Semi-Supervised Learning with Graphs

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Semi-supervised Learning

- classification
- classifiers need labeled data to train
- labeled data scarce, unlabeled data abundant
- *Traditional classifiers cannot use unlabeled data.*

My interest (semi-supervised learning): Develop classification methods that can use both labeled and unlabeled data.

Motivating examples

- speech recognition (sound $\longrightarrow$ sentence)
  - labeled data: transcription, 10 to 400 times real-time
  - unlabeled data: sounds alone, easy to get (radio, call center)
- parsing ("I saw a falcon with a telescope." $\longrightarrow$ tree)
  - labeled data: treebank, English 40,000/5, Chinese 4,000/2 years
  - unlabeled data: sentences without annotation, everywhere.
- personalized news (article $\longrightarrow$ interested?)
  - user patience
- video surveillance (image $\longrightarrow$ identity)
  - named images availability

unlabeled data useful?

The message

Unlabeled data can improve classification.

Why unlabeled data might help

example: classify astronomy vs. travel articles

- articles represented by content word occurrence vectors
- article similarity measured by content word overlap

	d_1	d_3	d_4	d_2
asteroid	•	•		
bright	•	•		
comet		•		
year				
zodiac				
⋮				
airport				
bike				
camp			•	
yellowstone			•	•
zion				•

Why labeled data alone might fail

	d_1	d_3	d_4	d_2
asteroid	●			
bright	●			
comet				
year				
zodiac		●		
⋮				
airport			●	
bike			●	
camp				
yellowstone				●
zion				●

- no overlap!
- tends to happen when labeled data is scarce

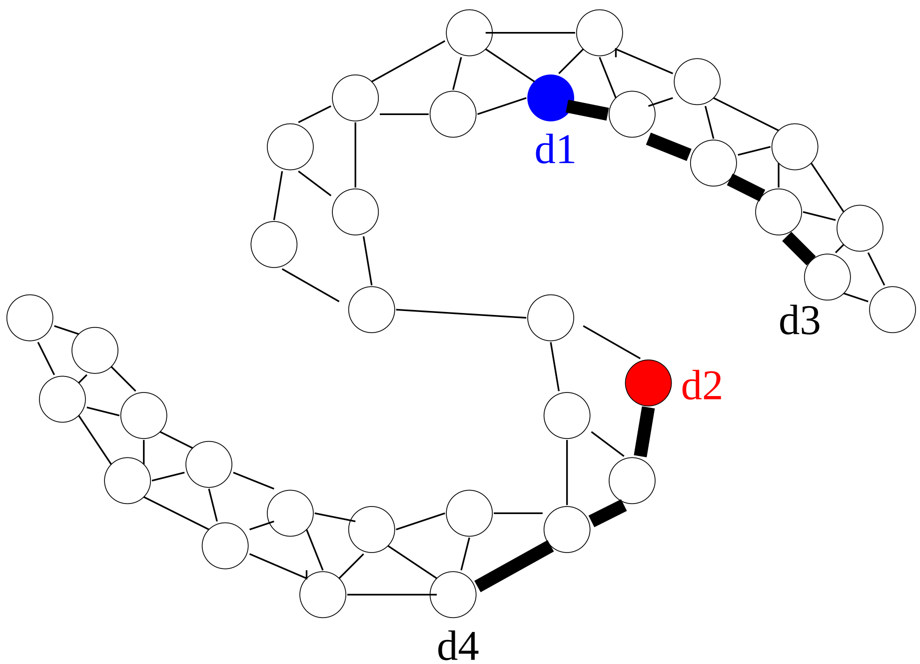
Unlabeled data are stepping stones

	d_1	d_5	d_6	d_7	d_3	d_4	d_8	d_9	d_2
asteroid	●								
bright	●	●							
comet		●	●						
year			●	●					
zodiac				●	●				
⋮									
airport						●			
bike						●	●		
camp							●	●	
yellowstone								●	●
zion									●

- observe *direct* similarity from features: $d_1 \sim d_5$, $d_5 \sim d_6$ etc.
- assume similar features $\Rightarrow$ same label
- labels propagate via unlabeled articles, *indirect* similarity

Unlabeled data are stepping stones

- arrange l labeled and u unlabeled(=test) points in a graph
  - nodes: the $n = l + u$ points
  - edges: the direct similarity W_{ij}, e.g. number of overlapping words. (in general: a decreasing function of the distance $||x_i - x_j||$)
- want to infer indirect similarity (with all paths)



One way to use labeled and unlabeled data

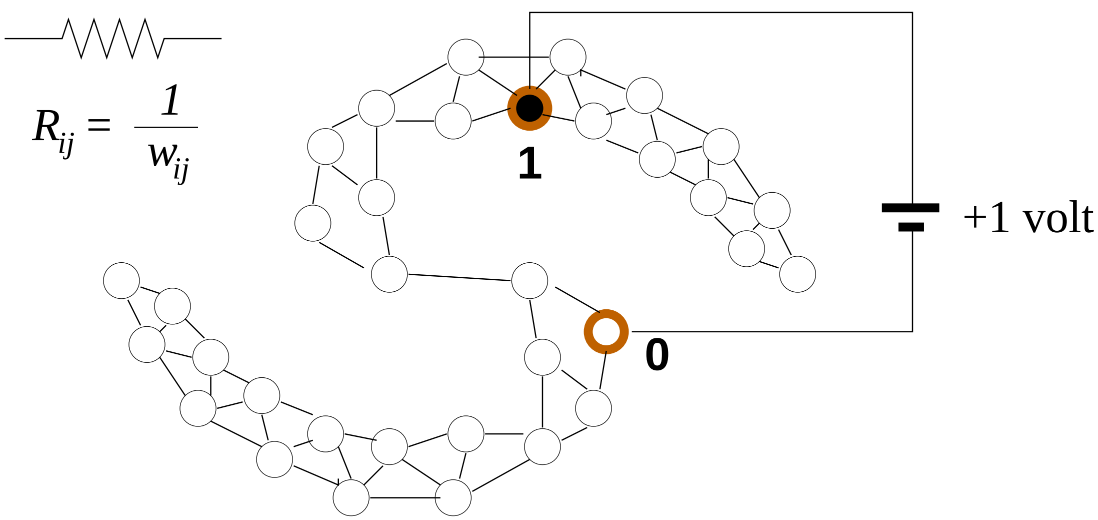
(Zhu and Ghahramani, 2002)

