



Aalto University
School of Science
and Technology

Structured output prediction for multilabel classification

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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>

Multilabel classification

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

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

- ▶ 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} , $f : \mathcal{X} \rightarrow \mathcal{Y}$.

Concerns

- ▶ Exponential Search space!

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

- ▶ 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.

$x_0 =$



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

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.

$\mathbf{x}_0 =$



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

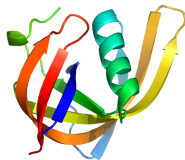
Flat classification approach

- ▶ The scheme is proposed in [Tsoumakas et al., 2010]
- ▶ The output variable \mathbf{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.

$\mathbf{x}_0 =$



$G =$

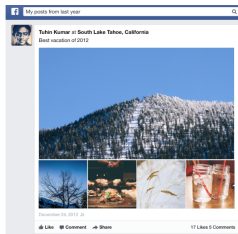
- 1: Channels/Pores
- 2: Electrochemical Potential-driven Transporters
 - 2.A: Porters (uniporters, symporters, antiporters)
 - 2.B: Nonribosomally synthesized porters
 - 2.C: Ion-gradient-driven energizers
 - 2.D: Transcompartment Lipid Carrier
 - 2.D.1: The PI4P/PS Counter Transporter (P/P-CT) Family
- 3: Primary Active Transporters
- 4: Group Translocators
- 5: Transmembrane Electron Carriers
- 8: Accessory Factors Involved in Transport
- 9: Incompletely Characterized Transport Systems

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Output correlation structure (cont.)

- Social network, information can spread through multiple users.

$x_0 =$



$G =$



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

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], M²CRF [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 $(\mathbf{x}, \mathbf{y}) \in \mathcal{X} \times \mathcal{Y}$.
- ▶ \mathcal{X} is an arbitrary input space.
- ▶ \mathcal{Y} is an output space of a collection of ℓ -dimensional *multilabels*.

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

- ▶ y_i is a *microlabel* and $y_i \in \{1, \dots, r_i\}$, $r_i \in \mathbb{Z}$.
- ▶ 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 $\phi(\mathbf{x}, \mathbf{y})$.
- ▶ \mathbf{w} is the weight vector operates in the joint feature space.
- ▶ Define a linear score function $F(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{w}, \phi(\mathbf{x}, \mathbf{y}) \rangle$.
- ▶ \mathbf{w} ensures that example \mathbf{x}_i with correct multilabel \mathbf{y}_i achieves higher score than with any other incorrect multilabel $\mathbf{y}' \in \mathcal{Y}$.

Prediction

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

$$\mathbf{y}_w(\mathbf{x}) = \underset{\mathbf{y} \in \mathcal{Y}}{\operatorname{argmax}} \langle \mathbf{w}, \phi(\mathbf{x}, \mathbf{y}) \rangle. \quad (1)$$

- ▶ Search space is exponential in size, $|\mathcal{Y}| = 2^\ell$.
- ▶ (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 *a priori*.



- ▶ $\varphi(\mathbf{x}) \in \mathbb{R}^d$ is the input feature map, e.g., bag-of-words of a document.
- ▶ $\psi(\mathbf{y}) \in \mathbb{R}^{|E|}$ 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 $\psi(\mathbf{y})$

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

$\underbrace{\hspace{10em}}_{(v_1, v_3)} \quad \underbrace{\hspace{10em}}_{(v_1, v_2)} \quad \underbrace{\hspace{10em}}_{(v_3, v_4)}$

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

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

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



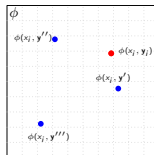
- The score function can be factorized by the output graph G

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

Optimization problem

- Max-margin learning for \mathbf{w}

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



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

$$\min_{\mathbf{w}, \xi_k} \quad \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{k=1}^m \xi_k \quad (2)$$

$$\begin{aligned} \text{s.t.} \quad & \langle \mathbf{w}, \phi(\mathbf{x}_k, \mathbf{y}_k) \rangle - \langle \mathbf{w}, \phi(\mathbf{x}_k, \mathbf{y}) \rangle \geq \ell(\mathbf{y}_k, \mathbf{y}) - \xi_k, \\ & \xi_k \geq 0, \forall \mathbf{y} \in \mathcal{Y}, k \in \{1, \dots, m\}. \end{aligned}$$

