# DSC 140A

## Probabilistic Modeling & Machine Learning

Lecture 14 | 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

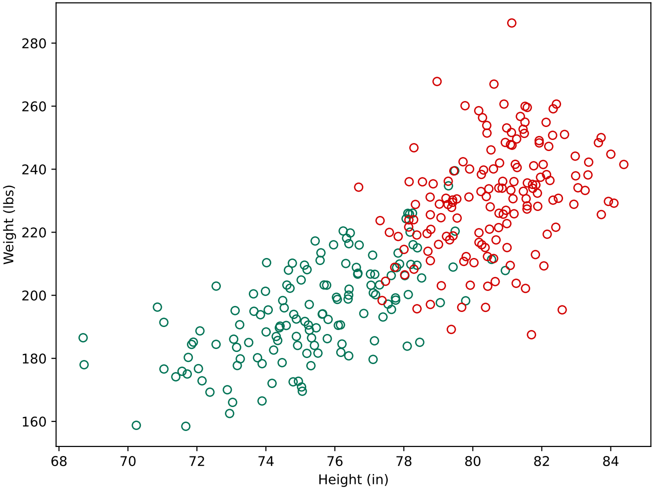
- **Guard** and **Forward** are two positions in basketball.

- 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.



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

# Bayes in ≥ 2 Dimensions

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

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

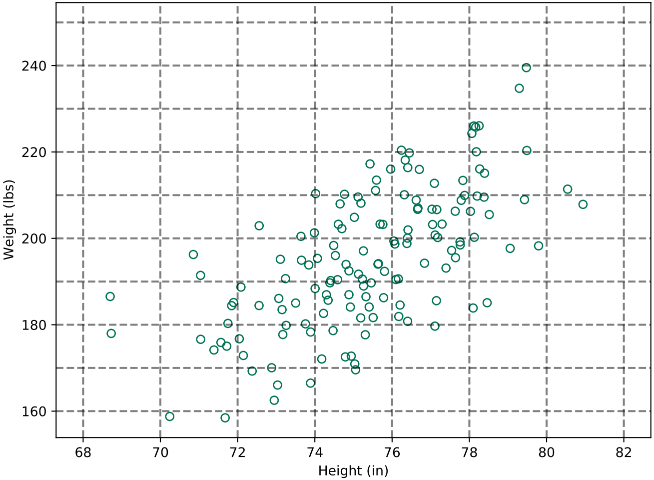
- With $k$ features, pick $y$ maximizing:

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

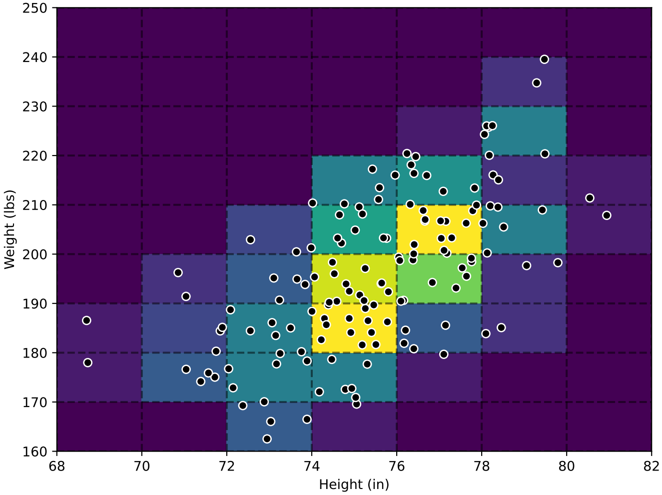
- $\vec{x}$ is the **feature vector**. Here: $(\text{height}, \text{weight})^T$

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

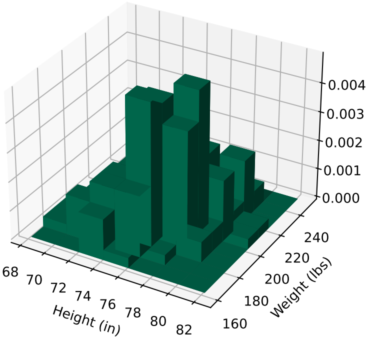
# Estimating with Histograms



# 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.

# DSC 140A

Probabilistic Modeling & Machine Learning

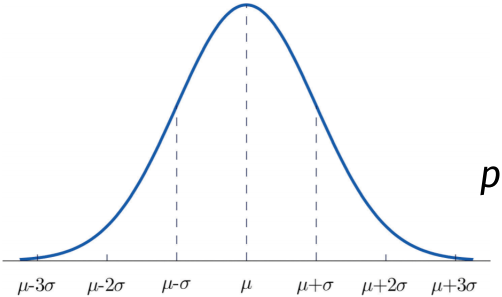
Lecture 14 | Part 2

## 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** $p(x_1, x_2, \ldots, x_d)$?
- Since we assumed $X_1, \ldots, X_d$ are independent:

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

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_1-\mu_1)^2/\sigma^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_2-\mu_2)^2/\sigma^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_d-\mu_d)^2/\sigma^2}\right)$$

# 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:

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

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_1-\mu_1)^2/\sigma^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_2-\mu_2)^2/\sigma^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_d-\mu_d)^2/\sigma^2}\right)$$

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

# 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:

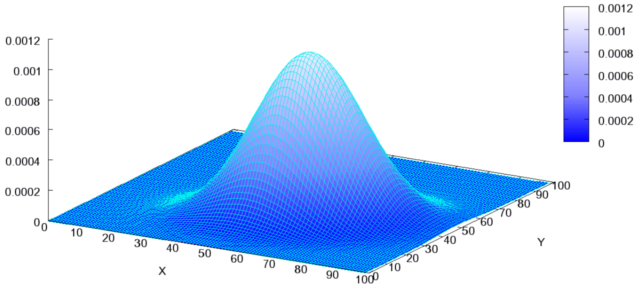
$$p(x_1, x_2, \dots, x_d) = p(x_1)p(x_2)\cdots p(x_d)$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_1-\mu_1)^2/\sigma^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_2-\mu_2)^2/\sigma^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(x_d-\mu_d)^2/\sigma^2}\right)$$

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

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

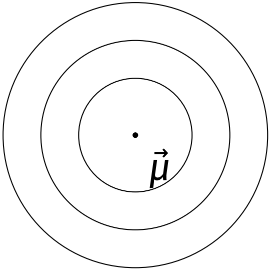
# Setting #1


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

# 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 $X_1, \dots, X_d$ are independent, Gaussian.
- But they now have different variances:

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

# Setting #2

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

$$= \left(\frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{1}{2}(x_1-\mu_1)^2/\sigma_1^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{1}{2}(x_2-\mu_2)^2/\sigma_2^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma_d^2}} e^{-\frac{1}{2}(x_d-\mu_d)^2/\sigma_d^2}\right)$$

# Setting #2

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

$$= \left(\frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{1}{2}(x_1-\mu_1)^2/\sigma_1^2}\right) \cdot \left(\frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{1}{2}(x_2-\mu_2)^2/\sigma_2^2}\right) \cdots \left(\frac{1}{\sqrt{2\pi\sigma_d^2}} e^{-\frac{1}{2}(x_d-\mu_d)^2/\sigma_d^2}\right)$$

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

# 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:

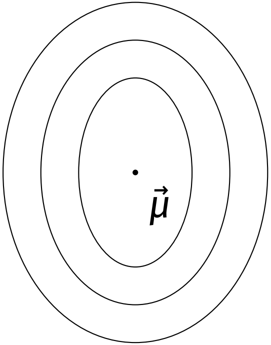
$$p(\vec{x}) = \frac{1}{(2\pi)^{d/2}|C|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu})^T C^{-1} (\vec{x} - \vec{\mu})\right)$$

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

# Setting #2: **Axis-Aligned** Gaussians

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

- Contours are axis-aligned (hy-per)ellipses.
- C is the **covariance matrix**.
  - Diagonal.
  - Entries are variances.



# Setting #3: General Gaussians

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

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

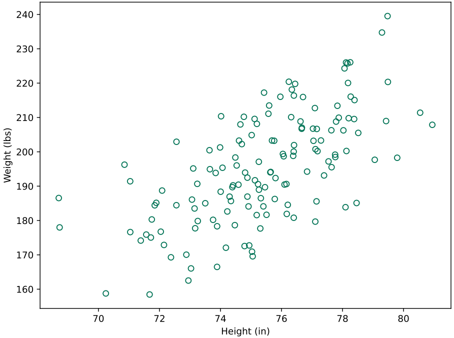
$$\text{Cov}(X_i, X_j) = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)]$$

- **Note**:

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

# 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:

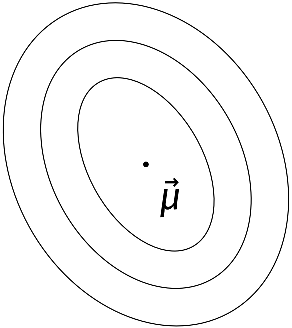
$$C = \begin{pmatrix} \mathrm{Var}(X_1) & \mathrm{Cov}(X_1, X_2) & \cdots & \mathrm{Cov}(X_1, X_d) \\ \mathrm{Cov}(X_2, X_1) & \mathrm{Var}(X_2) & \cdots & \mathrm{Cov}(X_2, X_d) \\ \cdots & \cdots & \cdots & \cdots \\ \mathrm{Cov}(X_d, X_1) & \mathrm{Cov}(X_d, X_2) & \cdots & \mathrm{Var}(X_d) \end{pmatrix}$$

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

# Setting #3: General Gaussians

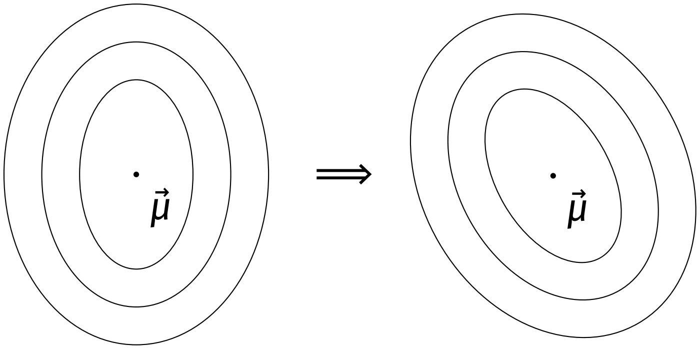
$$p(\vec{x}) = \frac{1}{(2\pi)^{d/2}|C|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu})^T C^{-1}(\vec{x} - \vec{\mu})\right)$$

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



# General Gaussians: Another View

- A **general** Gaussian is an **axis-aligned** Gaussian that has been rotated:



# General Gaussians: Another View

- Which matrices are **valid** covariance matrices?
- 1. If $C$ is the rotation of some diagonal covariance matrix $C_0$. That is, $C = RC_0$
- 2. Equivalently, $C$ is symmetric, positive semi-definite.

# 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, from least to most general:

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

# DSC 140A

## Probabilistic Modeling & Machine Learning

Lecture 14 | 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**.

# 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 $\mu$ is:

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

# 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: $\sigma^2$.

- The density function becomes:

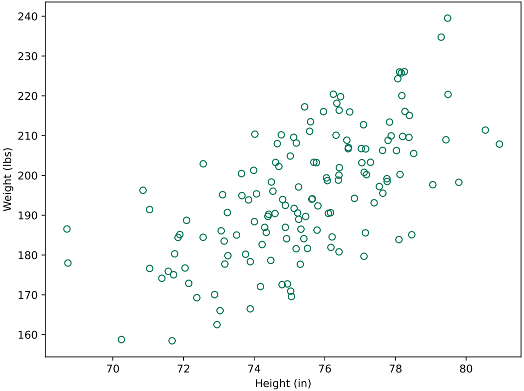
$$p(\vec{x}) = \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{(\vec{x} - \vec{\mu})^T(\vec{x} - \vec{\mu})}{2\sigma^2}\right)$$

- The maximum likelihood estimator:

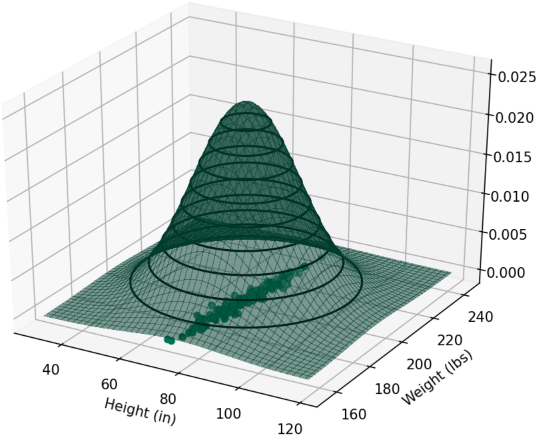
$$\sigma^2_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n} \|\vec{x}^{(i)} - \vec{\mu}_{\text{MLE}}\|^2$$

