



Graphs in Machine Learning

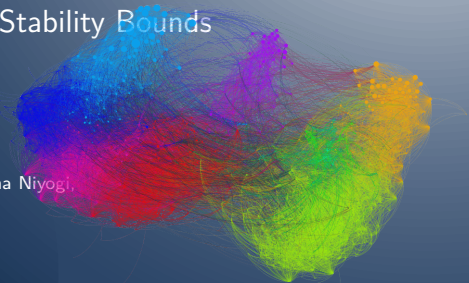
SSL Regularization and Stability

Regularized, Soft Harmonic, and Stability Bounds

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Inria & ENS Paris-Saclay, MVA

Partially based on material by: Mikhail Belkin, Partha Niyogi,
Olivier Chapelle, Bernhard Schölkopf



SSL with Graphs: Regularized Harmonic Functions

$$f_i = p_i^{(+1)} - p_i^{(-1)}$$

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

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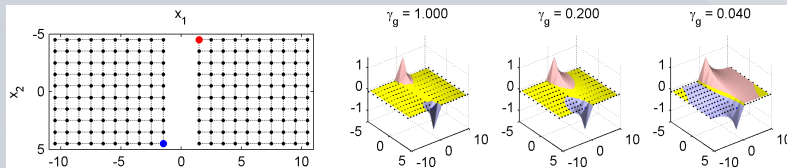
How does γ_g influence HS?

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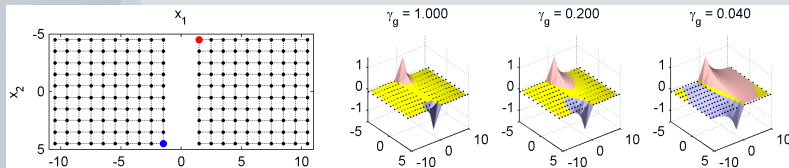


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What happens to sneaky outliers?

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

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

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

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

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

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Closed form **soft harmonic solution**:

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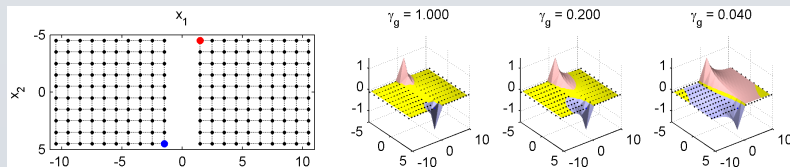
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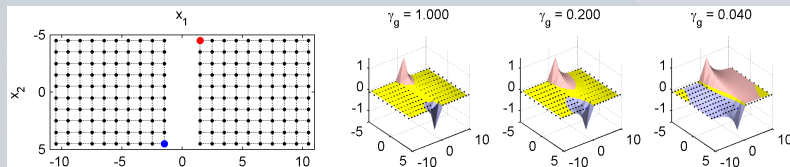


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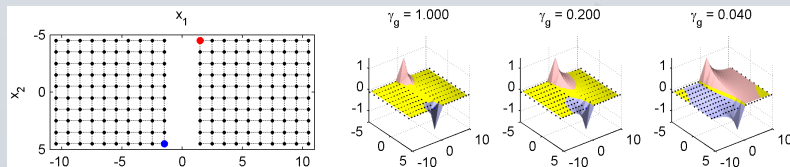
What are the differences between hard and soft?

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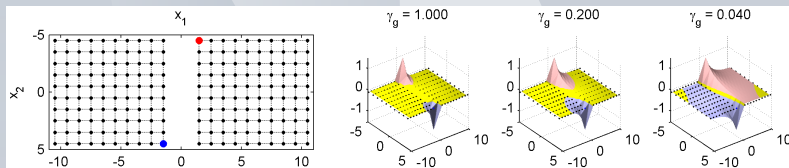
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Provable generalization guarantees for the soft one.

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

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$$\mathcal{C}_1 = \mathbf{C}_1^{-1} \mathbf{Q} + \mathbf{I} \text{ and } \mathcal{C}_2 = \mathbf{C}_2^{-1} \mathbf{Q} + \mathbf{I}$$

What is the maximal difference in the solutions?

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

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

$$\|\mathbf{f}_2^* - \mathbf{f}_1^*\|_2$$

SSL with Graphs: Stability Bounds

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

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

SSL with Graphs: Stability Bounds

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SSL with Graphs: Stability Bounds

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SSL with Graphs: Stability Bounds

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

SSL with Graphs: Stability Bounds

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

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

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

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

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

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

SSL with Graphs: Stability Bounds

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

SSL with Graphs: Stability Bounds

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

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

Take $c_l = 1$

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

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

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

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

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

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

SSL with Graphs: Stability Bounds

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

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

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

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

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

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

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

SSL with Graphs: Stability Bounds

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

SSL with Graphs: Stability Bounds

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SSL with Graphs: Stability Bounds

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

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SSL with Graphs: Stability Bounds

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

This algorithm is β -stable!

SSL with Graphs: Regularized Harmonic Functions

Larger implications of random walks

random walk relates to **commute distance**

SSL with Graphs: Regularized Harmonic Functions

Larger implications of random walks

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

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

SSL with Graphs: Regularized Harmonic Functions

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Do we have this property for HS?

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Solutions?

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Solutions? 1) γ_g

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Solutions? 1) γ_g 2) amplified commute distance

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

SSL with Graphs: Regularized Harmonic Functions

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Solution: **Manifold Regularization**

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`https://misovalko.github.io/mva-ml-graphs.html`