Graphs in Machine Learning

Daniele Calandriello

DeepMind Paris, France

Collaborators: Achraf Azize,
Michal Valko

Partially based on material by: Gary Miller,
Mikhail Belkin, Branislav Kveton,
Doyle & Schnell, Daniel Spielman

Previous Lecture

- spectral graph theory
- Laplacians and their properties
  - symmetric and asymmetric normalization
  - random walks
- geometry of the data and the connectivity
- spectral clustering

This Lecture

- manifold learning with Laplacians eigenmaps
- inductive and transductive semi-supervised learning
- graph-based semi-supervised learning
- graph based manifold regularization

$$\mathbb{R}^d \longrightarrow \mathbb{R}^m$$

manifold learning

...discworld

Manifold Learning: Recap

problem: definition reduction/manifold learning

Given $\{\mathbf{x}_i\}_{i=1}^{N}$ from $\mathbb{R}^d$ find $\{\mathbf{y}_i\}_{i=1}^{N}$ in $\mathbb{R}^m$, where $m \ll d$.

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  - feature extraction

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  - often assuming $\mathcal{M} \subset \mathbb{R}^d$
  - linear vs. nonlinear dimensionality reduction

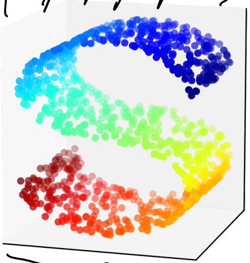
Manifold Learning: Linear vs. Non-linear

What do we know about linear vs. nonlinear methods?

Manifold Learning: Linear vs. Nonlinear

What do we know about linear vs. nonlinear methods?

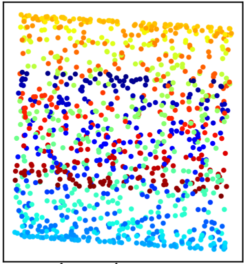
↳ no division that properly separates → we want non linear proj



colour ↳ closeness

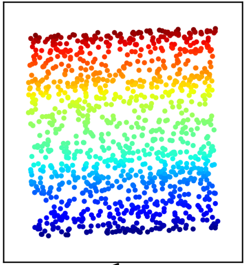
we want 2D projection to conserve clustering

PCA projection



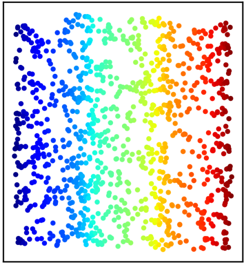
↳ not good

LLE projection



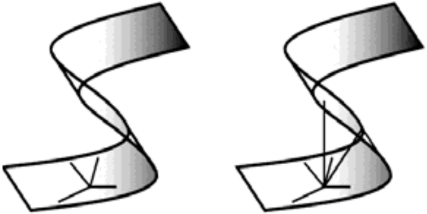
↳ better, non linear

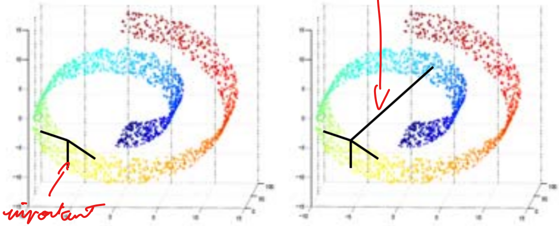
IsoMap projection



Manifold Learning: Preserving (just) local distances

not very important.

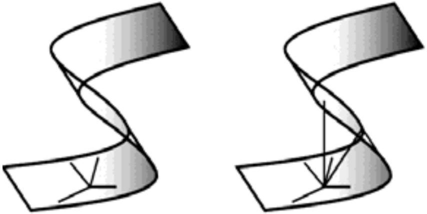


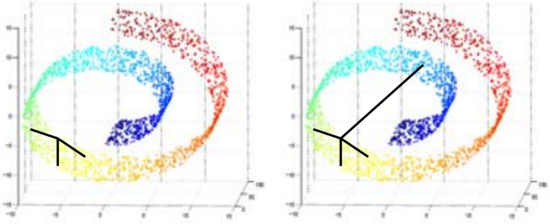


important distance

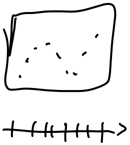
A manifold is a space that is non linear but locally is.

Manifold Learning: Preserving (just) local distances





euclidian distant $d(\mathbf{y}_i, \mathbf{y}_j) = d(\mathbf{x}_i, \mathbf{x}_j)$ only if $d(\mathbf{x}_i, \mathbf{x}_j)$ is small



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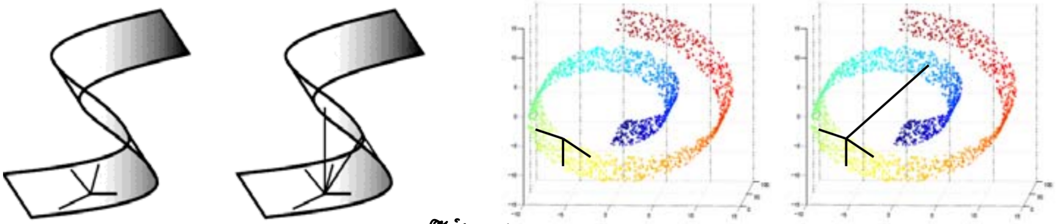

projection point orig one

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1-D $$\min \sum_{ij} w_{ij}(y_i - y_j)^2$$

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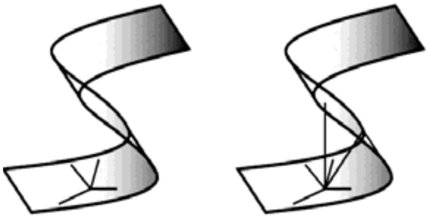

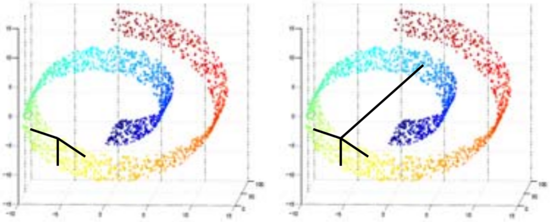

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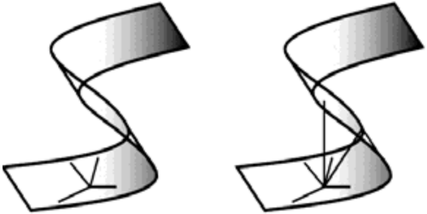

