CSC 411 Lecture 14: Probabilistic Models II

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Overview

- Bayesian parameter estimation
- MAP estimation
- Gaussian discriminant analysis

Data Sparsity

- Maximum likelihood has a pitfall: if you have too little data, it can overfit.
- E.g., what if you flip the coin twice and get H both times?

$$\theta_{\mathrm{ML}} = \frac{N_H}{N_H + N_T} = \frac{2}{2+0} = 1$$

- Because it never observed T, it assigns this outcome probability 0. This problem is known as data sparsity.
- If you observe a single T in the test set, the log-likelihood is $-\infty$.

Bayesian Parameter Estimation

- In maximum likelihood, the observations are treated as random variables, but the parameters are not.
- The Bayesian approach treats the parameters as random variables as well.
- To define a Bayesian model, we need to specify two distributions:
  - The prior distribution $p(\boldsymbol{\theta})$, which encodes our beliefs about the parameters *before* we observe the data
  - The likelihood $p(\mathcal{D} \mid \boldsymbol{\theta})$, same as in maximum likelihood
- When we update our beliefs based on the observations, we compute the posterior distribution using Bayes' Rule:

$$p(\boldsymbol{\theta} \mid \mathcal{D}) = \frac{p(\boldsymbol{\theta}) p(\mathcal{D} \mid \boldsymbol{\theta})}{\int p(\boldsymbol{\theta}') p(\mathcal{D} \mid \boldsymbol{\theta}') \, \mathrm{d}\boldsymbol{\theta}'}.$$

- We rarely ever compute the denominator explicitly.

Bayesian Parameter Estimation

- Let's revisit the coin example. We already know the likelihood:

$$L(\theta) = p(\mathcal{D}) = \theta^{N_H}(1-\theta)^{N_T}$$

- It remains to specify the prior $p(\theta)$.
  - We can choose an uninformative prior, which assumes as little as possible. A reasonable choice is the uniform prior.
  - But our experience tells us 0.5 is more likely than 0.99. One particularly useful prior that lets us specify this is the beta distribution:

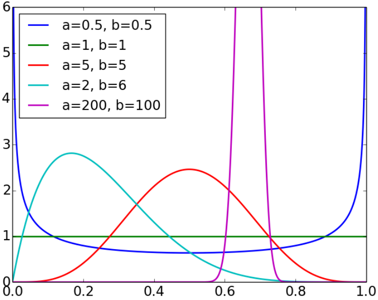
$$p(\theta; a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\,\theta^{a-1}(1-\theta)^{b-1}.$$

  - This notation for proportionality lets us ignore the normalization constant:

$$p(\theta; a, b) \propto \theta^{a-1}(1-\theta)^{b-1}.$$

Bayesian Parameter Estimation

- Beta distribution for various values of a, b:



- Some observations:
  - The expectation $\mathbb{E}[\theta] = a/(a+b)$.
  - The distribution gets more peaked when a and b are large.
  - The uniform distribution is the special case where $a = b = 1$.
- The main thing the beta distribution is used for is as a prior for the Bernoulli distribution.

Bayesian Parameter Estimation

- Computing the posterior distribution:

$$\begin{aligned} p(\boldsymbol{\theta} \mid \mathcal{D}) &\propto p(\boldsymbol{\theta}) p(\mathcal{D} \mid \boldsymbol{\theta}) \\ &\propto \left[\theta^{a-1}(1-\theta)^{b-1}\right]\left[\theta^{N_H}(1-\theta)^{N_T}\right] \\ &= \theta^{a-1+N_H}(1-\theta)^{b-1+N_T}. \end{aligned}$$

- This is just a beta distribution with parameters $N_H + a$ and $N_T + b$.
- The posterior expectation of θ is:

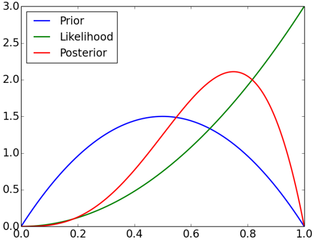
$$\mathbb{E}[\theta \mid \mathcal{D}] = \frac{N_H + a}{N_H + N_T + a + b}$$

- The parameters a and b of the prior can be thought of as pseudo-counts.
    - The reason this works is that the prior and likelihood have the same functional form. This phenomenon is known as conjugacy, and it's very useful.

