Structured output prediction for multilabel classification

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Multilabel classification

- *Multilabel classification* is an important research field in machine learning.
- Input variable $\mathbf{x} \in \mathcal{X}$ is in d dimensional input space $\mathcal{X} = \mathbb{R}^d$.
- Output variable $\mathbf{y} = (y_1, \cdots, y_l) \in \mathcal{Y}$ is a binary vector consist of l binary variables $y_j \in \{+1, -1\}$.
- $\mathbf{y}$ is called a multilabel, y_j is called a microlabel.
- Output space is composed by a Cartesian product of l sets

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

- For example, in document classification, a document $\mathbf{x}$ can be classified as "news", "movie", and "science"

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

- The goal is to find a mapping function $f \in \mathcal{H}$ that predicts the best values of an output given an input $f : \mathcal{X} \to \mathcal{Y}$.

Central problems in multilabel classification

▶ The size of the output space (searching space) is exponential in the number of microlabels.

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

▶ The dependency of microlabels needs to be exploited to improve the prediction performance.

　▶ If a document is about "movie", then it is more likely to be about "art" than "science".

Real world applications

▶ Social network, information can spread through multiple users.

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

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

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

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

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

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

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

Flat multilabel classification approaches

- The categorization is proposed in [Tsoumakas et al., 2010]

- Problem transformation
  - Model the multilabel classification as a collection of single-label classification problems and solve each problem independently.
  - For example, ML-KNN [Zhang and Zhou, 2007], CC [Read et al., 2009, Read et al., 2011], IBLR [Cheng and Hüllermeier, 2009].

- Algorithm adaptation
  - Modify the single-label classification algorithm for multilabel classification problems.
  - For example, ADABOOST.MH [Schapire and Singer, 1999, Esuli et al., 2008], CORRLOG [Bian et al., 2012], MTL [Argyriou et al., 2008].

- These approaches does not model the dependency structure explicitly.

Structured output prediction

- Model the dependency structure with an output graph defined on microlabels.
- The categorization is proposed in [Su, 2015].
- Hierarchical classification
  - The output graph is a rooted tree or a DAG defining different levels of granularities.
  - For example, SSVM [Tsochantaridis et al., 2004, Tsochantaridis et al., 2005].
- Graph labeling
  - The output graph takes a more general form (e.g., a tree, a chain).
  - For example, 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*.

Contributions

- Structured output prediction models when the output graph is known.
  - SPIN for network influence prediction [Su et al., 2014].
  - MMCRF to work with general output graph structures [Su et al., 2010].

- Structured output prediction models working with unknown output graph.

  - MVE to combine multiple structured output predictors with 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 trees [Marchand et al., 2014].

- Codes for developed models are available from http://hongyusu.github.io.

Outline

- Preliminaries
- Structured output learning with known output graph
- Structured output learning with unknown output graph
- Future work
- Experimental results

Preliminaries

- Training examples come in pairs $(\mathbf{x}, \mathbf{y}) \in \mathcal{X} \times \mathcal{Y}$.

- $\mathbf{x} \in \mathcal{X}$ is an arbitrary input space.

- $\mathcal{Y}$ is an output space of a collection of ℓ-dimensional *multilabels*.

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

- 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 $\phi(\mathbf{x}, \mathbf{y})$.

- $\mathbf{w}$ is the weight vector in the joint feature space.

- Define a linear score function $F(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{w}, \phi(\mathbf{x}, \mathbf{y}) \rangle$.

- $\mathbf{w}$ makes sure example $\mathbf{x}$ with correct multilabel $\mathbf{y}$ achieves higher score than with any other incorrect multilabel $\mathbf{y}' \in \mathcal{Y}$.

Inference problem

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

$$\mathbf{y_w}(\mathbf{x}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) \rangle. \qquad (1)$$

▶ Search space $|\mathcal{Y}| = 2^{\ell}$ is exponential in size.

