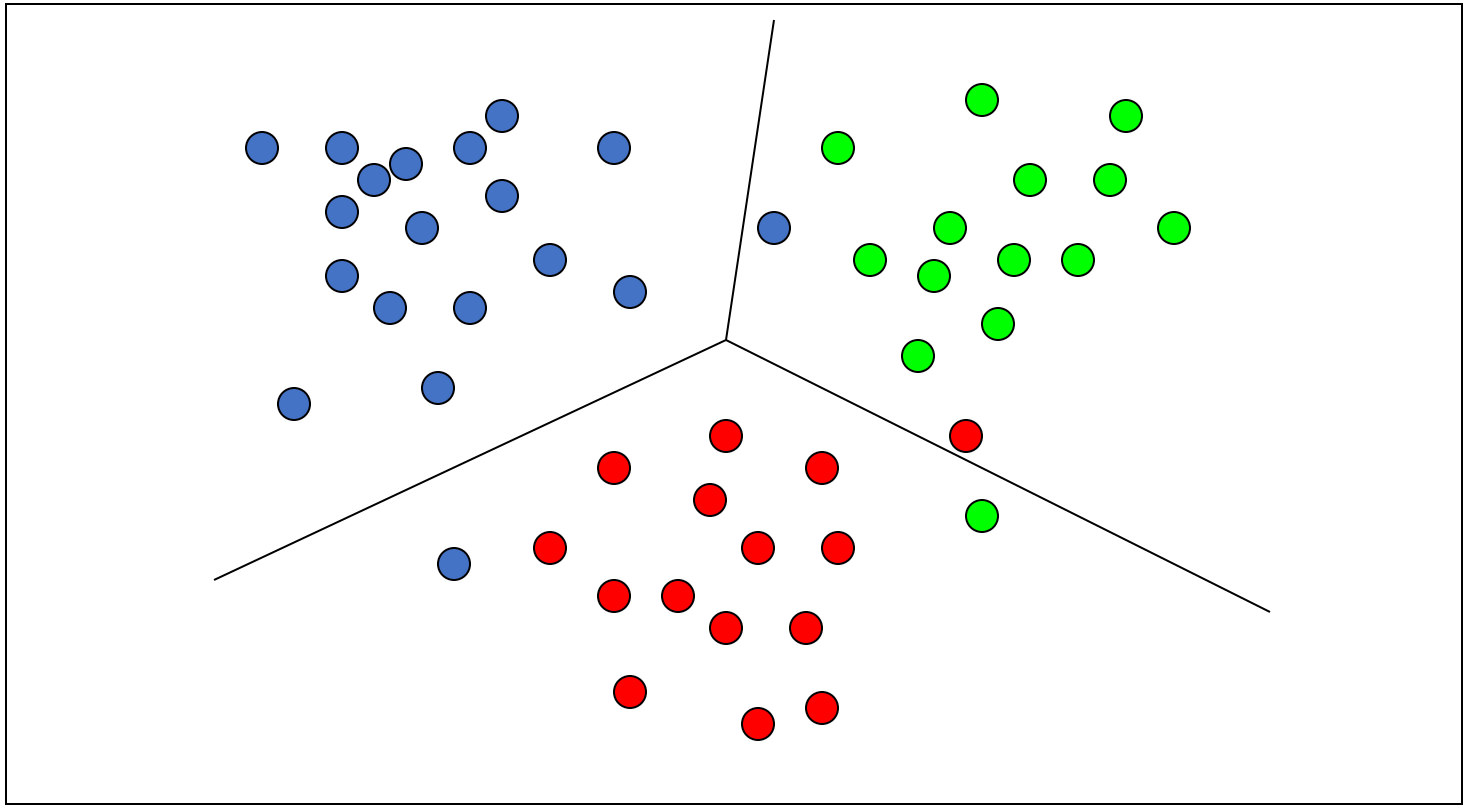
The Gaussian Distribution are shifted versions of each other



