Large Graph Limits of Learning Algorithms

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In preparation

Talk Overview

Learning and Inverse Problems

Graph Laplacian

Inverse Problem Formulation

Large Graph Limits

Probability

Conclusions

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Regression

- Let $D \subset \mathbb{R}^d$ be a bounded open set.
- Let $D' \subset D$.

Ill-Posed Inverse Problem

Find $u : D \mapsto \mathbb{R}$ given

$$y(x) = u(x), \quad x \in D'.$$

- Strong prior information needed.

Classification

- Let $D \subset \mathbb{R}^d$ be a bounded open set.
- Let $D' \subset D$.

Ill-Posed Inverse Problem

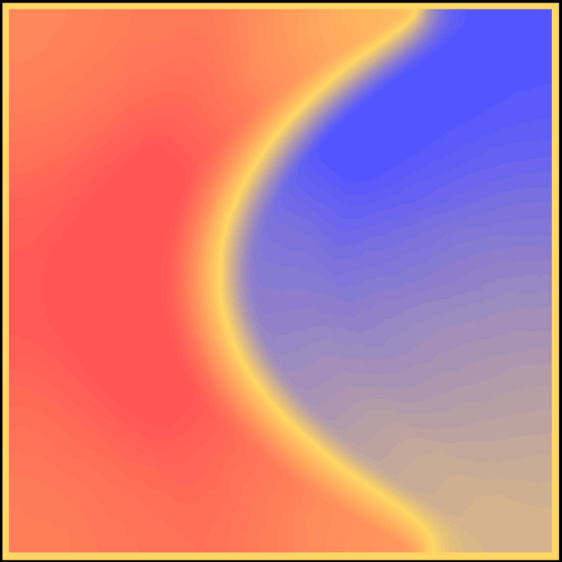
Find $u : D \mapsto \mathbb{R}$ given

$$y(x) = \text{sign}\big(u(x)\big), \quad x \in D'.$$

- Even stronger prior information needed.

$y = \text{sign}(u)$. Red$= 1$. Blue$= -1$. Yellow: no information.

Reconstruction of the function u on D



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Graph Laplacian

Graph Laplacian:

- Similarity graph G with n vertices $Z = \{1, \ldots, n\}$.
- Weighted adjacency matrix $W = \{w_{j,k}\}$, $\Big(w_{j,k} = \eta_\varepsilon(x_j - x_k).\Big)$
- Diagonal $D = \text{diag}\{d_{jj}\}$, $d_{jj} = \sum_{k \in Z} w_{j,k}$.
- $L = s_n(D - W)$ (unnormalized).

Spectral Properties:

- L is positive semi-definite: $\langle u, Lu \rangle_{\mathbb{R}^n} \propto \sum_{j \sim k} w_{j,k} |u_j - u_k|^2$.
- $Lq_j = \lambda_j q_j$;
- Fully connected $\Rightarrow$ $\lambda_1 > \lambda_0 = 0$. Fiedler Vector: q_1.

Example: Voting Records

U.S. House of Representatives 1984, 16 key votes. For each congress representative we have an associated feature vector $x_j \in \mathbb{R}^{16}$ such as

$$x_j = (1, -1, 0, \cdots, 1)^T;$$

1 is "yes", -1 is "no" and 0 abstain/no-show. Here $d = 16$ and $n = 435$.

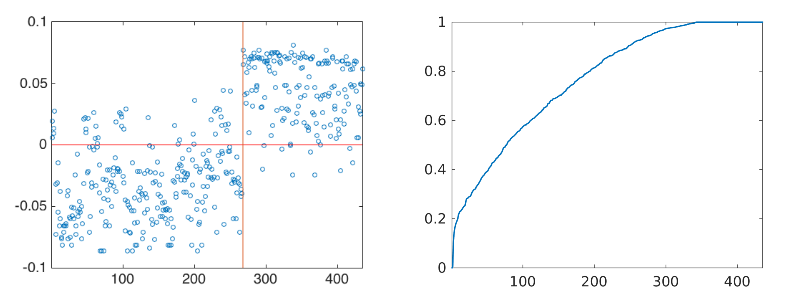

Figure: Strong Prior Information: Fiedler Vector and Spectrum (Normalized)

