Graphs in Machine Learning

Michal Valko

Inria Lille - Nord Europe, France

TA: Pierre Perrault

Partially based on material by: Mikhail Belkin, Branislav Kveton

Previous Lecture

- Graph-based semi-supervised learning
- SSL with MinCuts
- Gaussian random fields and harmonic solution
- Regularization of harmonic solution
- Soft-harmonic solution
- Inductive and transductive semi-supervised learning
- Manifold regularization
- Max-Margin Graph Cuts
- Theory of Laplacian-based manifold methods
- Transductive learning stability based bounds

This Lecture

- Theory of Laplacian-based manifold methods
- Transductive learning stability based bounds
- Online Semi-Supervised Learning
- Online incremental k-centers
- Examples of applications of online SSL
- Analysis of online SSL
- SSL learnability
- When does graph-based SSL provably help?
- Scaling harmonic functions to millions of samples

Previous Lab Session

- 24. 10. 2018 by Pierre Perrault
- Content
  - Graph Construction
  - Test sensitivity to parameters: σ, k, ε
  - Spectral Clustering
  - Spectral Clustering vs. k-means
  - Image Segmentation
- Short written report
- Questions to piazza (without giving away solutions)
- *Deadline:* 7. 11. 2018 Today!

Next Lab Session

- 14. 11. 2018 by Pierre Perrault
- Content
  - Semi-supervised learning
  - Graph quantization
  - Online face recognizer
- AR: record a video with faces
- Install VM (in case you have not done it yet for TD1)
- Short written report
- Questions to piazza
- *Deadline:* 28. 11. 2018

Final Class projects

- detailed description on the class website
- preferred option: you come up with the topic
- theory/implementation/review or a combination
- one or two people per project (exceptionally three)
- grade 60%: report + short presentation of the **team**
- deadlines
  - 21. 11. 2018 - strongly recommended DL for taking projects
  - 28. 11. 2018 - hard DL for taking projects
  - 07. 01. 2019 - submission of the project report
  - 11. 01. 2019 or later - project presentation
- list of suggested topics on piazza

SSL with Graphs: Generalization Bounds

Bounding **transductive** **error**

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

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 $|\ell_i^\star| \leq 1$.

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

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

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

This algorithm is β-stable!

SSL with Graphs: Generalization Bounds

Bounding transductive error

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

By the generalization bound of Belkin [BMN04]

$$R_P(\boldsymbol{\ell}^\star) \leq \widehat{R}_P(\boldsymbol{\ell}^\star) + \underbrace{\beta + \sqrt{\frac{2\ln(2/\delta)}{n_l}}(n_l\beta + 4)}_{\text{transductive error } \Delta_T(\beta, n_l, \delta)}$$

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

holds with probability $1 - \delta$, where

$$R_P(\boldsymbol{\ell}^\star) = \frac{1}{N}\sum_i (\ell_i^\star - y_i)^2$$

$$\widehat{R}_P(\boldsymbol{\ell}^\star) = \frac{1}{n_l}\sum_{i \in l} (\ell_i^\star - y_i)^2.$$

SSL with Graphs: Generalization Bounds

Bounding transductive error

$$R_P(\boldsymbol{\ell}^\star) \;\leq\; \widehat{R}_P(\boldsymbol{\ell}^\star) + \underbrace{\beta + \sqrt{\frac{2\ln(2/\delta)}{n_l}}(n_l\beta + 4)}_{\text{transductive error } \Delta_T(\beta, n_l, \delta)}$$

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

Does the bound say anything useful?

1) The error is controlled.

2) Practical when error $\Delta_T(\beta, n_l, \delta)$ decreases at rate $O(n_l^{-\frac{1}{2}})$.

Achieved when $\beta = O(1/n_l)$. That is, $\gamma_g = \Omega(n_l^{\frac{3}{2}})$.

We have an idea how to set γ_g!