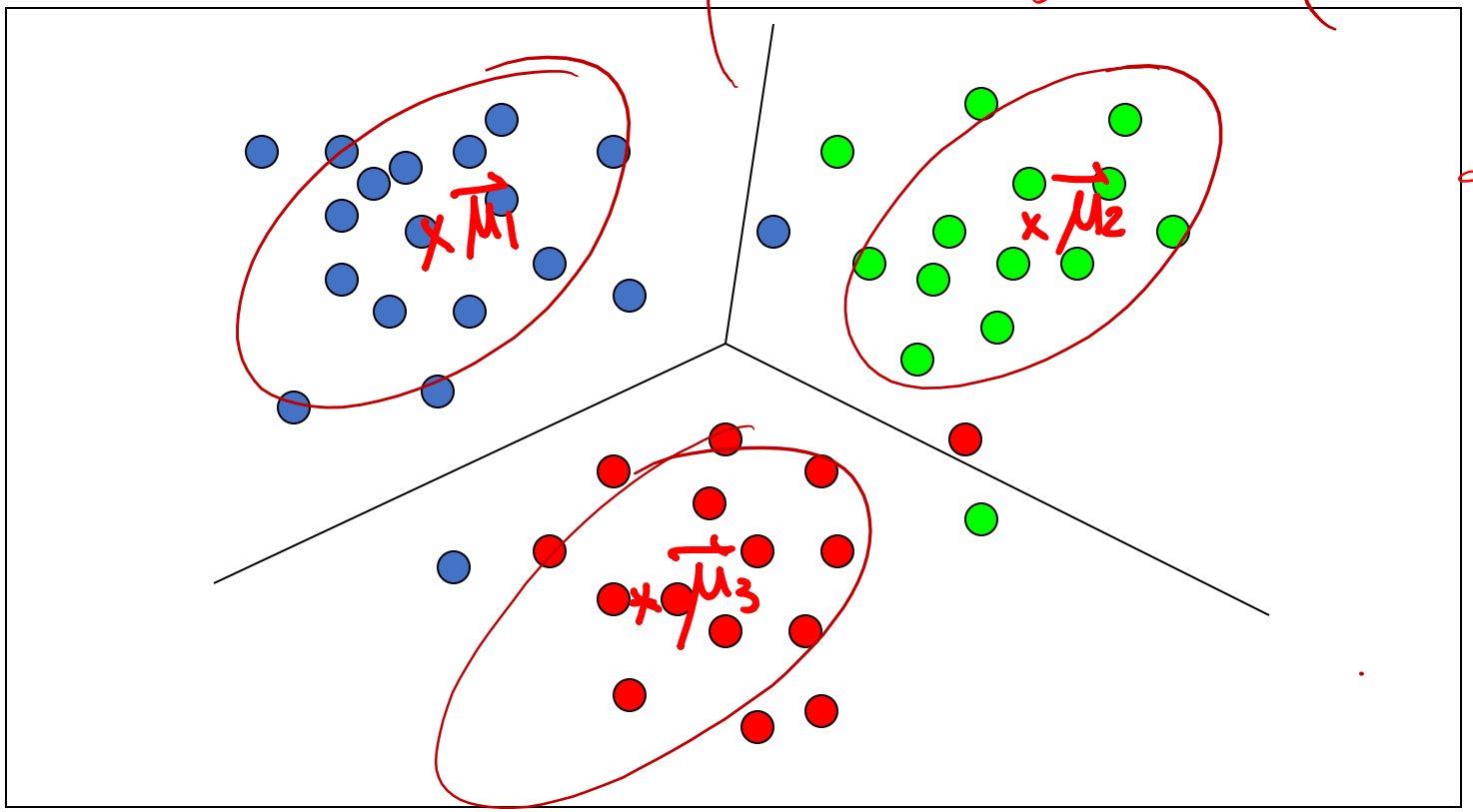


Visualization (three classes)

$\Sigma_1 = \Sigma_2 = \cdots = \Sigma_L \Rightarrow$ linear



Visualization (three classes)



$$\underset{k}{\operatorname{argmax}} P(C_k \mid X) = \underset{k}{\operatorname{argmax}} P(X, C_k) = \underset{k}{\operatorname{argmax}} P(X \mid C_k) P(C_k)$$

$$= \underset{k}{\operatorname{argmax}} \log\{P(X \mid C_k) P(C_k)\}$$

Decision Boundary Points ➔

Satisfying: $p(C_i \mid X) = p(C_j \mid X)$

$$\frac{p(C_i \mid X)}{p(C_j \mid X)} = 1$$

$$\Rightarrow \log \frac{p(C_i \mid X)}{p(C_j \mid X)} = 0$$

$$\underset{k}{\operatorname{argmax}} P(C_k \mid X) = \underset{k}{\operatorname{argmax}} P(X, C_k) = \underset{k}{\operatorname{argmax}} P(X \mid C_k) P(C_k)$$

$$= \underset{k}{\operatorname{argmax}} \log\{P(X \mid C_k) P(C_k)\}$$

$$= \underset{k}{\operatorname{argmax}} \log P(X \mid C_k) + \log P(C_k) \Rightarrow \pi_k$$