Example of Underlying Gaussian (Voting Records)

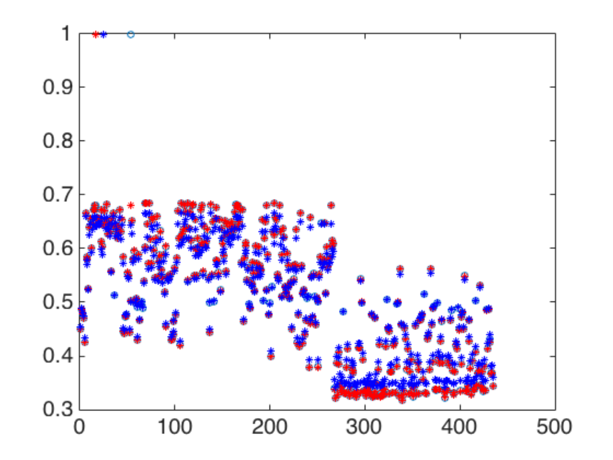

Figure: Two point correlation of $\mathrm{sign}(u)$ for 3 Democrats

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Problem Statement (Optimization)

Semi-Supervised Learning

- **Input**:
  - Unlabelled data $\{x_j \in \mathbb{R}^d, \quad j \in Z := \{1, \ldots, n\}\}$;
  - Labelled data $\{y_j \in \{\pm 1\}, \quad j \in Z' \subset Z\}$.
- **Output**:
  - Labels $\{y_j \in \{\pm 1\}, \quad j \in Z\}$.

Classification based on $\mathrm{sign}(u)$, u the optimizer of:

$$J(u; y) = \frac{1}{2}\langle u, C^{-1}u\rangle_{\mathbb{R}^n} + \Phi(u; y).$$

- u is an $\mathbb{R}-$valued function on the graph nodes.
- $C = (L + \tau^2 I)^{-\alpha}$ $\Big($from unlabelled data: $w_{j,k} = \eta_\varepsilon(x_j - x_k)$.$\Big)$
- $\Phi(u; y)$ links real-valued u to the binary-valued labels y.

Problem Statement (Bayesian Formulation)

Semi-Supervised Learning

- **Input**:
  - Unlabelled data $\{x_j \in \mathbb{R}^d, \quad j \in Z := \{1, \dots, n\}\}$; **prior**
  - Labelled data $\{y_j \in \{\pm 1\}, \quad j \in Z' \subseteq Z\}$. **likelihood**
- **Output**:
  - Labels $\{y_j \in \{\pm 1\}, \quad j \in Z\}$. **posterior**

Connection between probability and optimization:

$$J^{(n)}(u; y) = \frac{1}{2}\langle u, C^{-1}u\rangle_{\mathbb{R}^n} + \Phi^{(n)}(u; y).$$

$$\begin{aligned}
\mathbb{P}(u|y) &\propto \exp\big(-J^{(n)}(u; y)\big) \\
&\propto \exp\big(-\Phi^{(n)}(u; y)\big) \times \mathsf{N}(0, C) \\
&\propto \mathbb{P}(y|u) \times \mathbb{P}(u).
\end{aligned}$$

Probit

Rasmussen and Williams, 2006. (MIT Press)

Bertozzi, Luo, Stuart and Zygalakis, 2017. (SIAM-JUQ)

Probit Model

$$\mathsf{J}_{\mathrm{p}}^{(n)}(u;y) = \frac{1}{2}\langle u, C^{-1}u\rangle_{\mathbb{R}^n} + \Phi_{\mathrm{p}}^{(n)}(u;y).$$

Here

$$C = (L+\tau^2 I)^{-\alpha},$$

$$\Phi_{\mathrm{p}}^{(n)}(u;y) := -\sum_{j\in Z'} \log\big(\Psi(y_j\, u_j\ ;\gamma)\big)$$

where Ψ is the smoothed Heaviside function:

$$\Psi(v;\gamma) = \frac{1}{\sqrt{2\pi\gamma^2}}\int_{-\infty}^{v} \exp\big(-t^2/2\gamma^2\big)\mathrm{d}t.$$