- input: $n \times n$ graph weights W (important!)
  labels $Y_l \in \{0,1\}^l$
- create matrix $P_{ij} = W_{ij} / \sum W_{i\cdot}$
- repeat until f converges
  - clamp labeled data $f_l = Y_l$
  - propagate $f \leftarrow Pf$
- f converges to a unique solution, the *harmonic function*.
  $0 \le f \le 1$, "soft labels"

An electric network interpretation

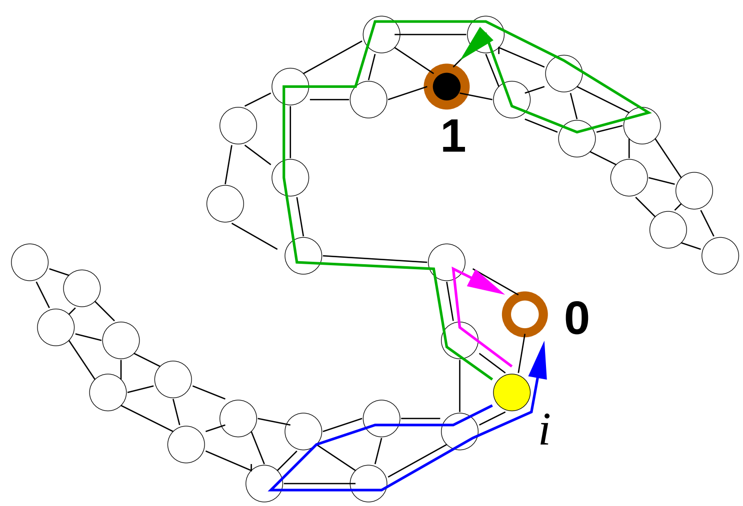
(Zhu, Ghahramani and Lafferty, ICML2003)

- harmonic function f is the voltage at the nodes
  - edges are resistors with $R = 1/W$
  - 1 volt battery connects to labeled nodes
- indirect similarity: similar voltage if many paths exist



A random walk interpretation of harmonic functions

- harmonic function $f_i = P(\text{hit label 1} \mid \text{start from } i)$
  - random walk from node i to j with probability P_{ij}
  - stop if we hit a labeled node
- indirect similarity: random walks have similar destinations



Closed form solution for the harmonic function

- define diagonal degree matrix D, $D_{ii} = \sum W_{i\cdot}$
  define graph *Laplacian* matrix $\Delta = D - W$

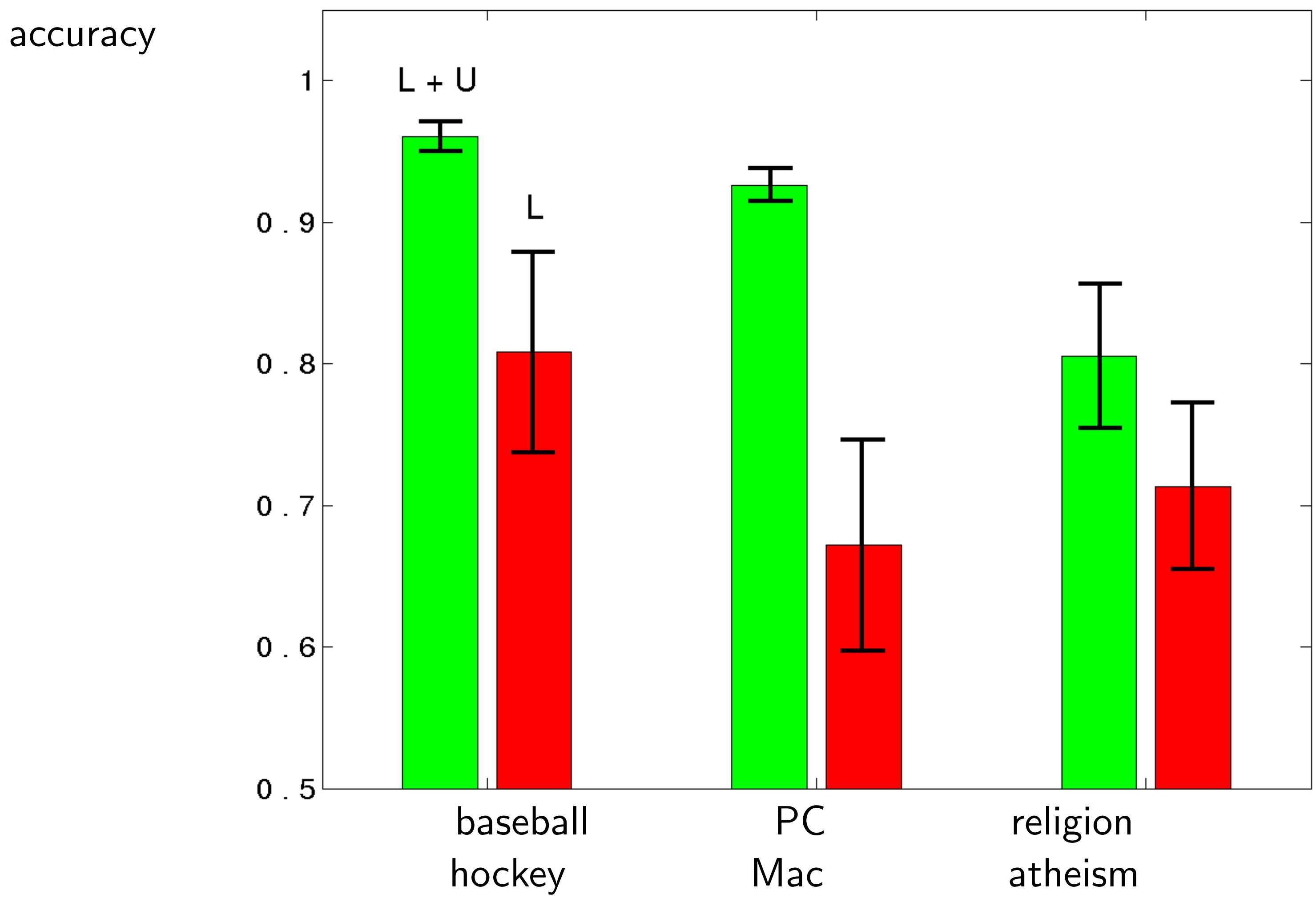
$$\boxed{f_u = -\Delta_{uu}{}^{-1} \Delta_{ul} Y_l}$$