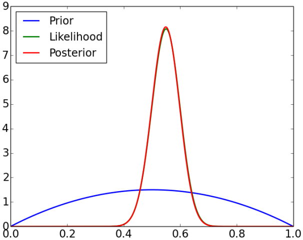
Bayesian Parameter Estimation

Bayesian inference for the coin flip example:

Small data setting
$N_H = 2, \; N_T = 0$



Large data setting
$N_H = 55, \; N_T = 45$



When you have enough observations, the data overwhelm the prior.

Bayesian Parameter Estimation

- What do we actually do with the posterior?
- The posterior predictive distribution is the distribution over future observables given the past observations. We compute this by marginalizing out the parameter(s):

$$p(\mathcal{D}' \,|\, \mathcal{D}) = \int p(\boldsymbol{\theta} \,|\, \mathcal{D}) p(\mathcal{D}' \,|\, \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta}. \tag{1}$$

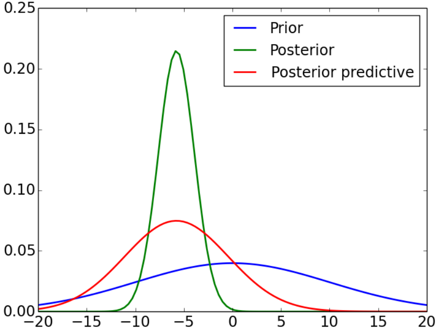
- For the coin flip example:

$$\begin{aligned} \theta_{\text{pred}} &= \Pr(x' = H \,|\, \mathcal{D}) \\ &= \int p(\theta \,|\, \mathcal{D}) \Pr(x' = H \,|\, \theta) \, \mathrm{d}\theta \\ &= \int \mathrm{Beta}(\theta; N_H + a, N_T + b) \cdot \theta \, \mathrm{d}\theta \\ &= \mathbb{E}_{\mathrm{Beta}(\theta; N_H + a, N_T + b)}[\theta] \\ &= \frac{N_H + a}{N_H + N_T + a + b}, \end{aligned} \tag{2}$$

Bayesian Parameter Estimation

Bayesian estimation of the mean temperature in Toronto

- Assume observations are i.i.d. Gaussian with known standard deviation σ and unknown mean μ
- Broad Gaussian prior over μ, centered at 0
- We can compute the posterior and posterior predictive distributions analytically (full derivation in notes)
- Why is the posterior predictive distribution more spread out than the posterior distribution?



Bayesian Parameter Estimation

Comparison of maximum likelihood and Bayesian parameter estimation

- The Bayesian approach deals better with data sparsity
- Maximum likelihood is an optimization problem, while Bayesian parameter estimation is an integration problem
  - This means maximum likelihood is much easier in practice, since we can just do gradient descent
  - Automatic differentiation packages make it really easy to compute gradients
  - There aren't any comparable black-box tools for Bayesian parameter estimation (although Stan can do quite a lot)

Maximum A-Posteriori Estimation

- Maximum a-posteriori (MAP) estimation: find the most likely parameter settings under the posterior
- This converts the Bayesian parameter estimation problem into a maximization problem

$$\begin{aligned}
\hat{\boldsymbol{\theta}}_{\mathrm{MAP}} &= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta} \,|\, \mathcal{D}) \\
&= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta}, \mathcal{D}) \\
&= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta}) \, p(\mathcal{D} \,|\, \boldsymbol{\theta}) \\
&= \arg\max_{\boldsymbol{\theta}} \; \log p(\boldsymbol{\theta}) + \log p(\mathcal{D} \,|\, \boldsymbol{\theta})
\end{aligned}$$

