Online Similarity Prediction of Networked Data from Known and Unknown Graphs

Claudio Gentile, Mark Herbster, Stephen Pasteris

Universita' dell'Insubria, University College London

13 June 2013

通 と イ ヨ と イ ヨ と

What is Learning?

Supervised Learning

Given data S = {(x₁, y₁), ..., (x_l, y_l)}, infer a function f such that f(x_i) ≈ y_i for all possible instances x_i.

Unsupervised Learning

- Given data $S = \{x_1, ..., x_l\}$, model the data. e.g:
 - Fit a probability distribution to the space of all possible instances.
 - Map the instances to a low dimensional manifold in the instance space, such that the mapped instance is close to the original instance.

Semi-Supervised Learning

• Given data $S = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_l, y_l), \mathbf{x}_{l+1}, ..., \mathbf{x}_n\}$, infer a function f such that $f(x_i) \approx y_i$ for all possible instances \mathbf{x}_i . Utilises both supervised and unsupervised methods.

Batch Learning

 \bullet Learner is given the data set ${\mathcal S}$ and then performs the learning task

Online Learning

- We are given an initial data set \mathcal{S} .
- Learning proceeds in rounds. On each round:
 - Learner is queried (with some instance).
 - 2 Correct answer is given, which updates the data set S.

・ロト ・御ト ・モト ・モト

In this paper we focus on online, semi-supervised learning.

Model

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.
- Aim: Minimize mistakes

Classification			
Instance:			
Prediction:			
Outcome:			
Mistakes:			

Model

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.
- Aim: Minimize mistakes

Classification			
Instance:	×		
Prediction:			
Outcome:			
Mistakes:			

Model

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.
- Aim: Minimize mistakes

Classification			
Instance:			
Prediction:	Bart		
Outcome:			
Mistakes:			

Model

On each round:

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.

Classification			
Instance:			
Prediction:	Bart		
Outcome:	Bart		
Mistakes:			

Model

On each round:

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.

Classification			
Instance:			
Prediction:	Bart		
Outcome:	Bart		
Mistakes:	0		

Model

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.
- Aim: Minimize mistakes

Classification				
Instance:		2		
Prediction:	Bart			
Outcome:	Bart			
Mistakes:	0			

Model

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.
- Aim: Minimize mistakes

Classification				
Instance:		2		
Prediction:	Bart	Bart		
Outcome:	Bart			
Mistakes:	0			

Model

On each round:

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.

Classification				
Instance:				
Prediction:	Bart	Bart		
Outcome:	Bart	Lisa		
Mistakes:	0			

Model

On each round:

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.

Classification				
Instance:				
Prediction:	Bart	Bart		
Outcome:	Bart	Lisa		
Mistakes:	0	1		

Model

On each round:

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.

Classification				
Instance:			*	
Prediction:	Bart	Bart		
Outcome:	Bart	Lisa		
Mistakes:	0	1		

Model

On each round:

- Nature presents an instance.
- Learner predicts the class.
- Nature reveals the class.

Classification					
Instance:	×	2	*		
Prediction:	Bart	Bart	Lisa	Maggie	Maggie
Outcome:	Bart	Lisa	Lisa	Maggie	Bart
Mistakes:	0	1	1	1	2

We have a labelled line graph with n vertices:

Suppose a priori:

- We know no labels
- We know that the cutsize is at most 1.

Let \mathcal{H} be the set of all 2n consistent classifiers:













◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへで





Prediction: Majority vote amongst classifiers in \mathcal{H} : Red or Blue Update: Remove inconsistent classifiers from \mathcal{H} .





































◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへで

• $|\mathcal{H}|$ is initially 2*n*.

.

- When a mistake is made at least half the classifiers are removed from \mathcal{H} .
- \bullet The correct classifier is never removed from ${\cal H}$ so we always have $|{\cal H}|\geq 1$

◆□▶ ◆□▶ ◆注▶ ◆注▶ 注 のへで

Hence: No more than $\log_2(2n)$ mistakes made.

