ML4 B&I: Introduction to Machine Learning

Lecture 7- Clustering Algorithms

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Vector Institute, Fall 2022

Overview

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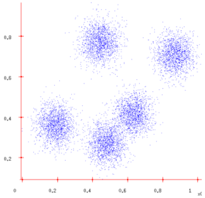
- Those methods made an interesting assumption that data depends on some latent variables that are never observed. Such models are called latent variable models.
  - For PCA, these correspond to the code vectors (representation).
- Today's lecture:
  - First, introduce K-means, a simple algorithm for clustering, i.e. grouping data points into clusters
  - Then, we will reformulate clustering as a latent variable model, apply the EM algorithm

Clustering

- Sometimes the data form clusters, where samples within a cluster are similar to each other, and samples in different clusters are dissimilar:



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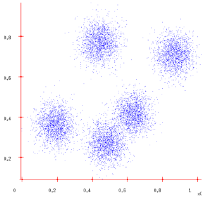

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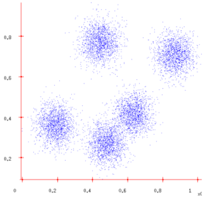

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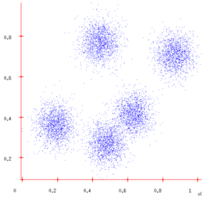

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- E.g. clustering machine learning papers based on topic (deep learning, Bayesian models, etc.)
    - But topics are never observed (unsupervised).

K-means intuition

- K-means assumes there are k clusters, and each point is close to its cluster center, or mean (the mean of points in the cluster).
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    - Chicken and egg problem!
- Very simple (and useful) heuristic - start randomly and alternate between the two!

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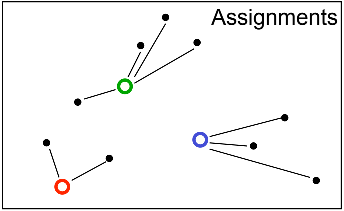
- The algorithm iteratively alternates between two steps:
  - Assignment step: Assign each data point to the closest cluster



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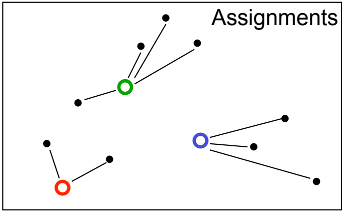
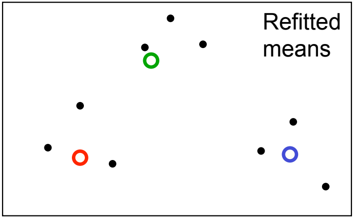
  - Refitting step: Move each cluster center to the center of gravity of the data assigned to it





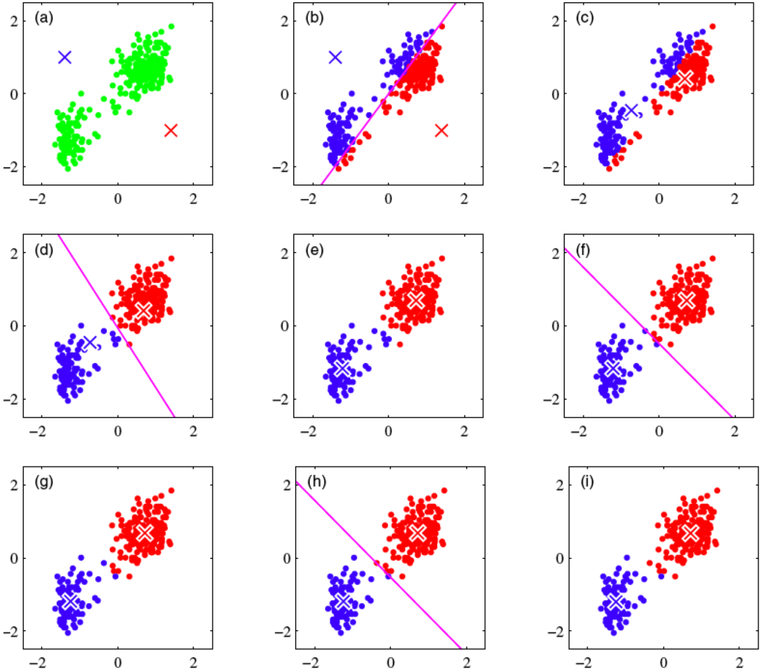


Figure from Bishop

Simple demo: http://syskall.com/kmeans.js/

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  - Refitting: Each center is set to mean of data assigned to it