- Δ graph version of the continuous Laplacian operator
  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$
- harmonic: $\Delta f = 0$ with Dirichlet boundary conditions on labeled data

Properties of the harmonic function

- currents in-flow $=$ out-flow at any node (Kirchoff's law)
- min energy $E(f) = \sum_{i \sim j} W_{ij}(f_i - f_j)^2 = f^\top \Delta f$
- average of neighbors: $f_u(i) = \frac{\sum_{j \sim i} W_{ij} f(j)}{\sum_{j \sim i} W_{ij}}$
- uniquely exists
- $0 \leq f \leq 1$

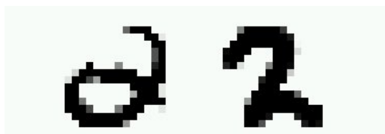
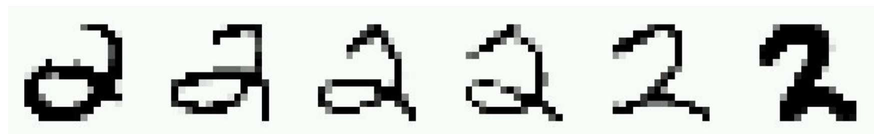
Text categorization with harmonic functions



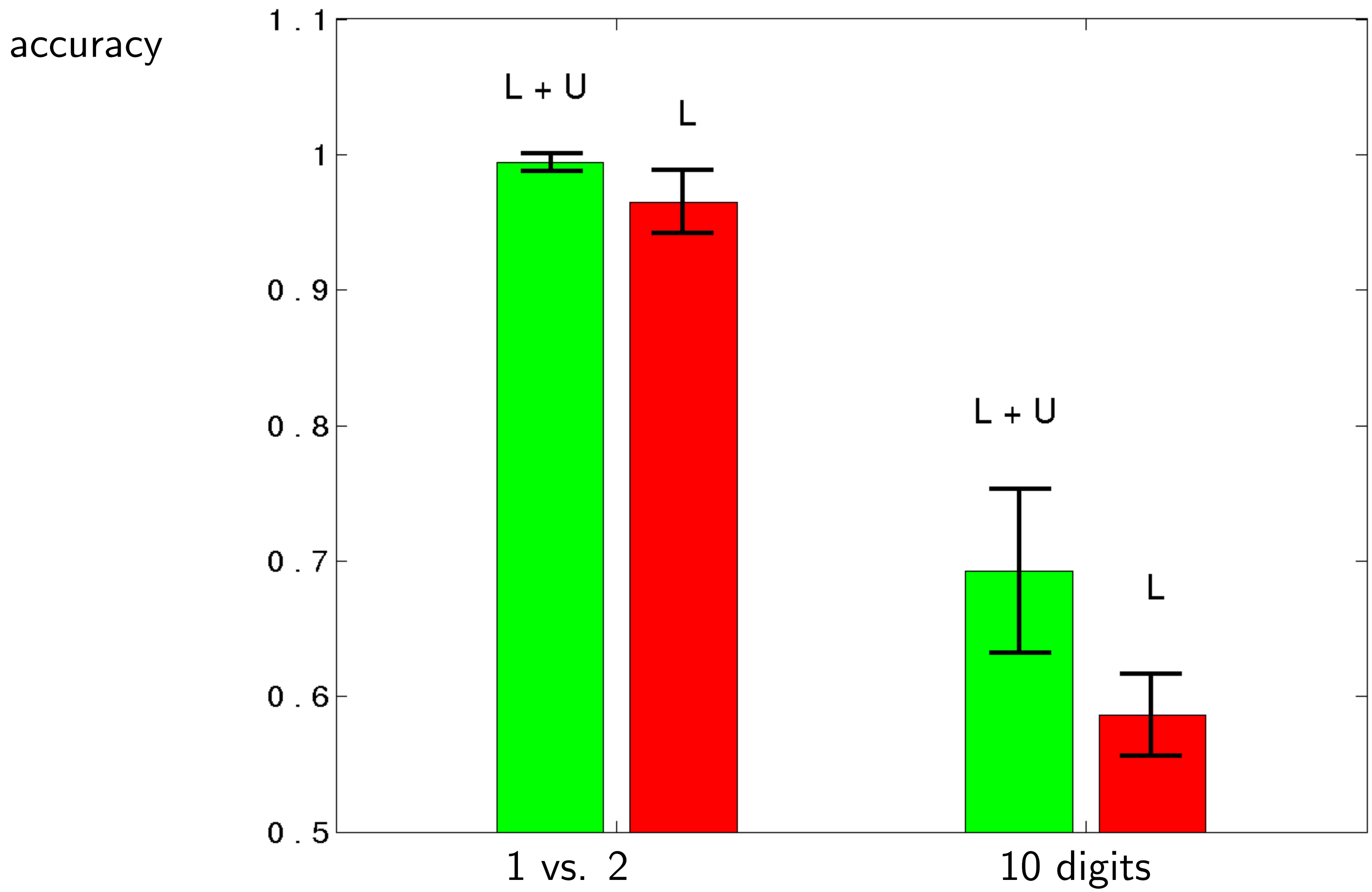
50 labeled articles, about 2000 unlabeled articles. 10NN graph.