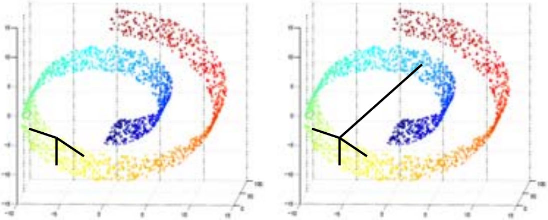

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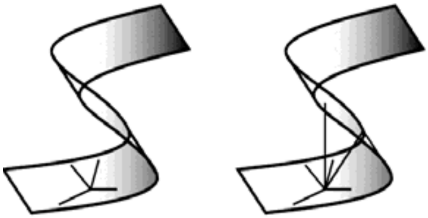

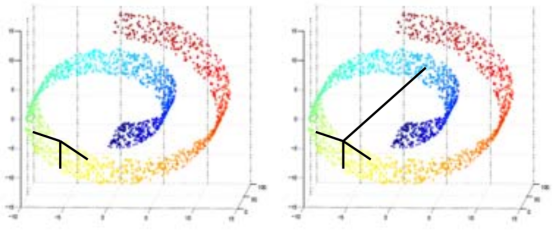

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m-D $$\min_{\mathbf{y}} \sum_{ij} w_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|^2$$

Manifold Learning: Laplacian Eigenmaps to 1D

Laplacian Eigenmaps 1D objective

$$\min_{\mathbf{f}} \mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f} \quad \text{s.t.} \quad f_i \in \mathbb{R}, \quad \mathbf{f}^\mathsf{T}\mathbf{D}\mathbf{1} = 0, \quad \mathbf{f}^\mathsf{T}\mathbf{D}\mathbf{f} = \mathbf{1}$$

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What is the solution?

Manifold Learning: Laplacian Eigenmaps

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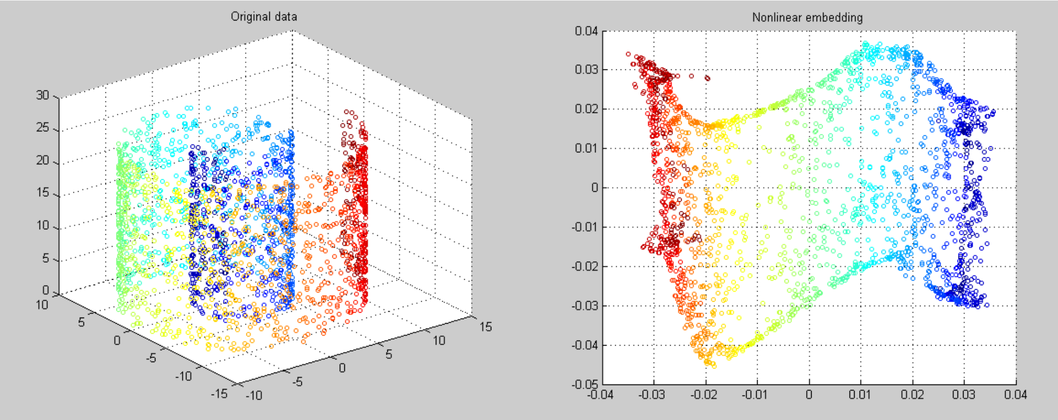
Note$_1$: we need to get $m+1$ smallest eigenvectors
Note$_2$: $\mathbf{f}_1$ is useless

`http://web.cse.ohio-state.edu/~mbelkin/papers/LEM_NC_03.pdf`

Manifold Learning: Example



`http://www.mathworks.com/matlabcentral/fileexchange/36141-laplacian-eigenmap-~-diffusion-map-~-manifold-learning`

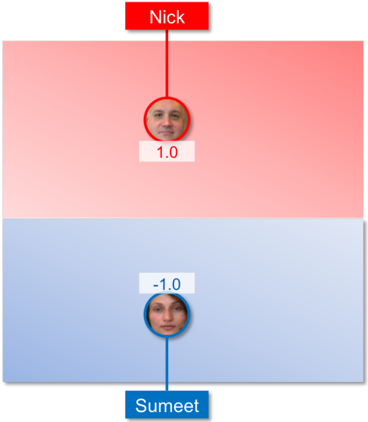
SSL

semi-supervised learning

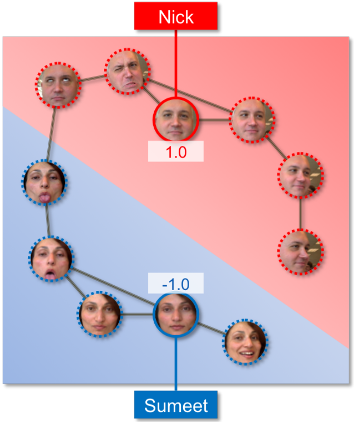
...our running example for learning with graphs

Semi-supervised learning: How is it possible?

Take unlabelled data and try to associate unlabelled data to labelled data



SUPERVISED



SEMI-SUPERVISED

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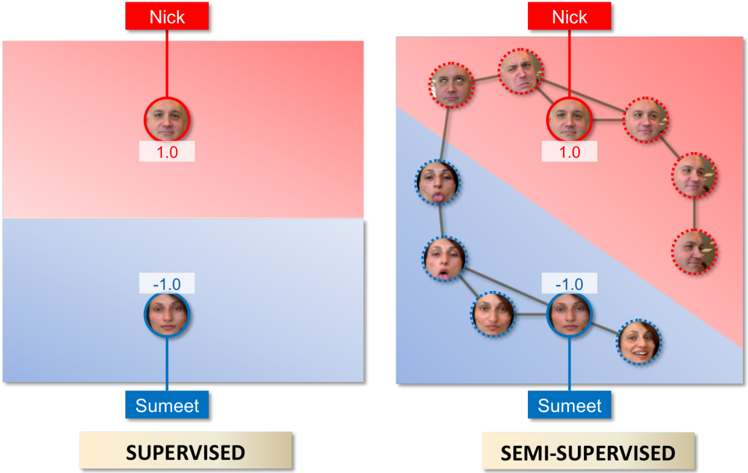

This is how children learn! hypothesis

Semi-supervised learning (SSL) labeled data

SSL problem: definition

Given $\{\mathbf{x}_i\}_{i=1}^{N}$ from $\mathbb{R}^d$ and $\{y_i\}_{i=1}^{n_l}$, with $n_l \ll N$, find $\{y_i\}_{i=n_l+1}^{N}$ (**transductive**) or find f predicting y well beyond that (**inductive**).

total nber of data

Semi-supervised learning (SSL)

