



Aalto University  
School of Science  
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# 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](http://www.hongyusu.com) and [my technical blog](http://www.hongyusu.com/pages.html).

<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  $\ell$  variables.
- ▶  $y$ : *multilabel*,  $y_j$ : *microlabel*.
- ▶ Output space  $\mathcal{Y}$  is composed by a tensor product of  $\ell$  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.

$\mathbf{x}_0 =$

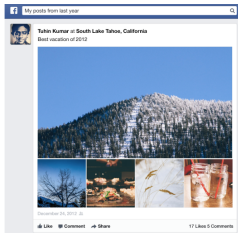


$$\mathbf{y} = ( \underbrace{+1}_{\alpha\text{-channel}}, \underbrace{+1}_{\beta\text{-barrel}}, \underbrace{+1}_{\text{holins}}, \underbrace{-1}_{\text{vesicle fusion pores}}, \underbrace{-1}_{\text{Phosphotransfer-driven Group}} )$$

# 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.

$\mathbf{x}_0 =$



$G =$

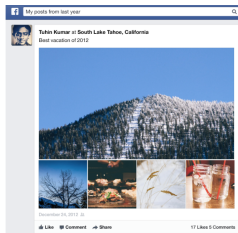
- 1: Channels/Pores
- 2: Electrochemical Potential-driven Transporters
  - 2.A: Porters (uniporters, symporters, antiporters)
  - 2.B: Nonribosomally synthesized porters
  - 2.C: Ion-gradient-driven energizers
  - 2.D: Transcompartment Lipid Carrier
    - 2.D.1: The PI4P/PS Counter Transporter (P/P-CT)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

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

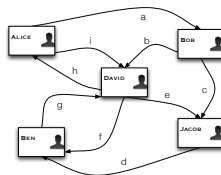
# Output correlation structure (cont.)

- Social network, information can spread through multiple users.

$x_0 =$



$G =$



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

# 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], MMCRF [Rousu et al., 2007, Su et al., 2010], SPIN [Su et al., 2014].
- ▶ These approaches assume the output graph is known *a priori*.
- ▶ More general, there is no pre-defined output graph!

# 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].
- ▶ Codes are available from <http://github.com/hongyusu>.

# The rest of the talk

- ▶ Preliminaries
- ▶ Structured output prediction
  - ▶ Undirected graph
  - ▶ DAG
  - ▶ 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  $\ell$ -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  $\phi$  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  $\psi(\mathbf{y})$

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



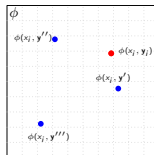
- The score function can be factorized by the output graph  $G$

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

# 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

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

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

- ▶ (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 optimization

- ▶ (4) is optimized by conditional gradient decent.
- ▶ In each iteration it optimizes  $\mu_k$  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  $\mu_k$  is given by  $g_k = \ell_k - \sum_j K \mu_j$ .
- ▶ Compute the maximal feasible solution  $\mu_k^*$  as an update direction

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

- ▶ (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  $\mu_k \leftarrow \mu_k + \tau(\mu_k^* - \mu_k)$ .



# Exact line search

- ▶ Line search gives the optimal feasible solution as a stationary point ( $\tau$ )

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

- ▶  $\tau = 0$  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  $\mu^t$

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

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

# Short summary

- We have seen so far.

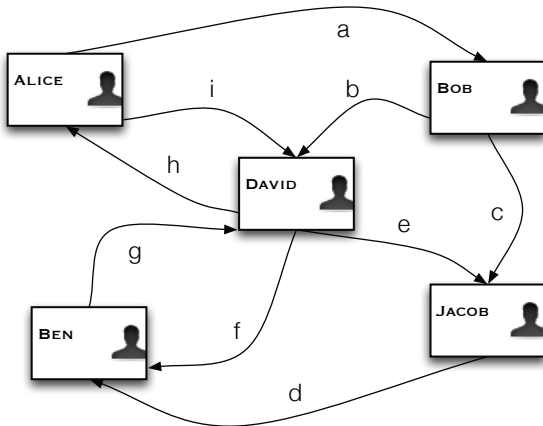
Output graph	Inference problem	Inference algorithm
Tree	Polynomial	DP [Rousu et al., 2007]
Graph	$\mathcal{NP}$ -hard	LBP [Su et al., 2010]

- What if the output graph is DAG ?