Model

On each round:

- Nature presents an instance pair.
- Learner predicts similarity of pair.
- Nature reveals similarity.

Similiarity			
Instance:			
Prediction:			
Outcome:			
Mistakes:			

Model

On each round:

- Nature presents an instance pair.
- Learner predicts similarity of pair.
- Nature reveals similarity.

Similiarity			
Instance:	*		
Prediction:			
Outcome:			
Mistakes:			

Model

On each round:

- Nature presents an instance pair.
- Learner predicts similarity of pair.
- Nature reveals similarity.

Similiarity			
Instance:	*		
Prediction:	Similar		
Outcome:			
Mistakes:			

Model

On each round:

- Nature presents an instance pair.
- Learner predicts similarity of pair.
- Nature reveals similarity.

Similiarity			
Instance:	*		
Prediction:	Similar		
Outcome:	Similar		
Mistakes:			

Model

On each round:

- Nature presents an instance pair.
- Learner predicts similarity of pair.
- Nature reveals similarity.

Similiarity			
Instance:	*		
Prediction:	Similar		
Outcome:	Similar		
Mistakes:	0		
Similarity

Model

On each round:

- Nature presents an instance pair.
- Learner predicts similarity of pair.
- Nature reveals similarity.

Aim: Minimize mistakes

Similiarity			
Instance:	*		
Prediction:	Similar		
Outcome:	Similar		
Mistakes:	0		

Similarity

Model

On each round:

- Nature presents an instance pair.
- Learner predicts similarity of pair.
- Nature reveals similarity.

Aim: Minimize mistakes

Similiarity								
Instance:	*		Ř	2				
Prediction:	similar	disim.	disim.	similar	similar			
Outcome:	similar	disim.	similar	similar	disim.			
Mistakes:	0	0	1	1	2			

Connection Between Classification and Similarity

Notation

- A **concept** *y* is a mapping from instances into *K*-classes.
- $\mathbb{B}_A(y)$ the maximal mistakes by algorithm A wrt concept y.

Theorem

Given classification algorithm C there exists similarity algorithm S such that for any concept y:

$\mathbb{B}_{\mathcal{S}}(y) \leq 5 \mathbb{B}_{\mathcal{C}}(y) \log_2 K$

Given similarity algorithm S there exists classification algorithm C such that for any concept y:

 $\mathbb{B}_{\mathcal{C}}(y) \leq \mathbb{B}_{\mathcal{S}}(y) + K$

Construction requires exponential-time!

◆□▶ ◆舂▶ ★逹▶ ★逹▶ ─ 臣 ─

Ingredients (basic)

- Linear classifiers via "metric"-learning kernel [XNJR02,SSN04]
- Online algs: Matrix Perceptron and Matrix Winnow [W07]

Ingredients (fancy) :

Aim: optimal mistake bounds or poly-log-time predictions

- Prediction on a graph framework [CGVZ10,HLP09]
- ② Expected mistake bound with random spanning trees
- Inearization with path graph embedding
- 8 Reduced diameter and fast prediction with binary support tree

Results: Matrix winnow (optimality) Matrix perceptron (speed)

Similarity prediction on a graph

- The graph is labeled by $y : \text{vertices} \rightarrow \{\bullet, \bullet, \bullet\}$
- Instances are pairs of vertices, for example (v, w)



 $\begin{aligned} & \Phi(y) = 3 & (\text{cut}) \\ & R(v, w) = 2 & (\text{eff. resistance}) \\ & \varphi_r(y) = 2\frac{1}{2} & (\text{eff. resistance-weighted cut}) \end{aligned}$



- We have a finite dimensional inner product space \mathcal{V} .
- Instances are vectors in \mathcal{V} .
- There exists a hyperplane $\mathcal H$ which classifies instances.