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Some facts about SSL

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- now it helps now, now it does not (sic)
  - provable cases when it helps
- inductive or transductive/out-of-sample extension

http://olivier.chapelle.cc/ssl-book/discussion.pdf

SSL: Overview: Self-Training

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Input: $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{n_l}$ and $\mathcal{U} = \{\mathbf{x}_i\}_{i=n_l+1}^{N}$

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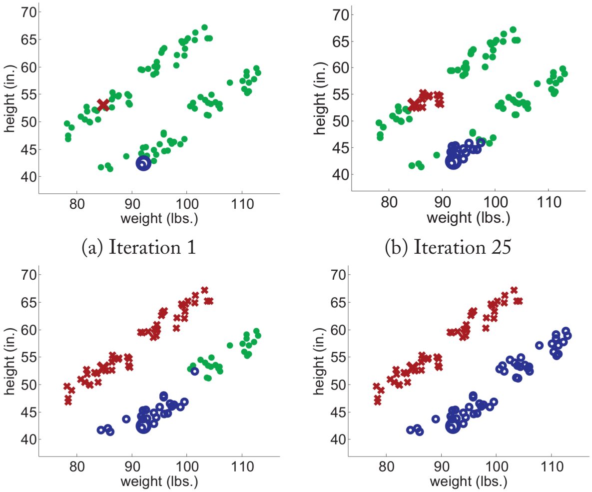
What are the properties of self-training?

- its a wrapper method
- heavily depends on the the internal classifier
- some theory exist for specific classifiers
- nobody uses it anymore ($\neq$ self supervised)
- errors propagate (unless the clusters are well separated)

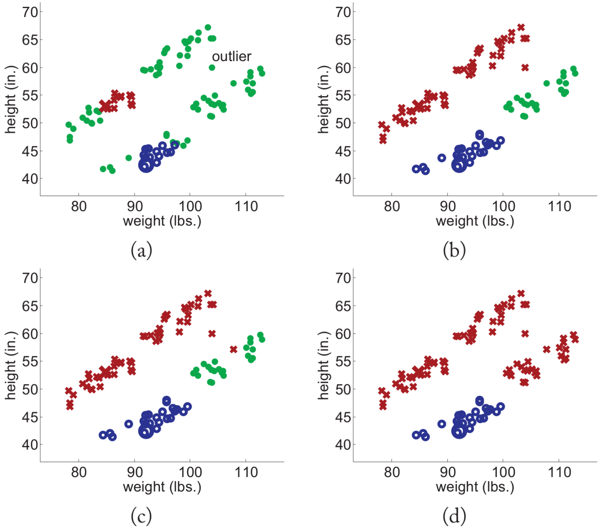
SSL: Self-Training (Good Case)



(a) Iteration 1 (b) Iteration 25

(c) Iteration 74 (d) Final labeling of all instances

SSL: Self-Training (Bad Case)



(a) (b)

(c) (d)

SSL($\mathcal{G}$)

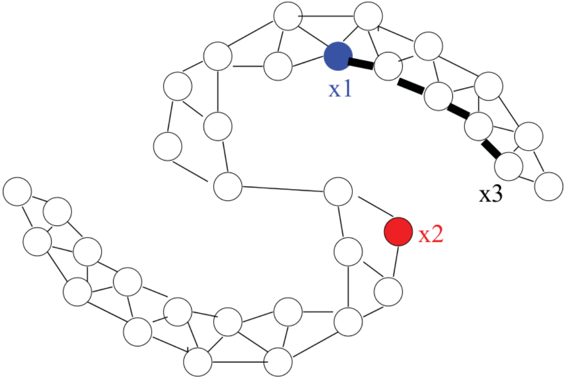
semi-supervised learning with graphs and harmonic functions

...our running example for learning with graphs

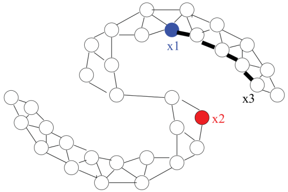
SSL with Graphs: Prehistory

Blum/Chawla: Learning from Labeled and Unlabeled Data using Graph Mincuts
`http://www.aladdin.cs.cmu.edu/papers/pdfs/y2001/mincut.pdf`

*following some insights from vision research in 1980s



SSL with Graphs: MinCut



MinCut SSL: an idea similar to MinCut clustering

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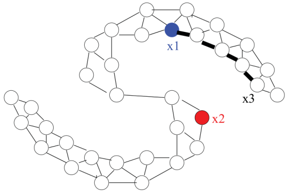
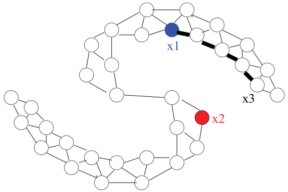


MinCut SSL: an idea similar to MinCut clustering
Where is the link?

SSL with Graphs: MinCut



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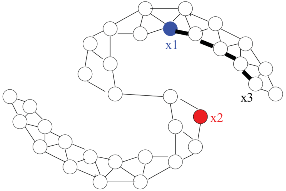
Where is the link? connected classes, not necessarily compact

SSL with Graphs: MinCut



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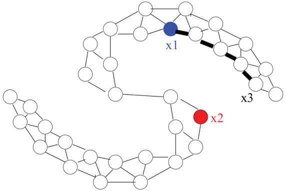
Where is the link? connected classes, not necessarily compact

What is the formal statement?

SSL with Graphs: MinCut



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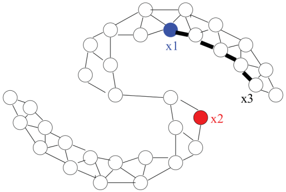
What is the formal statement? We look for $f(\mathbf{x}) \in \{\pm 1\}$

$$\mathrm{cut} = \sum_{i,j=1}^{n_l+n_u} w_{ij} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j)\right)^2 = \Omega(f)$$

SSL with Graphs: MinCut



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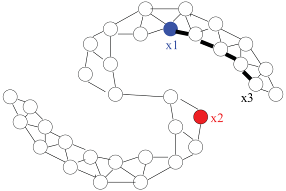

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Why $\left(f(\mathbf{x}_i) - f(\mathbf{x}_j)\right)^2$ and not $|f(\mathbf{x}_i) - f(\mathbf{x}_j)|$? It does not matter.