SSL with Graphs: Generalization Bounds

Combining inductive + transductive error

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

$$R_P(f) \;\leq\; \frac{1}{n}\sum_i \mathcal{L}(f(\mathbf{x}_i), \operatorname{sgn}(\ell_i^\star)) + \widehat{R}_P(\boldsymbol{\ell}^\star) + \Delta_T(\beta, n_l, \delta) + \Delta_I(h, N, \eta)$$

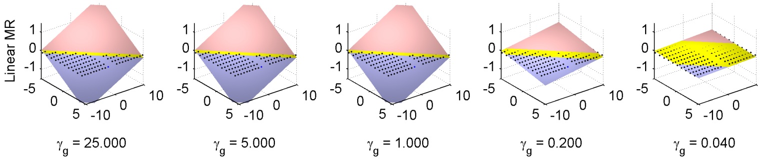
We need to account for ε. With probability $1 - (\eta + \delta)$.

$$R_P(f) \leq \frac{1}{n}\sum_{i:|\ell_i^\star|\geq\varepsilon} \mathcal{L}(f(\mathbf{x}_i), \operatorname{sgn}(\ell_i^\star)) + \frac{2\varepsilon n_\varepsilon}{N} + \widehat{R}_P(\boldsymbol{\ell}^\star) + \Delta_T(\beta, n_l, \delta) + \Delta_I(h, N, \eta)$$

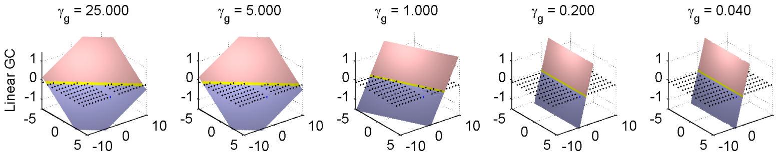
We should have $\varepsilon \leq n_l^{-1/2}$!

SSL with Graphs: LapSVMs and MM Graph Cuts

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

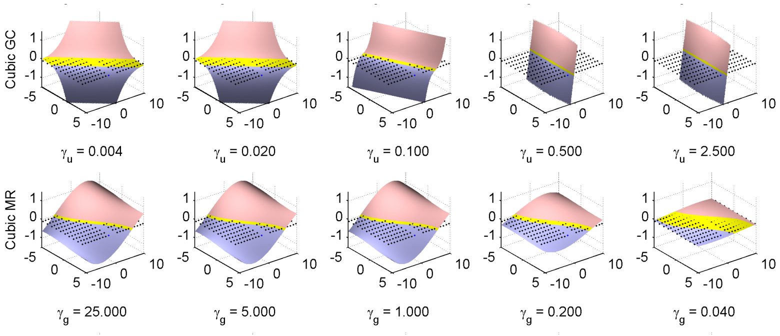


MMGC for 2D data and **linear** $\mathcal{K}$ works as we want



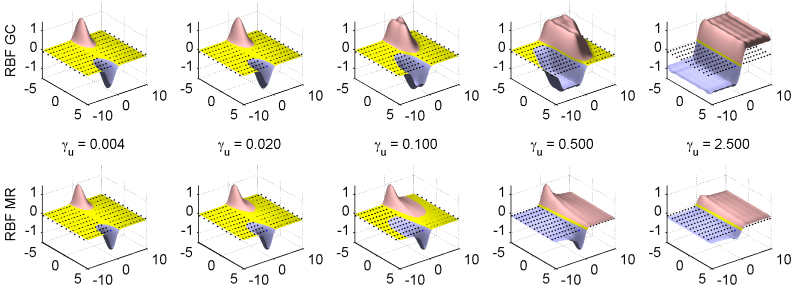
SSL with Graphs: LapSVMs and MM Graph Cuts

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

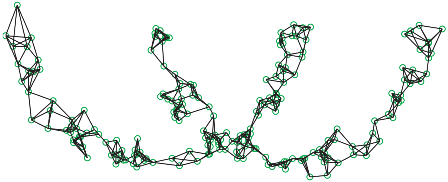


SSL with Graphs: LapSVMs and MM Graph Cuts

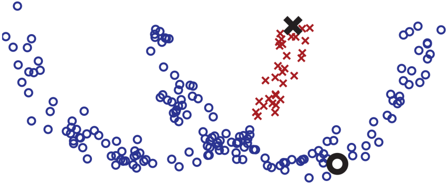
MMGC and MR for 2D data and RBF $\mathcal{K}$



SSL with Graphs



(a) 4-NN graph



(b) Harmonic function predictions

Graph-based SSL is obviously sensitive to graph construction!

