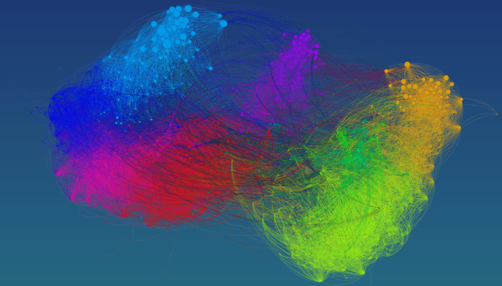
Graphs in Machine Learning

Michal Valko

Inria Lille - Nord Europe, France

TA: Pierre Perrault

Partially based on material by: Branislav Kveton, Partha Niyogi, Rob Fergus



Last Lecture

- Inductive and transductive semi-supervised learning
- Manifold regularization
- 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

This Lecture

- Analysis of online SSL
- SSL Learnability
- When does graph-based SSL provably help?
- Scaling harmonic functions to millions of samples

Previous Lab Session

- 13. 11. 2017 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:* 27. 11. 2017

Next Lab Session/Lecture

- 27. 11. 2016 by Pierre Perrault
- Content (this time lecture in class + coding at home)
  - Large-scale graph construction and processing (in class)
  - Scalable algorithms:
    - Online face recognizer (to code in Matlab)
    - Iterative label propagation (to code in Matlab)
    - Graph sparsification (presented in class)
- AR: record a video with faces
- Short written report
- Questions to piazza
- *Deadline:* 11. 12. 2016

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
  - 20. 11. 2017 - strongly recommended DL for taking projects
  - 27. 11. 2017 - hard DL for taking projects
  - 08. 01. 2018 - submission of the project report
  - 09. 01. 2018 or later - project presentation
- list of suggested topics on piazza

DELTA: MVA internship + PhD proposal

Dynamically Evolving Long-Term Autonomy

- join project between 4 partners, UPF Barcelona, MUL Austria, ULG Belgium, and Inria
- Jonsson, Neu, Gomez, Valko, Kaufmann, Lazaric, Auer, Ortner, Cornelusse, Ernst
- **PhD position at SequeL team at Inria**
- project starts on 1.1.2018, PhD student expected to start September/October 2018
- 4 postdocs, one in each center
- Inria will lead the effort on adaptive planning with a model that can adapt to changes. Inria will work with MUL on the hierarchical state partitioning
- contact: (Emilie Kaufmann & Michal Valko) @ SequeL @ Inria

Online SSL with Graphs: Analysis

What can we guarantee?

Three sources of error

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

All together:

$$\frac{1}{N}\sum_{t=1}^{N}(\ell^{\mathrm{q}}_t[t]-y_t)^2 \le \frac{9}{2N}\sum_{t=1}^{N}(\ell^\star_t-y_t)^2+\frac{9}{2N}\sum_{t=1}^{N}(\ell^{\mathrm{o}}_t[t]-\ell^\star_t)^2+\frac{9}{2N}\sum_{t=1}^{N}(\ell^{\mathrm{q}}_t[t]-\ell^{\mathrm{o}}_t[t])$$

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

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

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

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

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

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

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

How should we set γ_g?

Online SSL with Graphs: Analysis

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

Idea: If $\mathbf{L}$ and $\mathbf{L}^{\mathrm{o}}$ 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 $\mathbf{v} \in \mathbb{R}^{n\times 1}$, $\lambda_m(A)\|\mathbf{v}\|_2 \leq \|A\mathbf{v}\|_2 \leq \lambda_M(A)\|\mathbf{v}\|_2$

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

Difference between offline and online solutions:

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

Again, how should we set γ_g?

Online SSL with Graphs: Analysis

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

How are the quantized and full solution different?

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

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

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

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

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

Online SSL with Graphs: Analysis

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

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

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

$||\cdot||_F$ 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 $(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t])^2$

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 $(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t])^2$

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 $(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t])^2$

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** $(\ell_t^{\mathrm{q}}[t]-\ell_t^{\mathrm{o}}[t])^2$

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 of $\mathcal{O}(N^{-1/2})$ with $\gamma_g=\Omega(N^{1/8})$.