▶ (1) is called *inference* problem which is $\mathcal{NP}$-hard for most output feature maps.

▶ We aim at using an output 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.
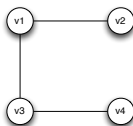- G models potential pairwise correlations.

- $\varphi(\mathbf{x}) \in \mathbb{R}^d$ 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 output feature map

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

- Multilabel $\mathbf{y}$

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

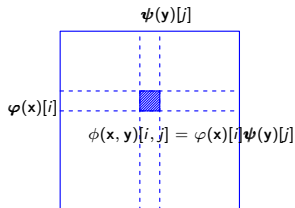- Output feature map $\boldsymbol{\psi}(\mathbf{y})$

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

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

Joint feature map

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

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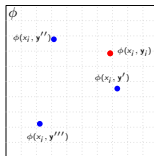

▶ The score function can be factorized by the output graph G

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

Optimization problem

▶ To learn parameter **w**, we aim to maximize the magin between correct pair $(\mathbf{x}_i, \mathbf{y}_i)$ and all the other incorrect pairs $(\mathbf{x}_i, \mathbf{y}), \mathbf{y} \in \mathcal{Y}/\mathbf{y}_i$ in the joint feature space ϕ.

▶ The model is max-margin conditional random field MMCRF [Rousu et al., 2007, Su et al., 2010].

▶ The primal optimization problem is defined as

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

$$\text{s.t.} \quad \langle \mathbf{w}, \phi(\mathbf{x}_k, \mathbf{y}_k) \rangle - \langle \mathbf{w}, \phi(\mathbf{x}_k, \mathbf{y}) \rangle \geq \ell(\mathbf{y}_k, \mathbf{y}) - \xi_k,$$

$$\xi_k \geq 0, \forall \, \mathbf{y} \in \mathcal{Y}, k \in \{1, \ldots, m\}.$$

▶ $\ell(\mathbf{y}, \mathbf{y}_i)$ 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

$$\max_{\alpha \geq 0} \quad \alpha^\intercal \ell - \frac{1}{2} \alpha^\intercal K \alpha \tag{3}$$

$$\text{s.t.} \quad \sum_{\mathbf{y} \in \mathcal{Y}} \alpha(i, \mathbf{y}) \leq C, \; \forall i \in \{1, \cdots, m\}.$$

- (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]

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

- 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 variable is $m \times 4|E|$.

Conditional gradient optimization

▶ (4) is optimized by conditional gradient decent which 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 a feasible solution μ_k^* as an update direction

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

▶ (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 (τ)

$$\max_{\tau} \quad g(\mu_k + \tau\Delta\mu_k) \qquad (6)$$

$$\text{s.t.} \quad 0 \leq \tau \leq 1.$$

- $\tau = 0$ corresponds to no update.
- Feasible maximum update is achieved at $\tau = 1$.
- The cost of computing (8) is significantly smaller than the cost of computing (5).

Compute duality gap

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

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

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

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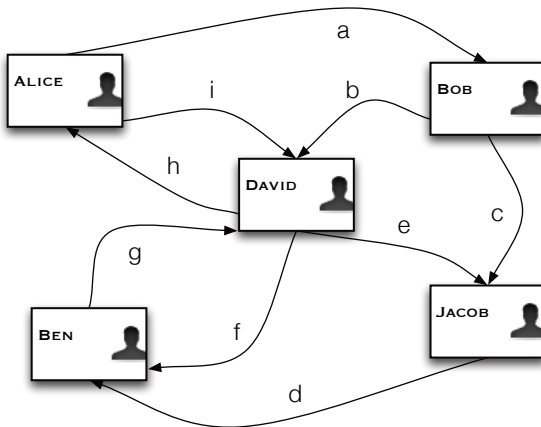- Duality gap at μ^t

