Active Learning in Graph-Based Semi-Supervised Learning

Kevin Miller, Andrea Bertozzi

University of California, Los Angeles

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Setup

Observe *labeled data* $\mathcal{D}_\ell = \{(\mathbf{x}_i, y_i)\}_{i \in \mathcal{L}}$ and *unlabeled data* $\mathcal{X}_\mathcal{U} = \{\mathbf{x}_j\}_{j \in \mathcal{U}}$.

- $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\} = \mathcal{X}_\mathcal{L} \cup \mathcal{X}_\mathcal{U}$
- $\mathcal{L}$: labeled indices
- $\mathcal{U}$: unlabeled indices
- $Z = \mathcal{L} \cup \mathcal{U}$

Semi-Supervised Learning

From the given data, can we accurately infer the labelings on $\mathcal{U}$?

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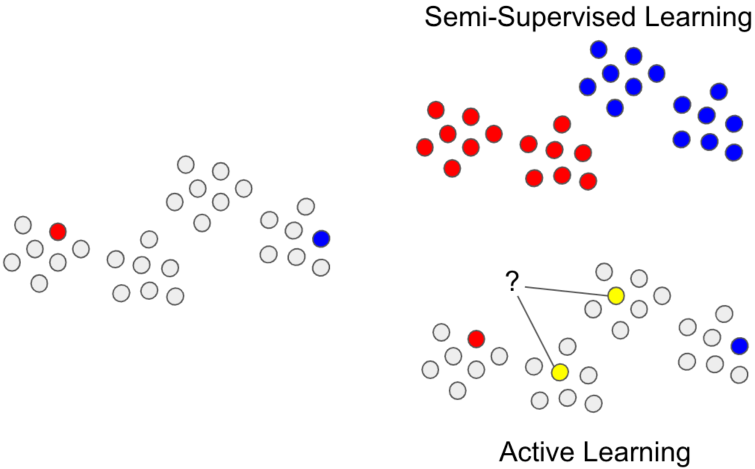
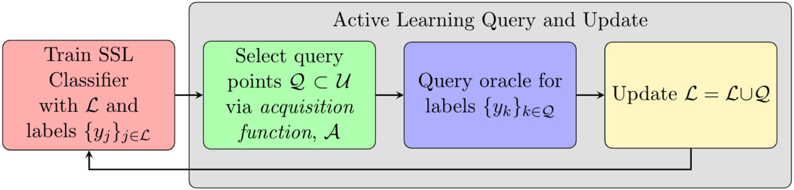
Semi-Supervised Learning

From the given data, can we accurately infer the labelings on $\mathcal{U}$?

Active Learning

From the given data, can we judiciously "choose" unlabeled points $\mathcal{Q} \subset \mathcal{U}$ to label that will improve the output of the underlying learning model?


Semi-Supervised Learning
?
Active Learning


Train SSL Classifier with $\mathcal{L}$ and labels $\{y_j\}_{j\in\mathcal{L}}$
Active Learning Query and Update
Select query points $\mathcal{Q} \subset \mathcal{U}$ via *acquisition function*, $\mathcal{A}$
Query oracle for labels $\{y_k\}_{k\in\mathcal{Q}}$
Update $\mathcal{L} = \mathcal{L} \cup \mathcal{Q}$

Given data $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$, construct *similarity graph* $G(Z, W)$, where

- $Z = \{1, 2, \ldots, N\}$
- $W_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$
- $d_i = \sum_{j \in Z} W_{ij}$
- degree matrix $D = \mathrm{diag}(d_1, d_2, \ldots, d_N)$

Graph Laplacians

- $L = D - W$, *unnormalized*
- $L_n = I - D^{-1/2} W D^{-1/2}$, *normalized*
- $L_{rw} = I - D^{-1} W$, *random walk*

Binary Graph-Based SSL

Consider family of graph-based SSL models, using a perturbed *graph Laplacian* $L_\tau = L + \tau^2 I$:

$$\hat{\mathbf{u}} = \underset{\mathbf{u}\in\mathbb{R}^N}{\arg\min}\, \frac{1}{2}\langle \mathbf{u}, L_\tau \mathbf{u}\rangle + \sum_{j\in\mathcal{L}} \ell(u_j, y_j) =: \underset{\mathbf{u}\in\mathbb{R}^N}{\arg\min}\, J_\ell(\mathbf{u};\mathbf{y}), \tag{1}$$

for different loss functions ℓ with parameter γ:

- $\ell(x, y) = (x-y)^2/2\gamma^2$, (Regression)
- $\ell(x, y) = \ln(1 + e^{-xy/\gamma})$, (Logistic)
- $\ell(x, y) = -\ln \Psi_\gamma(xy)$, (Probit)

where $\Psi_\gamma(t) = \int_{-\infty}^{t} \psi_\gamma(s)ds$ is CDF of log-concave PDF $\psi_\gamma(s)$.

Multiclass Graph-Based SSL

With perturbed graph Laplacian L_τ and n_c the number of classes,

$$\hat{U} = \underset{U \in \mathbb{R}^{N \times n_c}}{\arg\min} \ \frac{1}{2}\langle U, L_\tau U \rangle_F + \sum_{j \in \mathcal{L}} \ell(\mathbf{u}^j, \mathbf{y}^j) =: \underset{U \in \mathbb{R}^{N \times n_c}}{\arg\min} \ \mathcal{J}_\ell(U; Y),$$

for different loss functions ℓ with parameter γ:

- $\ell(\mathbf{s}, \mathbf{t}) = \frac{1}{2\gamma^2}\|\mathbf{s} - \mathbf{t}\|_2^2$, (Multiclass Regression)
- $\ell(\mathbf{s}, \mathbf{t}) = -\sum_{c=1}^{n_c} t_c \ln(s_c)$, (Cross-Entropy)

Probabilistic and Bayesian Perspective

Optimizer $\hat{\mathbf{u}}$ can be viewed as *maximum a posteriori* (MAP) estimator

$$\arg\min_{\mathbf{u}} J_\ell(\mathbf{u};\mathbf{y}) \iff \arg\max_{\mathbf{u}} \ \exp(-J_\ell(\mathbf{u};\mathbf{y}))$$

$$= \arg\max_{\mathbf{u}} \ \underbrace{\exp\left(-\frac{1}{2}\langle \mathbf{u}, L_\tau \mathbf{u}\rangle\right)}_{prior} \underbrace{\exp\left(-\sum_{j\in\mathcal{L}} \ell(u_j, y_j)\right)}_{likelihood}$$

$$= \arg\max_{\mathbf{u}} \ \mathbb{P}(\mathbf{u}|\mathbf{y})$$

for a posterior distribution $\mathbb{P}(\mathbf{u}|\mathbf{y}) \propto \exp(-J_\ell(\mathbf{u};\mathbf{y}))$.

- Different loss functions give different likelihoods

Harmonic Functions (HF) Model

Assuming hard constraints for labeling[1], have conditional distribution:

$$\mathbf{u}_{\mathcal{U}}|\mathbf{y} \sim \mathcal{N}(\mathbf{u}_{hf}, L_{\mathcal{U},\mathcal{U}}^{-1}), \quad \mathbf{u}_{hf} = -L_{\mathcal{U},\mathcal{U}}^{-1} L_{\mathcal{U},\mathcal{L}}\mathbf{y}$$

with $\mathbf{u}_{\mathcal{L}} = \mathbf{y}$.

Gaussian Regression (GR) Model

With $\ell(x, y) = (x-y)^2/2\gamma^2$, then likelihood/prior/posterior is Gaussian.

$$\begin{aligned}\mathbb{P}(\mathbf{u}|\mathbf{y}) &\propto \exp\left(-\frac{1}{2}\langle \mathbf{u}, L_\tau \mathbf{u}\rangle\right)\exp\left(-\frac{1}{2\gamma^2}\sum_{j\in\mathcal{L}}(u_j - y_j)^2\right)\\ &\sim \mathcal{N}(\mathbf{m}, C),\ \mathbf{m} = \frac{1}{\gamma^2}CP^T\mathbf{y},\ C^{-1} = L + \frac{1}{\gamma^2}P^TP,\end{aligned}$$

where $P : \mathbb{R}^N \to \mathbb{R}^{|\mathcal{L}|}$ is projection onto labeled set $\mathcal{L}$.

