Unsupervised and Semi-Supervised learning

Overview - Un/Semi/Fully Supervised learning

Assume we have data

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

.

The data can be

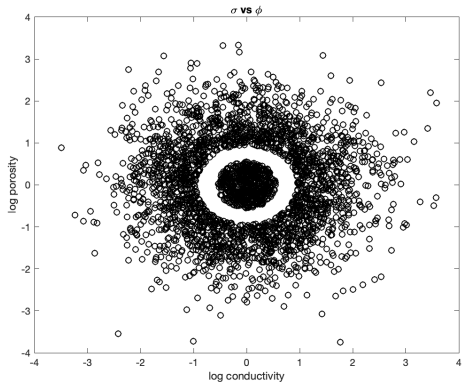
- Images
- Text
- Sound
- Set of numbers (climate, pressure ...)

We can think of (at least) 3 goals

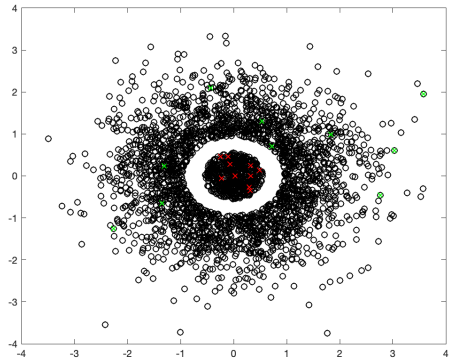
- Cluster the data (unsupervised)
- Give meaning to each cluster, label it (semisupervised)
- Find a functional relation between the cluster and its label (supervised)

Overview - Un/Semi/Fully Supervised learning

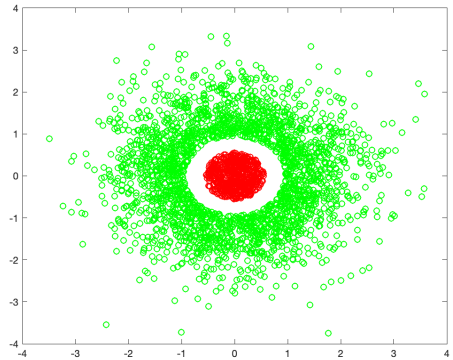
Example - rock conductivity verses porosity data



Unsupervised



Semisupervised



Supervised

- How many types of rocks we have: **Unsupervised learning**
- What are their names (Granite, Basalt): **Semisupervised learning**
- Given σ, ϕ 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

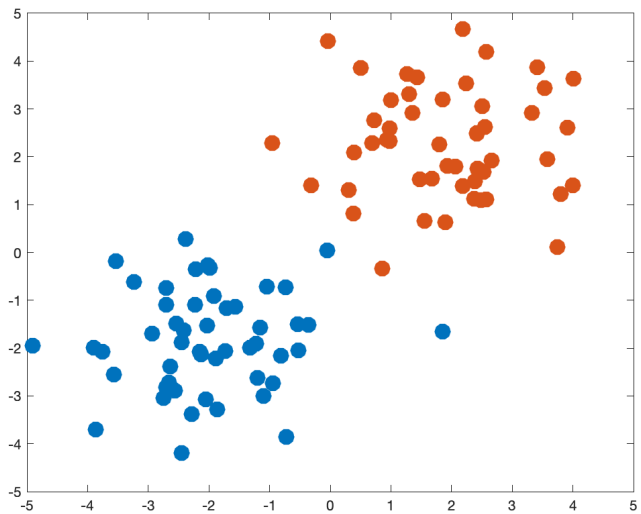
In this module we focus on semisupervised learning and a bit on unsupervised learning.
Main questions

- 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 $D(\mathbf{x}, \mathbf{y}) \rightarrow [0, \infty)$ with the following properties

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

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?)

