Graphical Semisupervised Learning

Applications and Theory

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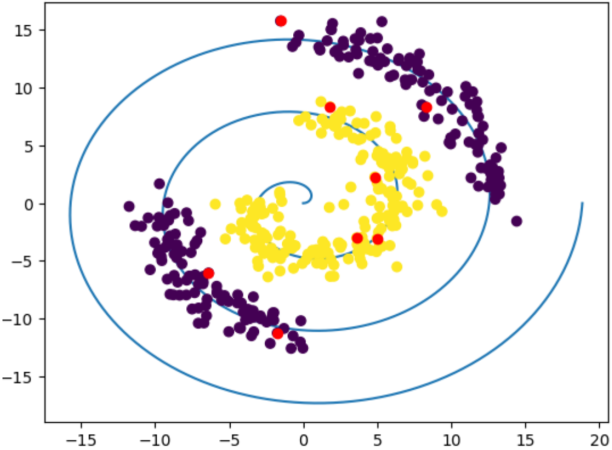
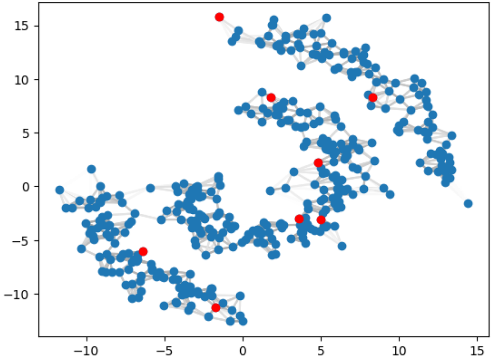
SSL

Given $\{x_i, y_i\}_{i=1}^{M}$ and $\{x_i\}_{i=M+1}^{N}$, we predict $y_i(x_i)$ for $i = M+1, \ldots, N$ where $M \ll N$.



GSSL

We construct our graphs by KNN or Proximity graph construction.



Optimization Problem
Loss functions

- General optimization

$$\vec{f}^* = \underset{\vec{f} \in \mathbb{R}^m}{\arg\min}\, \mathcal{L}(\vec{f}, y) + \lambda \vec{f}^T C^{-1} \vec{f}$$

where $\mathcal{L}$ is a loss function:

- Probit loss

$$\mathcal{L}(\vec{f}, y) = -\sum_{j=1}^{M} \log \Psi(\vec{f}_j y_j)$$

- Regression loss

$$\mathcal{L}(\vec{f}, y) = \sum_{j=1}^{M} \left(\vec{f}_j - y_j\right)^2$$

Optimization Problem
Matérn kernel-regularization

- General optimization

$$\vec{f}^* = \underset{\vec{f} \in \mathbb{R}^m}{\arg\min}\, \mathcal{L}(\vec{f}, y) + \lambda \vec{f}^T C^{-1} \vec{f}$$

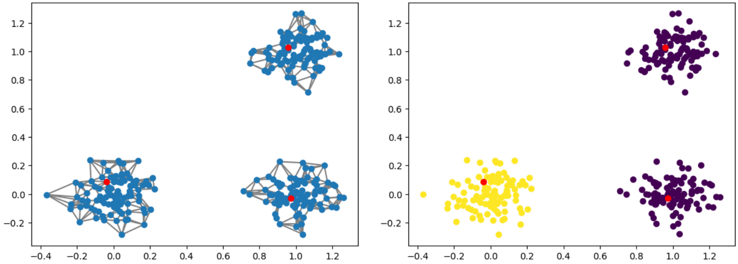
where $C = (L + \tau^2 I)^{-\alpha}$, where L is the graph Laplacian.

- C embeds the spectral geometric information in our regression problem:

$$C = \tau^{-2\alpha} \sum_{q=1}^{Q} \mathbb{1}_{G_q} \mathbb{1}_{G_q}^T + O(1)$$

Results
Three Cluster Case

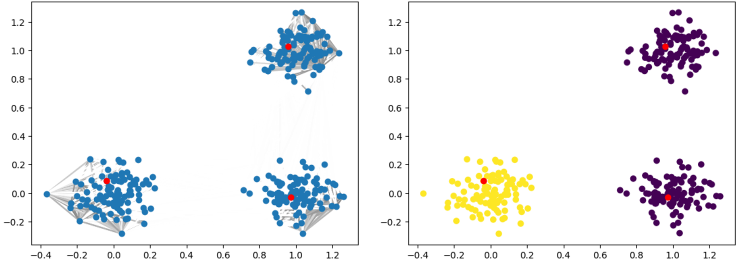
Using the K-Nearest Neighbors Graph with Uniform Weights



Loss Function	Classification Accuracy (over 50 trials)
Probit	100.0%
Regression	100.0%

Results
Three Cluster Case

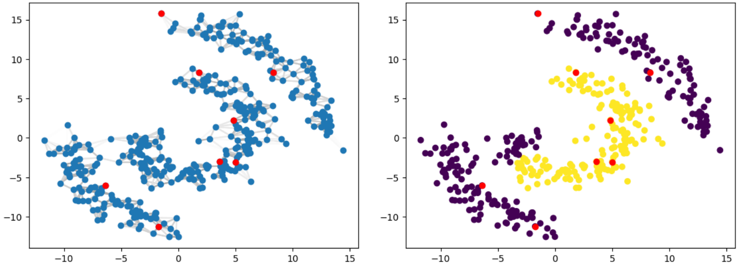
Using the Proximity Graph with RBF Weights



Loss Function	Classification Accuracy (over 50 trials)
Probit	100.0%
Regression	100.0%

Results
Spiral Case

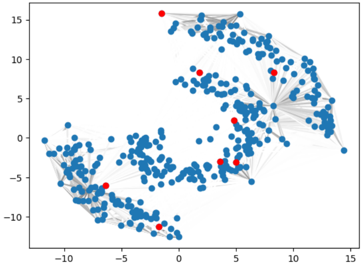
Using the K-Nearest Neighbors Graph with RBF Weights

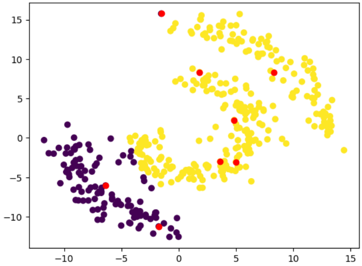


Loss Function	Classification Accuracy (over 50 trials)
Probit	96.3%
Regression	95.8%

Results
Spiral Case

Using the Proximity Graph with RBF Weights





Loss Function	Classification Accuracy (on 1 trial)
Probit	73.0%
Regression	63.0%

Conclusions and Further Questions

- Conclusions
  - For well separated clusters, the method is effective, even without careful tuning
  - Not the case for more difficult scenarios
- Challenges Encountered
  - Tuning of parameters - especially for real data
  - Majority labelling
- Next Steps
  - Plan to apply this approach to MNIST to test on real data
  - Anticipate tuning challenges for more difficult pairs of numbers

Bibliography

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