DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 13 | Part 1

Bayes with Multiple Features

Recap

- **Bayes Classifier:** predict y that maximizes $\mathbb{P}(Y = y \mid X = x)$

- **Alternatively:** predict y that maximizes

$$p_X(x \mid Y = y)\mathbb{P}(Y = y)$$

- We must estimate these probabilities/densities.

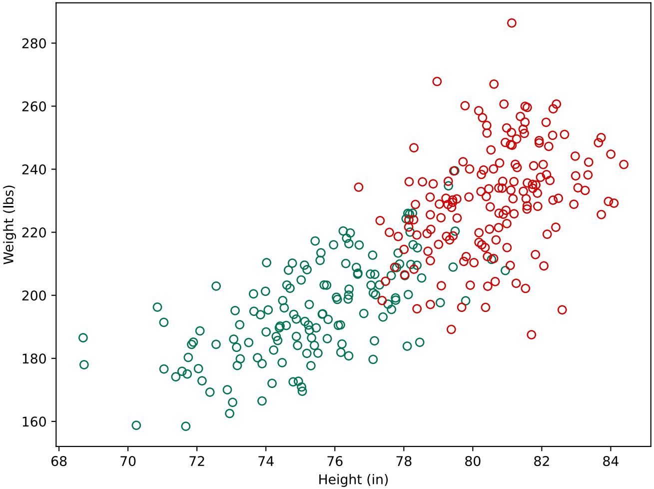
Example: NBA Players

- **Guard** and **Forward** are two positions in basketball.
- Forwards tend to be larger than guards.

Example: NBA Players

- Suppose we have a data set of n NBA players:
  - X_1: the player's height
  - X_2: the player's weight
  - Y: the player's position (1 = guard, 0 = forward)

- **Given:** a new player's height and weight, predict their position.


280
260
240
220
200
180
160
Weight (lbs)
68
70
72
74
76
78
80
82
84
Height (in)

Bayes in ≥ 2 Dimensions

- With one feature, Bayes said to pick y maximizing:

$$p_X(x \mid Y = y)\mathbb{P}(Y = y)$$

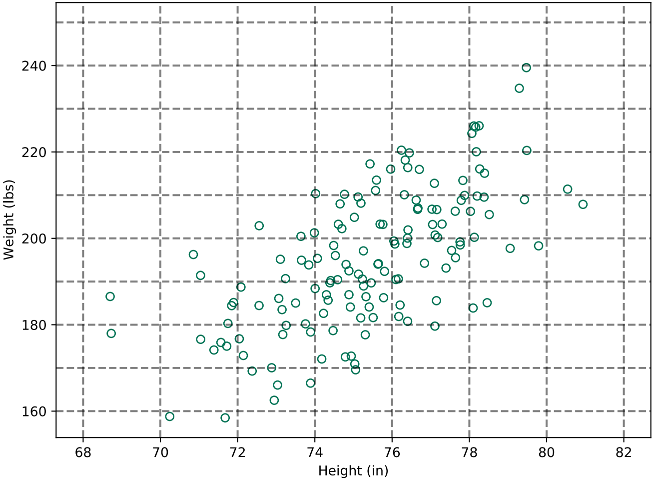
- With k features, pick y maximizing:

$$p_{\vec{X}}(\vec{x} \mid Y = y)\mathbb{P}(Y = y)$$

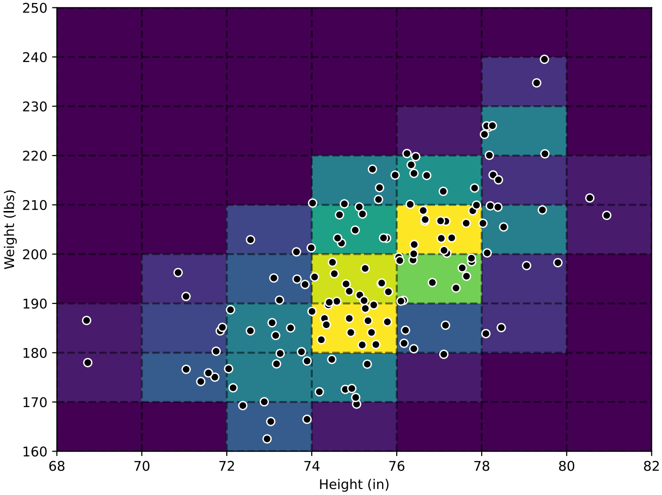
- $\vec{x}$ is the **feature vector**. Here: $(\text{height}, \text{weight})^T$

- We need to estimate density $p(\vec{x} \mid Y = y)$ for each class.

