

Graphs in Machine Learning

Daniele Calandriello

DeepMind Paris, France

Collaborators: Achraf Azize,
Michal Valko

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



Previous lecture

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

This lecture *Deeper in the theory*

- ▶ transductive learning stability based bounds
- ▶ analysis of inductive and transductive semi-supervised learning
- ▶ online semi-supervised Learning
- ▶ online incremental k -centers
- ▶ Analysis of online SSL
- ▶ SSL learnability
- ▶ When does graph-based SSL provably help?

SSL(\mathcal{G})

semi-supervised learning with
graphs and harmonic functions

...our running example for learning with graphs

Checkpoint 2

Unconstrained regularization in general ($\mathbf{C} = \text{diag}(\{c_l, c_u\})$, $\mathbf{Q} = \mathbf{L} + \gamma_g \mathbf{I}$):

conducting case
with N datapoints
(m labelled and $n - m$ unlabelled)

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

Checkpoint 2

+ $\frac{1}{2}$
- $\frac{1}{2}$
0
↓

Unconstrained regularization in general ($\mathbf{C} = \text{diag}(\{c_l, c_u\})$, $\mathbf{Q} = \mathbf{L} + \gamma_g \mathbf{I}$):

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

diag

contain Laplacian and γ_g
that are regularizers

Out of sample extension: Laplacian SVMs

↳ predict new datapoints that are arriving

$$f^* = \arg \min_{f \in \mathcal{H}_K} \sum_i^{n_l} \max(0, 1 - y f(\mathbf{x})) + \gamma_1 \|f\|_K^2 + \gamma_2 \mathbf{f}^\top \mathbf{L} \mathbf{f}$$

Transductive Generalization Bounds

check stability

True risk vs. empirical risk

true risk $\rightarrow R_N(f) = \frac{1}{N} \sum_i (f_i - y_i)^2$

empirical risk $\rightarrow \hat{R}_N(f) = \frac{1}{n_I} \sum_{i \in I} (f_i - y_i)^2$

Transductive Generalization Bounds

True risk vs. empirical risk

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We look for **transductive** bounds in the form

$$R_N(f) \leq \hat{R}_N(f) + \text{errors}$$

what we want: empirical rule & true rule

Transductive Generalization Bounds

Bounding transductive error using stability analysis (in our case Belkin [BMN04])

<http://www.cs.nyu.edu/~mohri/pub/str.pdf>

http://web.cse.ohio-state.edu/~mbelkin/papers/RSS_COLT_04.pdf

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one false point as cliff

(Informal) let β be the maximal difference $\|\ell_2^* - \ell_1^*\|_\infty \leq \beta$ between solutions

$$\ell_1^* = (\mathbf{C}_1^{-1} \mathbf{Q} + \mathbf{I})^{-1} \mathbf{y}_1 \text{ and } \ell_2^* = (\mathbf{C}_2^{-1} \mathbf{Q} + \mathbf{I})^{-1} \mathbf{y}_2$$

for two datasets differing in exactly one *labeled* point. Then w.p. $1 - \delta$

The rest are coming from the unlabeled points

Transductive Generalization Bounds

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stability considerations, if β big is not stable

$$R_N(\ell^*) \leq \widehat{R}_N(\ell^*) + \underbrace{\beta + \sqrt{\frac{2 \ln(2/\delta)}{n_I} (n_I \beta + 4)}}_{\text{transductive error } \Delta_T(\beta, n_I, \delta)}.$$

Transductive Generalization Bounds

Stability analysis from last class

$$\|\ell_2^* - \ell_1^*\|_\infty$$

Transductive Generalization Bounds

Stability analysis from last class

$$\|\ell_2^* - \ell_1^*\|_\infty \leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right) \left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)}$$

*the stability
depends on the
labels, laplacian
and symmetry*

Transductive Generalization Bounds

Stability analysis from last class

$$\begin{aligned}\|\ell_2^* - \ell_1^*\|_\infty &\leq \frac{\|\mathbf{y}_2 - \mathbf{y}_1\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1} + \frac{\lambda_M(\mathbf{Q})\|\mathbf{C}_1^{-1} - \mathbf{C}_2^{-1}\|_2 \cdot \|\mathbf{y}_1\|_2}{\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_2)} + 1\right)\left(\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C}_1)} + 1\right)} \\ &\leq 2 \left[\frac{\sqrt{2}}{\gamma_g + 1} + \sqrt{2n_I} \frac{1 - c_u}{c_u} \frac{\lambda_M(\mathbf{L}) + \gamma_g}{\gamma_g^2 + 1} \right] \stackrel{\text{def}}{=} \beta\end{aligned}$$

reg of laplacian

Transductive Generalization Bounds

Stability analysis from last class

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Soft HFS is β -stable!

Transductive Generalization Bounds

$$R_N(\ell^*) \leq \hat{R}_N(\ell^*) + \beta + \sqrt{\frac{2 \ln(2/\delta)}{n_I}}(n_I\beta + 4), \quad \beta \leq 2 \left[\frac{\sqrt{2}}{\gamma_g + 1} + \sqrt{2n_I} \frac{1 - c_u}{c_u} \frac{\lambda_M(\mathbf{L}) + \gamma_g}{\gamma_g^2 + 1} \right]$$

Does the bound say anything useful?

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Does the bound say anything useful?

- 1) The error is controlled. as it is not infinite we can regularize a lot or get more data.

Transductive Generalization Bounds

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We have an idea how to set γ_g !

What about inductive error?

SSL with Graphs: Laplacian SVMs

$$f^* = \arg \min_{f \in \mathcal{H}_{\mathcal{K}}} \sum_i^{n_I} \max(0, 1 - y f(\mathbf{x})) + \gamma_1 \|f\|_{\mathcal{K}}^2 + \gamma_2 \mathbf{f}^\top \mathbf{L} \mathbf{f}$$

$\mathcal{H}_{\mathcal{K}}$ is nice and expressive.

SSL with Graphs: Laplacian SVMs

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Can there be a problem with certain $\mathcal{H}_{\mathcal{K}}$?

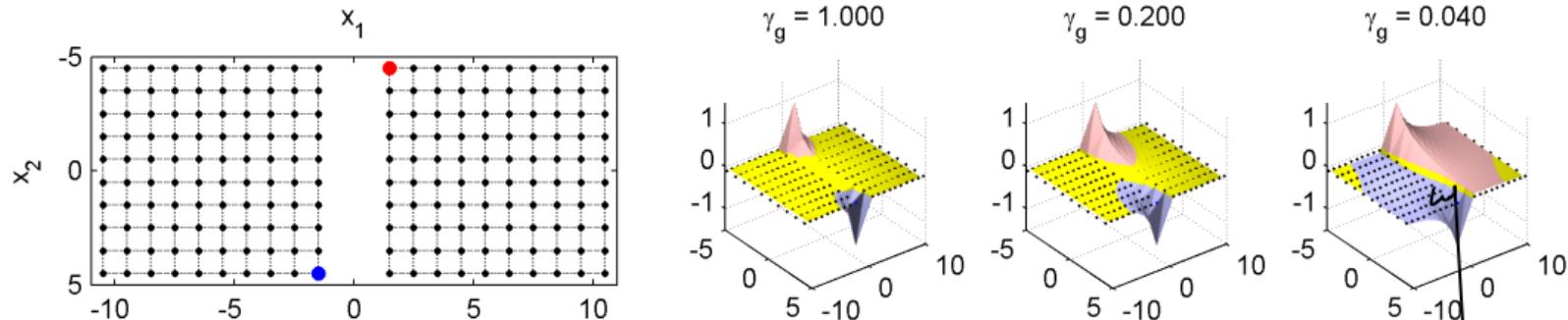
SSL with Graphs: Laplacian SVMs

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$\mathcal{H}_{\mathcal{K}}$ is nice and expressive.

Can there be a problem with certain $\mathcal{H}_{\mathcal{K}}$?

We look for f only in $\mathcal{H}_{\mathcal{K}}$. If it is simple (e.g., **linear**) minimization of $\mathbf{f}^T \mathbf{L} \mathbf{f}$ can perform badly.



SSL with Graphs: Laplacian SVMs

Linear \mathcal{K} \equiv functions $f(x_i) = \alpha_1 x_{i1} + \alpha_2 x_{i2}$. - \rightarrow space of function with 2 param α_1, α_2 $\in \mathbb{R}$

SSL with Graphs: Laplacian SVMs

Linear $\mathcal{K} \equiv$ functions $f(x_i) = \alpha_1 x_{i1} + \alpha_2 x_{i2}$.

$$\min_{\alpha_1, \alpha_2} \sum_i^{n_I} V(f, \mathbf{x}_i, y_i) + \gamma_1$$

SSL with Graphs: Laplacian SVMs

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$$\min_{\alpha_1, \alpha_2} \sum_i^{n_I} V(f, \mathbf{x}_i, y_i) + \gamma_1 [\alpha_1^2 + \alpha_2^2] + \gamma_2 \mathbf{f}^\top \mathbf{L} \mathbf{f}$$

SSL with Graphs: Laplacian SVMs

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For this simple case (only vertical/horizontal edges) we can write down $\mathbf{f}^\top \mathbf{L} \mathbf{f}$ explicitly.

SSL with Graphs: Laplacian SVMs

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$$\mathbf{f}^\top \mathbf{L} \mathbf{f} = \frac{1}{2} \sum_{i,j} w_{ij} (f(\mathbf{x}_i) - f(\mathbf{x}_j))^2$$

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SSL with Graphs: Laplacian SVMs

2D data and linear \mathcal{K} objective

$$\min_{\alpha_1, \alpha_2} \sum_i^{n_f} V(f, \mathbf{x}_i, y_i) + \left(\gamma_1 + \frac{\gamma_2 \Delta}{2} \right) [\alpha_1^2 + \alpha_2^2]$$

SSL with Graphs: Laplacian SVMs

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Setting $\bar{\gamma} = \left(\gamma_1 + \frac{\gamma_2 \Delta}{2} \right)$:

SSL with Graphs: Laplacian SVMs

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SSL with Graphs: Laplacian SVMs

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What does this objective function correspond to?

The Laplacian should add margins but it fails here or I don't

SSL with Graphs: Laplacian SVMs

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SSL with Graphs: Laplacian SVMs

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The only influence of unlabeled data is through $\bar{\gamma}$.