Decision Boundary points

$$\log \frac{P(C_k \mid X)}{P(C_\ell \mid X)} = 0 = \log \frac{P(X \mid C_k)}{P(X \mid C_\ell)} + \log \frac{\pi_k}{\pi_\ell}$$

$$= \log P(X \mid C_k) - \log P(X \mid C_\ell) + \log \frac{\pi_k}{\pi_\ell}$$

$$\log \frac{P(C_k \mid X)}{P(C_l \mid X)} = \log \frac{P(X \mid C_k)}{P(X \mid C_l)} + \log \frac{P(C_k)}{P(C_l)}$$

Decision Boundary Points of LDA classifier ➔

$$= \log \frac{\pi_k}{\pi_\ell} - \frac{1}{2}(\mu_k + \mu_\ell)^T \mathbf{\Sigma}^{-1}(\mu_k - \mu_\ell) \qquad (4.9)$$
$$+ x^T \mathbf{\Sigma}^{-1}(\mu_k - \mu_\ell),$$

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Decision Boundary Points of LDA classifier ➔

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$$+ x^T \mathbf{\Sigma}^{-1}(\mu_k - \mu_\ell),$$

The above is derived from the following :

$$-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k) = x^T \Sigma^{-1} \mu_k - \frac{1}{2}\mu_k^T \Sigma^{-1} \mu_k - \frac{1}{2} x^T \Sigma^{-1} x$$

$$\log \frac{P(C_k \mid X)}{P(C_l \mid X)} = \log \frac{P(X \mid C_k)}{P(X \mid C_l)} + \log \frac{P(C_k)}{P(C_l)}$$

Decision Boundary Points of LDA classifier ➔

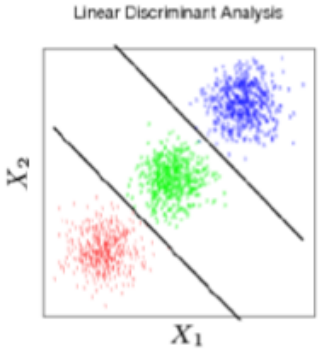
$$= \log \frac{\pi_k}{\pi_\ell} - \frac{1}{2}(\mu_k + \mu_\ell)^T \Sigma^{-1}(\mu_k - \mu_\ell) \quad (4.9)$$
$$+ x^T \Sigma^{-1}(\mu_k - \mu_\ell), = 0$$

b

a

$\Rightarrow$ $x^T a + b = 0 \Rightarrow$ a linear line decision boundary

LDA Classification Rule (also called as Linear discriminant function:)



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$$= \arg\max_k \left[-\log((2\pi)^{p/2}|\Sigma|^{1/2}) - \frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k) + \log(\pi_k) \right]$$

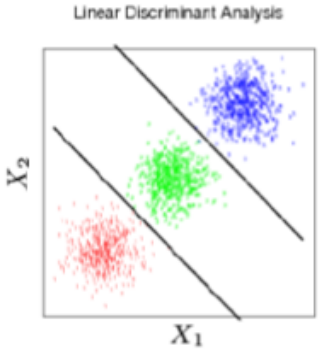
$$= \arg\max_k \left[-\frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k) + \log(\pi_k) \right]$$

- Note

Linear Discriminant Function for LDA

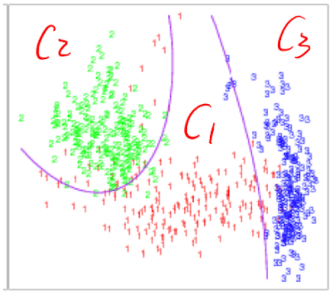
Not-naïve Gaussian BC

- LDA: Linear Discriminant Analysis



- QDA: Quadratic Discriminant Analysis

Quadratic decision Boundary



(2) If covariance matrix are not the same

e.g. ➔ QDA (Quadratic Discriminant Analysis)

- Estimate the covariance matrix Σ_k separately for each class k, $k = 1, 2, ..., K$.
- *Quadratic discriminant function*:

$$\delta_k(x) = -\frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k) + \log\pi_k \ .$$

- Classification rule:

$$\log p(x|C_k)p(C_k)$$

$$\hat{G}(x) = \arg\max_k \delta_k(x) \ .$$

- Decision boundaries are quadratic equations in x.
- QDA fits the data better than LDA, but has more parameters to estimate.

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$\{\Sigma_1, \Sigma_2, ..\Sigma_K, \mu_1, \mu_2, ..\mu_K\}$

- Classification rule:

$$\hat{G}(x) = \arg\max_k \delta_k(x) \ .$$

$\delta_k(x) - \delta_\ell(x) = 0$

Total # para

$K(p+p^2)$

$\{\mu_k, \Sigma_k\}$

- Decision boundaries are quadratic equations in x.
- QDA fits the data better than LDA, but has more parameters to estimate.