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

Marginal-dual optimization

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

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

- ▶ (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]

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

- ▶ The margin-dual optimization problem is

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

- ▶ 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

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

- ▶ 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

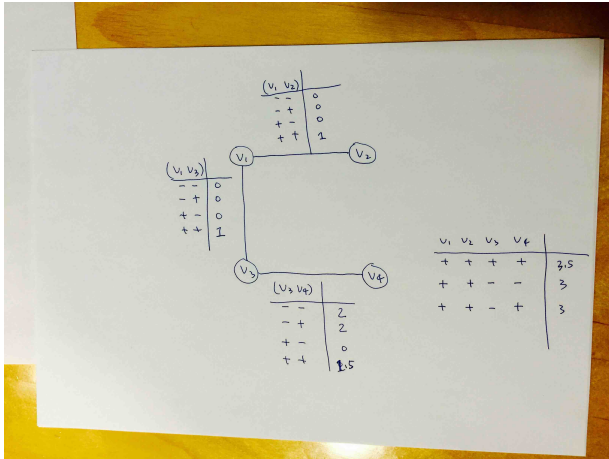
$$\mu_k^* = \operatorname{argmax}_{\mu_k \in \mathcal{M}} \mu_k^\top g_k = \operatorname{argmax}_{\mu_k \in \mathcal{M}} \sum_e \mu(k, e)^\top g(k, e). \quad (5)$$

- ▶ 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 happening?



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

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

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

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

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

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

Short summary

- We have seen so far.

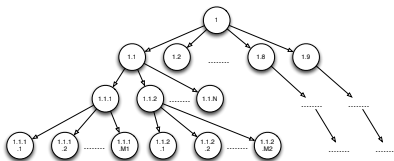
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- What if the solution corresponds to some special structure?

Exponential reduction in search space

Transporter protein classification [Su et al., 2015]

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



- ▶ It seems: $|\mathcal{Y}| = 2^{3145}$, DP on G .
- ▶ A valid annotation is a path from root to leaf, $|\mathcal{Y}| = 2000$
- ▶ The primal optimization problem is defined as

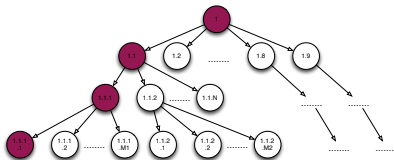
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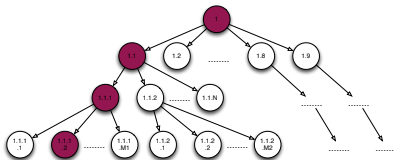
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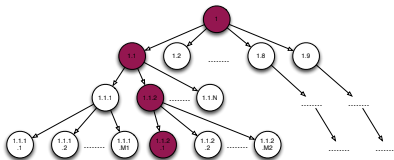
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Actual model

- ▶ In stead of conditional gradient descent, we can do gradient descent for all training examples.
- ▶ Multi-view data: 30 set of features, $\{\phi(\mathbf{x}_i)_k\}_{k=1}^{30}$.
- ▶ Multiple kernel learning ALIGNF.
- ▶ Results:

| | 0/1 | | | | | |
|--------|---------------|------|-------|-----------------|------|-------|
| | <i>Linear</i> | | | <i>Gaussian</i> | | |
| | SVM | MMR | MMCRF | SVM | MMR | MMCRF |
| 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

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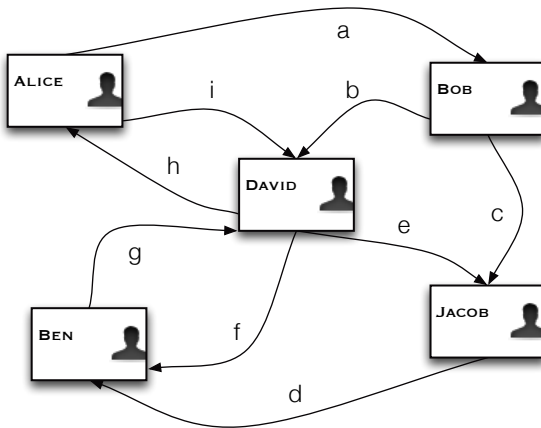
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| Pattern | Exponential reduction | [Su et al., 2015] |

- What if the output graph is DAG ?