SSL with Graphs: MinCut

We look for $f(\mathbf{x}) \in \{\pm 1\}$ to minimize the cut $\Omega(\mathbf{f})$

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SSL with Graphs: MinCut

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orig loss

mincut loss

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$$V(\mathbf{x}, y, f(\mathbf{x})) = \infty \sum_{i=1}^{n_l} (f(\mathbf{x}_i) - y_i)^2$$

SSL with Graphs: MinCut

Final objective function:

$$\min_{\mathbf{f}\in\{\pm 1\}^{n_l+n_u}} \infty \sum_{i=1}^{n_l} (f(\mathbf{x}_i) - y_i)^2 + \lambda \sum_{i,j=1}^{n_l+n_u} w_{ij} (f(\mathbf{x}_i) - f(\mathbf{x}_j))^2$$

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Can we solve it?

SSL with Graphs: MinCut

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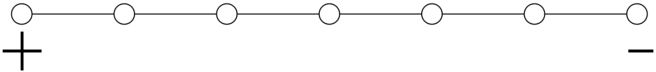

SSL with Graphs: MinCut

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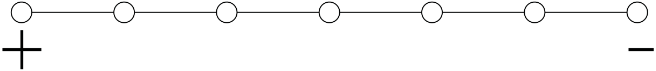

There are six solutions.

SSL with Graphs: MinCut

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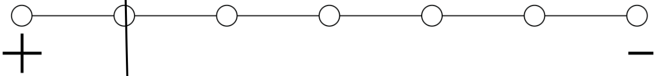

There are six solutions. All equivalent.

SSL with Graphs: MinCut

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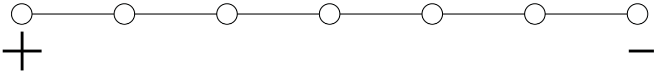

There are six solutions. All equivalent.

We need a better way to reflect the confidence.

SSL with Graphs: Harmonic Functions

Zhu/Ghahramani/Lafferty: Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions (ICML 2013) http://mlg.eng.cam.ac.uk/zoubin/papers/zgl.pdf

*a seminal paper that convinced people to use graphs for SSL

L looks for extra constraint to get a unique solution

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Idea 1: Look for a **unique** solution.

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Idea 1: Look for a **unique** solution.

Idea 2: Find a smooth one.

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Idea 1: Look for a **unique** solution.

Idea 2: Find a smooth one. (**harmonic** solution) $\rightsquigarrow$ used in physics to characterize In & Out = 0. Appears when have energy flow.

SSL with Graphs: Harmonic Functions

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Harmonic SSL

1): As before, we constrain f to match the supervised data:

$$f(\mathbf{x}_i) = y_i \qquad \forall i \in \{1, \ldots, n_l\}$$

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SSL with Graphs: Harmonic Functions

The harmonic solution is obtained from the mincut one ...

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...if we just relax the integer constraints to be real ...

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SSL with Graphs: Harmonic Functions

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...or equivalently (note that $f(\mathbf{x}_i) = f_i$) ...

$$\min_{\mathbf{f}\in\mathbb{R}^{n_l+n_u}} \sum_{i,j=1}^{n_l+n_u} w_{ij} (f(\mathbf{x}_i) - f(\mathbf{x}_j))^2$$

$$s.t. \quad y_i = f(\mathbf{x}_i) \quad \forall i = 1, \ldots, n_l$$

SSL with Graphs: Harmonic Functions

Properties of the relaxation from ± 1 to $\mathbb{R}$

- there is a closed form solution for $\mathbf{f}$
- this solution is unique
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SSL with Graphs: Harmonic Functions

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SSL with Graphs: Harmonic Functions

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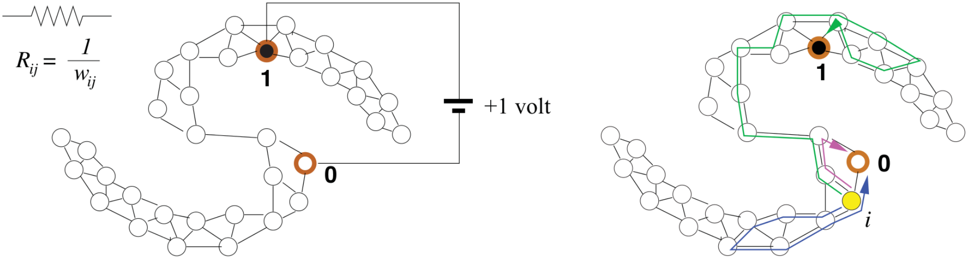
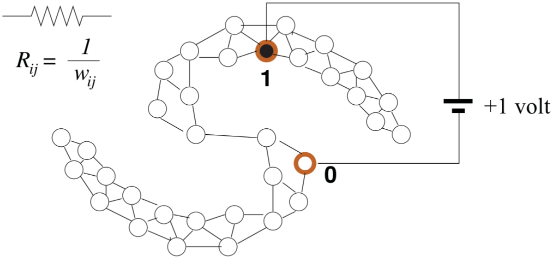
- electric-network interpretation
- random-walk interpretation

SSL with Graphs: Harmonic Functions



(a) The electric network interpretation   (b) The random walk interpretation

SSL with Graphs: Harmonic Functions



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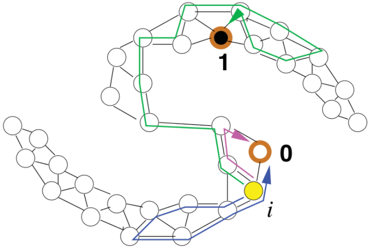
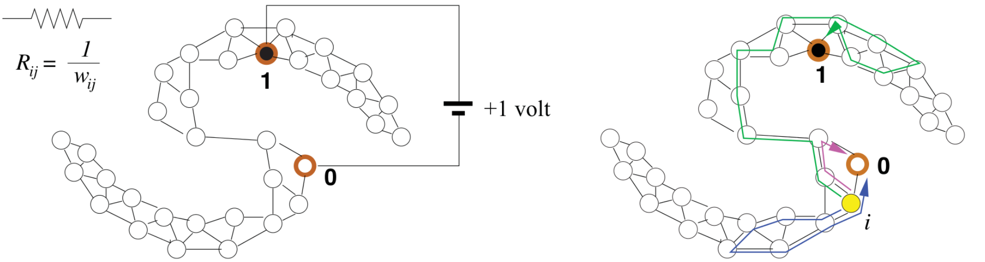


(b) The random walk interpretation

Random walk interpretation:

1) start from the vertex you want to label and randomly walk

SSL with Graphs: Harmonic Functions



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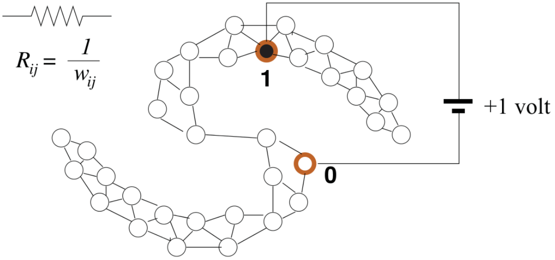
SSL with Graphs: Harmonic Functions