(3) Regularized Discriminant Analysis

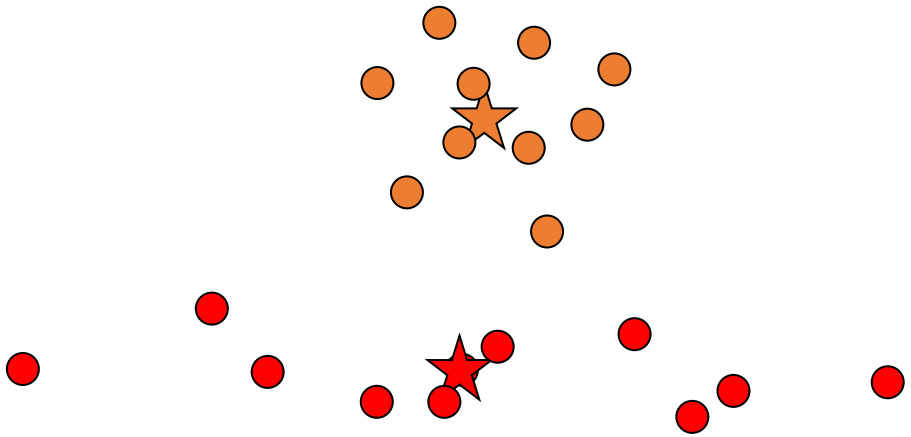
- A compromise between LDA and QDA.
- Shrink the separate covariances of QDA toward a common covariance as in LDA.
- Regularized covariance matrices:

$$\hat{\Sigma}_k(\alpha) = \alpha\hat{\Sigma}_k + (1-\alpha)\hat{\Sigma} .$$

- The quadratic discriminant function $\delta_k(x)$ is defined using the shrunken covariance matrices $\hat{\Sigma}_k(\alpha)$.
- The parameter α controls the complexity of the model.

More: Decision Boundary of Gaussian naïve Bayes Classifiers ???

Orange Team

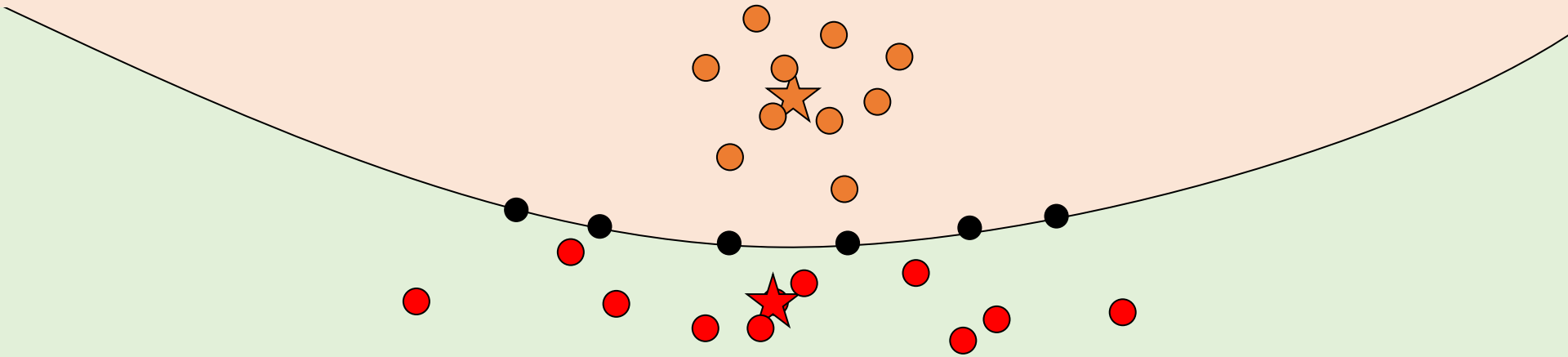


Green Team

Naïve Gaussian Bayes Classifier is not a linear classifier!

Gaussian Naïve Bayes Classifier

Orange Team



Green Team

Naïve Gaussian Bayes Classifier is not a linear classifier!

Decision Boundary of Gaussian naïve Bayes Classifiers ???