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 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

```
while new unlabeled example x_t comes do
    Add x_t to graph G(W)
    Update L_t
    Infer labels
        f_u = (L_uu + γ_g I)^{-1} (W_ul f_l)
    Predict ŷ_t = sgn(f_u(t))
end while
```

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

Predict $\widehat{y}_t = \mathrm{sgn}(\mathbf{f}_u(t))$

What is wrong with this solution?

The cost and memory of the operations.

What can we do?

Online SSL with Graphs

Let's keep only k vertices!

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

Each centroid represents *several* others.

Diagonal $\mathbf{V} \equiv$ **multiplicity**. We have $\mathbf{V}_{ii}$ copies of centroid i.

Can we compute it compactly? Compact harmonic solution.

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

Proof? Using electric circuits.

Why do we keep the multiplicities?

Online SSL with Graphs

Online HFS with Graph Quantization

Input
  k number of representative nodes
Initialization
  $\mathbf{V}$ matrix of multiplicities with 1 on diagonal
while new unlabeled example $\mathbf{x}_t$ comes **do**
  Add $\mathbf{x}_t$ to graph G
  if $\#$ nodes $> k$ **then**
    quantize G
  end if
  Update $\mathbf{L}_t$ of $G(\mathbf{VWV})$
  Infer labels
  Predict $\widehat{y}_t = \text{sgn}\left(\mathbf{f}_u\left(t\right)\right)$
end while

Online SSL with Graphs: Graph Quantization

An idea: incremental k-centers

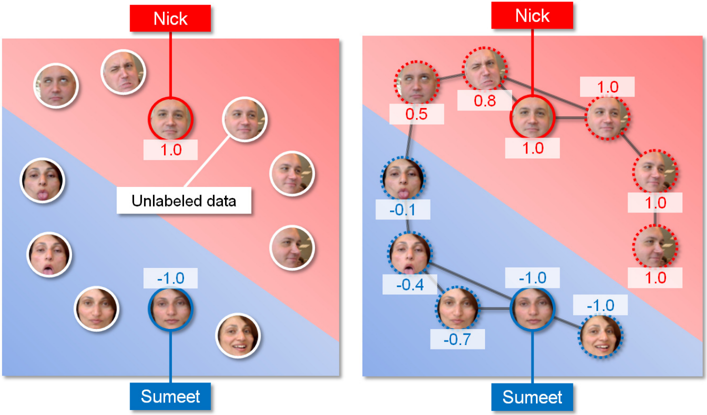
Doubling algorithm of Charikar et al. [Cha+97]

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

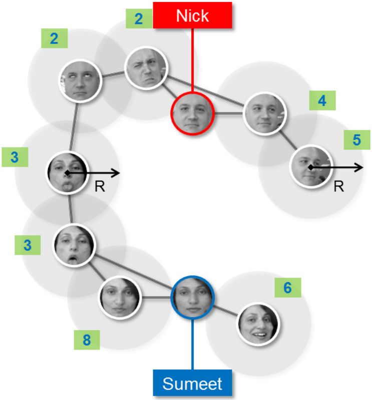
- Distance $\mathbf{c}_i, \mathbf{c}_j \in C_t$ is at least $\geq R$
- For each new $\mathbf{x}_t$, distance to some $\mathbf{c}_i \in C_t$ is less than R.
- $|C_t| \leq k$
- if not possible, R is doubled

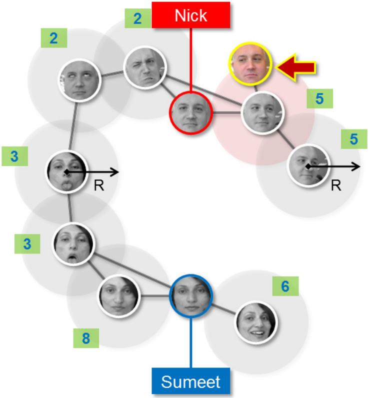
Online SSL with Graphs: Graph Quantization