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

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

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:

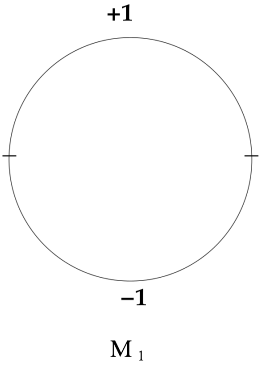
- SL: does not know about $\mathcal{M}$ and only knows $(\mathbf{x}_i, y_i)$
- SSL: perfect knowledge of $\mathcal{M} \equiv$ humongous amounts of $\mathbf{x}_i$

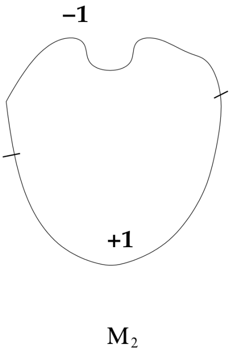
http://people.cs.uchicago.edu/~niyogi/papersps/ssminimax2.pdf

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 $m_p = \mathbb{E}\left[y\,|x\right]$ when $x \in \mathcal{M}$
Algorithm A and **labeled examples** $\overline{z} = \{z_i\}_{i=1}^{n_l} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n_l}$
Minimax rate

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

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

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

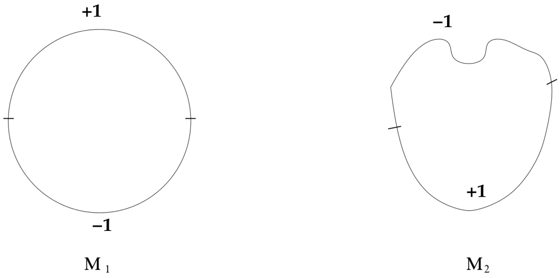
(SSL) When A is allowed to know $\mathcal{M}$

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

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 $\mathcal{H}_\mathcal{M}$?

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

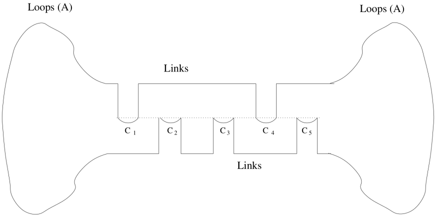
SSL with Graphs: What is behind it?

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

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

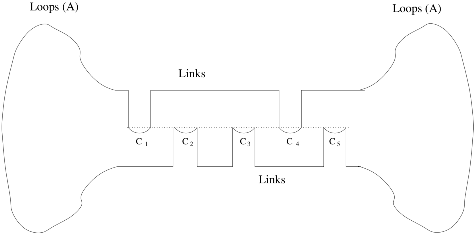
We consider 2^d manifolds of the form

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



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

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

Scaling SSL with Graphs to Millions

Semi-supervised learning with graphs

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

Let us see the same in eigenbasis of $\mathbf{L} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\mathsf{T}$, i.e., $\mathbf{f} = \mathbf{U}\boldsymbol{\alpha}$

$$\boldsymbol{\alpha}^\star = \min_{\boldsymbol{\alpha}\in\mathbb{R}^N} (\mathbf{U}\boldsymbol{\alpha}-\mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{U}\boldsymbol{\alpha}-\mathbf{y}) + \boldsymbol{\alpha}^\mathsf{T}\mathbf{\Lambda}\boldsymbol{\alpha}$$

What is the problem with scalability?

Diagonalization of $N \times N$ matrix

What can we do? Let's take only first k eigenvectors $\mathbf{f} = \mathbf{U}\boldsymbol{\alpha}$!

Scaling SSL with Graphs to Millions

$\mathbf{U}$ is now a $n \times k$ matrix

$$\boldsymbol{\alpha}^\star = \min_{\boldsymbol{\alpha} \in \mathbb{R}^N} (\mathbf{U}\alpha - \mathbf{y})^\mathsf{T}\mathbf{C}(\mathbf{U}\alpha - \mathbf{y}) + \alpha^\mathsf{T}\boldsymbol{\Lambda}\alpha$$

Closed form solution is $(\boldsymbol{\Lambda} + \mathbf{U}^\mathsf{T}\mathbf{C}\mathbf{U})\alpha = \mathbf{U}^\mathsf{T}\mathbf{C}\mathbf{y}$

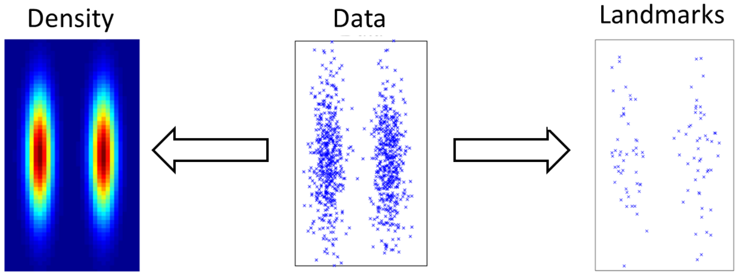
What is the size of this system of equation now?

Cool! Any problem with this approach?

Are there any reasonable assumptions when this is feasible?

Let's see what happens when $N \to \infty$!

Scaling SSL with Graphs to Millions



Limit as n $\rightarrow \infty$

Reduce n

Linear in number of data-points

Polynomial in number of landmarks

https://cs.nyu.edu/~fergus/papers/fwt_ssl.pdf

Scaling SSL with Graphs to Millions

What happens to L when $N \to \infty$?