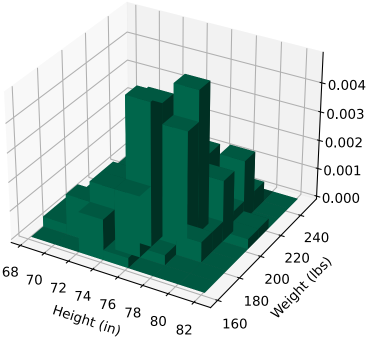
Estimating with Histograms



Estimating with Histograms



Estimating with Histograms



Predicting with Histograms

To predict the class of an input $\vec{x}$:

1. Use histograms to estimate $p_{\vec{X}}(\vec{x} \mid Y = y)$ for each class separately.

2. Predict the class y maximizing

$$p_{\vec{X}}(\vec{x} \mid Y = y)\mathbb{P}(Y = y)$$

Histogram Estimators

- Histogram density estimators are very flexible.
- But suffer heavily from **curse of dimensionality.**
- Not feasible for estimating density in more than a few dimensions.

Today

- **Last time:** we saw the **parametric** approach to density estimation.
  - Pick a parametric distribution (e.g., Gaussian)
  - Find parameters by maximizing likelihood

- We saw how to do this for one-dimensional data.

- **Today:** multidimensional data.

In particular...

- **Today:** multivariate Gaussian density estimation.
- That is: fitting multivariate Gaussians to data with maximum likelihood.

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Probabilistic Modeling & Machine Learning

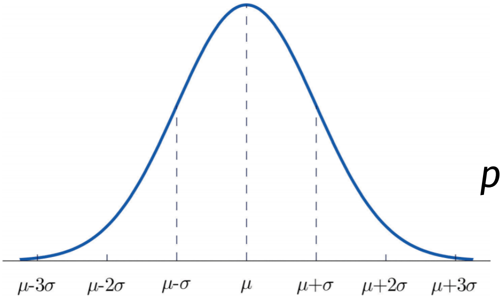
Lecture 13 | Part 2

Multivariate Gaussians

Multivariate Gaussians

- In 1 dimension, a Gaussian seemed to describe distribution of heights.
- Does a **multivariate** Gaussian describe distribution of heights and weights?

“Deriving” Multivariate Gaussians



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

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu)^2/\sigma^2}$$

Setting #1

- Suppose we have d independent random variables $X_1, \ldots, X_d$.
- Assume that each is Gaussian; different mean, but **same** variance:

$$X_1 \sim \mathcal{N}(\mu_1, \sigma^2), \quad X_2 \sim \mathcal{N}(\mu_2, \sigma^2), \ldots, \quad X_d \sim \mathcal{N}(\mu_d, \sigma^2).$$

Setting #1

- What is the **joint density** $p(x_1, x_2, \dots, x_d)$?

- Since we assumed $X_1, \dots, X_d$ are independent:

$$p(x_1, x_2, \dots, x_d) = \overset{\mu_1, \sigma^2}{p(x_1)}\,\overset{\mu_2, \sigma^2}{p(x_2)} \cdots p(x_d)$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_1)^2/\sigma^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_2)^2/\sigma^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_d)^2/\sigma^2}\right)$$

Setting #1

- What is the **joint density** $p(x_1, x_2, \ldots, x_d)$?

- Since we assumed $X_1, \ldots, X_d$ are independent:

$$p(x_1, x_2, \ldots, x_d) = p(x_1)p(x_2)\cdots p(x_d)$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_1)^2/\sigma^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_2)^2/\sigma^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_d)^2/\sigma^2}\right)$$

$$= \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{(x_1 - \mu_1)^2 + (x_2 - \mu_2)^2 + \ldots + (x_d - \mu_d)^2}{2\sigma^2}\right)$$

x_1 x_2

Setting #1

- What is the **joint density** $p(x_1, x_2, \ldots, x_d)$?

- Since we assumed $X_1, \ldots, X_d$ are independent:

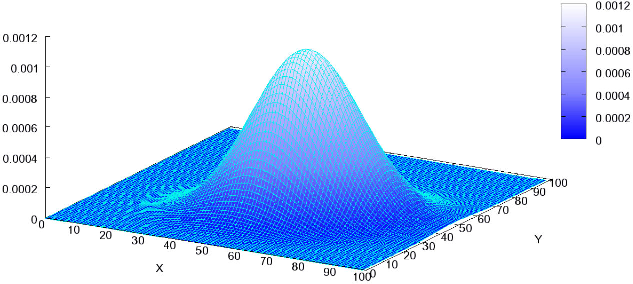
$$p(x_1, x_2, \ldots, x_d) = p(x_1)p(x_2)\cdots p(x_d)$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_1)^2/\sigma^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_2)^2/\sigma^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x-\mu_d)^2/\sigma^2}\right)$$

$$= \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{(x_1-\mu_1)^2 + (x_2-\mu_2)^2 + \ldots + (x_d-\mu_d)^2}{2\sigma^2}\right)$$

$$= \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{\|\vec{x}-\vec{\mu}\|^2}{2\sigma^2}\right)$$

