CSC 411: Lecture 09: Naive Bayes

Class based on Raquel Urtasun & Rich Zemel's lectures

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Today

- Classification – Multi-dimensional (Gaussian) Bayes classifier
- Estimate probability densities from data
- Naive Bayes classifier

Generative vs Discriminative

Two approaches to classification:

- Discriminative classifiers estimate parameters of decision boundary/class separator directly from labeled examples
  - learn $p(y|\mathbf{x})$ directly (logistic regression models)
  - learn mappings from inputs to classes (least-squares, neural nets)
- Generative approach: model the distribution of inputs characteristic of the class (Bayes classifier)
  - Build a model of $p(\mathbf{x}|y)$
  - Apply Bayes Rule

Bayes Classifier

- Aim to diagnose whether patient has diabetes: classify into one of two classes (yes C=1; no C=0)
- Run battery of tests
- Given patient's results: $\mathbf{x} = [x_1, x_2, \cdots, x_d]^T$ we want to update class probabilities using Bayes Rule:

$$p(C|\mathbf{x}) = \frac{p(\mathbf{x}|C)p(C)}{p(\mathbf{x})}$$

- More formally

$$\text{posterior} = \frac{\text{Class likelihood} \times \text{prior}}{\text{Evidence}}$$

- How can we compute $p(\mathbf{x})$ for the two class case?

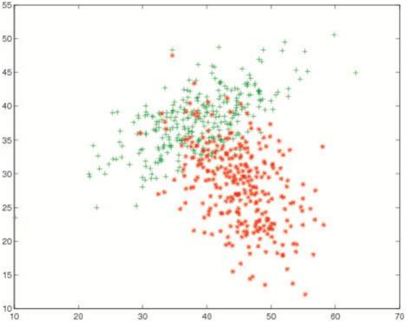
$$p(\mathbf{x}) = p(\mathbf{x}|C=0)p(C=0) + p(\mathbf{x}|C=1)p(C=1)$$

Classification: Diabetes Example

- Last class we had a single observation per patient: white blood cell count

$$p(C = 1|x = 48) = \frac{p(x = 48|C = 1)p(C = 1)}{p(x = 48)}$$

- Add second observation: Plasma glucose value
- Now our input $\mathbf{x}$ is 2-dimensional



Gaussian Discriminant Analysis (Gaussian Bayes Classifier)

- Gaussian Discriminant Analysis in its general form assumes that $p(\mathbf{x}|t)$ is distributed according to a multivariate normal (Gaussian) distribution
- Multivariate Gaussian distribution:

$$p(\mathbf{x}|t = k) = \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} \exp\left[-(\mathbf{x} - \boldsymbol{\mu}_k)^T \Sigma_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)\right]$$

  where $|\Sigma_k|$ denotes the determinant of the matrix, and d is dimension of $\mathbf{x}$
- Each class k has associated mean vector $\boldsymbol{\mu}_k$ and covariance matrix Σ_k
- Typically the classes share a single covariance matrix Σ ("share" means that they have the same parameters; the covariance matrix in this case): $\Sigma = \Sigma_1 = \cdots = \Sigma_k$

Multivariate Data

- Multiple measurements (sensors)
- d inputs/features/attributes
- N instances/observations/examples

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_d^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_d^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(N)} & x_2^{(N)} & \cdots & x_d^{(N)} \end{bmatrix}$$

Multivariate Parameters

- Mean

$$\mathbb{E}[\mathbf{x}] = [\mu_1, \cdots, \mu_d]^T$$

- Covariance

$$\Sigma = Cov(\mathbf{x}) = \mathbb{E}[(\mathbf{x} - \mu)^T (\mathbf{x} - \mu)] = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{bmatrix}$$

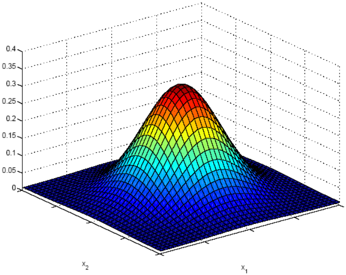
- Correlation $= Corr(\mathbf{x})$ is the covariance divided by the product of standard deviation

$$\rho_{ij} = \frac{\sigma_{ij}}{\sigma_i \sigma_j}$$

Multivariate Gaussian Distribution

- $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$, a Gaussian (or normal) distribution defined as