SSL with Graphs: Laplacian SVMs

2D data and linear \mathcal{K} objective

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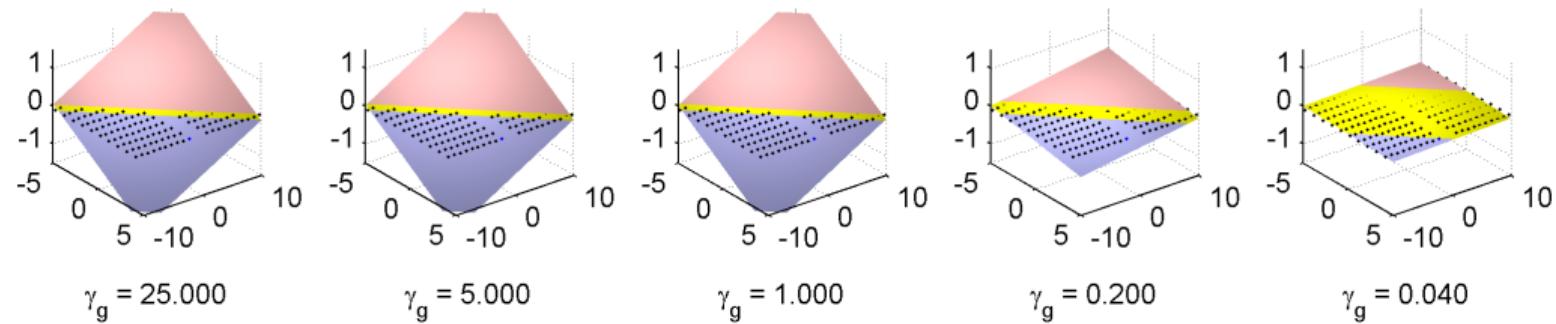
What does this objective function correspond to?

The only influence of unlabeled data is through $\bar{\gamma}$.

The same value of the objective as for supervised learning for some γ **without the unlabeled data!** This is not good.

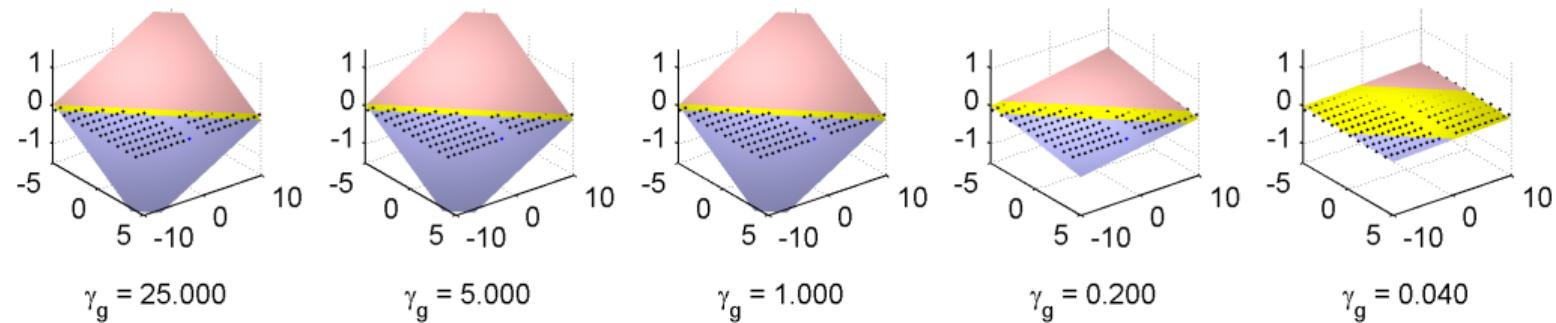
SSL with Graphs: Laplacian SVMs

LSVM for 2D data and linear \mathcal{K} only changes the slope



SSL with Graphs: Laplacian SVMs

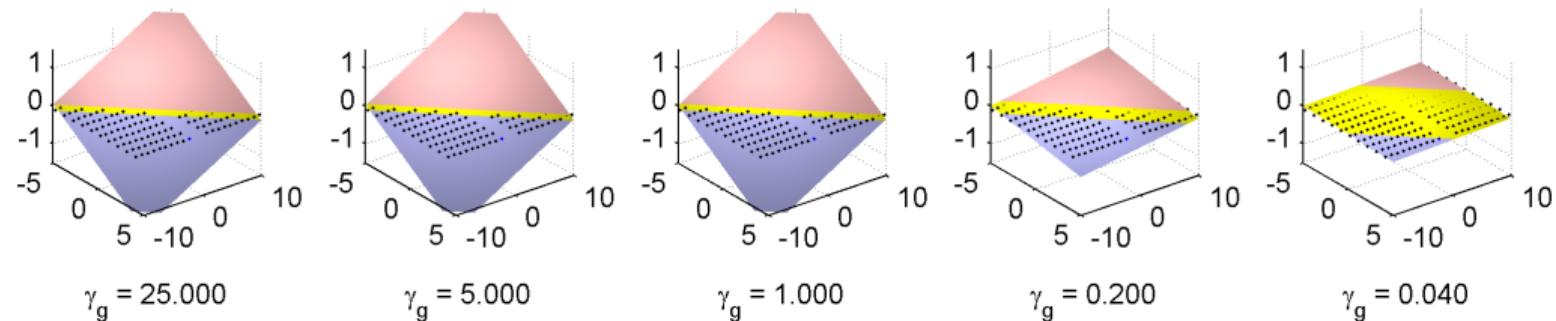
LSVM for 2D data and linear \mathcal{K} only changes the slope



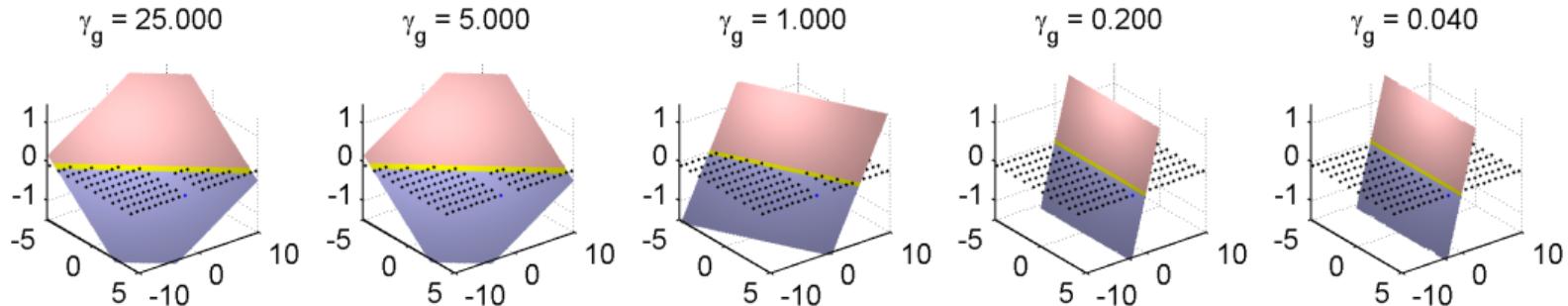
What would we like to see?

SSL with Graphs: Laplacian SVMs

LSVM for 2D data and linear \mathcal{K} only changes the slope

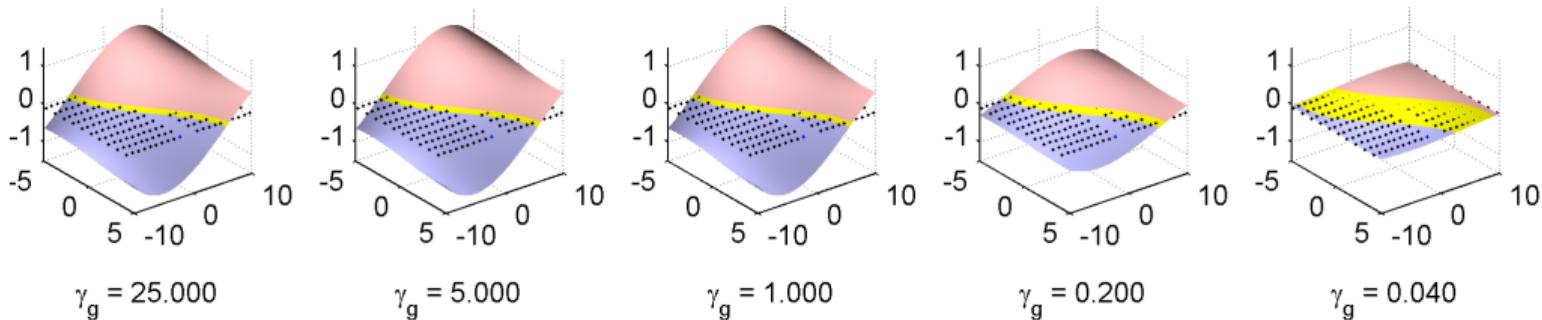


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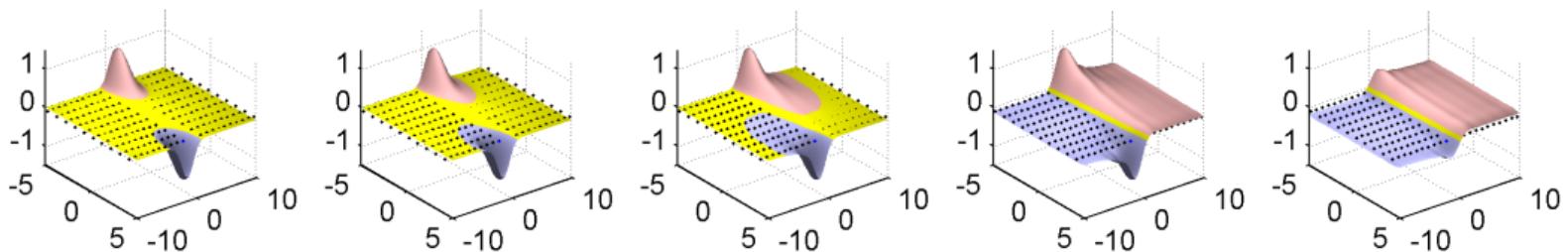
SSL with Graphs: LapSVMs

LapSVM for 2D data and **cubic** \mathcal{K} is also not so good



SSL with Graphs: LapSVMs

LapSVM for 2D data and RBF \mathcal{K}



SSL with Graphs: Max-Margin Graph Cuts

Let's take the confident data and use them as true!

SSL with Graphs: Max-Margin Graph Cuts

Let's take the confident data and use them as true!

$$f^* = \min_{f \in \mathcal{H}_K} \sum_{i: |\ell_i^*| \geq \varepsilon} V(f, \mathbf{x}_i, \text{sgn}(\ell_i^*)) + \gamma \|f\|_K^2$$

$$\text{s.t. } \ell^* = \arg \min_{\ell \in \mathbb{R}^N} \ell^\top (\mathbf{L} + \gamma_g \mathbf{I}) \ell$$

$$\text{s.t. } \ell_i = y_i \text{ for all } i = 1, \dots, n_I$$

involve more thing in error.