We have data $\mathbf{x}_i \in \mathbb{R}$ sampled from $p(\mathbf{x})$.

When $n \to \infty$, instead of vectors $\mathbf{f}$, we consider functions $F(x)$.

Instead of $\mathbf{L}$, we define $\mathcal{L}_p$ - **weighted smoothness operator**

$$\mathcal{L}_p(F) = \frac{1}{2}\int (F(\mathbf{x}_1) - F(\mathbf{x}_2))^2 W(\mathbf{x}_1, \mathbf{x}_2) p(\mathbf{x}_1) p(\mathbf{x}_2) \,\mathrm{d}\mathbf{x}_1\mathbf{x}_2$$

$$\text{with } W(\mathbf{x}_1, \mathbf{x}_2) = \frac{\exp(-\|\mathbf{x}_1 - \mathbf{x}_2\|^2)}{2\sigma^2}$$

$\mathbf{L}$ defined the eigenvectors of increasing smoothness.

What defines $\mathcal{L}_p$? **Eigenfunctions!**

Scaling SSL with Graphs to Millions

$$\mathcal{L}_p(F) = \frac{1}{2}\int \left(F(\mathbf{x}_1) - F(\mathbf{x}_2)\right)^2 W(\mathbf{x}_1, \mathbf{x}_2) p(\mathbf{x}_1)\, p(\mathbf{x}_2)\, \mathrm{d}x_1 x_2$$

First eigenfunction

$$\Phi_1 = \underset{F:\int F^2(\mathbf{x})p(\mathbf{x})D(\mathbf{x})\,\mathrm{d}x=1}{\arg\min} \mathcal{L}_p(F)$$

where $D(\mathbf{x}) = \int_{\mathbf{x}_2} W(\mathbf{x}, \mathbf{x}_2)\, p(\mathbf{x}_2)\, \mathrm{d}\mathbf{x}_2$

What is the solution? $\Phi_1(\mathbf{x}) = 1$ because $\mathcal{L}_p(1) = 0$

How to define Φ_2? same, constraining to be orthogonal to Φ_1

$$\int F(\mathbf{x})\, \Phi_1(\mathbf{x})\, p(\mathbf{x})\, D(\mathbf{x})\, \mathrm{d}x = 0$$

Scaling SSL with Graphs to Millions

Eigenfunctions of $\mathcal{L}_p$

Φ_3 as before, orthogonal to Φ_1 and Φ_2 etc.

How to define eigenvalues? $\lambda_k = \mathcal{L}_p(\Phi_k)$

Relationship to the discrete Laplacian

$$\frac{1}{N^2}\mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f} = \frac{1}{2N^2}\sum_{ij} W_{ij}(f_i - f_j)^2 \xrightarrow[N\to\infty]{} \mathcal{L}_p(F)$$

http://www.informatik.uni-hamburg.de/ML/contents/people/luxburg/publications/Luxburg04_diss.pdf
http://arxiv.org/pdf/1510.08110v1.pdf

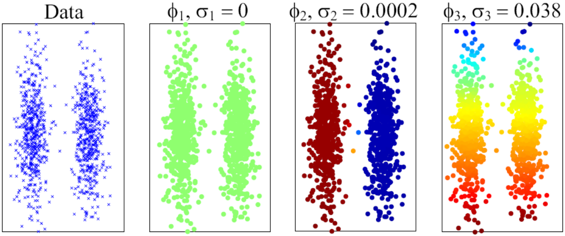
Isn't estimating eigenfunctions $p(\mathbf{x})$ more difficult?

Are there some "easy" distributions?

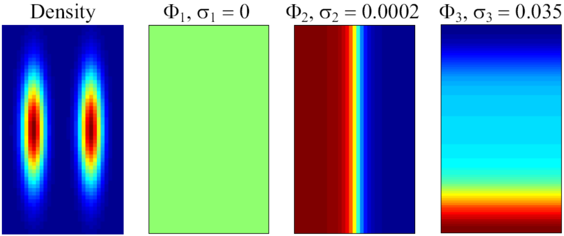
Can we compute it numerically?

Scaling SSL with Graphs to Millions

Eigenvectors



Eigenfunctions

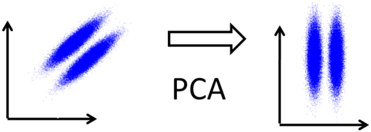


Scaling SSL with Graphs to Millions

Factorized data distribution What if

$$p(\mathbf{s}) = p(s_1)\, p(s_2) \ldots p(s_d)$$

In general, this is not true. But we can rotate data with $\mathbf{s} = \mathbf{Rx}$.



Treating each factor individually

$p_k \stackrel{\text{def}}{=}$ marginal distribution of s_k

$\Phi_i(s_k) \stackrel{\text{def}}{=}$ eigenfunction of $\mathcal{L}_{p_k}$ with eigenvalue λ_i

Then: $\Phi_i(s) = \Phi_i(s_k)$ is eigenfunction of $\mathcal{L}_p$ with λ_i

We only considered single-coordinate eigenfunctions.