Digit recognition with harmonic functions

- pixel-wise Euclidean distance

	
not similar	indirectly similar with stepping stones

Digit recognition with harmonic functions



50 labeled images, about 4000 unlabeled images, 10NN graph

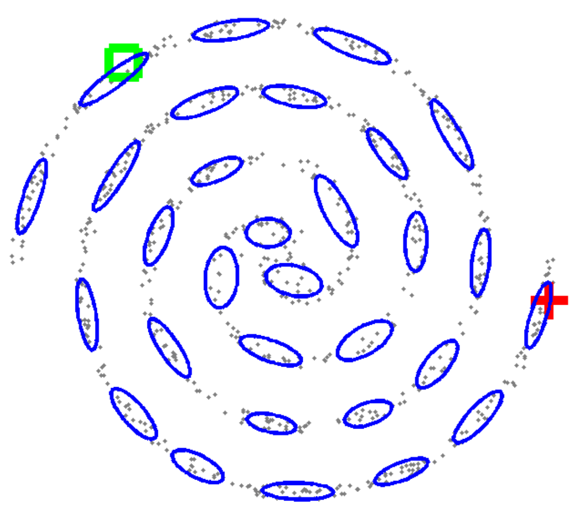
Practical concerns about harmonic functions

- does it scale?
  - closed form involves matrix inversion $f_u = -\Delta_{uu}{}^{-1} \Delta_{ul} Y_l$
  - $O(u^3)$, e.g. millions of crawled web pages
- solution 1: use iterative methods
  - the label propagation algorithm (slow)
  - loopy belief propagation
  - conjugate gradient
- solution 2: reduce problem size
  - use a random small unlabeled subset *(Delalleau et al. 2005)*
  - *harmonic mixtures*
- can it handle new points (induction)?

Harmonic mixtures

(Zhu and Lafferty, 2005)

- fit unlabeled data with a mixture model, e.g.
  - Gaussian mixtures for images
  - multinomial mixtures for documents

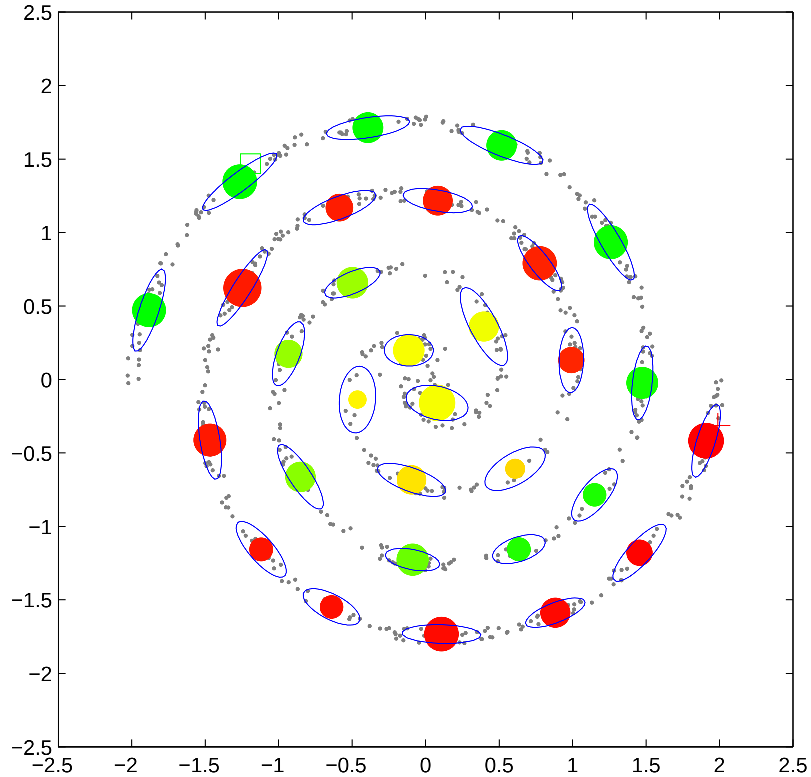


- use EM or other methods
- M mixture components, here $M = 30 \ll u \approx 1000$
- learn soft labels for the *mixture components*, not the unlabeled points

Harmonic mixtures
learn labels for mixture components

- assume mixture component labels $\lambda_1, \cdots, \lambda_M$
- labels on unlabeled points determined by the mixture model
  - The mixture model defines *responsibility* R: $R_{im} = p(m|x_i)$
  - $f(i) = \sum_{m=1}^{M} R_{im}\lambda_m$
- learn λ such that f is closest to harmonic
  - minimize energy $E(f) = f^\top \Delta f$
  - convex optimization
  - closed form solution $\lambda = -\left(R^\top \Delta_{uu} R\right)^{-1} R^\top \Delta_{ul} Y_l$

Harmonic mixtures



mixture component labels λ follow the graph

Harmonic mixtures computational savings

- computation on unlabeled data
  - harmonic mixtures

$$f_u = -R(\underbrace{R^\top \Delta_{uu} R}_{M \times M})^{-1} R^\top \Delta_{ul} Y_l$$

  - original harmonic function

$$f_u = -(\underbrace{\Delta_{uu}}_{u \times u})^{-1} \Delta_{ul} Y_l$$

- harmonic mixtures $O(M^3)$, much cheaper than $O(u^3)$

> Harmonic mixtures can handle large problems.
> Also induction $f(x) = \sum_{m=1}^{M} R_{xm} \lambda_m$