Level Set

Iglesias, Lu and Stuart, 2016. (IFB)

Level Set Model

$$\mathsf{J}_{\mathrm{ls}}^{(n)}(u;y) = \frac{1}{2}\langle u, C^{-1}u\rangle_{\mathbb{R}^n} + \Phi_{\mathrm{ls}}^{(n)}(u;y).$$

Here

$$C = (L + \tau^2 I)^{-\alpha},$$

and

$$\Phi_{\mathrm{ls}}^{(n)}(u;y) := \frac{1}{2\gamma^2}\sum_{j\in Z'}\left|y_j - \mathrm{sign}\left(u_j\right)\right|^2.$$

Sampling Algorithm

Cotter, Roberts, Stuart, White, 2013. (Statis. Sci.)

The preconditioned Crank-Nicolson (pCN) Method

1: Define: $\alpha(u,v) = \min\{1, \exp(\Phi(u) - \Phi(v)\}$. $C = (L + \tau^2 I)^{-\alpha}$
2: **while** $k < M$ **do**
3: $\quad v^{(k)} = \sqrt{1-\beta^2}u^{(k)} + \beta\xi^{(k)}$, where $\xi^{(k)} \sim \mathsf{N}(0, C)$.
4: $\quad$ Calculate acceptance probability $\alpha(u^{(k)}, v^{(k)})$.
5: $\quad$ Accept: $u^{(k+1)} = v^{(k)}$ with probability $\alpha(u^{(k)}, v^{(k)})$, otherwise
6: $\quad$ Reject: $u^{(k+1)} = u^{(k)}$.
7: **end while**

Bertozzi, Luo, Stuart, 2018. (In preparation.)

$$\mathbb{E}(\alpha(u,v)) = O(Z_0^2), \quad Z_0 = \mu(\{S(u(j)) = y(j) \,|\, j \in Z'\})$$

Example of UQ (Hyperspectral)

Here $d = 129$ and $N \approx 3 \times 10^5$. Use Nyström .

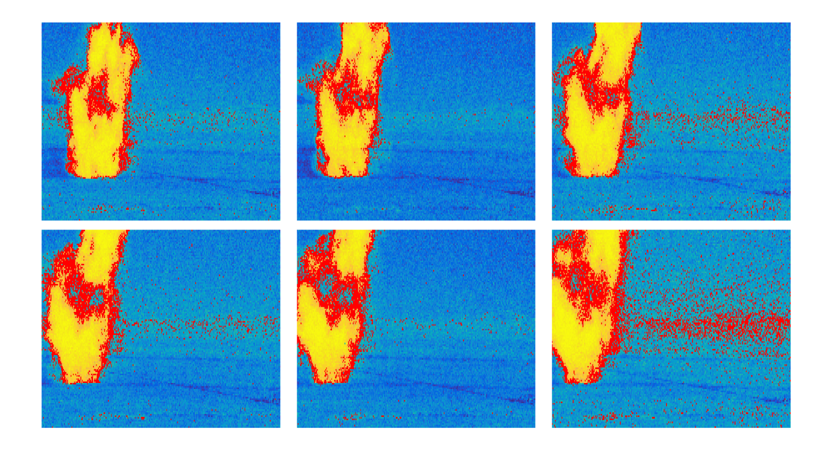

Figure: Spectral Approximation. Uncertain classification in red.

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Limit Theorem for the Dirichlet Energy

Garcia-Trillos and Slepčev, 2016. (ACHA)

Unlabelled data $\{x_j\}$ sampled i.i.d. from density ρ supported on bounded $D \subset \mathbb{R}^d$. Let

$$\mathcal{L}u = -\frac{1}{\rho}\nabla \cdot \left(\rho^2 \nabla u\right) \quad x \in D, \quad \frac{\partial u}{\partial n} = 0, \quad x \in \partial D.$$

Theorem 2

Let $s_n = \frac{2}{C(\eta)n\varepsilon^2}$. Then under connectivity conditions on $\varepsilon = \varepsilon(n)$ in η_ε, the scaled Dirichlet energy $\Gamma-$ converges in the TL^2 metric:

$$\frac{1}{n}\langle u, Lu\rangle_{\mathbb{R}^n} \to \langle u, \mathcal{L}u\rangle_{L^2_\rho} \quad \text{as} \quad n \to \infty.$$

Limit Theorem for Probit

Dunlop, Slepčev, Stuart and Thorpe, In preparation, 2018.