    $$\mathbf{m}_k = \frac{\sum_n r_k^{(n)} \mathbf{x}^{(n)}}{\sum_n r_k^{(n)}}.$$

Why K-means Converges

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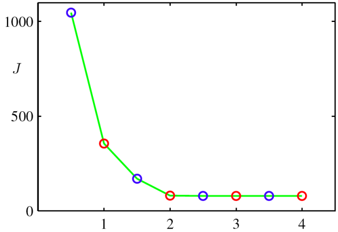
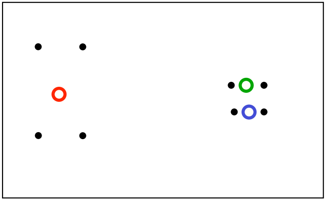


- Sum of squared distances after each assignment step (blue) and refitting step (red). The algorithm converged after the third step.

Local Minima

- This is a non-convex algorithm so it is not guaranteed to converge to the global minimum
- There is nothing to prevent k-means getting stuck at local minima.
- We could try many random starting points

A bad local optimum



K-means for Vector Quantization

Figure from Bishop

- Given image, construct "dataset" of pixels represented by their RGB pixel intensities
- Run k-means, replace each pixel by its cluster center

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  - Allows a cluster to use more information about the data in the refitting step.
  - How do we decide on the soft assignments?
  - We already saw this in multi-class classification:
    - 1-of-K encoding vs softmax assignments

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  - Assignment: Each data point n given soft "degree of assignment" to each cluster mean k, based on responsibilities

$$r_k^{(n)} = \frac{\exp[-\beta\|\mathbf{m}_k - \mathbf{x}^{(n)}\|^2]}{\sum_j \exp[-\beta\|\mathbf{m}_j - \mathbf{x}^{(n)}\|^2]}$$

$$\Longrightarrow \mathbf{r}^{(n)} = \mathrm{softmax}(-\beta\{\|\mathbf{m}_k - \mathbf{x}^{(n)}\|^2\}_{k=1}^{K})$$

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  - Refitting: Model parameters, means, are adjusted to match sample means of datapoints they are responsible for:

$$\mathbf{m}_k = \frac{\sum_n r_k^{(n)} \mathbf{x}^{(n)}}{\sum_n r_k^{(n)}}$$

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Some remaining issues

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These aren't straightforward to address with K-means. Instead, in the sequel, we'll reformulate clustering using a generative model.

As $\beta \to \infty$, soft k-Means becomes k-Means! (Exercise)

Questions about K-means

- Why does update set $\mathbf{m}_k$ to mean of assigned points?
- What if we used a different distance measure?
- How can we choose the best distance?
- How to choose K?
- Will it converge?

Hard cases – unequal spreads, non-circular spreads, in-between points

A Generative View of Clustering

- Next: probabilistic formulation of clustering
- We need a sensible measure of what it means to cluster the data well
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- We need a sensible measure of what it means to cluster the data well
  - This makes it possible to judge different methods
  - It may help us decide on the number of clusters
- An obvious approach is to imagine that the data was produced by a generative model
  - Then we adjust the model parameters according to a maximum likelihood criteria.

The Generative Model

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- Can also be written:

$$p(z = k) = \pi_k$$

$$p(\mathbf{x}|z = k) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \mathbf{I})$$

Clusters from Generative Model

- This defines joint distribution $p(z, \mathbf{x}) = p(z)p(\mathbf{x}|z)$ with parameters $\{\pi_k, \boldsymbol{\mu}_k\}_{k=1}^{K}$

