# Discriminative Experimental Design

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# Outline

# Active Learning

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**Input:** Labeled data set $\mathcal{L}$; Unlabeled data set $\mathcal{U}$
**Output:** Learning model

Step 1: Train a learning model based on $\mathcal{L}$;
Step 2:
For $t = 1, \ldots, t_{\text{max}}$
2.1: Select an unlabeled data set $\mathcal{S}$ from $\mathcal{U}$ based on some unlabeled data selection criterion;
2.2: Query an oracle to label $\mathcal{S}$;
2.3: $\mathcal{L} \leftarrow \mathcal{L} \cup \mathcal{S}, \mathcal{U} \leftarrow \mathcal{U} \setminus \mathcal{S}$;
2.4: Re-train the learning model based on $\mathcal{L}$;

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  - A projection method to solve the optimization problem.
  - The good performance on some benchmark datasets.

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- $\phi(\cdot)$: The feature mapping corresponding to some kernel function $k(\cdot, \cdot)$

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# Least-Square SVM Revisited

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- The objective function of least-square SVM is formulated as:

$$\min_{\mathbf{w}} \sum_{i=1}^{l} (\mathbf{w}^T \phi(\mathbf{x}_i) - y_i)^2 + \lambda \|\mathbf{w}\|_2^2. \quad (1)$$

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- Here the square loss is similar to the square hinge loss $L'(s,t) = \max(0, 1 - st)^2$.
- The function score for a data point is defined as:

$$y = \frac{1}{\mathbf{w}^T \phi(\mathbf{x})},$$

# The Objective Function

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- According to the analysis in TED, the estimation error satisfies

$$\mathrm{cov}(\mathbf{w} - \mathbf{w}^\star) \propto \mathbf{C}_\mathbf{w} = \left(\frac{\partial^2 J(\mathbf{w})}{\partial \mathbf{w} \partial \mathbf{w}^T}\right)^{-1} = \left(\phi(\mathbf{X})\mathbf{Y}_\mathbf{X}^2\phi(\mathbf{X})^T + \lambda \mathbf{I}_{d'}\right)^{-1}$$

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Definition

Discriminative Experimental Design:

$$\begin{aligned} \max_{\mathbf{X},\mathbf{Y}_{\mathbf{X}}} \quad & \operatorname{tr}\left[\mathbf{Y}_{\mathbf{V}}\mathbf{K}_{\mathbf{VX}}\mathbf{Y}_{\mathbf{X}}(\lambda \mathbf{I}_t + \mathbf{Y}_{\mathbf{X}}\mathbf{K}_{\mathbf{X}}\mathbf{Y}_{\mathbf{X}})^{-1}\mathbf{Y}_{\mathbf{X}}\mathbf{K}_{\mathbf{XV}}\mathbf{Y}_{\mathbf{V}}\right] \\ \text{s.t.} \quad & \mathbf{X} \subset \mathbf{V}, |\mathbf{X}| = t, \mathbf{Y}_{\mathbf{X}} \subset \mathbf{Y}_{\mathbf{V}}. \end{aligned} \tag{3}$$

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- The optimization problem of linear DED:

$$\begin{aligned} \max_{\tilde{\mathbf{X}}} \quad & \mathrm{tr}\left[\tilde{\mathbf{V}}^T\tilde{\mathbf{X}}(\lambda\mathbf{I}_t + \tilde{\mathbf{X}}^T\tilde{\mathbf{X}})^{-1}\tilde{\mathbf{X}}^T\tilde{\mathbf{V}}\right] \\ \text{s.t.} \quad & \tilde{\mathbf{X}} \subset \tilde{\mathbf{V}}, |\tilde{\mathbf{X}}| = t. \end{aligned} \tag{4}$$

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- TED can be seen as a special case of DED.
- DED is a weighted version of TED.
  - The weights are related to function scores of the data points.

# Reformulation of DED

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- A selection indicator matrix $\mathbf{S} \in \{0,1\}^{n \times t}$ is defined as

$$s_{ij} = \begin{cases} 1 & \text{if } (\phi(\mathbf{X})\mathbf{Y_X})_{,j} \text{ is from } (\phi(\mathbf{V})\mathbf{Y_V})_{,i} \\ 0 & \text{otherwise} \end{cases}$$

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  - $\mathbf{S}^\star$ consists of the top $t$ eigenvectors of $\tilde{\mathbf{K}}_{\mathbf{V}}$.
  - $\mathbf{P} \in \mathbb{R}^{t\times t}$ is an orthogonal matrix.