Naive BC

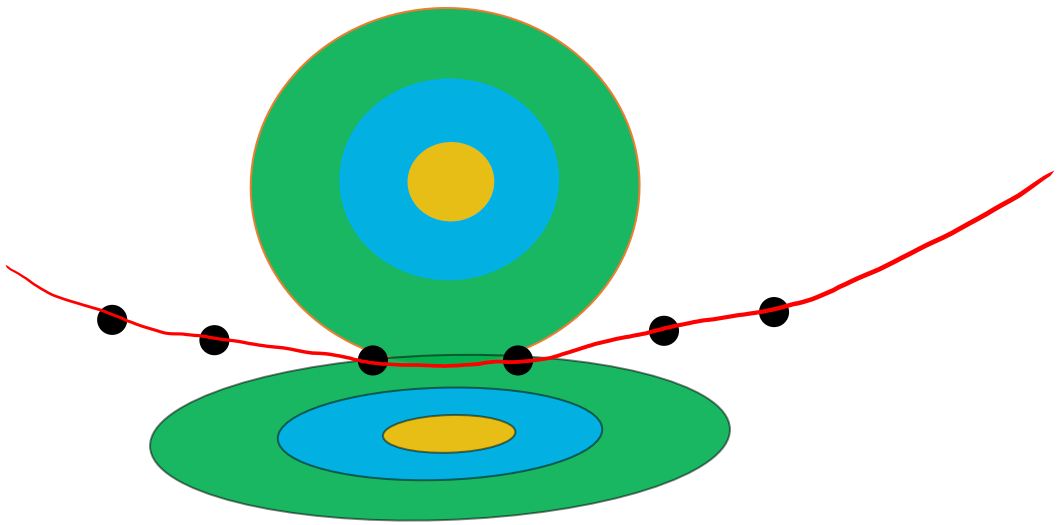
$\Sigma_1 \neq \Sigma_2$

diagonal

$\Sigma_1 = \Lambda_1$

$\Sigma_2 = \Lambda_2$

diagonal



Quadratic decision Boundary

Today: More Generative Bayes Classifiers

- ✓ Generative Bayes Classifier
- ✓ Naïve Bayes Classifier
- ✓ Gaussian Bayes Classifiers
  - Gaussian distribution
  - Naïve Gaussian BC
  - Not-naïve Gaussian BC ➔ LDA, QDA
- ✓ Discriminative vs. Generative classifier

Discriminative vs. Generative

Generative approach

- Model the joint distribution p(X, C) using

  $p(X \mid C = c_k)$ and $p(C = c_k)$

Discriminative approach

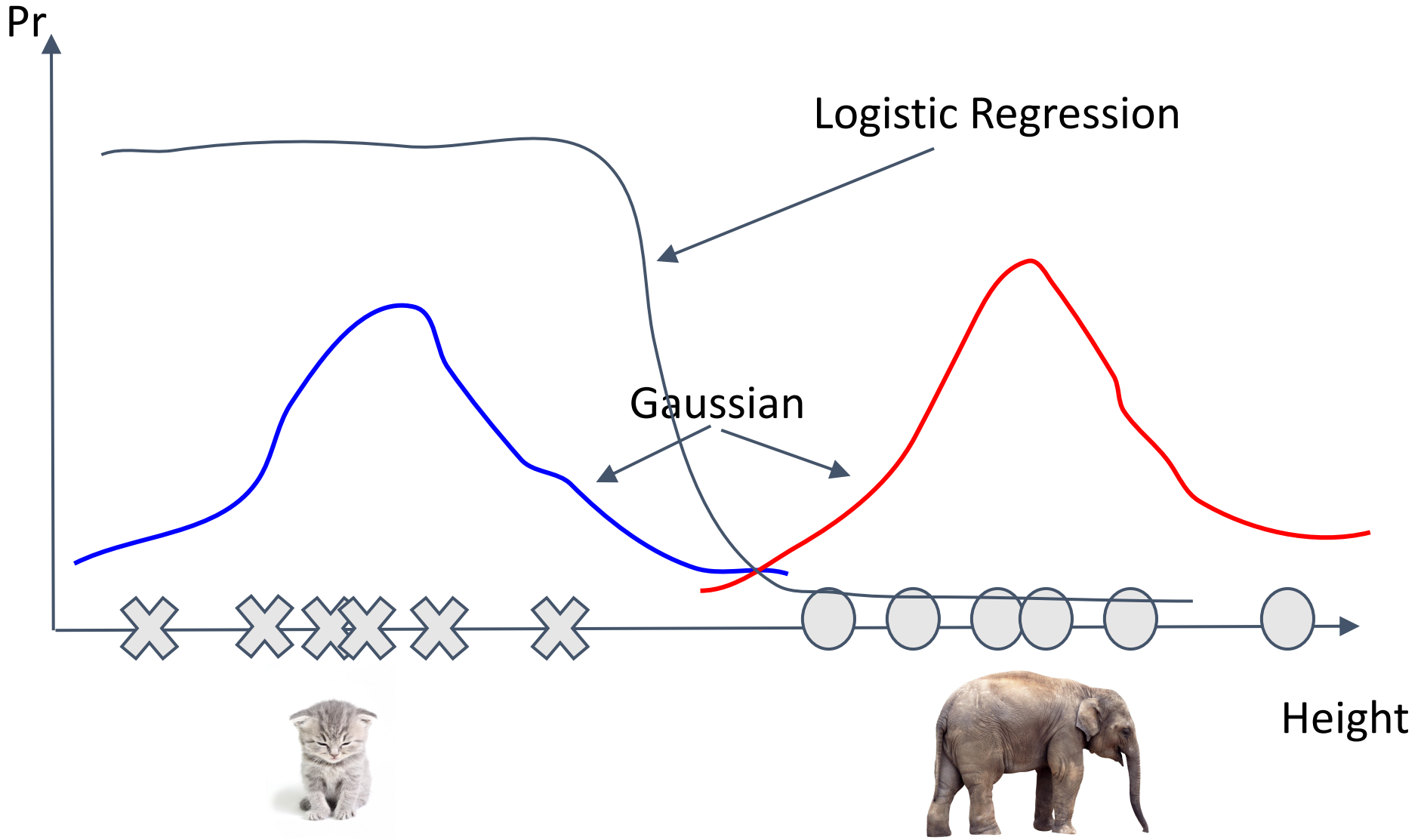
- Model the conditional distribution p(c| X) directly