Setting #1

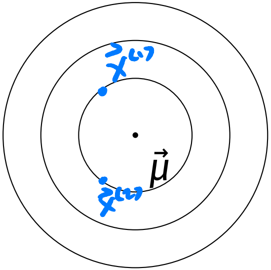


0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
X
Y
0 10 20 30 40 50 60 70 80 90 100
0 10 20 30 40 50 60 70 80 90 100

Setting #1: Spherical Gaussians

$$p(\vec{x}) = \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{1}{2}\frac{\|\vec{x}-\vec{\mu}\|^2}{\sigma^2}\right)$$

- Contours are (hyper)spheres.
- Every slice through middle gives same Gaussian.



Setting #2

- Still assume $X_1, \ldots, X_d$ are independent, Gaussian.
- But they now have different variances:

$$X_1 \sim \mathcal{N}(\mu_1, \sigma_1^2), \quad X_2 \sim \mathcal{N}(\mu_2, \sigma_2^2), \ldots, \quad X_d \sim \mathcal{N}(\mu_d, \sigma_d^2).$$

Setting #2

$$p(x_1, x_2, \dots, x_d) = p(x_1)p(x_2) \cdots p(x_d)$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{1}{2}(x-\mu_1)^2/\sigma_1^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{1}{2}(x-\mu_2)^2/\sigma_2^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma_d^2}} e^{-\frac{1}{2}(x-\mu_d)^2/\sigma_d^2}\right)$$

$$A = \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix} \quad A^{-1} = \begin{pmatrix} 1/a_1 & 0 \\ 0 & 1/a_2 \end{pmatrix} \quad C^{-1} = \begin{pmatrix} 1/\sigma_1^2 & & & 0 \\ & 1/\sigma_2^2 & & \\ & & \ddots & \\ 0 & & & 1/\sigma_d^2 \end{pmatrix}$$

Setting #2

$$\vec{x} = (x_1, x_2)^T \quad \mu = (\mu_1, \mu_2)^T$$

$$p(x_1, x_2, \ldots, x_d) = p(x_1)p(x_2)\cdots p(x_d)$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{1}{2}(x-\mu_1)^2/\sigma_1^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{1}{2}(x-\mu_2)^2/\sigma_2^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma_d^2}} e^{-\frac{1}{2}(x-\mu_d)^2/\sigma_d^2}\right)$$

$$= \frac{1}{(2\pi)^{d/2}\sigma_1 \cdot \sigma_2 \cdots \sigma_d} \exp\left(-\frac{1}{2}\left[\frac{(x_1-\mu_1)^2}{\sigma_1^2} + \frac{(x_2-\mu_2)^2}{\sigma_2^2} + \ldots + \frac{(x_d-\mu_d)^2}{\sigma_d^2}\right]\right)$$

$$C^{-1}(\vec{x} - \vec{\mu}) = \begin{pmatrix} 1/\sigma_1^2 & 0 \\ 0 & 1/\sigma_2^2 \end{pmatrix} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix} = \begin{pmatrix} (x_1 - \mu_1)/\sigma_1^2 \\ (x_2 - \mu_2)/\sigma_2^2 \end{pmatrix}$$

$\vec{x}^T A x$ $\quad \frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} =$

Setting #2

$$C^{-1}(\vec{x}-\vec{\mu}) = \begin{pmatrix} 1/\sigma_1^2 & 0 \\ 0 & 1/\sigma_2^2 \end{pmatrix} \begin{pmatrix} x_1-\mu_1 \\ x_2-\mu_2 \end{pmatrix} = \begin{pmatrix} (x_1-\mu_1)/\sigma_1^2 \\ (x_2-\mu_2)/\sigma_2^2 \end{pmatrix}$$

$$p(x_1, x_2, \ldots, x_d) = p(x_1)p(x_2)\cdots p(x_d)$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{1}{2}(x-\mu_1)^2/\sigma_1^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{1}{2}(x-\mu_2)^2/\sigma_2^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma_d^2}} e^{-\frac{1}{2}(x-\mu_d)^2/\sigma_d^2}\right)$$

$$= \frac{1}{(2\pi)^{d/2}\sigma_1 \cdot \sigma_2 \cdots \sigma_d} \exp\left(-\frac{1}{2}\left[\frac{(x_1-\mu_1)^2}{\sigma_1^2} + \frac{(x_2-\mu_2)^2}{\sigma_2^2} + \ldots + \frac{(x_d-\mu_d)^2}{\sigma_d^2}\right]\right)$$

$$(\vec{x}-\mu)^T C^{-1}(\vec{x}-\mu) = \begin{pmatrix} x_1-\mu_1 & x_2-\mu_2 \end{pmatrix} \begin{pmatrix} (x_1-\mu_1)/\sigma_1^2 \\ (x_2-\mu_2)/\sigma_2^2 \end{pmatrix} = (x_1-\mu_1)^2/\sigma_1^2 + (x_2-\mu_2)^2/\sigma_2^2$$

Setting #2

- Define

$$C = \begin{pmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \sigma_d^2 \end{pmatrix}$$

- Then:

$$p(\vec{x}) = \frac{1}{(2\pi)^{d/2}|C|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu})^T C^{-1} (\vec{x} - \vec{\mu})\right)$$

where $|C|$ is the **determinant** of C.