(日) (四) (문) (문) (문)

• Goal: Learn H.



- \bullet Predict according to ${\cal H}$
- \bullet If mistake is made then ${\cal H}$ is updated according to the new instance.

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへで



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへで



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.



- \bullet Predict according to ${\cal H}$
- $\bullet\,$ If mistake is made then ${\cal H}$ is updated according to the new instance.

Similarity prediction via linear classification

Inner-Product Space

 \mathcal{V} is the space of $n \times n$ matrices with:

$$\langle A, B \rangle := \mathsf{Trace}(A^{\mathsf{T}}B)$$

(1)

<ロト <四ト <注入 <注下 <注下 <

Encoding

A pair of vertices (v, w) is encoded as the matrix:

$$\sqrt{L^+}(e_v-e_w)(e_v-e_w)^T\sqrt{L^+}$$

Graph Laplacian: L; Basis vector: e_v

Similarity prediction via linear classification





 $M_P \leq \mathcal{O}([\Phi(y)R^G]^2)$ (Perceptron)

Resistance diameter: R^G ; Number of vertices: n

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへで

Construct: Random BST

- **O** Bounds ito resistance-weighted cut-size $[\mathbb{E}[\Phi^{G'}(y)] = \varphi_r^G(y)]$
- 2 Intermediate step $[\Phi^{G''}(y) \le 2\Phi^{G'}(y)]$
- Enables polylog time $[\Phi^{G''}(y) \le (\log n)\Phi^{G''}(y); R^{G''} = \log n]$



Construct: Random BST

- **9** Bounds ito resistance-weighted cut-size $[\mathbb{E}[\Phi^{G'}(y)] = \varphi_r^G(y)]$
- 2 Intermediate step $[\Phi^{G''}(y) \le 2\Phi^{G'}(y)]$
- Enables polylog time [\$\Phi^{G'''}(y) \le (log n)\$\Phi^{G'''}(y)\$; \$R^{G'''} = log n\$]
 Hence \$\mathbb{E}[\$\Phi^{G'''}(y)\$] \$\le 2\$\varphi_r\$^G(y)\$ log n\$



Construct: Random BST

- **9** Bounds ito resistance-weighted cut-size $[\mathbb{E}[\Phi^{G'}(y)] = \varphi_r^G(y)]$
- 2 Intermediate step $[\Phi^{G''}(y) \le 2\Phi^{G'}(y)]$
- Solution Enables polylog time $[\Phi^{G'''}(y) \le (\log n)\Phi^{G''}(y); R^{G'''} = \log n]$

• Hence $\mathbb{E}[\Phi^{G'''}(y)] \leq 2 \varphi_r^{-G}(y) \log r$



Construct: Random BST

- **9** Bounds ito resistance-weighted cut-size $[\mathbb{E}[\Phi^{G'}(y)] = \varphi_r^G(y)]$
- 2 Intermediate step $[\Phi^{G''}(y) \le 2\Phi^{G'}(y)]$
- So Enables polylog time $[\Phi^{G'''}(y) \le (\log n)\Phi^{G''}(y); R^{G'''} = \log n]$
- Hence $\mathbb{E}[\Phi^{G'''}(y)] \leq 2\varphi_r^G(y)\log n$



An optimal algorithm (Matrix Winnow + random BST)

Theorem

The mistakes of Winnow + random BST is bounded above $\forall y$:

 $\mathbb{E}[M] \leq \mathcal{O}(\varphi_r(\mathbf{y})\log^3(n))$

Direct implementation requires $\mathcal{O}(n^3)$ time per round.