e.g.,

$$P(C=1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 * X)}}$$

Ng, Jordan,. "On discriminative vs. generative classifiers 2002

Discriminative vs. Generative



LDA vs. Logistic Regression

- **LDA (Generative model)** linear
  - Assumes Gaussian class-conditional densities and a common covariance
  - Model parameters are estimated by maximizing the full log likelihood, parameters for each class are estimated independently of other classes, $Kp + \frac{p(p+1)}{2} + (K-1)$ parameters
  - Makes use of marginal density information $\Pr(x)$
  - Easier to train, low variance, more efficient if model is correct
  - Higher asymptotic error, but converges faster

- **Logistic Regression (Discriminative model)** linear
  - Assumes class-conditional densities are members of the (same) exponential family distribution
  - Model parameters are estimated by maximizing the conditional log likelihood, simultaneous consideration of all other classes, $(K-1)(p+1)$parameters
  - Ignores marginal density information $\Pr(x)$
  - Harder to train, robust to uncertainty about the data generation process
  - Lower asymptotic error, but converges more slowly

Ng, Jordan,. "On discriminative vs. generative classifiers 2002

LDA vs. Logistic Regression

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asymptotic classifiers

- Definitions
  - h_{gen} and h_{dis}: generative and discriminative classifiers
  - $h_{gen, inf}$ and $h_{dis, inf}$: same classifiers but trained on the entire population (asymptotic classifiers)
  - n → infinity, $h_{gen} \rightarrow h_{gen, inf}$ and $h_{dis} \rightarrow h_{dis, inf}$

Ng, Jordan,. "On discriminative vs. generative classifiers: A comparison of logistic regression and naive bayes." *Advances in neural information processing systems* 14 (2002): 841.

Discriminative vs. Generative

Proposition 1:

$$\epsilon\left(h_{dis,\inf}\right) \leq \epsilon\left(h_{gen,\inf}\right)$$

h_{true}

- p : number of dimensions
- n : number of observations
- ϵ : asymptotic generalization error

Proposition 1 states that aymptotically, the error of the discriminative logistic regression is smaller than that of the generative naive Bayes. This is easily shown

Logistic Regression vs. Naïve BC

Discriminative classifier (Logistic Regression)