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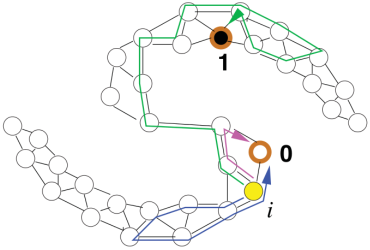

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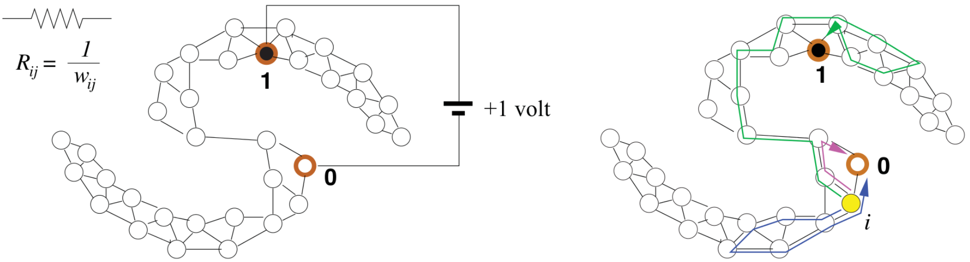
SSL with Graphs: Harmonic Functions



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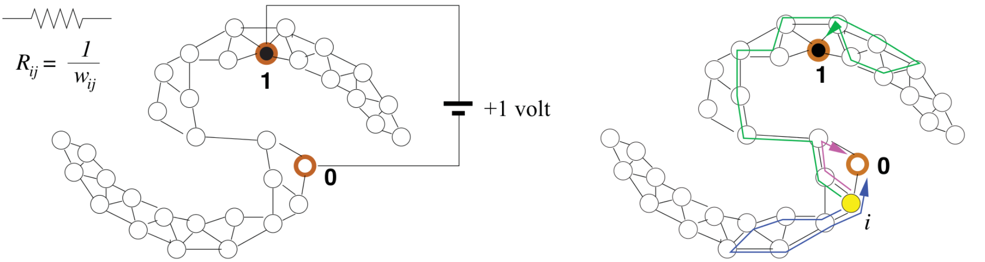
SSL with Graphs: Harmonic Functions



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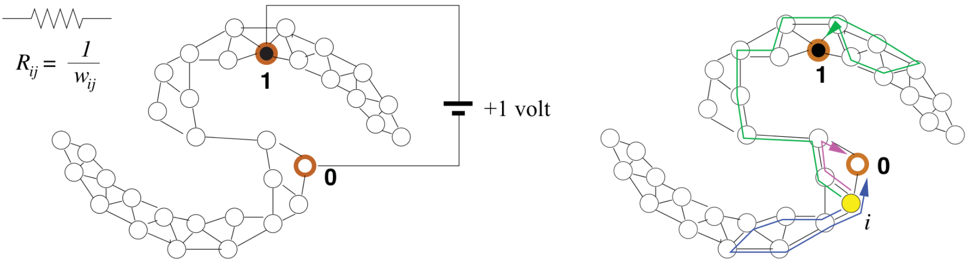
absorbing random walk

$f_i =$

SSL with Graphs: Harmonic Functions



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absorbing random walk

f_i = probability of reaching a positive labeled vertex

SSL with Graphs: Harmonic Functions

How to compute HS?

SSL with Graphs: Harmonic Functions

How to compute HS? **Option A:** iteration

SSL with Graphs: Harmonic Functions

How to compute HS? **Option A:** iteration/propagation

SSL with Graphs: Harmonic Functions

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SSL with Graphs: Harmonic Functions

How to compute HS? **Option A:** iteration/propagation

Step 1: Set $f(\mathbf{x}_i) = y_i$ for $i = 1, \ldots, n_l$
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$$f(\mathbf{x}_i) \leftarrow \frac{\sum_{i\sim j} f(\mathbf{x}_j) w_{ij}}{\sum_{i\sim j} w_{ij}} \qquad \forall i \in \{n_l + 1, \ldots, n_u + n_l\}$$

SSL with Graphs: Harmonic Functions

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SSL with Graphs: Harmonic Functions

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Pros:

- this will converge to the harmonic solution
- we can set the initial values for unlabeled nodes arbitrarily
- an interesting option for large-scale data

SSL with Graphs: Harmonic Functions

How to compute HS? **Option B:** Closed form solution

SSL with Graphs: Harmonic Functions

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SSL with Graphs: Harmonic Functions

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SSL with Graphs: Harmonic Functions

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$\mathbf{L}$ is a $(n_l + n_u) \times (n_l + n_u)$ matrix:

$$\mathbf{L} = \begin{bmatrix} \mathbf{L}_{ll} & \mathbf{L}_{lu} \\ \mathbf{L}_{ul} & \mathbf{L}_{uu} \end{bmatrix}$$

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How to compute this **constrained** minimization problem?

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How to compute this **constrained** minimization problem?

Yes, Lagrangian multipliers are an option, but . . .

SSL with Graphs: Harmonic Functions

Let us compute **harmonic** solution using **harmonic** property!

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$$(\mathbf{L}\mathbf{f})_u = \mathbf{0}_u$$

SSL with Graphs: Harmonic Functions

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In matrix notation

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SSL with Graphs: Harmonic Functions

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...from which we get

$$\mathbf{f}_u = \mathbf{L}_{uu}^{-1}(-\mathbf{L}_{ul}\mathbf{f}_l)$$

SSL with Graphs: Harmonic Functions

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SSL with Graphs: Harmonic Functions

Let us compute **harmonic** solution using **harmonic** property!

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Note that $\mathbf{f}_u$ does not depend on $\mathbf{L}_{ll}$.

SSL with Graphs: Harmonic Functions

Can we see that this calculates the probability of a random walk?

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SSL with Graphs: Regularized Harmonic Functions

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SSL with Graphs: Regularized Harmonic Functions

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What will this do to our predictions?

depends on the weigh on the edges

SSL with Graphs: Regularized Harmonic Functions

How do we represent the sink in $\mathbf{L}$ explicitly?

