

# Retrospective ICML99 Transductive Inference for Text Classification using Support Vector Machines

**Thorsten Joachims**

**Then:** Universität Dortmund, Germany  
**Now:** Cornell University, USA

# Outline

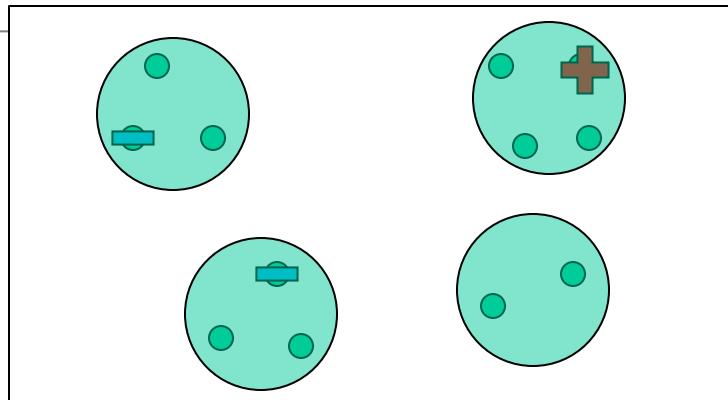
- **The paper in a nutshell**
- **Connections to other semi-supervised methods**
  - Co-training
  - Graph Mincuts
  - Normalized cuts
  - Harmonic functions
  - Manifold methods
  - Random walks
- **Post-mortem**
- **Valuable life lessons**

# Input

**Tom Mitchell**

**“What can we do with all the text data on the web?”**

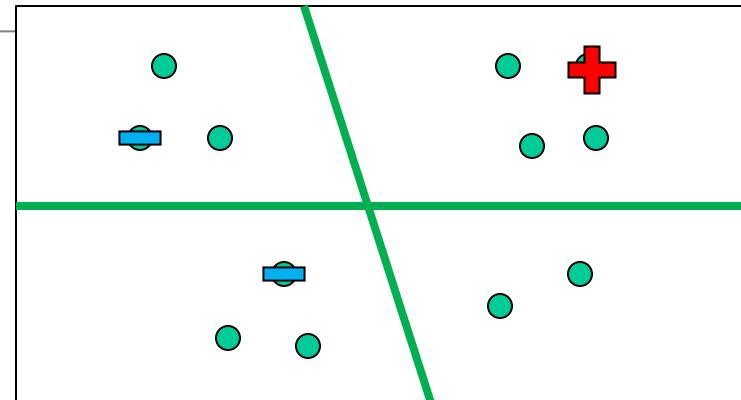
- [Blum/Mitchell] Co-training
  - Exploit redundant representations
- [Nigam/McCallum/Thrun/Mitchell] Semi-supervised Naïve Bayes
  - Generatively model clusters in  $P(X)$
  - Mixture model



**Vladimir Vapnik**

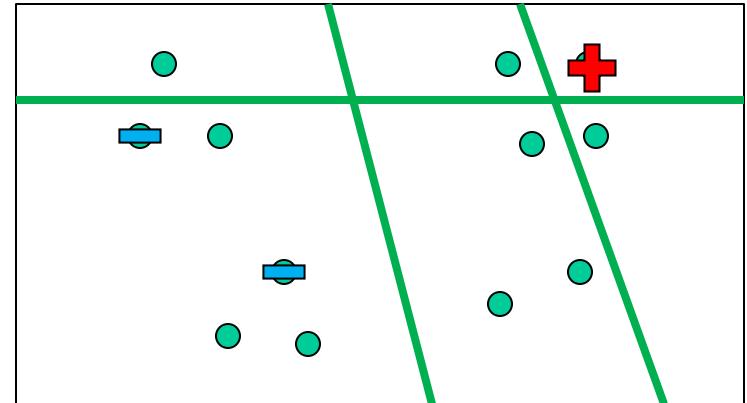
**Transduction: Predicting only at known locations is easier**

- Finite number of predictions vs. continuous function
- Define margin w.r.t. test points
- Generalization error bounds



# Transductive SVMs

- **Objective [Vapnik]: Max margin on training and test set**
- **Input:**
  - Location of examples:  $\{x_1 \dots x_n\}$
  - Labels for subset L of examples



