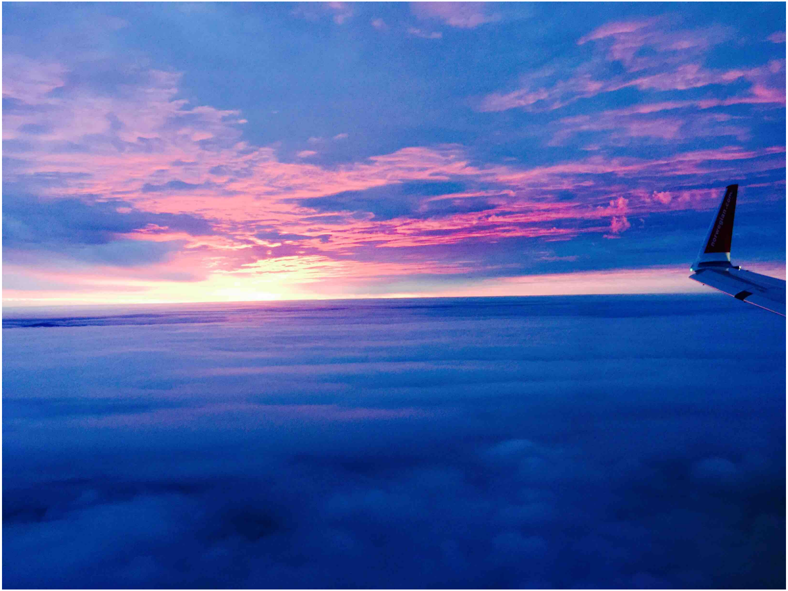

Aalto University
School of Science
and Technology

Structured output prediction for multilabel classification

Hongyu Su

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Department of Computer Science, Aalto University

December 1, 2015

An update-to-date version of this slide is available from my GitHub.

http://github.com/hongyusu

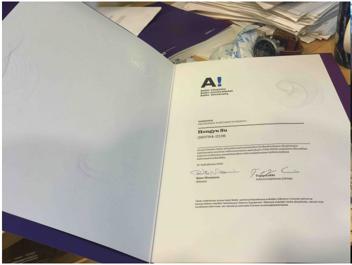
More about me

Take a look at my homepage and my technical blog.

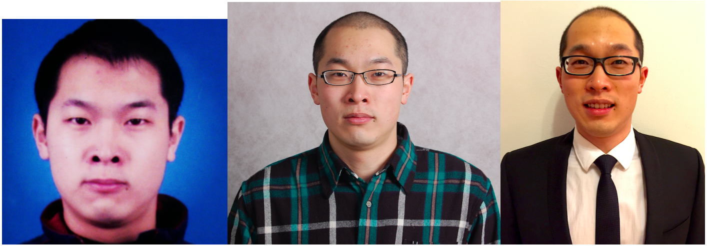
http://www.hongyusu.com
http://www.hongyusu.com/pages.html

About me

- Postdoc in Helsinki Institute for Information Technology and Aalto University since 2015.5.
- Research: build advance machine learning models to solve large scale data analysis problem (research project).
- Equivalent to: continuously learning, thinking, implementing, reporting.



Educations



- Bachelor in Computer Science and Engineering, Xidian University, 2007
- Master in Bioinformatics, University of Helsinki, 2010
- Phd in Information and Computer Science, Aalto University, 2015

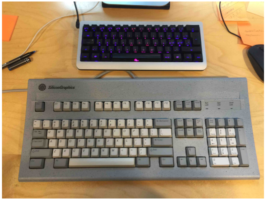
'Everything comes with a price. Some things just cost more than others.'
-Brom, *The Child thief*

Awards

- Chinese government awards for outstanding Phd candidate

A big fan of modern information technologies

- http://sentimentx.herokuapp.com
- http://tripassistant.herokuapp.com
- Know new technologies very well, e.g., deep learning, big data, Kafka, Spark, IoT.
- Maintain a techical blog at **www.hongyusu.com** on technology innovations.
- Double blade: new are not always good, e.g., I like old-fashion mechanical keyboard.



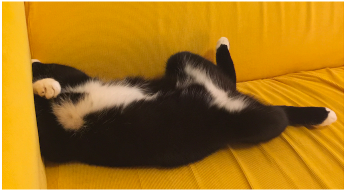
A big fan of sports

- I enjoy competitions and aggressive sport for example basketball.

- Now I try to discover unknown part of myself
  - Downhill snowboarding.
  - Bouldering (license)
  - Paragliding
  - Open water diving (license)
- A lot of gyms.

A cat person

- Pabulo

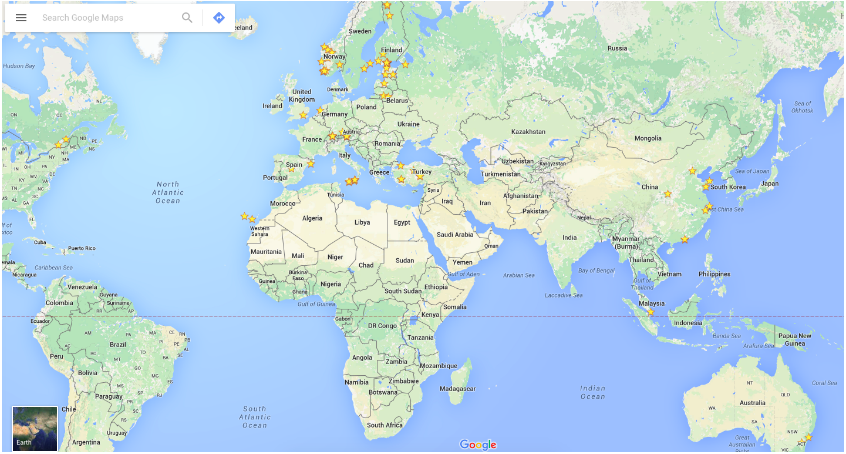


- Miu

- Cats are independent and make my life not very technical.

A hiker

I like to discover new places.



A photographer with a Flickr account

I like to memorize great moments.

A bottle collector

I like to taste new things.

Multilabel classification

- An important research field in machine learning.
- **Input**: $\mathbf{x} \in \boldsymbol{\mathcal{X}}$ lives in some input space $\boldsymbol{\mathcal{X}}$.
- **Output**: $\mathbf{y} = (y_1, \cdots, y_j, \cdots, y_l) \in \boldsymbol{\mathcal{Y}}$ is a vector of ℓ variables.
- $\mathbf{y}$: *multilabel*, y_j: *microlabel*.
- Output space $\boldsymbol{\mathcal{Y}}$ is composed by a tensor product of ℓ sets

$$\boldsymbol{\mathcal{Y}} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_\ell,\ \mathcal{Y}_i = \{+1, -1\}.$$

- For example, in document classification, a document $\mathbf{x}_0$ could be tagged with "news" "movie" "art" but not "sports" "politics" "finance".

$$\mathbf{y}_0 = (\underbrace{+1}_{\text{news}}, \underbrace{+1}_{\text{movie}}, \underbrace{-1}_{\text{sports}}, \underbrace{-1}_{\text{politics}}, \underbrace{-1}_{\text{finance}}, \underbrace{+1}_{\text{science}}, \underbrace{-1}_{\text{art}}).$$

- **Goal**: find a mapping function $f \in \mathcal{H}$ that predicts the best values of an output $\mathbf{y}$ given an input $\mathbf{x}$, $f : \boldsymbol{\mathcal{X}} \rightarrow \boldsymbol{\mathcal{Y}}$.

Concerns

- Exponential Search space!

$$\boldsymbol{\mathcal{Y}} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_\ell,\ \mathcal{Y}_i = \{+1, -1\} \quad |\boldsymbol{\mathcal{Y}}| = 2^\ell.$$

- Dependency of microlabels!
  - If a document is tagged with "movie", then it is more likely to be in the category of "art" than "science".

$$\mathbf{y} = (\underbrace{?}_{\text{news}}, \underbrace{?}_{\text{movie}}, \underbrace{?}_{\text{sports}}, \underbrace{?}_{\text{politics}}, \underbrace{?}_{\text{finance}}, \underbrace{?}_{\text{science}}, \underbrace{?}_{\text{art}}).$$

Motivated by applications

- Document classification, an article can be assigned to multiple categories.