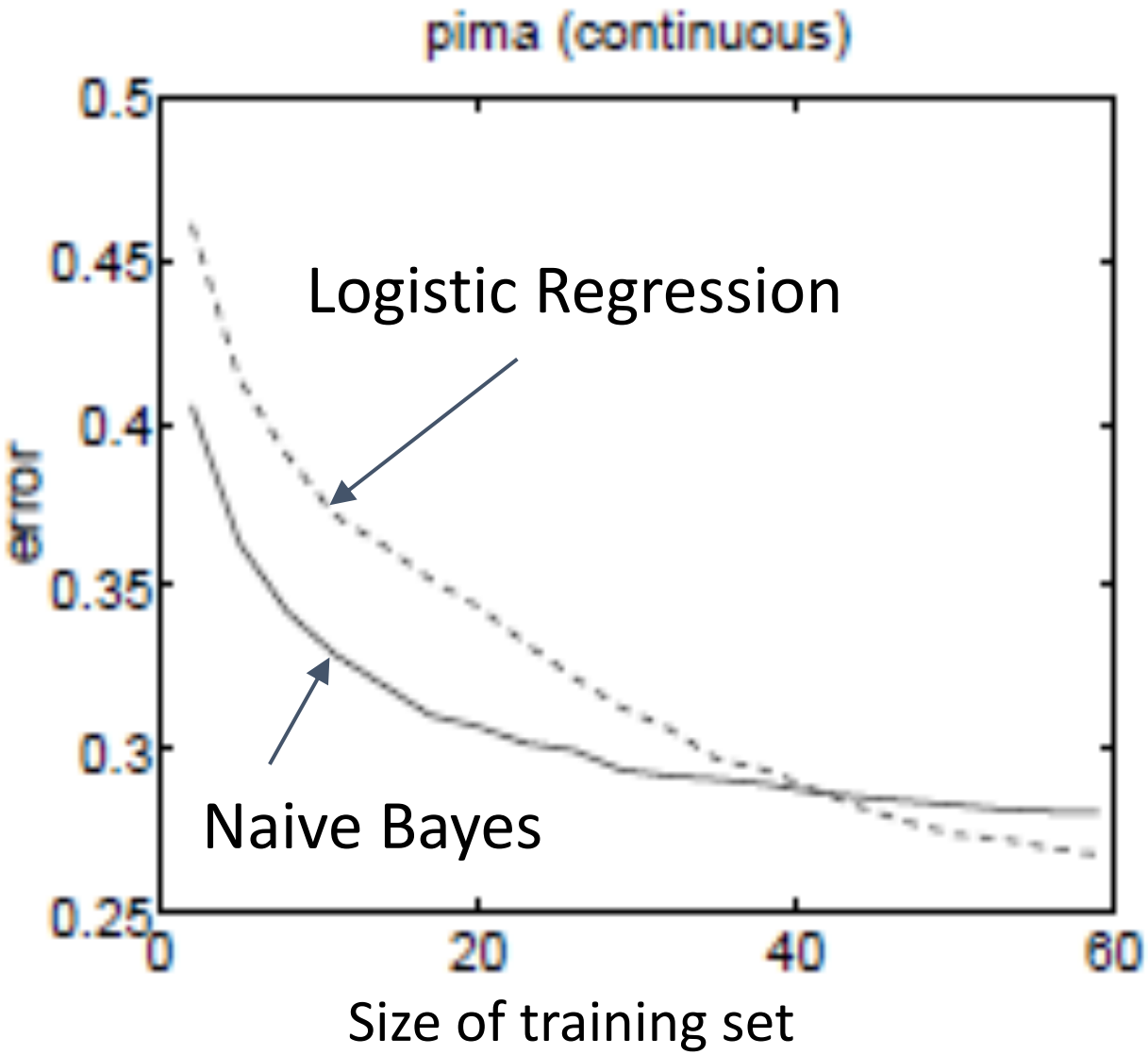
- Smaller asymptotic error
- Slow convergence ~ O(p)

Generative classifier (Naive Bayes)