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left[-(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)\right]$$



- Mahalanobis distance $(\mathbf{x}-\mu_k)^T\Sigma^{-1}(\mathbf{x}-\mu_k)$ measures the distance from $\mathbf{x}$ to μ in terms of Σ
- It normalizes for difference in variances and correlations

Bivariate Normal

$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\qquad$ $\Sigma = 0.5 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\qquad$ $\Sigma = 2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

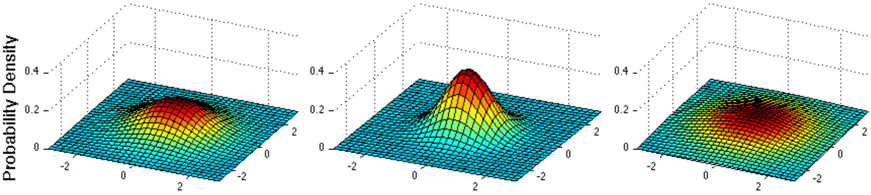


Figure: Probability density function

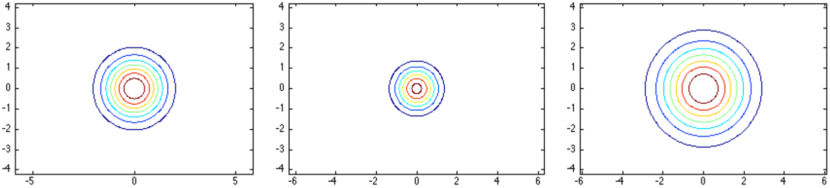
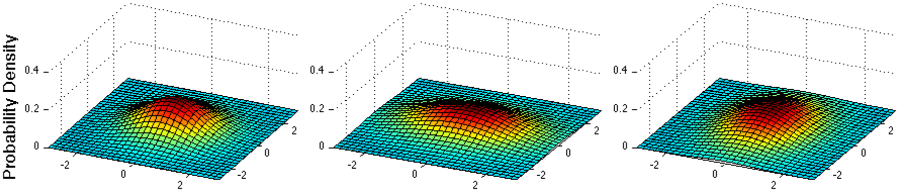


Figure: Contour plot of the pdf

Bivariate Normal

$var(x_1) = var(x_2)$ $\quad$ $var(x_1) > var(x_2)$ $\quad$ $var(x_1) < var(x_2)$



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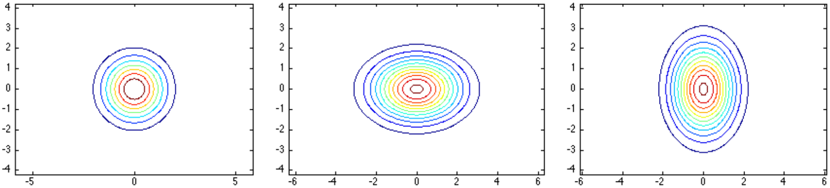
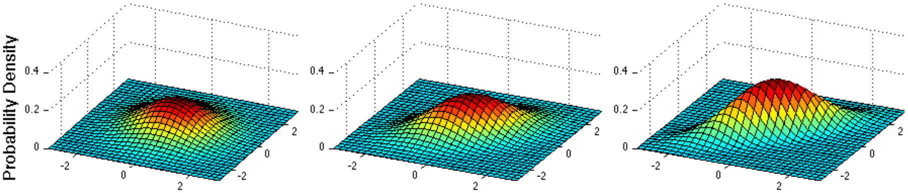


Figure: Contour plot of the pdf

Bivariate Normal

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$$



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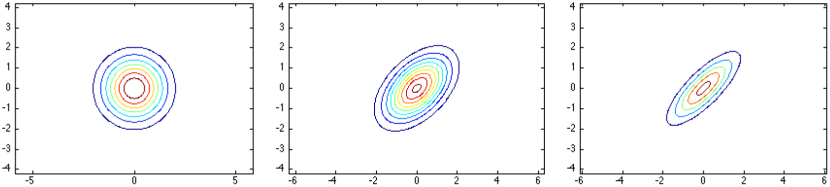