If we have problems of
to belong to a class
we put it in our
problem.

SSL with Graphs: Max-Margin Graph Cuts

Let's take the confident data and use them as true!

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Wait, but this is what we did not like in self-training!

SSL with Graphs: Max-Margin Graph Cuts

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Wait, but this is what we did not like in self-training!

Will we get into the same trouble?

SSL with Graphs: Max-Margin Graph Cuts

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$$\begin{aligned} f^* &= \min_{f \in \mathcal{H}_{\mathcal{K}}} \sum_{i: |\ell_i^*| \geq \varepsilon} V(f, \mathbf{x}_i, \text{sgn}(\ell_i^*)) + \gamma \|f\|_{\mathcal{K}}^2 \\ \text{s.t. } \ell^* &= \arg \min_{\ell \in \mathbb{R}^N} \ell^\top (\mathbf{L} + \gamma_g \mathbf{I}) \ell \\ \text{s.t. } \ell_i &= y_i \text{ for all } i = 1, \dots, n_I \end{aligned}$$

Wait, but this is what we did not like in self-training!

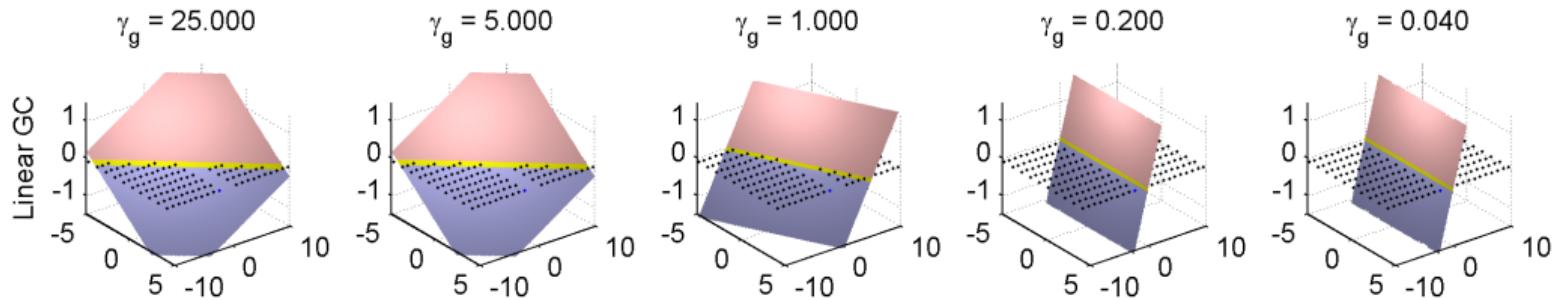
Will we get into the same trouble?

Representer theorem is still cool:

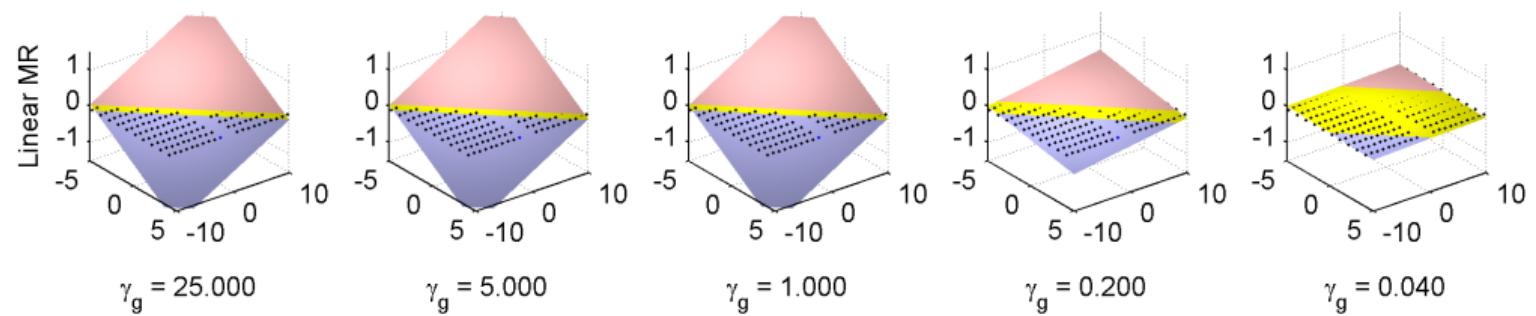
$$f^*(\mathbf{x}) = \sum_{i: |f_i^*| \geq \varepsilon} \alpha_i^* \overset{\text{confidence}}{\downarrow} \mathcal{K}(\mathbf{x}_i, \mathbf{x})$$

SSL with Graphs: LapSVMs and MM Graph Cuts

MMGC for 2D data and **linear** \mathcal{K} works as we want

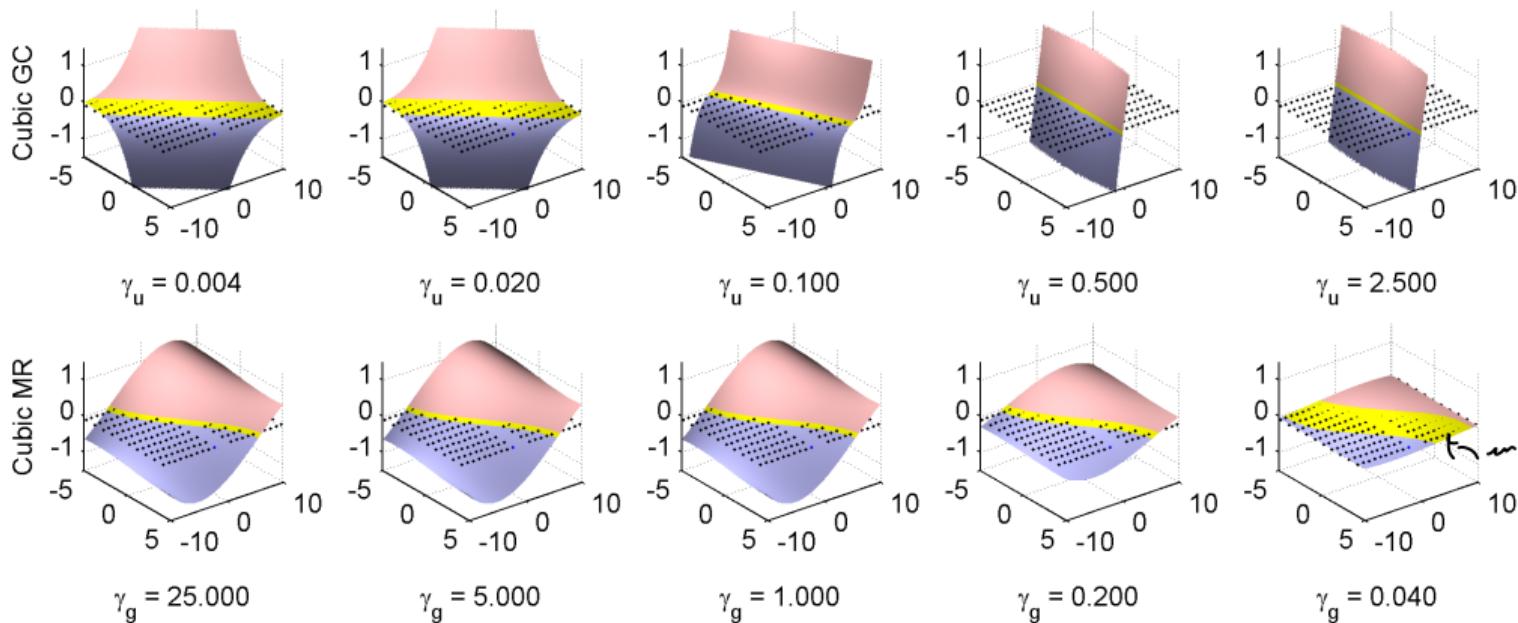


LapSVM for 2D data and **linear** \mathcal{K} only changes the slope



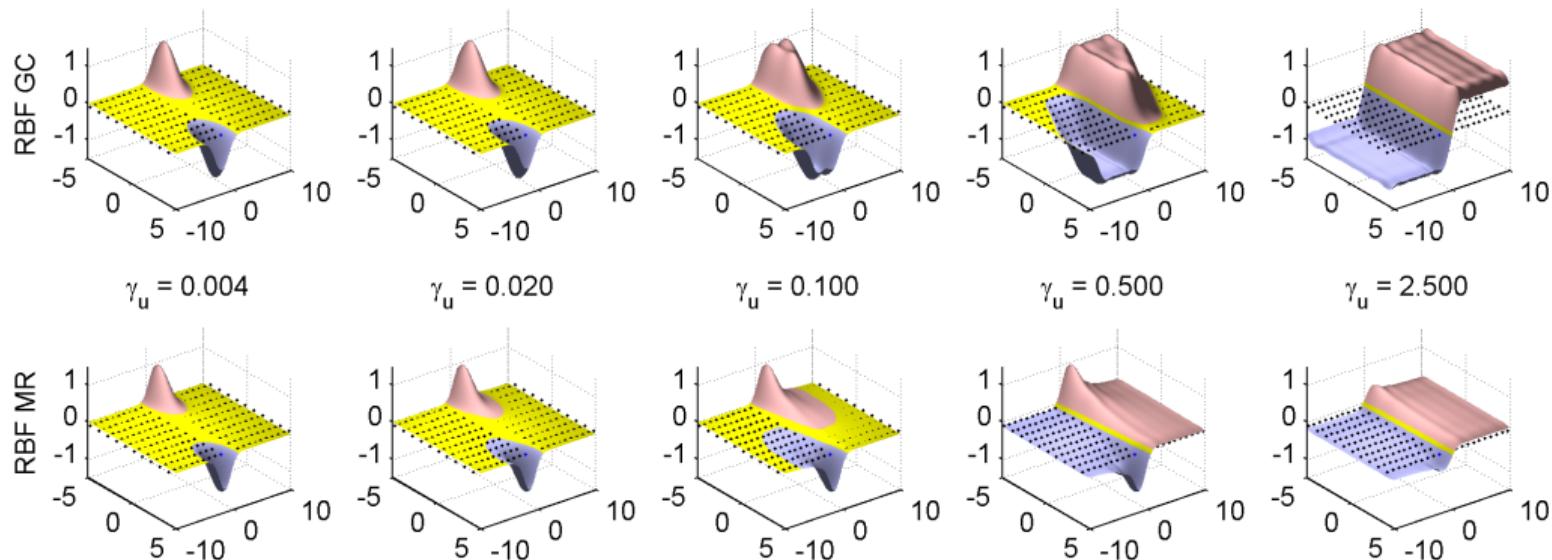
SSL with Graphs: LapSVMs and MM Graph Cuts

MMGC for 2D data and **cubic** \mathcal{K} is good



SSL with Graphs: LapSVMs and MM Graph Cuts

MMGC and LapSVM for 2D data and RBF \mathcal{K}



Inductive Generalization Bounds

We may want to bound the **classification risk** *commissum from hypothesis space*

$$R_P(f, \mathcal{L}) = \mathbb{E}_{P(x)} [\mathcal{L}(f(x), y(x))]$$

↳ dampfend

Three steps:

- 1) From expected to empirical error (SLT)
- 2) Convexify classification loss into squared loss
- 3) From empirical loss to inductive bound

Inductive Generalization Bounds

Using classical SLT tools (Equations 3.15 and 3.24 [Vap95]), with probability $1 - \eta$

$$R_P(f) \leq \frac{1}{N} \sum_i \mathcal{L}(f(\mathbf{x}_i), y_i) + \Delta_I(h, N, \eta).$$

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$N \equiv$ number of samples

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How to bound $\mathcal{L}(f(\mathbf{x}_i), y_i)$?

