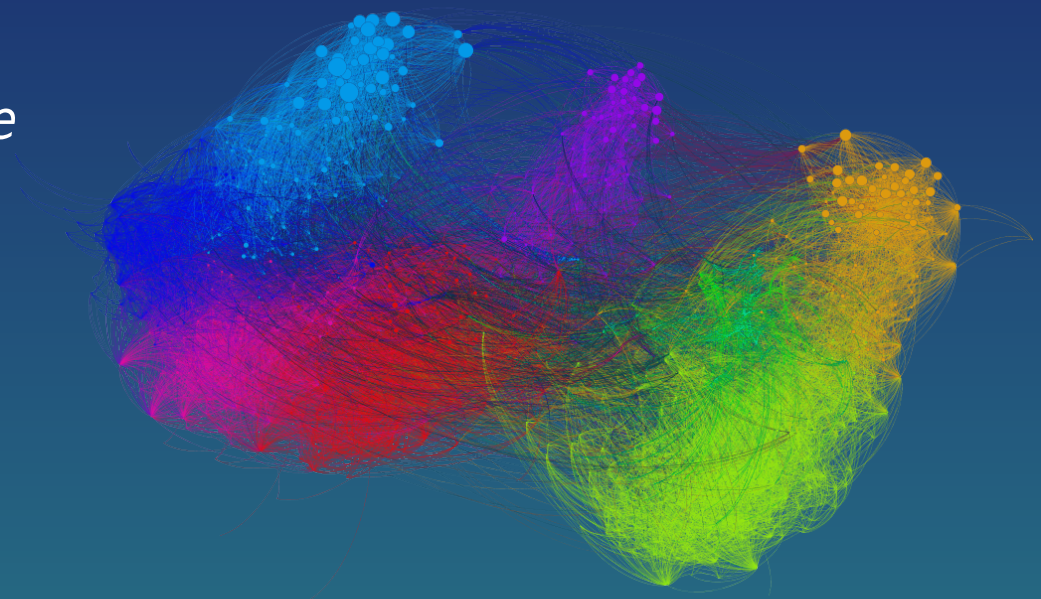
Graphs in Machine Learning

Michal Valko

Inria Lille - Nord Europe, France

Partially based on material by: Mikhail Belkin, Jerry Zhu, Olivier Chapelle, Branislav Kveton



October 26, 2015

MVA 2015/2016

Previous Lecture

- resistive networks
  - recommendation score as a resistance?
  - Laplacian and resistive networks
  - computation of effective resistance
- geometry of the data and the connectivity
- spectral clustering
  - connectivity vs. compactness
  - MinCut, RatioCut, NCut
  - spectral relaxations

Previous Lab Session

- 19. 10. 2015 by Daniele.Calandriello@inria.fr
- Content
  - Graph Construction
  - Test sensitivity to parameters: σ, k, ε
  - Spectral Clustering
  - Spectral Clustering vs. k-means
  - Image Segmentation
- Short written report (graded, all reports around 40% of grade)
- Check the course website for the policies
- Questions to piazza
- *Deadline:* 2. 11. 2015, 23:59

`http://researchers.lille.inria.fr/~calandri/ta/graphs/td1_handout.pdf`

This Lecture

- Manifold learning with Laplacian Eigenmaps
- Gaussian random fields and harmonic solution
- Graph-based semi-supervised learning and manifold regularization
- Transductive learning
- Inductive and transductive semi-supervised learning
- Manifold regularization

Ph.D. position in Lille and Amsterdam

PhD position in Theoretical Machine Learning is offered at Inria Lille. Possibility of a joint PhD with CWI, Amsterdam. Lille is 1h away from Paris, 34min from Brussels, 1h30 from London and 2h30 from Amsterdam, all by (fast) train. (And Amsterdam is in Amsterdam.)

The topic is to explore which regularities are "learnable" from data. Specifically, the focus is on the problem of forecasting, that is, predicting the probabilities of future outcomes of a series of events given the past. The question to be addressed is: under which assumptions on the stochastic mechanism generating the data is it possible to construct a consistent forecaster?

The student will be advised by Daniil.Ryabko@inria.fr, to whom all inquiries should be directed.

The topic is highly mathematical. Please do not apply if you don't like **proving theorems.**

Manifold Learning: Recap

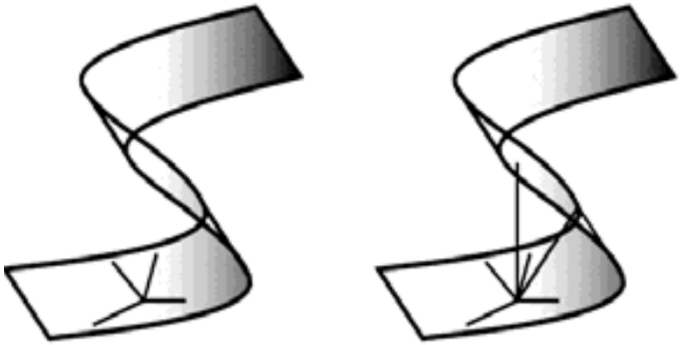
problem: definition reduction/manifold learning

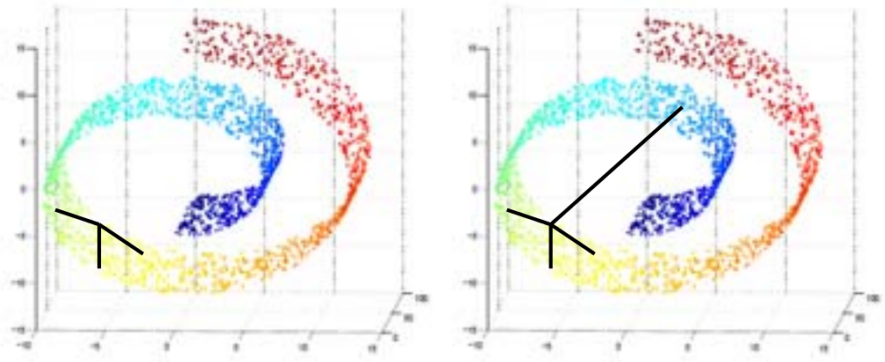
Given $\{\mathbf{x}_i\}_{i=1}^n$ from $\mathbb{R}^d$ find $\{\mathbf{y}_i\}_{i=1}^n$ in $\mathbb{R}^m$, where $m \ll d$.

- What do we know about the **dimensionality reduction**
  - representation/visualization (2D or 3D)
  - an old example: globe to a map
  - often assuming $\mathcal{M} \subset \mathbb{R}^d$
  - feature extraction
  - linear vs. nonlinear dimensionality reduction
- What do we know about linear vs. nonlinear methods?
  - linear: ICA, PCA, SVD, ...
  - nonlinear often preserve only **local** distances

Manifold Learning: Linear vs. Non-linear

Manifold Learning: Preserving (just) local distances





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

$$\min \sum_{ij} w_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|^2$$

Looks familiar?