$D^{\pm}$ two disjoint bounded subsets of D, define $D' = D^{+} \cup D^{-}$ and

$$y(x) = +1, \ x \in D^{+}; \quad y(x) = -1, \ x \in D^{-}.$$

Assume that $\#D_n/n \to$ const. as $n \to \infty$. For $\alpha > 0$, define $\mathcal{C} = (\mathcal{L} + \tau^2 I)^{-\alpha}$.
Recall $\mathcal{L}u = -\frac{1}{\rho}\nabla \cdot (\rho^2 \nabla u)$, and no flux boundary conditions.

Theorem 3

Let $s_n = \frac{2}{C(\eta)n\varepsilon^2}$. Then under connectivity conditions on $\varepsilon = \varepsilon(n)$ the scaled probit objective function $\Gamma-$converges in the TL^2 metric:

$$\frac{1}{n}\mathsf{J}_{\mathrm{p}}^{(n)}(u;y) \to \mathsf{J}_{\mathrm{p}}(u;y) \quad \text{as} \quad n \to \infty,$$

$$\mathsf{J}_{\mathrm{p}}(u;y) = \frac{1}{2}\langle u, \mathcal{C}^{-1}u\rangle_{L^2_\rho} + \Phi_{\mathrm{p}}(u;y),$$

$$\Phi_{\mathrm{p}}(u;y) := -\int_{D'} \log\Big(\Psi(y(x)\,u(x)\ ;\gamma)\Big)\rho(x)\mathrm{d}x.$$

Limit Theorem for Probit

Dunlop, Slepčev, Stuart and Thorpe, In preparation, 2018.

Assume now that $\#D_n$ is fixed as $n \to \infty$.

Theorem 4

Let $s_n = \frac{2}{C(\eta)n\varepsilon^2}$ with $\varepsilon = \varepsilon(n, \alpha)$. Suppose that either

1. $\alpha > d/2$ and $\varepsilon(n, \alpha)n^{\frac{1}{2\alpha}} \to \infty$; or
2. $\alpha < d/2$.

Then with probability one, sequences of minimizers of $\mathsf{J}_{\mathrm{p}}^{(n)}$ converge to zero in the TL^2 metric.

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Example (PDE Two Moons – Unlabelled Data)

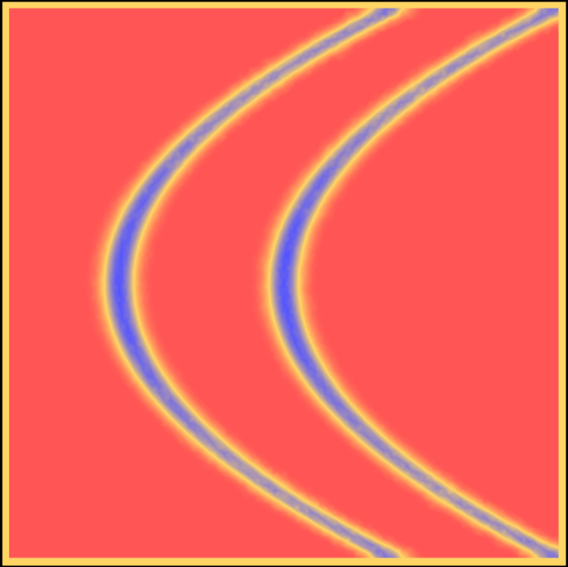

Figure: Sampling density ρ of unlabelled data.

Example (PDE Two Moons – Label Data)

Figure: Labelled Data.

Example (PDE Two Moons – Fiedler Vector of $\mathcal{L}$)

Figure: Fiedler Vector.

