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Machine learning – Block 6

Måns Magnusson
Department of Statistics, Uppsala University

Autumn 2023

- Practicalities
- Introduction to unsupervised learning
 - Latent variables
- Clustering
 - k-means
- Mixture models
- Expectation Maximization
- probabilistic PCA



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This week's lectures

- Practicalities
 - Introduction to unsupervised learning
 - Latent variables
 - Clustering
 - k-means
 - Mixture models
 - Expectation Maximization
 - probabilistic PCA
- Introduction to unsupervised learning
 - k-means
 - Mixture of Gaussians
 - Expectation-Maximization
 - Probabilistic PCA



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Practicalities

- **Practicalities**
- Introduction to unsupervised learning
 - Latent variables
- Clustering
 - k-means
- Mixture models
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- probabilistic PCA

- Some rearranging of lectures next week.



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Assignment 5

- **Practicalities**

- Introduction to unsupervised learning

- Latent variables

- Clustering

- k-means

- Mixture models

- Expectation Maximization

- probabilistic PCA

- ...



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Section 2

Introduction to unsupervised learning



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Supervised and Unsupervised learning

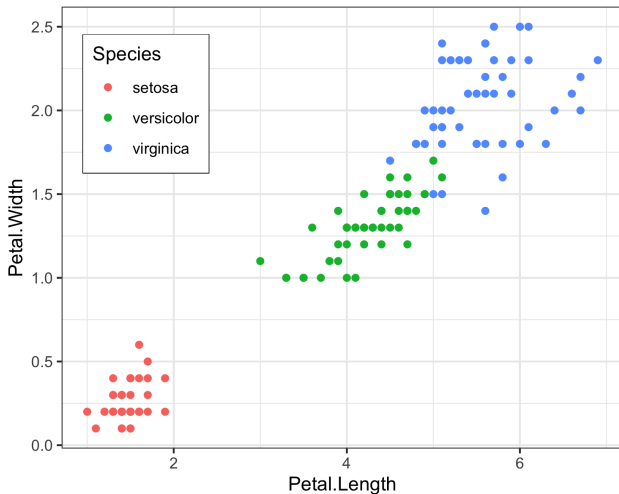


Figure: The Supervised Problem



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Supervised and Unsupervised learning

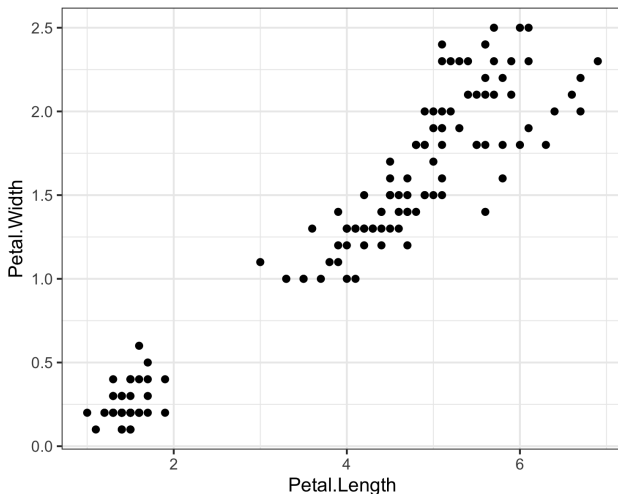


Figure: The Unsupervised Problem



In **supervised** learning:

- We have *training* data

$$\mathbf{d} = \{(y_i, \mathbf{x}_i), i = 1, \dots, n\}.$$

- We train a model $p(y|x)$ to **predict** y
- We only care about the loss function during training

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Supervised and Unsupervised learning

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- We only care about the loss function during training

In **unsupervised** learning:

- We have *training* data

$$\mathbf{d} = \{(\mathbf{x}_i), i = 1, \dots, n\}.$$

- We train a model $p(x)$ to **explain/model** x
- Our loss function (or model) can be the goal



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Unsupervised learning

Goal: Build a good (probabilistic) model $p(x)$ for x

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Unsupervised learning

Goal: Build a good (probabilistic) model $p(x)$ for x

Other names for $p(x)$:

- **Data** model
 $p(x)$ is our *data* generating mechanism
- **Generative** model
We can *generate* samples from $p(x)$.