Maximum A-Posteriori Estimation

- Joint probability in the coin flip example:

$$\begin{aligned}\log p(\theta, \mathcal{D}) &= \log p(\theta) + \log p(\mathcal{D} \mid \theta) \\ &= \mathrm{const} + (a-1)\log\theta + (b-1)\log(1-\theta) + N_H \log\theta + N_T \log(1-\theta) \\ &= \mathrm{const} + (N_H + a - 1)\log\theta + (N_T + b - 1)\log(1-\theta)\end{aligned}$$

- Maximize by finding a critical point

$$0 = \frac{\mathrm{d}}{\mathrm{d}\theta}\log p(\theta, \mathcal{D}) = \frac{N_H + a - 1}{\theta} - \frac{N_T + b - 1}{1-\theta}$$

- Solving for θ,

$$\hat{\theta}_{\mathrm{MAP}} = \frac{N_H + a - 1}{N_H + N_T + a + b - 2}$$

Maximum A-Posteriori Estimation

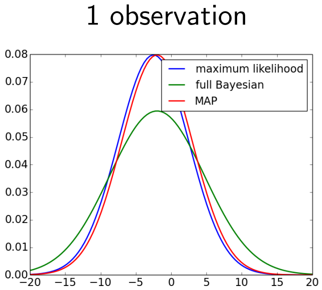
Comparison of estimates in the coin flip example:

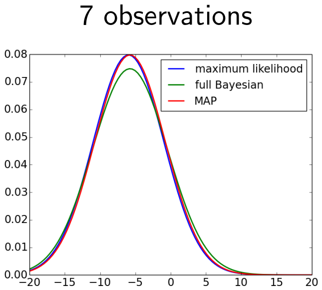
	Formula	$N_H = 2, N_T = 0$	$N_H = 55, N_T = 45$
$\hat{\theta}_{\mathrm{ML}}$	$\frac{N_H}{N_H+N_T}$	1	$\frac{55}{100} = 0.55$
θ_{pred}	$\frac{N_H+a}{N_H+N_T+a+b}$	$\frac{4}{6} \approx 0.67$	$\frac{57}{104} \approx 0.548$
$\hat{\theta}_{\mathrm{MAP}}$	$\frac{N_H+a-1}{N_H+N_T+a+b-2}$	$\frac{3}{4} = 0.75$	$\frac{56}{102} \approx 0.549$

$\hat{\theta}_{\mathrm{MAP}}$ assigns nonzero probabilities as long as $a, b > 1$.

Maximum A-Posteriori Estimation

Comparison of predictions in the Toronto temperatures example





Gaussian Discriminant Analysis

Motivation

- Generative models - model $p(\mathbf{x}|t = k)$
- Instead of trying to separate classes, try to model what each class "looks like".
- Recall that $p(\mathbf{x}|t = k)$ may be very complex

$$p(x_1, \cdots, x_d, y) = p(x_1|x_2, \cdots, x_d, y) \cdots p(x_{d-1}|x_d, y)p(x_d, y)$$

- Naive bayes used a conditional independence assumption. What else could we do? Choose a simple distribution.
- Today we will discuss fitting Gaussian distributions to our data.

Bayes Classifier

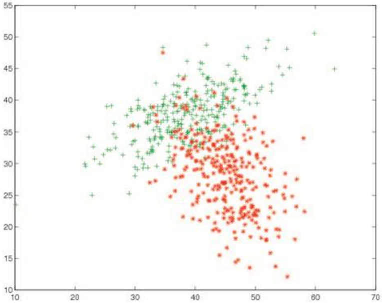
- Let's take a step back...
- Bayes Classifier

$$
\begin{aligned}
h(\mathbf{x}) &= \arg\max p(t = k|\mathbf{x}) = \arg\max \frac{p(\mathbf{x}|t = k)p(t = k)}{p(\mathbf{x})} \\
&= \arg\max p(\mathbf{x}|t = k)p(t = k)
\end{aligned}
$$

- Talked about Discrete $\mathbf{x}$, what if $\mathbf{x}$ is continuous?