## Hard Margin:

$$\min_y \min_w \frac{1}{2} w^T w$$

$$s.t. \quad \forall i : y_i [w^T x + b] \geq 1$$

$$\forall i \in L : y_i = 1 / -1$$

$$y \in \{+1, -1\}$$

$$y^T 1 = c$$

## Soft Margin:

$$\min_y \min_w \frac{1}{2} w^T w + C \sum \xi_i$$

$$s.t. \quad \forall i : y_i [w^T x + b] \geq 1 - \xi_i$$

$$\forall i \in L : y_i = 1 / -1$$

$$y \in \{+1, -1\}$$

$$y^T 1 = c$$

Class  
balance  
constraint

# Text and Margins

	nuclear	physics	atom	pepper	basil	salt	and
D1	1						1
D2	1	1	1				1
D3				1			1
D4					1	1	1
D5					1	1	1
D6						1	1

## Altavista (1999)

- hits(pepper & salt) → 327K
- hits(pepper & physics) → 4.2K
- hits(physics) > hits(salt)

## Google (2009)

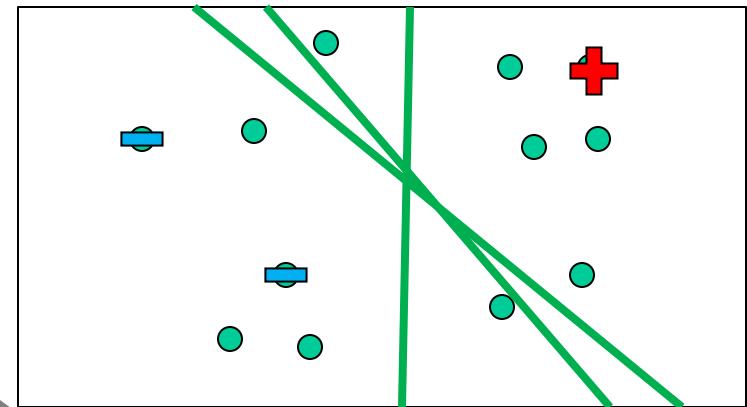
- hits(pepper & salt) → 159M
- hits(pepper & physics) → 1.3M
- hits(physics) = 107M > hits(salt) = 56M

Prof. Michael Pepper → Prof. Sir Michael Pepper

# Training Algorithm

- **Algorithm (<http://svmlight.joachims.org>)**

- Assign labels to test examples (s.t. class balance constraint)
- Train supervised SVM
- DO
  - Find pair of test labels to flip
  - Retrain supervised SVM
- WHILE objective decreased



**Soft Margin:**

Smoothed objective to avoid local optima  
Smoothing reduced as optimization progresses