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Unsupervised learning

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 $p(x)$ is our *data* generating mechanism
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We can *generate* samples from $p(x)$.

Common use cases for unsupervised learning:

- Generate new observations from $p(x)$
- Study structure in large data
- Anomaly detection
- Create representations for downstream tasks

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The Learning Problem

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- **Goal:** A model that can "explain" the data well
 - Two main approaches:
 - **Clustering:** Finding similar **observations** (rows)
 - **Dimensionality reduction:** Finding similar **variables** (columns)



The Learning Problem

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- **Goal:** A model that can "explain" the data well
- Two main approaches:
 - **Clustering:** Finding similar **observations** (rows)
 - **Dimensionality reduction:** Finding similar **variables** (columns)
- Commonly, we use parametric probabilistic models $p(x|\theta)$ where θ is unknown
- **Learning problem:** Learn θ to explain the data as good as possible



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Example: Autoencoder

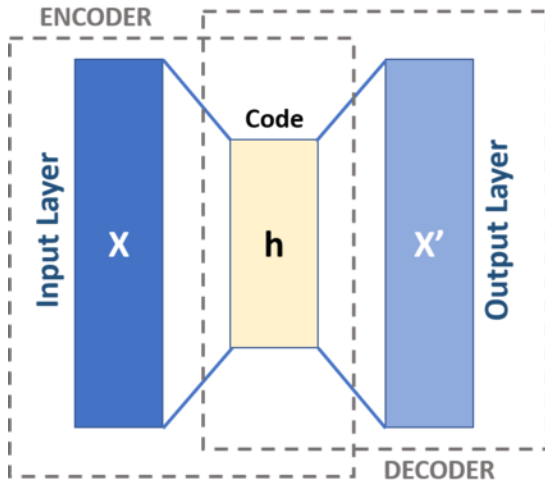


Figure: A Neural Autoencoder (Wikipedia)



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- Autoencoder uses the difference between the original and reconstructed output

$$L(x) = (d(e(h|x)|h) - x)^2,$$

where $d(x|h)$ is the decoder and $e(h|x)$ is the encoder.



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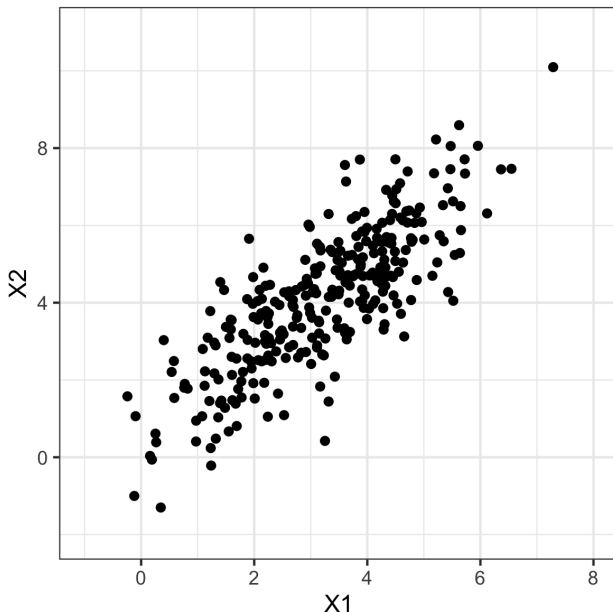
where $d(x|h)$ is the decoder and $e(h|x)$ is the encoder.

- In probabilistic models we can use the log-likelihood (\mathcal{L})
Sometimes called **perplexity** or **surprise**.
 - **High** \mathcal{L} : The observation is **well** explained by the model
 - **Low** \mathcal{L} : The observation is **badly** explained by the model
- Evaluate log-likelihood on a **held-out validation set**



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Example: Bivariate Gaussian model





Example: Bivariate Gaussian model

We assume a $p(x)$ is a Multivariate Gaussian model and estimate μ, Σ from data.