$\mathbf{x}_0 =$


"All the News That's Fit to Print."

The New York Times.

TITANIC SINKS FOUR HOURS AFTER HITTING ICEBERG; 866 RESCUED BY CARPATHIA, PROBABLY 1250 PERISH; ISMAY SAFE, MRS. ASTOR MAYBE, NOTED NAMES MISSING

$$\mathbf{y} = (\underbrace{+1}_{\text{news}}, \underbrace{+1}_{\text{economics}}, \underbrace{-1}_{\text{sports}}, \underbrace{-1}_{\text{politics}}, \underbrace{-1}_{\text{movie}}, \underbrace{-1}_{\text{science}}, \underbrace{-1}_{\text{art}})$$

Motivated by applications (cont.)

- Image annotation, an image can associate with multiple tags.

$\mathbf{x}_0 =$ 

$$\mathbf{y} = (\underbrace{+1}_{\text{boat}}, \underbrace{+1}_{\text{sea}}, \underbrace{-1}_{\text{sun}}, \underbrace{-1}_{\text{beach}}, \underbrace{-1}_{\text{people}}, \underbrace{+1}_{\text{ice}}, \underbrace{+1}_{\text{land}})$$

Motivated by applications (cont.)

- Drug discovery, a drug can be effective for multiple symptoms.

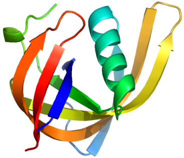
$\mathbf{x}_0 =$

$$\mathbf{y} = (\underbrace{+1}_{\text{heart}}, \underbrace{+1}_{\text{stroke}}, \underbrace{+1}_{\text{blood}}, \underbrace{+1}_{\text{fever}}, \underbrace{-1}_{\text{digest}}, \underbrace{-1}_{\text{liver}}, \underbrace{+1}_{\text{swelling}})$$

Motivated by applications (cont.)

- Protein function, a protein have multiple function in biological system.

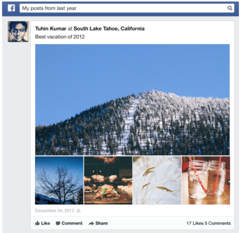
$\mathbf{x}_0 =$



$$\mathbf{y} = (\underbrace{+1}_{\alpha-\text{channel}}, \underbrace{+1}_{\beta-\text{barrel}}, \underbrace{+1}_{\text{holins}}, \underbrace{-1}_{\text{vesicle fusion pores}}, \underbrace{-1}_{\text{Phosphotransfer-driven Group}})$$

Motivated by applications (cont.)

- Social network, information can spread through multiple users.

$\mathbf{x}_0 =$ 

$$\mathbf{y} = (\underbrace{+1}_{\text{Ted}}, \underbrace{-1}_{\text{Alice}}, \underbrace{+1}_{\text{David}}, \underbrace{-1}_{\text{Mark}}, \underbrace{+1}_{\text{Alex}}, \underbrace{-1}_{\text{Zoe}}, \underbrace{-1}_{\text{Frank}})$$

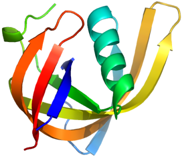
Flat classification approach

- The scheme is proposed in [Tsoumakas et al., 2010]
- The output variable **y** is assumed to be a flat vector.
- Problem transformation
  - Model the problem as a collection of single-label classification problems and solve each problem independently.
  - E.g., ML-KNN [Zhang and Zhou, 2007], CC [Read et al., 2011], IBLR [Cheng and Hüllermeier, 2009].
- Algorithm adaptation
  - Adapt single-label classification models to multilabel classification problems.
  - E.g., CORRLOG [Bian et al., 2012], MTL [Argyriou et al., 2008], ADABOOST.MH [Schapire and Singer, 1999, Esuli et al., 2008].
- These approaches do not model the dependency structure of microlabels.

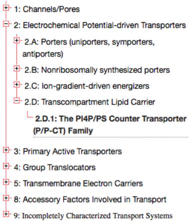
Output correlation structure

- Protein function, a protein have multiple function in biological system.

$\mathbf{x}_0 =$



$G =$

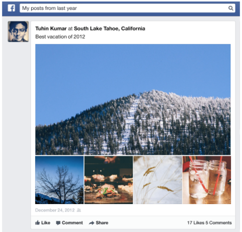


$$\mathbf{y} = (\underbrace{+1}_{\alpha-\text{channel}}, \underbrace{+1}_{\beta-\text{barrel}}, \underbrace{+1}_{\text{holins}}, \underbrace{-1}_{\text{vesicle fusion pores}}, \underbrace{-1}_{\text{Phosphotransfer-driven Group}})$$

Output correlation structure (cont.)

- Social network, information can spread through multiple users.

$\mathbf{x}_0 =$



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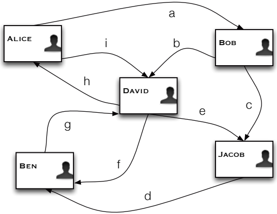


$$\mathbf{y} = (\underbrace{+1}_{\text{Ted}}, \underbrace{-1}_{\text{Alice}}, \underbrace{+1}_{\text{David}}, \underbrace{-1}_{\text{Mark}}, \underbrace{+1}_{\text{Alex}}, \underbrace{-1}_{\text{Zoe}}, \underbrace{-1}_{\text{Frank}})$$

Structured output prediction approach

- The scheme is proposed in [Su, 2015].
- Models the dependency by an *output graph* defined on microlabels.
- Hierarchical classification
  - The output graph is a rooted tree defining different levels of granularities.
  - E.g., SSVM [Tsochantaridis et al., 2004, Tsochantaridis et al., 2005].
- Graph labeling
  - The output graph has a more general form (e.g., a tree, a chain).
  - E.g., CRF [Lafferty et al., 2001, Taskar et al., 2002], M^3N [Taskar et al., 2004], MMCRF [Rousu et al., 2007, Su et al., 2010], SPIN [Su et al., 2014].
- These approaches assume the output graph is known *apriori*.
- More general, there is no pre-defined output graph!

My contributions

- SOP models developed for observed output graph.
  - Extend MMCRF to general output graph structures [Su et al., 2010].
  - SPIN on DAG for network influence prediction [Su et al., 2014].
  - SOP model for transporter protein classification [Su et al., 2015].
- SOP models developed for unknown output graph.
  - MVE to combine multiple structured output predictors by ensemble [Su and Rousu, 2011].
  - AMM and MAM to aggregate the inference results from multiple structured output predictors [Su and Rousu, 2013, Su and Rousu, 2015].
  - RTA to perform joint learning and inference over a collection of random spanning tree predictors [Marchand et al., 2014].
  - Joint learning and inference with sparse structure selection [Cousins et al., 2015a, Cousins et al., 2015b].
- Dissertation **Multilabel classification through structured output learning** [Su, 2015].
- Codes are available from http://github.com/hongyusu.

The rest of the talk

- Preliminaries
- Structured output prediction
  - Undirected graph
  - DAG
  - Special pattern
  - Unknown output graph
- Experimental evaluations
- Conclusions and future work

Preliminaries

- Training examples come in pairs $(\mathbf{x}, \mathbf{y}) \in \boldsymbol{\mathcal{X}} \times \boldsymbol{\mathcal{Y}}$.
- $\boldsymbol{\mathcal{X}}$ is an arbitrary input space.
- $\boldsymbol{\mathcal{Y}}$ is an output space of a collection of ℓ-dimensional *multilabels*.

$$\mathbf{y} = (y_1, \cdots, y_\ell) \in \boldsymbol{\mathcal{Y}}.$$

- y_i is a *microlabel* and $y_i \in \{1, \cdots, r_i\}$, $r_i \in \mathbb{Z}$.
- For example, multilabel binary classification $y_i \in \{-1, +1\}$.
- We are given a set of m training examples $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^m$.
- Each example $(\mathbf{x}, \mathbf{y})$ is mapped into a joint feature space $\boldsymbol{\phi}(\mathbf{x}, \mathbf{y})$.
- $\mathbf{w}$ is the weight vector operates in the joint feature space.
- Define a linear score function $F(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) \rangle$.
- $\mathbf{w}$ ensures that example $\mathbf{x}_i$ with correct multilabel $\mathbf{y}_i$ achieves higher score than with any other incorrect multilabel $\mathbf{y}' \in \boldsymbol{\mathcal{Y}}$.

