Scalable Active Learning by Approximated Error Reduction

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Outline

01 Background

02 Scalable Active Learning

03 Experiment and Conclusion

Outline

01 **Background**

- The aim and limitation of existing active learning.

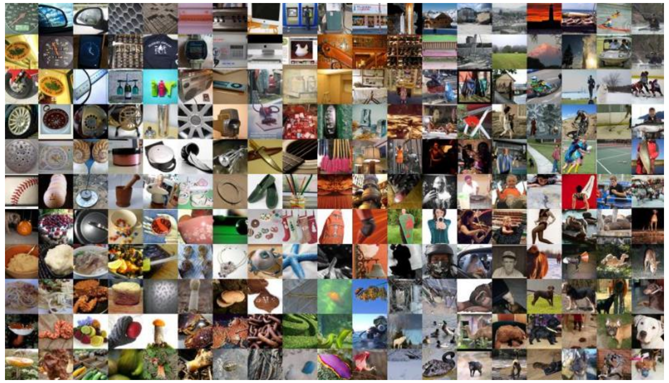
02 Scalable Active Learning

03 Experiment and Conclusion

Background

Classification

- Identifying the categories of unlabeled instances
  - computer vision, handwriting recognition, speech recognition, document classification

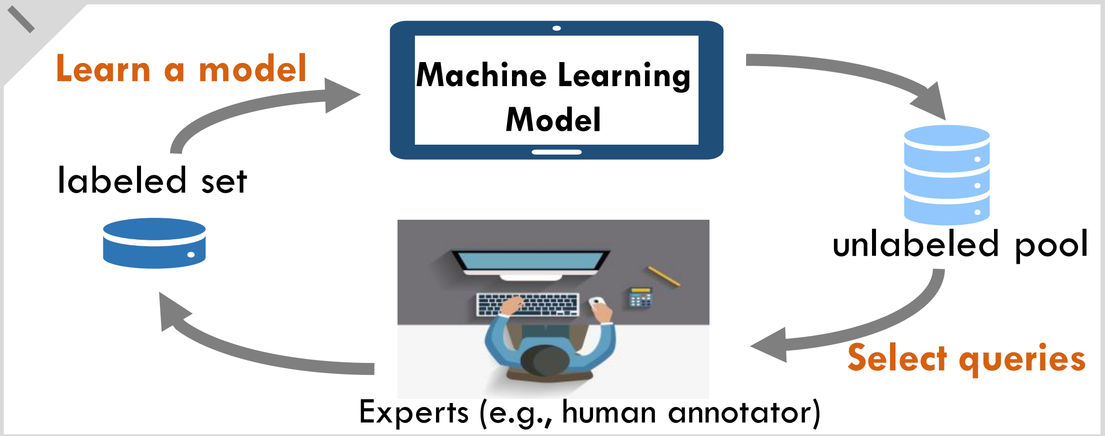


- Difficulties of this problem
  - Quality of labeled instances
  - Expensive costs of collecting labels

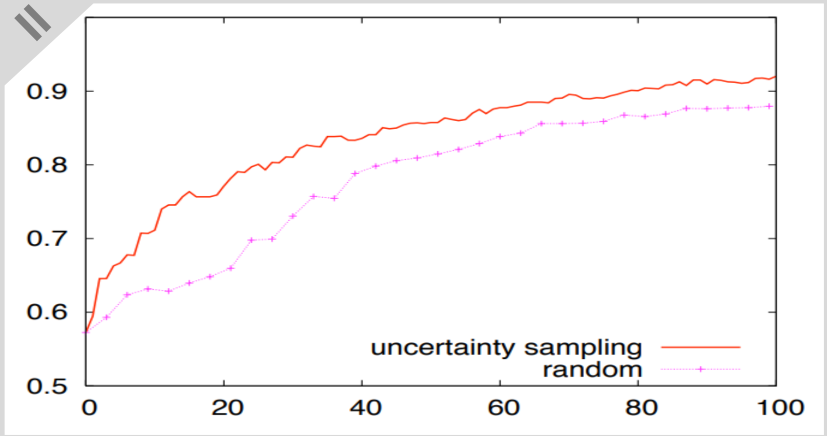
} **Active Learning**

Background

Active Learning



Procedures of Active Learning

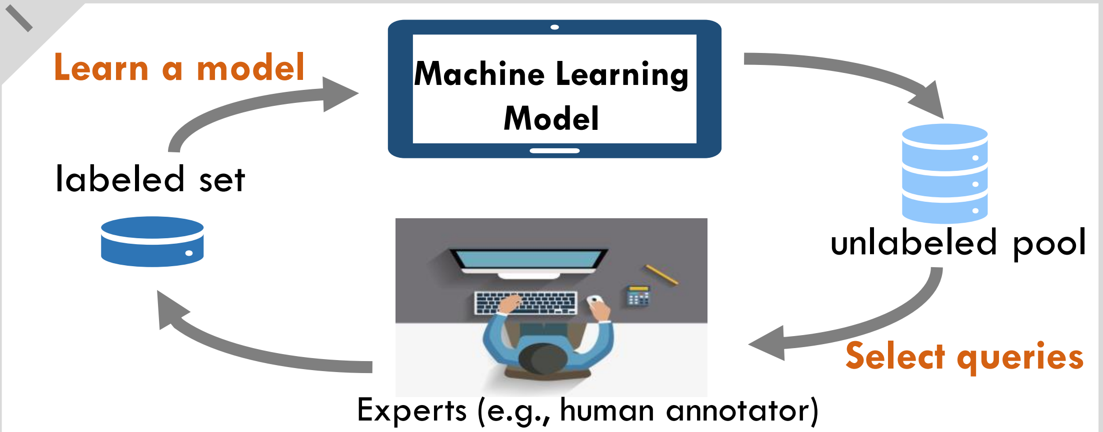


Performance of Active Learning

- Common procedures in the cycle.
  - Label prediction based on current **semi-supervised classifier**.
  - Measure estimation based on **query selection criterion**.
  - Query labeling by experts.