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Example: Bivariate Gaussian model

We assume a $p(x)$ is a Multivariate Gaussian model and estimate μ, Σ from data.

$$\hat{\mu} = [3.19, 4.11]$$

$$\hat{\Sigma} = \begin{bmatrix} 1.95 & 2.05 \\ 2.05 & 3.36 \end{bmatrix}$$

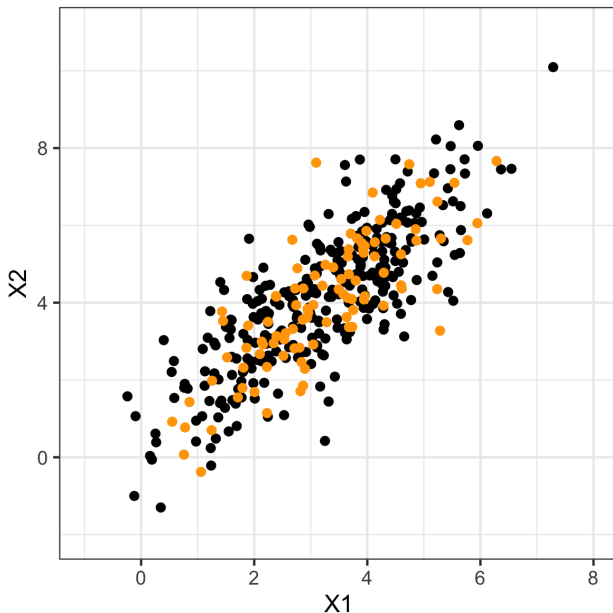
We can now **generate new data** from $\hat{p}(x)$ as $\text{MVN}(\hat{\mu}, \hat{\Sigma})$.

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Example: Bivariate Gaussian model





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Latent variables

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- An **unobserved** or **hidden** variable or "factor"



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- An **unobserved** or **hidden** variable or "factor"
- A parameter specific to some or a few observations or features



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- An **unobserved** or **hidden** variable or "factor"
- A parameter specific to some or a few observations or features
- Often these latent variables can be of **main interest**



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Example: Hidden Markov Model

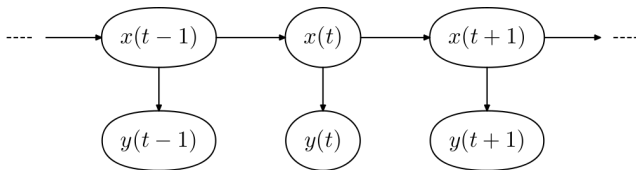


Figure: A Hidden Markov Model (Wikipedia).

Here: x is **unobserved/latent** and y is **observed**.



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Example: Factor Analysis

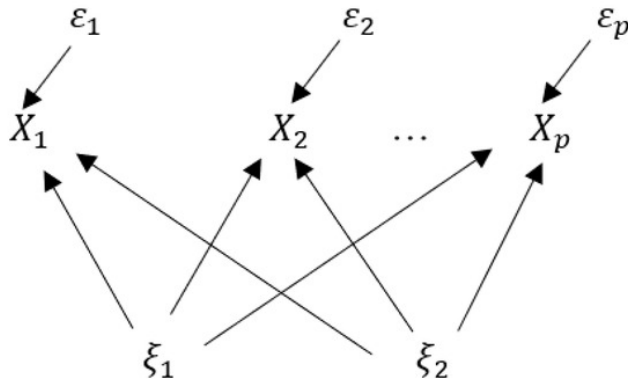


Figure: A Factor Analysis Model (Eshima, Tabata and Borroni, 2018, edited).