$$f(\mathbf{w}^t) - g(\mu^t) = C\left(\ell - K^{\Delta\boldsymbol{\phi}}\mu^t\right) - \mu^t\left(\ell - K^{\Delta\boldsymbol{\phi}}\mu^t\right)$$

$$= C^\mathsf{T}\nabla g(\mu^t) - \mu^{t\mathsf{T}}\nabla g(\mu^t)$$

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

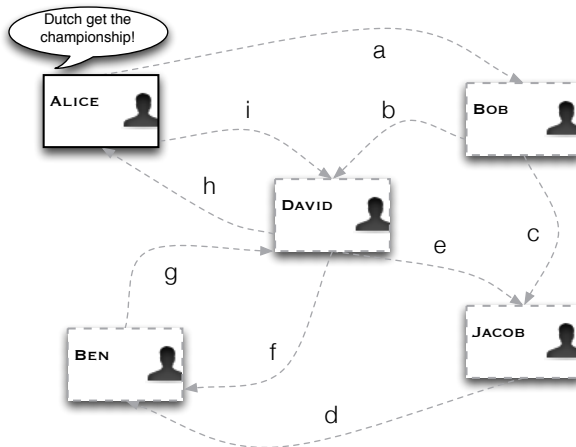# Output graph is directed

Predicting network response

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

Output graph is directed
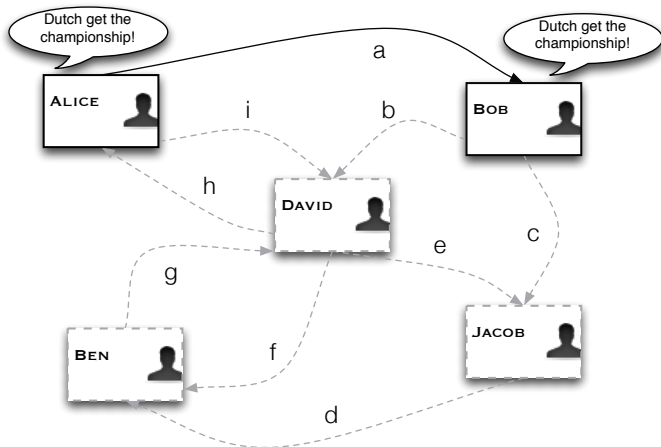
Predicting network response

Alice tweets a message after World Cup final.

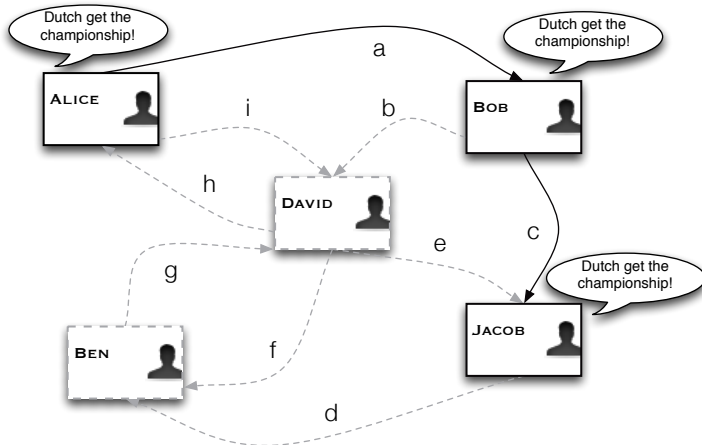# Output graph is directed

Predicting network response

Bob sees the message and retweets the message from Alice.

Output graph is directed

Predicting network response

Jacob retweets the message from Bob.