Figure: Contour plot of the pdf

Bivariate Normal

$Cov(x_1, x_2) = 0$ $\qquad$ $Cov(x_1, x_2) > 0$ $\qquad$ $Cov(x_1, x_2) < 0$

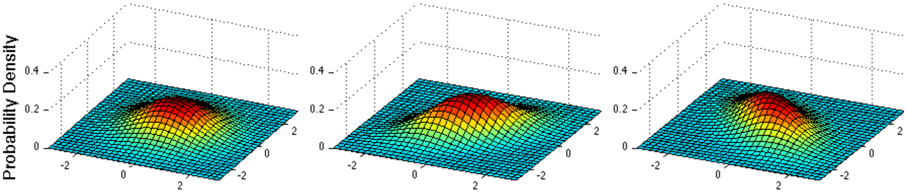


Figure: Probability density function

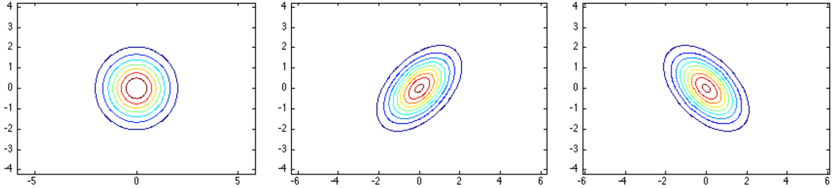


Figure: Contour plot of the pdf

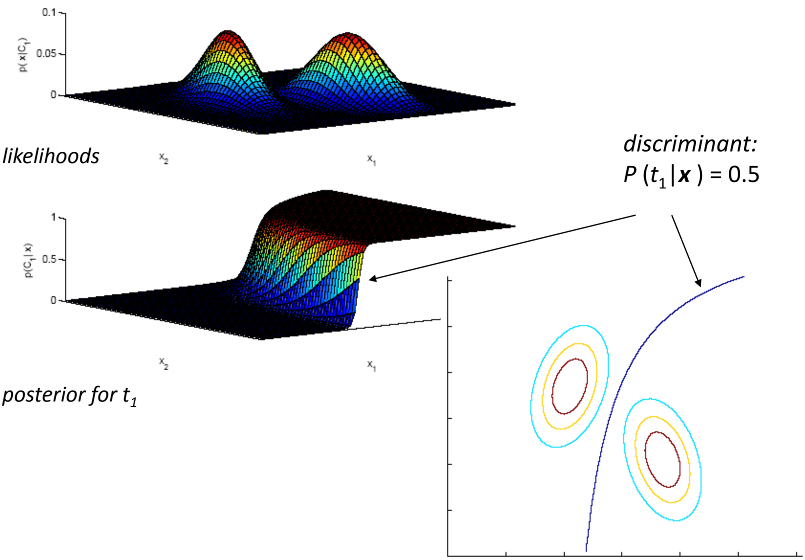
Gaussian Discriminant Analysis (Gaussian Bayes Classifier)

- GDA (GBC) decision boundary is based on class posterior:

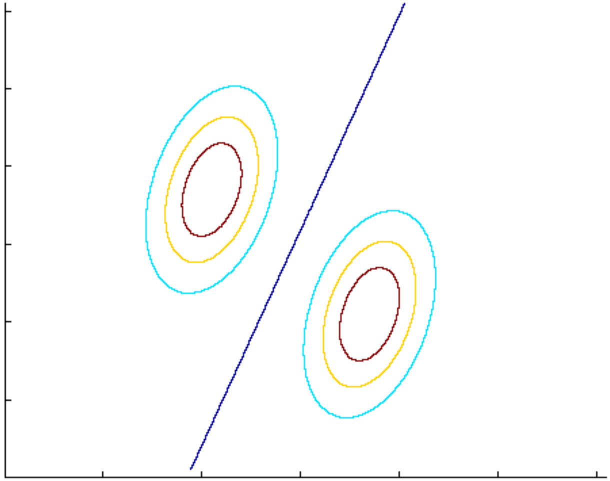
$$
\begin{aligned}
\log p(t_k|\mathbf{x}) &= \log p(\mathbf{x}|t_k) + \log p(t_k) - \log p(\mathbf{x}) \\
&= -\frac{d}{2}\log(2\pi) - \frac{1}{2}\log|\Sigma_k^{-1}| - \frac{1}{2}(\mathbf{x}-\mu_k)^T\Sigma_k^{-1}(\mathbf{x}-\mu_k) + \\
&\quad + \log p(t_k) - \log p(\mathbf{x})
\end{aligned}
$$