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Section 3

Clustering



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Clustering

- Separate observations x_i into **groups** or **segments**

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Clustering

- Separate observations x_i into **groups** or **segments**
- What is a cluster "is" depends on the **model/(dis)similarity**.
- (Dis)similarity:

$$D(x_i, x_j) = \sum_{k=1}^P d_k(x_{i,k}, x_{j,k})$$

- A common dissimilarity is the squared distance

$$d_k(x_{i,k}, x_{j,k}) = (x_{i,k} - x_{j,k})^2$$



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- Clustering can be divided into:
 - **Hard** clustering
 - **Soft** clustering



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- Clustering can also be divided into:
 - **Hierarchical** clustering
 - **Flat** clustering



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- Clustering can also be divided into:
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 - **Flat** clustering
- There is a ton of different algorithms and methods...



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k-means

- Popular in practice and a classic in unsupervised machine learning

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k-means

- Popular in practice and a classic in unsupervised machine learning
- Hard, flat clustering
- Simple and effective



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k-means

- Popular in practice and a classic in unsupervised machine learning
- Hard, flat clustering
- Simple and effective
- **Model:** x_i "is close to" one of m_1, \dots, m_K vectors
- **Loss function:**

$$L_{\mathbf{m}}(x) = \min_{\mathbf{m}} (x_i - m_k)^2$$



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- **Hyperparameter:** K (the number of clusters)
- **Parameters:** \mathbf{m} (a $K \times P$ matrix).



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- A **difficult** problem: K^n possibilities



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k-means algorithm

Algorithm 10.1 *K-Means Clustering*

1. Randomly assign a number, from 1 to K , to each of the observations. These serve as initial cluster assignments for the observations.
 2. Iterate until the cluster assignments stop changing:
 - (a) For each of the K clusters, compute the cluster *centroid*. The k th cluster centroid is the vector of the p feature means for the observations in the k th cluster.
 - (b) Assign each observation to the cluster whose centroid is closest (where *closest* is defined using Euclidean distance).
-

Figure: The k-means cluster algorithm (Garreth et al, 2013, Alg. 10.1).



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k-means clustering

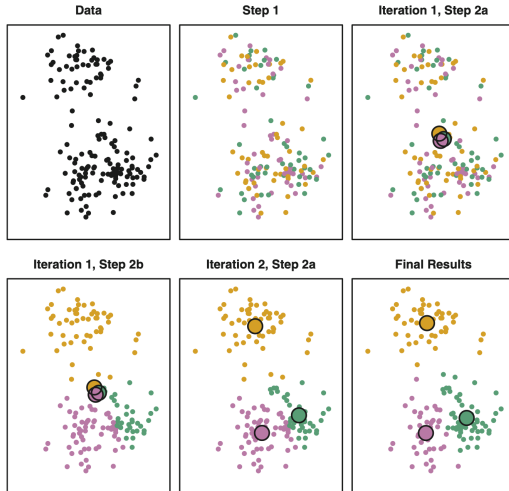


Figure: The k-means cluster algorithm (Garreth et al, 2013, Fig. 10.6).



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- k-means finds **local modes**
- Re-run algorithm with many **different starting values**
- Choose the best by the **best loss**



k-means clustering

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 - There exists many developments
 - scaling to large data



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 - approaches to find a good K



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k-means clustering



Figure: The k-means cluster algorithm (Garreth et al, 2013, Fig. 10.7).



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Problems with k-means

- Clusters might
 - overlap
 - have different forms

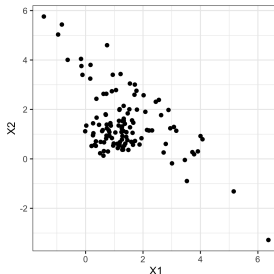


Figure: Two clusters with different shapes.



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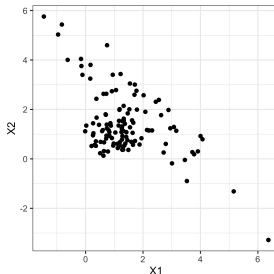


Figure: Two clusters with different shapes.