Background

Active Learning



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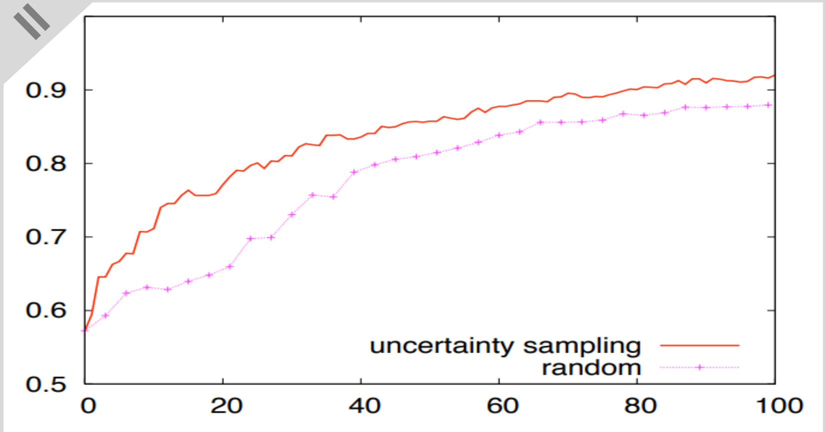

Performance of Active Learning

- Common procedures in the cycle.
  - Label prediction based on current **semi-supervised classifier**.
  - Measure estimation based on **query selection criterion**.
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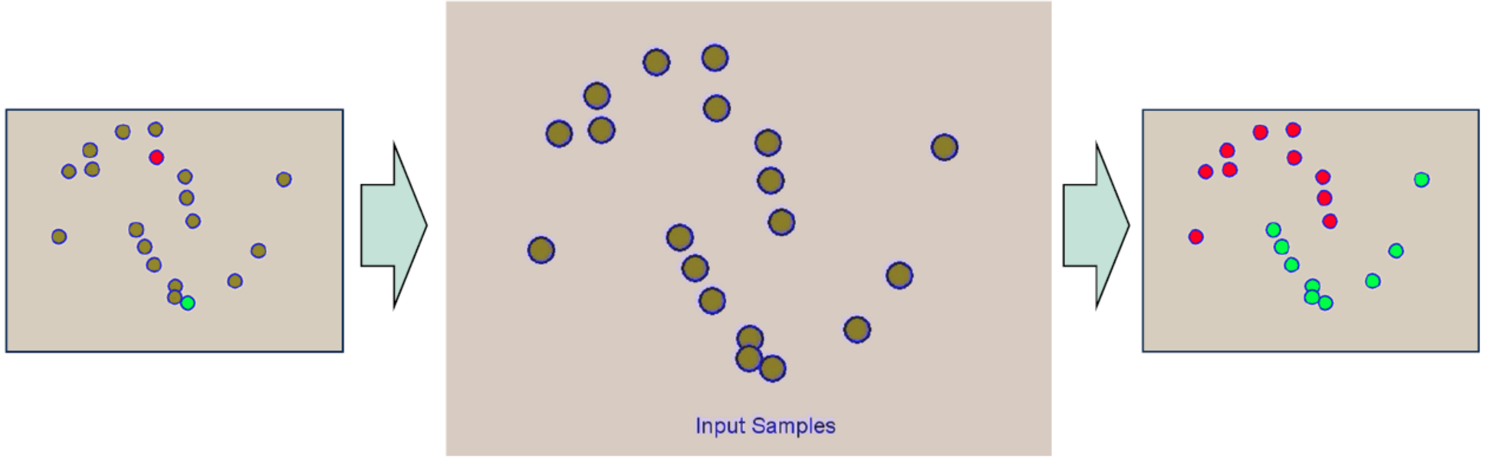
} **Keypoints**

Background

- **Semi-Supervised Classifier** (learn from labeled and unlabeled data)
  - Graph-based Classifier
    - Illustration:



    - Graph Construction + Label Propagation
    - Advantages:
      - Easy for explanation; Analytic solution …

Background

Semi-Supervised Classifier

Graph-based Classifier

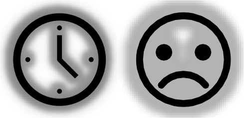
- **Formulation:**

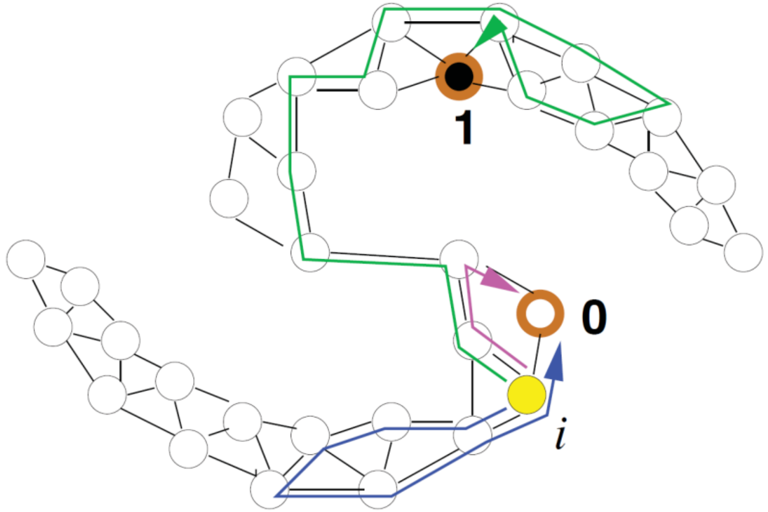
$$minimize \ \sum_i^n \|\boldsymbol{f}_i - \boldsymbol{y}_i\|^2 + \frac{\lambda}{2}\sum_{i,j=1}^n W_{ij}\left\|\frac{1}{\sqrt{D_{ii}}}\boldsymbol{f}_i - \frac{1}{\sqrt{D_{jj}}}\boldsymbol{f}_j\right\|^2 \Rightarrow \ minimize \ \|\mathbf{F}-\mathbf{Y}\|_F^2 + \lambda \mathrm{tr}[\mathbf{F}^T(\mathbf{I}-\mathbf{W})\mathbf{F}]$$

- Optimal Solution:

$$\underline{\mathbf{F} = [\mathbf{I} + \lambda(\mathbf{I}-\mathbf{W})]^{-1}\mathbf{Y}}$$

- **Procedure:**
  - I Label Propagation
    - matrix inversion with a cubic cost $O(N^3)$.
  - II Graph Construction
    - adjacency matrix with a quadratic cost $O(N^2)$.