- Decision: take the class with the highest posterior probability

Decision Boundary



Decision Boundary when Shared Covariance Matrix



Learning

- Learn the parameters using maximum likelihood

$$
\begin{aligned}
\ell(\phi, \mu_0, \mu_1, \Sigma) &= -\log \prod_{n=1}^{N} p(\mathbf{x}^{(n)}, t^{(n)} | \phi, \mu_0, \mu_1, \Sigma) \\
&= -\log \prod_{n=1}^{N} p(\mathbf{x}^{(n)} | t^{(n)}, \mu_0, \mu_1, \Sigma) p(t^{(n)} | \phi)
\end{aligned}
$$

- What have we assumed?

More on MLE

- Assume the prior is Bernoulli (we have two classes)

$$p(t|\phi) = \phi^t (1-\phi)^{1-t}$$

- You can compute the ML estimate in closed form

$$\begin{aligned}
\phi &= \frac{1}{N}\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = 1] \\
\mu_0 &= \frac{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = 0] \cdot \mathbf{x}^{(n)}}{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = 0]} \\
\mu_1 &= \frac{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = 1] \cdot \mathbf{x}^{(n)}}{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = 1]} \\
\Sigma &= \frac{1}{N}\sum_{n=1}^{N} (\mathbf{x}^{(n)} - \mu_{t^{(n)}})(\mathbf{x}^{(n)} - \mu_{t^{(n)}})^T
\end{aligned}$$

Gaussian Discriminative Analysis vs Logistic Regression

- If you examine $p(t=1|\mathbf{x})$ under GDA, you will find that it looks like this:

$$p(t|\mathbf{x}, \phi, \mu_0, \mu_1, \Sigma) = \frac{1}{1 + \exp(-\mathbf{w}^T\mathbf{x})}$$

  where $\mathbf{w}$ is an appropriate function of $(\phi, \mu_0, \mu_1, \Sigma)$
- So the decision boundary has the same form as logistic regression!
- When should we prefer GDA to LR, and vice versa?

Gaussian Discriminative Analysis vs Logistic Regression

- GDA makes stronger modeling assumption: assumes class-conditional data is multivariate Gaussian
- If this is true, GDA is asymptotically efficient (best model in limit of large N)
- But LR is more robust, less sensitive to incorrect modeling assumptions
- Many class-conditional distributions lead to logistic classifier
- When these distributions are non-Gaussian, in limit of large N, LR beats GDA

Simplifying the Model

What if $\mathbf{x}$ is high-dimensional?

- For Gaussian Bayes Classifier, if input $\mathbf{x}$ is high-dimensional, then covariance matrix has many parameters
- Save some parameters by using a shared covariance for the classes
- Any other idea you can think of?

Naive Bayes

- **Naive Bayes** is an alternative generative model: Assumes features independent given the class

$$p(\mathbf{x}|t = k) = \prod_{i=1}^{d} p(x_i|t = k)$$

- Assuming likelihoods are Gaussian, how many parameters required for Naive Bayes classifier?
- Important note: Naive Bayes does not assume a particular distribution

Naive Bayes Classifier

Given

- prior $p(t = k)$
- assuming features are conditionally independent given the class
- likelihood $p(x_i | t = k)$ for each x_i