# Example: NBA Data

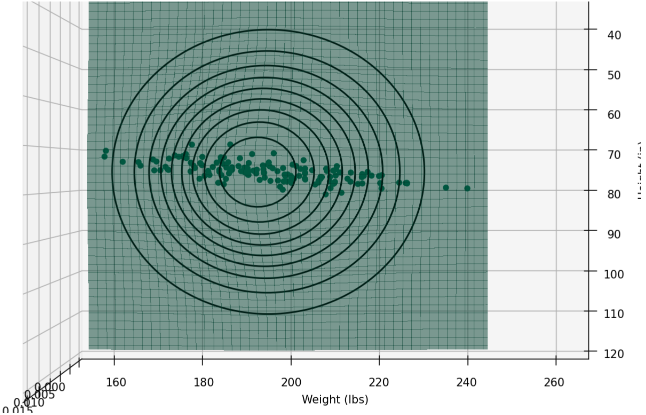
- What if we fit a spherical Gaussian to the NBA data?



# Fitting Spherical Gaussians



# Fitting Spherical Gaussians



# Example: NBA Data

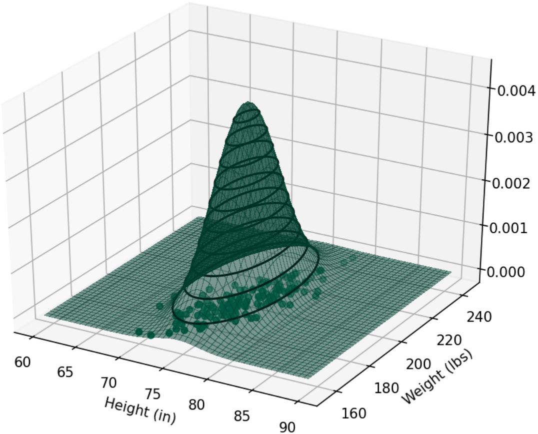
- Spherical Gaussians are not well-suited to this data.
- Perhaps if the data were **standardized...**
- Instead, try axis-aligned Gaussians.

# Fitting Axis-Aligned Gaussians

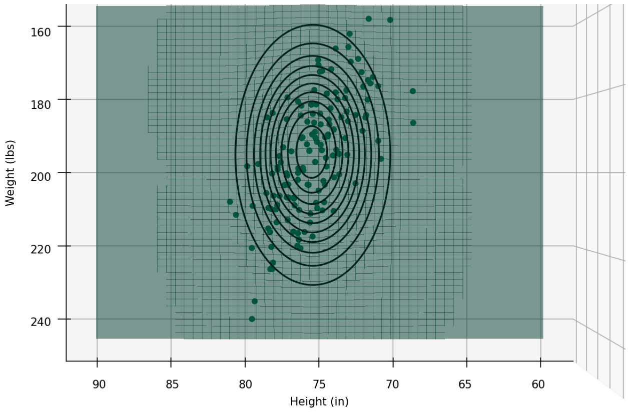
- Variance for each axis: $\sigma_1^2$ and $\sigma_2^2$.
- Maximum likelihood estimates:

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

# 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 $X$:

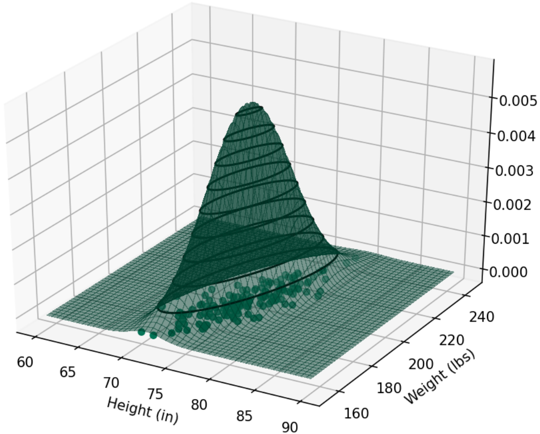
$$X = \begin{pmatrix} \text{height } 1 - \text{mean height} & \text{weight } 1 - \text{mean weight} \\ \text{height } 2 - \text{mean height} & \text{weight } 2 - \text{mean weight} \\ \dots & \dots \\ \text{height } n - \text{mean height} & \text{weight } n - \text{mean weight} \end{pmatrix}$$

# Computing the Covariance Matrix

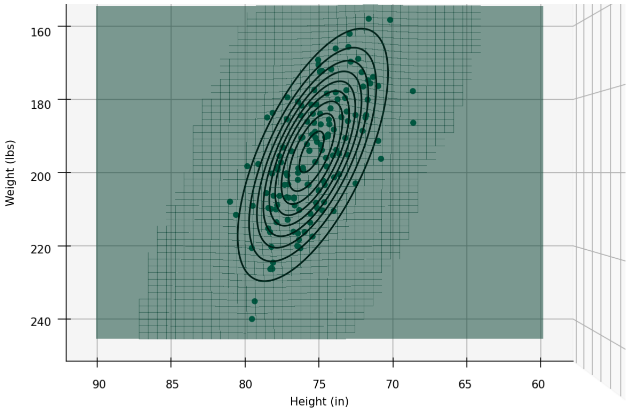
The empirical covariance matrix is then:

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

# Fitting General Gaussians



# Fitting General Gaussians



# Up next...

Making predictions using these fitted Gaussians.