Output graph is directed

Predicting network response

Ben retweets the message from Jacob.
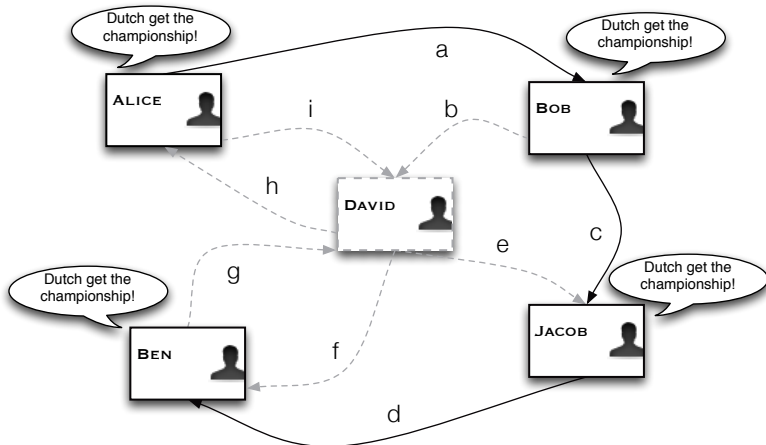
Output graph is directed

Predicting network response

David does not like soccer.
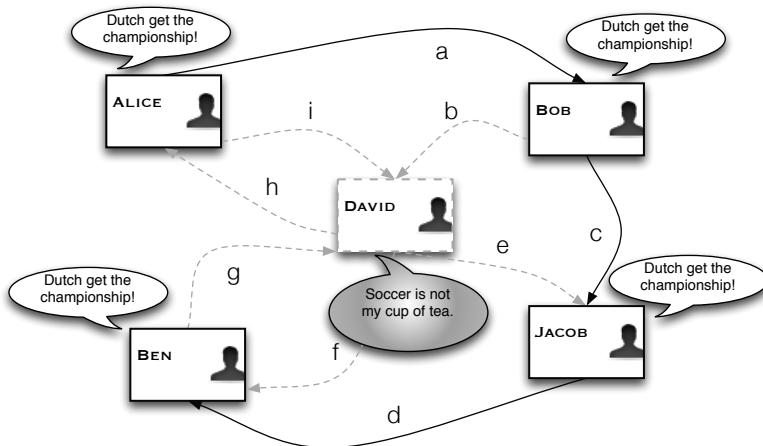
Network Response Problem

- Definition:
  - Given a complex network $G = (E, V)$, and an action **x** performed on the network.
  - 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? $E_{\mathbf{x}} = \{a, c, d\}$
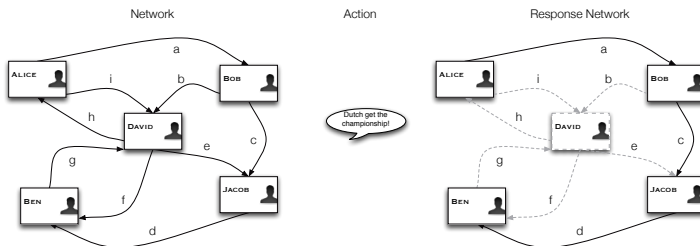
Direct output graph

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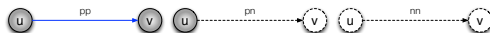
- *Input feature*: Encode $\mathbf{x}$ as $\boldsymbol{\varphi}(\mathbf{x})$ (e.g. bag-of-word of a tweet).
- *Output feature*: Encode $G_\mathbf{y}$ as $\boldsymbol{\psi}(\mathbf{y})$ (e.g. a set of edges and their labels)

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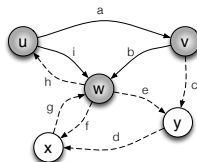
Structure Output Prediction Model

- 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.
  - $\boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) = \boldsymbol{\varphi}(\mathbf{x}) \otimes \boldsymbol{\psi}(\mathbf{y})$ 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

$$\min_{\mathbf{w}, \xi} \quad \frac{1}{2} \|\mathbf{w}\|_2^2 + C \sum_{i=1}^{m} \xi_i$$

$$\text{s.t.} \quad F(\mathbf{x}_i, \mathbf{y}_i; \mathbf{w}) > \max_{G'_{\mathbf{x}_i} \in \mathcal{H}(G)} (F(\mathbf{x}_i, \mathbf{y}'_i,)$$

$$+ \ell_G(\mathbf{y}_i, \mathbf{y}'_i)) - \xi_i, \xi_i \geq 0, \forall i \in \{1, \cdots, m\},$$

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 $\mathbf{x}$

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

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.