Inductive Generalization Bounds

For any $y_i \in \{-1, 1\}$ and ℓ_i^*

$$\frac{1}{N} \sum_i \mathcal{L}(f(\mathbf{x}_i), y_i)$$

Inductive Generalization Bounds

For any $y_i \in \{-1, 1\}$ and ℓ_i^*

$$\begin{aligned} & \frac{1}{N} \sum_i \mathcal{L}(f(\mathbf{x}_i), y_i) \\ & \stackrel{\text{convexity}}{\leq} \frac{1}{N} \sum_i \mathcal{L}(f(\mathbf{x}_i), \operatorname{sgn}(\ell_i^*)) + \underbrace{\frac{1}{N} \sum_i (\ell_i^* - y_i)^2}_{\text{unbiased}} \end{aligned}$$

for the SVM and GFS

Inductive Generalization Bounds

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$$\begin{aligned} & \frac{1}{N} \sum_i \mathcal{L}(f(\mathbf{x}_i), y_i) \\ & \stackrel{\text{convexity}}{\leq} \frac{1}{N} \sum_i \mathcal{L}(f(\mathbf{x}_i), \text{sgn}(\ell_i^*)) + \frac{1}{N} \sum_i (\ell_i^* - y_i)^2 \\ & \stackrel{\text{stability bound}}{\leq} \left(\frac{1}{N} \sum_i \mathcal{L}(f(\mathbf{x}_i), \text{sgn}(\ell_i^*)) \right) + \widehat{R}_P(\ell^*) + \Delta_T(\beta, n_l, \delta) \end{aligned}$$

Inductive Generalization Bounds

Combining **inductive** + **transductive** error

With probability $1 - (\eta + \delta)$.

$$\begin{aligned} R_P(f) &\leq \frac{1}{N} \sum_i \mathcal{L}(f(\mathbf{x}_i), \text{sgn}(\ell_i^*)) + \\ &\quad \widehat{R}_P(\ell^*) + \Delta_T(\beta, n_I, \delta) + \Delta_I(h, N, \eta) \end{aligned}$$

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We need to account for ε . With probability $1 - (\eta + \delta)$.
→ into making sure the rest don't blow up

$$\begin{aligned} R_P(f) &\leq \frac{1}{N} \sum_{i: |\ell_i^*| \geq \varepsilon} \mathcal{L}(f(\mathbf{x}_i), \text{sgn}(\ell_i^*)) + \frac{2\varepsilon n_\varepsilon}{N} + \\ &\quad \widehat{R}_P(\ell^*) + \Delta_T(\beta, n_I, \delta) + \Delta_I(h, N, \eta) \end{aligned}$$

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*in order
to get balance term* ↵ We should have $\varepsilon \leq n_I^{-1/2}!$

SSL with Graphs: What is behind it?

Why and when it helps?

semi-supervised
↑ , ↑ supervised

Can we guarantee benefit of SSL over SL?

$$SL \rightarrow \frac{1}{\sqrt{mL}} \quad SGL = \frac{1}{\sqrt{mL}} \times \beta^L \quad \uparrow \text{can be lower than } 1$$

SSL with Graphs: What is behind it?

Why and when it helps?

Can we guarantee benefit of SSL over SL?

Are there cases when **manifold** SSL is provably helpful?

Say \mathcal{X} is supported on manifold \mathcal{M} . Compare two cases:

- ▶ SL: does not know about \mathcal{M} and only knows (\mathbf{x}_i, y_i)
- ▶ SSL: perfect knowledge of \mathcal{M}

SSL has access to the manifold of the data

SSL with Graphs: What is behind it?

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<http://people.cs.uchicago.edu/~niyogi/papersps/ssminimax2.pdf>

SSL with Graphs: What is behind it?

Set of learning problems - collections \mathcal{P} of probability distributions:

$$\mathcal{P}$$

SSL with Graphs: What is behind it?

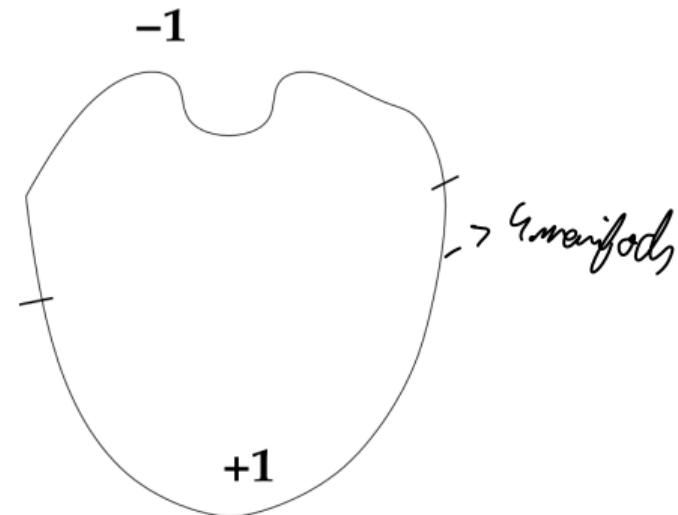
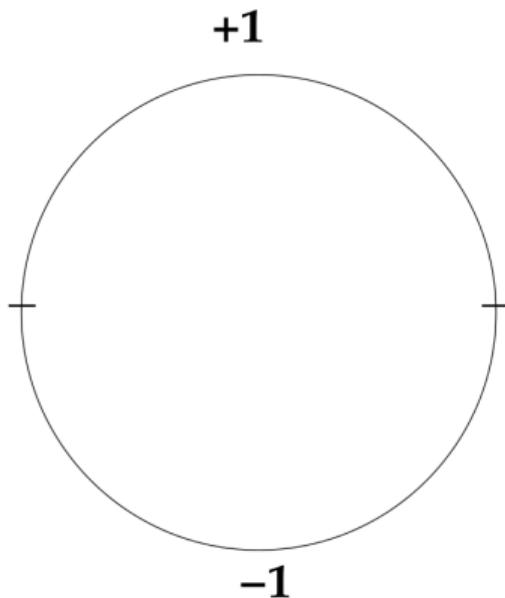
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Minimax rate

$$R(n_l, \mathcal{P}) = \inf_A \sup_{p \in \mathcal{P}} \mathbb{E}_{\bar{z}} \left[\|A(\bar{z}) - m_p\|_{L^2(p_{\mathbf{X}})} \right]$$

(worst manifold but best algo)

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were you think the manifold

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(SSL) When A is allowed to know \mathcal{M}

$$Q(n_l, \mathcal{P}) = \sup_{\mathcal{M}} \inf_A \sup_{p \in \mathcal{P}_{\mathcal{M}}} \mathbb{E}_{\bar{z}} \left[\|A(\bar{z}) - m_p\|_{L^2(p_{\mathbf{X}})} \right]$$

↳ because we can check the manifold

SSL with Graphs: What is behind it?

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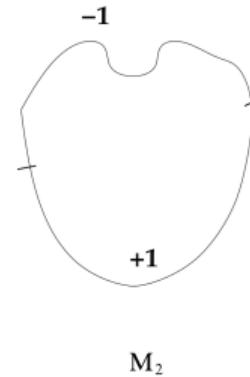
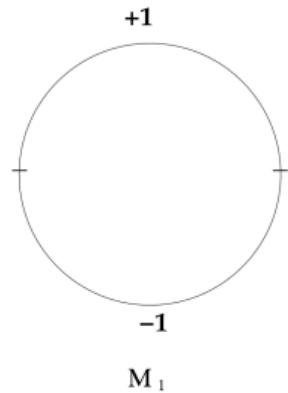
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In which cases there is a gap between $Q(n_l, \mathcal{P})$ and $R(n_l, \mathcal{P})$?

SSL with Graphs: What is behind it?

Hypothesis space \mathcal{H} : half of the circle as $+1$ and the rest as -1

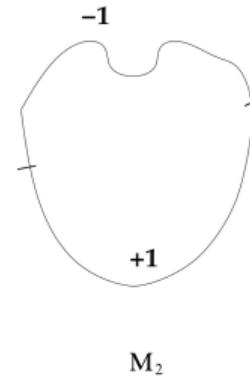
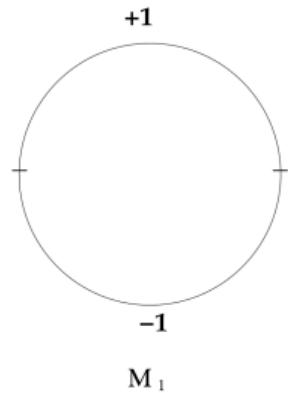


M_1

M_2

SSL with Graphs: What is behind it?

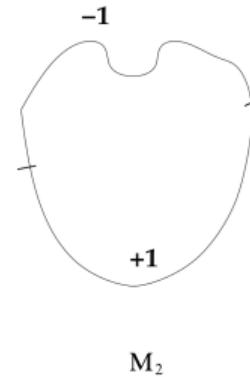
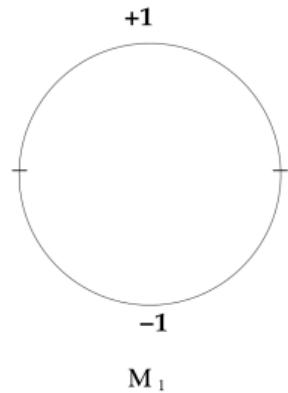
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Case 1: \mathcal{M} is known to the learner ($\mathcal{H}_{\mathcal{M}}$)

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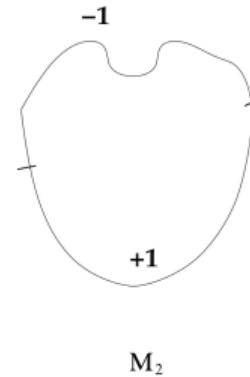
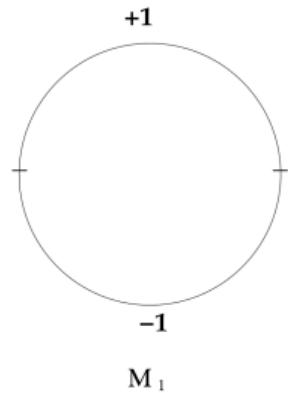
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SSL with Graphs: What is behind it?