Background

Query Selection Criterion

A. Expected Error Reduction (EER)

- **Definition**: choose the instance with the largest error reduction ⇒ tradeoff on error reduction
- **Formulation**:

$$\underbrace{\operatorname{argmax}_k \; \hat{\mathcal{E}}(f)}_{\text{current estimated error}} - \underbrace{\hat{\mathcal{E}}(f^{+y_{k,i}})}_{\text{expected generalization error}}, \quad \text{where } k \in 1{:}N, i \in 1{:}C.$$

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- **Procedure**:

At each iteration,
  For each unlabeled instance
    Suppose this instance is labeled, and re-train the classifier.
    Re-infer the soft labels exactly for hard labels.
    Estimate the expected error.
  End
Select the instance whose expected error reduction is largest.

Background

Query Selection Criterion

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Select the instance whose expected error reduction is largest.

- **Cost:**

$O(N + t_{train}) \times N$, where t_{train} is the time cost of training the classifier, e.g., $O(N^3)$ for many SSL classifier.

Query Selection Criterion

A. Expected Error Reduction (EER)

B. Uncertainty Sampling

- **Definition**: choose the instance with the largest uncertainty.
- **Procedure**:

> At each iteration,
> ~~For each unlabeled instance~~ avoid model retraining.
> Infer the labels of unlabeled instances.
> Estimate the uncertainty.
> ~~End~~
> Select the instance with the largest uncertainty.

- Analysis:
  - Cost: reduce the time cost to $O(N)$ without re-training.
  - Effectiveness: ignore the influence of labels; outliers may be selected.

Background

Limitations

- Semi-supervised Classifier
  - A. Graph-based Classifier
    - Large time cost of **graph construction** and **mode training.**
- Query Selection Criterion
  - A. Expected Error Reduction

    (Perform well at either tuning decision boundaries or discovering new classes)
    - Large time cost of **model re-training** and **label re-inference**.
  - B. Uncertainty Sampling
    - Ignore the **influence** of labels on the **classifier** and **other instances**.

Scalable Active Learning

Outline

Scalable Active Learning

Motivations

Efficient Semi-Supervised Classifier

- Reduce the time cost of graph-based learning.
- Keep a high classification accuracy.

Scalable Query Selection Criterion

- Cut down the time cost of query selection.
- Keep the high quality of selected instances.

Motivations

Efficient Semi-Supervised Classifier

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Scalable Query Selection

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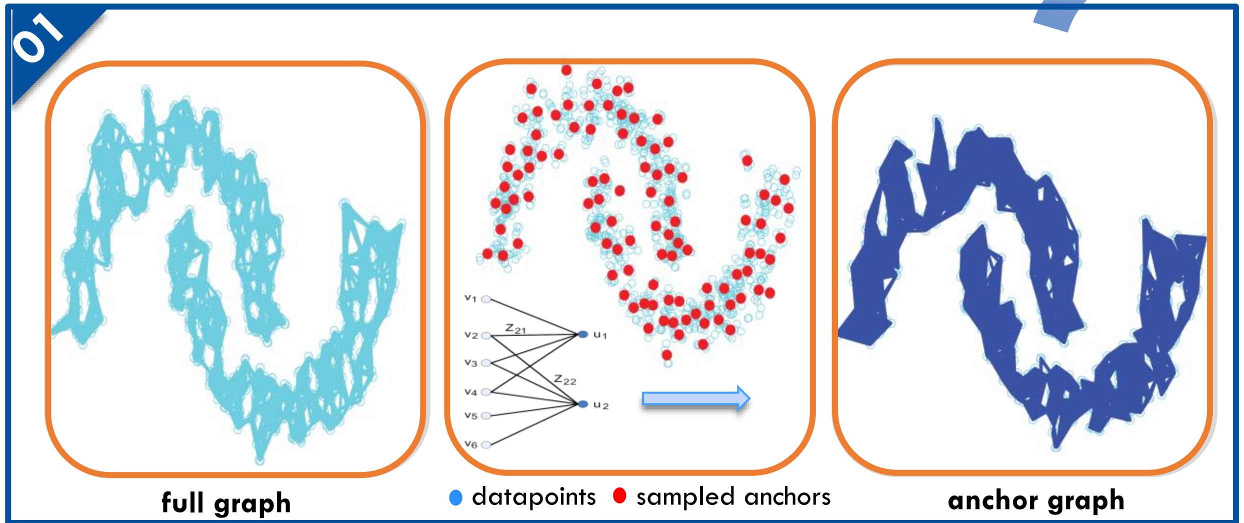
Scalable Active Learning