Manifold Learning: Laplacian Eigenmaps

Step 1: Solve generalized eigenproblem:

$$\mathbf{Lf} = \lambda \mathbf{Df}$$

Step 2: Assign m new coordinates:

$$\mathbf{x}_i \mapsto \left(f_2\left(i\right), \ldots, f_{m+1}\left(i\right)\right)$$

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: Laplacian Eigenmaps to 1D

Laplacian Eigenmaps 1D objective

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

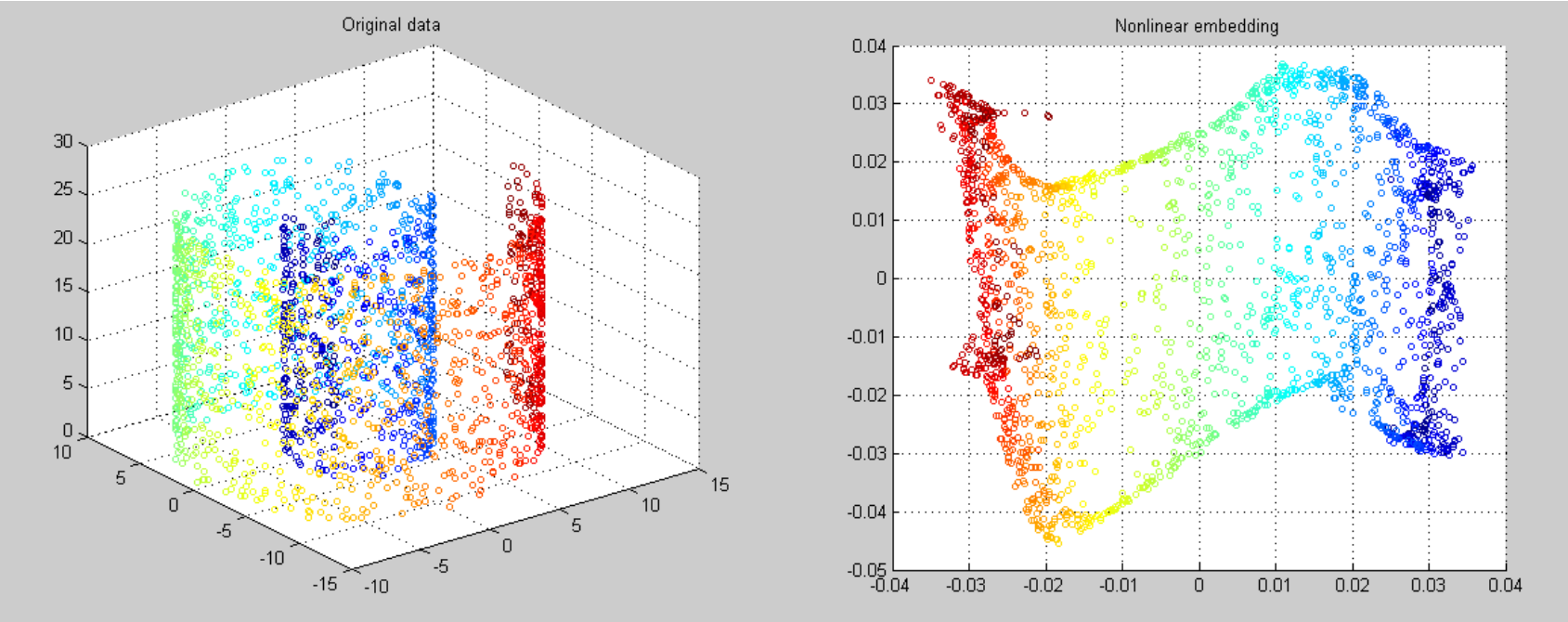
The meaning of the constraints is similar as for spectral clustering:

$\mathbf{f}^\top \mathbf{D}\mathbf{f} = \mathbf{1}$ is for scaling

$\mathbf{f}^\top \mathbf{D}\mathbf{1} = 0$ is to not get $\mathbf{v}_1$

What is the solution?

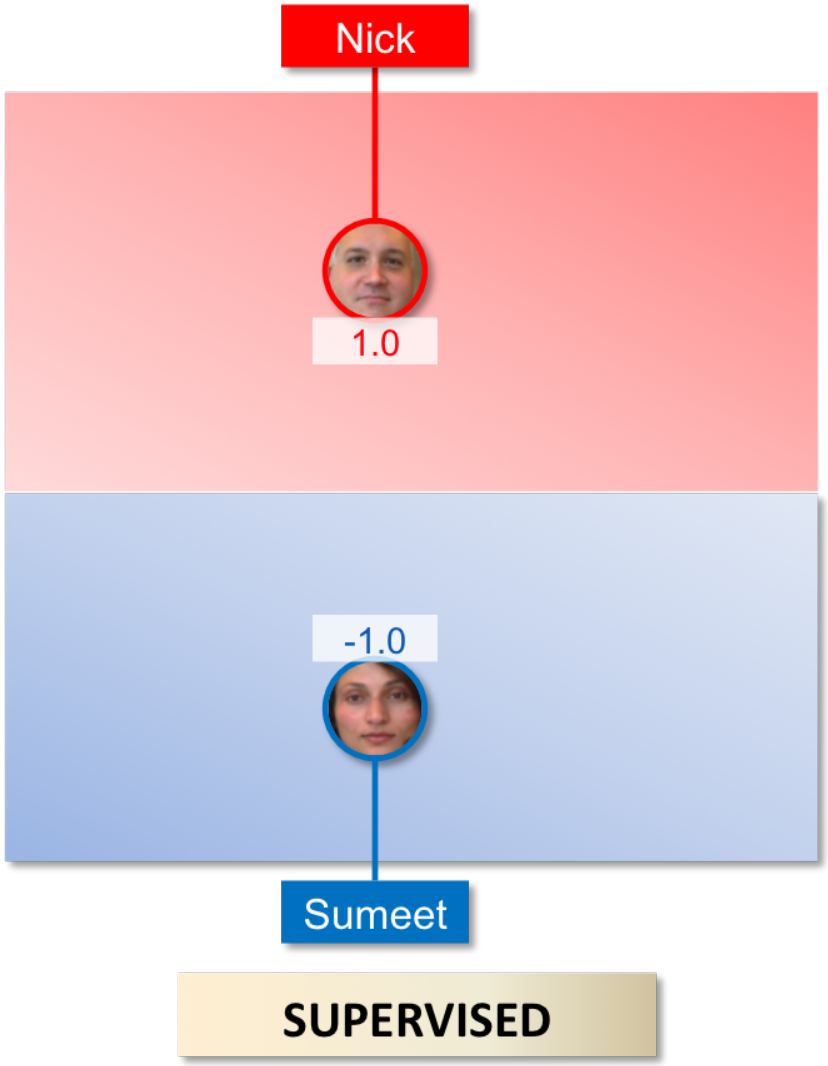
Manifold Learning: Example

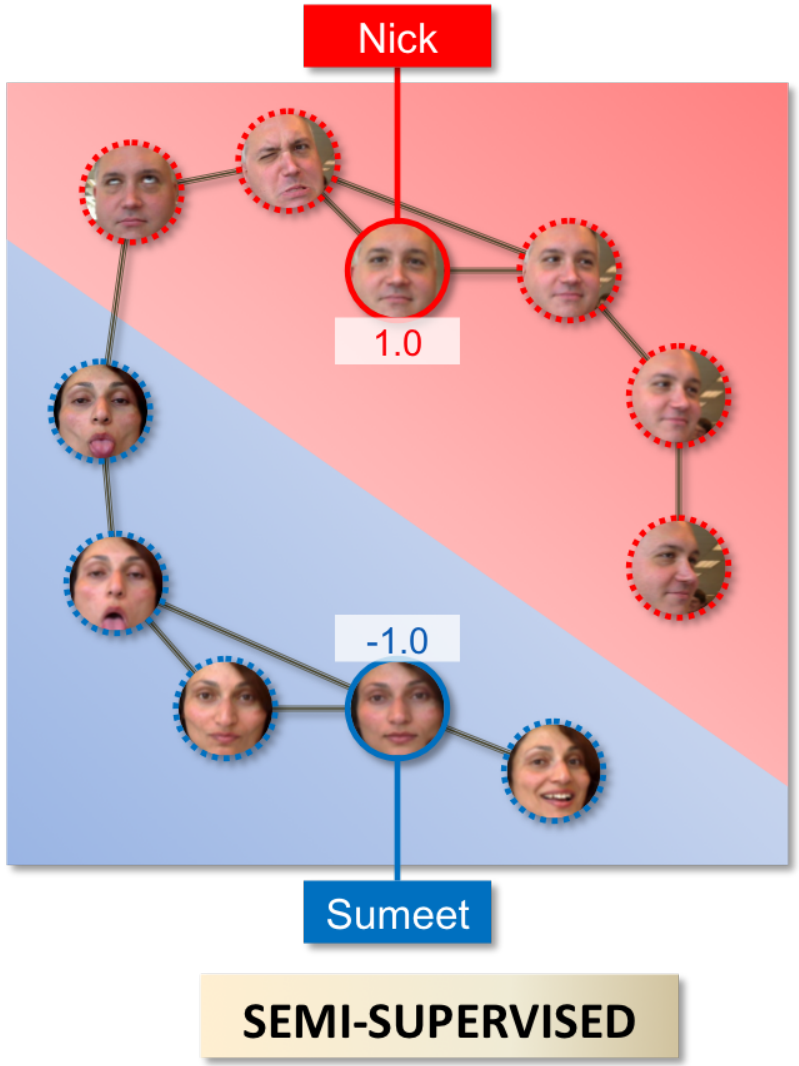


http://www.mathworks.com/matlabcentral/fileexchange/

36141-laplacian-eigenmap--~-diffusion-map--~-manifold-learning

Semi-supervised learning: How is it possible?