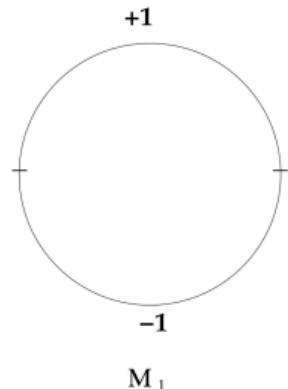
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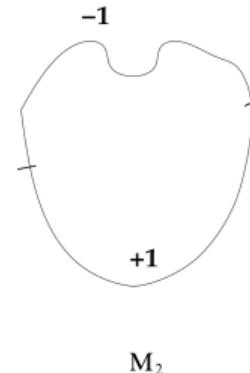
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M_1



M_2

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$$\text{Optimal rate } Q(n, \mathcal{P}) \leq 2 \sqrt{\frac{3 \log n_I}{n_I}}$$

SSL with Graphs: What is behind it?

Case 2: \mathcal{M} is **unknown** to the learner

SSL with Graphs: What is behind it?

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$$R(n_l, \mathcal{P}) = \inf_{\mathcal{A}} \sup_{p \in \mathcal{P}} \mathbb{E}_{\bar{z}} \left[\|A(\bar{z}) - m_p\|_{L^2(p_{\mathbf{x}})} \right] =$$

SSL with Graphs: What is behind it?

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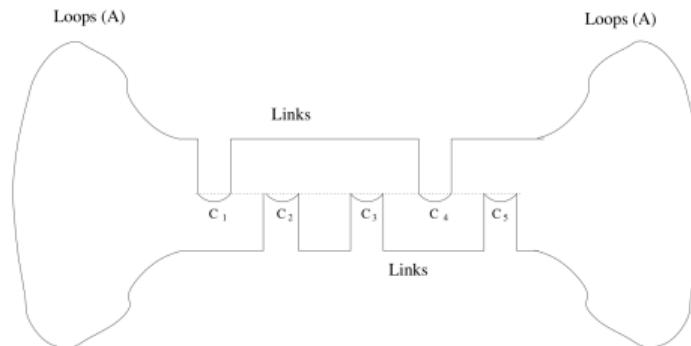
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We consider 2^d manifolds of the form

$$\mathcal{M} = \text{Loops} \cup \text{Links} \cup C \text{ where } C = \cup_{i=1}^d C_i$$



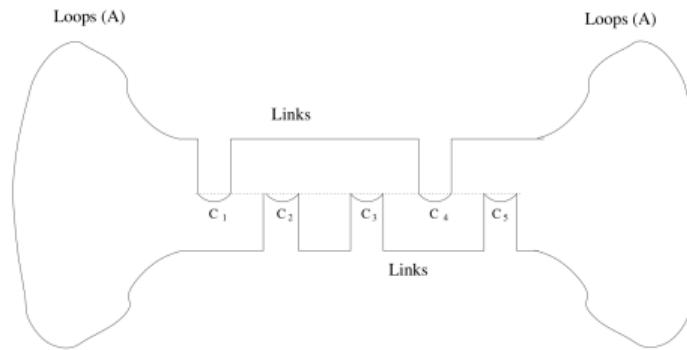
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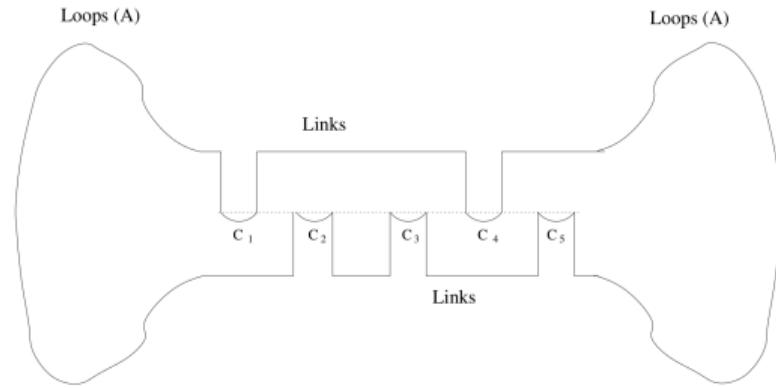
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Main idea: d segments in C , $d - l$ with no data, 2^l possible choices for labels, which helps us to lower bound $\|A(\bar{z}) - m_p\|_{L^2(p_X)}$

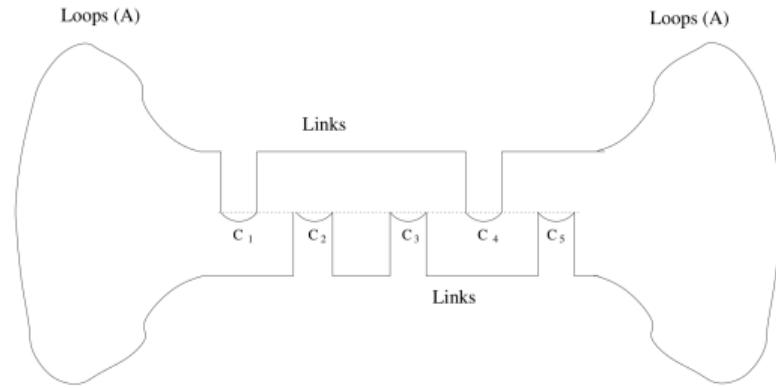
SSL with Graphs: What is behind it?



Knowing the manifold helps

- ▶ C_1 and C_4 are close

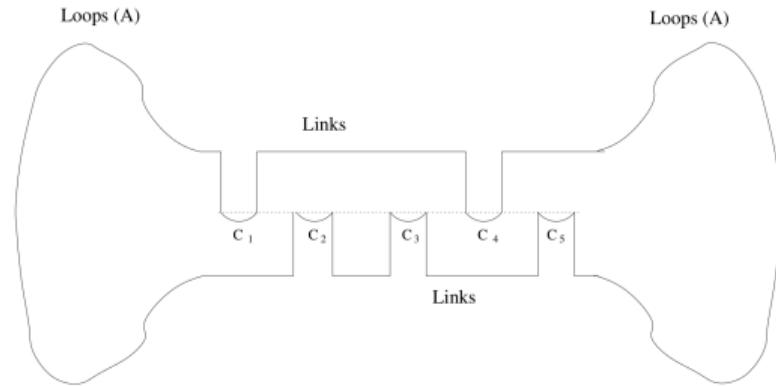
SSL with Graphs: What is behind it?



Knowing the manifold helps

- ▶ C_1 and C_4 are close
- ▶ C_1 and C_3 are far

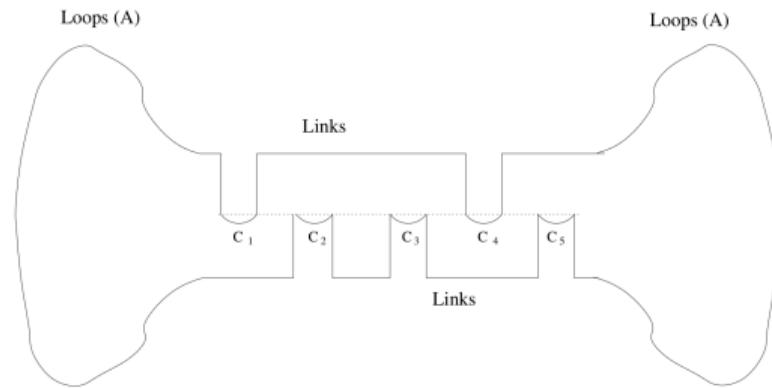
SSL with Graphs: What is behind it?



Knowing the manifold helps

- ▶ C_1 and C_4 are close
- ▶ C_1 and C_3 are far
- ▶ we also need: **target function varies smoothly**

SSL with Graphs: What is behind it?



Knowing the manifold helps

- ▶ C_1 and C_4 are close
- ▶ C_1 and C_3 are far
- ▶ we also need: **target function varies smoothly**
- ▶ altogether: **closeness on manifold \rightarrow similarity in labels**

SSL with Graphs: What is behind it?

What does it mean to know M ?

SSL with Graphs: What is behind it?

What does it mean to **know** \mathcal{M} ?

Different degrees of knowing \mathcal{M}

- ▶ set membership oracle: $x \stackrel{?}{\in} \mathcal{M}$
- ▶ approximate oracle
- ▶ knowing the harmonic functions on \mathcal{M}
- ▶ knowing the Laplacian $\mathcal{L}_{\mathcal{M}}$
- ▶ knowing eigenvalues and *eigenfunctions*
- ▶ topological invariants, e.g., dimension
- ▶ metric information: geodesic distance

OnlineSSL(\mathcal{G})

when we can't access future x

...and we want the results in real time

Online SSL with Graphs

Offline learning setup

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**).

Online SSL with Graphs

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Online SSL with Graphs

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Online learning setup

At the beginning: $\{\mathbf{x}_i, y_i\}_{i=1}^{n_l}$ from \mathbb{R}^d

- what if we want to learn face while watching?
- also useful for computational reasons

Online SSL with Graphs

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At time t :

receive \mathbf{x}_t

Online SSL with Graphs

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Online learning setup

At the beginning: $\{\mathbf{x}_i, y_i\}_{i=1}^{n_l}$ from \mathbb{R}^d

At time t :

receive \mathbf{x}_t

predict y_t

Online SSL with Graphs

Online HFS: Straightforward solution

- 1: **while** new unlabeled example x_t comes **do**
- 2: Add x_t to graph $G(\mathbf{W})$

Online SSL with Graphs

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Online SSL with Graphs

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Online SSL with Graphs

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What is wrong with this solution?

Online SSL with Graphs

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What is wrong with this solution?

The cost and memory of the operations.

Online SSL with Graphs

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What is wrong with this solution?

The cost and memory of the operations.

Do not scale!

What can we do?

Online SSL with Graphs

Let's keep only k vertices!

Online SSL with Graphs

Let's keep only k vertices!