# Output graph is DAG

## Predicting network response [Su et al., 2014]

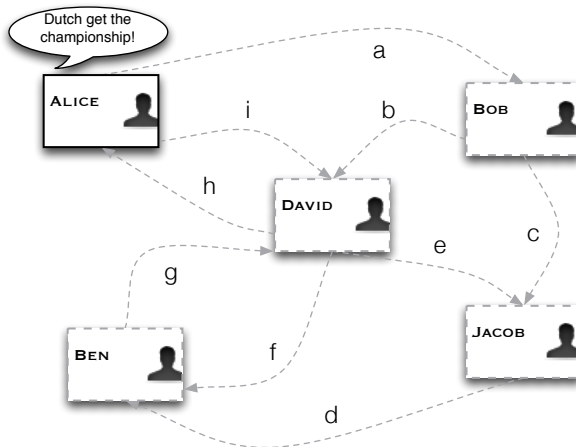
A twitter (follower-ship) network consists of five users.



# Output graph is DAG

Predicting network response [Su et al., 2014]

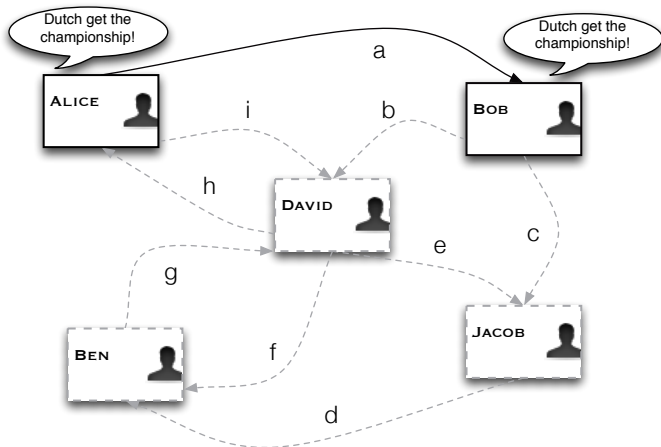
Alice tweets a message after World Cup final.



# Output graph is DAG

Predicting network response [Su et al., 2014]

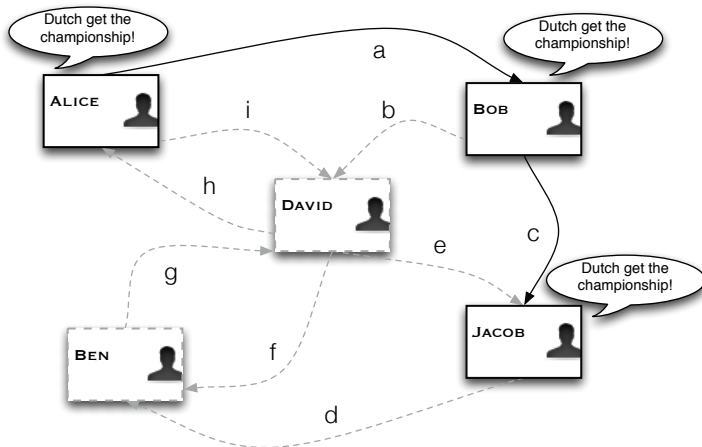
Bob sees the message and retweets the message from Alice.



# Output graph is DAG

Predicting network response [Su et al., 2014]

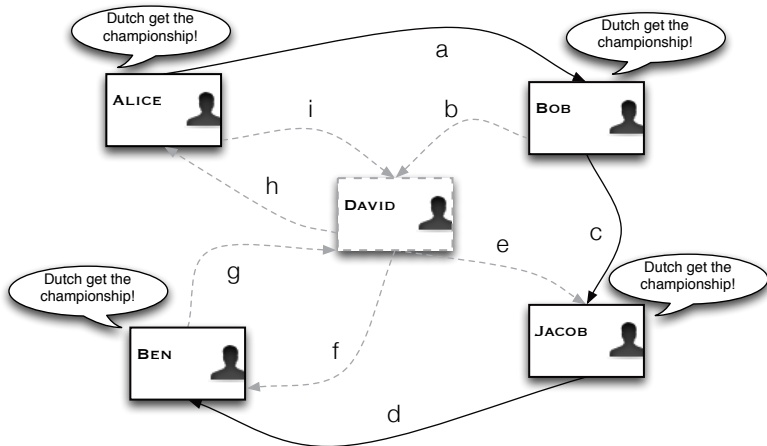
Jacob retweets the message from Bob.



# Output graph is DAG

Predicting network response [Su et al., 2014]

Ben retweets the message from Jacob.