Prediction

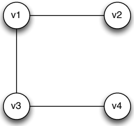
- The prediction $\mathbf{y}_{\mathbf{w}}(\mathbf{x})$ of an input $\mathbf{x}$ is the multilabel $\mathbf{y}$ that maximizes the score function

$$\mathbf{y}_{\mathbf{w}}(\mathbf{x}) = \underset{\mathbf{y} \in \boldsymbol{\mathcal{Y}}}{\mathbf{argmax}} \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) \rangle. \tag{1}$$

- Search space is exponential in size, $|\boldsymbol{\mathcal{Y}}| = 2^{\ell}$.
- (1) is called *inference* problem which is $\mathcal{NP}$-hard for most output feature maps.
- Often, we want a feature map in which the inference can be solved with a polynomial algorithm, e.g., dynamic programming.

Input/output feature maps

- We assume that the joint feature map ϕ is a potential function on a Markov network (undirected graph) $G = (E, V)$.
- A vertex $v_i \in V$ corresponds to a microlabel y_i, an edge $(v_i, v_j) \in E$ corresponds to the pairwise correlation of the microlabel y_i and y_j.
- G models potential pairwise correlations and is given *apriori*.

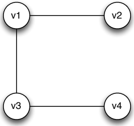


- $\varphi(\mathbf{x}) \in \mathbb{R}^d$ is the input feature map, e.g., bag-of-words of a document.
- $\psi(\mathbf{y}) \in \mathbb{R}^{4|E|}$ is the output feature map which maps the multilabel $\mathbf{y}$ into a collection of edges and labels

$$\varphi(\mathbf{y}) = (u_e)_{e \in E}, u_e \in \{-1, +1\}^2.$$

An example of $\psi(\mathbf{y})$

- Markov network (undirected graph) $G = (E, V)$



- Multilabel $\mathbf{y}$

$$\mathbf{y} = (y_1, y_2, y_3, y_4) = (+1, -1, +1, +1)$$

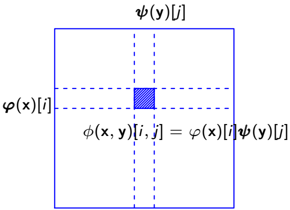
- Output feature map $\psi(\mathbf{y})$

$$\psi(\mathbf{y}) = (\underbrace{\underbrace{0}_{--}, \underbrace{0}_{-+}, \underbrace{0}_{+-}, \underbrace{1}_{++}}_{(v_1, v_3)}, \underbrace{\underbrace{0}_{--}, \underbrace{0}_{-+}, \underbrace{1}_{+-}, \underbrace{0}_{++}}_{(v_1, v_2)}, \underbrace{\underbrace{0}_{--}, \underbrace{0}_{-+}, \underbrace{0}_{+-}, \underbrace{1}_{++}}_{(v_3, v_4)})$$

Joint feature map $\phi(\mathrm{x}, \mathrm{y})$

- The joint feature is the Kronecker product of $\boldsymbol{\varphi}(\mathbf{x})$ and $\boldsymbol{\psi}(\mathbf{y})$

$$\boldsymbol{\phi}(\mathbf{x},\mathbf{y}) = (\boldsymbol{\phi}_e(\mathbf{x},\mathbf{y}))_{e\in E} = (\boldsymbol{\varphi}(\mathbf{x}) \otimes \boldsymbol{\psi}_e(\mathbf{y}_e))_{e\in E}.$$



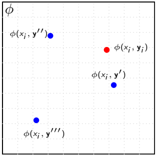
- The score function can be factorized by the output graph G

$$F(\mathbf{w},\mathbf{x},\mathbf{y}) = \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x},\mathbf{y})\rangle = \sum_{e\in E} \langle \mathbf{w}_e, \boldsymbol{\phi}_e(\mathbf{x},\mathbf{y}_e)\rangle.$$

Optimization problem

- Max-margin learning for **w**

$$\gamma(\mathbf{w}, \mathbf{x}_i) = F(\mathbf{w}, \mathbf{x}_i, \mathbf{y}_i) - \max_{\mathbf{y} \in \boldsymbol{\mathcal{Y}}/\mathbf{y}_i} F(\mathbf{w}, \mathbf{x}_i, \mathbf{y})$$



- The model is max-margin conditional random field MMCRF [Rousu et al., 2007, Su et al., 2010].
- The primal optimization problem is defined as

$$\begin{aligned} \min_{\mathbf{w}, \xi_k} \quad & \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{k=1}^{m} \xi_k \\ \text{s.t.} \quad & \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}_k, \mathbf{y}_k) \rangle - \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}_k, \mathbf{y}) \rangle \geq \ell(\mathbf{y}_k, \mathbf{y}) - \xi_k, \\ & \xi_k \geq 0, \forall\ \mathbf{y} \in \boldsymbol{\mathcal{Y}}, k \in \{1, \dots, m\}. \end{aligned} \tag{2}$$

- $\ell(\mathbf{y}, \mathbf{y}_k)$ scales the margin according to the multilabel **y**.

Marginal-dual optimization

- (2) is difficult as the number of the constraints is $m \times |\mathcal{Y}|$.
- The dual optimization problem is defined as

$$\begin{aligned} \max_{\alpha \geq 0} \quad & \alpha^\intercal \ell - \frac{1}{2}\alpha^\intercal K \alpha \\ \text{s.t.} \quad & \sum_{\mathbf{y} \in \mathcal{Y}} \alpha(k, \mathbf{y}) \leq C, \forall k \in \{1, \cdots, m\}. \end{aligned} \tag{3}$$

- (3) is also challenging due to the exponential number of dual variables.
- We use edge marginals to replace the dual variables [Taskar et al., 2004]

$$\mu(k, e, u_e) = \sum_{\mathbf{y}} \mathbf{1}_{\{\boldsymbol{\psi}_e(\mathbf{y}) = u_e\}} \alpha(k, \mathbf{y}).$$

- The margin-dual optimization problem is

$$\max_{\mu \in \mathcal{M}} \quad \mu^\intercal \ell - \frac{1}{2}\mu^\intercal K \mu. \tag{4}$$

- The number of marginal-dual variables is $m \times 4|E|$.

Conditional gradient descent

- (4) is optimized by conditional gradient decent.
- In each iteration it optimizes μ_k that corresponds to a single example while keeps others $(\mu_j, j \neq k)$ fixed

$$\max_{\mu_k \in \mathcal{M}} \quad \mu_k^{\intercal} \ell_k - \frac{1}{2} \sum_j \mu_k^{\intercal} K \mu_j, \, \forall k.$$

- Current gradient of μ_k is given by $g_i = \ell_i - \sum_j K \mu_j$.
- Compute the maximal feasible solution μ_k^* as an update direction

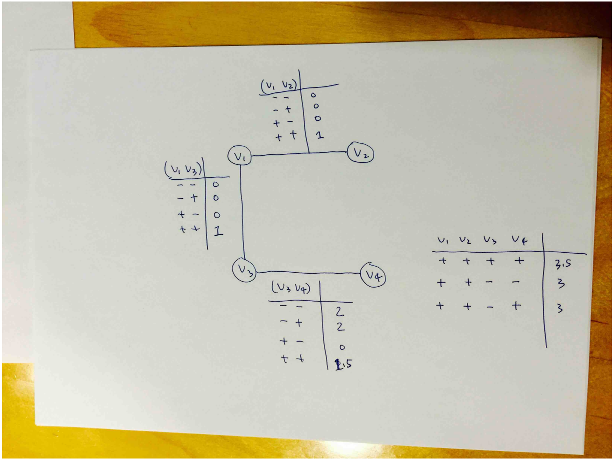
$$\mu_k^* = \operatorname*{argmax}_{\mu_k \in \mathcal{M}} \mu_k^{\intercal} g_k = \operatorname*{argmax}_{\mu_k \in \mathcal{M}} \sum_e \mu(k, e)^{\intercal} g(k, e). \tag{5}$$

- What is actually going on here?
- (5) is an instantiation of MAP problem

Output graph	Inference problem	Inference algorithm
Tree	Polynomial	DP [Rousu et al., 2007]
Graph	$\mathcal{NP}$-hard	LBP [Su et al., 2010]

- Perform the update via exact line search $\mu_k \leftarrow \mu_k + \tau(\mu_k^* - \mu_k)$.