Online SSL with Graphs: Graph Quantization

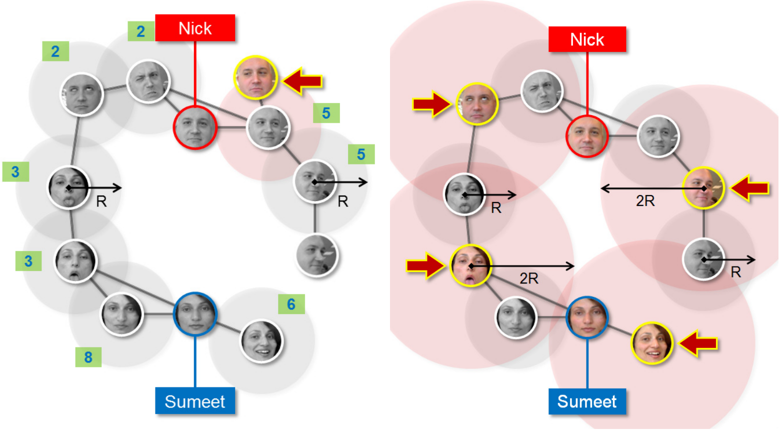


Online SSL with Graphs: Graph Quantization





Online SSL with Graphs: Graph Quantization



Online SSL with Graphs: Graph Quantization

Doubling algorithm [Cha+97]

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 $\mathbf{c}$?

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

Guarantees: $(1+\varepsilon)$-approximation algorithm.

Why not incremental k-means?

Online SSL with Graphs: Graph Quantization

Online k-centers

an unlabeled $\mathbf{x}_t$, a set of centroids C_{t-1}, multiplicities $\mathbf{v}_{t-1}$
if $(|C_{t-1}| = k+1)$ **then**
    $R \leftarrow mR$
    greedily repartition C_{t-1} into C_t such that:
        no two vertices in C_t are closer than R
        for any $\mathbf{c}_i \in C_{t-1}$ exists $\mathbf{c}_j \in C_t$ such that $d(\mathbf{c}_i, \mathbf{c}_j) < R$
    update $\mathbf{v}_t$ to reflect the new partitioning
else
    $C_t \leftarrow C_{t-1}$
    $\mathbf{v}_t \leftarrow \mathbf{v}_{t-1}$
end if
if $\mathbf{x}_t$ is closer than R to any $\mathbf{c}_i \in C_t$ **then**
    $\mathbf{v}_t(i) \leftarrow \mathbf{v}_t(i) + 1$
else
    $\mathbf{v}_t(|C_t|+1) \leftarrow 1$
end if

Online SSL with Graphs

Video examples

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

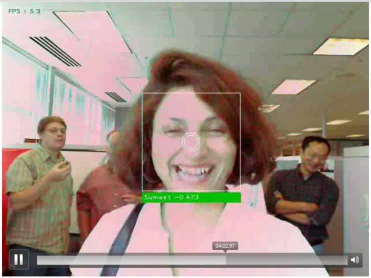
http://www.bkveton.com/videos/Ad.mp4

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

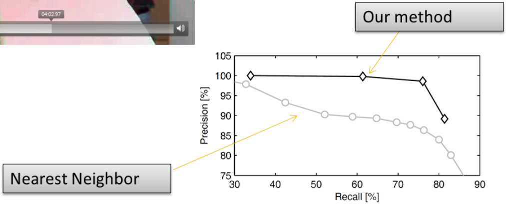
http://researchers.lille.inria.fr/~valko/hp/serve.php?what=publications/kveton2009nipsdemo.officespace.mov

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

SSL with Graphs: Some experimental results

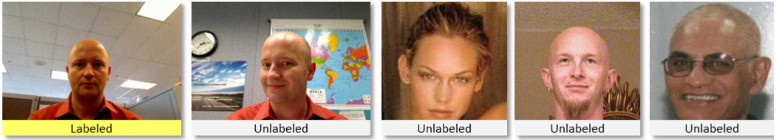


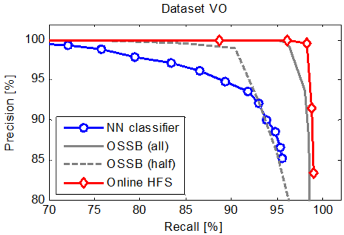
- 8 people classification
- Making funny faces
- 4 faces/person are labeled