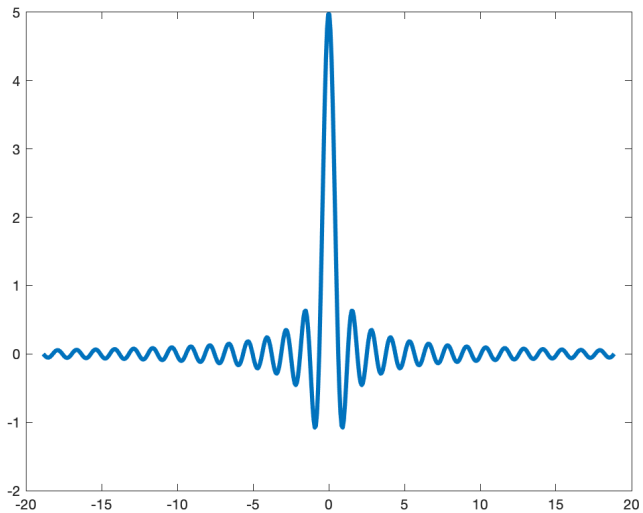
A simple modification weighted norms

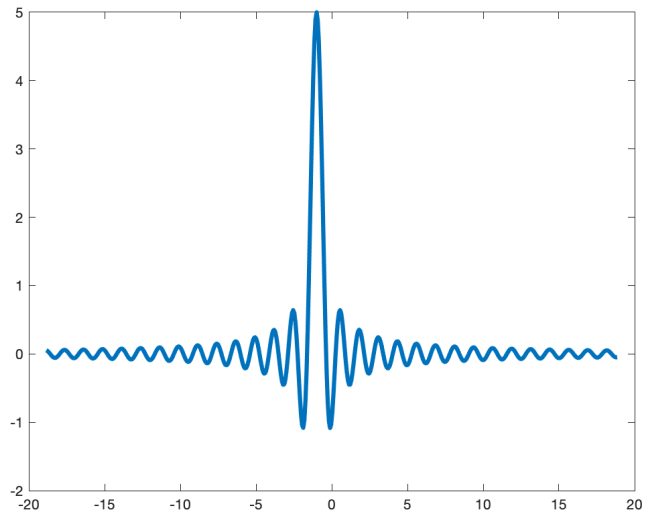
$$D(\mathbf{x}, \mathbf{y}) = \left(\sum \mathbf{w}_i |\mathbf{x}_i - \mathbf{y}_i|^p \right)^{\frac{1}{p}}$$