[1] Does not actually rigorously fit into Bayesian framework like others

Look-Ahead model with index k and label y_k:

$$\operatorname*{arg\,min}_{\mathbf{u}\in\mathbb{R}^N} J^k(\mathbf{u};\mathbf{y},y_k) := \operatorname*{arg\,min}_{\mathbf{u}\in\mathbb{R}^N} \ \frac{1}{2}\langle \mathbf{u}, L_\tau \mathbf{u}\rangle + \sum_{j\in\mathcal{L}} \ell(u_j, y_j) + \overbrace{\ell(u_k, y_k)}^{plus\ \ k}.$$

- For Gaussian model, look-ahead posterior distribution's parameters from the current posterior distribution
  - *without expensive model retraining* – **rank-one updates**

$$\textbf{GR:}\quad \mathbf{m}^{k,y_k} = \mathbf{m} + \tfrac{(y_k - m_k)}{\gamma^2 + C_{kk}} C_{:,k}, \qquad C^{k,y_k} = C - \tfrac{1}{\gamma^2 + C_{kk}} C_{:,k} C_{:,k}^T$$

Non-Gaussian, Probit

When likelihood not Gaussian, posterior $\mathbb{P}(\mathbf{u}|\mathbf{y})$ *is non-Gaussian..*

Problems:

- model classifier as mean $\mu = \mathbb{E}_{\mathbf{u}\sim\mathbb{P}}[\mathbf{u}]$? or MAP estimator $\hat{\mathbf{u}} = \arg\max \mathbb{P}(\mathbf{u}|\mathbf{y})$?
- compute mean, μ, and covariance $C = \mathbb{E}_{\mathbf{u}\sim\mathbb{P}}\left[(\mathbf{u}-\mu)(\mathbf{u}-\mu)^T\right]$? (*potentially expensive!*)
- Look-ahead updates??

With non-Gaussian models, we lose these nice properties. *What to do?*

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Let's approximate with Gaussian, and see what happens!

Laplace approximation is a popular technique for approximating non-Gaussian distributions $\mathbb{P}$ with a Gaussian distribution.

$$\mathbf{x} \sim \mathcal{N}(\hat{\mathbf{x}}, \hat{C}), \quad \hat{\mathbf{x}} = \underset{\mathbf{x} \in \mathbb{R}^N}{\arg\max}\ \mathbb{P}(\mathbf{x}), \quad \hat{C} = \left(-\nabla^2 \ln(\mathbb{P}(\mathbf{x}))|_{\mathbf{x}=\hat{\mathbf{x}}}\right)^{-1},$$

where

- $\hat{\mathbf{x}}$: MAP estimator of $\mathbb{P}$
- $\hat{C}$: Hessian matrix of the negative-log density of $\mathbb{P}$, evaluated at $\hat{\mathbf{x}}$

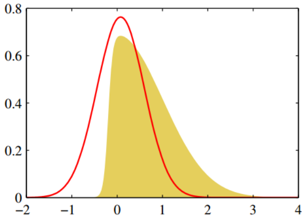

Figure 1: photo credit : http://wiljohn.top/2019/04/14/PRML4-4/

Spectral Truncation

Consider only first $M < N$ eigenvalues and eigenvectors of graph Laplacian, L:

$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_M, \quad \mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_M.$$

- $\Lambda_\tau = \operatorname{diag}\left(\lambda_1 + \tau^2, \ldots, \lambda_M + \tau^2\right)$
- $V = [\mathbf{v}_1 \;\; \mathbf{v}_2 \;\; \ldots \;\; \mathbf{v}_M] \in \mathbb{R}^{N \times M}$
- $\boldsymbol{\alpha} \in \mathbb{R}^M$ (binary), $A \in \mathbb{R}^{M \times n_c}$ (multiclass)