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

- 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.

So far in sides

▶ We develop structured output prediction model which model the label correlation with an output graph.

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 is hidden in many applications.
    - For example, a surveillance photo can be tagged with "building", "road", "pedestrian", and "vehicle".
- We study the problem in structured output learning when the output graph is not observed.
- In particular:
    - Assume the dependency can be expressed by a complete set of pairwise correlations.
    - Build a structured output learning model with a complete graph as the output graph.
    - Solve the $\mathcal{NP}$-hardinference problem on the complete graph by a polynomial time algorithm.
- 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 is a 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

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

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

- 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

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

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

- $U(G)$ 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 $n \in \Theta(\ell^2/\delta^2)$ 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]

$$\min_{\mathbf{w}_{T_i}, \xi_i} \quad \frac{1}{2} \sum_{i=1}^{n} ||\mathbf{w}_{T_i}||^2 + C \sum_{k=1}^{m} \xi_k$$

$$\text{s.t.} \quad \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \langle \mathbf{w}_{T_i}, \boldsymbol{\phi}_{T_t}(\mathbf{x}_k, \mathbf{y}_k) \rangle - \max_{\mathbf{y} \neq \mathbf{y}_k} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \langle \mathbf{w}_{T_t}, \boldsymbol{\phi}_{T_i}(\mathbf{x}_k, \mathbf{y}) \rangle \geq 1 - \xi_k,$$

$$\xi_k \geq 0, \forall \; k \in \{1, \ldots, m\}.$$

▶ The marginal-dual form is given by

$$\max_{\mu \in \mathcal{M}} \quad \sum_{i=1}^{n} \left(\mu_{T_i} \ell_{T_i} - \frac{1}{2} \mu_{T_i} K_{T_i}^{\Delta \boldsymbol{\phi}} \mu_{T_i} \right)$$

$$\text{s.t.} \quad \sum_{u_e} \mu_{T_i,e}(u_e) \leq C.$$

▶ 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

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

▶ 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

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

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

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

- 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 $\Theta(nK)$.

Exact line search for a single tree
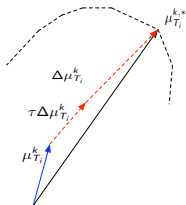
▶ Line search gives the optimal feasible solution as a stationary point (τ)

$$\max_{\tau} \quad f(\mu_{T_i}^k + \tau \Delta \mu_{T_i}^k) \qquad (8)$$

$$\textbf{s.t.} \quad 0 \leq \tau \leq 1.$$

▶ $\tau = 0$ corresponds to no update.

▶ Feasible maximum update is achieved at $\tau = 1$.

Optimization on a collection of n spanning trees
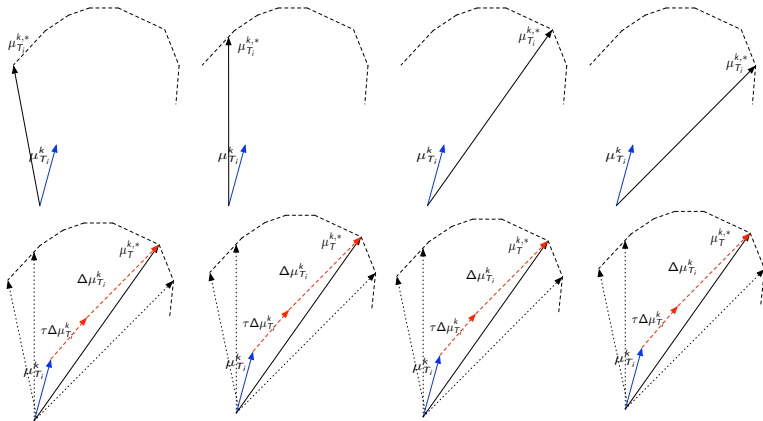
Exact line search for the collection of trees