◆□▶ ◆□▶ ◆注▶ ◆注▶ 注 のへで

Theorem

The mistakes of Perceptron + random BST is bounded $\forall y$ by

 $\mathbb{E}[M] \leq \mathcal{O}\left(\varphi_r(\mathbf{y})^2 \log^4(n)\right)$

There exists an $O(\log^2 n)$ time per round implementation

• An exponentially faster per-round prediction •

◆□▶ ◆□▶ ◆注▶ ◆注▶ 注 のへで

- **Receive:** vertex instance pair (v, w)
- Compute \mathcal{P} path from v to w (blue fill)
- **Predict:** $\hat{y} = \mathcal{I}[\sum_{i,j\in\mathcal{P}} F_{ij} > 4\log^2 n]$
- **Receive:** "similarity" label y_t ('0' is similar/'1' is dissimilar)
- Compute f (circled numbers)
- Determine S (bolded circles)
- Extend f to S
- Update: $\forall i, j \in S, F_{ij} \leftarrow F_{ij} + (2y_t 1)(f_i f_j)^2$



- **Receive:** vertex instance pair (*v*, *w*)
- Compute \mathcal{P} path from v to w (blue fill)
- **Predict:** $\hat{y} = \mathcal{I}[\sum_{i,j\in\mathcal{P}} F_{ij} > 4\log^2 n]$
- **Receive:** "similarity" label y_t ('0' is similar/'1' is dissimilar)
- Compute *f* (circled numbers)
- Determine *S* (bolded circles)
- Extend f to S
- Update: $\forall i, j \in S, F_{ij} \leftarrow F_{ij} + (2y_t 1)(f_i f_j)^2$



- Receive: vertex instance pair (v, w)
- Compute \mathcal{P} path from v to w (blue fill)

• **Predict:**
$$\hat{y} = \mathcal{I}[\sum_{i,j\in\mathcal{P}} F_{ij} > 4\log^2 n]$$

- **Receive:** "similarity" label y_t ('0' is similar/'1' is dissimilar)
- Compute f (circled numbers)
- Determine *S* (bolded circles)
- Extend f to S
- Update: $\forall i, j \in S, F_{ij} \leftarrow F_{ij} + (2y_t 1)(f_i f_j)^2$



- **Receive:** vertex instance pair (*v*, *w*)
- Compute \mathcal{P} path from v to w (blue fill)
- **Predict:** $\hat{y} = \mathcal{I}[\sum_{i,j\in\mathcal{P}} F_{ij} > 4\log^2 n]$
- **Receive:** "similarity" label y_t ('0' is similar/'1' is dissimilar)
- Compute f (circled numbers)
- Determine S (bolded circles)
- Extend f to S
- Update: $\forall i, j \in S, F_{ij} \leftarrow F_{ij} + (2y_t 1)(f_i f_j)^2$



- **Receive:** vertex instance pair (v, w)
- Compute \mathcal{P} path from v to w (blue fill)
- **Predict:** $\hat{y} = \mathcal{I}[\sum_{i,j\in\mathcal{P}} F_{ij} > 4\log^2 n]$
- **Receive:** "similarity" label y_t ('0' is similar/'1' is dissimilar)
- Compute f (circled numbers)
- Determine *S* (bolded circles)
- Extend f to S
- Update: $\forall i, j \in S, F_{ij} \leftarrow F_{ij} + (2y_t 1)(f_i f_j)^2$



- **Receive:** vertex instance pair (v, w)
- Compute \mathcal{P} path from v to w (blue fill)
- **Predict:** $\hat{y} = \mathcal{I}[\sum_{i,j\in\mathcal{P}} F_{ij} > 4\log^2 n]$
- **Receive:** "similarity" label y_t ('0' is similar/'1' is dissimilar)
- Compute f (circled numbers)
- Determine S (bolded circles)
- Extend f to a
- Update: $\forall i, j \in S, F_{ij} \leftarrow F_{ij} + (2y_t 1)(f_i f_j)^2$