Classification: Diabetes Example

- Observation per patient: White blood cell count & glucose value.



- How can we model $p(x|t = k)$? Multivariate Gaussian

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:

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

  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
- Σ_k has $\mathcal{O}(d^2)$ parameters - could be hard to estimate (more on that later).

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

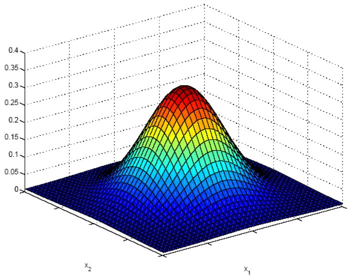
$$\Sigma = Cov(\mathbf{x}) = \mathbb{E}[(\mathbf{x} - \mu)^T(\mathbf{x} - \mu)] = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{bmatrix}$$

- For Gaussians - all you need to know to represent! (not true in general)

Multivariate Gaussian Distribution

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

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



- 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

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

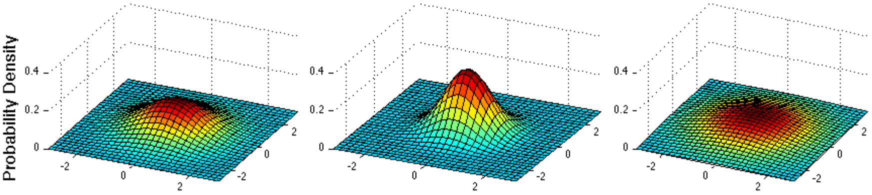


Figure: Probability density function

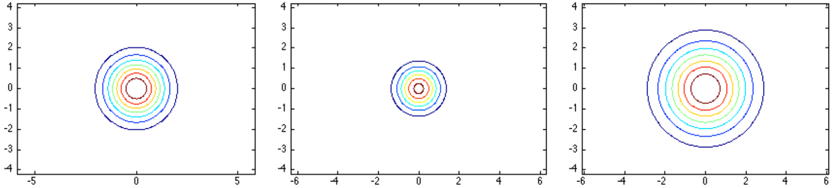
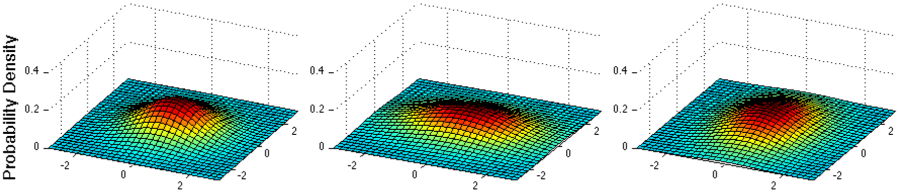


Figure: Contour plot of the pdf

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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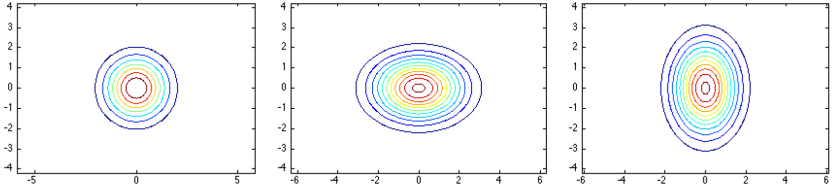
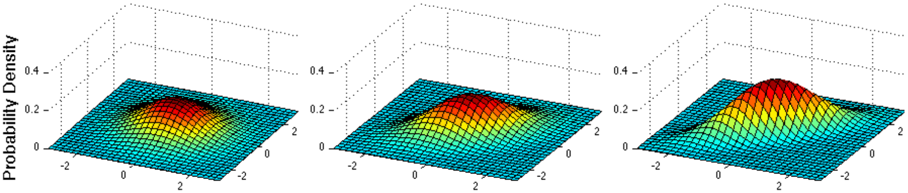