Criterion for selecting pair that guarantees descent

Criterion is efficiently computable

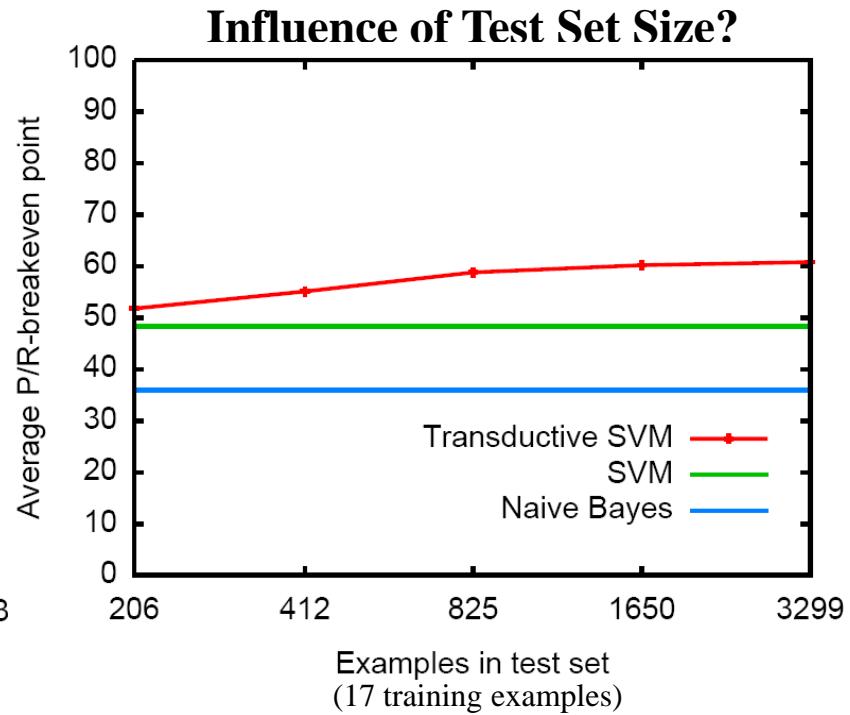
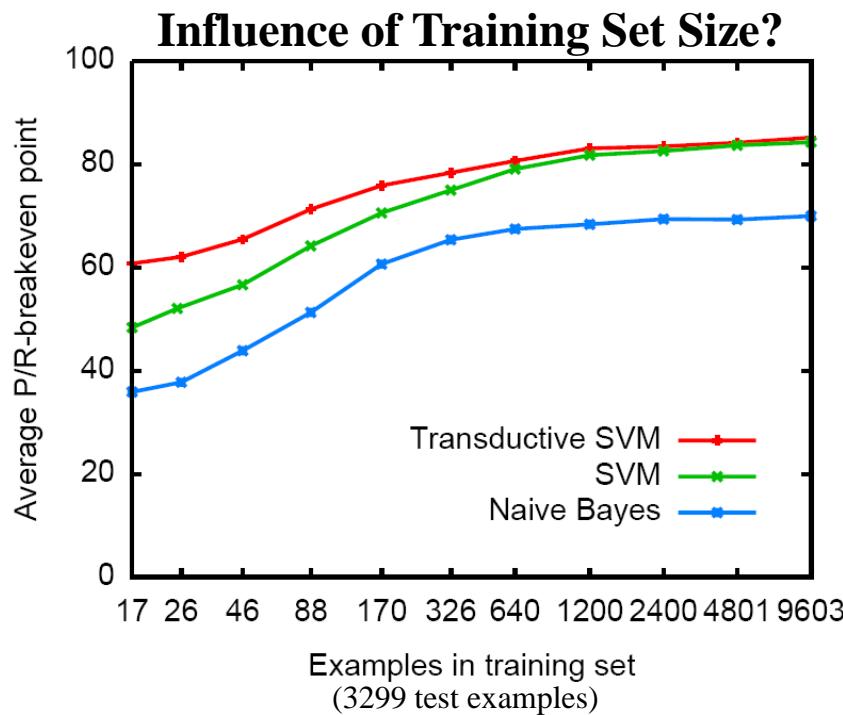
$$\forall i \in L : y_i = 1 / - 1$$

$$y \in \{+1, -1\}$$

$$y^T 1 = c$$

# Experiment: Reuters-21587

- **Setup**
  - Top 10 categories of Reuters-21587 dataset
  - ~12000 features after stemming and stopword removal
  - Macro-averaged precision/recall break-even point



# Experiment: WebKB

- **Setup**
  - 4 classes
  - 9 training examples, 3957 test examples
  - Precision/recall break-even point per class (and average)

	Bayes	SVM	TSVM
course	57.2	68.7	93.8
faculty	42.4	52.5	53.7
project	21.4	37.5	18.4
student	63.5	70.0	83.8
macro-average	46.1	57.2	62.4

# Other Approaches

- **Optimization Methods for TSVM Objective**
  - Semi-definite Programming relaxation (convex) [Xu et al.]
  - Gradient Descent in Primal [Chapelle/Zien]
  - Concave Convex Procedure [Collobert et al.]
- **Other Objectives**
  - Manifolds and Graph Kernels [Belkin/Niyogi] [Chapelle et al.]
  - Harmonic Functions and Gaussian Processes [Zhu et al.]
  - Random Walks [Szummer/Jaakola]
  - Graph Cuts [Blum/Chawla]
  - Kernels from Generative Models [Jaakola/Haussler]
- **Special Structure of Problem**
  - Co-Training [Blum/Mitchell]
  - Structured Output Prediction [Brefeld/Scheffer]
- **Transductive Error Bounds**
- **Much more...**

# Self-Consistency and Stability

- **Inductive Learner:**  $L_{\text{ind}}$
  - **Transductive Learner:**  $L_{\text{trans}}$  (based on  $L_{\text{ind}}$ )
  - **Assumption**
    - If whole sample was labeled, then  $L_{\text{ind}}$  would learn accurate classifier.
  - **Reasoning**
    - If assumption holds, then  $L_{\text{ind}}$  will have low leave-one-out error.
    - If  $L_{\text{trans}}$  returns a labeling on which  $L_{\text{ind}}$  would have high leave-one-out error, it cannot be the correct labeling.
- **Construct prior of  $L_{\text{trans}}$  via leave-one-out error of  $L_{\text{ind}}$ .**
- Margin wrt. test set bounds leave-one-out error of inductive SVM.
  - Ridge Regression [Chapelle et al.]
  - Graph-cuts [Blum/Chawla]