This is how children learn! hypothesis

Semi-supervised learning (SSL)

SSL problem: definition

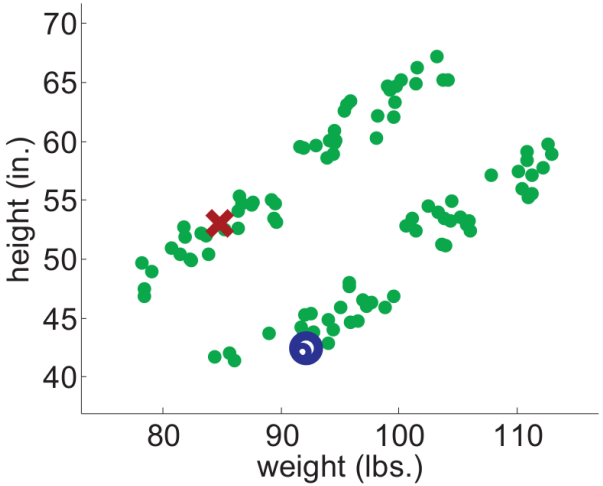
Given $\{\mathbf{x}_i\}_{i=1}^{n}$ from $\mathbb{R}^d$ and $\{y_i\}_{i=1}^{n_l}$, with $n_l \ll n$, find $\{y_i\}_{i=n_l+1}^{n}$ (transductive) or find f predicting y well beyond that (inductive).

Some facts about SSL

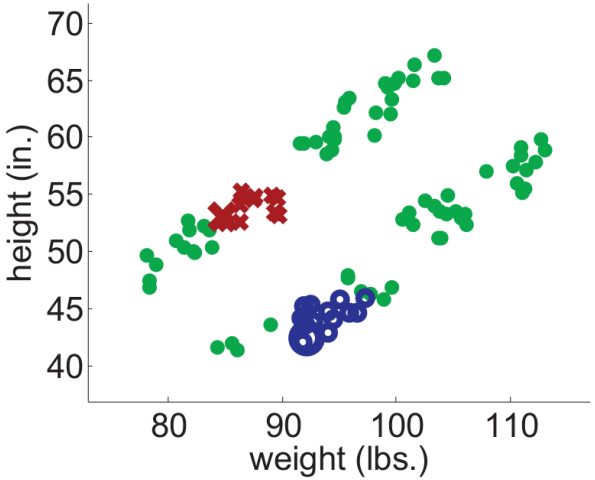
- assumes that the unlabeled data is useful
- works with data geometry assumptions
  - cluster assumption - low-density separation
  - manifold assumption
  - smoothness assumptions, generative models, ...
- now it helps now, now it does not (sic)
  - provable cases when it helps
- inductive or transductive/out-of-sample extension

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

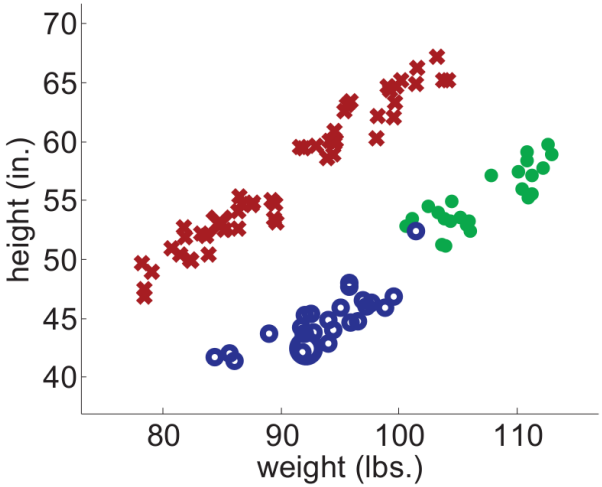
SSL: Self-Training



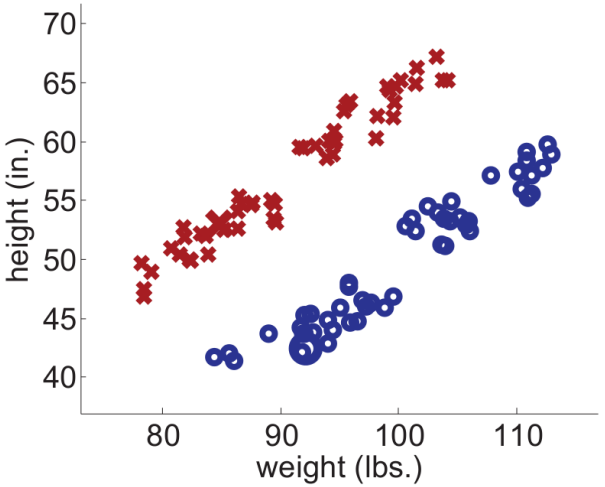
(a) Iteration 1



(b) Iteration 25



(c) Iteration 74



(d) Final labeling of all instances

SSL: Overview: Self-Training

SSL: Self-Training

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

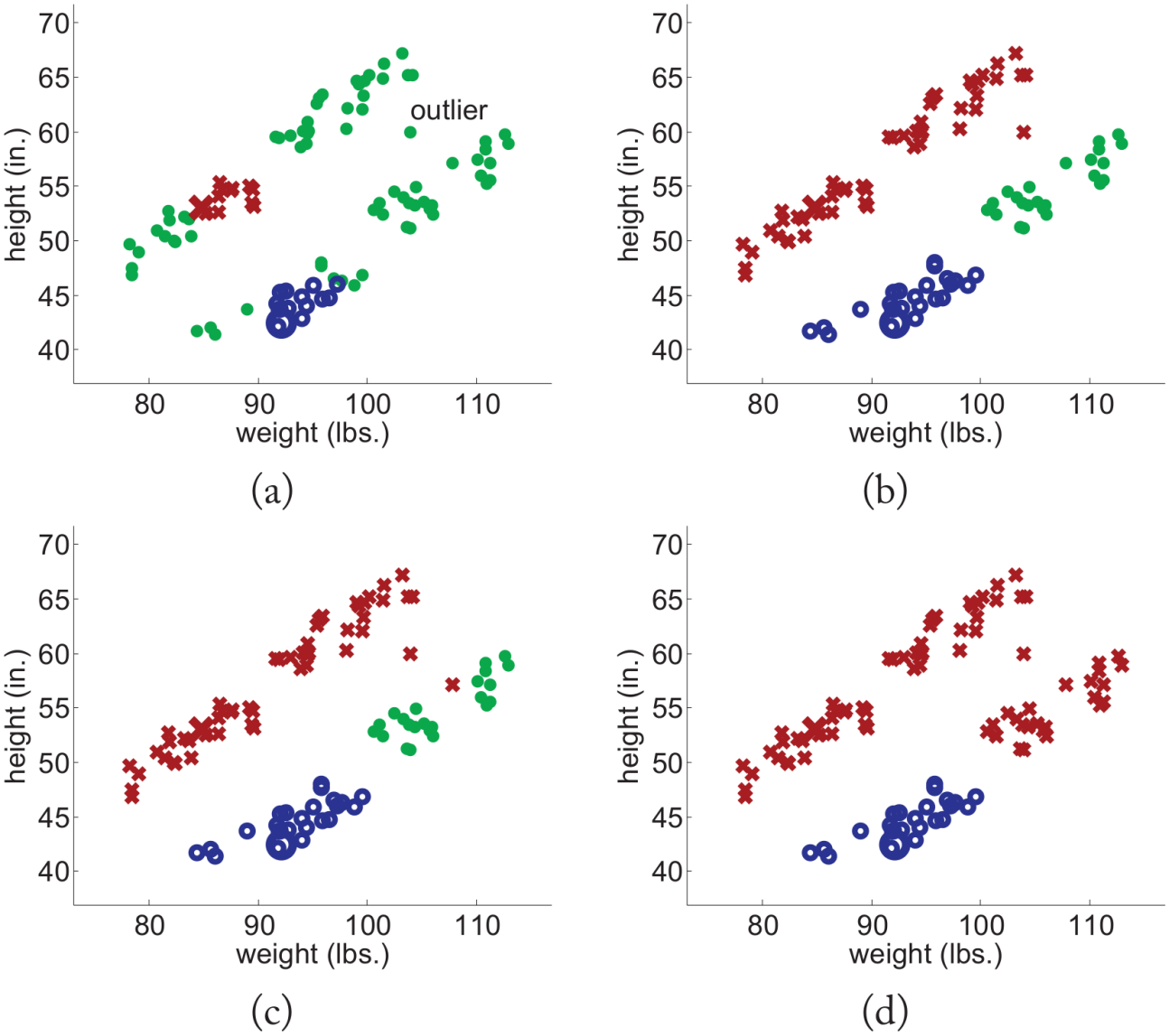
Repeat:

- train f using $\mathcal{L}$
- apply f to (some) $\mathcal{U}$ and add them to $\mathcal{L}$

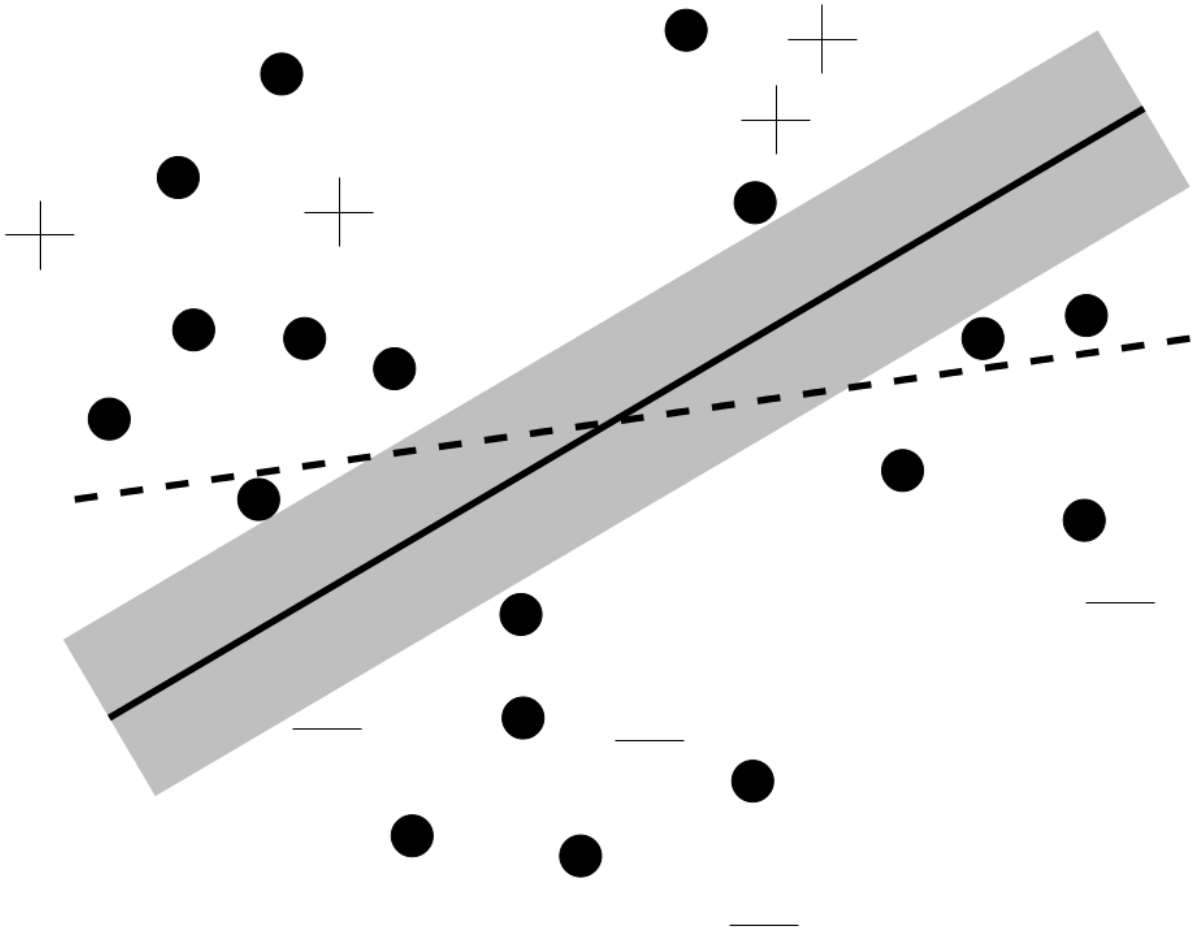
What are the properties of self-training?

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

SSL: Self-Training: Bad Case



SSL: Transductive SVM: S3VM



SSL: Transductive SVM: Classical SVM

Linear case: $f = \mathbf{w}^\top \mathbf{x} + b \quad \rightarrow \quad$ we look for $(\mathbf{w}, b)$

max-margin classification

$$\begin{aligned} \max_{\mathbf{w},b} \quad & \frac{1}{\|\mathbf{w}\|} \\ s.t. \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 \quad \forall i = 1, \ldots, n_l \end{aligned}$$

max-margin classification

$$\begin{aligned} \min_{\mathbf{w},b} \quad & \|\mathbf{w}\|^2 \\ s.t. \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 \quad \forall i = 1, \ldots, n_l \end{aligned}$$

SSL: Transductive SVM: Classical SVM

max-margin classification: separable case

$$\begin{aligned} \min_{\mathbf{w},b} \quad & \|\mathbf{w}\|^2 \\ s.t. \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 \quad \forall i = 1, \ldots, n_l \end{aligned}$$

max-margin classification: non-separable case

$$\begin{aligned} \min_{\mathbf{w},b} \quad & \lambda\|\mathbf{w}\|^2 + \sum_i \xi_i \\ s.t. \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \quad \forall i = 1, \ldots, n_l \\ & \xi_i \geq 0 \quad \forall i = 1, \ldots, n_l \end{aligned}$$

SSL: Transductive SVM: Classical SVM

max-margin classification: non-separable case

$$\begin{aligned} \min_{\mathbf{w},b} \quad & \lambda\|\mathbf{w}\|^2 + \sum_i \xi_i \\ s.t. \quad & y_i(\mathbf{w}^\mathsf{T}\mathbf{x}_i + b) \geq 1 - \xi_i \quad \forall i = 1, \ldots, n_l \\ & \xi_i \geq 0 \quad \forall i = 1, \ldots, n_l \end{aligned}$$