Figure: Contour plot of the pdf

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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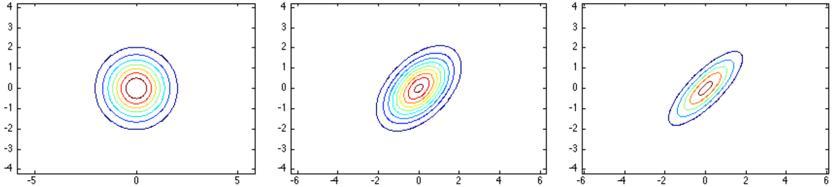

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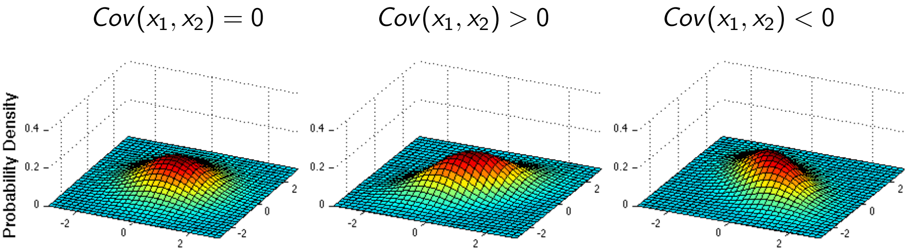

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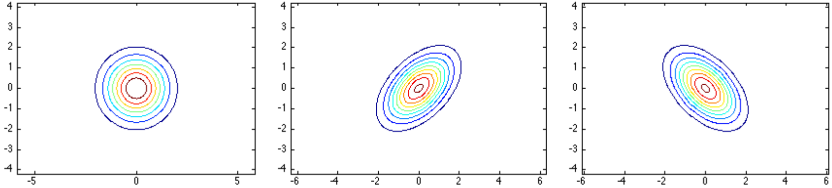

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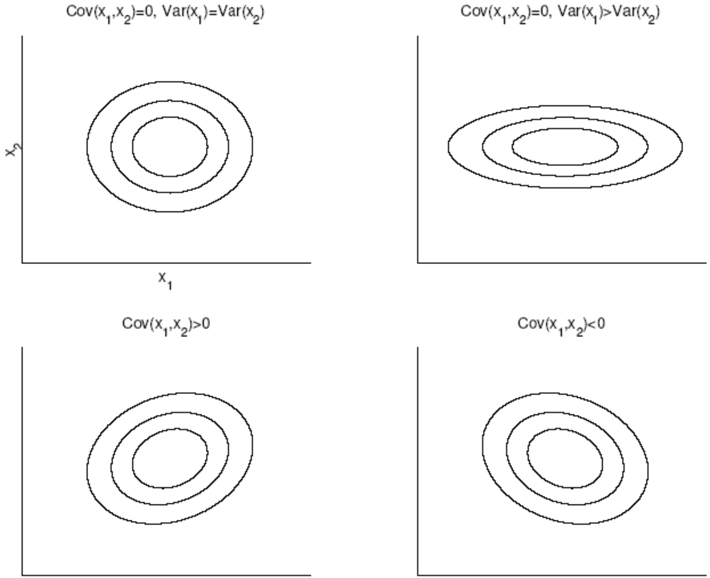
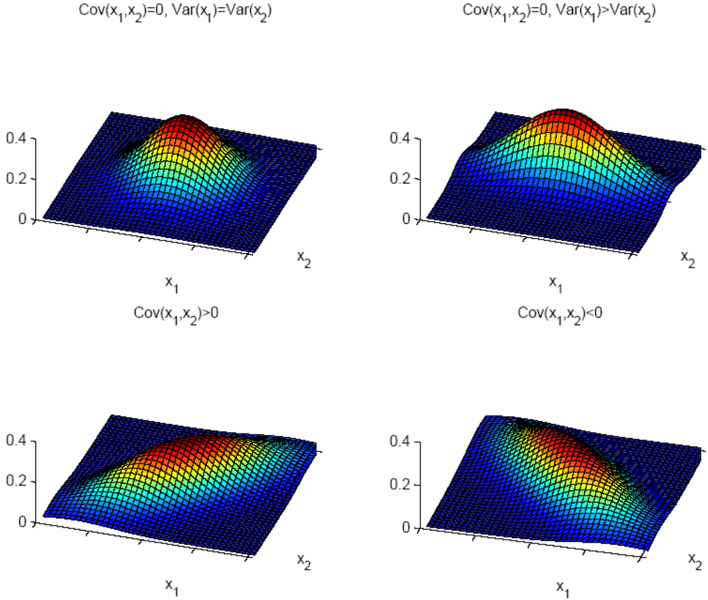
Bivariate Normal