# DSC 140A

## Probabilistic Modeling & Machine Learning

Lecture 14 | 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:

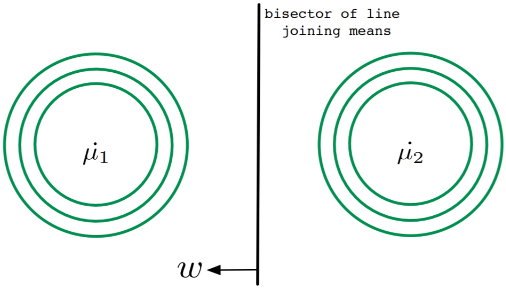
$$p(\vec{X} = \vec{x} \mid Y = y)\mathbb{P}(Y = y)$$

# 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 $y_2$.

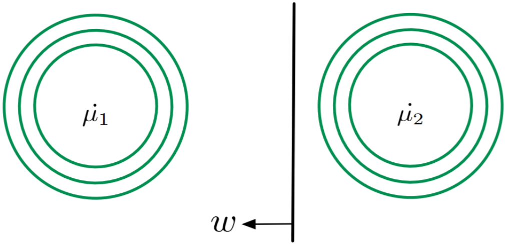
# Setting #1

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



# Setting #1

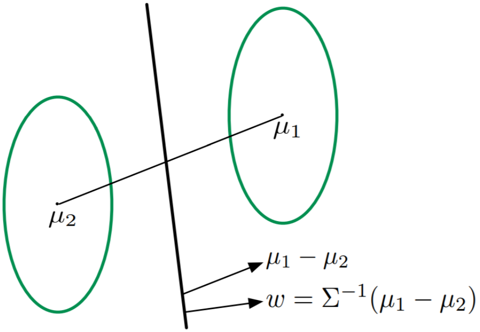
- If $\mathbb{P}(Y = y_1) > \mathbb{P}(Y = y_2)$:




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

# Setting #2

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



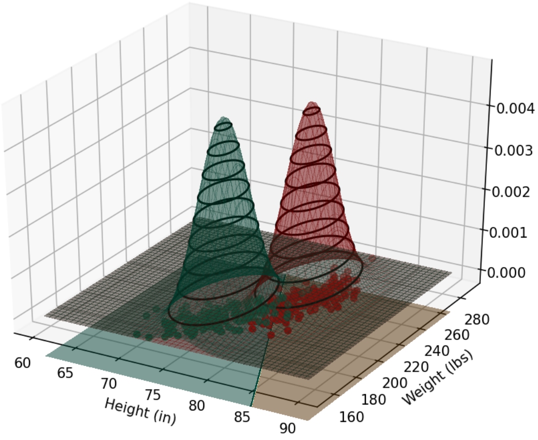

Predict class 1 if
$\vec{x} \cdot \vec{w} \geq \theta$.

# 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:

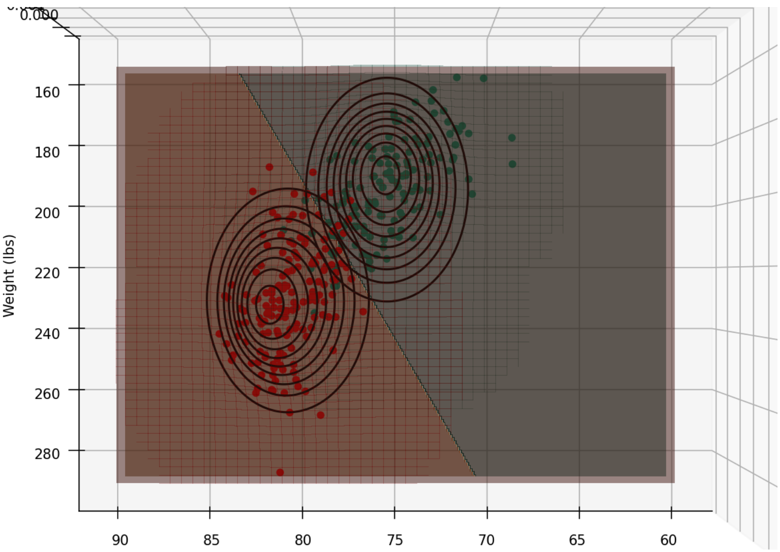
$$C = \frac{n_1 C_1 + n_2 C_2}{n_1 + n_2}$$