Limit memory to k centroids with $\tilde{\mathbf{W}}^q$ weights.
between each other (k^2 edges)

Online SSL with Graphs

Let's keep only k vertices!

Limit memory to k **centroids** with $\tilde{\mathbf{W}}^q$ weights. ↳ centroids will need to represent bunch of points
Each centroid represents several others.

Online SSL with Graphs

Let's keep only k vertices!

Limit memory to k centroids with $\widetilde{\mathbf{W}}^q$ weights.

Each centroid represents several others.

Diagonal $\mathbf{V} \equiv$ multiplicity. \hookrightarrow how many points in a centroid

Online SSL with Graphs

Let's keep only k vertices!

Limit memory to k **centroids** with $\widetilde{\mathbf{W}}^q$ weights.

Each centroid represents *several* others.

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Online SSL with Graphs

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Can we compute it compactly?

Online SSL with Graphs

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Can we compute it compactly? Compact harmonic solution. *We can (this is harmonic solve) replace with centroids.*

$$\ell^q = (\mathbf{L}_{uu}^q + \gamma_g \mathbf{V})^{-1} \mathbf{W}_{ul}^q \ell_l \quad \text{where} \quad \mathbf{W}^q = \mathbf{V} \widetilde{\mathbf{W}}^q \mathbf{V}$$

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Proof?

Online SSL with Graphs

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Proof? Using electric circuits.

Online SSL with Graphs

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Proof? Using electric circuits.

Why do we keep the multiplicities?

Online SSL with Graphs



Online HFS with Graph Quantization

- 1: **Input**
- 2: k number of representative nodes

Online SSL with Graphs

Online HFS with Graph Quantization

- 1: **Input**
- 2: k number of representative nodes
- 3: **Initialization**
- 4: \mathbf{V} matrix of multiplicities with 1 on diagonal

Online SSL with Graphs

Online HFS with Graph Quantization

- 1: **Input**
- 2: k number of representative nodes
- 3: **Initialization**
- 4: \mathbf{V} matrix of multiplicities with 1 on diagonal
- 5: **while** new unlabeled example \mathbf{x}_t comes **do**
- 6: Add \mathbf{x}_t to graph G
- 7: **if** # nodes > k **then**
- 8: quantize G
- 9: **end if**

Online SSL with Graphs

Online HFS with Graph Quantization

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- 2: k number of representative nodes
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- 8: quantize G
- 9: **end if**
- 10: Update \mathbf{L}_t of $G(\mathbf{VWV})$

Online SSL with Graphs

we don't want to do it (we want each label data to be in the graph)

Online HFS with Graph Quantization

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 - 4: \mathbf{V} matrix of multiplicities with 1 on diagonal
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 - 11: Infer labels
 - 12: Predict $\hat{y}_t = \text{sgn}(\mathbf{f}_u(t))$
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-

Online SSL with Graphs: Graph Quantization

An idea: incremental k -centers

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Doubling algorithm of Charikar et al. [Cha+97]

Online SSL with Graphs: Graph Quantization

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Doubling algorithm of Charikar et al. [Cha+97]

Keeps up to k centers $C_t = \{\mathbf{c}_1, \mathbf{c}_2, \dots\}$ with

Online SSL with Graphs: Graph Quantization

An idea: incremental k -centers

Doubling algorithm of Charikar et al. [Cha+97]

Keeps up to k centers $C_t = \{\mathbf{c}_1, \mathbf{c}_2, \dots\}$ with

- Distance $\mathbf{c}_i, \mathbf{c}_j \in C_t$ is at least $\geq R \rightarrow$ try to keep some variance

Online SSL with Graphs: Graph Quantization

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Doubling algorithm of Charikar et al. [Cha+97]

Keeps up to k centers $C_t = \{\mathbf{c}_1, \mathbf{c}_2, \dots\}$ with

- ▶ Distance $\mathbf{c}_i, \mathbf{c}_j \in C_t$ is at least $\geq R$
- ▶ For each new \mathbf{x}_t , distance to some $\mathbf{c}_i \in C_t$ is less than R . *→ every time a new point arrives, we want to have a center in radius R. If not, create a center*

Online SSL with Graphs: Graph Quantization

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- ▶ $|C_t| \leq k$

Online SSL with Graphs: Graph Quantization

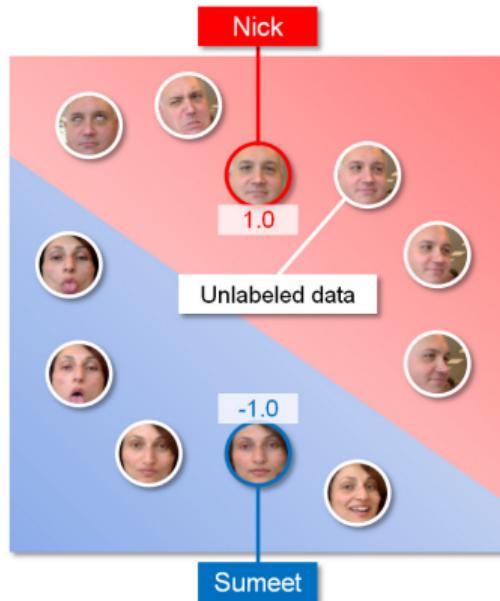
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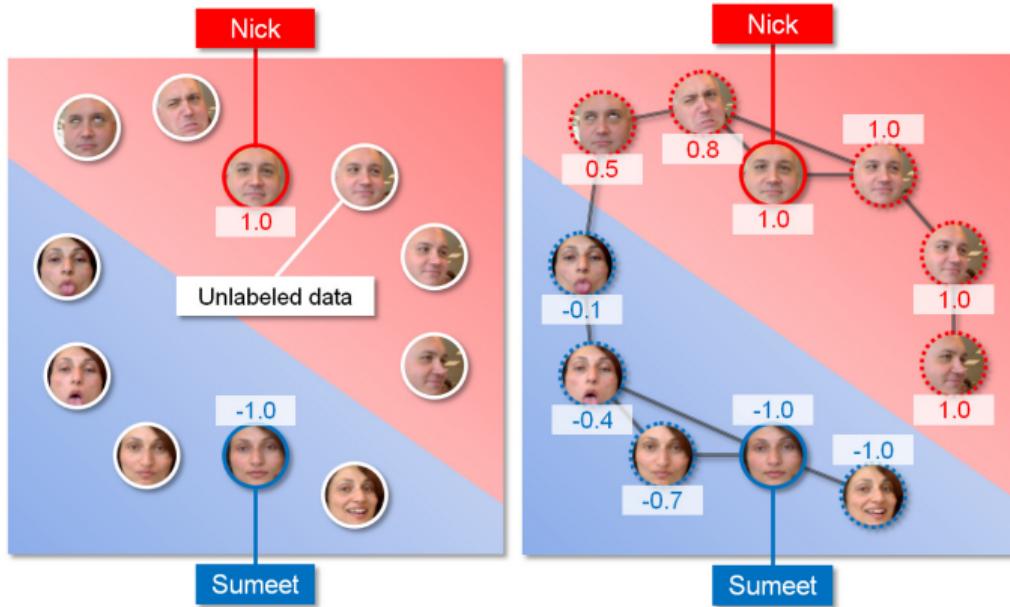
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- ▶ For each new \mathbf{x}_t , distance to some $\mathbf{c}_i \in C_t$ is less than R .
- ▶ $|C_t| \leq k$
- ▶ if not possible, R is doubled

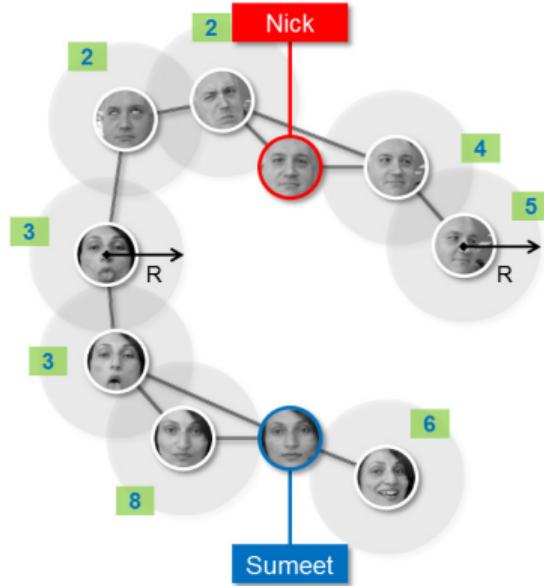
Online SSL with Graphs: Graph Quantization



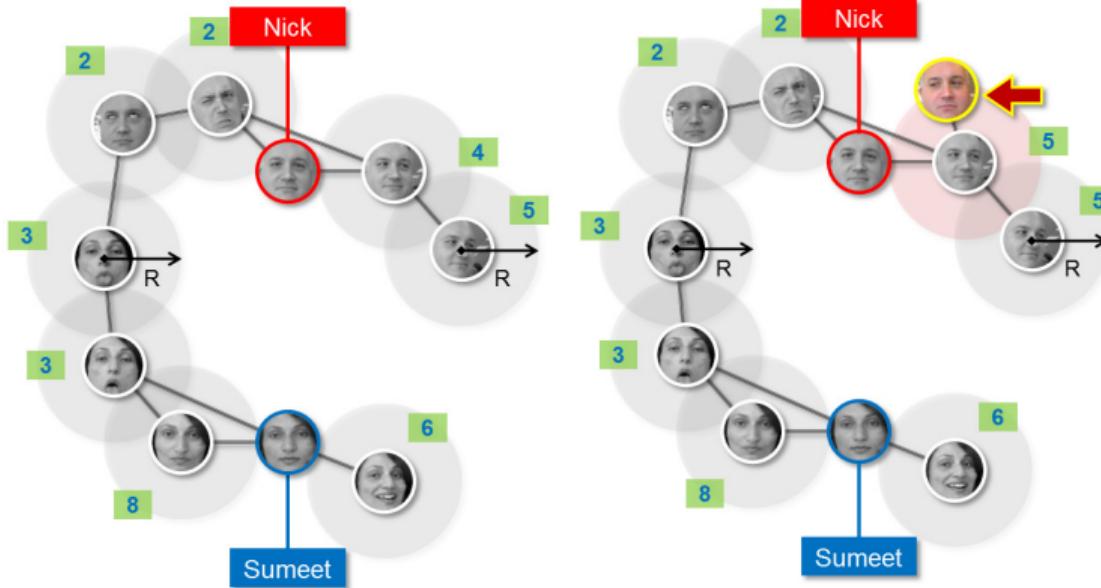
Online SSL with Graphs: Graph Quantization