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$$\begin{bmatrix} \mathbf{L}_{ll} + \gamma_G \mathbf{I}_{n_l} & \mathbf{L}_{lu} & -\gamma_G \mathbf{1}_{n_l \times 1} \\ \mathbf{L}_{ul} & \mathbf{L}_{uu} + \gamma_G \mathbf{I}_{n_u} & -\gamma_G \mathbf{1}_{n_u \times 1} \\ -\gamma_G \mathbf{1}_{1 \times n_l} & -\gamma_G \mathbf{1}_{1 \times n_u} & n\gamma_G \end{bmatrix} \begin{bmatrix} \mathbf{f}_l \\ \mathbf{f}_u \\ 0 \end{bmatrix} = \begin{bmatrix} \dots \\ \mathbf{0}_u \\ \dots \end{bmatrix}$$

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SSL with Graphs: Regularized Harmonic Functions

How do we represent the sink in **L** explicitly?

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...and therefore we simply add γ_G to the diagonal of **L**!

SSL with Graphs: Regularized Harmonic Functions

How do we compute this **regularized** random walk?

SSL with Graphs: Regularized Harmonic Functions

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$$\mathbf{f}_u = \left(\mathbf{L}_{uu} + \gamma_g \mathbf{I}\right)^{-1} \left(\mathbf{W}_{ul}\mathbf{f}_l\right)$$

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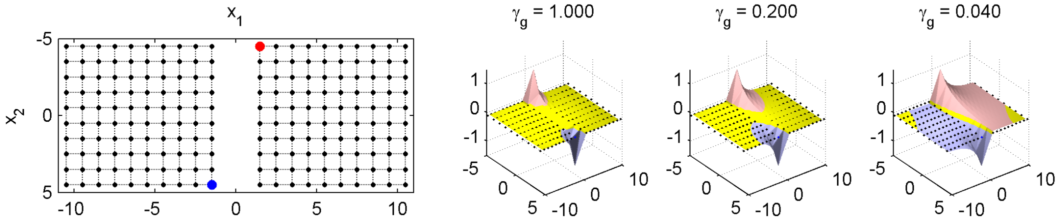

SSL with Graphs: Regularized Harmonic Functions

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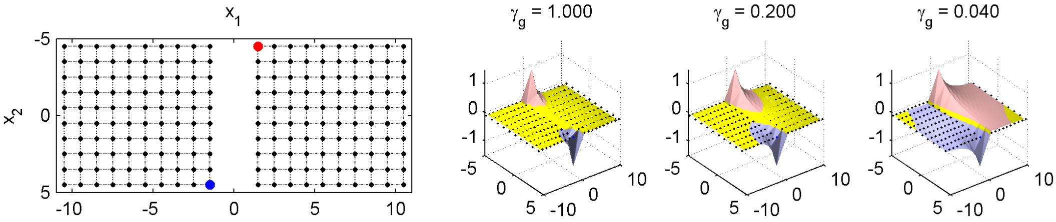

What happens to sneaky outliers?

SSL with Graphs: Soft Harmonic Functions

Regularized HS objective with $\mathbf{Q} = \mathbf{L} + \gamma_g \mathbf{I}$:

SSL with Graphs: Soft Harmonic Functions

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$$\min_{\mathbf{f} \in \mathbb{R}^{n_l + n_u}} \infty \sum_{i=1}^{n_l} (f(\mathbf{x}_i) - y_i)^2 + \lambda \mathbf{f}^\mathsf{T} \mathbf{Q} \mathbf{f}$$

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SSL with Graphs: Soft Harmonic Functions

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$\mathbf{C}$ is diagonal with $C_{ii} = \begin{cases} c_l & \text{for labeled examples} \\ c_u & \text{otherwise.} \end{cases}$

$\mathbf{y} \equiv$ pseudo-targets with $y_i = \begin{cases} \text{true label} & \text{for labeled examples} \\ 0 & \text{otherwise.} \end{cases}$

SSL with Graphs: Soft Harmonic Functions

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^n} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

Closed form **soft harmonic solution**:

SSL with Graphs: Soft Harmonic Functions

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SSL with Graphs: Soft Harmonic Functions

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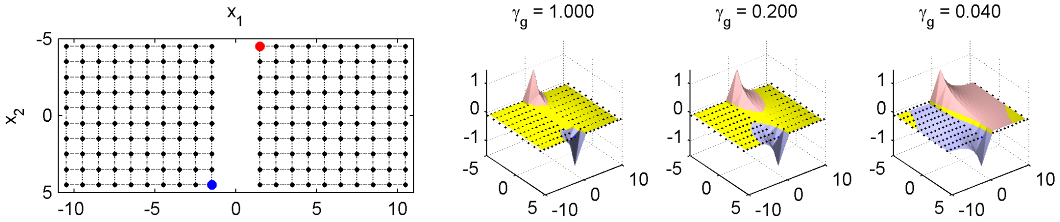

SSL with Graphs: Soft Harmonic Functions

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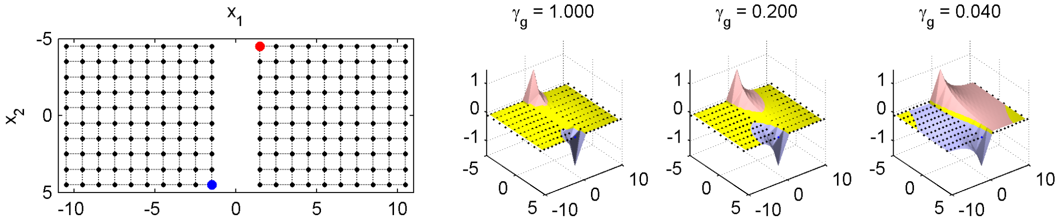

What are the differences between hard and soft?

SSL with Graphs: Soft Harmonic Functions

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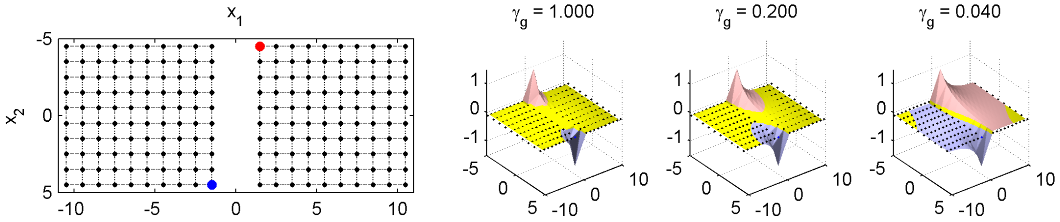

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Not much different in practice.