Output graph is DAG

Predicting network response [Su et al., 2014]

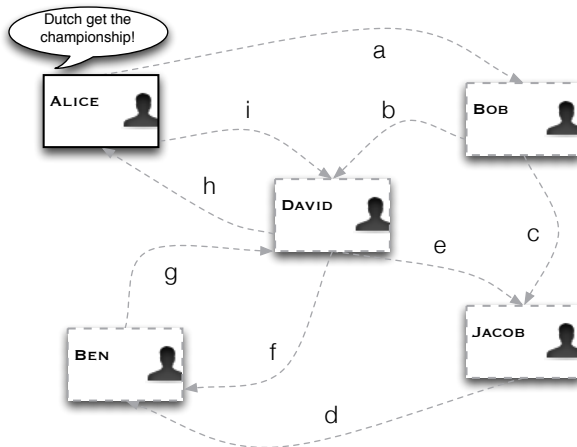
A Twitter (follower-ship) network consists of five users.



Output graph is DAG

Predicting network response [Su et al., 2014]

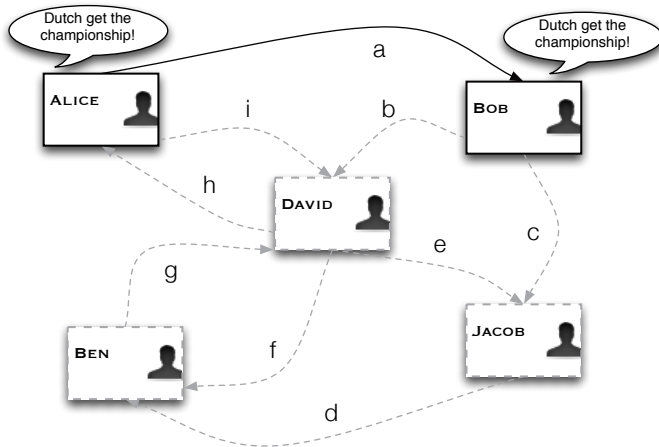
Alice tweets after World Cup final.



Output graph is DAG

Predicting network response [Su et al., 2014]

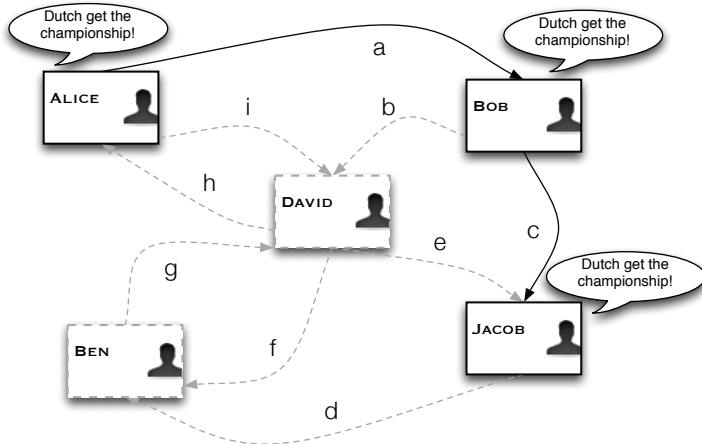
Bob saw the tweet and retweets from Alice.



Output graph is DAG

Predicting network response [Su et al., 2014]

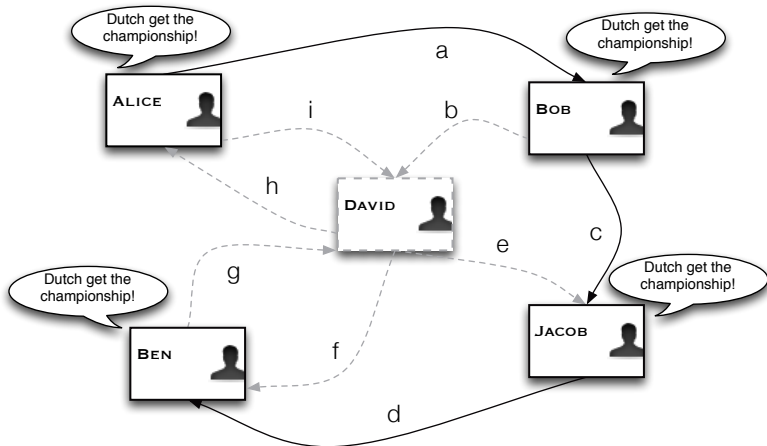
Jacob retweets from Bob.



