# Graphs in Machine Learning

## SSL Regularization and Stability

### Regularized, Soft Harmonic, and Stability Bounds

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

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

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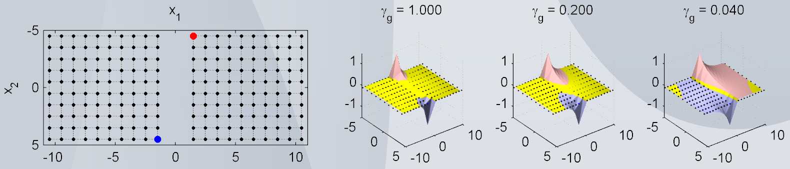

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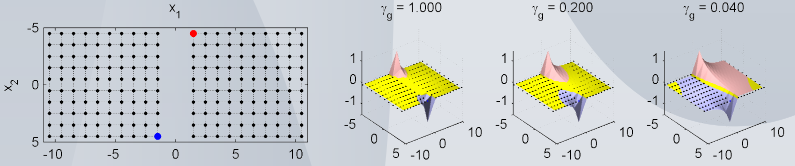


What happens to sneaky outliers?

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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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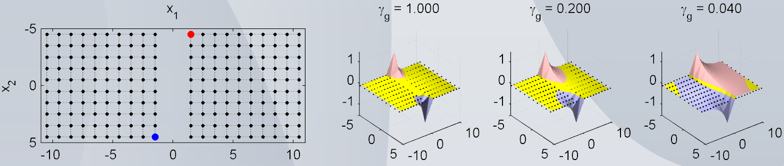

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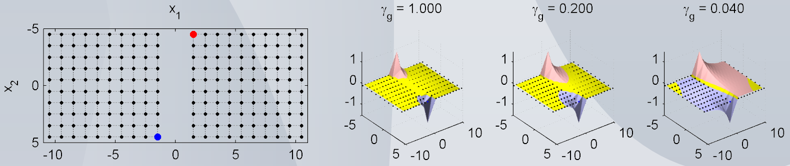


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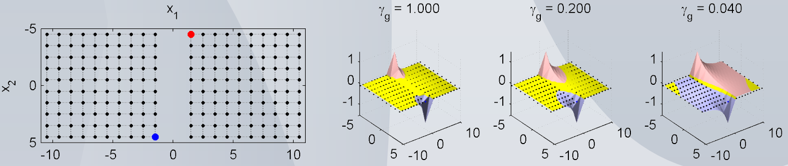


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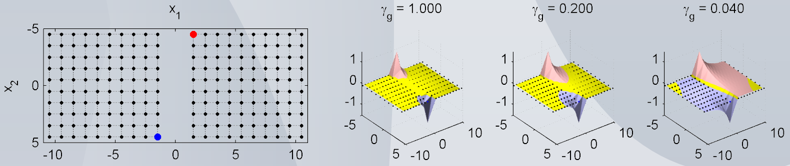


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Provable generalization guarantees for the soft one.

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\end{aligned}$$

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

# SSL with Graphs: Stability Bounds

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

Think about **stability** of this solution.
Consider two datasets differing in exactly one *labeled* point.
$\mathcal{C}_1 = \mathbf{C}_1^{-1}\mathbf{Q} + \mathbf{I}$ and $\mathcal{C}_2 = \mathbf{C}_2^{-1}\mathbf{Q} + \mathbf{I}$

What is the maximal difference in the solutions?

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

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# SSL with Graphs: Stability Bounds

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

Take $c_l = 1$

# SSL with Graphs: Stability Bounds

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

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

# SSL with Graphs: Stability Bounds

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

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

This algorithm is $\beta$-stable!

# SSL with Graphs: Regularized Harmonic Functions

**Larger implications of random walks**

random walk relates to **commute distance**

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Solutions?

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Solutions? 1) $\gamma_g$

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Solution: **Manifold Regularization**

# Michal Valko

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