# Redefining Margin

**Primal:**

$$\min_{\mathbf{y}} \min_{\mathbf{w}} \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

$$s.t. \quad \forall i : y_i \mathbf{w}^T \mathbf{x} \geq 1$$

$$\forall i \in L : y_i = 1 / -1$$

$$\mathbf{y} \in \{+1, -1\}$$

**Dual:**

$$\min_{\mathbf{y}} \max_{\alpha \geq 0} 1^T \alpha - \frac{1}{2} \alpha^T Y A Y \alpha$$

$$s.t. \quad \forall i : Y_{ii} = y_i$$

$$\forall i \in L : y_i = 1 / -1$$

$$\mathbf{y} \in \{+1, -1\}$$

$$\alpha_1 = \dots = \alpha_n$$

**Classification Rule / Margin:**

$$h(\mathbf{x}) = \text{sign} \left\{ \sum_{i=1}^n y_i \cancel{\alpha}_i K(\mathbf{x}, \mathbf{x}_i) \right\}$$

$$m(\mathbf{x}, \mathbf{y}) = 1 - y \sum_{i=1}^n y_i \cancel{\alpha}_i K(\mathbf{x}, \mathbf{x}_i)$$



Nearest Neighbor Rule



**Simplified Dual:**

$$\min_{\mathbf{y}} -\mathbf{y}^T A \mathbf{y}$$

$$s.t. \quad \forall i \in L : y_i = 1 / -1$$

$$\mathbf{y} \in \{+1, -1\}$$

Min bound on  
leave-one-out  
error of NN

# Connection to Graph Cuts

## [Blum/Chawla]

**Simplified Dual:**

$$\min_{\mathbf{y}} -\mathbf{y}^T \mathbf{A} \mathbf{y}$$

$$s.t. \forall i \in L : y_i = 1 / -1$$

$$\mathbf{y} \in \{+1, -1\}$$

**Graph Cut:**

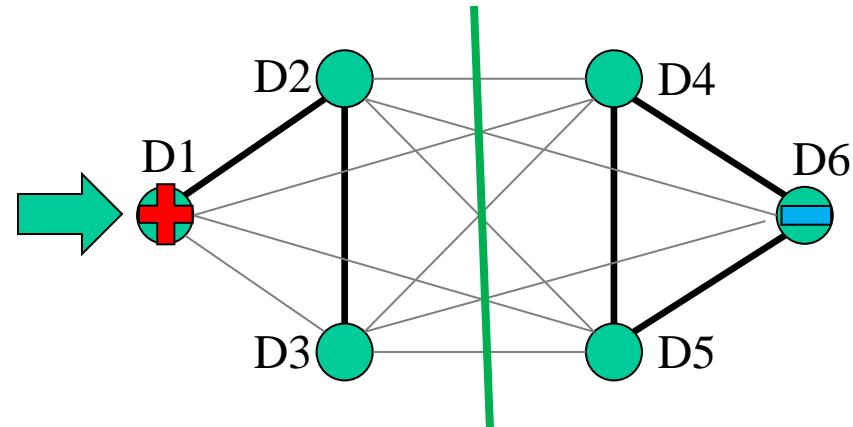
$$\min_{\mathbf{y}} \sum_{y_i \neq y_j} A_{ij} = \sum_{ij} A_{ij} (y_i - y_j)^2$$

$$s.t. \forall i \in L : y_i = 1 / -1$$

$$\mathbf{y} \in \{+1, -1\}$$

+

	nuclear	physics	atom	pepper	basil	salt	and
D1	1						1
D2	1	1	1				1
D3				1			1
D4				1	1		1
D5				1		1	1
D6					1	1	1



→ Fast algorithms for computing cuts for sparse graphs (e.g. k-NN)

# Connection to Harmonic Functions

## [Zhu/Ghahramani/Lafferty]

### Graph Cut:

$$\begin{aligned} \min_{\mathbf{y}} \sum_{ij} A_{ij} (y_i - y_j)^2 \\ \text{s.t. } \forall i \in L : y_i = 1 / -1 \\ \mathbf{y} \in \{+1, -1\} \end{aligned}$$