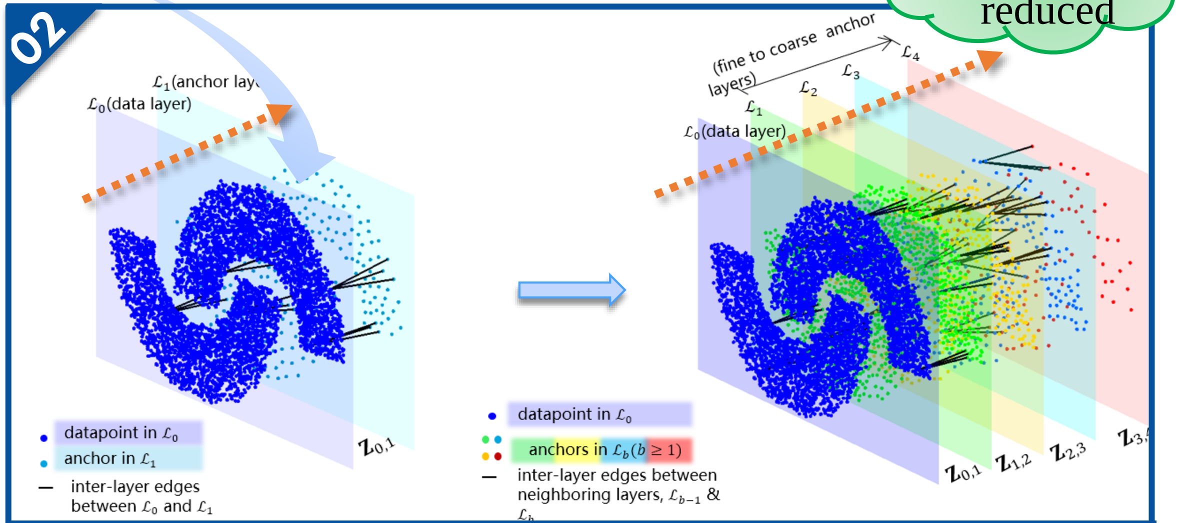
Efficient Semi-Supervised Classifier

- Hierarchical Anchor Graph
- Learning with Hierarchical Anchor Graph Regularization (HAGR)

Sizes are generally reduced



from Full-Graph to Anchor Graph

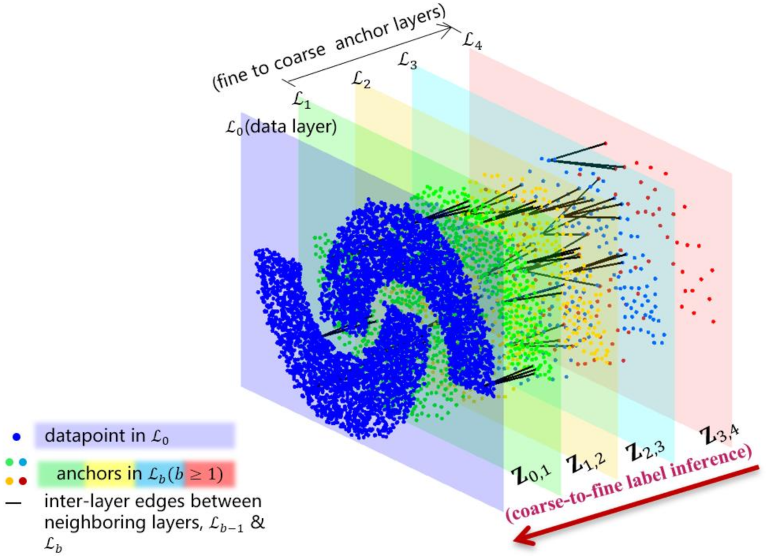


from Anchor Graph to Hierarchical Anchor Graph

Scalable Active Learning

Efficient Semi-Supervised Classifier

- Hierarchical Anchor Graph
- Learning with **H**ierarchical **A**nchor **G**raph **R**egularization **(HAGR)**
  - Formulation: $\sum_{i=1}^{l} \left\| \mathbf{Z}_{i.}^{\mathrm{H}}\mathbf{A} - \mathbf{y}_i \right\|^2 + \frac{\lambda}{2} \sum_{i,j}^{n} W_{ij} (\mathbf{Z}_{i.}^{\mathrm{H}}\mathbf{A} - \mathbf{Z}_{j.}^{\mathrm{H}}\mathbf{A})^2.$
    - **Label smoothing** (Laplacian matrix) based on the **finest** anchors with $\mathbf{W} = {\mathbf{Z}^{0,1}}^{\mathrm{T}}\mathbf{Z}^{0,1}$.
    - **Label inference** (hierarchically) from the **coarsest** anchors with $\mathbf{Z}^{\mathrm{H}} = \mathbf{Z}^{0,1}\mathbf{Z}^{1,2} \ldots \mathbf{Z}^{h-1,h}$.
  - Solution: $\mathbf{A} = \left({\mathbf{Z}_{\mathrm{L}}^{\mathrm{H}}}^{\mathrm{T}}\mathbf{Z}^{\mathrm{H}} + \lambda\tilde{\mathbf{L}}\right)^{-1} {\mathbf{Z}_{\mathrm{L}}^{\mathrm{H}}}^{\mathrm{T}}\mathbf{Y}_{\mathrm{L}}$
  - Time cost: reduced to $O(NN_h^2 + N_h^3)$.



Motivations

- Efficient Semi-Supervised Classifier
  - Cut down the computational cost of graph construction and model optimization.
  - Keeping a satisfying performance on the classification accuracy.

- Scalable Query Selection Criterion
  - Cut down the computational cost of query selection.
  - Keeping a satisfying performance on the quality of selected instances.

Scalable Active Learning

Scalable Query Selection

Approximated Error Reduction (AER)

Definition:

- an approximated estimation of expected error reduction with limited computations.

Formulation:

average estimated error

$$\text{argmax}_{\mathbf{x}_q} I_q \times \left(\frac{\mathcal{E}r_{\langle q\rangle}}{I_{\langle q\rangle}}\right)^{1-\varepsilon}$$

where I_q is the **expected impact** over **all instances**, ε is the hyper-parameter and $\frac{\mathcal{E}r_{\langle q\rangle}}{I_{\langle q\rangle}}$ is the **approximated ratio** between the **error reduction** and the **expected impact** over **nearby instances**.