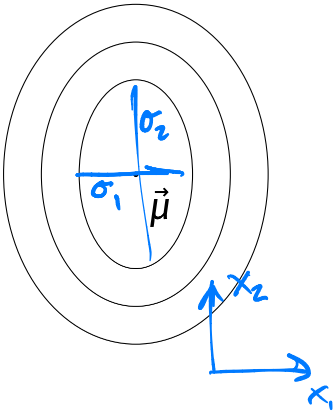
Setting #2: Axis-Aligned Gaussians

$\sigma_1^2 \quad \sigma_2^2$

$$p(\vec{x}) = \frac{1}{(2\pi)^{d/2}|C|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T C^{-1}(\vec{x}-\vec{\mu})\right)$$

- Contours are axis-aligned (hyper)ellipses.

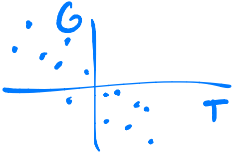
- C is the **covariance matrix**.
  - Diagonal.
  - Entries are variances.



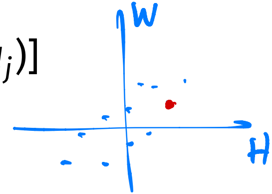
Setting #3: General Gaussians

- We have assumed that $X_1, \ldots, X_d$ are independent.

- Now assume that they're not. Define **covariance**:



$$\mathrm{Cov}(X_i, X_j) = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)]$$

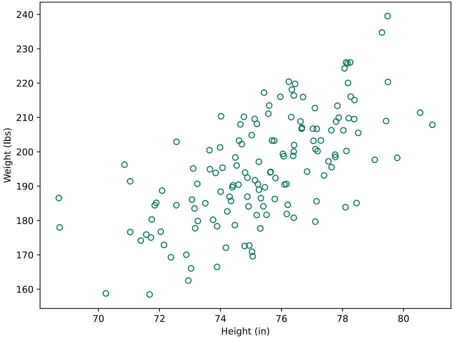


- **Note**:

$$\mathrm{Var}(\mathrm{X}_\mathrm{i}) = \mathrm{Cov}(X_i, X_i)$$

Covariance

- Covariance measures how much two quantities **vary together**.



$$\mathrm{Cov}(X_i, X_j) = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)]$$

Setting #3: General Gaussians

- Now the **covariance matrix** has off-diagonal elements:

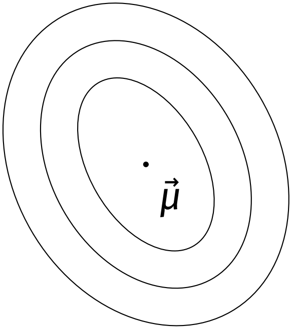
$$C = \begin{pmatrix} \mathrm{Var}(X_1) & \mathrm{Cov}(X_1, X_2) & \cdots & \mathrm{Cov}(X_1, X_d) \\ \mathrm{Cov}(X_2, X_1) & \mathrm{Var}(X_2) & \cdots & \mathrm{Cov}(X_2, X_d) \\ \cdots & \cdots & \cdots & \cdots \\ \mathrm{Cov}(X_d, X_1) & \mathrm{Cov}(X_d, X_2) & \cdots & \mathrm{Var}(X_d) \end{pmatrix}$$

- Since $\mathrm{Cov}(X_i, X_j) = \mathrm{Cov}(X_j, X_i)$, C is symmetric.

Setting #3: General Gaussians

$$p(\vec{x}) = \frac{1}{(2\pi)^{d/2}|C|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T C^{-1}(\vec{x}-\vec{\mu})\right)$$

Contours are general (hyper)ellipses.
C need not be diagonal.



Overview

- The probability density function for a multivariate Gaussian distribution is:

$$p(\vec{x}) = \frac{1}{(2\pi)^{d/2}|C|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu})^T C^{-1}(\vec{x} - \vec{\mu})\right)$$

- Here, C is the **covariance matrix**.

Overview

- There are three cases:

1. C is diagonal, with all the same entries.
2. C is diagonal, with different entries.
3. C is not diagonal.

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Probabilistic Modeling & Machine Learning

Lecture 13 | Part 3

Fitting Multivariate Gaussians

Fitting Multivariate Gaussians

- Suppose $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}$ came from a multivariate Gaussian.
- What were the parameters of that Gaussian?
- We can use the principle of **maximum likelihood**.