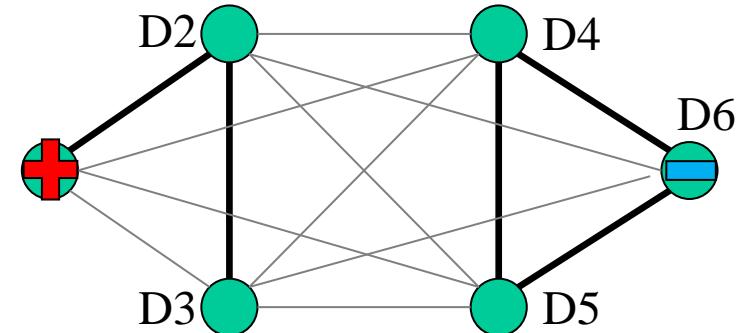
relax

### Harmonic:

$$\begin{aligned} \min_{\mathbf{y}} \sum_{ij} A_{ij} (y_i - y_j)^2 \\ \text{s.t. } \forall i \in L : y_i = 1 / -1 \\ \mathbf{y} \in [+1, -1] \end{aligned}$$

### Interpretations:

- Gaussian process
  - Electric network
  - Probability that random walk hits positively labeled node first
- Connection to [Szummer/Jaakkola]



→ Closed form solution and/or very efficient iterative methods

# Connection to Normalized Cuts [Joachims]

## Graph Cut:

$$\begin{aligned} \min_{\mathbf{y}} \quad & \sum_{ij} A_{ij} (y_i - y_j)^2 \\ \text{s.t. } & \forall i \in L : y_i = 1 / -1 \\ \mathbf{y} \in & \{+1, -1\} \end{aligned}$$

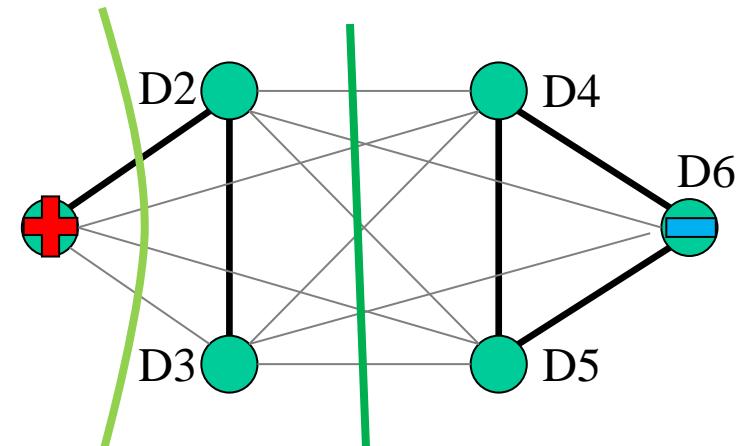
norm

## Normalized (Ratio) Cut:

$$\begin{aligned} \min_{\mathbf{y}} \quad & \sum_{ij} A_{ij} (y_i - y_j)^2 / \sum_{ij} (y_i - y_j)^2 \\ \text{s.t. } & \forall i \in L : y_i = 1 / -1 \\ \mathbf{y} \in & \{+1, -1\} \end{aligned}$$

## Interpretations:

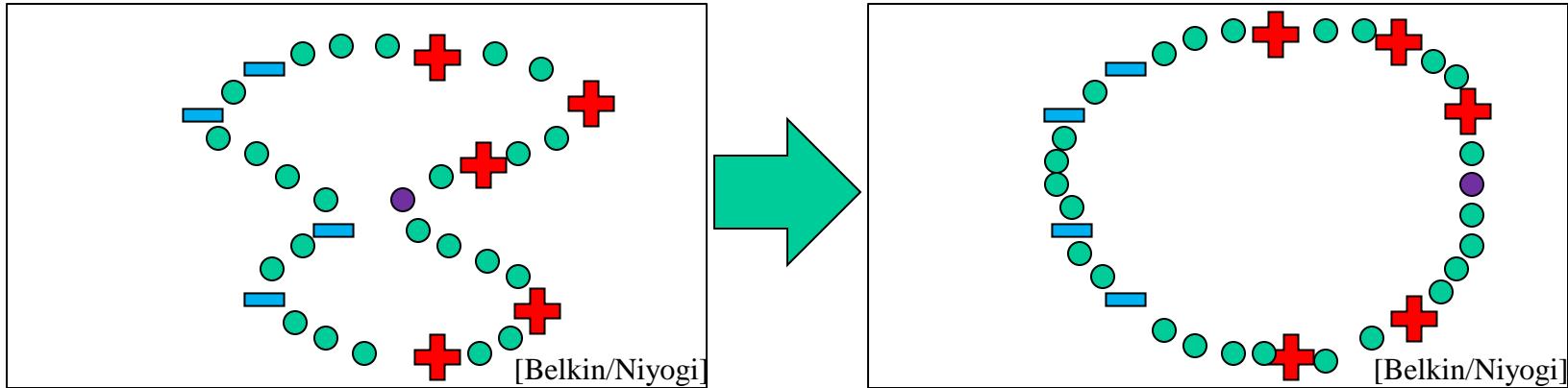
- Minimize average weight of cut edge
- Spectral relaxation has efficient solution  
→ Normalized cuts [Shi/Malik]
- “Supervised” normalized cut  
→ Supervised clustering [Yu/Gross/Shi]