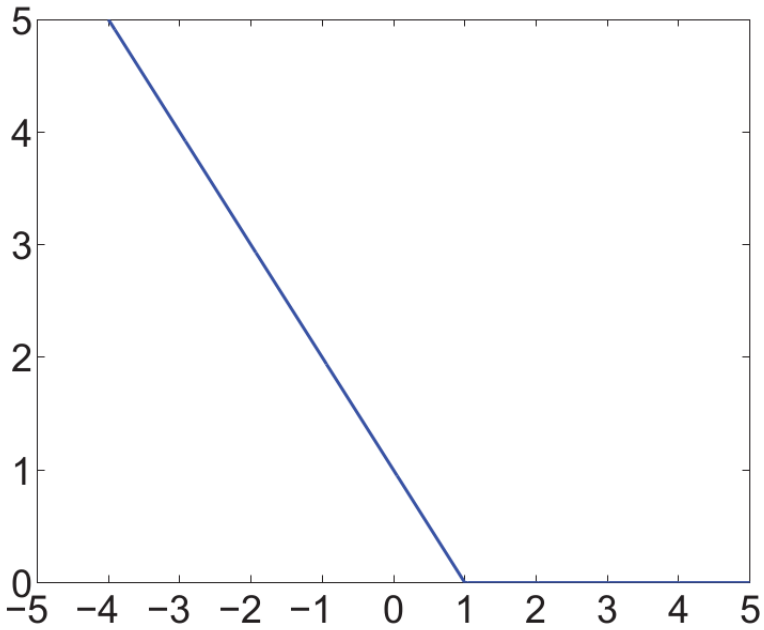
Unconstrained formulation using **hinge loss**:

$$\min_{\mathbf{w},b} \sum_i^{n_l} \max\left(1 - y_i\left(\mathbf{w}^\mathsf{T}\mathbf{x}_i + b\right), 0\right) + \lambda\|\mathbf{w}\|^2$$

In general?

$$\min_{\mathbf{w},b} \sum_i^{n_l} V(\mathbf{x}_i, y_i, f\left(\mathbf{x}_i\right)) + \lambda\Omega(f)$$

SSL: Transductive SVM: Classical SVM: Hinge loss



(a) the hinge loss

$$V(\mathbf{x}_i, y_i, f(\mathbf{x}_i)) = \max(1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b), 0)$$

SSL: Transductive SVM: Unlabeled Examples

$$\min_{\mathbf{w},b} \sum_{i}^{n_l} \max\left(1 - y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right), 0\right) + \lambda \|\mathbf{w}\|^2$$

How to incorporate unlabeled examples?

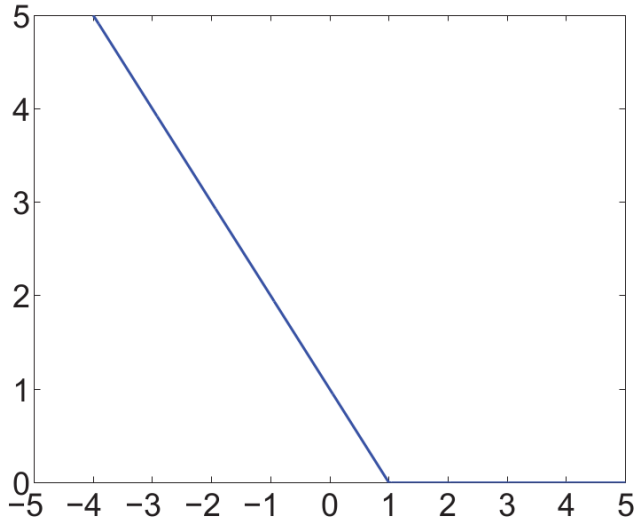
No y's for unlabeled $\mathbf{x}$.

Prediction of f for (any) $\mathbf{x}$? $\widehat{y} = \operatorname{sgn}\left(f\left(\mathbf{x}\right)\right) = \operatorname{sgn}\left(\mathbf{w}^\top \mathbf{x} + b\right)$

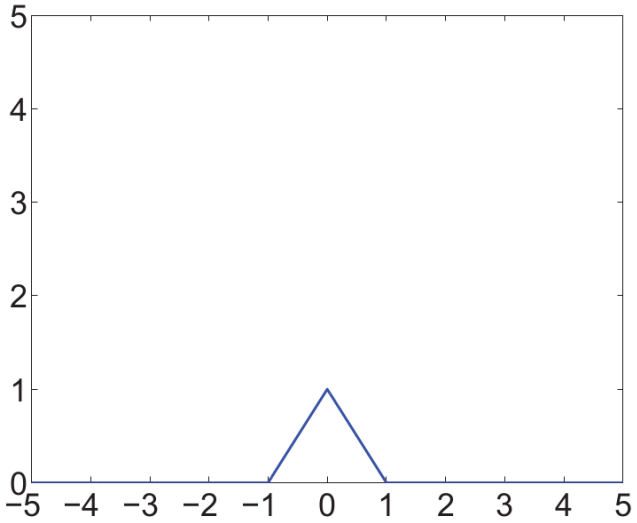
Pretending that $\operatorname{sgn}\left(f\left(\mathbf{x}\right)\right)$ is the true label ...

$$\begin{aligned} V(\mathbf{x}, \widehat{y}, f\left(\mathbf{x}\right)) &= \max\left(1 - \widehat{y}\left(\mathbf{w}^\top \mathbf{x} + b\right), 0\right) \\ &= \max\left(1 - \operatorname{sgn}\left(\mathbf{w}^\top \mathbf{x} + b\right)\left(\mathbf{w}^\top \mathbf{x} + b\right), 0\right) \\ &= \max\left(1 - \left|\mathbf{w}^\top \mathbf{x} + b\right|, 0\right) \end{aligned}$$

SSL: Transductive SVM: Hinge and Hat Loss



(a) the hinge loss



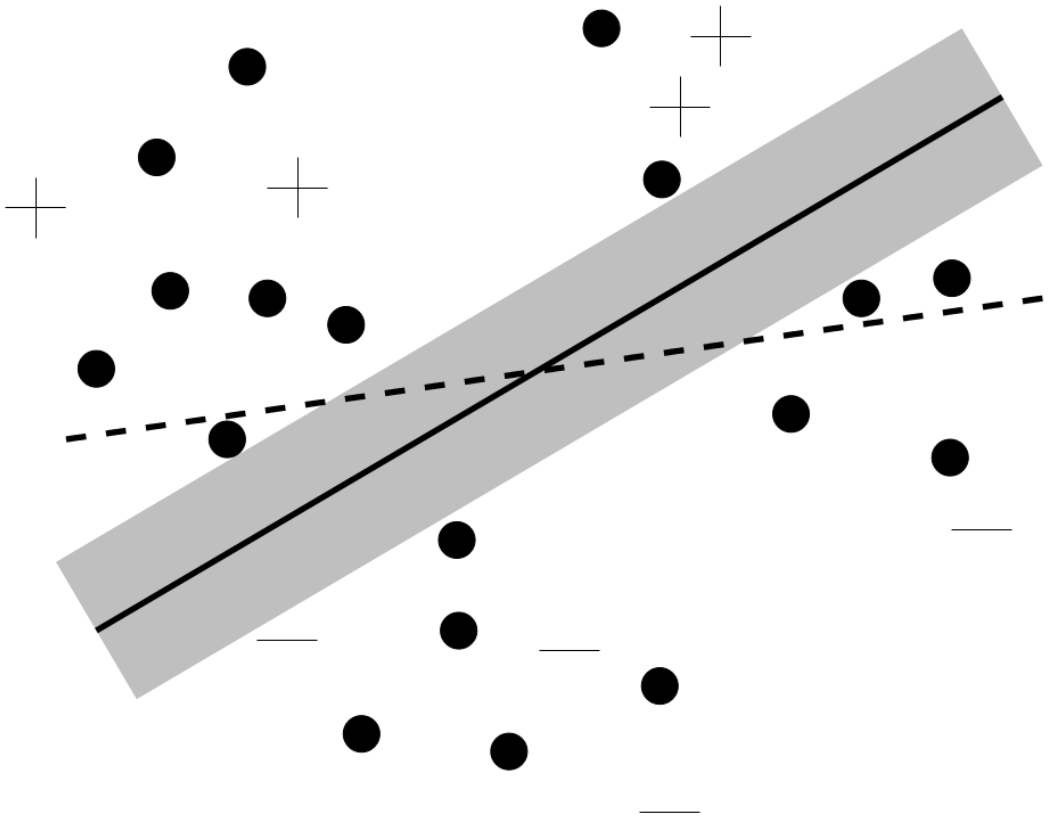
(b) the hat loss

What is the difference in the objectives?