$\mathbb{R}^d$ $\frac{\partial}{C_{12}}$

What are the parameters?

$$p(\vec{x}) = \frac{1}{(2\pi)^{d/2}|C|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T C^{-1}(\vec{x}-\vec{\mu})\right)$$

- $\vec{\mu}$: controls Gaussian's location
- C: controls Gaussian's shape

Estimating $\vec{\mu}$

- The maximum likelihood estimator for μ is:

$$\vec{\mu}_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n} \vec{x}^{(i)}$$

$\mathbb{R}^d$

Estimating C

- First: make assumptions on covariance matrix.

- In order from strict to weak:
  - Spherical: C is diagonal, with all the same entries.
  - Axis-Aligned: C is diagonal, with different entries.
  - General: C is not diagonal.

- The weaker the assumptions, the more parameters to estimate.

Fitting Spherical Gaussians

- Only one variance parameter: σ^2.

- The density function becomes:

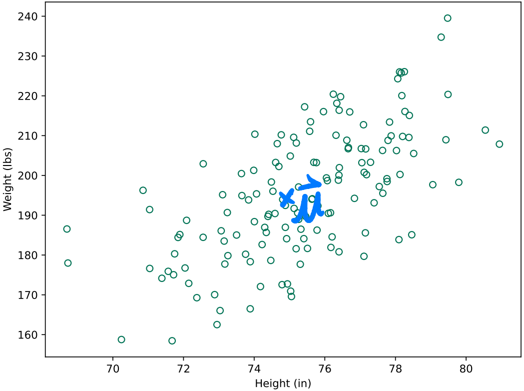
$$p(\vec{x}) = \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{(\vec{x} - \vec{\mu})^T (\vec{x} - \vec{\mu})}{2\sigma^2} \right)$$

- The maximum likelihood estimator:

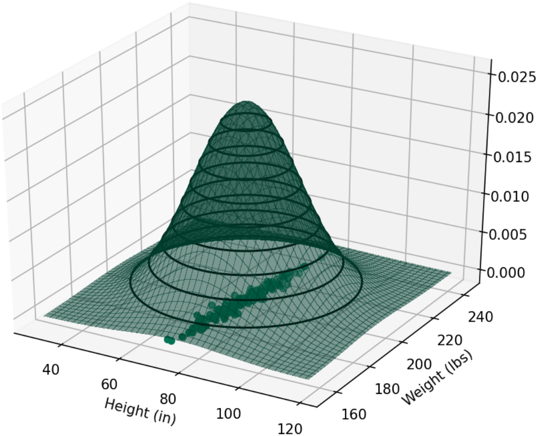
$$\sigma^2_{\text{MLE}} = \frac{1}{n} \sum_{i=1}^{n} \|\vec{x}^{(i)} - \vec{\mu}_{\text{MLE}}\|^2$$

Example: NBA Data

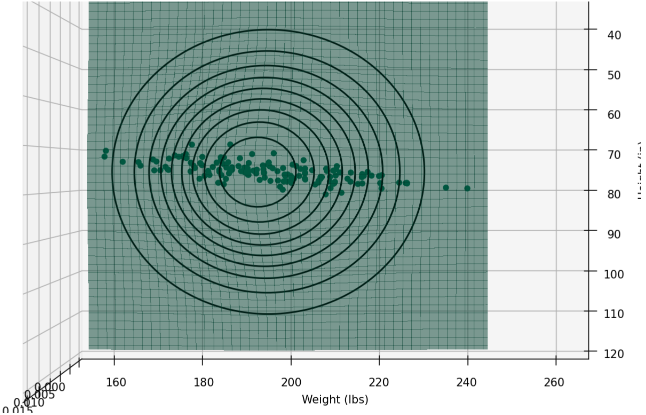
- What if we fit a spherical Gaussian to the NBA data?



Fitting Spherical Gaussians



Fitting Spherical Gaussians



Example: NBA Data

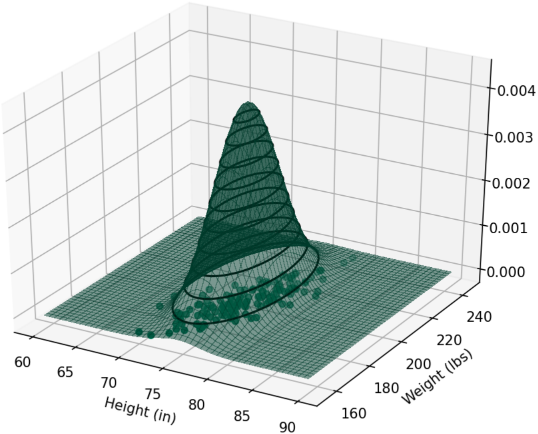
- Spherical Gaussians are not well-suited to this data.
- Perhaps if the data were **standardized...**
- Instead, try axis-aligned Gaussians.