SSL with Graphs: Soft Harmonic Functions

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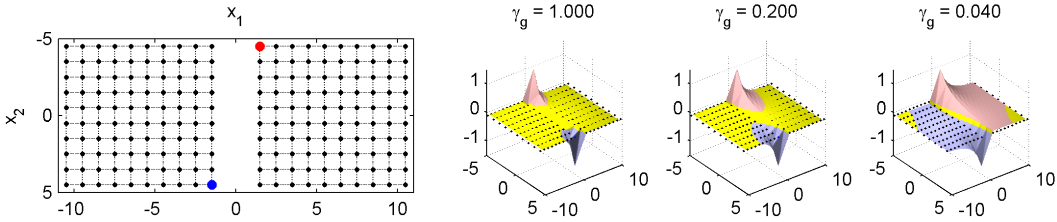

What are the differences between hard and soft?

Not much different in practice.

Provable generalization guarantees for the soft one.

SSL with Graphs: Stability Bounds

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^N} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

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Think about **stability** of this solution.

SSL with Graphs: Stability Bounds

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Think about **stability** of this solution.
Consider two datasets differing in exactly one *labeled* point.

SSL with Graphs: Stability Bounds

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^N} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

Think about **stability** of this solution.
Consider two datasets differing in exactly one *labeled* point. $\mathcal{C}_1 = \mathbf{C}_1^{-1}\mathbf{Q} + \mathbf{I}$ and $\mathcal{C}_2 = \mathbf{C}_2^{-1}\mathbf{Q} + \mathbf{I}$

SSL with Graphs: Stability Bounds

$$\mathbf{f}^\star = \min_{\mathbf{f} \in \mathbb{R}^N} (\mathbf{f} - \mathbf{y})^\mathsf{T} \mathbf{C} (\mathbf{f} - \mathbf{y}) + \mathbf{f}^\mathsf{T} \mathbf{Q} \mathbf{f}$$

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SSL with Graphs: Stability Bounds

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What is the maximal difference in the solutions?

$$\mathbf{f}_2^\star - \mathbf{f}_1^\star$$

SSL with Graphs: Stability Bounds

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What is the maximal difference in the solutions?

$$\mathbf{f}_2^\star - \mathbf{f}_1^\star = \mathcal{C}_2^{-1}\mathbf{y}_2 - \mathcal{C}_1^{-1}\mathbf{y}_1$$

SSL with Graphs: Stability Bounds

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^N} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

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What is the maximal difference in the solutions?

$$\begin{aligned}\mathbf{f}_2^\star - \mathbf{f}_1^\star &= \mathcal{C}_2^{-1}\mathbf{y}_2 - \mathcal{C}_1^{-1}\mathbf{y}_1 \\ &= \mathcal{C}_2^{-1}(\mathbf{y}_2 - \mathbf{y}_1) - \left(\mathcal{C}_1^{-1} - \mathcal{C}_2^{-1}\right)\mathbf{y}_1\end{aligned}$$

SSL with Graphs: Stability Bounds

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\mathbf{f}_2^\star - \mathbf{f}_1^\star &= \mathcal{C}_2^{-1}\mathbf{y}_2 - \mathcal{C}_1^{-1}\mathbf{y}_1 \\
&= \mathcal{C}_2^{-1}(\mathbf{y}_2 - \mathbf{y}_1) - \left(\mathcal{C}_1^{-1} - \mathcal{C}_2^{-1}\right)\mathbf{y}_1 \\
&= \mathcal{C}_2^{-1}(\mathbf{y}_2 - \mathbf{y}_1) - \left(\mathcal{C}_1^{-1}\left[\left(\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\right)\mathbf{Q}\right]\mathcal{C}_2^{-1}\right)\mathbf{y}_1
\end{aligned}$$

SSL with Graphs: Stability Bounds

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SSL with Graphs: Stability Bounds

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\end{aligned}$$

Note that $\mathbf{v} \in \mathbb{R}^{N\times 1}$, $\lambda_m(A)\|\mathbf{v}\|_2 \le \|A\mathbf{v}\|_2 \le \lambda_M(A)\|\mathbf{v}\|_2$

SSL with Graphs: Stability Bounds

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SSL with Graphs: Stability Bounds

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$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_2 \le \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)}$$

SSL with Graphs: Stability Bounds

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^N} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

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Note that $\mathbf{v} \in \mathbb{R}^{N\times 1}$, $\lambda_m(A)\|\mathbf{v}\|_2 \le \|A\mathbf{v}\|_2 \le \lambda_M(A)\|\mathbf{v}\|_2$

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_2 \le \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)} + \lambda_M(\mathbf{Q})$$

SSL with Graphs: Stability Bounds

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$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_2 \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)} + \lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2$$

SSL with Graphs: Stability Bounds

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^N} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

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$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_2 \le \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{}$$

SSL with Graphs: Stability Bounds

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Note that $\mathbf{v} \in \mathbb{R}^{N\times 1}$, $\lambda_m(A)\|\mathbf{v}\|_2 \le \|A\mathbf{v}\|_2 \le \lambda_M(A)\|\mathbf{v}\|_2$

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_2 \le \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)\lambda_m(\mathcal{C}_1)}$$

SSL with Graphs: Stability Bounds

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^N} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

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SSL with Graphs: Stability Bounds

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$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_2 \le \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)\lambda_m(\mathcal{C}_1)}$$

Using $\lambda_m(\mathcal{C}) \ge \frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C})} + 1$

SSL with Graphs: Stability Bounds

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^N} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_2 \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\lambda_m(\mathcal{C}_2)\lambda_m(\mathcal{C}_1)}$$

Using $\lambda_m(\mathcal{C}) \geq \frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C})} + 1$

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_2 \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \leq {\color{red}\beta} \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \leq \beta \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

Now, let us plug in the values for our problem.

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \leq \beta \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

Now, let us plug in the values for our problem.

Take $c_l = 1$

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \leq \beta \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

Now, let us plug in the values for our problem.

Take $c_l = 1$ and $c_l > c_u$.

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \leq \color{red}{\beta} \color{black}{\leq} \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

Now, let us plug in the values for our problem.

Take $c_l = 1$ and $c_l > c_u$. We have $|y_i| \leq 1$

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \leq {\color{red}\beta} \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

Now, let us plug in the values for our problem.

Take $c_l = 1$ and $c_l > c_u$. We have $|y_i| \leq 1$ and $|f_i^\star| \leq 1$.

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \le \beta \le \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

Now, let us plug in the values for our problem.

Take $c_l = 1$ and $c_l > c_u$. We have $|y_i| \le 1$ and $|f_i^\star| \le 1$.

$$\beta \le 2\left[\frac{\sqrt{2}}{\lambda_m(\mathbf{Q}) + 1} + \sqrt{2n_l}\frac{1 - c_u}{c_u}\frac{\lambda_M(\mathbf{Q})}{(\lambda_m(\mathbf{Q}) + 1)^2}\right]$$

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \leq \beta \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

Now, let us plug in the values for our problem.