Output graph is DAG

Predicting network response [Su et al., 2014]

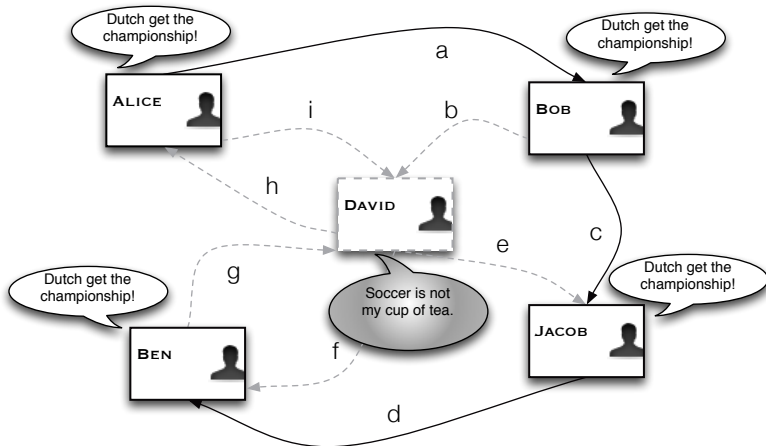
Ben retweets from Jacob.



Output graph is DAG

Predicting network response [Su et al., 2014]

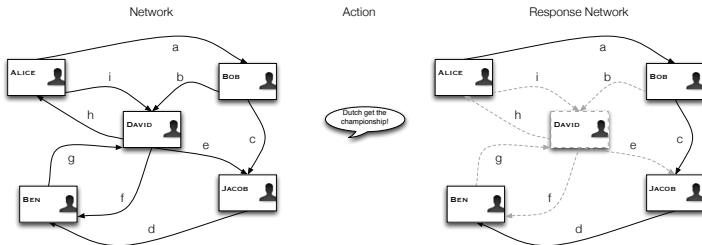
David is not a fan.



Network response problem

► Definition:

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



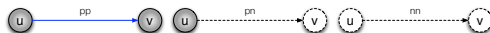
- **Applications:** Information propagation, idea formation, disease spreads, adoption of new technologies.

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.

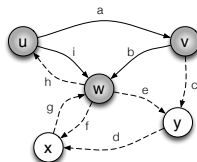


- ▶ Notation of edge labels:



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

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



Structure output prediction model

- ▶ Compatibility score for (\mathbf{x}, \mathbf{y}) : $F(\mathbf{x}, \mathbf{y}, \mathbf{w}) = \langle \mathbf{w}, \phi(\mathbf{x}, \mathbf{y}) \rangle$
 - ▶ \mathbf{w} is the feature weight to be learned.
 - ▶ $\phi(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x}) \otimes \psi(\mathbf{y})$ 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

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

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}

$$H^*(\mathbf{x}) = \operatorname{argmax}_{H \in \mathcal{H}(G)} \sum_{e \in E_H} s_{y_e}(e, \mathbf{x}, \mathbf{w}). \quad (8)$$

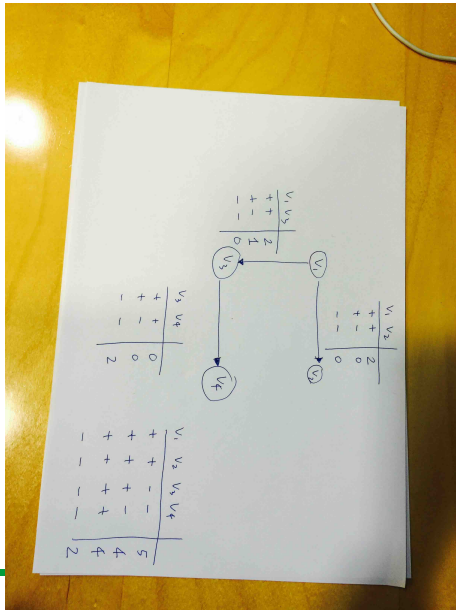
Lemma

Finding the graph that maximizes Eq. (8) is an \mathcal{NP} -hard problem.

Proof.

Reduction from MAX-CUT problem. □

What is happening?



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.

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

- ▶ 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.