We can solve these problems using **probabilistic models**



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Section 4

Mixture models



The **finite mixture model** can be expressed as:

$$y_i = \sum_{k=1}^K \pi_k \phi_k(\theta_k),$$

- The parts of a (finite) mixture model:
 - The number of components: K

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 - The parameters of component k : θ_k

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- Usually, we
 - set K , and
 - use the same density for all k .



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- Usually, we
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- We can simulate data from the model as **compound probability distribution**:
 1. Simulate cluster assignments for all i :

$$z_i \sim \text{Categorical}(\pi)$$



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Finite Mixture Models

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 1. Simulate cluster assignments for all i :

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2. Generate y_i conditioned on z_i :

$$y_i \sim \phi_{z_i}(\theta_{z_i})$$



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Finite Mixture Models

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- Cluster assignments z_i are the **latent variables**



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- The (finite) Gaussian mixture model:

$$y_i = \sum_{k=1}^K \pi_k \mathcal{N}(\mu_k, \Sigma_k),$$

where μ_k and Σ_k depend on the dimensionality of y_i .



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where μ_k and Σ_k depend on the dimensionality of y_i .

- GMM is a **universal approximator** of densities



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Example: Simulate data from a GMM

1. Generate cluster assignments:

$$z_i \sim \text{Categorical}(\pi = [0.4, 0.6])$$

2. Generate observation conditioned on cluster assignment:

$$y_i \sim \mathcal{N}(\mu_k, \Sigma_k),$$

where

$$\mu_1 = [2, 2], \mu_2 = [1, 1] \text{ and}$$

$$\Sigma_1 = \begin{bmatrix} 3 & -2.7 \\ -2.7 & 3 \end{bmatrix}, \Sigma_2 = \begin{bmatrix} 0.2 & 0 \\ 0 & 0.2 \end{bmatrix}$$



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Simulated data from a GMM

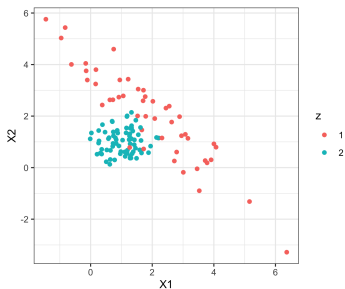


Figure: Simulated mixture data with the latent variable z .



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Simulated data from a GMM

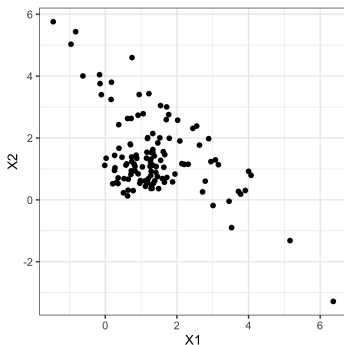


Figure: Simulated mixture data with the latent variable z .



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Mixtures of Multinomial distributions

What **distribution** (ϕ) should I use?

- Practicalities
- Introduction to unsupervised learning
 - Latent variables
- Clustering
 - k-means
- **Mixture models**
- Expectation Maximization
- probabilistic PCA



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Mixtures of Multinomial distributions

What **distribution** (ϕ) should I use?

Depends on your **data** (y).

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Mixtures of Multinomial distributions

What **distribution** (ϕ) should I use?

Depends on your **data** (y).

$$y_i = \sum_{k=1}^K \pi_k \text{Multinomial}(\mathbf{p}_k)$$

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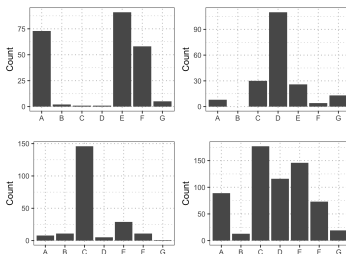


Figure: Mixture of Multinomials.



- We are interested in estimating θ_k and π_k for the model

$$y_i = \sum_{k=1}^K \pi_k \phi(\theta_k),$$

- If we add a cluster indicators z it is simpler...

