# Unsupervised and Semi-Supervised learning

# Overview - Un/Semi/Fully Supervised learning

Assume we have data

$$\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_n]$$

.

The data can be

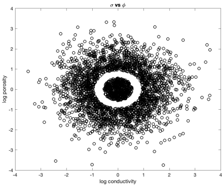
- Images
- Text
- Sound
- Set of numbers (climate, pressure ...)

We can think of (at least) 3 goals

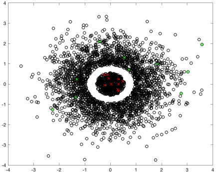
- Cluster the data (unsupervised)
- Give meaning to each cluster, label it (semisupervised)
- Find a functional relation between the cluster and its label (supervised)

# Overview - Un/Semi/Fully Supervised learning

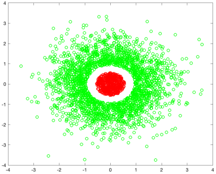
## Example - rock conductivity verses porosity data




Unsupervised



Semisupervised



Supervised

- How many types of rocks we have: **Unsupervised learning**
- What are their names (Granite, Basalt): **Semisupervised learning**
- Given $\sigma, \phi$ can we find a function $f(\sigma, \phi) = \text{rock type}$: **Supervised learning**

# Overview - Un/Semi/Fully Supervised learning

- Supervised learning requires a large labeled data set
- Gives an "explanation" (a model) between data and label
- Un/Semisupervised is more modest
- No model, just label
- Can be followed by supervised learning

# Overview - Un/Semi/Fully Supervised learning

- What kind of cars are in the picture
- What is their colour
- What is their size
- Which direction are they going

Types of learning

- Unsupervised learning may cluster cars in irrelevant manner
- Semi-supervised we label a few cars and ask the computer the label the rest
- In supervised learning someone labeled all the cars

# Overview - Un/Semi Supervised learning

In this module we focus on semisupervised learning and a bit on unsupervised learning.

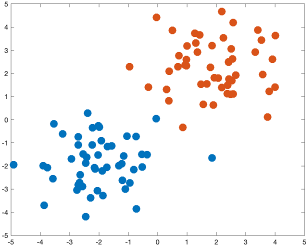
Main questions

- Given a data set cluster the data into a few groups
- Assuming that a few data are labeled, label the rest

# Un/Semisupervised learning: General principle

**Main assumption:**
Given the data set $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_n]$, if $\mathbf{y}_i$ is "close" to $\mathbf{y}_j$ then they belong to the same class.

What is close?



# Measuring closeness - metrics

The question is how to measure the closeness of two vectors in our space.
Assume a function $D(\mathbf{x}, \mathbf{y}) \to [0, \infty)$ with the following properties

- $D(\mathbf{x}, \mathbf{y}) \geq 0$
- $D(\mathbf{x}, \mathbf{y}) = 0 \quad \to \quad \mathbf{x} = \mathbf{y}$
- $D(\mathbf{x}, \mathbf{y}) = D(\mathbf{y}, \mathbf{x})$
- $D(\mathbf{x}, \mathbf{z}) \leq D(\mathbf{x}, \mathbf{y}) + D(\mathbf{y}, \mathbf{z})$

In many cases we will not keep all the above but will keep most of them

# Measuring closeness - metrics

Most obvious metric based on a norm

$$D(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_p = \left(\sum |\mathbf{x}_i - \mathbf{y}_i|^p\right)^{\frac{1}{p}}$$

- Most used is the 2-norm (why?)
- $p = \infty$ is called the max norm (why?)

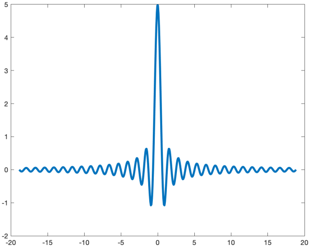
A simple modification weighted norms

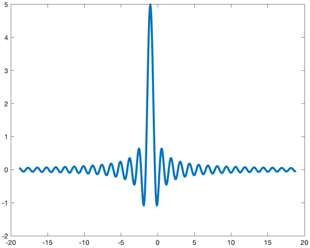
$$D(\mathbf{x}, \mathbf{y}) = \left(\sum \mathbf{w}_i |\mathbf{x}_i - \mathbf{y}_i|^p\right)^{\frac{1}{p}}$$

where $\mathbf{w} > 0$ is a vector of positive weights.
Allow us to focus on some parts of the vectors and scale it if needed

# Measuring closeness - metrics

Are these signals similar?




Measure is very sensitive to translation

# Measuring closeness - metrics

Which of these images are closer

# Measuring closeness - metrics

Many different definitions of distance based on the application

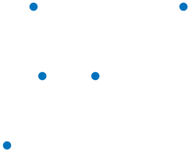
- Normed distance
- Hamming distance - for strings
- Wasserstein metric - for probabilities (also applied to images)
- Riemannian metrics - for data that "lives" on manifolds

Choosing the right distance is the key for the application
In many cases - chicken and egg. If we know the right distance then we know how to cluster.