Hinge loss penalizes?

Hat loss penalizes?

SSL: Transductive SVM: S3VM



This is what we wanted!

SSL: Transductive SVM: Formulation

Main SVM idea stays the same: penalize the margin

$$\min_{\mathbf{w},b} \sum_{i=1}^{n_l} \max\left(1 - y_i\left(\mathbf{w}^\mathsf{T}\mathbf{x}_i + b\right), 0\right) + \lambda_1 \|\mathbf{w}\|^2 + \lambda_2 \sum_{i=l+1}^{n_l+n_u} \max\left(1 - |\mathbf{w}^\mathsf{T}\mathbf{x}_i + b|, 0\right)$$

What is the loss and what is the regularizer?

$$\min_{\mathbf{w},b} \sum_{i=1}^{n_l} \max\left(1 - y_i\left(\mathbf{w}^\mathsf{T}\mathbf{x}_i + b\right), 0\right) + \lambda_1 \|\mathbf{w}\|^2 + \lambda_2 \sum_{i=l+1}^{n_l+n_u} \max\left(1 - |\mathbf{w}^\mathsf{T}\mathbf{x}_i + b|, 0\right)$$

Think of **unlabeled data** as the **regularizers** for your classifiers!

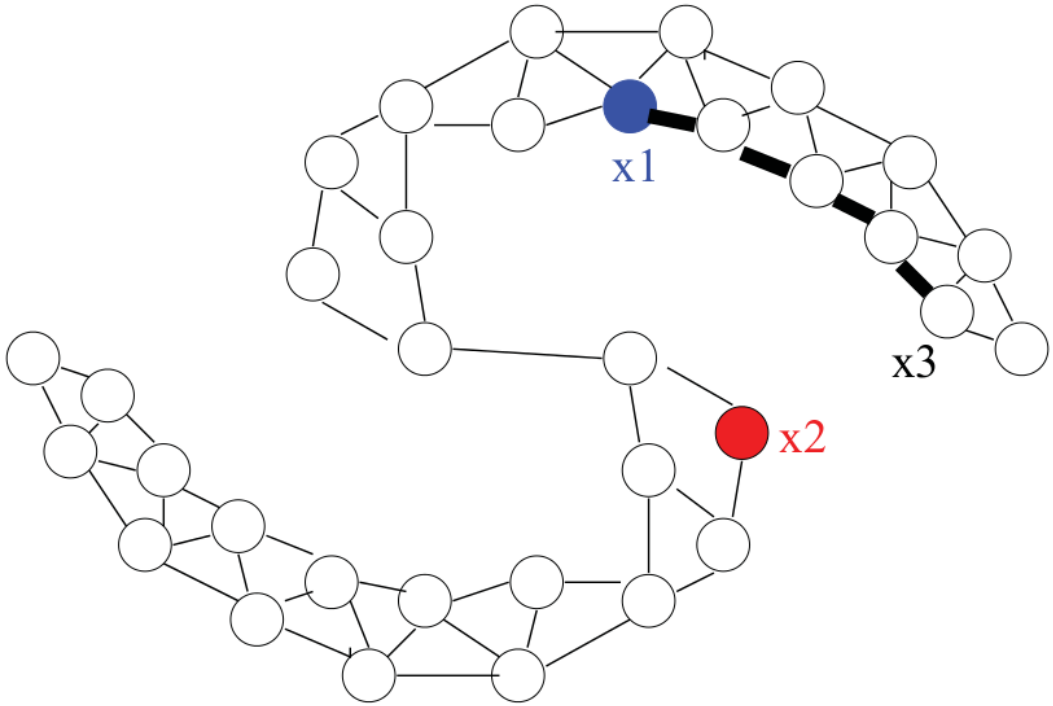
Practical hint: Additionally enforce the class balance.

What it the main issue of TSVM?

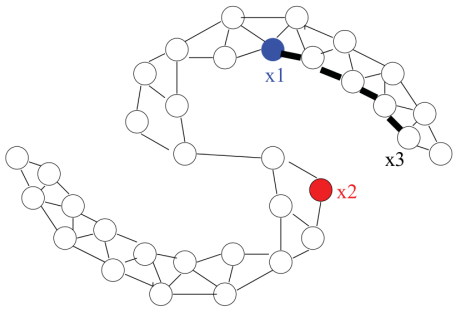
SSL with Graphs: Prehistory

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

Where is the link?

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

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

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

SSL with Graphs: MinCut

We look for $f(\mathbf{x}) \in \{\pm 1\}$

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

Clustering was unsupervised, here we have supervised data.

Recall the general objective-function framework:

$$\min_{\mathbf{w},b} \sum_{i}^{n_l} V(\mathbf{x}_i, y_i, f(\mathbf{x}_i)) + \lambda \Omega(\mathbf{f})$$

It would be nice if we match the prediction on labeled data:

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

SSL with Graphs: MinCut

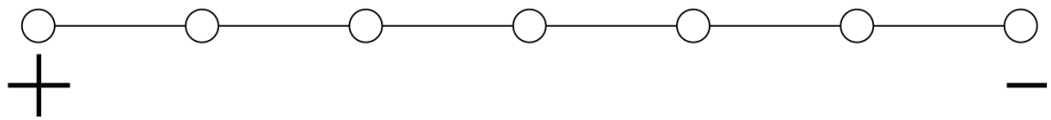
Final objective function:

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

This is an integer program :(

Can we solve it?

Are we happy?



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

`http://mlg.eng.cam.ac.uk/zoubin/papers/zgl.pdf`

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

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

Idea 2: Find a smooth one. (**harmonic** solution)

Harmonic SSL

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

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

2): We enforce the solution f to be harmonic.

$$f(\mathbf{x}_i) = \frac{\sum_{i \sim j} f(\mathbf{x}_j) w_{ij}}{\sum_{i \sim j} w_{ij}} \qquad \forall i \in \{n_l + 1, \dots, n_u + n_l\}$$

SSL with Graphs: Harmonic Functions

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

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

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

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

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

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

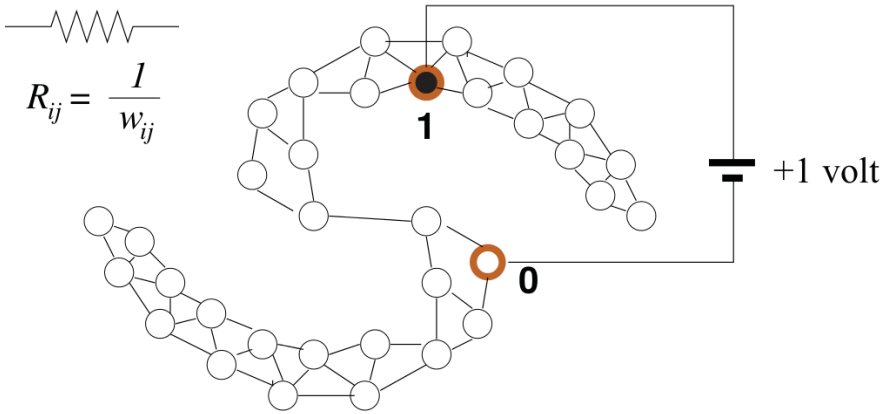
$$s.t. \quad y_i = f(\mathbf{x}_i) \quad \forall i = 1, \ldots, n_l$$

SSL with Graphs: Harmonic Functions

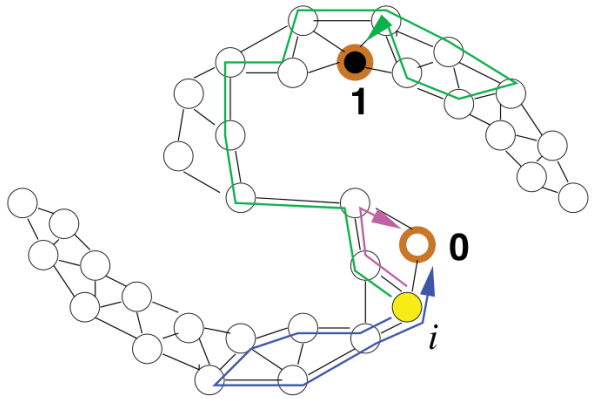
Properties of the relaxation from ± 1 to $\mathbb{R}$