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

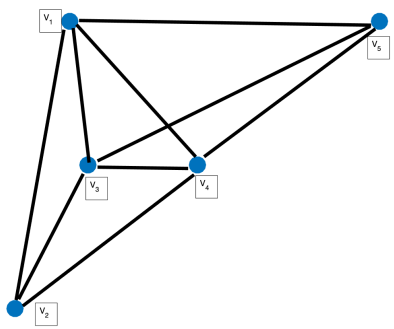
A vertex set $\mathcal{V}$

Using metrics - graphical models

A graph is

A vertex set $\mathcal{V}$

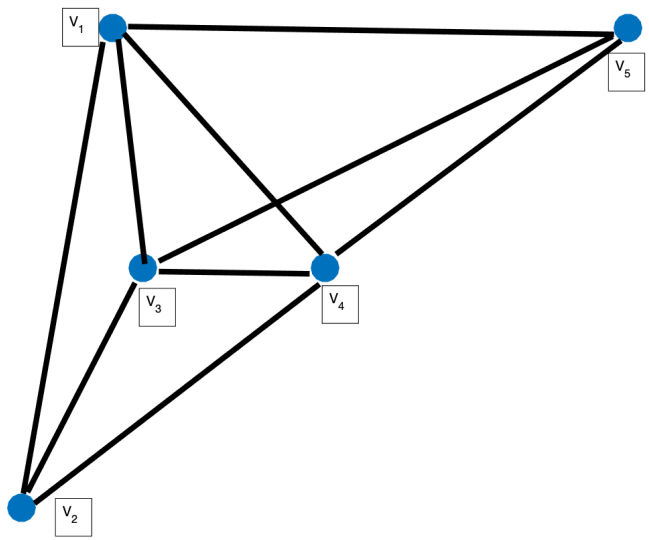
Edge set $\mathcal{E}$



The adjacency matrix

The adjacency matrix is defined as

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

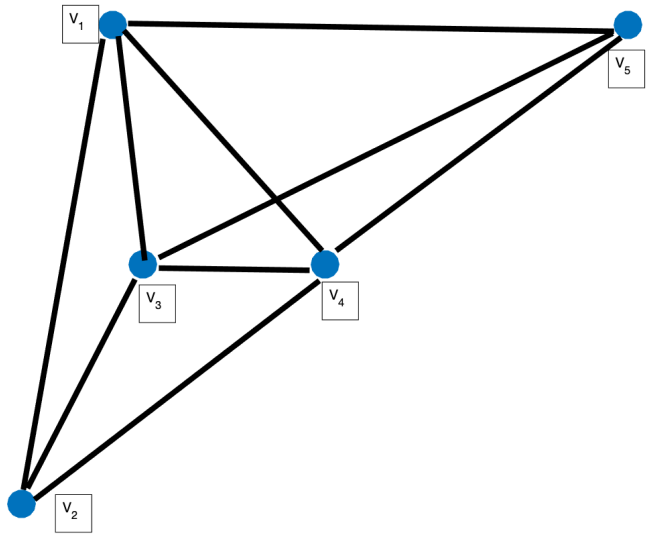


$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \end{pmatrix}$$

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

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

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 $0 \leq w_{ij}$.

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

Typical choice for $\mathbf{w}$ is

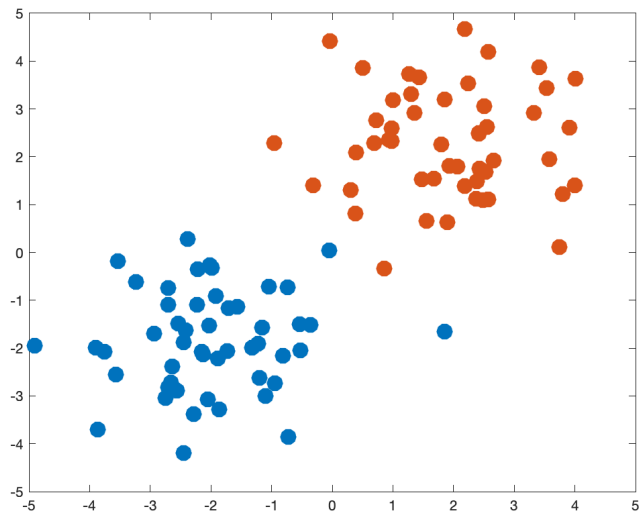
$$\mathbf{w}_{ij} = \exp\left(-\frac{\|\mathbf{v}_i - \mathbf{v}_j\|^2}{\sigma}\right)$$

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 $\mathbf{v} = [1, \ldots, 1]^\top$ (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

$$\begin{aligned} \min_{\mathbf{u} \neq \gamma \mathbf{e}} \quad & \frac{1}{2} \mathbf{u}^\top \mathbf{L} \mathbf{u} \\ \text{subject to} \quad & \|\mathbf{u}\| = 1 \end{aligned}$$

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

$$\begin{aligned} \min_{\mathbf{u} \neq \gamma \mathbf{e}} \quad & \frac{1}{2} \mathbf{u}^\top \mathbf{L} \mathbf{u} \\ \text{subject to} \quad & \|\mathbf{u}\| = 1 \end{aligned}$$

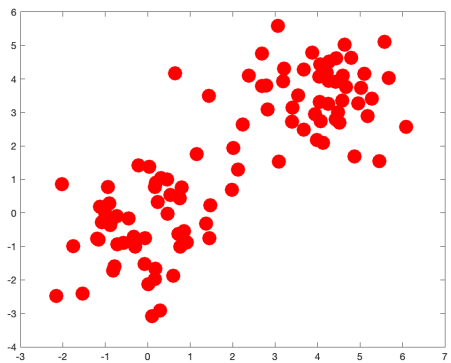
- For small problems use eig solver of a dense matrix
- For large problem use iterative methods - inverse iteration, Krylov methods, randomized linear algebra

Power method

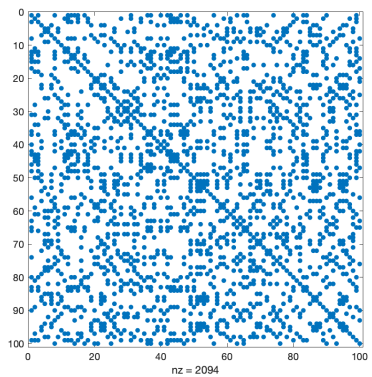
$$\mathbf{v}_k = \mathbf{L}^{-\dagger} \mathbf{u}_k \qquad \mathbf{u}_{k+1} = \frac{\mathbf{v}_k}{\|\mathbf{v}_k\|}$$