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- We are interested in estimating θ_k and π_k for the model

$$y_i = \sum_{k=1}^K \pi_k \phi(\theta_k),$$

- If we add a cluster indicators \mathbf{z} it is simpler...
- Two approaches:
 - Gibbs sampler (Bayesian)

$$p(\mathbf{z}, \theta, \pi | \mathbf{y})$$



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Estimating Mixtures Models

- We are interested in estimating θ_k and π_k for the model

$$y_i = \sum_{k=1}^K \pi_k \phi(\theta_k),$$

- If we add a cluster indicators \mathbf{z} it is simpler...
- Two approaches:
 - Gibbs sampler (Bayesian)

$$p(\mathbf{z}, \theta, \pi | \mathbf{y})$$

- Expectation maximization (Frequentist)



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Estimating Mixtures Models

- Hence we want to maximize the log-likelihood

$$\mathcal{L}(\pi, \theta) = \sum_{i=1}^N \log \left(\sum_{k=1}^K \pi_k \phi(y_i | \theta_k) \right)$$

- This is difficult, although if we only knew \mathbf{z} ...



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Estimating Mixtures Models

- Hence we want to maximize the log-likelihood

$$\mathcal{L}(\pi, \theta) = \sum_{i=1}^N \log \left(\sum_{k=1}^K \pi_k \phi(y_i | \theta_k) \right)$$

- This is difficult, although **if we only knew \mathbf{z}** ...

$$\begin{aligned} \mathcal{L}_{\text{full}}(\pi, \theta, \mathbf{z}) &= \sum_{i=1}^N \log \left(\sum_{k=1}^K I(z_i = k) \phi(y_i | \theta_k) \right) + \\ &\quad \log(\pi_k^{I(z_i=k)}) \\ &= \sum_{i=1}^N \sum_{k=1}^K I(z_i = k) \log \phi(y_i | \theta_k) + \\ &\quad I(z_i = k) \log(\pi_k) \end{aligned}$$

- So if we knew \mathbf{z} it is essentially just maximizing \mathcal{L} for each cluster separately.



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The Expectation

- Practicalities
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Maximization**
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- But, we don't know z .



The Expectation

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- But, we don't know \mathbf{z} .
- Although, we could compute the **expected** cluster assignment

$$\gamma_i = E_{\mathbf{z}_i}(\mathcal{L}_{\text{full}} | \theta, y_i) .$$



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- Although, we could compute the **expected** cluster assignment

$$\gamma_i = E_{\mathbf{z}_i}(\mathcal{L}_{\text{full}} | \theta, y_i).$$

- γ_i can be seen as observation *is* **weights** for each cluster
- γ_i is sometimes referred to as the **responsibility**.



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The Maximization

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- Now, given γ we can (hopefully) easier maximize θ .



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The Maximization

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- Now, given γ we can (hopefully) easier maximize θ .
- We maximize $\mathcal{L}_{\text{full}}$ given γ and y .



The Maximization

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- Now, given γ we can (hopefully) easier maximize θ .
 - We maximize $\mathcal{L}_{\text{full}}$ given γ and y .
 - We usually choose ϕ (the density) so the maximization
 - is a nice analytical expression.
 - end up with a weighted MLE.



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Example: EM for a Gaussian Mixture

Algorithm 8.1 *EM Algorithm for Two-component Gaussian Mixture.*

1. Take initial guesses for the parameters $\hat{\mu}_1, \hat{\sigma}_1^2, \hat{\mu}_2, \hat{\sigma}_2^2, \hat{\pi}$ (see text).
2. *Expectation Step*: compute the responsibilities

$$\hat{\gamma}_i = \frac{\hat{\pi} \phi_{\hat{\theta}_2}(y_i)}{(1 - \hat{\pi}) \phi_{\hat{\theta}_1}(y_i) + \hat{\pi} \phi_{\hat{\theta}_2}(y_i)}, \quad i = 1, 2, \dots, N. \quad (8.42)$$

