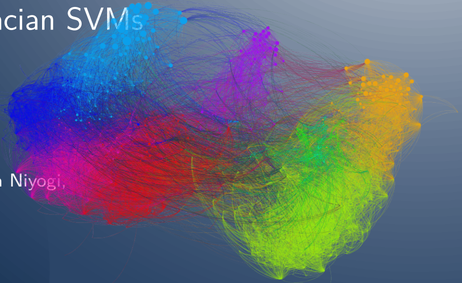
Graphs in Machine Learning

SSL Manifold Regularization

Manifold Regularization and Laplacian SVMs

Michal Valko

Inria & ENS Paris-Saclay, MVA



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

SSL with Graphs: Manifold Regularization

General (S)SL objective:

$$\min_f \sum_i^{n_l} V(\mathbf{x}_i, y_i, f(\mathbf{x}_i)) + \lambda\Omega(f)$$

Want to control f, also for the out-of-sample data, i.e., **everywhere**.

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For general **kernels**:

$$\min_{f\in\mathcal{H}_\mathcal{K}} \sum_{i}^{n_l} V(\mathbf{x}_i, y_i, f(\mathbf{x}_i)) + \lambda_1 \|f\|_\mathcal{K}^2 + \lambda_2 \mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f}$$

SSL with Graphs: Manifold Regularization

$$f^\star = \underset{f \in \mathcal{H}_\mathcal{K}}{\arg\min} \sum_{i}^{n_l} V\left(\mathbf{x}_i, y_i, f\right) + \lambda_1 \|f\|_\mathcal{K}^2 + \lambda_2 \mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f}$$

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SSL with Graphs: Laplacian SVMs

$$f^\star = \operatorname*{arg\,min}_{f \in \mathcal{H}_\mathcal{K}} \sum_{i}^{n_l} \max\left(0, 1 - yf\left(\mathbf{x}\right)\right) + \gamma_A \|f\|_\mathcal{K}^2 + \gamma_I \mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f}$$

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Allows us to learn a function in **RKHS**, i.e., **RBF** kernels.

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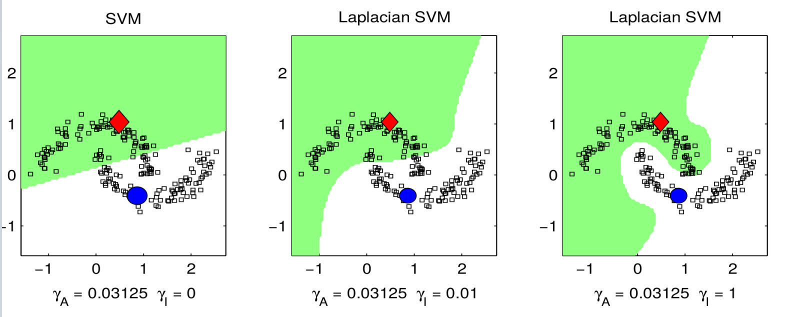

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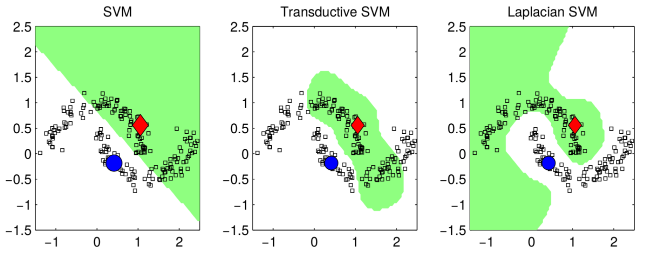

Checkpoint 1

Semi-supervised learning with graphs:

$$\min_{\mathbf{f} \in \{\pm 1\}^{n_l+n_u}} (\infty) \sum_{i=1}^{n_l} w_{ij} \left(f(\mathbf{x}_i) - y_i\right)^2 + \lambda \sum_{i,j=1}^{n_l+n_u} \left(f(\mathbf{x}_i) - f(\mathbf{x}_j)\right)^2$$

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Regularized harmonic Solution:

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

Checkpoint 2

Unconstrained regularization in general:

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

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Out of sample extension: Laplacian SVMs

$$f^\star = \arg\min_{f\in\mathcal{H}_\mathcal{K}} \sum_i^{n_l} \max\left(0, 1 - yf\left(\mathbf{x}\right)\right) + \lambda_1 \|f\|_\mathcal{K}^2 + \lambda_2 \mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f}$$

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