- there is a closed form solution for f
- this solution is unique
- globally optimal
- it is either constant or has a maximum/minimum on a boundary
- $f(\mathbf{x}_i)$ may not be discrete
  - but we can threshold it
- electric networks interpretation
- random walk interpretation

SSL with Graphs: Harmonic Functions



(a) The electric network interpretation



(b) The random walk interpretation

Random walk interpretation:

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

2) $P(j|i) = \frac{w_{ij}}{\sum_k w_{ik}} \quad \equiv \quad \mathbf{P} = \mathbf{D}^{-1}\mathbf{W}$

3) finish when the labeled vertex is hit

absorbing random walk

f_i = probability of reaching a positive labeled vertex

SSL with Graphs: Harmonic Functions

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

Step 1: Set $f(\mathbf{x}_i) = y_i$ for $i = 1, \ldots, n_l$
Step 2: Propagate iteratively (only for unlabeled)

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

Properties:

- 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

Define $\mathbf{f} = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_{n_l+n_u})) = (f_1, \ldots, f_{n_l+n_u})$

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

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

$$\mathbf{L} = \begin{bmatrix} \mathbf{L}_{ll} & \mathbf{L}_{lu} \\ \mathbf{L}_{u1} & \mathbf{L}_{uu} \end{bmatrix}$$

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

SSL with Graphs: Harmonic Functions

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

How did we formalize the harmonic property of a circuit?

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

In matrix notation

$$\begin{bmatrix} \mathbf{L}_{ll} & \mathbf{L}_{lu} \\ \mathbf{L}_{ul} & \mathbf{L}_{uu} \end{bmatrix} \begin{bmatrix} \mathbf{f}_l \\ \mathbf{f}_u \end{bmatrix} = \begin{bmatrix} \dots \\ \mathbf{0}_u \end{bmatrix}$$

$\mathbf{f}_l$ is constrained to be $\mathbf{y}_l$ and for $\mathbf{f}_u$ .....

$$\mathbf{L}_{ul}\mathbf{f}_l + \mathbf{L}_{uu}\mathbf{f}_u = \mathbf{0}_u$$

. . . from which we get

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

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

SSL with Graphs: Harmonic Functions

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

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

Note that $\mathbf{P} = \mathbf{D}^{-1}\mathbf{W}$. Then equivalently

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

Split the equation into +ve & -ve part:

$$\begin{aligned} f_i &= (\mathbf{I} - \mathbf{P}_{uu})^{-1}_{iu}\mathbf{P}_{ul}\mathbf{f}_l \\ &= \underbrace{\sum_{j:y_j=1} (\mathbf{I} - \mathbf{P}_{uu})^{-1}_{iu}\mathbf{P}_{uj}}_{p_i^{(+1)}} - \underbrace{\sum_{j:y_j=-1} (\mathbf{I} - \mathbf{P}_{uu})^{-1}_{iu}\mathbf{P}_{uj}}_{p_i^{(-1)}} \\ &= p_i^{(+1)} - p_i^{(-1)} \end{aligned}$$

SSL with Graphs: Regularized Harmonic Functions

$$f_i = p_i^{(+1)} - p_i^{(-1)} \qquad \Longrightarrow \quad f_i = \underbrace{|f_i|}_{\text{confidence}} \times \underbrace{\text{sgn}(f_i)}_{\text{label}}$$

What if a nasty outlier sneaks in?

The prediction for the outlier can be hyperconfident :(

How to control the confidence of the inference?

Allow the random walk to **die**!

We add a **sink** to the graph.

sink = artificial label node with value 0

We connect it to every other vertex.

What will this do to our predictions?

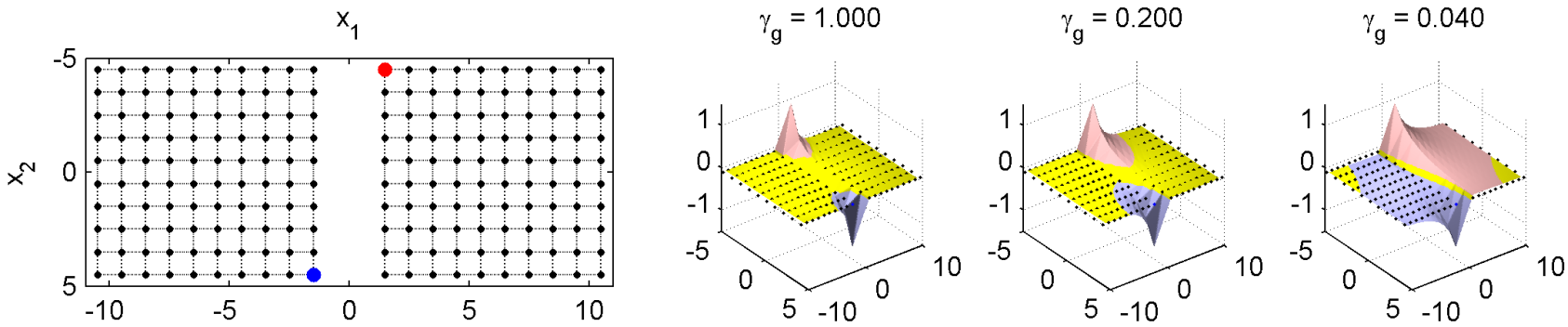
depends on the weigh on the edges

SSL with Graphs: Regularized Harmonic Functions

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

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

How does γ_g influence HS?



What happens to sneaky outliers?

SSL with Graphs: Harmonic Functions

Why don't we represent the sink in $\mathbf{L}$ explicitly?

Formally, to get the harmonic solution on the graph with sink ...

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

$$\mathbf{L}_{ul}\mathbf{f}_l + (\mathbf{L}_{uu} + \gamma_G \mathbf{I}_{n_u})\,\mathbf{f}_u = \mathbf{0}_u$$

... which is the same if we disregard the last column and row ...

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

... and therefore we simply add γ_G to the diagonal of $\mathbf{L}$!

SSL with Graphs: Soft Harmonic Functions

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

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

What if we do not really believe that $f(\mathbf{x}_i) = y_i$, $\forall i$?

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

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

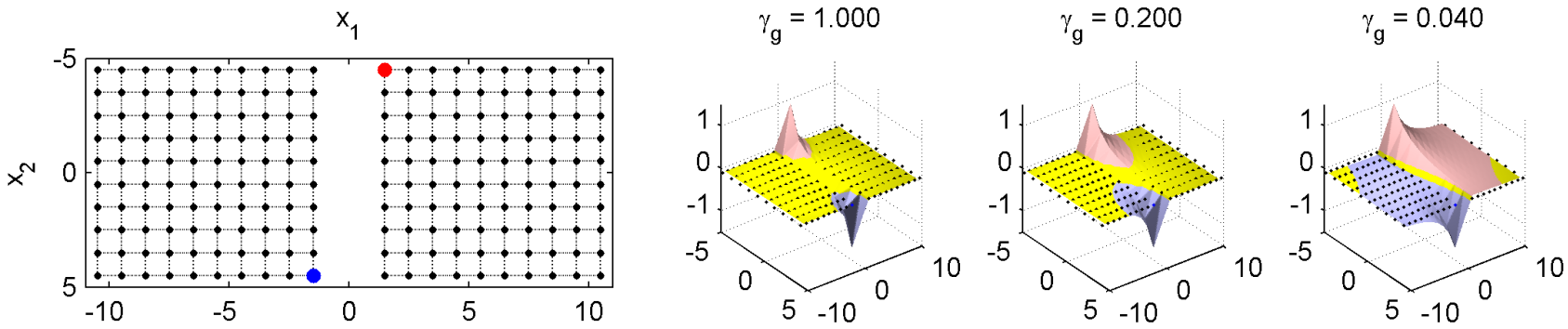
$\mathbf{y} \equiv$ pseudo-targets with $y_i = \begin{cases} \text{true label} & \text{for labeled examples} \\ 0 & \text{otherwise.} \end{cases}$

SSL with Graphs: Soft Harmonic Functions

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

Closed form **soft harmonic solution**:

$$\mathbf{f}^\star = (\mathbf{C}^{-1}\mathbf{Q} + \mathbf{I})^{-1}\mathbf{y}$$



What are the differences between hard and soft?