Scaling SSL with Graphs to Millions

How to approximate 1D density? Histograms!

Algorithm of Fergus et al. [FWT09] for eigenfunctions

- Find $\mathbf{R}$ such that $\mathbf{s} = \mathbf{Rx}$
- For each "independent" s_k approximate $p(s_k)$
- Given $p(s_k)$ numerically solve for eigensystem of $\mathcal{L}_{p_k}$

$$\left(\widetilde{\mathbf{D}} - \mathbf{P}\widetilde{\mathbf{W}}\mathbf{P}\right)\mathbf{g} = \lambda \mathbf{P}\widehat{\mathbf{D}}\mathbf{g} \qquad \text{(generalized eigensystem)}$$

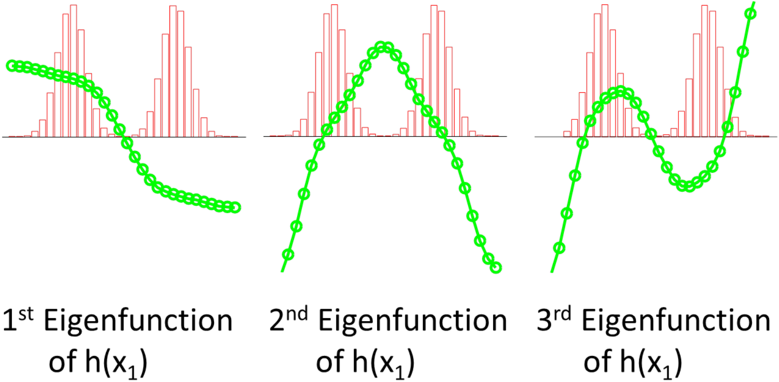
  $\mathbf{g}$ - vector of length $B \equiv$ number of bins
  $\mathbf{P}$ - density at discrete points
  $\widetilde{\mathbf{D}}$ - diagonal sum of $\mathbf{P}\widetilde{\mathbf{W}}\mathbf{P}$
  $\widehat{\mathbf{D}}$ - diagonal sum of $\mathbf{P}\widetilde{\mathbf{W}}$

- Order eigenfunctions by increasing eigenvalues

https://cs.nyu.edu/~fergus/papers/fwt_ssl.pdf

Scaling SSL with Graphs to Millions

Numerical 1D Eigenfunctions



https://cs.nyu.edu/~fergus/papers/fwt_ssl.pdf

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Computational complexity for $N \times d$ dataset

Typical harmonic approach

one diagonalization of $N \times N$ system

Numerical eigenfunctions with B bins and k eigenvectors

d eigenvector problems of $B \times B$

$$\left(\widetilde{\mathbf{D}} - \mathbf{P}\widetilde{\mathbf{W}}\mathbf{P}\right)\mathbf{g} = \lambda \mathbf{P}\widehat{\mathbf{D}}\mathbf{g}$$

one $k \times k$ least squares problem

$$(\mathbf{\Lambda} + \mathbf{U}^\mathsf{T}\mathbf{C}\mathbf{U})\alpha = \mathbf{U}^\mathsf{T}\mathbf{C}\mathbf{y}$$

some details: several approximation, eigenvectors only linear combinations single-coordinate eigenvectors, ...

When d is not too big then N can be in millions!

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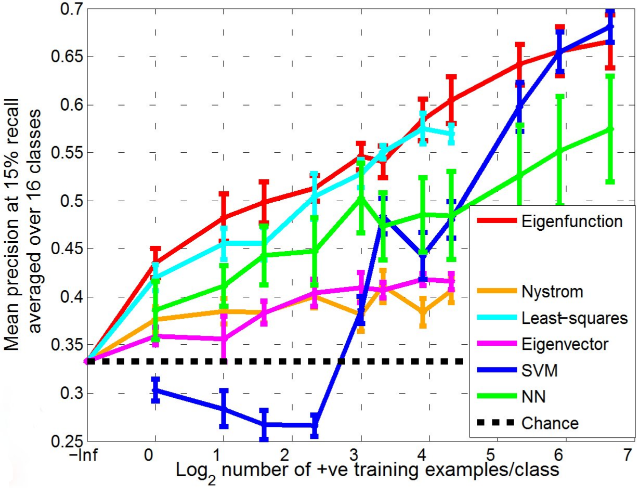

CIFAR experiments `https://cs.nyu.edu/~fergus/papers/fwt_ssl.pdf`

Michal Valko
michal.valko@inria.fr
ENS Paris-Saclay, MVA 2017/2018
SequeL team, Inria Lille — Nord Europe
`https://team.inria.fr/sequel/`