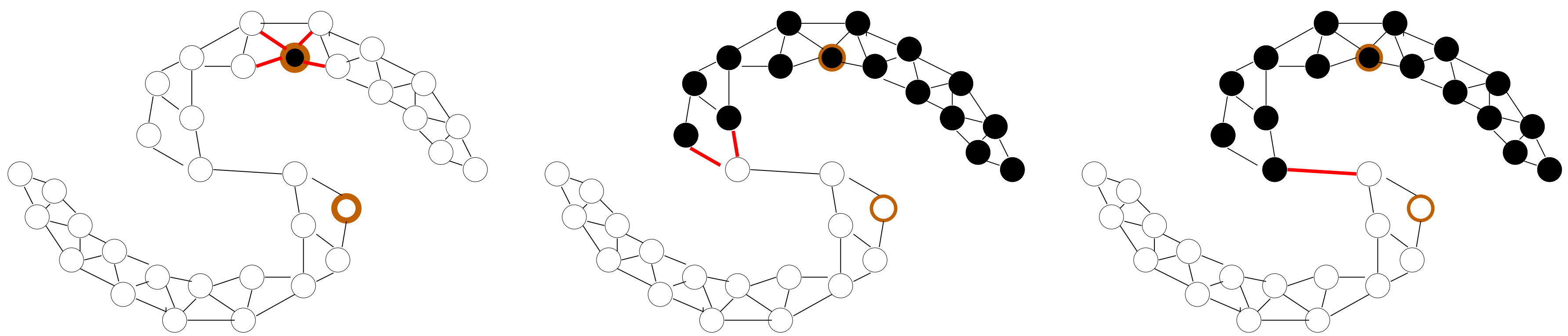
From harmonic functions to kernels

- harmonic functions too specialized?
- I will show you the *kernel* behind harmonic function
  - general, important concept in machine learning.
  - used in many learning algorithms, e.g. support vector machines
  - on the graph: symmetric, positive semi-definite $n \times n$ matrix
- I will then give you an even better kernel.

but first a short detour . . .

The probabilistic model behind harmonic function

- random field $p(f) \propto \exp\left(-E(f)\right)$
- energy $E(f) = \sum_{i \sim j} W_{ij}(f_i - f_j)^2 = f^\top \Delta f$
- low energy $=$ good label propagation



$E(f) = 4$ $E(f) = 2$ $E(f) = 1$

- if $f \in \{0, 1\}$ discrete, standard Markov random fields (Boltzmann machines), inference hard

The probabilistic model behind harmonic function Gaussian random fields

(Zhu, Ghahramani and Lafferty, ICML2003)

- continuous relaxation $f \in \mathbb{R} \Rightarrow$ Gaussian random field
- Gaussian random field $p(f)$ is a n-dimensional Gaussian with inverse covariance matrix Δ.

$$p(f) \quad \propto \quad \exp\left(-E(f)\right) = \exp\left(-f^\top \Delta f\right)$$

- *harmonic functions are the mean of Gaussian random fields*
- Gaussian random fields $=$ Gaussian processes on finite data
- covariance matrix $=$ kernel matrix in Gaussian processes

The kernel behind harmonic functions

$$K = \Delta^{-1}$$

- K_{ij} = indirect similarity
  - The direct similarity W_{ij} may be small
  - But K_{ij} will be large if many paths between i, j
- K can be used with many kernel machines
  - K + support vector machine = semi-supervised SVM
  - kernel built on both labeled and unlabeled data
  - additional benefit: handles noisy labeled data

Kernels should encourage smooth eigenvectors

- graph spectrum $\Delta = \sum_{k=1}^{n} \lambda_k \phi_k \phi_k^\top$
- small eigenvalue, smooth eigenvector
  $\sum_{i \sim j} W_{ij} (\phi_k(i) - \phi_k(j))^2 = \lambda_k$
- kernels *encourage* smooth eigenvectors with large weights

$$\begin{array}{rr} \text{Laplacian} & \Delta = \sum_k \lambda_k \phi_k \phi_k^\top \\ \text{harmonic kernel} & K = \Delta^{-1} = \sum_k \frac{1}{\lambda_k} \phi_k \phi_k^\top \end{array}$$

- smooth functions good for semi-supervised learning

$$||f||_K = f^\top K^{-1} f = f^\top \Delta f = \sum_{i \sim j} W_{ij} (f_i - f_j)^2$$

General semi-supervised kernels

- Δ^{-1} not the only semi-supervised kernel, may not be the best
- General principle for creating semi-supervised kernels

$$K = \sum_i r(\lambda_i) \phi_i \phi_i^\top$$

- $r(\lambda)$ should be large when λ is small, to encourage smooth eigenvectors.
- Specific choices of $r()$ lead to known kernels
  - harmonic function kernel $r(\lambda) = 1/\lambda$
  - diffusion kernel $r(\lambda) = \exp(-\sigma^2 \lambda)$
  - random walk kernel $r(\lambda) = (\alpha - \lambda)^p$
- *Is there a best $r()$?* Yes, as measured by kernel alignment.

Alignment measures kernel quality

- measures kernel by its alignment to the labeled data Y_l

$$\text{align}(K, Y_l) = \frac{\langle K_{ll}, Y_l {Y_l}^\top \rangle}{\| K_{ll} \| \cdot \| Y_l {Y_l}^\top \|}$$

- extension of cosine angle between vectors
- high alignment related to good generalization performance
- leads to a convex optimization problem

Finding the best kernel

(Zhu, Kandola, Ghahramani and Lafferty, NIPS2004)

- the *order constrained* semi-supervised kernel

$$\begin{array}{rc} \max_{r} & \text{align}(K, Y_l) \\ \text{subject to} & K = \sum_i r_i \phi_i \phi_i^\top \\ & r_1 \geq \cdots \geq r_n \geq 0 \end{array}$$

- order constraints $r_1 \geq \cdots \geq r_n$ encourage smoothness
- convex optimization
- r nonparametric

The order constrained kernel improves alignment and accuracy

text categorization (religion vs. atheism), 50 labeled and 2000 unlabeled articles.