Take $c_l = 1$ and $c_l > c_u$. We have $|y_i| \leq 1$ and $|f_i^\star| \leq 1$.

$$\beta \leq 2\left[\frac{\sqrt{2}}{\lambda_m(\mathbf{Q}) + 1} + \sqrt{2n_l}\frac{1 - c_u}{c_u}\frac{\lambda_M(\mathbf{Q})}{(\lambda_m(\mathbf{Q}) + 1)^2}\right]$$

$\mathbf{Q}$ is reg. $\mathbf{L}$: $\lambda_m(\mathbf{Q}) = \lambda_m(\mathbf{L}) + \gamma_g$

SSL with Graphs: Stability Bounds

$$\|\mathbf{f}_2^\star - \mathbf{f}_1^\star\|_\infty \le \beta \le \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

Now, let us plug in the values for our problem.

Take $c_l = 1$ and $c_l > c_u$. We have $|y_i| \le 1$ and $|f_i^\star| \le 1$.

$$\beta \le 2\left[\frac{\sqrt{2}}{\lambda_m(\mathbf{Q}) + 1} + \sqrt{2n_l}\frac{1 - c_u}{c_u}\frac{\lambda_M(\mathbf{Q})}{(\lambda_m(\mathbf{Q}) + 1)^2}\right]$$

$\mathbf{Q}$ is reg. $\mathbf{L}$: $\lambda_m(\mathbf{Q}) = \lambda_m(\mathbf{L}) + \gamma_g$ and $\lambda_M(\mathbf{Q}) = \lambda_M(\mathbf{L}) + \gamma_g$

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This algorithm is β-stable!

SSL with Graphs: Regularized Harmonic Functions

Larger implications of random walks

random walk relates to **commute distance**

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random walk relates to **commute distance** which should satisfy

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The goal of these solutions: **make them remember!**

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Solution: **Manifold Regularization**

SSL with Graphs: Manifold Regularization

General (S)SL objective:

$$\min_f \sum_i^{n_l} V(\mathbf{x}_i, y_i, f(\mathbf{x}_i)) + \lambda \Omega(f)$$

Want to control f, also for the out-of-sample data, i.e., **everywhere**.

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For general **kernels**:

$$\min_{f \in \mathcal{H}_\mathcal{K}} \sum_i^{n_l} V(\mathbf{x}_i, y_i, f(\mathbf{x}_i)) + \lambda_1 \|f\|_\mathcal{K}^2 + \lambda_2 \mathbf{f}^\mathsf{T} \mathbf{L} \mathbf{f}$$

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Representer theorem for manifold regularization

The minimizer $f^\star$ has a **finite** expansion of the form

$$f^\star(\mathbf{x}) = \sum_{i=1}^{n_l+n_u} \alpha_i \mathcal{K}(\mathbf{x}, \mathbf{x}_i)$$

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LapRLS Laplacian Regularized Least Squares

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LapRLS Laplacian Regularized Least Squares

$$V(\mathbf{x}, y, f) = \max(0, 1 - yf(\mathbf{x}))$$

LapSVM Laplacian Support Vector Machines

SSL with Graphs: Laplacian SVMs

$$f^\star = \arg\min_{f \in \mathcal{H}_\mathcal{K}} \sum_{i}^{n_l} \max\left(0, 1 - yf\left(\mathbf{x}\right)\right) + \gamma_A \|f\|_\mathcal{K}^2 + \gamma_I \mathbf{f}^\mathsf{T} \mathbf{L} \mathbf{f}$$

SSL with Graphs: Laplacian SVMs

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Allows us to learn a function in **RKHS**, i.e., **RBF** kernels.

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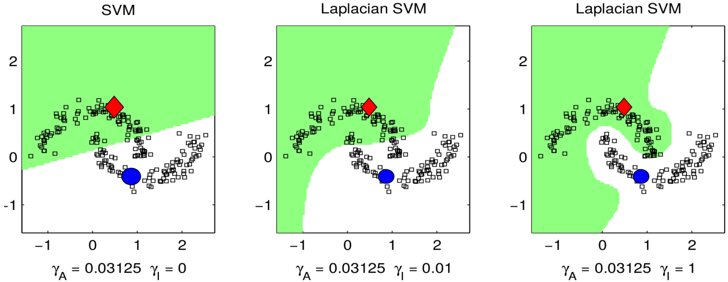

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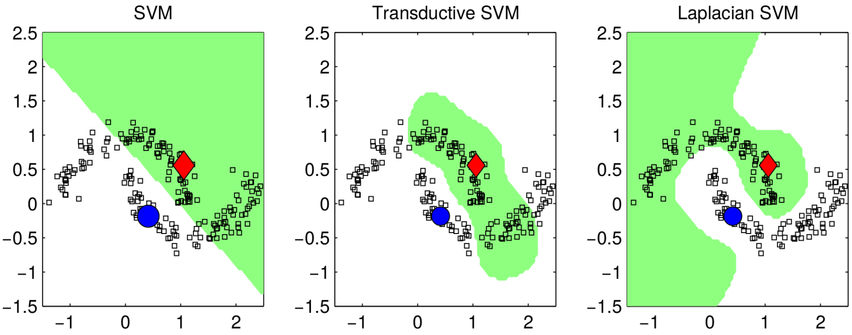

Checkpoint 1

Semi-supervised learning with graphs:

$$\min_{\mathbf{f}\in\{\pm 1\}^{n_l+n_u}} (\infty)\sum_{i=1}^{n_l} w_{ij}\left(f(\mathbf{x}_i) - y_i\right)^2 + \lambda \sum_{i,j=1}^{n_l+n_u} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j)\right)^2$$

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Regularized harmonic Solution:

$$\mathbf{f}_u=\left(\mathbf{L}_{uu}+\gamma_g\mathbf{I}\right)^{-1}\left(\mathbf{W}_{ul}\mathbf{f}_l\right)$$

Checkpoint 2

Unconstrained regularization in general:

$$\mathbf{f}^\star = \min_{\mathbf{f}\in\mathbb{R}^N} (\mathbf{f}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{f}-\mathbf{y}) + \mathbf{f}^\mathsf{T}\mathbf{Q}\mathbf{f}$$

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Out of sample extension: Laplacian SVMs

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Daniele Calandriello

dcalandriello@google.com

ENS Paris-Saclay, MVA 2022/2023

https://sites.google.com/view/daniele-calandriello/