We will use $L_2$ distance for conveniency.

# Using metrics - graphical models

A graph is



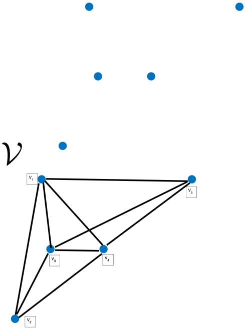
A vertex set $\mathcal{V}$

# Using metrics - graphical models

A graph is

A vertex set $\mathcal{V}$

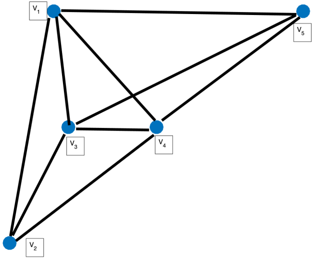
Edge set $\mathcal{E}$



# The adjacency matrix

The adjacency matrix is defined as

$$\mathbf{A}_{ij} = \begin{cases} 1 & \text{if there is an edge} \\ 0 & \text{otherwise} \\ 0 & \text{if } i = j \end{cases}$$

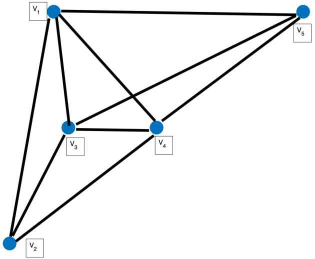



$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{pmatrix}$$

# The graph Laplacian

The degree matrix

$$\mathbf{D} = \mathrm{diag}\left(\sum_j \mathbf{A}ij\right)$$




$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

# The graph Laplacian

The graph Laplacian

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

$$\mathbf{L} = \begin{pmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 & 0 \\ -1 & -1 & 4 & -1 & -1 \\ -1 & -1 & -1 & 4 & -1 \\ -1 & 0 & -1 & -1 & 3 \end{pmatrix}$$

Note

$$(\mathbf{Lv})_i = \sum_{i \neq j} \mathbf{v}_i - \mathbf{v}_j \quad \text{and} \quad \mathbf{v}^\top \mathbf{L} \mathbf{v} = \sum_{e_{ij}} (\mathbf{v}_i - \mathbf{v}_j)^2$$

# The weighted graph Laplacian

In the Laplacian above every neighbour gets the same weight. Define the weighted Laplacian, where each edge $e_{ij}$ is associated with a weight $0 \leq w_{ij}$.

$$(\mathbf{L}\mathbf{v})_i = \sum_{i \neq j} \mathbf{w}_{ij}(\mathbf{v}_i - \mathbf{v}_j) \quad \text{and} \quad \mathbf{v}^\top \mathbf{L}\mathbf{v} = \sum_{e_{ij}} \mathbf{w}_{ij}(\mathbf{v}_i - \mathbf{v}_j)^2$$

Typical choice for $\mathbf{w}$ is

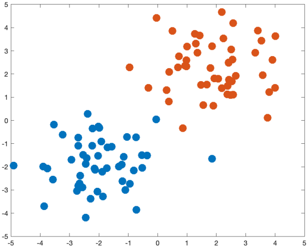
$$\mathbf{w}_{ij} = \exp\left(-\frac{\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sigma}\right)$$

More appropriate choice

$$\mathbf{w}_{ij} = \exp\left(-\frac{D(\mathbf{v}_i, \mathbf{v}_j)}{\sigma}\right)$$

# The eigenvalues and eigenvectors of the Laplacian

The smallest eigenvalue is always 0 with eigenvector $\mathbf{v} = [1, \dots, 1]^\top$ (why)
The second to smallest eigenvalue that is not zero is the Fiedler eigenvalue.




It gets the (approximate) value 1 on the first group and $-1$ (approximately) on the second group.

# The eigenvalues and eigenvectors of the Laplacian

The second eigenvalue is the solution to the optimization problem

$$\begin{array}{ll} \min\limits_{\mathbf{u} \neq \gamma \mathbf{e}} & \frac{1}{2}\mathbf{u}^\top \mathbf{L} \mathbf{u} \\ \text{subject to} & \|\mathbf{u}\| = 1 \end{array}$$

**Interpretation**

Try to find the non-constant vector with the minimal energy
The solution should be "smooth" on the graph

# The eigenvalues and eigenvectors of the Laplacian

The second eigenvalue is the solution to the optimization problem

$$\begin{array}{ll} \min\limits_{\mathbf{u} \neq \gamma \mathbf{e}} & \frac{1}{2}\mathbf{u}^\top \mathbf{L} \mathbf{u} \\ \text{subject to} & \|\mathbf{u}\| = 1 \end{array}$$