Fitting Axis-Aligned Gaussians

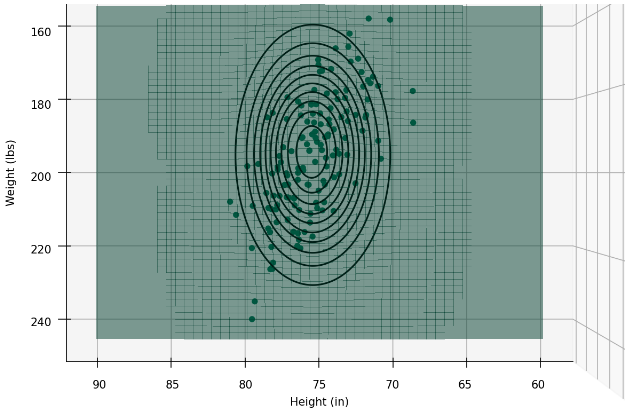
- Variance for each axis: σ_1^2 and σ_2^2.
- Maximum likelihood estimates:

$$\sigma_1^2 = \text{sample variance of heights}$$
$$\sigma_2^2 = \text{sample variance of weights}$$

Fitting Axis-Aligned Gaussians



Fitting Axis-Aligned Gaussians



Example: NBA Data

- Axis-aligned Gaussian does not capture correlation between height and weight.
- Try general Gaussian with full covariance.

Fitting General Gaussians

- Must compute covariance for each pair of dimensions.

- Maximum likelihood estimate for covariance of feature *i* and *j*:

$$C_{ij} = \left(\frac{1}{n} \sum_{k=1}^{n} \vec{x}_i^{(k)} \vec{x}_j^{(k)} \right) - \mu_i \mu_j$$

Computing the Covariance Matrix

Step 1. Make matrix with heights in first column, weights in second:

$$\begin{pmatrix} \text{height 1} & \text{weight 1} \\ \text{height 2} & \text{weight 2} \\ \dots & \dots \\ \text{height } n & \text{weight } n \end{pmatrix}$$

Computing the Covariance Matrix

Step 2. Subtract sample mean height, mean weight from each column. Call this matrix X:

$$X = \begin{pmatrix} \text{height 1} - \text{mean height} & \text{weight 1} - \text{mean weight} \\ \text{height 2} - \text{mean height} & \text{weight 2} - \text{mean weight} \\ \dots & \dots \\ \text{height } n - \text{mean height} & \text{weight } n - \text{mean weight} \end{pmatrix}$$

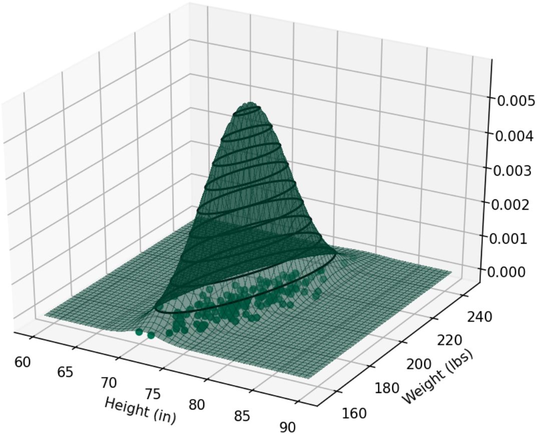
Computing the Covariance Matrix

The empirical covariance matrix is then:

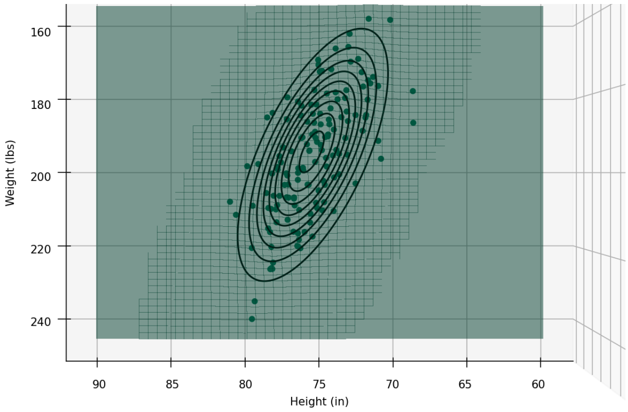
$$C = \frac{1}{n} X^T X$$

$$C_{ij} = \left(\frac{1}{n} \sum_{k=1}^{n} \vec{x}_i^{(k)} \vec{x}_j^{(k)} \right) - \mu_i \mu_j$$

Fitting General Gaussians



Fitting General Gaussians



Up next...

Making predictions using these fitted Gaussians.