Interpretation:

- $\textit{error reduction} = \textit{expected impact} \times \frac{\textit{expected error reduction}}{\textit{expected Impact}}$.
- $\textit{approximated error reduction} = \textit{expected impact} \times \left(\frac{\textit{expected error reduction}}{\textit{expected Impact}}\right)^{1-\varepsilon}_{\textit{nearby datapoints}}$.
- Setting ϵ as **average estimated error** within (0, 1) ⇒ **Adaptive tradeoff between two terms with the error decreasing**.

Scalable Active Learning

Scalable Query Selection

Approximated Error Reduction (AER)

Formulation:

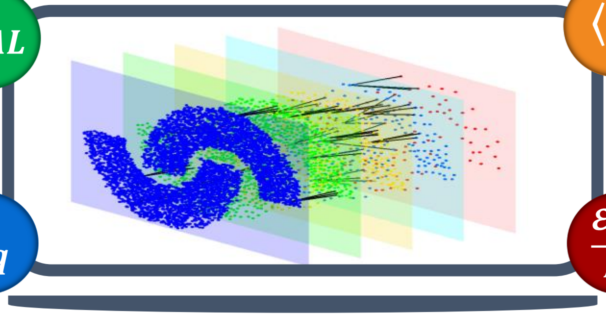
$$\mathrm{argmax}_{\mathbf{x}_q}\ I_q \times \left(\frac{\mathcal{E}r_{\langle q\rangle}}{I_{\langle q\rangle}}\right)^{1-\varepsilon},\ q \in S_{AL}$$

where I_q is the expected impact over all instances, $\frac{\mathcal{E}r_{\langle q\rangle}}{I_{\langle q\rangle}}$ is the approximated ratio between the error reduction and the expected impact over nearby instances, and ε is the tradeoff parameter.

Keypoints:

Candidate set S_{AL}

$\langle q\rangle$ Nearby datapoints of the candidate $\mathbf{x}_q$



Expected impact over all instances I_q

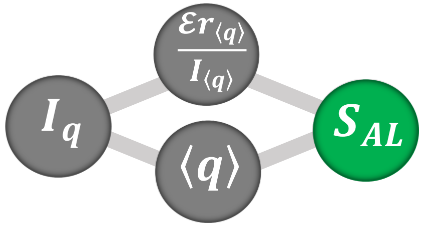
$\frac{\mathcal{E}r_{\langle q\rangle}}{I_{\langle q\rangle}}$ Approximated ratio over nearby datapoints

Scalable Active Learning

Scalable Query Selection

Approximated Error Reduction (**AER**)

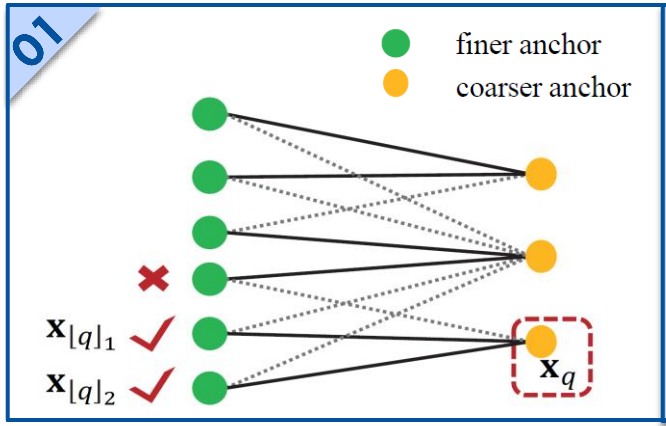
Keypoints:



Candidate set

Details:

Hierarchical expansion of candidates



Hierarchical Expansion

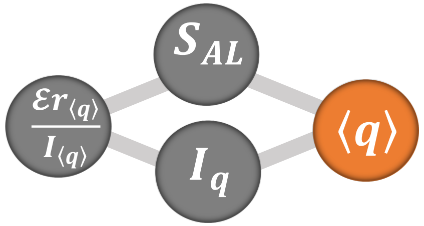
1. Initialize candidates with all the coarsest anchors.
2. Once $\mathbf{x}_q$ is labeled, the connected finer anchors whose nearest coarser anchor is $\mathbf{x}_q$, is added into the candidate set.

Scalable Active Learning

Scalable Query Selection

Approximated **E**rror **R**eduction (**AER**)

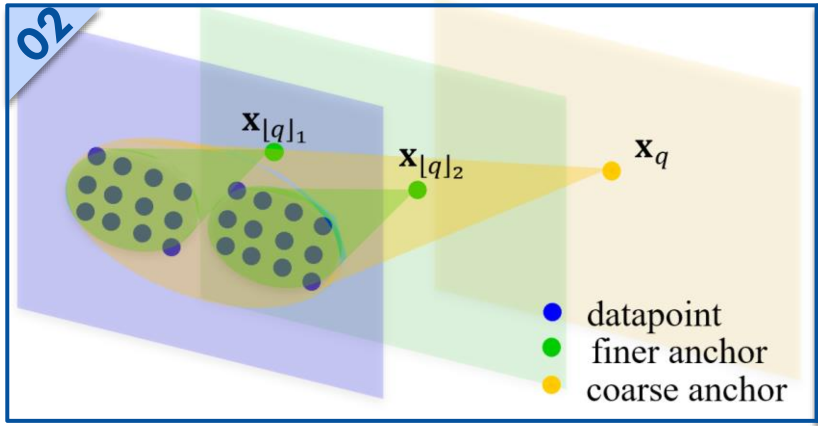
Keypoints:



Nearby datapoints of x_q

Details:

Hierarchical assignment of nearby datapoints



Hierarchical Assignment

Once the current anchor $\mathbf{x}_q$ is labeled, its nearby datapoints ⟨q⟩ are re-assigned to the nearest finer anchors $x_{\lfloor q\rfloor_1}$ and $x_{\lfloor q\rfloor_2}$.