- **Receive:** vertex instance pair (v, w)
- Compute \mathcal{P} path from v to w (blue fill)
- Predict: $\hat{y} = \mathcal{I}[\sum_{i,j\in\mathcal{P}} F_{ij} > 4\log^2 n]$
- **Receive:** "similarity" label y_t ('0' is similar/'1' is dissimilar)
- Compute f (circled numbers)
- Determine S (bolded circles)
- Extend f to S
- Update: $\forall i, j \in S, F_{ij} \leftarrow F_{ij} + (2y_t 1)(f_i f_j)^2$



- **Receive:** vertex instance pair (v, w)
- Compute \mathcal{P} path from v to w (blue fill)
- Predict: $\hat{y} = \mathcal{I}[\sum_{i,j\in\mathcal{P}} F_{ij} > 4\log^2 n]$
- **Receive:** "similarity" label y_t ('0' is similar/'1' is dissimilar)
- Compute f (circled numbers)
- Determine S (bolded circles)
- Extend f to $\mathcal S$
- Update: $\forall i, j \in S, F_{ij} \leftarrow F_{ij} + (2y_t 1)(f_i f_j)^2$



What if the graph is unknown?

◆□▶ ◆□▶ ◆三▶ ◆三▶ ○○ のへで
Unknown graph

Model: progressive graph disclosure

- Nature presents a vertex pair & a path connecting the vertices
- Learner predicts similarity of pair.
- Nature reveals similarity.

Algorithm sketch



Theorem

There exists a p-norm perceptron-based algorithm such that $M < O(\Phi(\gamma)^4 \log(n))$

Unknown graph

Model: progressive graph disclosure

- Nature presents a vertex pair & a path connecting the vertices
- Learner predicts similarity of pair.
- Nature reveals similarity.

Algorithm sketch



Theorem

There exists a p-norm perceptron-based algorithm such that $M < O(\Phi(\gamma)^4 \log(n))$

Unknown graph

Model: progressive graph disclosure

- Nature presents a vertex pair & a path connecting the vertices
- Learner predicts similarity of pair.
- Nature reveals similarity.

Algorithm sketch



Theorem

There exists a p-norm perceptron-based algorithm such that $M < O(\Phi(\gamma)^4 \log(n))$

• Established an equivalence between classification and similarity

- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- Established an equivalence between classification and similarity
- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- Established an equivalence between classification and similarity
- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- Established an equivalence between classification and similarity
- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- Established an equivalence between classification and similarity
- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- Established an equivalence between classification and similarity
- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- Established an equivalence between classification and similarity
- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- Established an equivalence between classification and similarity
- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- Established an equivalence between classification and similarity
- Modeled as a graph labeling problem
- Designed a randomized BST graph-approximation
- Optimal to log-factors prediction with Matrix Winnow
- Fast poly-log-time prediction with the Matrix Perceptron
- Introduced a novel "unknown" graph framework

- Weaken assumption: $sim(a, b) \& sim(b, c) \Longrightarrow sim(a, c)$
- Structurally richer graph approximations with fast algorithms
- Tight lower and upper bounds in the unknown graph setting

- [CGVZ10] N. Cesa-Bianchi, C Gentile, F. Vitale, and G. Zappella. Random spanning trees and the prediction of weighted graphs. In *ICML* 2010.
 - [HKS12] E. Hazan, S. Kale, and S. Shalev-Shwartz. Near-Optimal Algorithms for Online Matrix Prediction In *COLT*, 2002.
 - [HLP09] M. Herbster, G. Lever, and M. Pontil. Online prediction on large diameter graphs. In *NIPS* 2009.
 - [SSN04]S. Shalev-Shwartz, Y. Singer, and A. Ng. Online and batch learning of pseudo-metrics. In *ICML* 2004.
- [XNJR02] E. P. Xing, A. Y. Ng, M. I. Jordan, and J. Russell S. Distance metric learning with application to clustering with side-information. In *NIPS* 2002.
 - [W07] M. K. Warmuth. Winnowing subspaces. In *ICML* 2007.