- alignment

kernel	order	harmonic	RBF
alignment	*0.31*	0.17	0.04

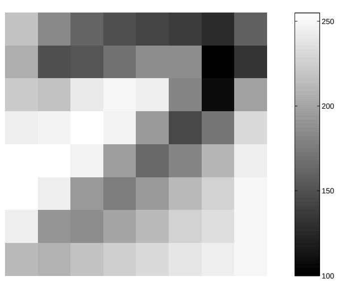
- accuracy with support vector machines

kernel	order	harmonic	RBF
accuracy	*84.5*	80.4	69.3

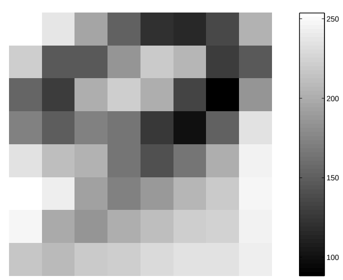
We now have good kernels for semi-supervised learning.

Other research (1)
Graph hyperparameter learning

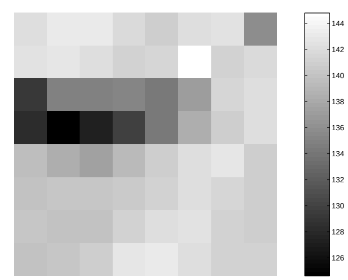
- what if we don't know W_{ij}?
- set up hyperparameters $W_{ij} = \exp\left(-\sum_d \frac{(x_{id}-x_{jd})^2}{\alpha_d}\right)$
- learn α with e.g. Bayesian evidence maximization



average 7



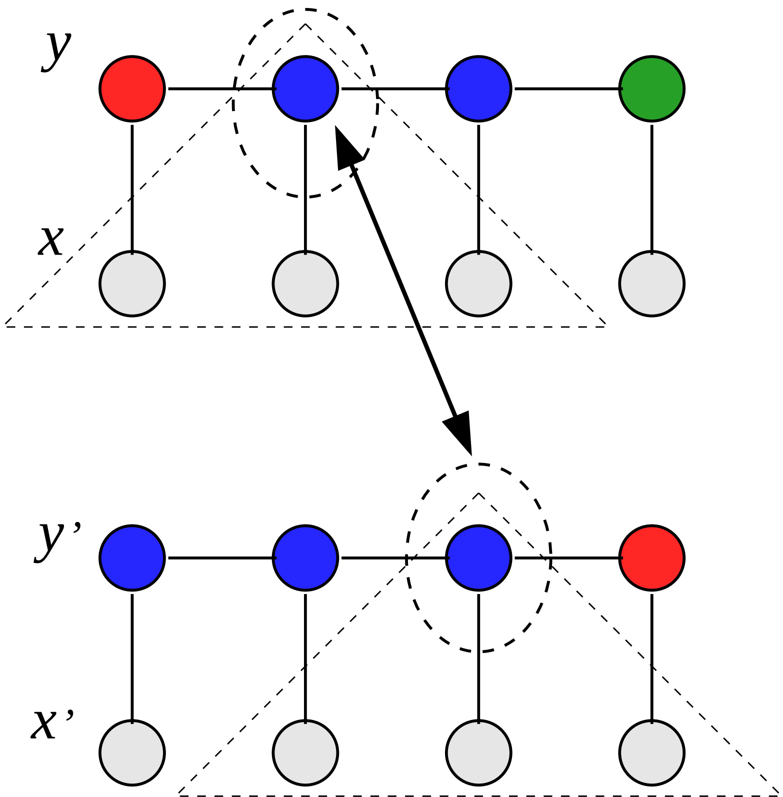
average 9



learned α

Other research (2)
Sequences and other structured data

(Lafferty, Zhu and Liu, 2004)

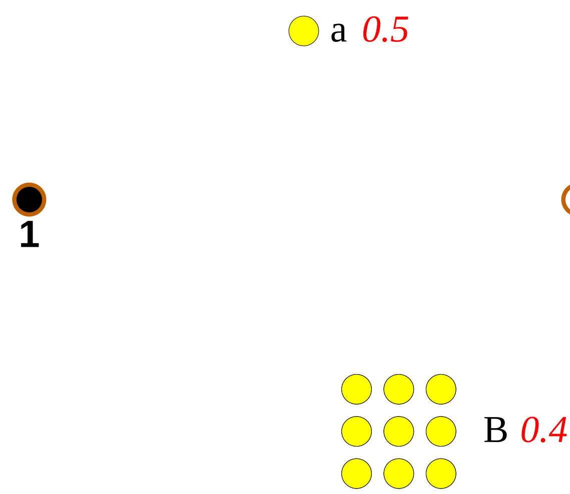


- what if $x_1 \cdots x_n$ form sequences? speech, natural language processing, biosequence analysis, etc.
- conditional random fields (CRF)
- kernel CRF
- kernel CRF $+$ semi-supervised kernels

Other research (3)
Active learning

(Zhu, Lafferty and Ghahramani, 2003b)

- what if the computer can ask for labels?
- smart queries: not necessarily the most ambiguous points



- active learning + semi-supervised learning, fast algorithm

Related work in semi-supervised learning

based on different assumptions

method	assumptions	references
graph	similar feature, same label	this talk
	mincuts	(Blum and Chawla, 2001)
	normalized Laplacian	(Zhou et al., 2003)
	regularization	(Belkin et al., 2004)
mixture model, EM	generative model	(Nigam et al., 2000)
transductive SVM	low density separation	(Joachims, 1999)
co-training	feature split	(Blum and Mitchell, 1998)

Semi-supervised learning has so far received relatively little attention in statistics literature.