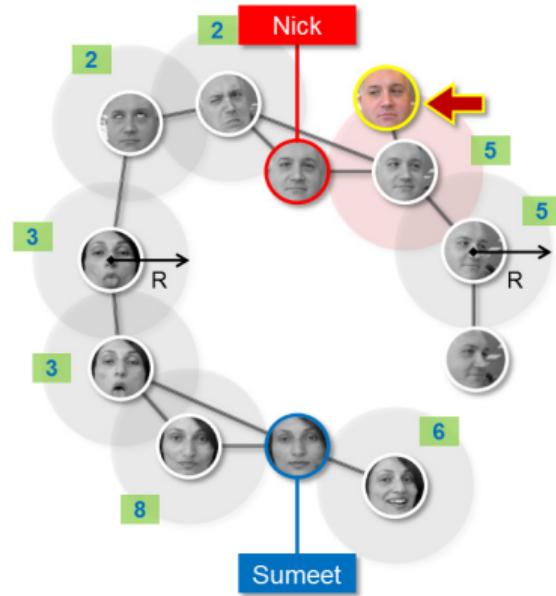
Online SSL with Graphs: Graph Quantization



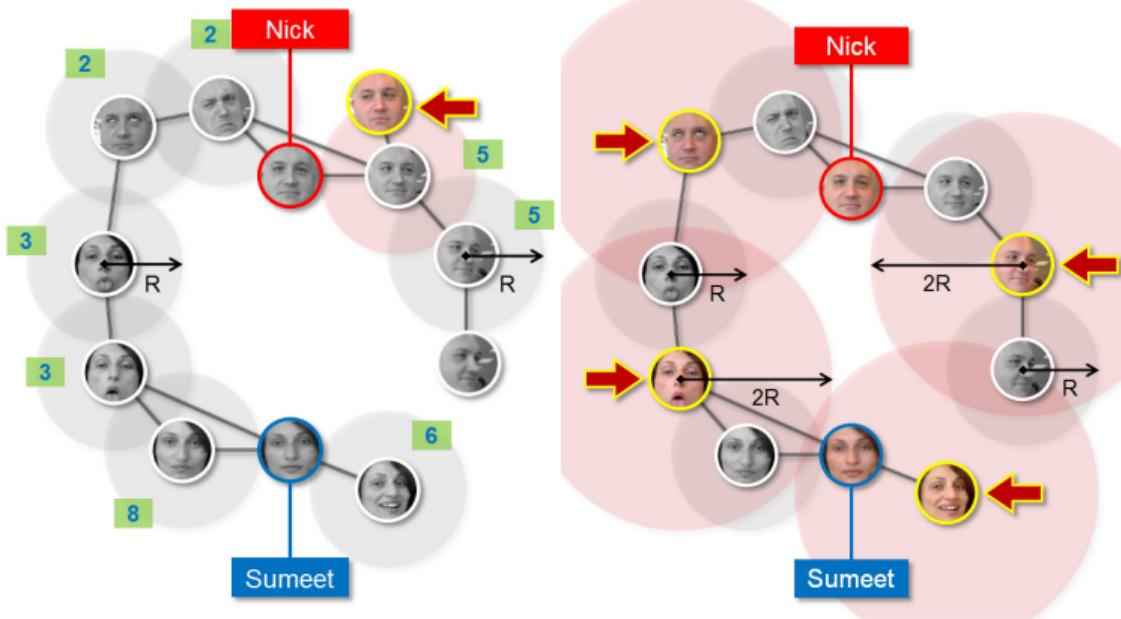
Online SSL with Graphs: Graph Quantization



Online SSL with Graphs: Graph Quantization



Online SSL with Graphs: Graph Quantization



Online SSL with Graphs: Graph Quantization

Online k -centers

- 1: an unlabeled \mathbf{x}_t , a set of centroids C_{t-1} , multiplicities \mathbf{v}_{t-1}

Online SSL with Graphs: Graph Quantization

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- 3: $R \leftarrow mR$

Online SSL with Graphs: Graph Quantization

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- 6: for any $\mathbf{c}_i \in C_{t-1}$ exists $\mathbf{c}_j \in C_t$ such that $d(\mathbf{c}_i, \mathbf{c}_j) < R$

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Online SSL with Graphs: Graph Quantization

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- 9: $C_t \leftarrow C_{t-1}$
- 10: $\mathbf{v}_t \leftarrow \mathbf{v}_{t-1}$
- 11: **end if**
- 12: **if** \mathbf{x}_t is closer than R to any $\mathbf{c}_i \in C_t$ **then**
- 13: $\mathbf{v}_t(i) \leftarrow \mathbf{v}_t(i) + 1$
- 14: **else**

Online SSL with Graphs: Graph Quantization

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 - 13: $\mathbf{v}_t(i) \leftarrow \mathbf{v}_t(i) + 1$
 - 14: **else**
 - 15: $\mathbf{v}_t(|C_t| + 1) \leftarrow 1$
 - 16: **end if**
-

Online SSL with Graphs: Graph Quantization

Doubling algorithm [Cha+97]

Online SSL with Graphs: Graph Quantization

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To reduce growth of R , we use $R \leftarrow m \times R$, with $m \geq 1$

Online SSL with Graphs: Graph Quantization

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C_t is changing. How far can x be from some c ?

Online SSL with Graphs: Graph Quantization

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R

Online SSL with Graphs: Graph Quantization

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$$R + \frac{R}{m}$$

Online SSL with Graphs: Graph Quantization

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$$R + \frac{R}{m} + \frac{R}{m^2}$$

Online SSL with Graphs: Graph Quantization

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To reduce growth of R , we use $R \leftarrow m \times R$, with $m \geq 1$

C_t is changing. How far can \mathbf{x} be from some \mathbf{c} ?

$$R + \frac{R}{m} + \frac{R}{m^2} + \dots = R \left(1 + \frac{1}{m} + \frac{1}{m^2} + \dots \right)$$

Online SSL with Graphs: Graph Quantization

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Guarantees

Online SSL with Graphs: Graph Quantization

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Guarantees: 8-approximation algorithm.

Online SSL with Graphs: Graph Quantization

Doubling algorithm [Cha+97]

If linear O(1) reforms O(6³⁴)
then $R \cdot m_{\text{online}} \leq 2 \times 0.6^{34}$

To reduce growth of R , we use $R \leftarrow m \times R$, with $m \geq 1$

C_t is changing. How far can x be from some c ?

$$R + \frac{R}{m} + \frac{R}{m^2} + \dots = R \left(1 + \frac{1}{m} + \frac{1}{m^2} + \dots \right) = \frac{Rm}{m - 1}$$

Guarantees: 8-approximation algorithm.

Why not incremental k-means?

We can move stability with the presented variances

Online SSL with Graphs

Video examples

<http://www.bkveton.com/videos/Coffee.mp4>

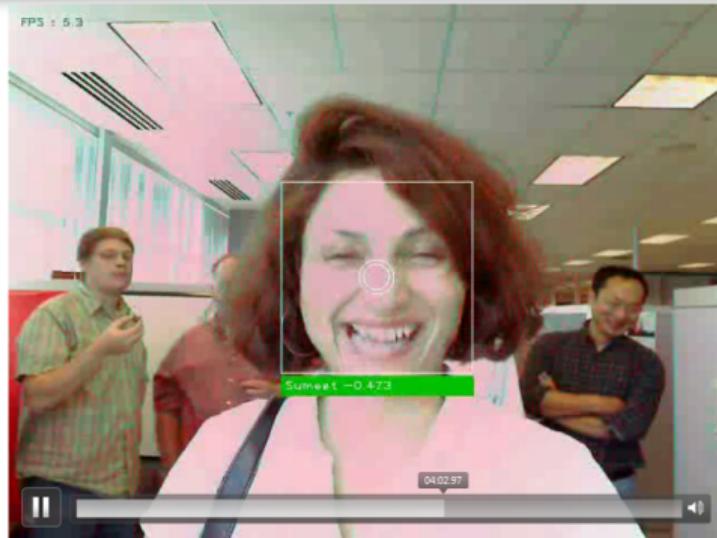
<http://www.bkveton.com/videos/Ad.mp4>

<http://researchers.lille.inria.fr/~valko/hp/serve.php?what=publications/kveton2009nipsdemo.adaptation.mov>

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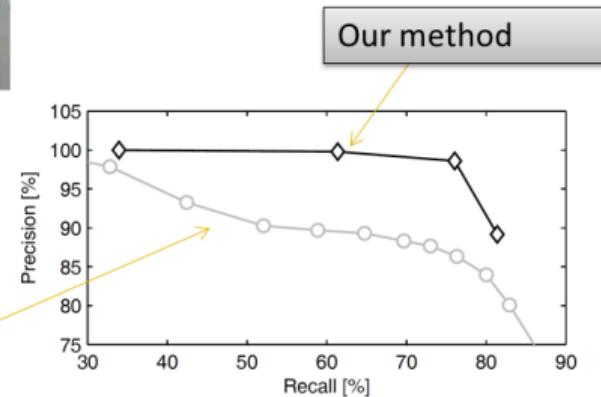
<http://researchers.lille.inria.fr/~valko/hp/publications/press-intel-2015.mp4>

SSL with Graphs: Some experimental results



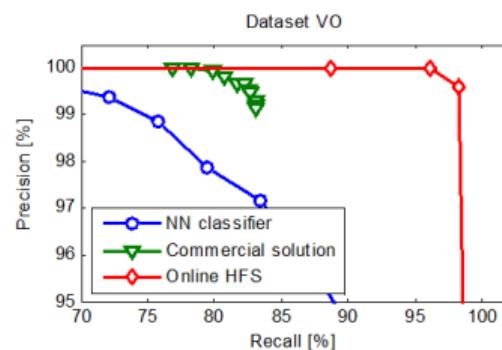
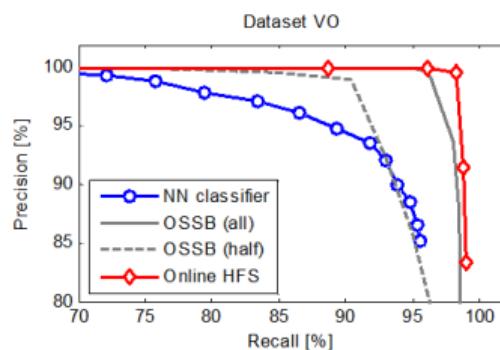
Nearest Neighbor

- 8 people classification
- Making funny faces
- 4 faces/person are labeled



SSL with Graphs: Some experimental results

- One person moves among various indoor locations
- 4 labeled examples of a person in the cubicle