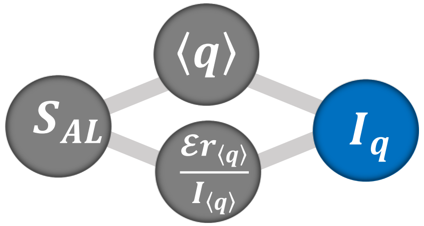
the coarser candidates requires more nearby datapoints to estimate their approximated ratio effectively.

Scalable Active Learning

Scalable Query Selection

Approximated Error Reduction (**AER**)

Keypoints:



Expected impact over all instances

Details:

Only soft labels are required.

Fast computation of the expected impact

03

HAGR: $I_q = \sum_{r=1}^{C} f_{qr} \left\| \mathbf{Z}^{\mathrm{H}} \left(\mathbf{A}^{+\hat{y}_{qr}} - \mathbf{A} \right) \right\|_{\mathrm{F}}^{2}$

$$\left\| \mathbf{Z}^{\mathrm{H}} \left(\mathbf{A}^{+\hat{y}_{qr}} - \mathbf{A} \right) \right\|_{\mathrm{F}}^{2}$$
$$= \mathrm{trace}\left[\left(\mathbf{A}^{+\hat{y}_{qr}} - \mathbf{A} \right) \boldsymbol{\Delta} \left(\mathbf{A}^{+\hat{y}_{qr}} - \mathbf{A} \right) \right]$$

$$\mathbf{A} = \left(\mathbf{Z}_q^{\mathrm{H}^{\mathrm{T}}} \mathbf{Z}_q^{\mathrm{H}} + \mathbf{M} \right)^{-1} \left(\mathbf{Z}_q^{\mathrm{H}^{\mathrm{T}}} \mathbf{Y}_q + \mathbf{Z}_{\mathrm{L}}^{\mathrm{H}^{\mathrm{T}}} \mathbf{Y}_{\mathrm{L}} \right)$$
$$\boxed{\boldsymbol{\Delta} = \mathbf{Z}_{\mathrm{L}}^{\mathrm{H}^{\mathrm{T}}} \mathbf{Z}_{\mathrm{L}}^{\mathrm{H}}} \qquad \mathbf{M} = \mathbf{Z}_{\mathrm{L}}^{\mathrm{H}^{\mathrm{T}}} \mathbf{Z}_{\mathrm{L}}^{\mathrm{H}} + \lambda \tilde{\mathbf{L}}$$

remaining time cost to data size is avoided

Fast Computation

Let $\tilde{\mathbf{M}} =$ ... $, \alpha_q = \mathbf{Z}_q^{\mathrm{H}^{\mathrm{T}}} \mathbf{M} \mathbf{Z}_q^{\mathrm{H}}, \beta_q = \frac{1}{1+\alpha_q}$,

then $\left(\mathbf{Z}_q^{\mathrm{H}}\right.$ ... $\left. \mathbf{Z}_q^{\mathrm{H}^{\mathrm{T}}} \mathbf{Z}_q^{\mathrm{H}} \mathbf{M} \right)$

matrix inversion lemma

Time Cost:

For N_q candidates, the time cost of expected impact estimation is $O\left(N_h^2 N_q + N_h^3 + N_h N_q C + N_h^2 C + N_q C^2\right) \approx O(N_h^2 N_q)$.

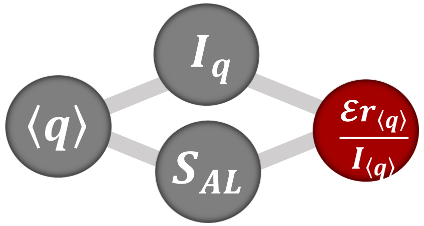
direct matrix operations !

Scalable Active Learning

□ Scalable Query Selection

Approximated **E**rror **R**eduction (**AER**)

Keypoints:



Approximated ratio

Details:

Fast estimation of the approximated ratio

04 expected impact over $\langle q\rangle$

$$I_{\langle q\rangle} \approx \frac{I_q}{1+\mu}$$

μ:degree of the impact overflow to nearby datapoints.

expected error reduction over $\langle q\rangle$

$$\mathcal{E}r_{\langle q\rangle} = \sum_{i=1}^{N_{\langle q\rangle}} \eta_i \ell(f_i, \hat{f}_i) \approx \eta \sum \ell(f_i, \hat{f}_i)$$

η:degree of the expected error will be reduced.

Fast Estimation

$$\frac{\mathcal{E}r_{\langle q\rangle}}{I_{\langle q\rangle}} = \eta \cdot \frac{\mathcal{E}_{\langle q\rangle}}{\frac{I_q}{1+\mu}}$$

$$= \eta(1+\mu) \times \frac{\mathcal{E}_{\langle q\rangle}}{I_q}$$

Time Cost:

For N_q candidates, the time cost of approximated ratio estimation is $O(NC)$.

Scalable Active Learning

Scalable Query Selection

Approximated Error Reduction (AER)

Objective formulation:

$$\text{argmax}_{\mathbf{x}_q} I_q \times \left(\frac{\mathcal{E}r_{\langle q\rangle}}{I_{\langle q\rangle}}\right)^{1-\varepsilon}, q \in S_{AL}$$

S_{AL} $\langle q\rangle$ I_q $\frac{\mathcal{E}r_{\langle q\rangle}}{I_{\langle q\rangle}}$

Final formulation:

$$\textbf{argmax}_{\mathbf{x}_q} \boldsymbol{I_q^{\varepsilon}} \times \boldsymbol{\mathcal{E}_{\langle q\rangle}}^{\mathbf{1-\varepsilon}}, \boldsymbol{q \in S_{AL}}$$

average estimated error

uncertainty over nearby instances

expected impact over all instances

Pros:

AER enables an efficient estimation of error reduction without re-inferring labels of instances.