What is happing?



Exact line search

- Line search gives the optimal feasible solution as a stationary point (τ)

$$\begin{aligned} \max_{\tau} \quad & g(\mu_k + \tau \Delta \mu_k) \\ \text{s.t.} \quad & 0 \leq \tau \leq 1. \end{aligned} \tag{6}$$

- $\tau = 0$ corresponds to no update.
- Feasible maximum update is achieved at $\tau = 1$.
- The cost of computing (6) is significantly smaller than the cost of computing (5).

Duality gap

- We use duality gap to measure the progress of the optimization.
- Primal and marginal-dual objective functions

$$f(\mathbf{w}) = \frac{1}{2}||\mathbf{w}||^2 + C\sum_{k=1}^{m}(\ell_k - \langle \mathbf{w}, \Delta\boldsymbol{\phi}(\mathbf{x}_k, \mathbf{y}_k)\rangle)$$

$$g(\mu) = \sum_{k=1}^{m}\mu_k\ell_k - \frac{1}{2}\sum_{k=1}^{m}\sum_{j=1}^{m}\mu_k K^{\Delta\boldsymbol{\phi}}(\mathbf{x}_k, \mathbf{y}_k; \mathbf{x}_j, \mathbf{y}_j)\mu_j$$

- $\max_{\mu} g(\mu) \leq \min_{\mathbf{w}} f(\mathbf{w})$, gap is minimized at optimal.
- Duality gap at μ^t

$$\begin{aligned} f(\mathbf{w}^t) - g(\mu^t) &= C\left(\ell - K^{\Delta\boldsymbol{\phi}}\mu^t\right) - \mu^t\left(\ell - K^{\Delta\boldsymbol{\phi}}\mu^t\right) \\ &= C^{\intercal}\nabla g(\mu^t) - \mu^{t\intercal}\nabla g(\mu^t) \end{aligned}$$

1. Estimate the marginal-dual objective by linear approximation $\nabla g(\mu^t)$.
2. Marginal-dual objective value at μ^t is computed by $\mu^{t\intercal}\nabla g(\mu^t)$.
3. Primal objective value is estimate by $C^{\intercal}\nabla g(\mu^t)$.

Short summary

- We have seen so far.

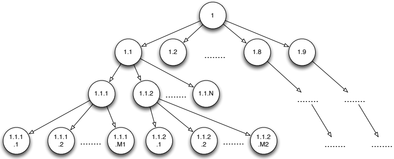
Output graph	Inference problem	Inference algorithm
Tree	Polynomial	DP [Rousu et al., 2007]
Graph	$\mathcal{NP}$-hard	LBP [Su et al., 2010]

- What if the solution $\mathbf{y}$ corresponds to some special structure?

Pattern and Exponential reduction

Transporter protein classification [Su et al., 2015]

- 12456 protein, $\mathbf{x}_i, \forall i \in \{1, \cdots, 12456\}$.
- 3145 transporter function classes, $\mathbf{y} = (y_1, \cdots, y_{3145})$.
- A hierarchical structured G defined on 3145 classes.



- **Task**: predict $\mathbf{y}_0$ given $\mathbf{x}_0$.
- It seems: $|\mathcal{Y}| = 2^{3145}$, DP on G.
- **Pattern**:
  - a valid annotation is a path from root to leave.
  - exponential reduction of search space $|\mathcal{Y}| = 2^{3145} \rightarrow |\mathcal{Y}| \approx 2000$.

Pattern and Exponential reduction

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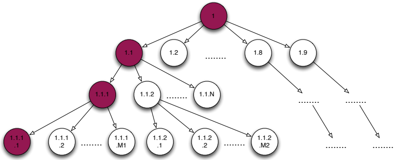

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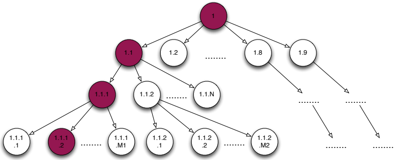

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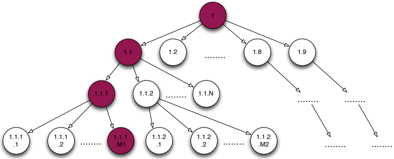
Pattern and Exponential reduction

Transporter protein classification [Su et al., 2015]

- 12456 protein, $\mathbf{x}_i, \forall i \in \{1, \cdots, 12456\}$.
- 3145 transporter function classes, $\mathbf{y} = (y_1, \cdots, y_{3145})$.
- A hierarchical structured G defined on 3145 classes.



- **Task**: predict $\mathbf{y}_0$ given $\mathbf{x}_0$.
- It seems: $|\mathcal{Y}| = 2^{3145}$, DP on G.
- **Pattern**:
  - a valid annotation is a path from root to leave.
  - exponential reduction of search space $|\mathcal{Y}| = 2^{3145} \rightarrow |\mathcal{Y}| \approx 2000$.

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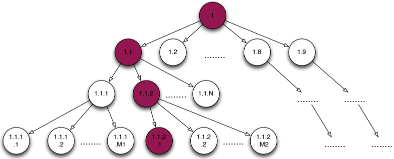

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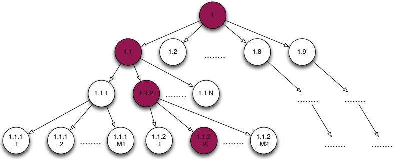

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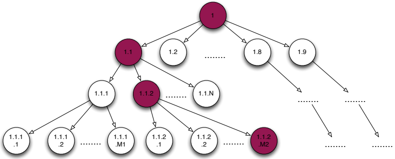

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Actual model

- The primal optimization problem is defined as

$$\begin{aligned} \min_{\mathbf{w},\xi_k} \quad & \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{k=1}^{m}\xi_k \\ \text{s.t.} \quad & \langle \mathbf{w}, \phi(\mathbf{x}_k, \mathbf{y}_k)\rangle - \langle \mathbf{w}, \phi(\mathbf{x}_k, \mathbf{y})\rangle \geq \ell(\mathbf{y}_k, \mathbf{y}) - \xi_k, \\ & \xi_k \geq 0, \forall\, \mathbf{y} \in \mathcal{Y}, k \in \{1,\ldots,m\}. \end{aligned}$$

- In stead of CGD, we do gradient descent for all examples in each iteration.
- Multi-view data: 30 set of features, $\{\phi(\mathbf{x}_i)_k\}_{k=1}^{30}$.
- Multiple kernel learning (MKL): ALIGN, ALIGNF.
- Experiments:

	0/1 (full annotation)					
	Linear			*Gaussian*		
	SVM	MMR	SOP	SVM	MMR	SOP
UNIF	53.3	12.0	66.8	23.2	68.1	69.7
ALIGN	54.8	12.4	63.3	16.0	71.9	74.2
ALIGNF	60.5	17.5	64.3	32.9	68.4	71.2

Table : Prediction performance with kernels from MKL.

Short summary

- We have seen so far.

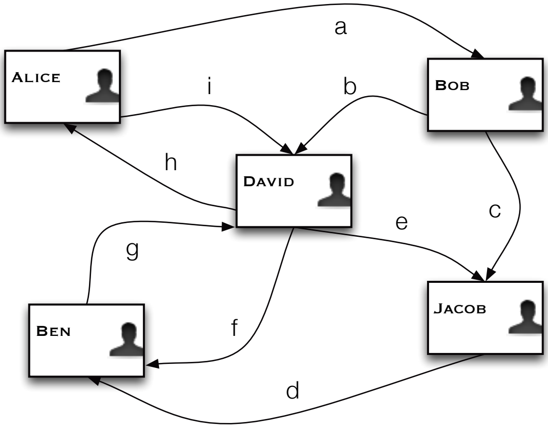
Output graph	Inference problem	Inference algorithm
Tree	Polynomial	DP [Rousu et al., 2007]
Graph	$\mathcal{NP}$-hard	LBP [Su et al., 2010]
$\rightarrow$Pattern	Linear?	Reduction [Su et al., 2015]

- What if the output graph is DAG ?