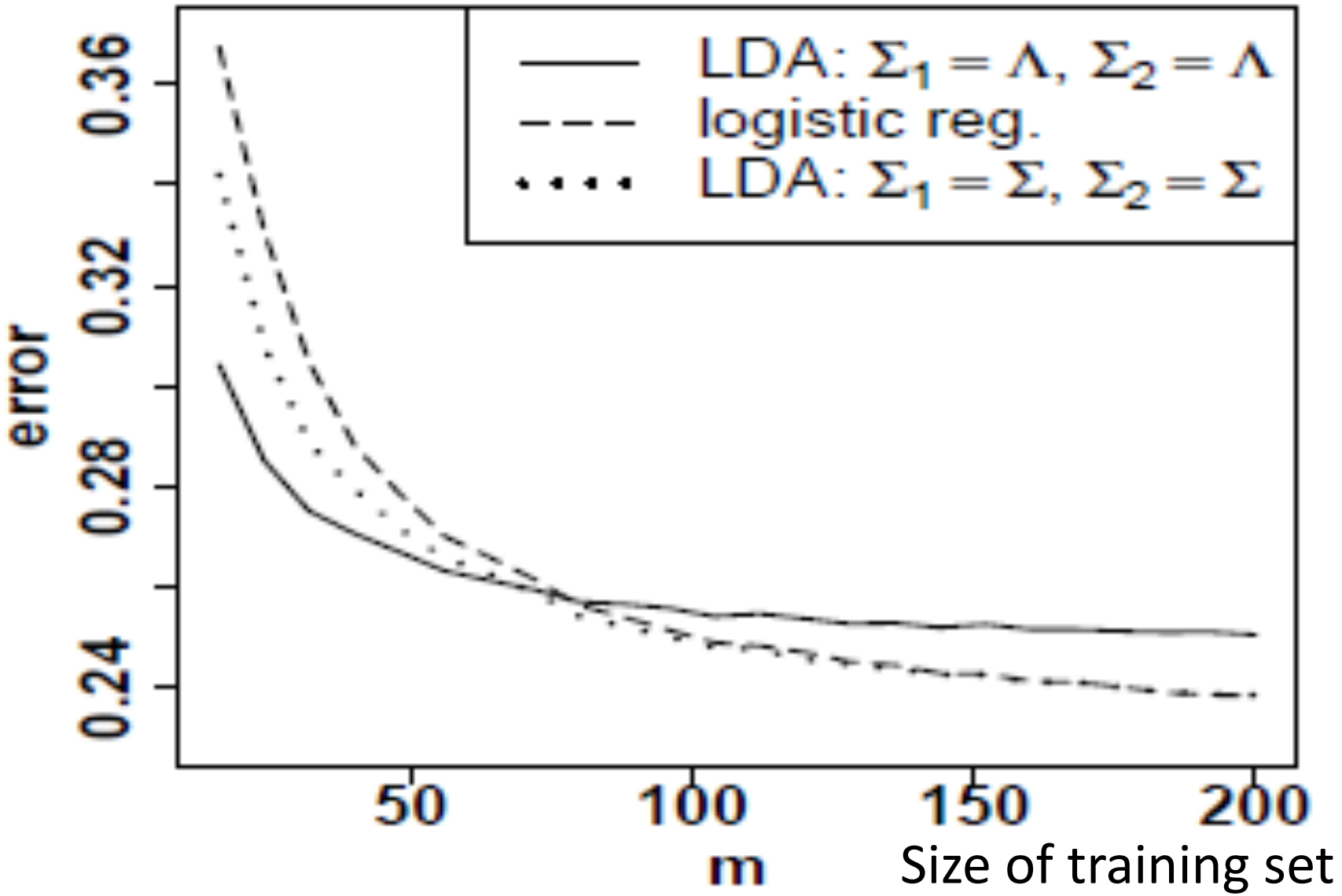
- Larger asymptotic error
- Can handle missing data (EM)
- Fast convergence ~ O(lg(p))

the speed at which a convergent sequence approaches its limit is called the rate of convergence.

Ng, Jordan,. "On discriminative vs. generative classifiers: A comparison of logistic regression and naive bayes." *Advances in neural information processing systems* 14 (2002): 841.



Logistic regression / vs. Naïve LDA / vs. LDA



Xue, Jing-Hao, and D. Michael Titterington. "Comment on “On discriminative vs. generative classifiers: A comparison of logistic regression and naive Bayes”."*Neural processing letters* 28.3 (2008): 169-187.

Summary: Discriminative vs. Generative

- Empirically, generative classifiers approach their asymptotic error faster than discriminative ones
  - Good for small training set
  - Handle missing data well (EM)

- Empirically, discriminative classifiers have lower asymptotic error than generative ones
  - Good for larger training set

$$\underset{k}{\operatorname{argmax}}\, P(C\_k \mid X) = \underset{k}{\operatorname{argmax}}\, P(X,C) = \underset{k}{\operatorname{argmax}}\, P(X \mid C)P(C)$$

Generative Bayes Classifier

Task

↓

Representation

↓

Score Function

↓

Search/Optimization

↓

Models, Parameters

classification

↓

Prob. models p(X|C)

$P(X_1, \cdots, X_p \mid C)$

↓

EPE with 0-1 loss ➔ MAP Rule

↓

Many options

↓

Prob. Models' Parameter

Bernoulli Naïve

$$p(W_i = true \mid c_k) = p_{i,k}$$

Gaussian Naive

$$\hat{P}(X_j \mid C = c_k) = \frac{1}{\sqrt{2\pi\sigma_{jk}}} \exp\left(-\frac{(X_j - \mu_{jk})^2}{2\sigma_{jk}^2}\right)$$

Multinomial

$$P(W_1 = n_1, \ldots, W_v = n_v \mid c_k) = \frac{N!}{n_{1k}!\, n_{2k}!\, .. n_{vk}!} \theta_{1k}^{n_{1k}} \theta_{2k}^{n_{2k}} .. \theta_{vk}^{n_{vk}}$$

References

- Prof. Tan, Steinbach, Kumar's "Introduction to Data Mining" slide
- Prof. Andrew Moore's slides
- Prof. Eric Xing's slides
- Prof. Ke Chen NB slides
- Hastie, Trevor, et al. *The elements of statistical learning*. Vol. 2. No. 1. New York: Springer, 2009.