Bivariate Normal



Gaussian Discriminant Analysis (Gaussian Bayes Classifier)

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

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

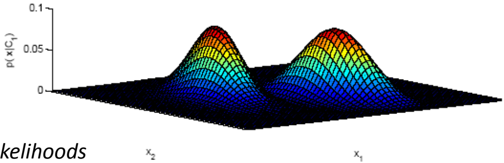
- Decision boundary:

$$(\mathbf{x}-\mu_k)^T\Sigma_k^{-1}(\mathbf{x}-\mu_k) = (\mathbf{x}-\mu_\ell)^T\Sigma_\ell^{-1}(\mathbf{x}-\mu_\ell) + Const$$

$$\mathbf{x}^T\Sigma_k^{-1}\mathbf{x} - 2\mu_k^T\Sigma_k^{-1}\mathbf{x} = \mathbf{x}^T\Sigma_\ell^{-1}\mathbf{x} - 2\mu_\ell^T\Sigma_\ell^{-1}\mathbf{x} + Const$$

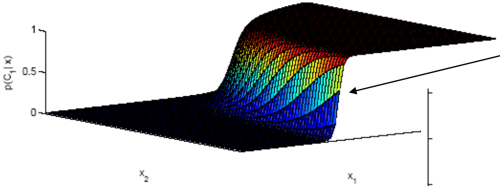
- Quadratic function in $\mathbf{x}$
- What if $\Sigma_k = \Sigma_\ell$?

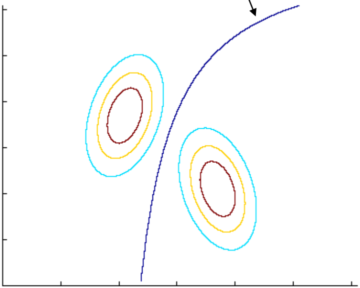
Decision Boundary



likelihoods

discriminant:
$P\,(t_1|\boldsymbol{x}\,) = 0.5$





posterior for t_1

Learning

- Learn the parameters for each class using maximum likelihood
- 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

$$\phi = \frac{1}{N}\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = 1]$$

$$\mu_k = \frac{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = k] \cdot \mathbf{x}^{(n)}}{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = k]}$$

$$\Sigma_k = \frac{1}{\sum_{n=1}^{N} \mathbb{1}[t^{(n)} = k]} \sum_{n=1}^{N} \mathbb{1}[t^{(n)} = k](\mathbf{x}^{(n)} - \mu_{t^{(n)}})(\mathbf{x}^{(n)} - \mu_{t^{(n)}})^T$$

Simplifying the Model

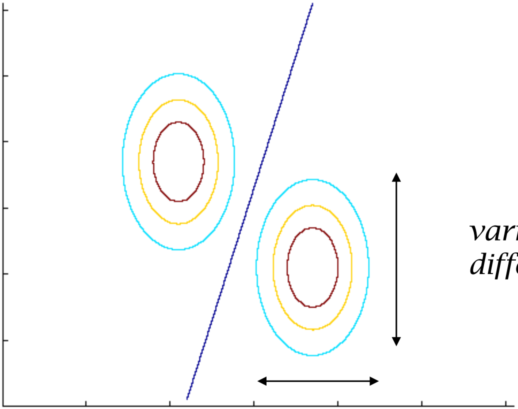
What if $\mathbf{x}$ is high-dimensional?