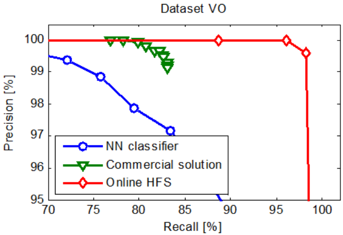


SSL with Graphs: Some experimental results

- 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)

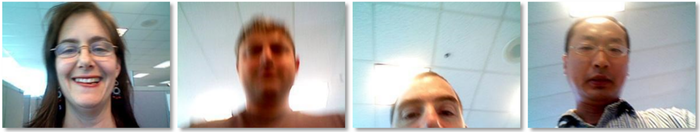
Online HFS yields better results than a commercial solution at 20% of the computational cost

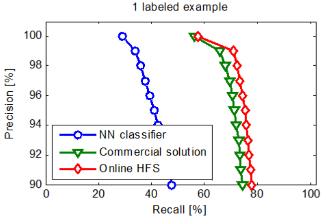
SSL with Graphs: Some experimental results

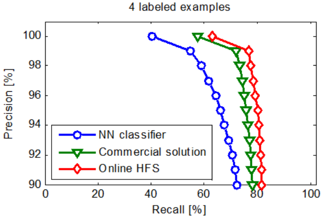
- **Logging in** with faces instead of password
- Able to **learn** and improve

SSL with Graphs: Some experimental results

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







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

Online SSL with Graphs: Analysis

What can we guarantee?

Three sources of error

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

All together:

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

Since for any a, b, c, $d \in [-1, 1]$:

$$(a-b)^2 \leq \frac{9}{2}\left[(a-c)^2 + (c-d)^2 + (d-b)^2\right]$$

Online SSL with Graphs: Analysis

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

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

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

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

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

$$R(\boldsymbol{\ell}^\star) = \frac{1}{N}\sum_t (\ell_t^\star - y_t)^2 \quad \text{and} \quad \widehat{R}(\boldsymbol{\ell}^\star) = \frac{1}{n_l}\sum_{t \in l} (\ell_t^\star - y_t)^2$$

How should we set γ_g?

Online SSL with Graphs: Analysis

Bounding online error $(\ell^{\text{o}}_t[t] - \ell^\star_t)^2$

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

since they get closer to zero

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

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

$$\|\boldsymbol{\ell}\|_2 \le \frac{\|\mathbf{y}\|_2}{\lambda_m(\mathbf{C}^{-1}\mathbf{Q} + \mathbf{I})} = \frac{\|\mathbf{y}\|_2}{\frac{\lambda_m(\mathbf{Q})}{\lambda_M(\mathbf{C})} + 1} \le \frac{\sqrt{n_l}}{\gamma_g + 1}$$

Difference between offline and online solutions:

$$(\ell^{\text{o}}_t[t] - \ell^\star_t)^2 \le \|\boldsymbol{\ell}^{\text{o}}[t] - \boldsymbol{\ell}^\star\|_\infty^2 \le \|\boldsymbol{\ell}^{\text{o}}[t] - \boldsymbol{\ell}^\star\|_2^2 \le \left(\frac{2\sqrt{n_l}}{\gamma_g + 1}\right)^2$$

Again, how should we set γ_g?

Online SSL with Graphs: Analysis

Bounding **quantization error** $\left(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t]\right)^2$

How are the quantized and full solution different?