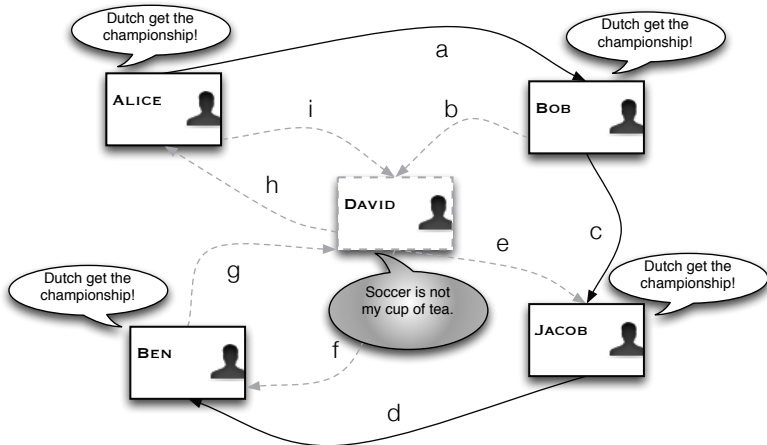




# Output graph is DAG

Predicting network response [Su et al., 2014]

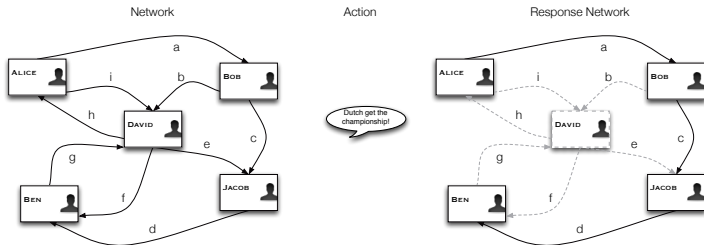
David is not a fan.



# Network response problem

- Definition:

- Given a complex network  $G = (E, V)$ , and an action  $x$  performed on the network.
- 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



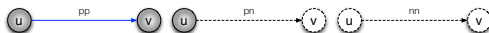
- Information propagation, idea formation, disease spreads, adoption of new technologies.

# 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.



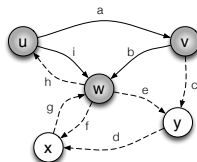
- Notation of edge labels:



- 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)

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

$\underbrace{++ \quad +- \quad --}_{a} \quad \underbrace{++ \quad +- \quad --}_{b} \quad \underbrace{++ \quad +- \quad --}_{c}$



# 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  $\mathbf{x}$

$$H^*(\mathbf{x}) = \operatorname{argmax}_{H \in \mathcal{H}(G)} \sum_{e \in E^H} s_{y_e}(e, \mathbf{x}, \mathbf{w}). \quad (7)$$

## Lemma

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

## Proof.

Reduction from MAX-CUT problem. □

# 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]
→ 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  $\phi$  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.
- ▶  $\varphi(\mathbf{x})$  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  $\ell$ .

# 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  $\mu_{T_i}$  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  $\text{RTA}$  is defined as finding the multilabel  $\mathbf{y}_{\mathcal{T}}(\mathbf{x})$  that maximizes the sum of scores over a collection of trees

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

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

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

- ▶ 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

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

- ▶ 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  $\Theta(nK)$ .

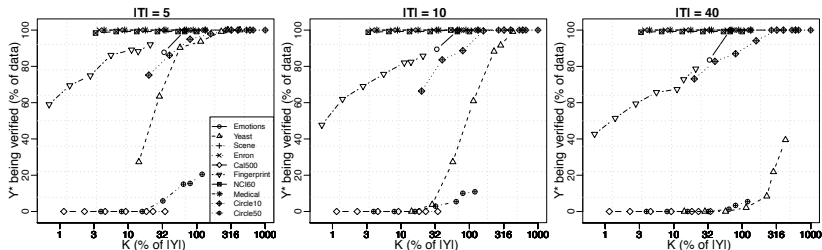
# Short summary

- We have seen so far.