Some key contributions

- harmonic function formulations for semi-supervised learning
- solving large scale problems with harmonic mixtures
- semi-supervised kernels by spectral transformation of the graph Laplacian
- kernelizing conditional random fields
- combining active learning and semi-supervised learning

Summary

Unlabeled data can improve classification.

The methods have reached the stage where we can apply them to real-world tasks.

Future Plans

- continue the research on semi-supervised learning
  - structured data, ranking, clustering, explore different assumptions
- application to human language tasks
  - speech recognition, document categorization, information retrieval, sentiment analysis
- explore novel machine learning approaches
  - text mixed with other modalities, e.g. images; speech and multimodal user interfaces; graphics; vision
- collaboration

Thank You

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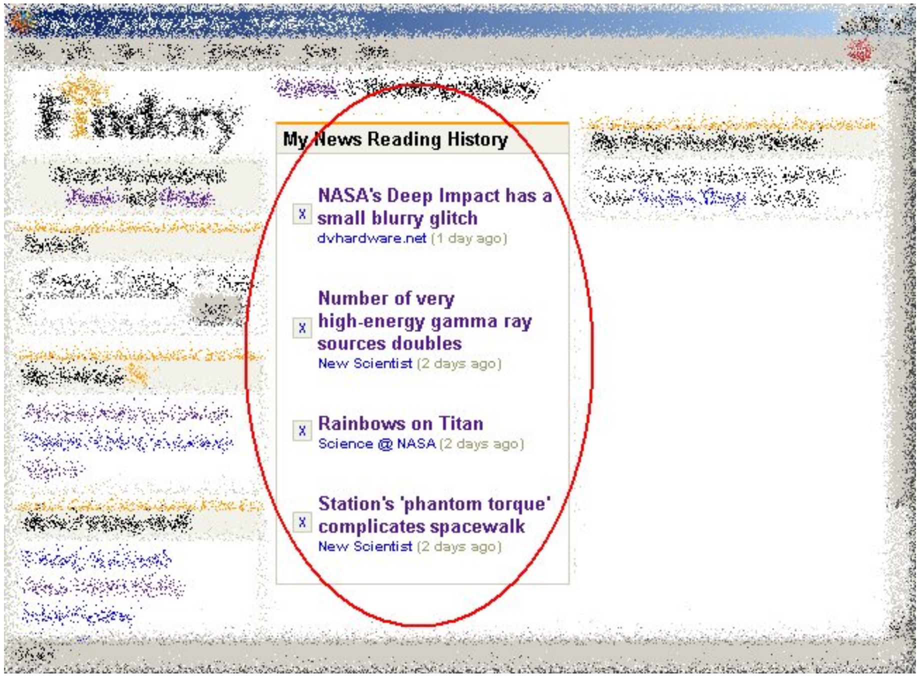
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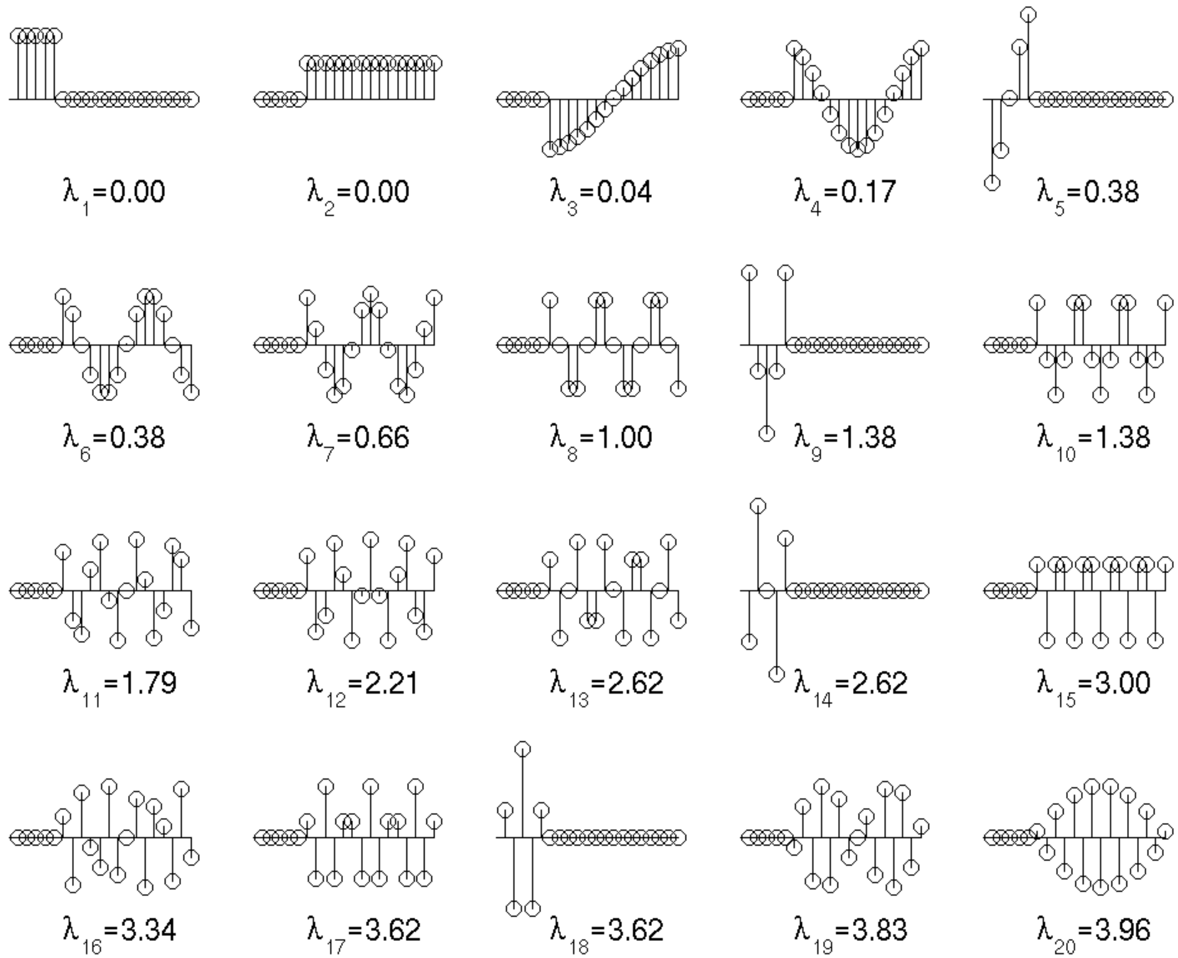
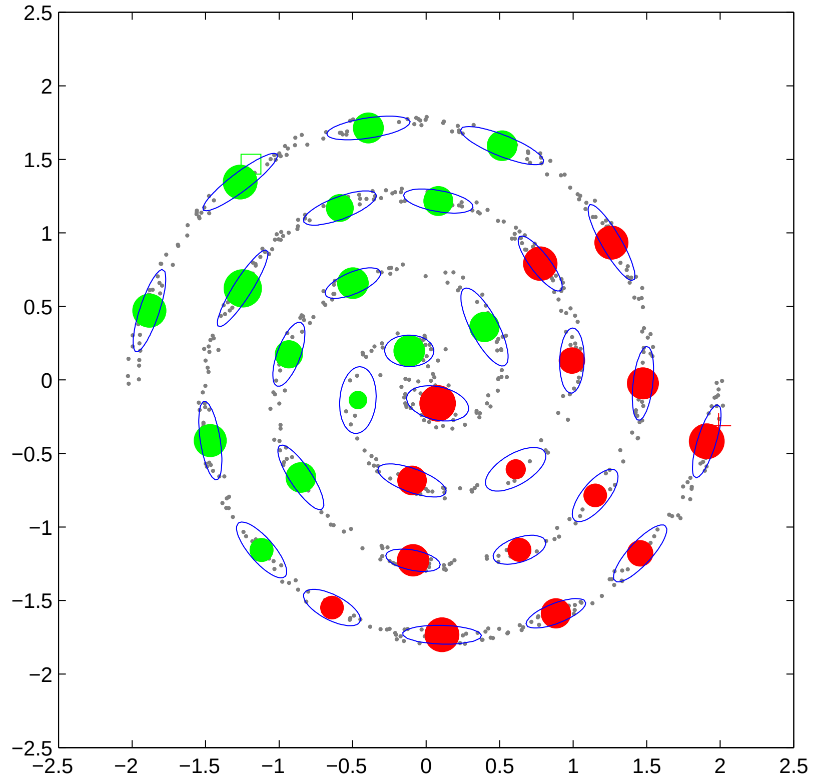
Graph spectrum $\Delta = \sum_{i=1}^{n} \lambda_i \phi_i \phi_i^\top$