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

In **Q**! $\mathbf{Q}^{\mathrm{o}}$ (online) vs. $\mathbf{Q}^{\mathrm{q}}$ (quantized)

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

Let $\mathbf{Z}^{\mathrm{q}} = \mathbf{C}^{-1}\mathbf{Q}^{\mathrm{q}} + \mathbf{I}$ and $\mathbf{Z}^{\mathrm{o}} = \mathbf{C}^{-1}\mathbf{Q}^{\mathrm{o}} + \mathbf{I}$.

$$\begin{aligned}\ell^{\mathrm{q}} - \ell^{\mathrm{o}} &= (\mathbf{Z}^{\mathrm{q}})^{-1}\mathbf{y} - (\mathbf{Z}^{\mathrm{o}})^{-1}\mathbf{y} = (\mathbf{Z}^{\mathrm{q}}\mathbf{Z}^{\mathrm{o}})^{-1}(\mathbf{Z}^{\mathrm{o}} - \mathbf{Z}^{\mathrm{q}})\mathbf{y} \\ &= (\mathbf{Z}^{\mathrm{q}}\mathbf{Z}^{\mathrm{o}})^{-1}\mathbf{C}^{-1}(\mathbf{Q}^{\mathrm{o}} - \mathbf{Q}^{\mathrm{q}})\mathbf{y}\end{aligned}$$

Online SSL with Graphs: Analysis

Bounding quantization error $\left(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t]\right)^2$

$$\begin{aligned}\boldsymbol{\ell}^{\mathrm{q}} - \boldsymbol{\ell}^{\mathrm{o}} &= (\mathbf{Z}^{\mathrm{q}})^{-1}\mathbf{y} - (\mathbf{Z}^{\mathrm{o}})^{-1}\mathbf{y} = (\mathbf{Z}^{\mathrm{q}}\mathbf{Z}^{\mathrm{o}})^{-1}(\mathbf{Z}^{\mathrm{o}} - \mathbf{Z}^{\mathrm{q}})\mathbf{y} \\ &= (\mathbf{Z}^{\mathrm{q}}\mathbf{Z}^{\mathrm{o}})^{-1}\mathbf{C}^{-1}(\mathbf{Q}^{\mathrm{o}} - \mathbf{Q}^{\mathrm{q}})\mathbf{y}\end{aligned}$$

$$\|\boldsymbol{\ell}^{\mathrm{q}} - \boldsymbol{\ell}^{\mathrm{o}}\|_2 \leq \frac{\lambda_M(\mathbf{C}^{-1})\|(\mathbf{Q}^{\mathrm{q}} - \mathbf{Q}^{\mathrm{o}})\mathbf{y}\|_2}{\lambda_m(\mathbf{Z}^{\mathrm{q}})\lambda_m(\mathbf{Z}^{\mathrm{o}})}$$

$||\cdot||_F$ and $||\cdot||_2$ are compatible and y_i is zero when unlabeled:

$$\|(\mathbf{Q}^{\mathrm{q}} - \mathbf{Q}^{\mathrm{o}})\mathbf{y}\|_2 \leq \|\mathbf{Q}^{\mathrm{q}} - \mathbf{Q}^{\mathrm{o}}\|_F \cdot \|\mathbf{y}\|_2 \leq \sqrt{n_l}\|\mathbf{Q}^{\mathrm{q}} - \mathbf{Q}^{\mathrm{o}}\|_F$$

Furthermore, $\lambda_m(\mathbf{Z}^{\mathrm{o}}) \geq \dfrac{\lambda_m(\mathbf{Q}^{\mathrm{o}})}{\lambda_M(\mathbf{C})} + 1 \geq \gamma_g$ and $\lambda_M\left(\mathbf{C}^{-1}\right) \leq c_u^{-1}$

We get $\|\boldsymbol{\ell}^{\mathrm{q}} - \boldsymbol{\ell}^{\mathrm{o}}\|_2 \leq \dfrac{\sqrt{n_l}}{c_u\gamma_g^2}\|\mathbf{Q}^{\mathrm{q}} - \mathbf{Q}^{\mathrm{o}}\|_F$

Online SSL with Graphs: Analysis

Bounding quantization error $\left(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t]\right)^2$

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

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

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

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

Assume manifold $\mathcal{M}$

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

Online SSL with Graphs: Analysis

Bounding quantization error $\left(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t]\right)^2$

Bounding $\|\mathbf{L}^{\mathrm{q}} - \mathbf{L}^{\mathrm{o}}\|_F$ 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

What is the maximum volume of this packing*?