Not much different in practice.

Provable generalization guarantees for soft.

SSL with Graphs: Regularized Harmonic Functions

Larger implications of random walks

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

($\star$) Vertices in the same cluster of the graph have a small commute distance, whereas two vertices in different clusters of the graph have a "large" commute distance.

Do we have this property for HS? What if $n \to \infty$?

Luxburg/Radl/Hein: *Getting lost in space: Large sample analysis of the commute distance* `http://www.informatik.uni-hamburg.de/ML/contents/people/luxburg/publications/LuxburgRadlHein2010_PaperAndSupplement.pdf`

Solutions? 1) γ_g 2) amplified commute distance 3) $\mathbf{L}^p$ 4) $\mathbf{L}^\star$ ...

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

SSL with Graphs: Out of sample extension

Both **MinCut** and **HFS** only inferred the labels on unlabeled data.

They are **transductive**.

What if a new point $\mathbf{x}_{n_l+n_u+1}$ arrives? also called out-of-sample extension

Option 1) Add it to the graph and recompute HFS.

Option 2) Make the algorithms **inductive**!

Allow to be defined everywhere: $f : \mathcal{X} \mapsto \mathbb{R}$
Allow $f(\mathbf{x}_i) \neq y_i$. Why? To deal with noise.

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**.

$$\Omega(f) = \lambda_2 \mathbf{f}^\top \mathbf{L} \mathbf{f} + \lambda_1 \int_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})^2 \, \mathrm{d}\mathbf{x}$$

For general **kernels**:

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

SSL with Graphs: Manifold Regularization

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

Representer Theorem for Manifold Regularization

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

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

$V\left(\mathbf{x}, y, f\right) = \left(y - f\left(\mathbf{x}\right)\right)^2$

LapRLS Laplacian Regularized Least Squares

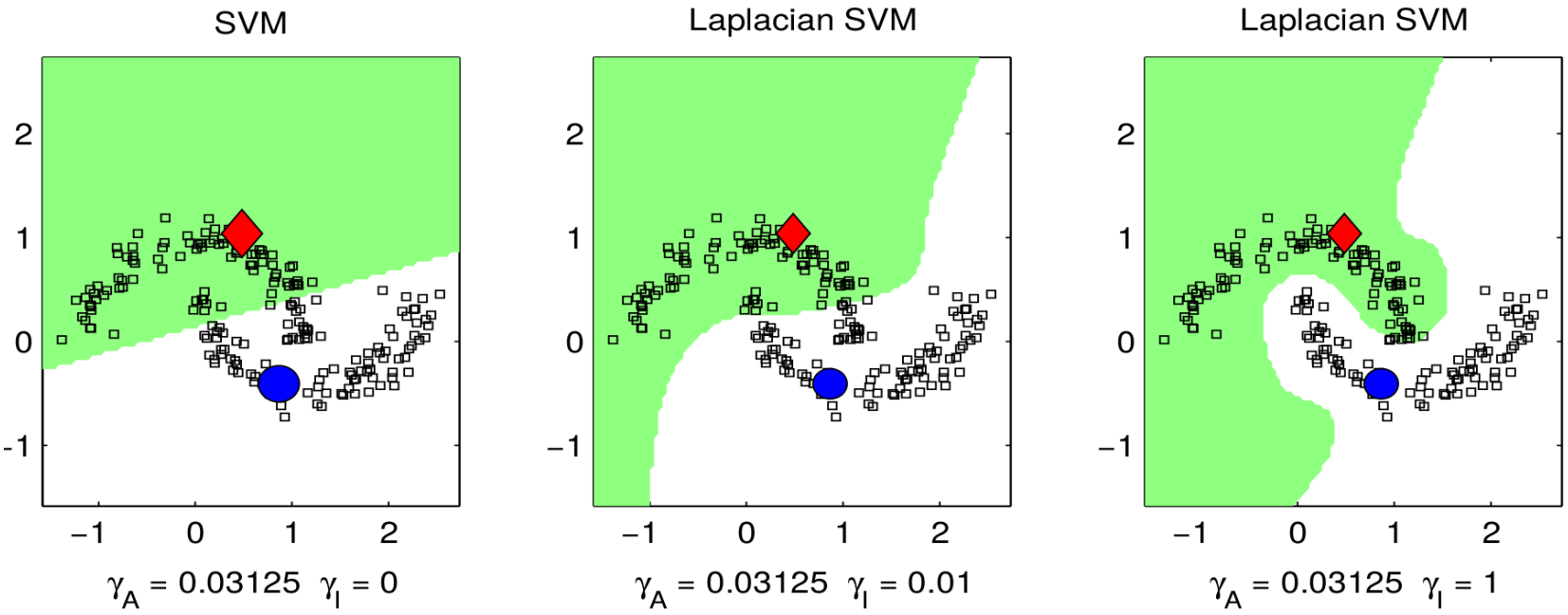
$V\left(\mathbf{x}, y, f\right) = \max\left(0, 1 - yf\left(\mathbf{x}\right)\right)$

LapSVM Laplacian Support Vector Machines

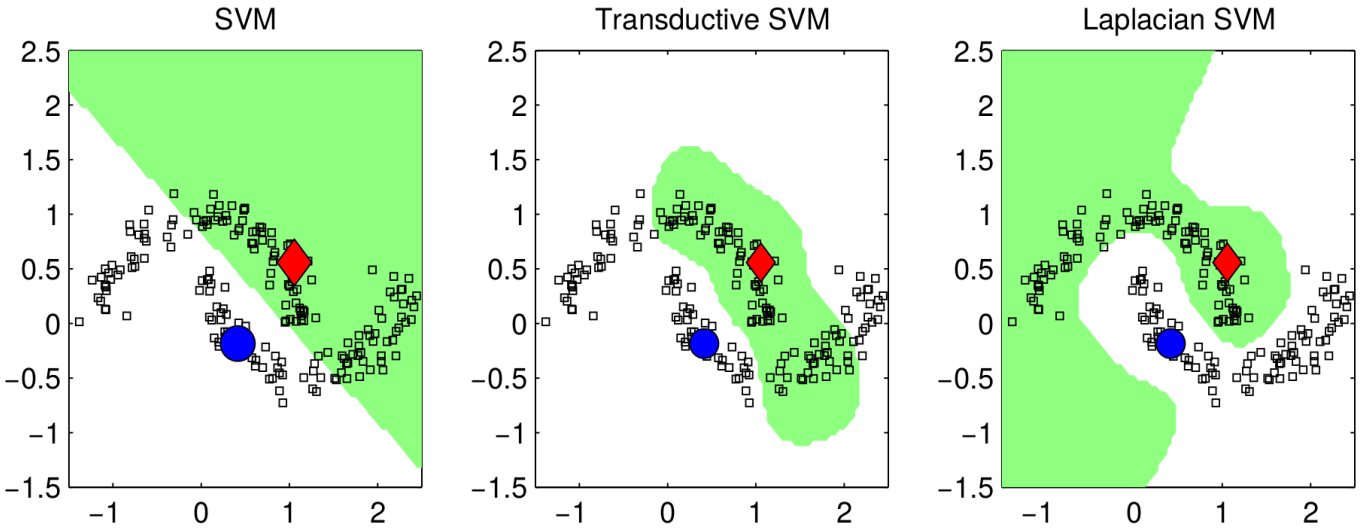
SSL with Graphs: Laplacian SVMs

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

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



SSL with Graphs: Laplacian SVMs



Michal Valko
michal.valko@inria.fr
sequel.lille.inria.fr

SequeL – Inria Lille

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