- 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?
- MLE in this case:

$$\Sigma = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}^{(n)} - \mu_{t^{(n)}})(\mathbf{x}^{(n)} - \mu_{t^{(n)}})^T$$

- Linear decision boundary.

Decision Boundary: Shared Variances (between Classes)



variances may be different

Gaussian Discriminative Analysis vs Logistic Regression

- Binary classification: If you examine $p(t = 1|\mathbf{x})$ under GDA and assume $\Sigma_0 = \Sigma_1 = \Sigma$, 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 $(\phi, \mu_0, \mu_1, \Sigma)$, $\phi = p(t = 1)$

- Same model 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 (what loss is it optimizing?)
- Many class-conditional distributions lead to logistic classifier
- When these distributions are non-Gaussian (a.k.a almost always), LR usually beats GDA
- GDA can handle easily missing features (how do you do that with LR?)

Naive Bayes

- **Naive Bayes**: 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?
- Equivalent to assuming Σ_k is diagonal.

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

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

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

- What decision boundaries do we get?

Decision Boundary: isotropic

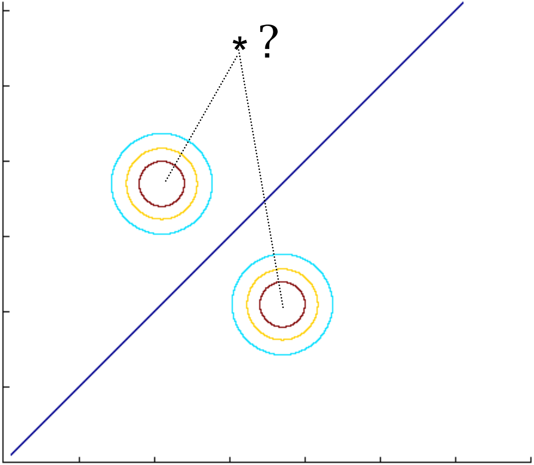
- In this case: $\sigma_{i,k} = \sigma$ (just one parameter), class priors equal (e.g., $p(t_k) = 0.5$ for 2-class case)
- Going back to class posterior for GDA:

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

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):

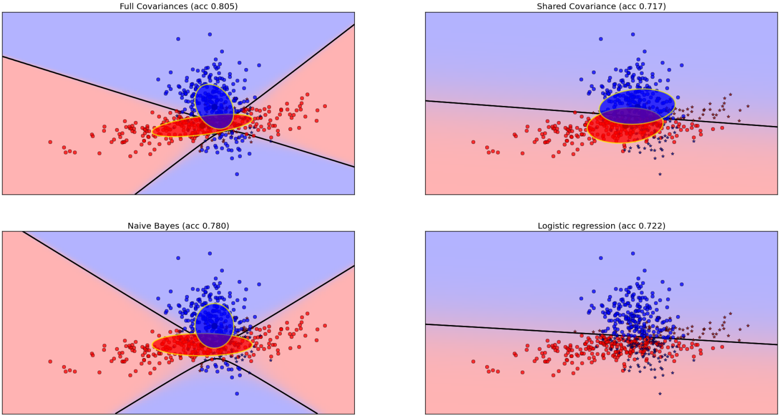
$$\log p(t_k|\mathbf{x}) = -\frac{1}{2\sigma^2}(\mathbf{x}-\mu_k)^T(\mathbf{x}-\mu_k)$$

Decision Boundary: isotropic



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

Example



Full Covariances (acc 0.805)
Shared Covariance (acc 0.717)
Naive Bayes (acc 0.780)
Logistic regression (acc 0.722)

Generative models - Recap

- GDA - quadratic decision boundary.
- With shared covariance "collapses" to logistic regression.
- Generative models:
  - Flexible models, easy to add/remove class.
  - Handle missing data naturally
  - More "natural" way to think about things, but usually doesn't work as well.
- Tries to solve a hard problem in order to solve a easy problem.