$kc_s r^s \leq V + Ac_{\mathcal{M}} r$ with $c_s, c_{\mathcal{M}}$ depending on dimension and $\mathcal{M}$.

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

$$r < \left(\left(V + Ac_{\mathcal{M}}\right) / \left(kc_s\right)\right)^{1/s} = \mathcal{O}\left(k^{-1/s}\right)$$

r-packing is a $2r$-covering:

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

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

Online SSL with Graphs: Analysis

Bounding quantization error $\left(\ell_t^{\mathrm{q}}[t] - \ell_t^{\mathrm{o}}[t]\right)^2$

If similarity is M-Lipschitz, $\mathbf{L}$ is normalized, $c_{ij}^{\mathrm{o}} = \sqrt{\mathbf{D}_{ii}^{\mathrm{o}}\mathbf{D}_{jj}^{\mathrm{o}}} > c_{min}N$

$|\mathbf{W}_{ij}^{\mathrm{q}} - \mathbf{W}_{ij}^{\mathrm{o}}| < 2MRm/(m-1)$ and $|c_{ij}^{\mathrm{q}} - c_{ij}^{\mathrm{o}}| < 2nMRm/(m-1)$:

$$\begin{aligned}
\mathbf{L}_{ij}^{\mathrm{q}} - \mathbf{L}_{ij}^{\mathrm{o}} &= \frac{\mathbf{W}_{ij}^{\mathrm{q}}}{c_{ij}^{\mathrm{q}}} - \frac{\mathbf{W}_{ij}^{\mathrm{o}}}{c_{ij}^{\mathrm{o}}} \\
&\leq \frac{\mathbf{W}_{ij}^{\mathrm{q}} - \mathbf{W}_{ij}^{\mathrm{o}}}{c_{ij}^{\mathrm{q}}} + \frac{\mathbf{W}_{ij}^{\mathrm{o}}(c_{ij}^{\mathrm{o}} - c_{ij}^{\mathrm{q}})}{c_{ij}^{\mathrm{o}}c_{ij}^{\mathrm{q}}} \\
&\leq \frac{4MRm}{(m-1)c_{min}N} + \frac{4M(NMRm)}{((m-1)c_{min}N)^2} \\
&= O\left(\frac{R}{N}\right)
\end{aligned}$$

Finally, $\|\mathbf{L}^{\mathrm{q}} - \mathbf{L}^{\mathrm{o}}\|_F^2 \leq N^2\mathcal{O}(R^2/N^2) = \mathcal{O}(k^{-2/s})$.

Are the assumptions reasonable?

Online SSL with Graphs: Analysis

Bounding **quantization error** $\left(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t]\right)^2$

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

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

This converges to zero at the rate $\mathcal{O}(N^{-1/2})$ with $\gamma_g = \Omega(N^{1/8})$.

With properly setting γ_g, e.g., $\gamma_g = \Omega(N^{1/8})$, we can have

$$\frac{1}{N}\sum_{t=1}^{N}\left(\ell_t^{\mathrm{q}}[t]-y_t\right)^2 = \mathcal{O}\left(N^{-1/2}\right).$$

What does that mean?

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:

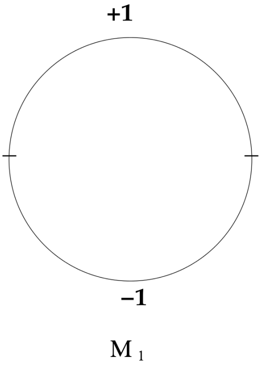
- SL: does not know about $\mathcal{M}$ and only knows $(\mathbf{x}_i, y_i)$
- SSL: perfect knowledge of $\mathcal{M}$ $\equiv$ humongous amounts of $\mathbf{x}_i$

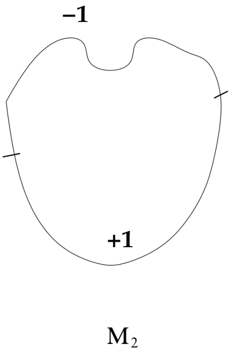
http://people.cs.uchicago.edu/~niyogi/papersps/ssminimax2.pdf

SSL with Graphs: What is behind it?