3. *Maximization Step*: compute the weighted means and variances:

$$\begin{aligned} \hat{\mu}_1 &= \frac{\sum_{i=1}^N (1 - \hat{\gamma}_i) y_i}{\sum_{i=1}^N (1 - \hat{\gamma}_i)}, & \hat{\sigma}_1^2 &= \frac{\sum_{i=1}^N (1 - \hat{\gamma}_i) (y_i - \hat{\mu}_1)^2}{\sum_{i=1}^N (1 - \hat{\gamma}_i)}, \\ \hat{\mu}_2 &= \frac{\sum_{i=1}^N \hat{\gamma}_i y_i}{\sum_{i=1}^N \hat{\gamma}_i}, & \hat{\sigma}_2^2 &= \frac{\sum_{i=1}^N \hat{\gamma}_i (y_i - \hat{\mu}_2)^2}{\sum_{i=1}^N \hat{\gamma}_i}, \end{aligned}$$

and the mixing probability $\hat{\pi} = \sum_{i=1}^N \hat{\gamma}_i / N$.

4. Iterate steps 2 and 3 until convergence.
-

Figure: The EM algorithm for a two component Gaussian mixture (Hastie et al 2008, Alg. 10.1)



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The EM algorithm

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- Expectation Maximization
- probabilistic PCA

- Properties of the EM algorithm:
 - The EM-algorithm will converge to a **local mode**



The EM algorithm

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- Properties of the EM algorithm:
 - The EM-algorithm will converge to a **local mode**
 - Each iteration will **always** increase the likelihood
 - Can be proven straight-forward using Jensens inequality



The EM algorithm

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- Properties of the EM algorithm:
 - The EM-algorithm will converge to a **local mode**
 - Each iteration will **always** increase the likelihood
 - Can be proven straight-forward using Jensens inequality
 - We can interpret the final γ_i as the **expected cluster**
Hence, the EM algorithm is a **soft clustering** approach.
- Expanding the likelihood with latent variables (z) is called **data augmentation**.
Note! Not the same as data augmentation in CNNs.



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Connections to other approaches

- Practicalities
- Introduction to unsupervised learning
 - Latent variables
- Clustering
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- Expectation Maximization
- probabilistic PCA

- If we set $z_i = \operatorname{argmax}(\gamma_i)$: **k-means**



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Connections to other approaches

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- If we set $z_i = \operatorname{argmax}(\gamma_i)$: **k-means**
- If we sample z_i according to γ : **stochastic EM**
- If we sample z_i conditional on θ : **Gibbs sampling**



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- Practicalities
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Section 6

probabilistic PCA



Dimensionality reduction

- Practicalities
- Introduction to unsupervised learning
 - Latent variables
- Clustering
 - k-means
- Mixture models
- Expectation Maximization
- probabilistic PCA

- So far focus has been on (clustering) **observations**
- Now, we will adress the other large area of UL:
dimensionality reduction



Dimensionality reduction

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- So far focus has been on (clustering) **observations**
- Now, we will adress the other large area of UL:
dimensionality reduction
- The starting point is **Principal Component Analysis (PCA)**
- PCA can be used for
 - **Reduce the dimensionality** of our data
 - **Produce lower-dimensional features** in a prediction model
 - **Discover underlying latent variables** (factors)



Dimensionality reduction

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- The starting point is **Principal Component Analysis (PCA)**
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 - **Produce lower-dimensional features** in a prediction model
 - **Discover underlying latent variables** (factors)
- More details in the **multivariate course**.



- Practicalities
- Introduction to unsupervised learning
 - Latent variables
- Clustering
 - k-means
- Mixture models
- Expectation Maximization
- probabilistic PCA

- **Basic idea:** We can summarize our data using K principal components (PC)
- The PCA "**model**" can be expressed as

$$X \approx b + WH^T,$$

where $H \in \mathbb{R}^{n \times k}$, $W \in \mathbb{R}^{k \times p}$, $b \in \mathbb{R}^p$ and $X \in \mathbb{R}^{n \times p}$.