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- The optimal solution $\mathbf{S}^{\star}\mathbf{P}$ is projected to the set $C_S$:

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- We propose a greedy method to select multiple largest elements in different rows.

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  - $(\mathbf{S}^\star)^T\mathbf{Q} = \mathbf{U}\Sigma\mathbf{R}^T$ be the singular value decomposition.

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- Performance measure: The area under the ROC curve (AUC).
- The size of queries $t$: 5
- The regularization parameters: 0.01.
- Five labeled data points are provided for each class before active learning starts.

# Results on Newsgroups Data

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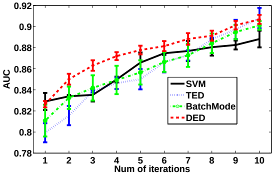
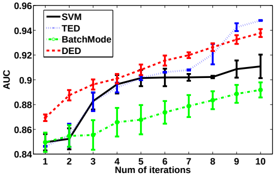
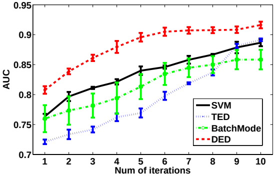


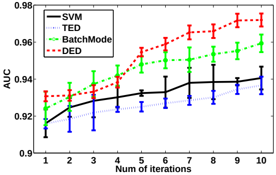

(e) Autos




(f) Motorcycles

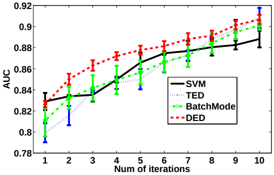



(g) Baseball

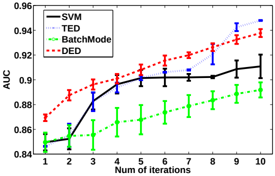



(h) Hockey

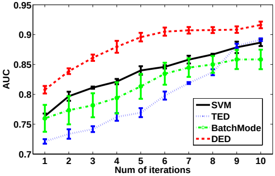
# Results on Newsgroups Data



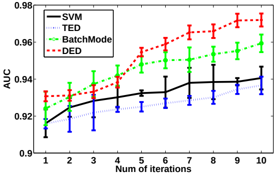

(i) Autos




(j) Motorcycles




(k) Baseball




(l) Hockey

- When the labeled data is scarce, data distribution information is very important.

# Results on Reuters Data

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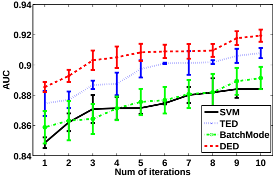
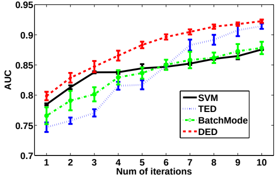
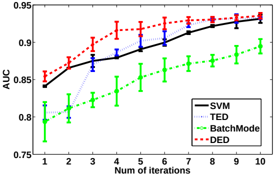


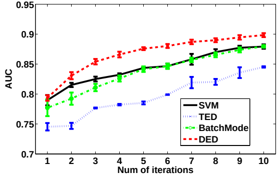

(q) CCAT




(r) ECAT




(s) GCAT




(t) MCAT

# Comparison on Two Optimization Techniques

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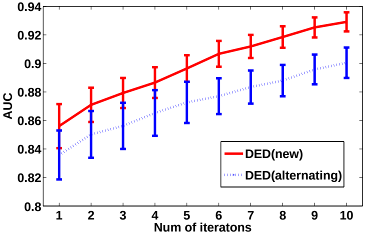
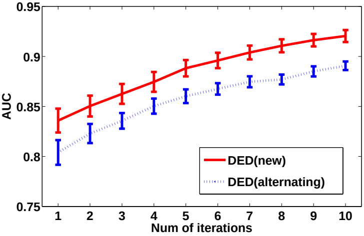



(w) Newsgroups data




(x) Reuters data

# Outline

# Conclusion

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Future Work:

# Conclusion

- A novel active learning method has been proposed.
- The data selection criterion utilizes discriminative information and data distribution information.

Future Work:

- The integration of active learning and semi-supervised learning

Thanks very much for your attention!