# Example



0.004
0.003
0.002
0.001
0.000
60
65
70
75
80
85
90
Height (in)
160
180
200
220
240
260
280
Weight (lbs)

# Example

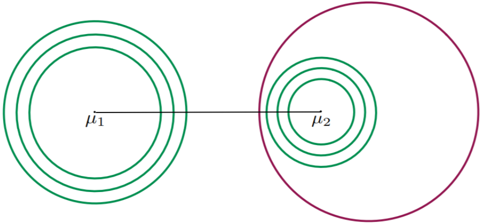


# Linear Discriminant Analysis

- 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.

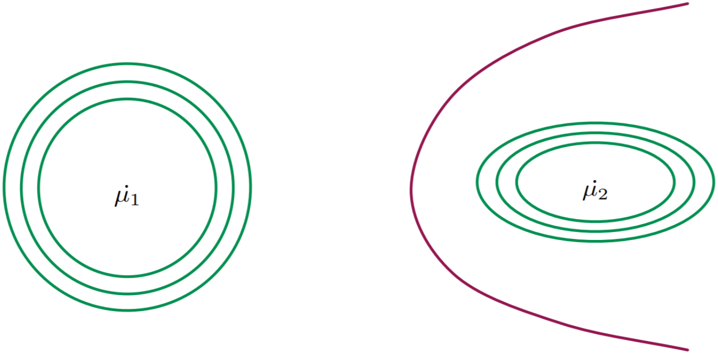
# Setting #3

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

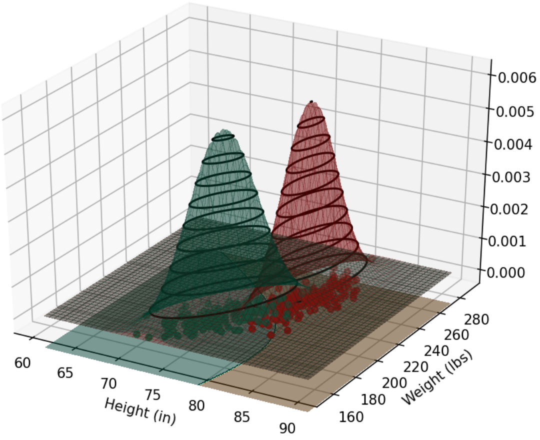


# Setting #3

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

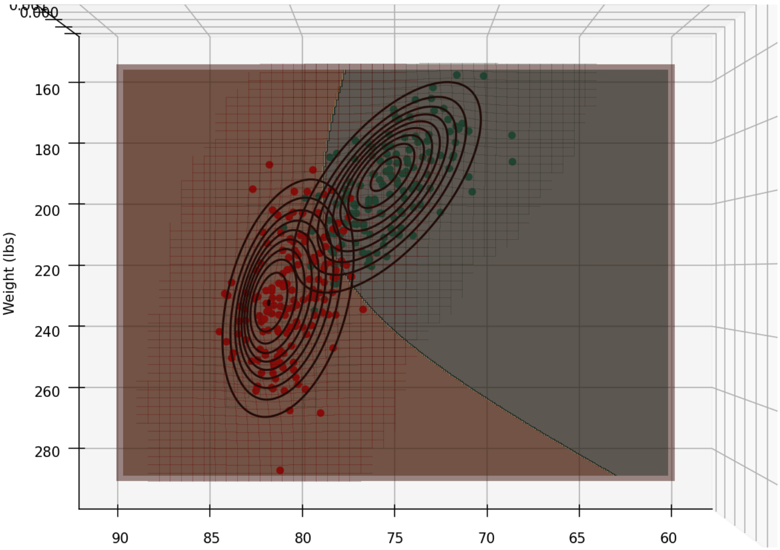


# Example



0.006
0.005
0.004
0.003
0.002
0.001
0.000
60
65
70
75
80
85
90
Height (in)
160
180
200
220
240
260
280
Weight (lbs)

# Example



# Quadratic Discriminant Analysis

- When covariance matrices are **not** equal, 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.