Example (PDE Two Moons – Posterior Labelling)

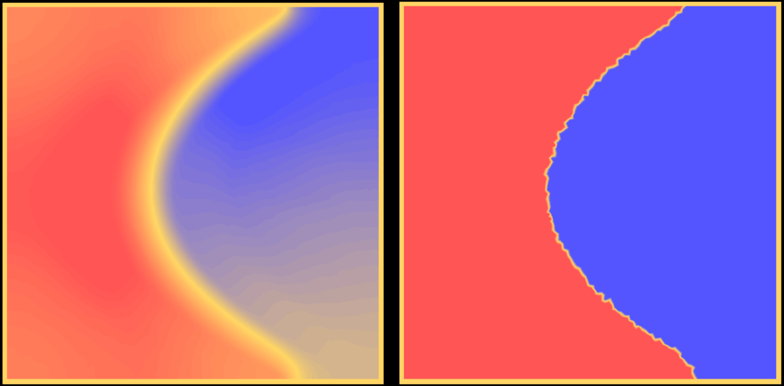

Figure: Posterior mode of u and $\mathrm{sign}(u)$.

Connecting Probit, Level Set and Regression

Dunlop, Slepčev, Stuart and Thorpe, In preparation, 2017.

Probit and Level Set Probabilistic Models

- Prior: Gaussian $\mathbb{P}(\mathrm{d}u) = \mathsf{N}(0, \mathcal{C})$.
- Probit Posterior: $\mathbb{P}_\gamma(\mathrm{d}u|y) \propto \exp\big(-\Phi_{\mathrm{p}}(u;y)\big)\mathbb{P}(\mathrm{d}u)$.
- Level Set Posterior: $\mathbb{P}_\gamma(\mathrm{d}u|y) \propto \exp\big(-\Phi_{\mathrm{ls}}(u;y)\big)\mathbb{P}(\mathrm{d}u)$.

Theorem 4

Let $\alpha > \frac{d}{2}$. We have $\mathbb{P}_\gamma(u|y) \Rightarrow \mathbb{P}(u|y)$ as $\gamma \to 0$ where

$$\mathbb{P}(\mathrm{d}u|y) \propto \mathbf{1}_A(u)\mathbb{P}(\mathrm{d}u), \quad \mathbb{P}(\mathrm{d}u) = \mathsf{N}(0, \mathcal{C})$$

$$A = \{u : \mathrm{sign}\big(u(x)\big) = y(x), \quad x \in D'\}.$$

Compare with regression (Zhu, Ghahramani, Lafferty 2003, (ICML):)

$$A \mapsto A_0 = \{u : u(x) = y(x), \quad x \in D'\}.$$

Example (MNIST: Human-in-the-loop labelling)

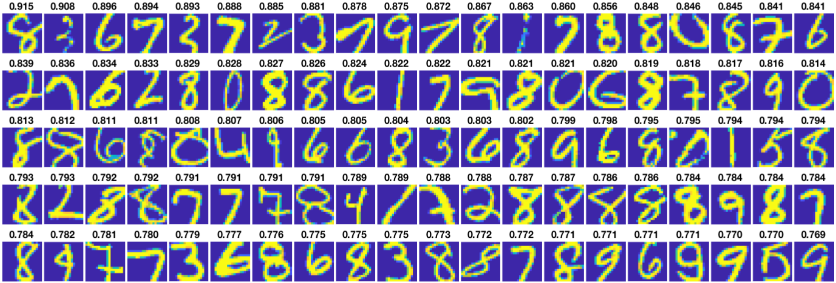

Figure: 100 most uncertain digits, 200 labels. Mean uncertainty: 14.0%

Example (MNIST)

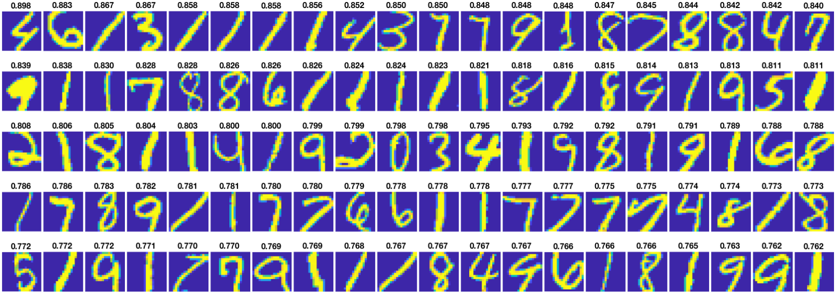

Figure: 100 most uncertain digits, 300 labels. Mean uncertainty: 10.3%

Example (MNIST)