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Probabilistic Modeling & Machine Learning

Lecture 13 | Part 4

Discriminant Analysis

Bayes Classifier with MV Gaussians

1. Fit Gaussian for $p(\vec{X} \mid Y = y)$ for each class, y.
2. For new point, predict y maximizing:

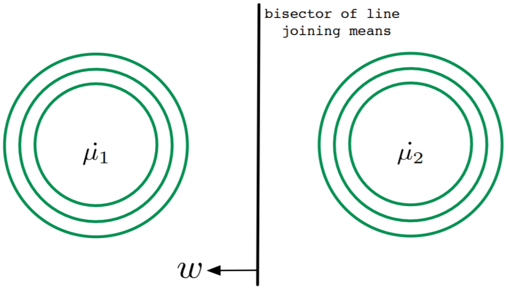
$$p(\vec{X} = \vec{x} \mid Y = y)\mathbb{P}(Y = y)$$

Decision Boundary

- For every point in space, we have a classification.
- The **decision boundary**: surface between different classifications.
  - On one side, prediction is y_1;
  - on the other, prediction is y_2.

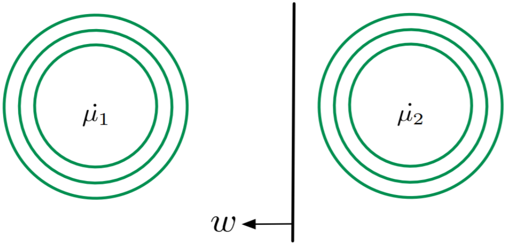
~~Setting~~ Case #1

- Assume:
  - classes equally likely: $\mathbb{P}(Y = 1) = \mathbb{P}(Y = 0)$
  - identical covariance matrices



Setting #1

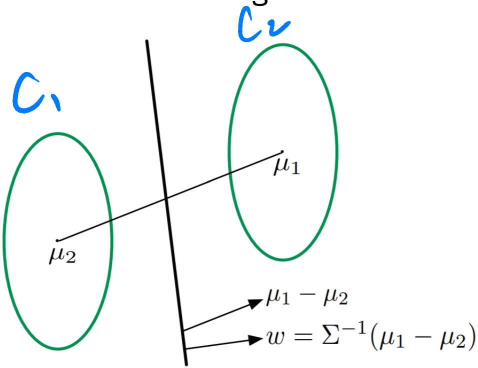
- If $\mathbb{P}(Y = y_1) > \mathbb{P}(Y = y_2)$:



Choose class 1 if $\vec{w} \cdot \frac{(\vec{\mu}_1 - \vec{\mu}_2)}{\sigma^2} \geq \theta$.

~~Setting~~ Case #2

- Assume:
  - covariance matrices identical, diagonal
  - that is: axis-aligned Gaussians



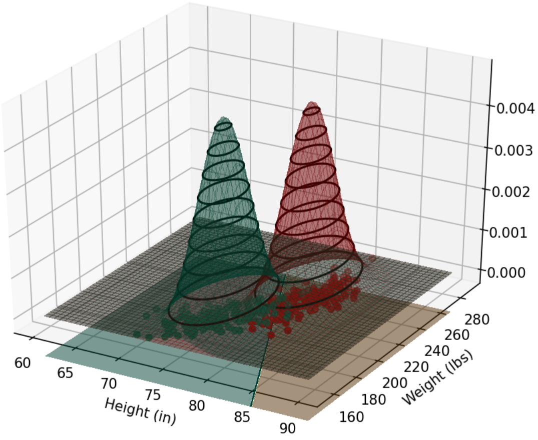
Predict class 1 if
$\vec{x} \cdot \vec{w} \geq \theta$.

Example

- Use to predict position given height and weight.
- How do we get one covariance matrix?
- Don't lump data together...
- Instead, compute covariance matrix for each class, perform weighted average:

$$C = \frac{n_1 C_1 + n_2 C_2}{n_1 + n_2}$$

Example



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Height (in)
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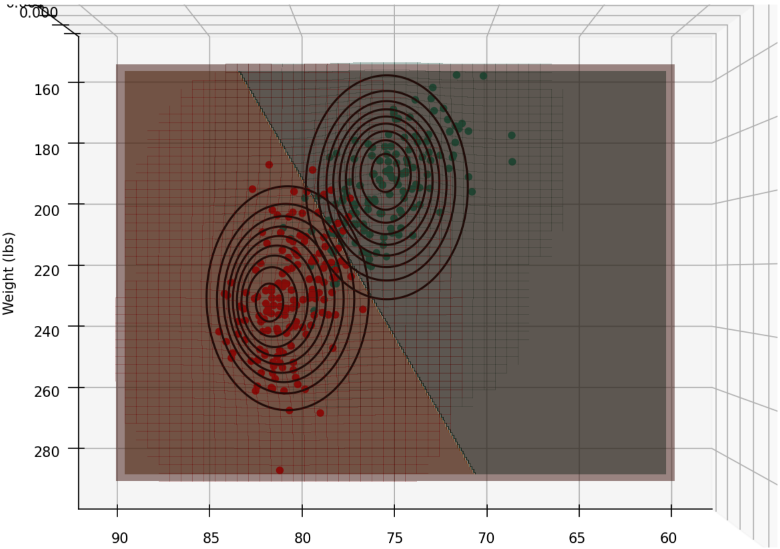
260
280
Weight (lbs)