The expected impact can be calculated for all candidates via direct matrix operations rather than multiple iterations.

Apart from the **similar time cost to** that of the **uncertainty sampling**, the remaining time cost of our AER-based approach is independent of data sizes during the query selection.

AER focuses on global impact first and pays attention to local uncertainty later, which provides an opportunity to achieve comparable or even higher accuracies than the EER-based approach.

Outline

Experiment and Conclusion

Experiment

- Efficient Semi-Supervised Learning on Hierarchical Anchor Graph
- Scalable Active Learning with Approximated Error Reduction

Classification error rates (%) on **USPS-Train** (7,291 samples) with $l = 100$ labeled samples. $m = 1000$ for four versions of AGR. The running time of `k-means` clustering is 7.65 seconds.

Method	Error Rate (%)	Running Time (seconds)
1NN	20.15 ± 1.80	0.12
LGC with 6NN graph	8.79 ± 2.27	403.02
GFHF with 6NN graph	5.19 ± 0.43	413.28
random `AnchorGraphReg`^{0}	11.15 ± 0.77	2.55
random `AnchorGraphReg`	10.30 ± 0.75	8.85
`AnchorGraphReg`^{0}	7.40 ± 0.59	10.20
`AnchorGraphReg`	$\mathbf{6.56 \pm 0.55}$	16.57

□ Experiment

- Efficient Semi-Supervised Learning on Hierarchical Anchor Graph
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Classification accuracies (%) with different number of labeled samples on the MNIST8M dataset.

# of labeled samples	1NN	LSVM	AGR -30,000	EAGR -30,000	HAGR -30,000-5,000	HAGR -300,000-30,000-5000
100	60.16 ± 1.96	59.67 ± 2.19	89.87 ± 1.78	90.27 ± 0.18	89.46 ± 1.24	$\mathbf{91.36 \pm 0.70}$
200	68.66 ± 1.29	64.46 ± 2.37	91.15 ± 0.59	91.76 ± 0.57	90.85 ± 0.50	$\mathbf{92.46 \pm 0.42}$
300	72.78 ± 0.81	66.79 ± 2.25	92.21 ± 0.51	92.37 ± 0.51	91.66 ± 0.42	$\mathbf{93.05 \pm 0.37}$
400	75.33 ± 0.60	68.33 ± 1.97	92.47 ± 0.44	92.73 ± 0.38	92.16 ± 0.36	$\mathbf{93.43 \pm 0.37}$
500	77.24 ± 0.55	70.65 ± 1.49	92.70 ± 0.41	93.05 ± 0.29	92.50 ± 0.29	$\mathbf{93.78 \pm 0.24}$
600	78.58 ± 0.54	72.64 ± 1.36	92.80 ± 0.34	93.17 ± 0.27	92.64 ± 0.26	$\mathbf{93.90 \pm 0.27}$
700	79.87 ± 0.70	73.80 ± 1.27	93.12 ± 0.31	93.41 ± 0.30	92.92 ± 0.28	$\mathbf{94.10 \pm 0.25}$
800	81.02 ± 0.50	73.87 ± 1.18	93.19 ± 0.23	93.51 ± 0.15	93.06 ± 0.16	$\mathbf{94.21 \pm 0.15}$
900	81.76 ± 0.49	73.97 ± 0.96	93.29 ± 0.36	93.63 ± 0.21	93.18 ± 0.26	$\mathbf{94.28 \pm 0.16}$
1000	82.51 ± 0.42	76.95 ± 1.13	93.49 ± 0.22	93.79 ± 0.15	93.37 ± 0.16	$\mathbf{94.39 \pm 0.12}$

The comparison of time costs (in seconds) of AGR, EAGR, and HAGR methods on the MNIST8M dataset.

Dataset	AGR-30,000	EAGR-30,000	HAGR-30,000-5000	HAGR-300,000-30,000-5,000
MNIST8M	665.07	662.60	104.97	137.54