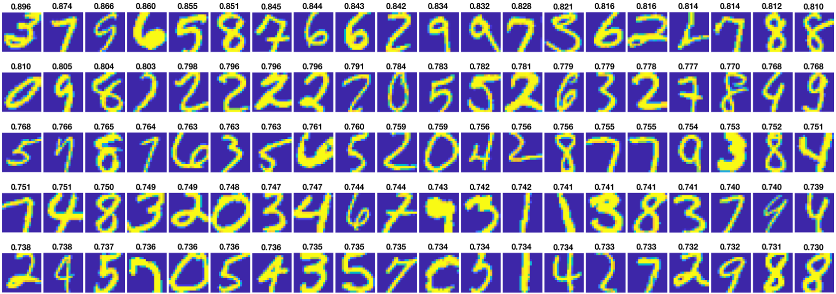

Figure: 100 most uncertain digits, 400 labels. Mean uncertainty: 8.1%

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Summary: Graph Based Learning

- Single optimization framework for classification algorithms.
- Single Bayesian framework for classification algorithms.
- Large graph limit reveals novel inverse problem structure.
- Links between probit, level set and regression.
- Gaussian measure conditioned on its sign.
- UQ for human-in-the-loop learning.
- Efficient MCMC algorithms.

References

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pCN

$$\alpha(u, v) = \min\{1, \exp(\Phi(u) - \Phi(v)\}.$$

The preconditioned Crank-Nicolson (pCN) Method

1: **while** $k < M$ **do**
2: $\quad v^{(k)} = \sqrt{1-\beta^2}u^{(k)} + \beta\xi^{(k)}$, where $\xi^{(k)} \sim \mathsf{N}(0, C)$.
3: $\quad$ Accept: $u^{(k+1)} = v^{(k)}$ with probability $\alpha(u^{(k)}, v^{(k)})$, otherwise
4: $\quad$ Reject: $u^{(k+1)} = u^{(k)}$.
5: **end while**

Why pCN?

- For given acceptance probability, β is independent of $N = |Z|$.
- Can exploit approximation of graph Laplacian (Nyström) and $\cdots$

Example of UQ (Two Moons)

Recall that $d = 10^2, N = 2 \times 10^3$.

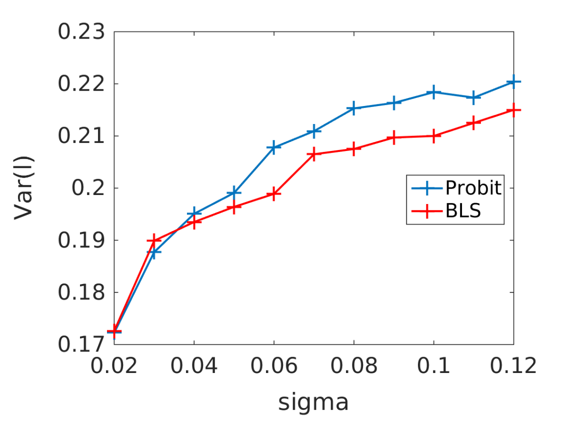

Figure: Average Label Posterior Variance vs σ, feature vector noise.

Example of UQ (MNIST)

Here $d = 784$ and $N = 4000$.

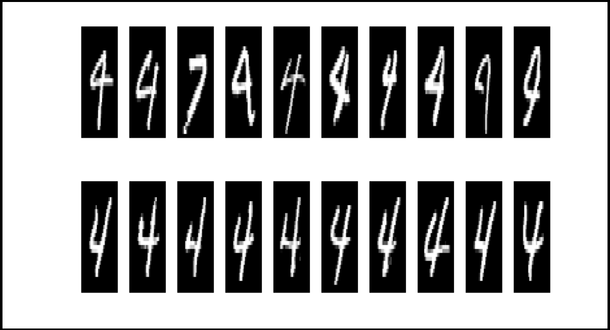

Figure: “Low confidence” vs “High confidence” nodes in MNIST49 graph.