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] |
| Pattern | Exponential 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 ϕ 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.
- ▶ $\varphi(\mathbf{x})$ is the input feature map, e.g., bag-of-words feature of an example \mathbf{x} .
- ▶ $\psi(\mathbf{y})$ is the output feature map which is a collection of edges and labels

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

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

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

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

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

Inference in terms of all spanning trees

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

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

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

- ▶ 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 $T \in \mathcal{S}(G)$.
- ▶ $\mathbf{w}_T = \{\mathbf{w}_{G,e}\}_{e \in T}$ is the projection of \mathbf{w}_G on $T \in \mathcal{S}(G)$.
- ▶ We can write $F(\mathbf{w}, \mathbf{x}, \mathbf{y})$ as a conic combination of all spanning trees

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

- ▶ $U(G)$ 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

$$F_{\mathcal{T}}(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \frac{1}{n} \sum_{i=1}^n a_{T_i} \langle \mathbf{w}_{T_i}, \phi_{T_i}(\mathbf{x}, \mathbf{y}) \rangle$$
$$\frac{1}{n} \sum_{i=1}^n a_{T_i}^2 = 1, \quad \frac{1}{n} \sum_{i=1}^n a_{T_i} < 1.$$

- ▶ When

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

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]

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

- ▶ 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

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

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

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

- ▶ 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

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

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

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

- ▶ 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 $\Theta(nK)$.

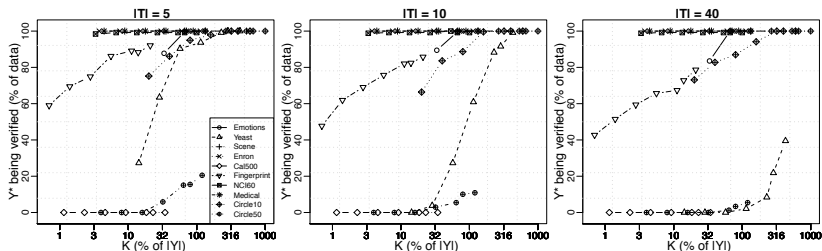
Short summary

- We have seen so far.

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

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 |

SPIN for context-sensitive prediction

- ▶ We assume action $\varphi(\mathbf{x})$ is known (e.g. bag-of-words 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 (10^3 s) | 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 |

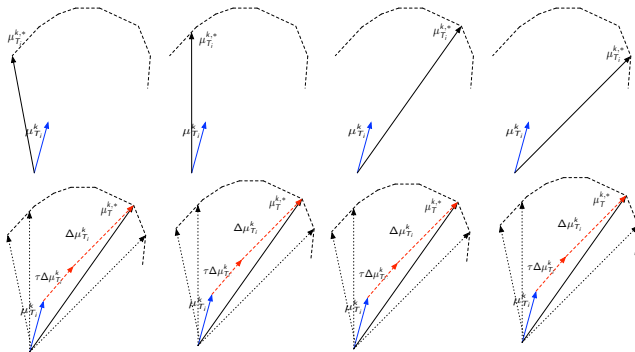
Conclusions

- ▶ Structured output learning is family of methods for multilabel classification.
- ▶ The output graph is often assume to be known *a priori*.
 - ▶ MMCRF assumes tree or general undirected graph as output graph.
 - ▶ SPIN assumes DAG as output graph.
- ▶ 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

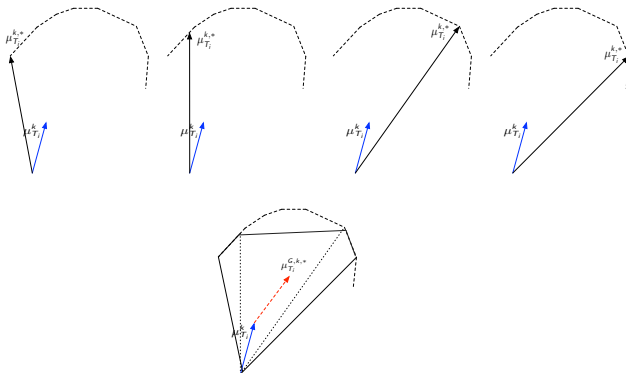
- From K-best inference algorithm
- To a Newton method: a conic combination of multiple update directions



Ongoing work

Optimization for RTA with Juho Rousu

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



Ongoing work

L_1 norm RTA with John Shawe-Taylor, Mario Marchand

- From conic combination of a collection of random spanning trees

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

- To convex combination of a collection of random spanning trees

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

- Optimization problem (tree selection!)

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

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