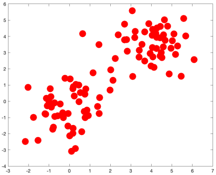
- For small problems use eig solver of a dense matrix
- For large problem use iterative methods - inverse iteration, Krylov methods, randomized linear algebra

Power method

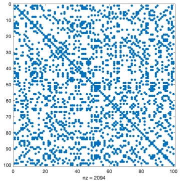
$$\mathbf{v}_k = \mathbf{L}^{-\dagger}\mathbf{u}_k \qquad \mathbf{u}_{k+1} = \frac{\mathbf{v}_k}{\|\mathbf{v}_k\|}$$

# The eigenvalues and eigenvectors of the Laplacian

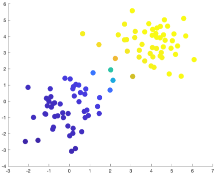
Example




Data




Graph Laplacian

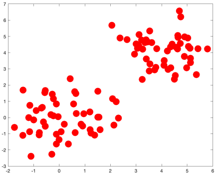



Fidler Vector

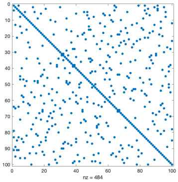
# The eigenvalues and eigenvectors of the Laplacian

Can be very sensitive to parameters

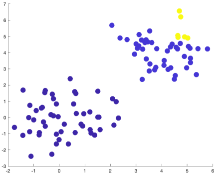
- Number of neiboghrs
- Choice of $\sigma$
- Distance measure



Data




Graph Laplacian



Fidler Vector

# From unsupervised to semisupervised learning

- In most cases it is possible to obtain a few labeled data
- Goal is to label the whole data given the labeled data
- Typically, results are much better and more robust than unsupervised learning

Assumption: we are given a set $\mathcal{S}$ where $\mathbf{p}_{\mathcal{S}}^{\mathrm{obs}}$ is the probability of each datum to belong to each class

# From unsupervised to semisupervised learning

**Incorporating probabilities - the softmax function**

- $\mathbf{p}^{\mathrm{obs}}$ is a probability, $0 \leq \mathbf{p}_i^{\mathrm{obs}} \leq 1$ and $\sum \mathbf{p}^{\mathrm{obs}} = 1$.
- $\mathbf{u}$ is unbounded
- Define $\mathbf{p}(\mathbf{u}) = \frac{\exp(\mathbf{u})}{\sum \exp(\mathbf{u})}$
- Use cross entropy to compare probabilities, $\mathbf{p}(\mathbf{u})$ and $\mathbf{p}^{\mathrm{obs}}$

$$\ell oss(\mathbf{u}, \mathbf{p}^{\mathrm{obs}}) = -\frac{1}{n}\mathbf{p}_{\mathrm{obs}}^{\top} \log(\mathbf{p}(\mathbf{u}))$$

# From unsupervised to semisupervised learning

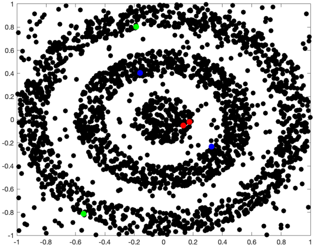
**New goal** - Fit the given labels **and** keep the vector smooth.

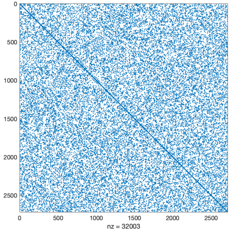
$$\min_{\mathbf{u}} \ \mathcal{E}(\mathbf{u}) = \ell oss(\mathbf{u}, \mathbf{p}^{\mathrm{obs}}) + \frac{\alpha}{2}\mathbf{u}^\top \mathbf{L}\mathbf{u}$$

- $\alpha$ tradeoff parameter
- Can be estimated using cross validation
- Solution using inexact Newton's method

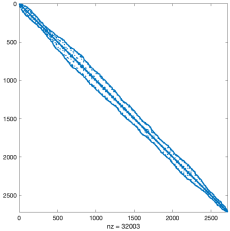
# From unsupervised to semisupervised learning

## Example - classifying nonlinear data



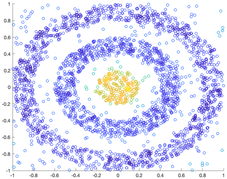



Graph Lap

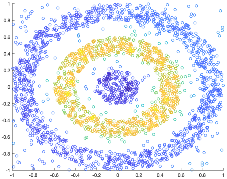



Reordered Graph Lap

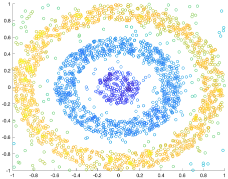
# From unsupervised to semisupervised learning



Class 1



Class 2



Class 3

# Semisupervised learning - challenges

- Choice of distance function
- Choice of hyper parameters
- Naive complexity $n^2$
- Sparse linear algebra, preconditioning, eigenvalue solvers