Saturation of Spectra in Applications

Karhunen-Loeve – if $Lq_j = \lambda_j q_j$ then $u \sim \mathsf{N}(0, C)$ is:

$$u = c^{\frac{1}{2}} \sum_{j=1}^{N-1} (\lambda_j + \tau^2)^{-\frac{\alpha}{2}} q_j z_j, z_j \sim \mathsf{N}(0, 1) \quad \text{i.i.d.} \tag{1}$$

- Spectrum of graph Laplacian often saturates as $j \to N - 1$.
- Spectral Projection $\iff$ $\lambda_k := \infty, k \geq \ell$.
- Spectral Approximation: set λ_k to some $\bar{\lambda} < \infty$.

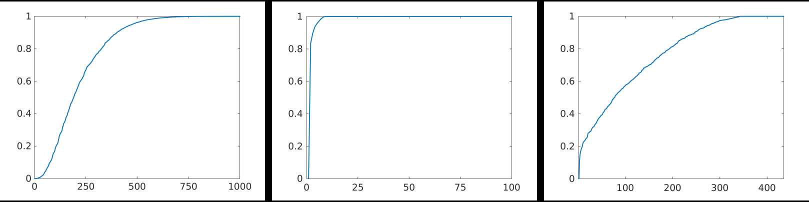

Figure: Two Moons, Hyperspectral, Voting Records.

Example of UQ (Voting)

Recall that $d = 16$ and $N = 435$.
Mean Absolute Error: *Projection*: 0.1577, *Approximation*: 0.0261.

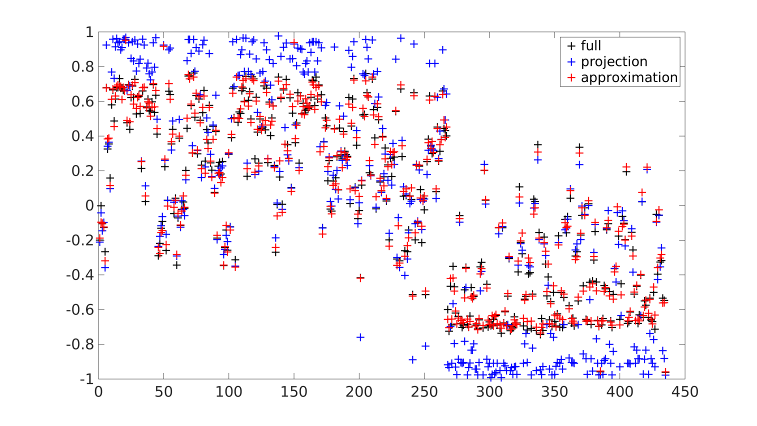

Figure: Mean Label Posterior. Compare Full (black), Spectral Approximation (red) and Spectral Projection (blue).

Example of UQ (Hyperspectral)

Here $d = 129$ and $N \approx 3 \times 10^5$. Use Nyström .

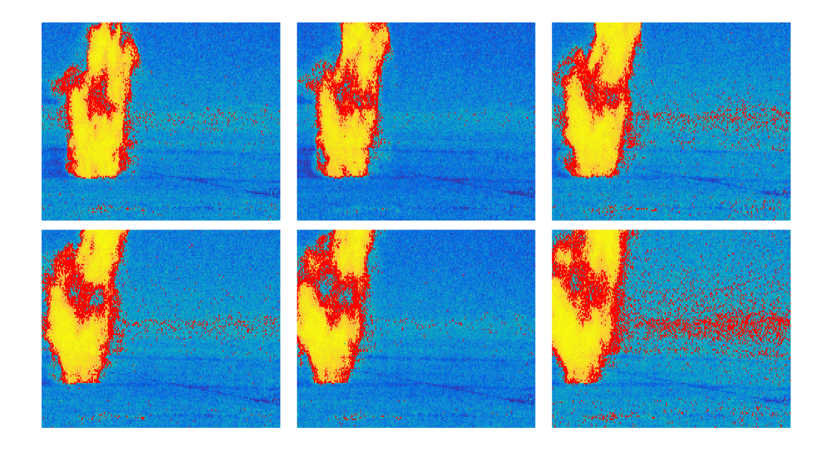

Figure: Spectral Approximation. Uncertain classification in red.