Learning component label with EM



Labels for the components do not follow the graph.

(Nigam et al., 2000)

Other research (2)
Sequences and other structured data

- KCRF: $p_f(\mathbf{y}|\mathbf{x}) = Z^{-1}(\mathbf{x}, f) \exp\left(\sum_c f(\mathbf{x}, \mathbf{y}_c)\right)$
- f induces regularized negative log loss on training data

$$R(f) = \sum_{i=1}^{l} - \log p_f(\mathbf{y}^{(i)}|\mathbf{x}^{(i)}) + \Omega(\| f \|_K)$$

- representer theorem for KCRFs: loss minimizer

$$f^\star(\mathbf{x}, \mathbf{y}_c) = \sum_{i=1}^{l} \sum_{c'} \sum_{\mathbf{y}'_{c'}} \alpha(i, \mathbf{y}'_{c'}) K((\mathbf{x}^{(i)}, \mathbf{y}'_{c'}), (\mathbf{x}, \mathbf{y}_c))$$

Other research (2)
Sequences and other structured data

- learn α to minimize $R(f)$, convex, sparse training
- special case $K((\mathbf{x}^{(i)}, \mathbf{y}'_{c'}), (\mathbf{x}, \mathbf{y}_c)) = \psi(K'(\mathbf{x}^{(i)}_{c'}, \mathbf{x}_c), \mathbf{y}'_{c'}, \mathbf{y}_c)$
- K' can be a semi-supervised kernel.

Other research (3)
Active Learning

- generalization error

$$\text{err} = \sum_{i \in U} \sum_{y_i = 0,1} (\text{sgn}(f_i) \neq y_i) \, P_{\text{true}}(y_i)$$

- approximation 1

$$P_{\text{true}}(y_i = 1) \leftarrow f_i$$

- estimated error

$$\widehat{\text{err}} = \sum_{i \in U} \min\left(f_i, 1 - f_i\right)$$

Other research (3)
Active Learning

- estimated error *after querying k with answer y_k*

$$\widehat{\text{err}}^{+(x_k,y_k)} = \sum_{i \in U} \min\left(f_i^{+(x_k,y_k)}, 1 - f_i^{+(x_k,y_k)}\right)$$

- approximation 2

$$\widehat{\text{err}}^{+x_k} = (1 - f_k)\widehat{\text{err}}^{+(x_k,0)} + f_k \widehat{\text{err}}^{+(x_k,1)}$$

- select query k^* to minimize the estimated error

$$k^* = \arg\min_k \widehat{\text{err}}^{+x_k}$$

Other research (3)
Active Learning

- 're-train' is fast with semi-supervised learning

$$f_u^{+(x_k,y_k)} = f_u + (y_k - f_k)\frac{(\Delta_{uu})^{-1}_{\cdot k}}{(\Delta_{uu})^{-1}_{kk}}$$