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

$$\mathcal{P} = \cup_{\mathcal{M}} \mathcal{P}_{\mathcal{M}} = \cup_{\mathcal{M}} \{p \in \mathcal{P} | p_{\mathcal{X}} \text{ is uniform on } \mathcal{M}\}$$





SSL with Graphs: What is behind it?

Set of problems $\mathcal{P} = \cup_{\mathcal{M}} \mathcal{P}_{\mathcal{M}} = \{p \in \mathcal{P} | p_{\mathcal{X}}$ is uniform on $\mathcal{M}\}$
Regression function $m_p = \mathbb{E}[y | x]$ when $x \in \mathcal{M}$
Algorithm A and **labeled examples** $\bar{z} = \{z_i\}_{i=1}^{n_l} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n_l}$
Minimax rate

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

Since $\mathcal{P} = \cup_{\mathcal{M}} \mathcal{P}_{\mathcal{M}}$

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

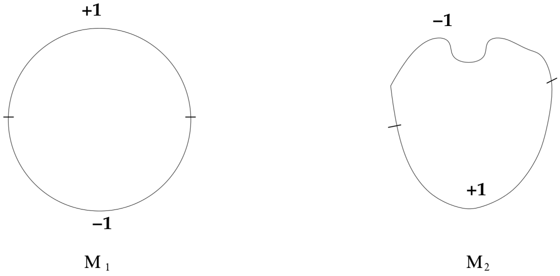
(SSL) When A is allowed to know $\mathcal{M}$

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

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



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

What is a VC dimension of $\mathcal{H}_{\mathcal{M}}$?

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

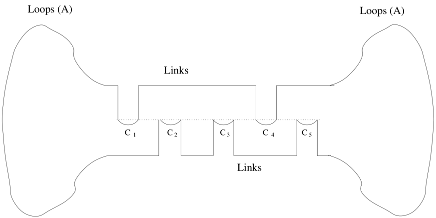
SSL with Graphs: What is behind it?

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

$$R(n_l, \mathcal{P}) = \inf_{A} \sup_{p \in \mathcal{P}} \mathbb{E}_{\bar{z}} \left[\| A(\bar{z}) - m_p \|_{L^2(p_{\mathbf{X}})} \right] = \Omega(1)$$

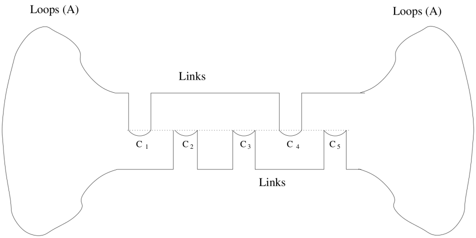
We consider 2^d manifolds of the form

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



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

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**

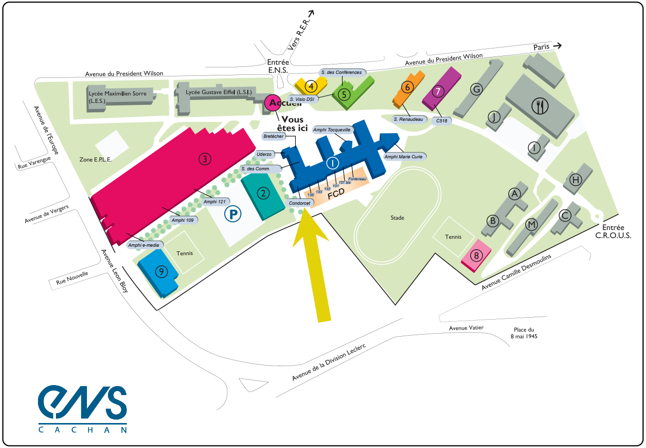
SSL with Graphs: What is behind it?

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

Different degrees of knowing $\mathcal{M}$

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

Next lecture: Wednesday, November 21th at 14:00!



Michal Valko

michal.valko@inria.fr

ENS Paris-Saclay, MVA 2018/2019

SequeL team, Inria Lille — Nord Europe

https://team.inria.fr/sequel/