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Binary: $(\mathbf{u} = V\boldsymbol{\alpha})$

$$\begin{aligned} J_\ell(\mathbf{u}; \mathbf{y}) &= \frac{1}{2}\langle \mathbf{u}, L_\tau \mathbf{u}\rangle + \sum_{j \in \mathcal{L}} \ell(u_j, y_j) \\ &\to \frac{1}{2}\langle \boldsymbol{\alpha}, \Lambda_\tau \boldsymbol{\alpha}\rangle + \sum_{j \in \mathcal{L}} \ell(\mathbf{e}_j^T V \boldsymbol{\alpha}, y_j) =: \tilde{J}_\ell(\boldsymbol{\alpha}; \mathbf{y}), \end{aligned}$$

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$$\to \frac{1}{2}\langle \boldsymbol{\alpha}, \Lambda_\tau \boldsymbol{\alpha}\rangle + \sum_{j \in \mathcal{L}} \ell(\mathbf{e}_j^T V\boldsymbol{\alpha}, y_j) =: \tilde{J}_\ell(\boldsymbol{\alpha}; \mathbf{y}),$$

Multiclass: $(U = VA)$

$$\mathcal{J}_\ell(U; Y) = \frac{1}{2}\langle U, L_\tau U\rangle_F + \sum_{j \in \mathcal{L}} \ell(\mathbf{u}^j, \mathbf{y}^j)$$

$$\to \frac{1}{2}\langle A, \Lambda_\tau A\rangle_F + \sum_{j \in \mathcal{L}} \ell(\mathbf{e}_j^T VA, \mathbf{y}^j) =: \tilde{\mathcal{J}}_\ell(A; Y).$$

$$\boldsymbol{\alpha}|\mathbf{y} \sim \mathcal{N}(\hat{\boldsymbol{\alpha}}, \hat{C}_{\hat{\boldsymbol{\alpha}}}), \qquad \hat{\boldsymbol{\alpha}} = \underset{\boldsymbol{\alpha}\in\mathbb{R}^M}{\arg\min}\ \tilde{J}_\ell(\boldsymbol{\alpha};\mathbf{y}),$$

and then calculate covariance of Laplace Approximation $\hat{C}_{\boldsymbol{\alpha}}$

$$\nabla_{\boldsymbol{\alpha}} \tilde{J}_\ell(\boldsymbol{\alpha};\mathbf{y}) = \Lambda_\tau \boldsymbol{\alpha} + \sum_{j\in\mathcal{L}} F(\mathbf{e}_j^T V\boldsymbol{\alpha}, y_j) V^T \mathbf{e}_j = \Lambda_\tau \boldsymbol{\alpha} + V^T \sum_{j\in\mathcal{L}} F(\mathbf{e}_j^T V\boldsymbol{\alpha}, y_j)\mathbf{e}_j,$$

$$\nabla^2_{\boldsymbol{\alpha}} \tilde{J}_\ell(\boldsymbol{\alpha};\mathbf{y}) = \Lambda_\tau + V^T \left(\sum_{j\in\mathcal{L}} F'(\mathbf{e}_j^T V\boldsymbol{\alpha}, y_j)\mathbf{e}_j\mathbf{e}_j^T\right) V,$$

$$\implies \hat{C}_{\boldsymbol{\alpha}} = \left(\nabla^2_{\boldsymbol{\alpha}} \tilde{J}_\ell(\boldsymbol{\alpha};\mathbf{y})\right)^{-1} = \left(\Lambda_\tau + V^T \left(\sum_{j\in\mathcal{L}} F'(\mathbf{e}_j^T V\boldsymbol{\alpha}, y_j)\mathbf{e}_j\mathbf{e}_j^T\right) V\right)^{-1}$$

How to approximate look-ahead model update, $\hat{\boldsymbol{\alpha}}^{k,y_k} = \arg\min \tilde{J}_\ell^{k,y_k}$?