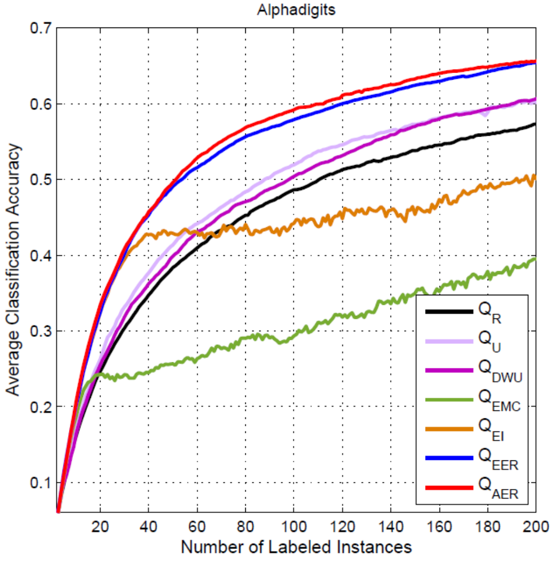
Experiment and Conclusion

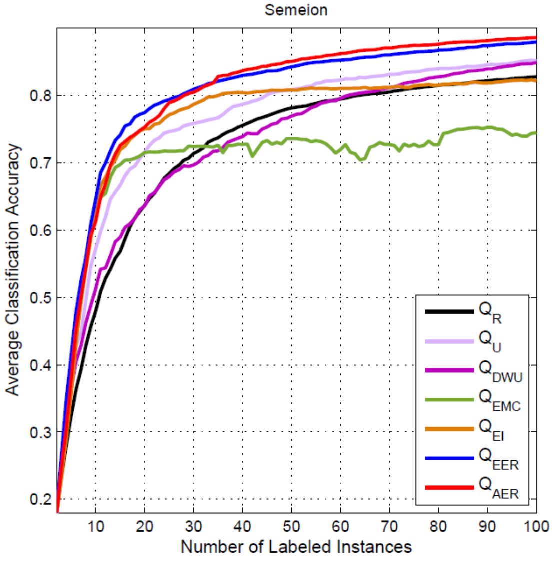
Experiment

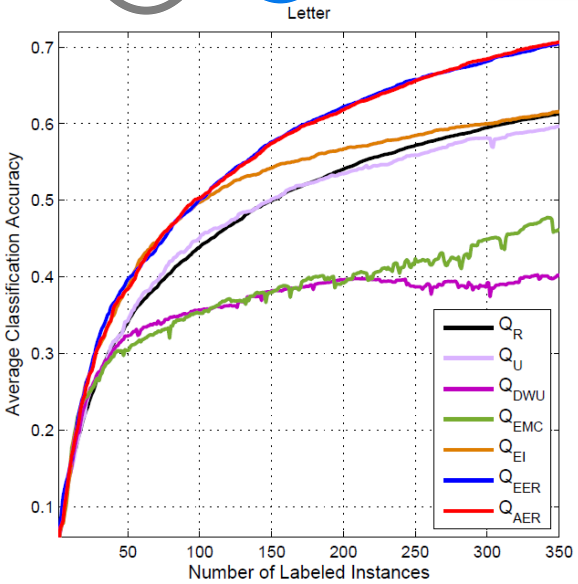
- Efficient Semi-Supervised Learning on Hierarchical Anchor Graph
- Scalable Active Learning with Approximated Error Reduction

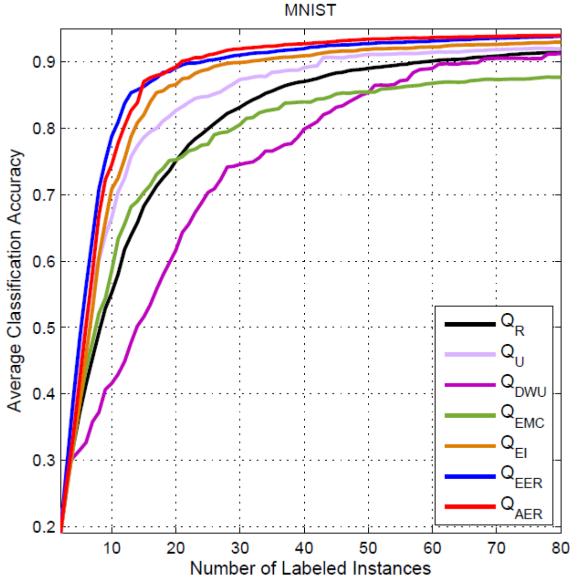
Dataset	Q_U	Q_{DWU}	Q_{EMC}	Q_{EI}	Q_{EER}	Q_{AER}
Alphadigits	0.01	0.03	0.04	0.04	1.80	0.04
Semeion	0.01	0.01	0.02	0.02	0.67	0.02
Letter	0.03	0.10	0.11	0.17	13.81	0.20
MNIST	0.04	0.18	0.15	0.17	30.16	0.21

Uncertainty
Model Change
Expected Error Reduction
Approximated Error Reduction





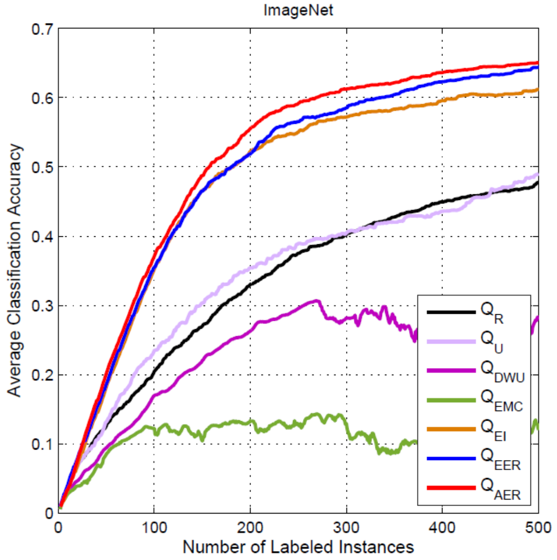


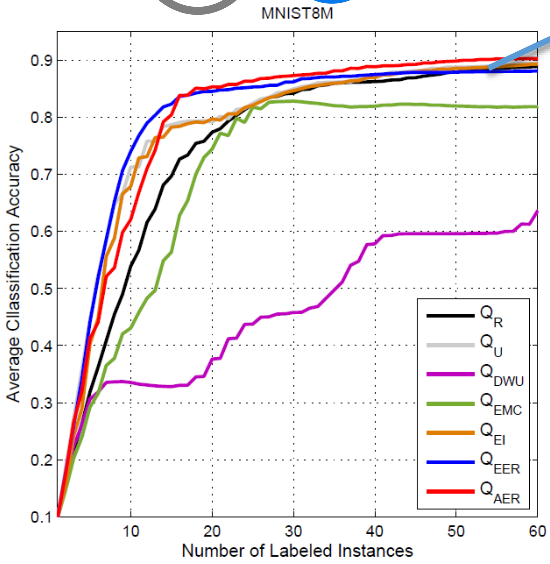


Experiment

- Efficient Semi-Supervised Learning on Hierarchical Anchor Graph
- Scalable Active Learning with Approximated Error Reduction

Dataset	Q_U	Q_{DWU}	Q_{EMC}	Q_{EI}	Q_{EER}	Q_{AER}
ImageNet	2.15	10.05	4.19	7.61	90.73	9.35
MNIST8M	4.22	14.47	10.97	12.19	198.73	16.15





Since AER pays attention to local region based on local uncertainty, it can leads to better performance than EER.

Uncertainty
Model Change
Expected Error Reduction
Approximated Error Reduction

Experiment and Conclusion

□ Conclusion

Our Work

- Semi-supervised classifier on hierarchical anchor graph.
- Query selection criterion with approximated error reduction.
- Scalable active learning for efficient classification.

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Thank you for attention!

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