Output graph is DAG

Predicting network response [Su et al., 2014]

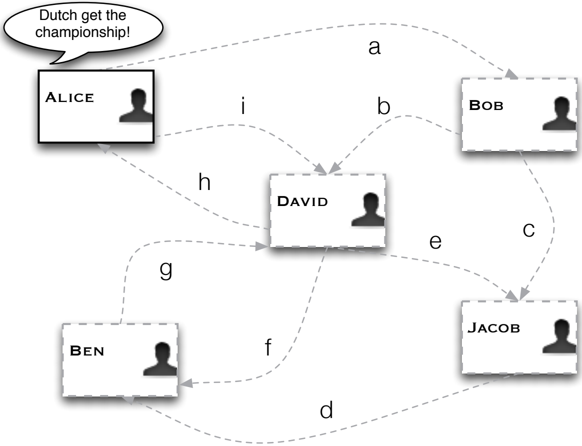
A Twitter (follower-ship) network consists of five users.



Output graph is DAG

Predicting network response [Su et al., 2014]

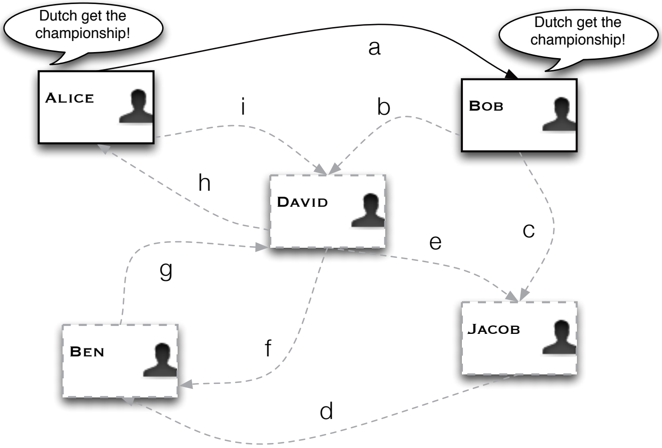
Alice tweets after World Cup final.



Output graph is DAG

Predicting network response [Su et al., 2014]

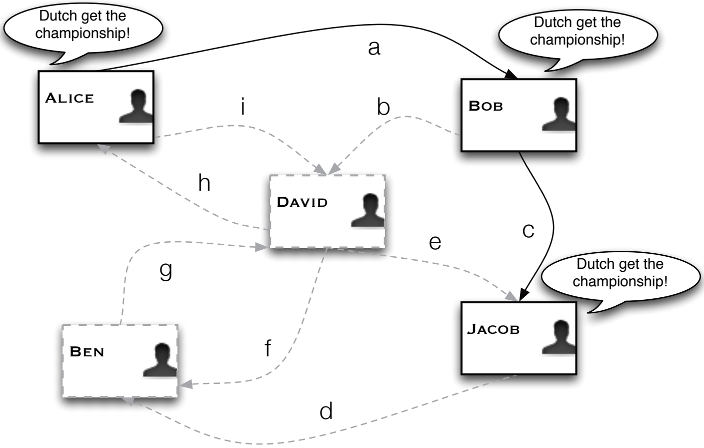
Bob saw the tweet and retweets from Alice.



Output graph is DAG

Predicting network response [Su et al., 2014]

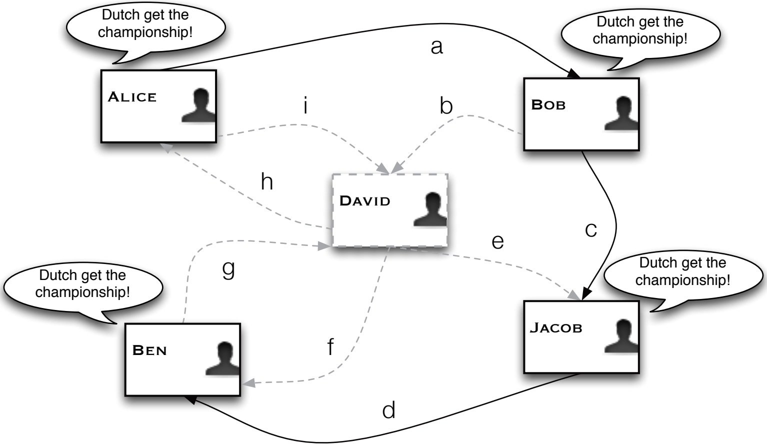
Jacob retweets from Bob.



Output graph is DAG

Predicting network response [Su et al., 2014]

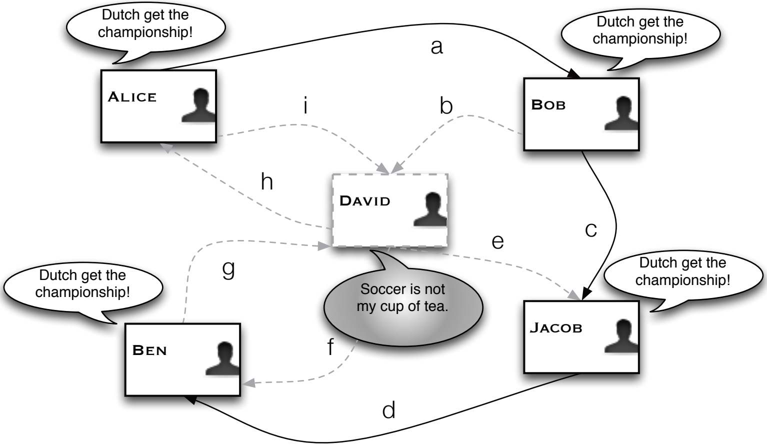
Ben retweets from Jacob.



Output graph is DAG

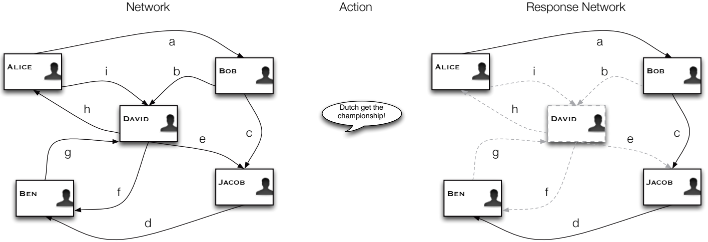
Predicting network response [Su et al., 2014]

David is not a fan.



Network response problem

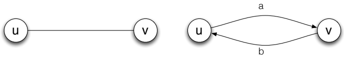
- Definition:
  - **Given**: a network $G = (E, V)$, and an action $\mathbf{x}$ performed on G.
  - **Task**: predict the subnetwork that responses to the action.
    - Which nodes $v \in V$ perform the action?
      $V_{\mathbf{x}} = \{Alice, Bob, Jacob, Ben\}$
    - Which directed edges $e \in E_{\mathbf{x}}$ relay the action from one node to its neighbors? $E_{\mathbf{x}} = \{a, c, d\}$



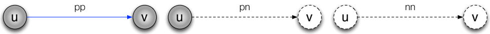
- **Applications**: Information propagation, idea formation, disease spreads, adoption of new technologies.

Direct output graph

- Model is defined on directed network.
  - Any undirected network can be seen as special case by replacing undirected edges with two directed ones.

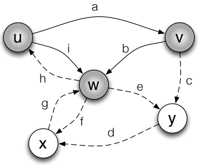


- Notation of edge labels:



- *Input feature*: Encode $\mathbf{x}$ as $\varphi(\mathbf{x})$ (e.g. bag-of-word of a tweet).
- *Output feature*: Encode $G_{\mathbf{y}}$ as $\psi(\mathbf{y})$ (e.g. a set of edges and their labels)

$$\psi(\mathbf{y}) =$$
$$(\underbrace{\underbrace{1}_{++},\underbrace{0}_{+-},\underbrace{0}_{--}}_{a},\underbrace{\underbrace{1}_{++},\underbrace{0}_{+-},\underbrace{0}_{--}}_{b},\underbrace{\underbrace{0}_{++},\underbrace{1}_{+-},\underbrace{0}_{--}}_{c},\cdots)$$



Structure output prediction model

- Compatibility score for $(\mathbf{x}, \mathbf{y})$: $F(\mathbf{x}, \mathbf{y}, \mathbf{w}) = \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) \rangle$
  - $\mathbf{w}$ is the feature weight to be learned.
  - $\boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x}) \otimes \psi(\mathbf{y})$ is joint feature map.
  - Intuition: given an action $\mathbf{x}$, the score of correct response graph $(\mathbf{x}, \mathbf{y})$ should be higher than any incorrect response graph $(\mathbf{x}, \mathbf{y}')$

$$F(\mathbf{x}, \mathbf{y}, \mathbf{w}) > F(\mathbf{x}, \mathbf{y}', \mathbf{w}), \quad \forall \mathbf{y}' \in \mathcal{H}(G).$$