→ Efficient solution of spectral relaxation

# Connection to Manifolds and Graph Kernels

## [Belkin/Niyogi] [Chapelle et al.]



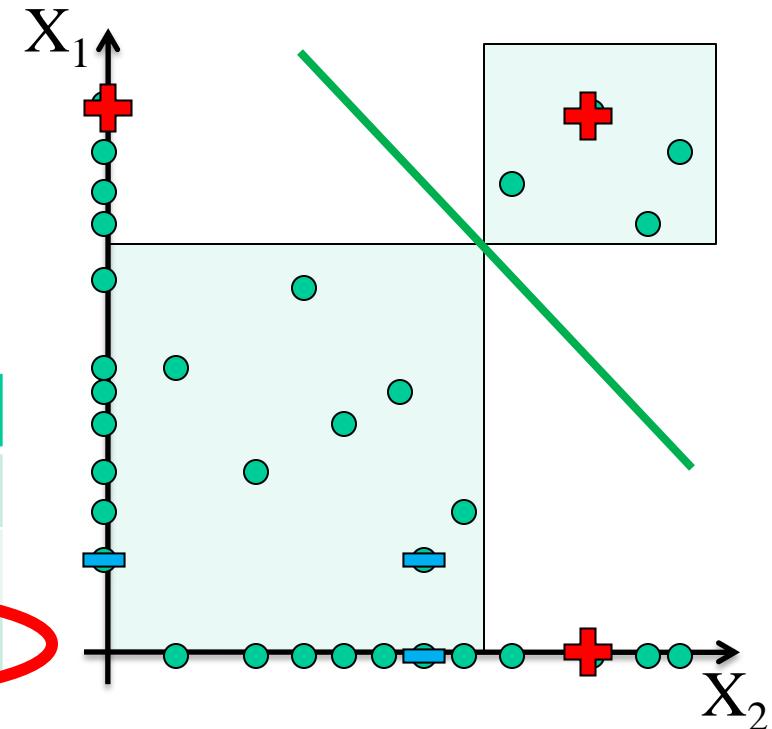
### Exploit Manifold Structure

- Smoothness criterion  $\sum_{ij} A_{ij}(y_i - y_j)^2 = \mathbf{y}^T L \mathbf{y}$  related to graph Laplacian  $L = D - A$
- Not Euclidian distance, but geodesic distance in local neighborhood graph
- Use eigenvectors  $U \Lambda U^T = L$  of graph Laplacian  $L$  to
  - explicitly re-represent data [Roweis/Saul] [Tennenbaum et al.]
  - define a kernel (e.g. to use in inductive SVM) [Kondor/Lafferty]

# Connection to Co-Training [Blum/Mitchell]

- **Idea:**
  - Exploit two sufficiently redundant representations
- **Example:**
  - Learn threshold on  $X_1 / X_2$
  - $\rightarrow$  Co-training implies margin
- **Experiment:**
  - Error rate on WebKB “course”

	SVM	TSVM	B&M
page	21.6	4.6	12.9
link	18.5	8.9	12.4
co-train	20.3	4.3	5.0



# Post Mortem

- **Why does Transductive Learning Work?**
  - Smoothness: labels change smoothly with structure of unlabeled data (clusters, manifold).
  - Self-Consistency: if all examples were labeled, supervised learner has low leave-one-out error.
- **Transduction vs. Semi-supervised?**
  - Transduction = semi-supervised
- **Discriminative vs. Generative?**
  - No need for density estimate of  $P(X)$
- **Use in Practice?**
  - Largest benefits for small training sets
  - Better mean, but (still) large variance
- **How can we use ALL the (text) data on the web?**