The decision rule

$$y = arg \max_k p(t = k) \prod_{i=1}^{d} p(x_i | t = k)$$

- If the assumption of conditional independence holds, NB is the optimal classifier
- If not, a heavily regularized version of generative classifier
- What's the regularization?
- Note: NB's assumptions (cond. independence) typically do not hold in practice. However, the resulting algorithm still works well on many problems, and it typically serves as a decent baseline for more sophisticated models

Gaussian Naive Bayes

- **Gaussian Naive Bayes** classifier assumes that the likelihoods are Gaussian:

$$p(x_i|t = k) = \frac{1}{\sqrt{2\pi}\sigma_{ik}} \exp\left[\frac{-(x_i - \mu_{ik})^2}{2\sigma_{ik}^2}\right]$$

  (this is just a 1-dim Gaussian, one for each input dimension)

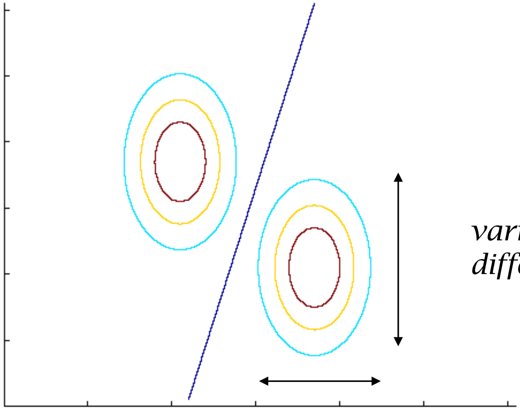
- Model the same as Gaussian Discriminative Analysis with diagonal covariance matrix

- Maximum likelihood estimate of parameters

$$\mu_{ik} = \frac{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = k] \cdot x_i^{(n)}}{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = k]}$$

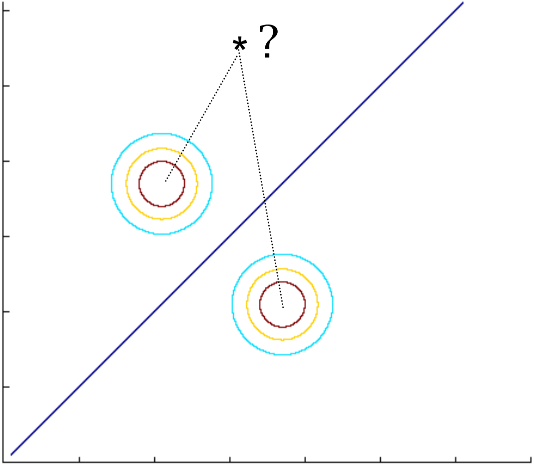
$$\sigma_{ik}^2 = \frac{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = k] \cdot (x_i^{(n)} - \mu_{ik})^2}{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = k]}$$

Decision Boundary: Shared Variances (between Classes)



variances may be different

Decision Boundary: isotropic



- Same variance across all classes and input dimensions, all class priors equal
- Classification only depends on distance to the mean. Why?

Decision Boundary: isotropic

- In this case: $\sigma_{i,k} = \sigma$ (just one parameter), class priors equal (e.g., $p(t_k) = 0.5$ for 2-class case)
- Going back to class posterior for GDA:

$$
\begin{aligned}
\log p(t_k|\mathbf{x}) &= \log p(\mathbf{x}|t_k) + \log p(t_k) - \log p(\mathbf{x}) \\
&= -\frac{d}{2}\log(2\pi) - \frac{1}{2}\log|\Sigma_k^{-1}| - \frac{1}{2}(\mathbf{x}-\mu_k)^T\Sigma_k^{-1}(\mathbf{x}-\mu_k) + \\
&\quad + \log p(t_k) - \log p(\mathbf{x})
\end{aligned}
$$

where we take $\Sigma_k = \sigma^2 I$ and ignore terms that don't depend on k (don't matter when we take max over classes):

$$
\log p(t_k|\mathbf{x}) = -\frac{1}{2\sigma^2}(\mathbf{x}-\mu_k)^T(\mathbf{x}-\mu_k)
$$

Spam Classification

- You have examples of emails that are spam and non-spam
- How would you classify spam vs non-spam?
- Think about it at home, solution in the next tutorial