- $\mathbf{w}$ is learned by solving structured output learning problem

$$\begin{aligned}
\min_{\mathbf{w}, \xi} \quad & \frac{1}{2}||\mathbf{w}||_2^2 + C \sum_{i=1}^{m} \xi_i \\
\textbf{s.t.} \quad & F(\mathbf{x}_i, \mathbf{y}_i; \mathbf{w}) > \max_{G'_{\mathbf{x}_i} \in \mathcal{H}(G)} (F(\mathbf{x}_i, \mathbf{y}'_i,) \\
& + \ell_G(\mathbf{y}_i, \mathbf{y}'_i)) - \xi_i, \xi_i \geq 0, \forall i \in \{1, \cdots, m\},
\end{aligned}$$

Inference problem

- To solve the optimization, we have to solve similar inference problem appeared both in training and in prediction.
- In prediction phase:
  - Given the feature weight $\mathbf{w}$ and the complex network G.
  - To find out a DAG $H^* = (V_H, E_H)$ that gives the maximal compatibility score for a given action $\mathbf{x}$

$$H^*(\mathbf{x}) = \underset{H \in \mathcal{H}(G)}{\mathbf{argmax}} \sum_{e \in E^H} s_{\mathbf{y}_e}(e, \mathbf{x}, \mathbf{w}). \tag{7}$$

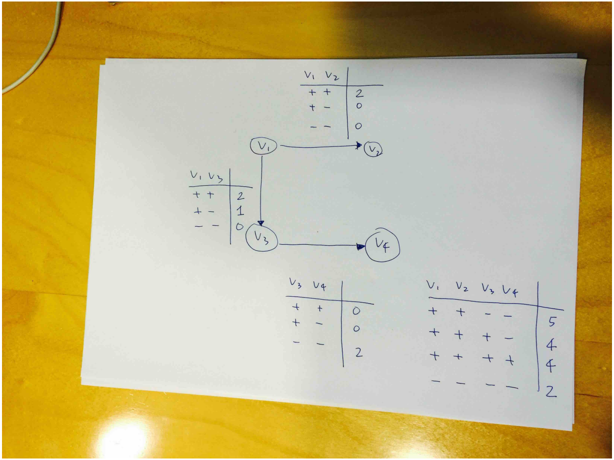
Lemma

Finding the graph that maximizes Eq. (7) is an $\mathcal{NP}$-hard problem.

Proof.

Reduction from MAX-CUT problem. □

What is happing?



Approximate inference via SDP relaxation

- We formulate the inference problem as *integer quadratic program* (IQP).
  - Introduce for each node $u \in V$ a binary variable $x_u \in \{-1, +1\}$.
  - Introduce a special variable $x_0 \in \{-1, +1\}$ to distinguish activated node.

$$
\begin{aligned}
\textbf{max} \quad & \frac{1}{4} \sum_{(u,v) \in E} [s_{pn}(u, v)(1 + x_0 x_u - x_0 x_v - x_u x_v) \\
& \qquad + s_{nn}(u, v)(1 - x_0 x_u - x_0 x_v + x_u x_v) \\
& \qquad + s_{pp}(u, v)(1 + x_0 x_u + x_0 x_v + x_u x_v)] \\
\textbf{s.t.} \quad & x_0, x_u, x_v \in \{-1, +1\}, \text{ for all } u, v \in V,
\end{aligned}
$$

- IQP is relaxed into *quadratic program* (QP) and solved by *semidefinite programming relaxation* (SDP).
- Optimization guarantee $E[Z] \geq (\alpha - \epsilon) Z_R$ with $\alpha > 0.796$, Z is objective achieved by SDP, Z_R is objective of IQP.

SPIN for context-sensitive prediction

- We assume action $\varphi(\mathbf{x})$ is known (e.g. bag-of-word of a tweet).
- Task is to predict the response network given the action.
- *Predicted Subgraph Coverage* (PSC) is the relative size of correctly predicted subgraph in terms of node labels.
- The result is shown in the following table.

Dataset	Node Accuracy			Node F_1 Score			Edge Acc		*PSC*		
	SVM	MMCRF	SPIN	SVM	MMCRF	SPIN	SVM	SPIN	SVM	MMCRF	SPIN
memeS	**73.4**	68.0	*72.2*	39.0	*39.8*	**47.1**	**62.7**	45.6	23.4	*25.3*	**33.6**
memeM	**82.1**	79.0	*81.5*	29.1	*30.1*	**38.0**	61.1	**68.8**	18.6	*18.8*	**28.3**
memeL	**89.9**	88.3	*89.8*	26.7	*27.1*	**35.0**	45.5	**80.0**	17.7	*18.9*	**27.6**
M700	91.9	**94.1**	*92.1*	*13.8*	7.3	**14.2**	26.3	**93.0**	*29.4*	23.9	**34.4**
M1k	94.1	**95.8**	*94.2*	**10.9**	3.5	*9.3*	26.6	**94.7**	*33.7*	16.6	**35.2**
M2k	*96.8*	**97.6**	96.7	**6.2**	1.4	*3.4*	25.3	**97.6**	**34.6**	9.6	*14.7*
L700	89.7	**92.4**	*89.7*	*16.2*	9.4	**17.3**	26.5	**90.4**	*9.5*	6.7	**12.5**
L1k	*92.4*	**94.4**	91.5	*12.4*	6.4	**13.9**	26.4	**92.3**	*6.1*	4.4	**8.4**
L2k	*92.5*	**94.5**	91.9	*12.3*	5.4	**12.7**	26.5	**93.2**	*6.0*	2.9	**7.2**
Geom.	85.5	*86.4*	**86.6**	*19.8*	12.6	**20.3**	32.6	**79.7**	*18.9*	14.2	**21.7**

SPIN for context-free prediction

- We assume action is unknown during prediction phase.
- Task is to predict directed edges (network skeleton) from a cascade of actions.
- The measure of success is *Precision@K*, where we ask for top-K percent edge predictions and compute the precision.
- The result is shown in the following table.

Dataset	Model	T (10^3s)	Precision @ K					
			10%	20%	30%	40%	50%	60%
memeS	SPIN	*5.50*	**82.9**	**81.0**	**76.0**	**74.0**	**74.0**	**70.0**
	ICM-EM	**0.01**	60.3	63.5	65.1	62.0	62.0	61.5
	NETRATE	5.83	*76.2*	*73.8*	*70.4*	*68.7*	*68.7*	*66.8*
memeM	SPIN	*5.52*	**82.7**	**72.1**	**70.5**	**69.2**	**69.2**	**67.9**
	ICM-EM	**0.02**	56.3	55.3	56.8	57.4	57.4	56.3
	NETRATE	13.93	*61.2*	*64.6*	*62.9*	*62.5*	*62.5*	*62.4*
memeL	SPIN	*4.75*	**82.2**	**73.6**	**69.1**	**66.7**	**66.7**	**65.9**
	ICM-EM	**0.01**	52.1	55.7	54.2	56.5	56.5	56.7
	NETRATE	12.63	*56.5*	*57.8*	*60.0*	*59.3*	*59.3*	*59.4*

Short summary

- We have seen so far.

Output graph	Inference problem	Inference algorithm
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Graph	$\mathcal{NP}$-hard	LBP [Su et al., 2010]
Pattern	Linear?	Reduction [Su et al., 2015]
$\rightarrow$ DAG	$\mathcal{NP}$-hard	SDP [Su et al., 2014]

- What if the output graph is not observed?

Research question

- The output graph G is hidden in many applications.
  - E.g., possible tags for a surveillance photo: "building", "road", "pedestrian", and "vehicle".
- Structured output learning when the output graph is not observed.
- In particular:
  - Dependency via a complete set of pairwise correlations.
  - Structured output learning with a complete graph.
  - Solve the $\mathcal{NP}$-hard inference problem via a polynomial time approximation algorithm.
- In general, a structured prediction model which performs max-margin learning on a random collection of spanning trees sampled from the output graph.