▶ The step size along the update direction τ is given by the exact line search

$$\max_{\tau} \quad \sum_{i=1}^{n} f(\mu_{T_i}^k + \tau \Delta \mu_{T_i}^k)$$

$$\text{s.t.} \quad 0 \leq \tau \leq 1.$$

▶ Problems with the *best update*

1. The best feasible solution on a single tree might not be the best feasible solution on a collection of trees

$$\mu_T^{k,*} \notin {\mu_{T_i}^{k,*}}_{i=1}^{n}.$$

2. κ-best inference algorithm

$$(\mu_{T_i}^{k,*_h})_{h=1}^{\kappa} = \underset{\mu \in \mathcal{M}}{\text{argmax}} \, \mu^{\mathsf{T}} g_{T_i}^k, \, \forall i$$

$$\mu_T^{k,*} \in {\mu_{T_i}^{k,*_h}}_{i=\{1,\cdots,n\},h\in\{1,\cdots,\kappa\}}.$$

Update with multiple directions
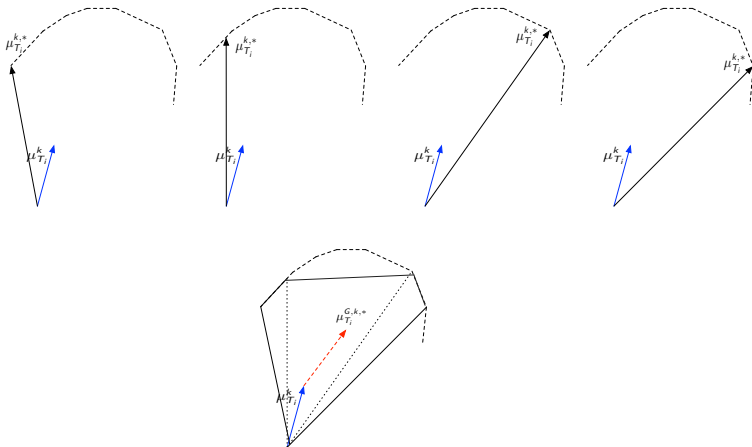
Newton method to compute τ

- We want to find τ that maximize the objective function given the update

$$\max_{\tau} \quad f(\mu^{G,k} + \Delta\mu^{G,k+1})$$

$$\text{s.t.} \quad 0 \leq \tau_i \leq 1,\ \sum_{i=1}^{n} \tau_i \leq 1,\ \forall i.$$

- The objective is quadratic with respect to τ.
- We use Newton method to find τ that maximize the objective.
- τ is projected into the feasible region.

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 $\Theta(nl^2)$.
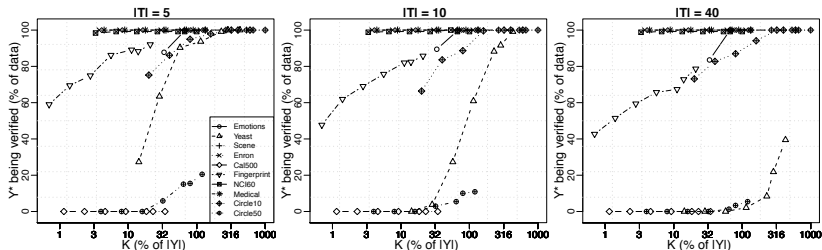
RTA on multilabel benchmark datasets

- ▶ 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-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 $(10^3 s)$	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*

Conclusion

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]
unknown	$\mathcal{NP}$-hard	RTA [Marchand et al., 2014]

Conclusion

- Structured output prediction is family of methods designed for multilabel classification problems.

- The output graph is often assume to known *apriori*.
  - 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.

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