The eigenvalues and eigenvectors of the Laplacian

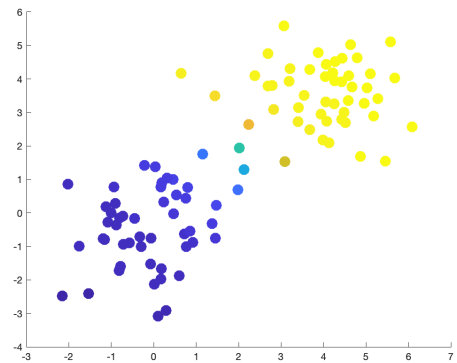
Example



Data



Graph Laplacian

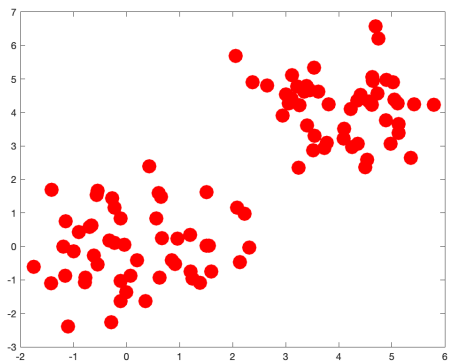


Fidler Vector

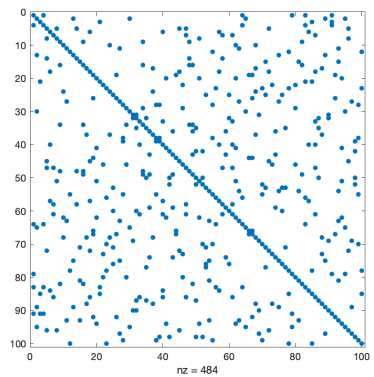
The eigenvalues and eigenvectors of the Laplacian

Can be very sensitive to parameters

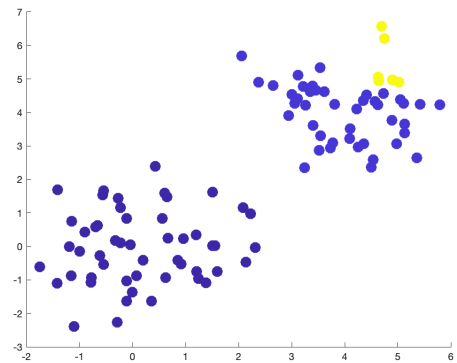
- Number of neiboghrs
- Choice of σ
- Distance measure



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 $\mathbf{p}_{\mathcal{S}}^{\text{obs}}$ is the probability of each datum to belong to each class

From unsupervised to semisupervised learning

Incorporating probabilities - the softmax function

- $\mathbf{p}^{\text{obs}}$ is a probability, $0 \leq \mathbf{p}_i^{\text{obs}} \leq 1$ and $\sum \mathbf{p}^{\text{obs}} = 1$.
- $\mathbf{u}$ 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 $\mathbf{p}^{\text{obs}}$

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

From unsupervised to semisupervised learning

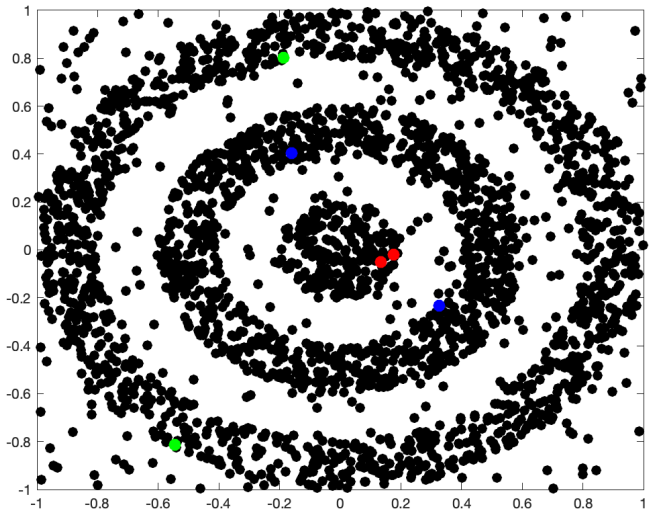
New goal - Fit the given labels **and** keep the vector smooth.