Complete graph as output graph

- We assume that the joint feature map $\boldsymbol{\phi}$ is a potential function on a Markov network (undirected graph) $G = (E, V)$.
- G : complete graph with $|V| = \ell$ nodes and $|E| = \frac{\ell(\ell-1)}{2}$ undirected edges.
- G models all pairwise correlations.
- $\boldsymbol{\varphi}(\mathbf{x})$ is the input feature map, e.g., bag-of-words feature of an example $\mathbf{x}$.
- $\boldsymbol{\psi}(\mathbf{y})$ is the output feature map which is a collection of edges and labels

$$\boldsymbol{\varphi}(\mathbf{y}) = (u_e)_{e \in E}, u_e \in \{-1, +1\}^2.$$

- The joint feature is the Kronecker product of $\boldsymbol{\varphi}(\mathbf{x})$ and $\boldsymbol{\psi}(\mathbf{y})$

$$\boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) = (\boldsymbol{\phi}_e(\mathbf{x}, \mathbf{y}))_{e \in E} = (\boldsymbol{\varphi}(\mathbf{x}) \otimes \boldsymbol{\psi}_e(\mathbf{y}_e))_{e \in E}.$$

- The score function can be factorized by the complete graph G

$$F(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) \rangle = \sum_{e \in E} \langle \mathbf{w}_e, \boldsymbol{\phi}_e(\mathbf{x}, \mathbf{y}_e) \rangle.$$

Inference in terms of all spanning trees

- Solving the following inference problem on a complete graph is $\mathcal{NP}$-hard

$$\mathbf{y}_{\mathbf{w}}(\mathbf{x}) = \operatorname*{argmax}_{\mathbf{y}\in\boldsymbol{\mathcal{Y}}} F(\mathbf{w},\mathbf{x},\mathbf{y}) = \operatorname*{argmax}_{\mathbf{y}\in\boldsymbol{\mathcal{Y}}} \sum_{e\in E} \langle \mathbf{w}_e, \boldsymbol{\phi}_e(\mathbf{x},\mathbf{y}_e)\rangle.$$

$$\phi_G(\mathbf{x},\mathbf{y}) = \{\phi_{G,e}(\mathbf{x},\mathbf{y}_e)\}_{e\in G}, \mathbf{w}_G = \{\mathbf{w}_{G,e}\}_{e\in G}, ||\phi_G(\mathbf{x},\mathbf{y})|| = ||\mathbf{w}_G|| = 1$$

- For a complete graph, there are $\ell^{\ell-2}$ unique spanning trees.
- $\phi_T(\mathbf{x},\mathbf{y}) = \{\phi_e(\mathbf{x},\mathbf{y})\}_{e\in T}$ is the projection of $\phi_G(\mathbf{x},\mathbf{y})$ on $T\in S(G)$.
- $\mathbf{w}_T = \{\mathbf{w}_{G,e}\}_{e\in T}$ is the projection of $\mathbf{w}_G$ on $T\in S(G)$.
- We can write $F(\mathbf{w},\mathbf{x},\mathbf{y})$ as a conic combination of all spanning trees

$$F(\mathbf{w},\mathbf{x},\mathbf{y}) = \mathop{\mathbf{E}}_{T\in U(G)} a_T \langle \mathbf{w}_T, \boldsymbol{\phi}_T(\mathbf{x},\mathbf{y})\rangle$$

$$\mathop{\mathbf{E}}_{T\in U(G)} a_T^2 = 1, \mathop{\mathbf{E}}_{T\in U(G)} a_T < 1.$$

- $U(G)$ is the uniform distribution over $\ell^{\ell-2}$ spanning trees.
- The number of spanning trees is exponentially dependent on the number of nodes ℓ.

A sample of n spanning trees

- Instead of using all spanning trees, we can just use n spanning trees

$$F_{\mathcal{T}}(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \frac{1}{n} \sum_{i=1}^{n} a_{T_i} \langle \mathbf{w}_{T_i}, \boldsymbol{\phi}_{T_i}(\mathbf{x}, \mathbf{y}) \rangle$$

$$\frac{1}{n} \sum_{i=1}^{n} a_{T_i}^2 = 1, \frac{1}{n} \sum_{i=1}^{n} a_{T_i} < 1.$$

- When

$$n \geq \frac{\ell^2}{\epsilon^2}(\frac{1}{16} + \frac{1}{2} \ln \frac{8\sqrt{n}}{\delta}),$$

  we have $|F_{\mathcal{T}}(\mathbf{w}, \mathbf{x}, \mathbf{y}) - F(\mathbf{w}, \mathbf{x}, \mathbf{y})| \leq \epsilon$, with high probability.
- A sample of $n \in \Theta(\ell^2/\epsilon^2)$ random spanning tree is sufficient to estimate the score function.
- Margin achieved by $F(\mathbf{w}, \mathbf{x}, \mathbf{y})$ is also preserved by the sample of n random spanning trees $F_{\mathcal{T}}(\mathbf{w}, \mathbf{x}, \mathbf{y})$ [Marchand et al., 2014].

Random spanning tree approximation RTA

- The optimization problem of RTA is defined as [Marchand et al., 2014]

$$
\begin{aligned}
\min_{\mathbf{w}_{T_i},\xi_i} \quad & \frac{1}{2}\sum_{i=1}^{n}||\mathbf{w}_{T_i}||^2 + C\sum_{k=1}^{m}\xi_k \\
\text{s.t.} \quad & \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\langle \mathbf{w}_{T_i}, \boldsymbol{\phi}_{T_t}(\mathbf{x}_k,\mathbf{y}_k)\rangle - \max_{\mathbf{y}\neq\mathbf{y}_k}\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\langle \mathbf{w}_{T_t}, \boldsymbol{\phi}_{T_i}(\mathbf{x}_k,\mathbf{y})\rangle \geq 1-\xi_k, \\
& \xi_k \geq 0\,, \forall\ k \in \{1,\dots,m\}.
\end{aligned}
$$

- The marginal-dual form is given by

$$
\begin{aligned}
\max_{\mu\in\mathcal{M}} \quad & \sum_{i=1}^{n}\left(\mu_{T_i}\ell_{T_i} - \frac{1}{2}\mu_{T_i}K_{T_i}^{\Delta\phi}\mu_{T_i}\right) \\
\text{s.t.} \quad & \sum_{u_e}\mu_{T_i,e}(u_e) \leq C.
\end{aligned}
$$

- Inside the summation, there is a structure output model with parameter μ_{T_i} defined on a spanning tree T_i.
- The problem is how to jointly optimize structured output models defined on n spanning trees.

Inference problem for a collection of trees

- The inference problem of RTA is defined as finding the multilabel $\mathbf{y}_{\mathcal{T}}(\mathbf{x})$ that maximizes the sum of scores over a collection of trees

$$\mathbf{y}_{\mathcal{T}}(\mathbf{x}) = \underset{\mathbf{y}\in\boldsymbol{\mathcal{Y}}}{\mathbf{argmax}}\, F_{\mathcal{T}}(\mathbf{x},\mathbf{y};\mathbf{w}_{\mathcal{T}}) = \underset{\mathbf{y}\in\boldsymbol{\mathcal{Y}}}{\mathbf{argmax}} \sum_{t=1}^{n} \langle \mathbf{w}_{T_t}, \phi_{T_t}(\mathbf{x},\mathbf{y})\rangle.$$

- The inference problem on each individual spanning tree can be solve efficiently in $\Theta(\ell)$ by *dynamic programming*

$$\mathbf{y}_{T_t}(\mathbf{x}) = \underset{\mathbf{y}\in\boldsymbol{\mathcal{Y}}}{\mathbf{argmax}}\, F_{T_t}(\mathbf{x},\mathbf{y};\mathbf{w}_{T_t}) = \underset{\mathbf{y}\in\boldsymbol{\mathcal{Y}}}{\mathbf{argmax}}\, \langle \mathbf{w}_{T_t}, \phi_{T_t}(\mathbf{x},\mathbf{y})\rangle.$$

- There is no guarantee that there exists a tree $T_t \in \mathcal{T}$ in which the maximizer of F_{T_t} is the maximizer of $F_{\mathcal{T}}$.