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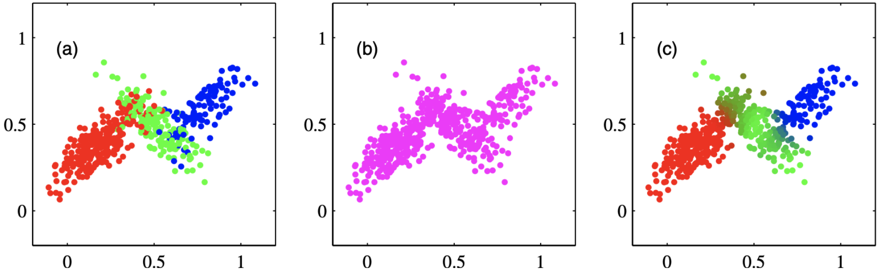
- $p(z = k|\mathbf{x})$ can be computed using Bayes rule

$$p(z = k|\mathbf{x}) = \frac{p(\mathbf{x} \,|\, z = k)p(z = k)}{p(\mathbf{x})}$$

and tells us the probability $\mathbf{x}$ came from the k^{th} cluster

The Generative Model

- 500 points drawn from a mixture of 3 Gaussians.



a) Samples from $p(\mathbf{x} \mid z)$ b) Samples from the marginal $p(\mathbf{x})$ c) Responsibilities $p(z \mid \mathbf{x})$

Maximum Likelihood with Latent Variables

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- As usual, define a cost, minimize it over parameters
- We don't observe the cluster assignments z, we only see the data $\mathbf{x}$

Gaussian Mixture Model (GMM)

What is $p(\mathbf{x})$?

$$p(\mathbf{x}) = \sum_{k=1}^{K} p(z=k)p(\mathbf{x}|z=k) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \mathbf{I})$$

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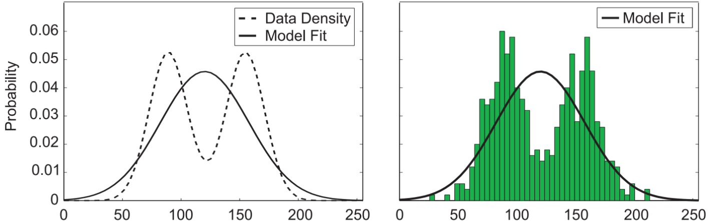
- In general, we would have different covariance for each cluster, i.e., $p(\mathbf{x}\,|\,z=k) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$. For this lecture, we assume $\boldsymbol{\Sigma}_k = \mathbf{I}$ for simplicity.
- If we allow arbitrary covariance matrices, GMMs are **universal approximators of densities** (if you have enough Gaussians). Even diagonal GMMs are universal approximators.

Visualizing a Mixture of Gaussians – 1D Gaussians

- If you fit a Gaussian to data:



[Slide credit: K. Kutulakos]

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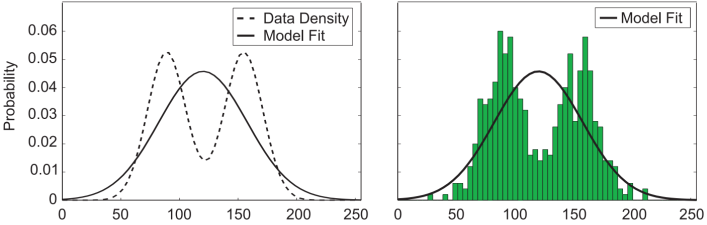
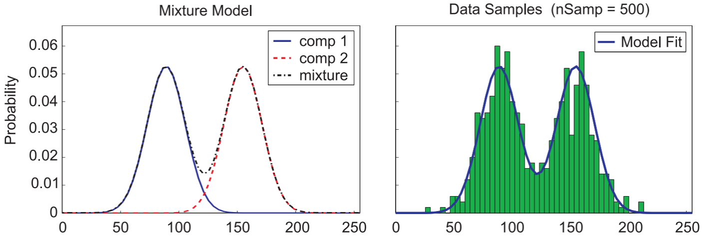


- Now, we are trying to fit a GMM (with $K = 2$ in this example):