- have $\hat{C}_{\hat{\boldsymbol{\alpha}}}$ (i.e. *inverse Hessian*)

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- have $\hat{C}_{\hat{\boldsymbol{\alpha}}}$ (i.e. *inverse Hessian*)

Try one step of Newton's method, *starting at* $\hat{\boldsymbol{\alpha}}$:

$$
\begin{aligned}
\tilde{\boldsymbol{\alpha}}^{k,y_k} &= \hat{\boldsymbol{\alpha}} - \left(\nabla^2_{\boldsymbol{\alpha}} \tilde{J}_\ell^{k,y_k}(\hat{\boldsymbol{\alpha}}; \mathbf{y}, y_k)\right)^{-1} \left(\nabla_{\boldsymbol{\alpha}} \tilde{J}_\ell^{k,y_k}(\hat{\boldsymbol{\alpha}}; \mathbf{y}, y_k)\right) \\
&= \dots \\
&= \hat{\boldsymbol{\alpha}} - \frac{F((\mathbf{v}^k)^T \hat{\boldsymbol{\alpha}}, y_k)}{1 + F'((\mathbf{v}^k)^T \boldsymbol{\alpha}, y_k)(\mathbf{v}^k)^T \hat{C}_{\hat{\boldsymbol{\alpha}}} \mathbf{v}^k} \hat{C}_{\hat{\boldsymbol{\alpha}}} \mathbf{v}^k
\end{aligned}
$$

where

$$
F(x, y) := \frac{\partial \ell}{\partial x}(x, y), \;\; F'(x, y) := \frac{\partial^2 \ell}{\partial x^2}(x, y).
$$

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where

$$F(x, y) := \frac{\partial \ell}{\partial x}(x, y), \;\; F'(x, y) := \frac{\partial^2 \ell}{\partial x^2}(x, y).$$

Simple update!

$*$ GR: this reduces to the exact look-ahead update!

Approximate Look-Ahead - Multiclass

Similar result for multiclass case, but a little lengthy to describe...

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$$\tilde{A}^{k,y_k} = \hat{A} - \underbrace{\left(\nabla_A^2 \tilde{\mathcal{J}}^{k,y_k}(\hat{A}; Y, \mathbf{y}^k)\right)^{-1} \left(\nabla_A \tilde{\mathcal{J}}^{k,y_k}(\hat{A}; Y, \mathbf{y}^k)\right)}_{\text{simplifies to be rank } n_c}$$

Model Change Acquisition Function

Calculating the approximate change in a model (i.e. classifier) from the addition of an index k and associated label y_k has been investigated previously[2].

[2] Cai, Zhang, and Zhou, "Maximizing Expected Model Change for Active Learning in Regression", 2013; Karzand and Nowak, "MaxiMin Active Learning in Overparameterized Model Classes", 2020.

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Employ approximate update (recalling that $V\boldsymbol{\alpha} = \mathbf{u}$):

$$\begin{aligned}
\mathcal{A}(k) &= \min_{y_k \in \{\pm 1\}} \|\hat{\mathbf{u}}^{k,y_k} - \hat{\mathbf{u}}\|_2 \approx \min_{y_k \in \{\pm 1\}} \left\|\tilde{\mathbf{u}}^{k,y_k} - \hat{\mathbf{u}}\right\|_2 = \min_{y_k \in \{\pm 1\}} \left\|\tilde{\boldsymbol{\alpha}}^{k,y_k} - \hat{\boldsymbol{\alpha}}\right\|_2 \\
&= \min_{y_k \in \{\pm 1\}} \left| \frac{F((\mathbf{v}^k)^T \hat{\boldsymbol{\alpha}}, y_k)}{1 + F'((\mathbf{v}^k)^T \hat{\boldsymbol{\alpha}}, y_k)(\mathbf{v}^k)^T \hat{C}_{\hat{\boldsymbol{\alpha}}} \mathbf{v}^k} \right| \left\|\hat{C}_{\hat{\boldsymbol{\alpha}}} \mathbf{v}^k\right\|_2 \\
&= \min_{y_k \in \{\pm 1\}} \left| \frac{F(\hat{u}_k, y_k)}{1 + F'(\hat{u}_k, y_k)(\mathbf{v}^k)^T \hat{C}_{\hat{\boldsymbol{\alpha}}} \mathbf{v}^k} \right| \left\|\hat{C}_{\hat{\boldsymbol{\alpha}}} \mathbf{v}^k\right\|_2,
\end{aligned}$$

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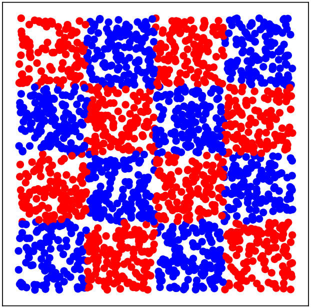
Binary Experiments



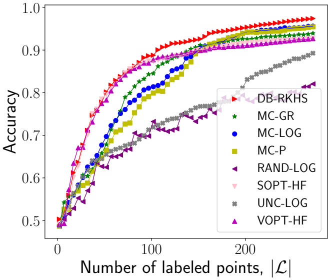
Checkerboard 2 Dataset. 2,000 points sampled uniformly at random from $[0,1]^2$.