Example

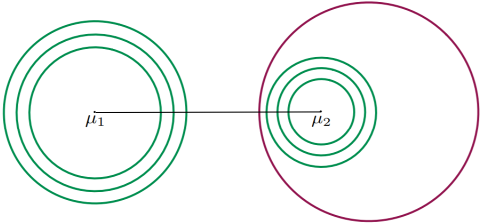


Linear Discriminant Analysis

- When covariance matrices are **equal**, decision boundary is linear.
- This procedure is called **linear discriminant analysis** (LDA).
- True even if the Gaussians have full covariance.

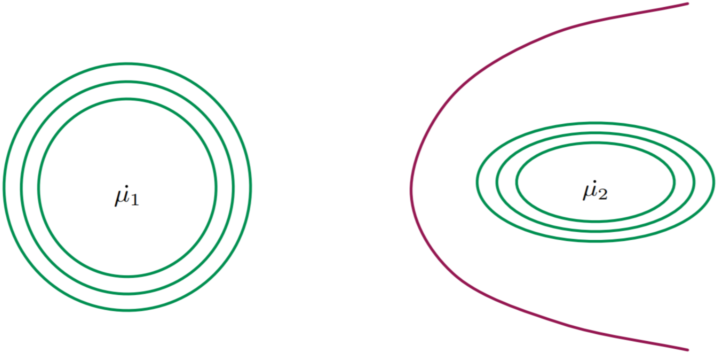
Setting #3

- Assume:
  - covariance matrices C_1, C_2 different, non-diagonal

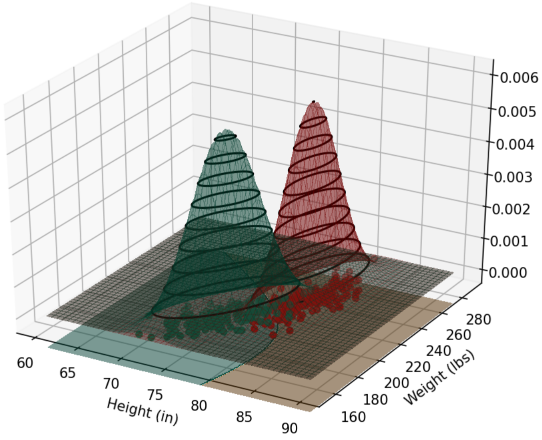


Setting #3

- Assume:
  - covariance matrices C_1, C_2 different, non-diagonal



Example



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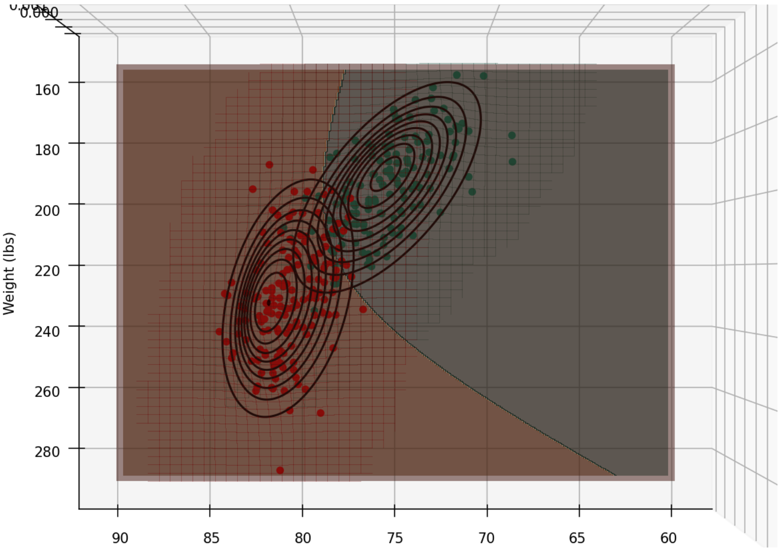
Example



Quadratic Discriminant Analysis

- When covariance matrices are unequal, decision boundary is quadratic (ellipsoidal, paraboloidal, hyperboloidal).

- This procedure is called **quadratic discriminant analysis** (QDA).

In practice...

- A full covariance requires estimating $\Theta(d^2)$ parameters; needs more data.
- Gaussian assumption may be a poor match for data.