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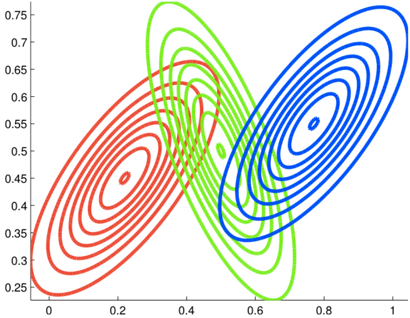
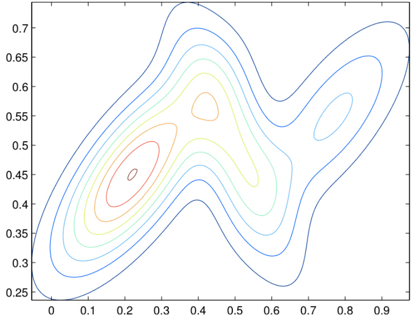
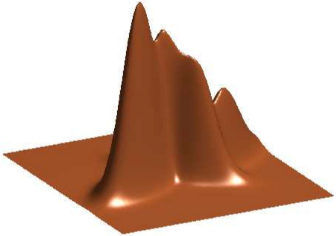
Visualizing a Mixture of Gaussians – 2D Gaussians







Fitting GMMs

Fitting a GMM is equivalent to minimizing the cost:

$$-\log p(\mathcal{D}) = -\sum_{n=1}^{N} \log p(\mathbf{x}^{(n)}) = -\sum_{n=1}^{N} \log \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}^{(n)} | \boldsymbol{\mu}_k, \mathbf{I}) \right)$$

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- Can we have a closed form update?

Maximum Likelihood

- We will alternate as in the previous part.
- If we observed the cluster assignments $z^{(n)}$'s:
- By minimizing $-\log p(\mathcal{D}_{\text{complete}})$, we would get this:

$$\hat{\boldsymbol{\mu}}_k = \frac{\sum_{n=1}^{N} \mathbb{I}[z^{(n)} = k]\, \mathbf{x}^{(n)}}{\sum_{n=1}^{N} \mathbb{I}[z^{(n)} = k]} = \text{class means}$$

$$\hat{\pi}_k = \frac{1}{N} \sum_{n=1}^{N} \mathbb{I}[z^{(n)} = k] = \text{class proportions}$$

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- We haven't observed the cluster assignments $z^{(n)}$, but we can compute their expectations!
- Conditional expectation (using Bayes rule) of z given $\mathbf{x}$

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$$\begin{aligned}\mathbb{E}[\mathbb{I}[z^{(n)} = k]|\mathbf{x}] &= ... \\ &= .. \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \mathbf{I})}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \mathbf{I})}\end{aligned}$$

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- This is still easy to optimize! Solution is similar to what we have seen:

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- Note: this only works if we treat $r_k^{(n)} = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\boldsymbol{\mu}_k, \mathbf{I})}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}^{(n)}|\boldsymbol{\mu}_j, \mathbf{I})}$ as fixed.

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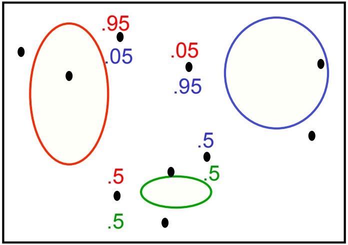

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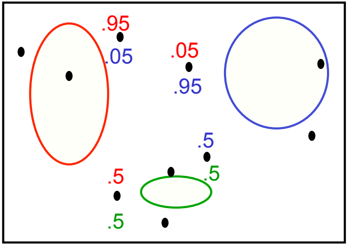