Output graph	Inference problem	Inference algorithm
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Graph	$\mathcal{NP}$ -hard	LBP [Su et al., 2010]
DAG	$\mathcal{NP}$ -hard	SDP [Su et al., 2014]
→unknown	$\mathcal{NP}$ -hard	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	<b>18.8</b>	77.8	74.5	71.3	69.6	<b>66.3</b>
YEAST	20.0	20.7	21.7	20.1	<b>19.8</b>	85.9	88.7	93.0	86.0	<b>77.7</b>
SCENE	9.8	11.6	18.4	17.0	<b>8.8</b>	47.2	55.2	72.2	94.6	<b>30.2</b>
ENRON	6.4	6.5	6.2	<b>5.0</b>	5.3	99.6	99.6	92.7	87.9	<b>87.7</b>
CAL500	<b>13.7</b>	13.8	<b>13.7</b>	<b>13.7</b>	13.8	100.0	100.0	100.0	100.0	100.0
FINGERPRINT	<b>10.3</b>	17.3	10.5	10.5	10.7	99.0	100.0	99.6	99.6	<b>96.7</b>
NCI60	15.3	16.0	14.6	<b>14.3</b>	14.9	56.9	53.0	63.1	60.0	<b>52.9</b>
MEDICAL	2.6	2.6	<b>2.1</b>	<b>2.1</b>	<b>2.1</b>	91.8	91.8	63.8	63.1	<b>58.8</b>
CIRCLE10	4.7	6.3	2.6	2.5	<b>0.6</b>	28.9	33.2	20.3	17.7	<b>4.0</b>
CIRCLE50	5.7	6.2	<b>1.5</b>	2.1	3.8	69.8	72.3	<b>38.8</b>	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	<b>73.4</b>	68.0	72.2	39.0	39.8	<b>47.1</b>	<b>62.7</b>	45.6	23.4	25.3	<b>33.6</b>
memeM	<b>82.1</b>	79.0	81.5	29.1	30.1	<b>38.0</b>	61.1	<b>68.8</b>	18.6	18.8	<b>28.3</b>
memeL	<b>89.9</b>	88.3	89.8	26.7	27.1	<b>35.0</b>	45.5	<b>80.0</b>	17.7	18.9	<b>27.6</b>
M700	91.9	<b>94.1</b>	92.1	13.8	7.3	<b>14.2</b>	26.3	<b>93.0</b>	29.4	23.9	<b>34.4</b>
M1k	94.1	<b>95.8</b>	94.2	<b>10.9</b>	3.5	9.3	26.6	<b>94.7</b>	33.7	16.6	<b>35.2</b>
M2k	96.8	<b>97.6</b>	96.7	<b>6.2</b>	1.4	3.4	25.3	<b>97.6</b>	<b>34.6</b>	9.6	14.7
L700	89.7	<b>92.4</b>	89.7	16.2	9.4	<b>17.3</b>	26.5	<b>90.4</b>	9.5	6.7	<b>12.5</b>
L1k	92.4	<b>94.4</b>	91.5	12.4	6.4	<b>13.9</b>	26.4	<b>92.3</b>	6.1	4.4	<b>8.4</b>
L2k	92.5	<b>94.5</b>	91.9	12.3	5.4	<b>12.7</b>	26.5	<b>93.2</b>	6.0	2.9	<b>7.2</b>
<b>Geom.</b>	85.5	86.4	<b>86.6</b>	19.8	12.6	<b>20.3</b>	32.6	<b>79.7</b>	18.9	14.2	<b>21.7</b>

# 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	<b>82.9</b>	<b>81.0</b>	<b>76.0</b>	<b>74.0</b>	<b>74.0</b>	<b>70.0</b>
	ICM-EM	<b>0.01</b>	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	<b>82.7</b>	<b>72.1</b>	<b>70.5</b>	<b>69.2</b>	<b>69.2</b>	<b>67.9</b>
	ICM-EM	<b>0.02</b>	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	<b>82.2</b>	<b>73.6</b>	<b>69.1</b>	<b>66.7</b>	<b>66.7</b>	<b>65.9</b>
	ICM-EM	<b>0.01</b>	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

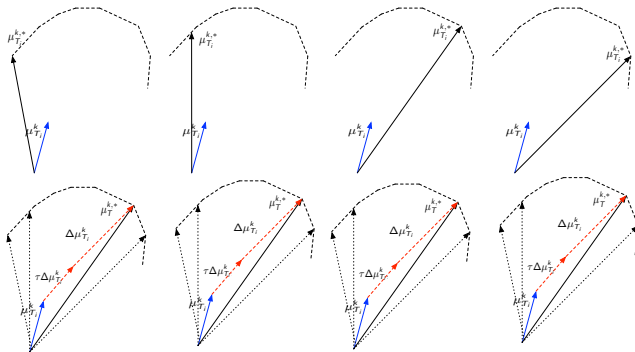
# Conclusions

- ▶ 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

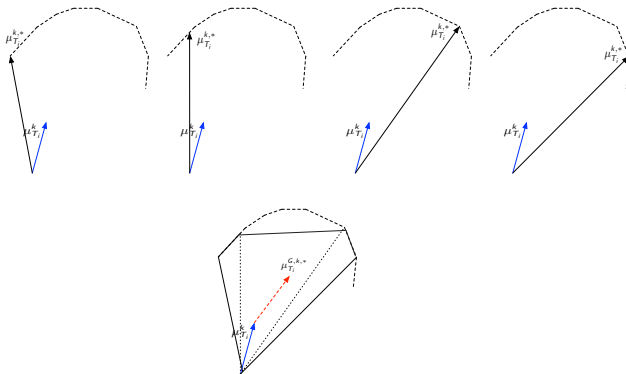
- From K-best inference algorithm
- To a Newton method: a conic combination of multiple update directions



# 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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