Fast inference for a collection of trees

- For each tree T_t, instead of computing the best multilabel $\mathbf{y}_{T_t}$, we compute K-best multilabels in $\Theta(K\ell)$ time

$$\mathcal{Y}_{T_t,K} = \{\mathbf{y}_{T_t,1}, \cdots, \mathbf{y}_{T_t,K}\}.$$

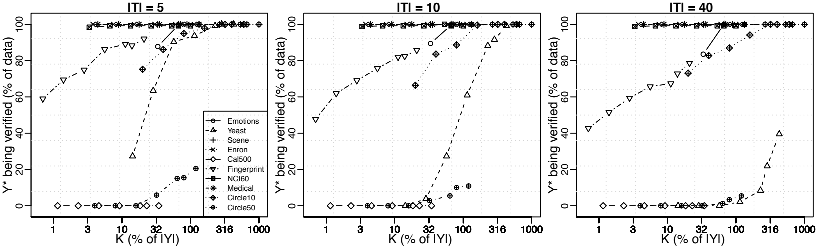
- Performing the same computation on all trees gives a candidate list of $n \times K$ multilabels (K best list) in $\Theta(nK\ell)$ time

$$\mathcal{Y}_{\mathcal{T},K} = \mathcal{Y}_{T_1,K} \cup \cdots \mathcal{Y}_{T_n,K}.$$

- We prove that with high probability the global best multilabel will exist in K best list.
- We have developed a condition to verify the global best multilabel from K best list in linear time $\Theta(nK)$.

RTA inference algorithm

- 10 datasets, $|\mathcal{T}| = \{5, 10, 40\}$, $K = \{2, 4, 8, 16, 32, 40, 60\}$.
- Y-axis is the percentage of examples with exact inference.
- X-axis is the value of K as the percentage of the number of microlabels.
- $K = 100\%|Y|$ corresponds to a complexity of $\Theta(n\ell^2)$.



RTA on multilabel benchmark datasets

- Prediction performance on multilabel benchmark datasets.
- Measurement of success is microlabel accuracy and multilabel accuracy.
- The result is shown in the following table.

Dataset	Microlabel Loss (%)					0/1 Loss (%)				
	SVM	MTL	MMCRF	MAM	RTA	SVM	MTL	MMCRF	MAM	RTA
Emotions	22.4	20.2	20.1	*19.5*	**18.8**	77.8	74.5	71.3	*69.6*	**66.3**
Yeast	*20.0*	20.7	21.7	20.1	**19.8**	*85.9*	88.7	93.0	86.0	**77.7**
Scene	*9.8*	11.6	18.4	17.0	**8.8**	*47.2*	55.2	72.2	94.6	**30.2**
Enron	6.4	6.5	6.2	**5.0**	*5.3*	99.6	99.6	92.7	*87.9*	**87.7**
Cal500	**13.7**	*13.8*	**13.7**	**13.7**	*13.8*	100.0	100.0	100.0	100.0	100.0
Fingerprint	**10.3**	17.3	*10.5*	*10.5*	10.7	99.0	100.0	*99.6*	*99.6*	**96.7**
NCI60	15.3	16.0	*14.6*	**14.3**	14.9	56.9	*53.0*	63.1	60.0	**52.9**
Medical	*2.6*	*2.6*	**2.1**	**2.1**	**2.1**	91.8	91.8	63.8	*63.1*	**58.8**
Circle10	4.7	6.3	2.6	*2.5*	**0.6**	28.9	33.2	20.3	*17.7*	**4.0**
Circle50	5.7	6.2	**1.5**	*2.1*	3.8	69.8	72.3	**38.8**	*46.2*	*52.8*

Short summary

- We have seem so far.

Output graph	Inference problem	Inference algorithm
Tree	Polynomial	DP [Rousu et al., 2007]
Graph	$\mathcal{NP}$-hard	LBP [Su et al., 2010]
Pattern	Linear?	Reduction [Su et al., 2015]
DAG	$\mathcal{NP}$-hard	SDP [Su et al., 2014]
$\rightarrow$unknown	$\mathcal{NP}$-hard	MVE AMM MAM [Su and Rousu, 2015] RTA [Marchand et al., 2014]

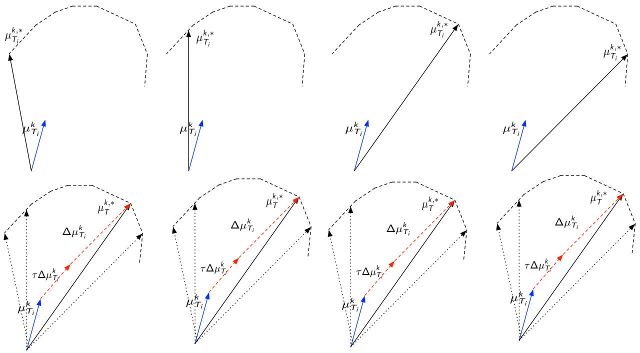
Conclusions

- Structured output learning is family of methods for multilabel classification.
- The output graph is often assume to be known *apriori*.
  - MMCRF assumes tree or general undirected graph as output graph.
  - SPIN assumes DAG as output graph.
  - Possible for exponential reduction of the search space.
- In addition, we focus on the problems where the output graph is unobserved.
  - MVE AMM MAM aggregates the inference results from based models.
  - RTA is a unified learning and inference framework.
    - Model all pairwise correlations with a complete graph.
    - Under margin assumption, the properties of a complete graph can be achieved by a collection of its spanning tree.
- All developed models are tested with real-world applications or benchmark datasets.
- Codes are available from http://hongyusu.github.io.

Ongoing work

Optimization for RTA with Juho Rousu

- From K-best inference algorithm
- To a Newton method: a conic combination of multiple update directions



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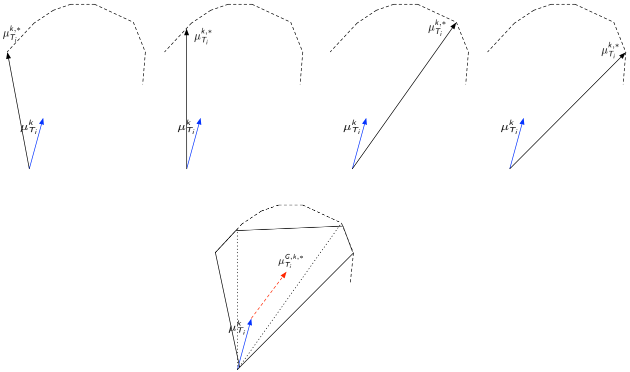

Ongoing work

L_1 norm RTA with John Shawe-Taylor, Mario Marchand

- From conic combination of a collection of random spanning trees

$$F(\mathbf{w},\mathbf{x},\mathbf{y}) = \mathop{\mathbf{E}}_{T\in U(G)} a_T \langle \mathbf{w}_T, \boldsymbol{\phi}_T(\mathbf{x},\mathbf{y})\rangle \quad \mathop{\mathbf{E}}_{T\in U(G)} a_T^2 = 1, \mathop{\mathbf{E}}_{T\in U(G)} a_T < 1.$$

- To convex combination of a collection of random spanning trees

$$F(\mathbf{w},\mathbf{x},\mathbf{y}) = \mathop{\mathbf{E}}_{T\in U(G)} a_T \langle \mathbf{w}_T, \boldsymbol{\phi}_T(\mathbf{x},\mathbf{y})\rangle \quad \mathop{\mathbf{E}}_{T\in U(G)} a_T = 1, \mathop{\mathbf{E}}_{T\in U(G)} a_T < 1.$$

- Optimization problem (tree selection!)

$$\begin{aligned}
\min_{\mathbf{w}_{T_i},\xi_i} \quad & \frac{1}{2}\left(\sum_{i=1}^{n} ||\mathbf{w}_{T_i}||\right)^2 + C\sum_{k=1}^{m}\xi_k \\
\textbf{s.t.} \quad & \frac{1}{n}\sum_{i=1}^{n}\langle \mathbf{w}_{T_i}, \boldsymbol{\phi}_{T_t}(\mathbf{x}_k,\mathbf{y}_k)\rangle - \max_{\mathbf{y}\neq\mathbf{y}_k}\frac{1}{n}\sum_{i=1}^{n}\langle \mathbf{w}_{T_t}, \boldsymbol{\phi}_{T_i}(\mathbf{x}_k,\mathbf{y})\rangle \geq 1-\xi_k, \\
& \xi_k \geq 0\,, \forall\ k \in \{1,\dots,m\}.
\end{aligned}$$

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