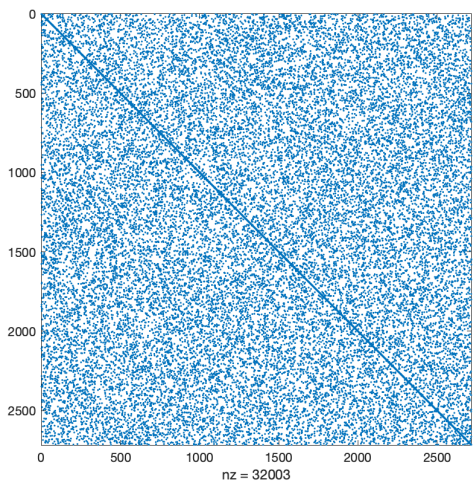
$$\min_{\mathbf{u}} \ \mathcal{E}(\mathbf{u}) = \ell oss(\mathbf{u}, \mathbf{p}^{\text{obs}}) + \frac{\alpha}{2}\mathbf{u}^\top \mathbf{L}\mathbf{u}$$

- α tradeoff parameter
- Can be estimated using cross validation
- Solution using inexact Newton's method

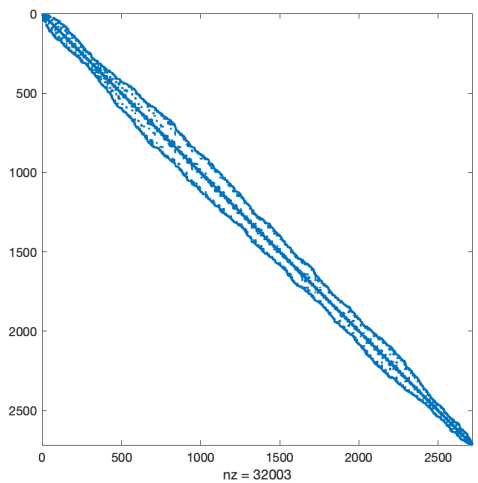
From unsupervised to semisupervised learning

Example - classifying nonlinear data



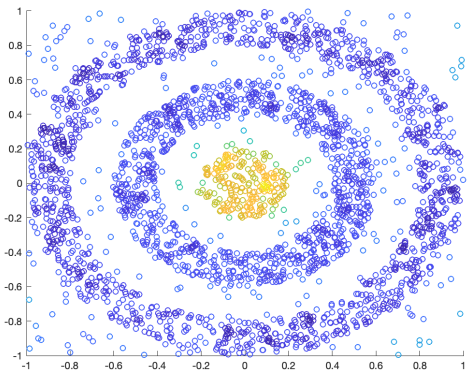


Graph Lap

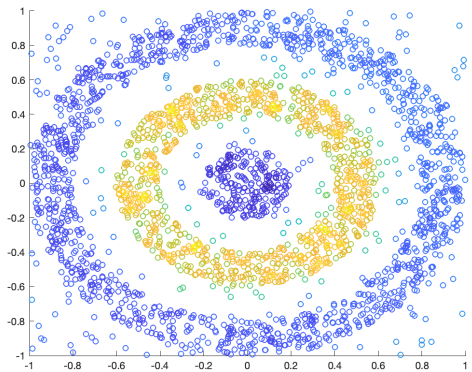


Reordered Graph Lap

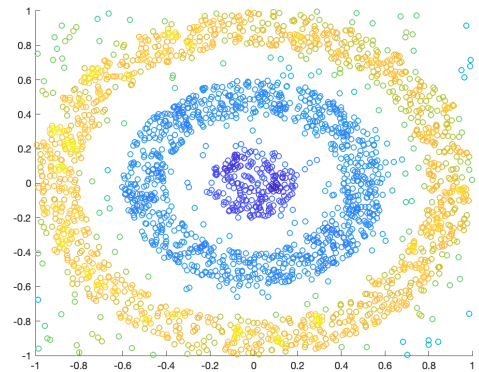
From unsupervised to semisupervised learning



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