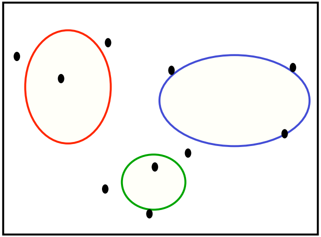

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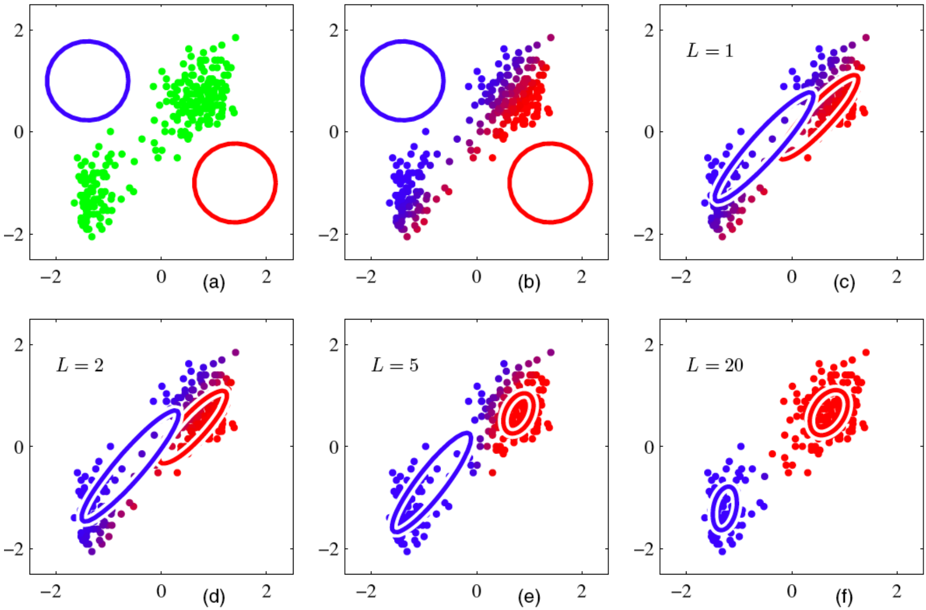
  - M-step: Re-estimate the parameters given current responsibilities

$$\begin{aligned}
\hat{\boldsymbol{\mu}}_k &= \frac{1}{N_k} \sum_{n=1}^N r_k^{(n)} \mathbf{x}^{(n)} \\
\hat{\pi}_k &= \frac{N_k}{N} \quad \text{with} \quad N_k = \sum_{n=1}^N r_k^{(n)}
\end{aligned}$$



2
0
−2
−2
0
(a)
2
(b)
L = 1
(c)
L = 2
(d)
L = 5
(e)
L = 20
(f)

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- We don't know $z^{(n)}$'s (they are latent), so we replaced $\mathbb{I}[z^{(n)} = k]$ with responsibilities $r_k^{(n)} = p(z^{(n)} = k | \mathbf{x}^{(n)})$.
- That is: we replaced $\mathbb{I}[z^{(n)} = k]$ with its expectation under $p(z^{(n)} | \mathbf{x}^{(n)})$ (E-step).

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- We ended up with the expected GMM cost which we maximized over parameters $\{\pi_k, \boldsymbol{\mu}_k\}_k$ (M-step)
- The EM algorithm alternates between:
  - The E-step: computing the $r_k^{(n)} = p(z^{(n)} = k|\mathbf{x}^{(n)})$ (i.e. expectations $\mathbb{E}[\mathbb{I}[z^{(n)} = k]|\mathbf{x}^{(n)}]$) given the current model parameters $\pi_k, \boldsymbol{\mu}_k$
  - The M-step: update the model parameters $\pi_k, \boldsymbol{\mu}_k$ to optimize the expected complete data log-likelihood

Relation to k-Means

- The K-Means Algorithm:
  1. Assignment step: Assign each data point to the closest cluster
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- The K-Means Algorithm:
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- The EM Algorithm:
  1. E-step: Compute the posterior probability over z given our current model
  2. M-step: Maximize the probability that it would generate the data it is currently responsible for.
- Can you find the similarities between the soft k-Means algorithm and EM algorithm with shared covariance $\frac{1}{\beta}\mathbf{I}$?
- Both rely on alternating optimization methods and can suffer from bad local optima.

Further Discussion

- We assumed the covariance of each Gaussian was I to simplify the math. This assumption can be removed, allowing clusters to have different spatial extents. The resulting algorithm is still very simple.

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- We assumed the covariance of each Gaussian was I to simplify the math. This assumption can be removed, allowing clusters to have different spatial extents. The resulting algorithm is still very simple.
- Problem with the previous minimization:
  - Non-convex
- EM is more general than what was covered in this lecture. Here, EM algorithm is used to find the optimal parameters under the GMMs.

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- A probabilistic view of clustering - Each cluster corresponds to a different Gaussian.

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- A probabilistic view of clustering - Each cluster corresponds to a different Gaussian.
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- General approach, can replace Gaussian with other distributions (continuous or discrete)
- More generally, mixture models are very powerful models, i.e. universal distribution approximators
- Optimization is done using the EM algorithm.

Conclusion

- We covered two clustering algorithms.
  - k-Means algorithm.
  - EM-algorithm.
- Tomorrow, we will conclude the course with a brief lecture on Fairness in ML.