- H can be seen as a **latent factors**



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- W can be seen as a **factor loadings**



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- H can be seen as a **latent factors**
- W can be seen as a **factor loadings**
- We assume that W is orthogonal: $W^T W = I$



- Practicalities
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- The PCA model

$$X \approx b + WH^T,$$

- The loss function, also called **reconstruction error**:

$$J(b, W, H) = \sum_i^N ||x_i - b + Wh_i^T||^2$$



- Practicalities
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- The PCA model

$$X \approx b + WH^T,$$

- The loss function, also called **reconstruction error**:

$$J(b, W, H) = \sum_i^N ||x_i - b + Wh_i^T||^2$$

- This can be minimized using **Singular Value Decomposition**



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PCA: Conceptual depiction

$$\begin{bmatrix} X \\ (n \times p) \end{bmatrix} \approx \begin{bmatrix} W \\ (p \times k) \end{bmatrix} \times \begin{bmatrix} H^T \\ (k \times n) \end{bmatrix}$$

Figure: Conceptual depiction of PCA.



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probabilistic PCA (pPCA)

- Practicalities
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- PCA is not a probabilistic model



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- PCA is not a probabilistic model
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$$x_i = b + Wh_i^T + \epsilon_i$$

where $\epsilon \sim N(\mathbf{0}, \Psi)$

- In pPCA, we assume $\Psi = \sigma^2 \mathbf{I}$
- We also assume that $h_i \sim N(0, I)$



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where $\epsilon \sim N(\mathbf{0}, \Psi)$

- In pPCA, we assume $\Psi = \sigma^2 \mathbf{I}$
- We also assume that $h_i \sim N(0, \mathbf{I})$
- We can integrate out H and get the model

$$x_i \sim N(b, WW^T + \Psi)$$



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probabilistic PCA

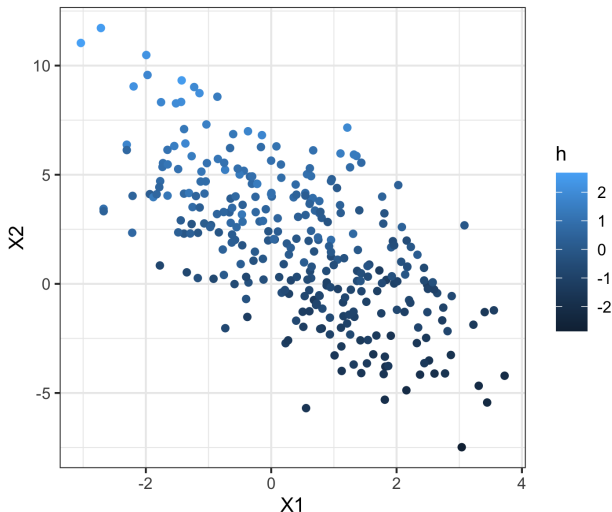


Figure: Data from a pPCA model with $W = (-1, 3)^T$, $b = (0.5, 2)$ and $\sigma^2 = 1$



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probabilistic PCA

- probabilistic PCA

$$x_i = b + Wh_i^T + \epsilon_i$$

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- probabilistic PCA

$$x_i = b + Wh_i^T + \epsilon_i$$

- We can now **estimate our parameters** using EM (or Bayesian methods)
- Enables us to **combine with other models** (e.g. mixture of pPCA)

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- **probabilistic PCA**



- probabilistic PCA

$$x_i = b + Wh_i^T + \epsilon_i$$

- We can now **estimate our parameters** using EM (or Bayesian methods)
- Enables us to **combine with other models** (e.g. mixture of pPCA)
- And as we will see next week, is the **basic building block** for many high-dimensional problems



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- probabilistic PCA

$$x_i = b + Wh_i^T + \epsilon_i$$

where $\epsilon \sim N(\mathbf{0}, \Psi)$

- pPCA is closely connected to PCA and Factor Analysis:
 - $\sigma_I \rightarrow 0$: pPCA \rightarrow PCA
 - $\Psi = \text{diag}(\sigma_1, \dots, \sigma_p, \dots, \sigma_P)$: pPCA \rightarrow Factor Analysis