Graph Construction:

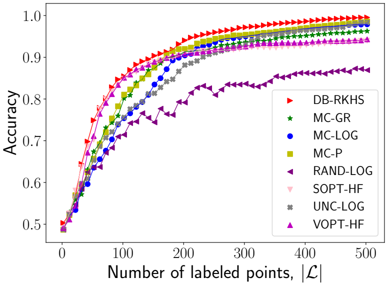
- 10 nearest neighbors, ZP scaling
- $M = 50$ eigenvalues

Experiments:

- initially label 1 per class
- Sequential
  - 200 active learning iterations, select $B = 1$ query points at each iteration
- Batch
  - 100 active learning iterations, select $B = 5$ query points at each iteration



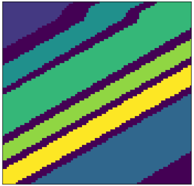
(a) Sequential, $B = 1$



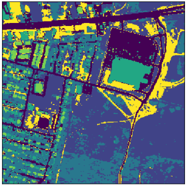
(b) Batch, $B = 5$

- **DB-RKHS** – “data-based” criterion, RKHS model. (Karzand and Nowak, 2020)
- **VOPT, SOPT** – V-Opt (Ji and Han, 2012), Σ-Opt (Ma et al, 2013)
- **UNC** – Uncertainty Sampling (Settles, 2012)
- **RAND** – Random choices

Multiclass Experiments - HSI



(c) Salinas A



(d) Urban

Graph Construction:

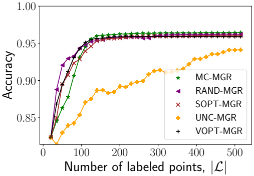
- 15 nearest neighbors, cosine similarity
- Zelnik-Perona scaling
- $M = 50$ eigenvalues

Experiments:

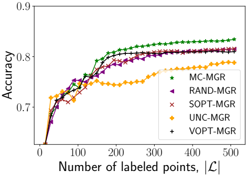
- initially label 2 per class
- Batch
  - 100 active learning iterations, select $B = 5$ query points at each iteration
  - MGR (Multiclass Gaussian Regression)
  - CE (Cross-Entropy)

Results - Multiclass

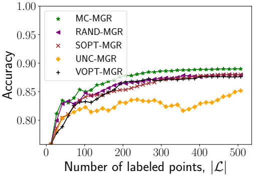
Multiclass GR Results:



(e) MNIST

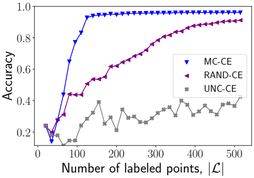


(f) Salinas A

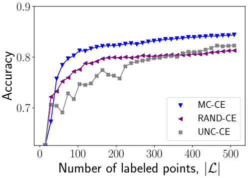


(g) Urban

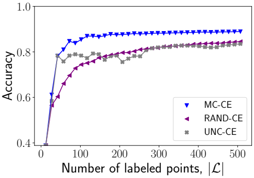
Cross-Entropy Results:



(h) MNIST



(i) Salinas A



(j) Urban

Future Directions

- Adapt this to more useful GBSSL models?
  - Currently only viable for convex loss functions (i.e. for Laplace Approximation)
  - e.g. graph MBO posterior is multimodal, so Laplace approximation meaningful?
- Other active learning criterion that take advantage of the nice model properties we have here?

Cai, Wenbin, Ya Zhang, and Jun Zhou. "Maximizing Expected Model Change for Active Learning in Regression". In: *2013 IEEE 13th International Conference on Data Mining*. ISSN: 2374-8486. Dec. 2013, pp. 51–60. DOI: 10.1109/ICDM.2013.104.

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