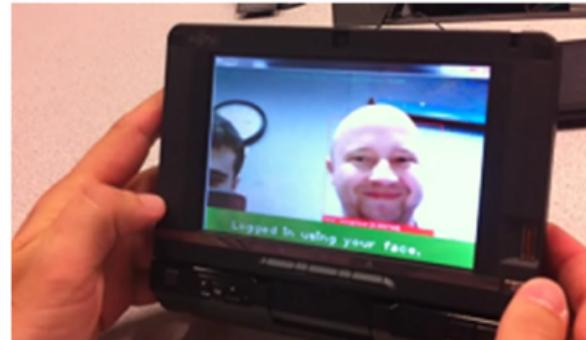


Online HFS outperforms OSSB (even when the weak learners are chosen using future data)

Online HFS yields better results than a commercial solution at 20% of the computational cost

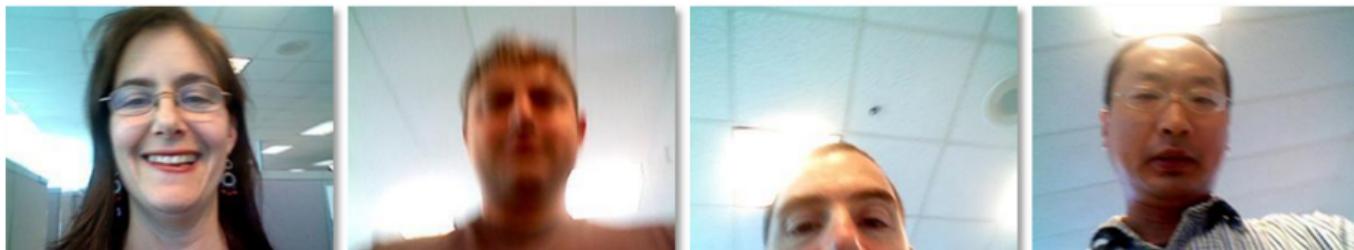
SSL with Graphs: Some experimental results

- **Logging in** with faces instead of password
- Able to **learn** and improve

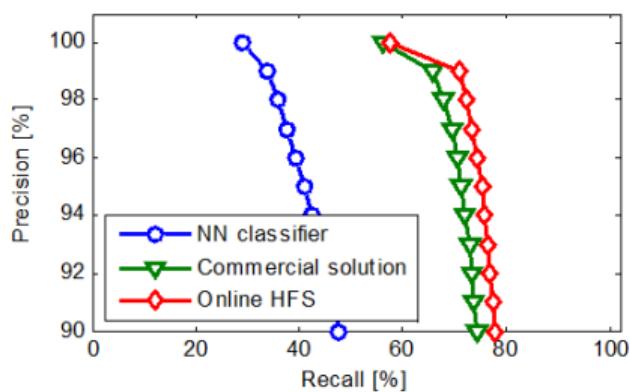


SSL with Graphs: Some experimental results

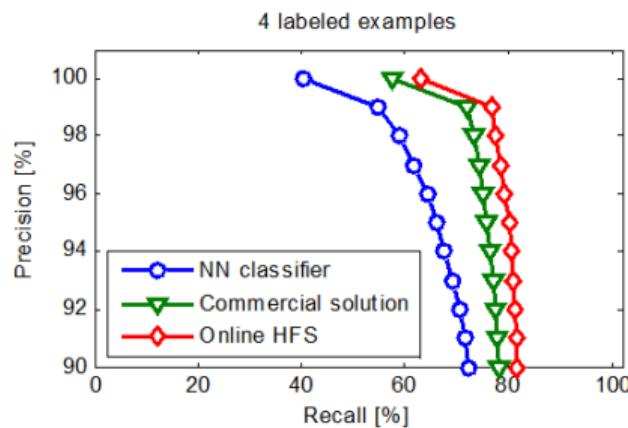
- 16 people log twice into a tablet PC at 10 locations



1 labeled example



4 labeled examples



Online SSL with Graphs: Analysis

Want to bound $\frac{1}{N} \sum_{t=1}^N (\ell_t^q[t] - y_t)^2$

What can we guarantee?

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Three sources of error

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Three sources of error

- ▶ generalization error — if all data: $(\ell_t^* - y_t)^2$ offline vs world
- ▶ online error — data only incrementally: $(\ell_t^o[t] - \ell_t^*)^2$ online as often
- ▶ quantization error — memory limitation: $(\ell_t^q[t] - \ell_t^o[t])^2$ \rightarrow quantize to online

Online SSL with Graphs: Analysis

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Three sources of error

- ▶ generalization error — if all data: $(\ell_t^* - y_t)^2$
- ▶ online error — data only incrementally: $(\ell_t^o[t] - \ell_t^*)^2$
- ▶ quantization error — memory limitation: $(\ell_t^q[t] - \ell_t^o[t])^2$

All together:

$$\frac{1}{N} \sum_{t=1}^N (\ell_t^q[t] - y_t)^2 \leq \frac{9}{2N} \sum_{t=1}^N (\ell_t^* - y_t)^2 + \frac{9}{2N} \sum_{t=1}^N (\ell_t^o[t] - \ell_t^*)^2 + \frac{9}{2N} \sum_{t=1}^N (\ell_t^q[t] - \ell_t^o[t])^2$$

Online SSL with Graphs: Analysis

Bounding transduction error $(\ell_t^* - y_t)^2$

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If all labeled examples I are i.i.d., $c_I = 1$ and $c_I \gg c_u$, then

$$R(\ell^*) \leq \widehat{R}(\ell^*) + \underbrace{\beta + \sqrt{\frac{2 \ln(2/\delta)}{n_I}}(n_I\beta + 4)}_{\text{transductive error } \Delta_T(\beta, n_I, \delta)}$$

$$\beta \leq 2 \left[\frac{\sqrt{2}}{\gamma_g + 1} + \sqrt{2n_I} \frac{1 - c_u}{c_u} \frac{\lambda_M(\mathbf{L}) + \gamma_g}{\gamma_g^2 + 1} \right]$$

holds with the probability of $1 - \delta$, where

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ie they are close

Idea: If \mathbf{L} and \mathbf{L}^o are regularized, then HFSs get closer together.

since they get closer to zero

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Recall $\ell = (\mathbf{C}^{-1}\mathbf{Q} + \mathbf{I})^{-1}\mathbf{y}$, where $\mathbf{Q} = \mathbf{L} + \gamma_g \mathbf{I}$

and also $\mathbf{v} \in \mathbb{R}^{n \times 1}$, $\lambda_m(A)\|\mathbf{v}\|_2 \leq \|A\mathbf{v}\|_2 \leq \lambda_M(A)\|\mathbf{v}\|_2$

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Difference between offline and online solutions:

$$(\ell_t^o[t] - \ell_t^*)^2$$

Online SSL with Graphs: Analysis

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Online SSL with Graphs: Analysis

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How are the quantized and full solution different?

$$\ell^* = \min_{\ell \in \mathbb{R}^N} (\ell - \mathbf{y})^\top \mathbf{C}(\ell - \mathbf{y}) + \ell^\top \mathbf{Q}\ell$$

Online SSL with Graphs: Analysis

Bounding quantization error $(\ell_t^q[t] - \ell_t^o[t])^2$

How are the quantized and full solution different?

With quantization, we replace a bunch of point with repetitions of centroid: i.e. the corresponding placement in blocks

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In Q!

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We have: $\ell^o = (\mathbf{C}^{-1}\mathbf{Q}^o + \mathbf{I})^{-1}\mathbf{y}$ vs. $\ell^q = (\mathbf{C}^{-1}\mathbf{Q}^q + \mathbf{I})^{-1}\mathbf{y}$

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With linear algebra we get

$$\|\ell^q - \ell^o\|_2 \leq \frac{\sqrt{n_I}}{c_u \gamma_g^2} \|\mathbf{Q}^q - \mathbf{Q}^o\|_F$$

Online SSL with Graphs: Analysis

Bounding quantization error $(\ell_t^q[t] - \ell_t^o[t])^2$

The quantization error depends on $\|\mathbf{Q}^q - \mathbf{Q}^o\|_F = \|\mathbf{L}^q - \mathbf{L}^o\|_F$.

When can we keep $\|\mathbf{L}^q - \mathbf{L}^o\|_F$ under control?

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Charikar guarantees distortion error of at most $Rm/(m-1)$

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Charikar guarantees distortion error of at most $Rm/(m-1)$

For what kind of data $\{\mathbf{x}_i\}_{i=1,\dots,n}$ is the distortion small?

Online SSL with Graphs: Analysis

distortion: how far away are 2d points
in category from centroids?

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Assume manifold \mathcal{M}

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Assume manifold \mathcal{M}

- ▶ all $\{\mathbf{x}_i\}_{i \geq 1}$ lie on a smooth d -dimensional compact \mathcal{M}
- ▶ with boundary of bounded geometry Def. 11 of Hein [HAL07]
 - ▶ has finite volume V
 - ▶ has finite surface area A
 - ▶ should not intersect itself
 - ▶ should not fold back onto itself

Online SSL with Graphs: Analysis

Bounding quantization error $(\ell_t^q[t] - \ell_t^o[t])^2$

Bounding $\|\mathbf{L}^q - \mathbf{L}^o\|_F$ when $\mathbf{x}_i \in \mathcal{M}$

Consider k -sphere packing* of radius r with centers contained in \mathcal{M} . *only the centers are packed,

not necessarily the entire ball

If k is large $\rightarrow r <$ injectivity radius of \mathcal{M} [HAL07]

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Consider k -sphere packing* of radius r with centers contained in \mathcal{M} . *only the centers are packed,

not necessarily the entire ball

If k is large $\rightarrow r <$ injectivity radius of \mathcal{M} [HAL07] and $r < 1$:

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$$\max_{i=1, \dots, N} \|\mathbf{x}_i - \mathbf{c}\|_2 \leq R \frac{m}{m-1} \leq 2 \mathcal{O} \left(k^{-1/d} \right) = \mathcal{O} \left(k^{-1/d} \right)$$

But what about $\|\mathbf{L}^q - \mathbf{L}^o\|_F$?

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If similarity is M -Lipschitz

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Are the assumptions reasonable?

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We showed $\|\mathbf{L}^q - \mathbf{L}^o\|_F^2 \leq \mathcal{O}(k^{-2/d}) = \mathcal{O}(1)$.

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$$\frac{1}{N} \sum_{t=1}^N (\ell_t^q[t] - \ell_t^o[t])^2 \leq \frac{n_I}{c_u^2 \gamma_g^4} \|\mathbf{L}^q - \mathbf{L}^o\|_F^2$$

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What does that mean?

Daniele Calandriello

dcalandriello@google.com

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