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Structured output prediction for multilabel classification

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Multilabel classification

- *Multilabel classification* is an important research field in machine learning.
- Input variable $\mathbf{x} \in \boldsymbol{\mathcal{X}}$ is in d dimensional input space $\boldsymbol{\mathcal{X}} = \mathbb{R}^d$.
- Output variable $\mathbf{y} = (y_1, \cdots, y_l) \in \boldsymbol{\mathcal{Y}}$ 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

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

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

Central problems in multilabel classification

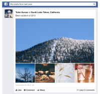
- The size of the output space (searching space) is exponential in the number of microlabels.

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

- 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.


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

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

- 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

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

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

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

Inference problem

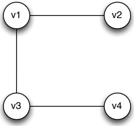
- The prediction $\mathbf{y}_\mathbf{w}(\mathbf{x})$ of an input $\mathbf{x}$ is the multilabel $\mathbf{y}$ that maximizes the score function

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

- Search space $|\boldsymbol{\mathcal{Y}}| = 2^{\ell}$ 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 $G = (E, V)$.
- 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.

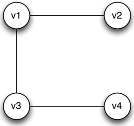


- $\varphi(\mathbf{x}) \in \mathbb{R}^d$ is the input feature map, e.g., bag-of-words of a document.
- $\boldsymbol{\psi}(\mathbf{y}) \in \mathbb{R}^{4|E|}$ is the output feature map which maps the multilabel $\mathbf{y}$ into a collection of edges and labels

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

An example of output feature map

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



- Multilabel $\mathbf{y}$

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

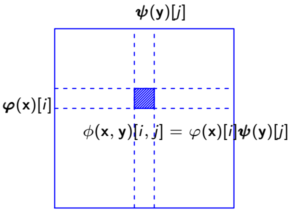
- Output feature map $\boldsymbol{\psi}(\mathbf{y})$

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

Joint feature map

- 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 output graph G

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

Primal optimization problem

- The primal optimization problem is defined as [Rousu et al., 2007, Su et al., 2010]

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

Structured output learning

- There is an *output graph* connecting multiple labels.
  - A set of nodes represents multiple labels.
  - A set of edges represents the correlation between labels.
- Hierarchical classification:
  - The output graph is a rooted tree or a directed graph defining different levels of granularities.
  - For example, SSVM, ...
- Graph labeling:
  - The output graph often takes a general form (e.g., a tree, a chain).
  - For example, M^3N, CRF, MMCRF, ...
- The output graph is assumed to be known *apriori*.

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 optimization problem and the inference problem ($\mathcal{NP}$-hard).

Today

- A structured prediction model which performs max-margin learning on a random sample of spanning tree.
- Two ways to combine the set of random spanning trees
  - conical combination in NIPS paper.
  - convex combination as future work.
- Derivations and the corresponding optimization problems.

Model

- Training examples comes in pair $S = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^m \in \boldsymbol{\mathcal{X}} \times \boldsymbol{\mathcal{Y}}$.
- A complete graph $G = (E, V)$ is used as the output graph.
- $\varphi(\mathbf{x})$ is the input feature map, e.g., a feature vector of d dimension.
- $\Gamma_G(\mathbf{y})$ is the output feature map of $\mathbf{y}$ on G of $4 \times |E|$ dimension

$$\Gamma_G(\mathbf{y}) = \{\Gamma_e(\mathbf{y}_e)\}_{e \in G},$$
$$\Gamma_e(\mathbf{y}_e) = [\mathbf{1}_{\mathbf{y}_e==00}, \mathbf{1}_{\mathbf{y}_e==01}, \mathbf{1}_{\mathbf{y}_e==10}, \mathbf{1}_{\mathbf{y}_e==11}]$$

- A joint feature map of $(\mathbf{x}_i, \mathbf{y}_i)$

$$\phi_G(\mathbf{x}_i, \mathbf{y}_i) = \varphi(\mathbf{x}_i) \otimes \Gamma_G(\mathbf{y}_i) = \{\phi_e(x_i, \mathbf{y}_{i,e})\}_{e \in G}.$$

- A compatibility score is defined as

$$F(\mathbf{x}, \mathbf{y}; \mathbf{w}_G) = \langle \mathbf{w}_G, \phi_G(\mathbf{x}, \mathbf{y}) \rangle = \sum_{e \in G} \langle \mathbf{w}_{G,e}, \phi_e(\mathbf{x}, \mathbf{y}_e) \rangle$$

Model (cont.)

- $\mathbf{w}$ ensures an input $\mathbf{x}_i$ with a correct multilabel $\mathbf{y}_i$ achieves a higher score than with any incorrect multilabel $\mathbf{y} \in \mathcal{Y}$.
- The predicted output $\mathbf{y}(\mathbf{x})$ for a given input $\mathbf{x}$ is computed by

$$\mathbf{y}(\mathbf{x}) = \operatorname*{\mathbf{argmax}}_{\mathbf{y} \in \boldsymbol{\mathcal{Y}}} F(\mathbf{x}, \mathbf{y}; \mathbf{w}_G) = \operatorname*{\mathbf{argmax}}_{\mathbf{y} \in \boldsymbol{\mathcal{Y}}} \sum_{e \in G} \langle \mathbf{w}_{G,e}, \phi_{G,e}(\mathbf{x}, \mathbf{y}_e) \rangle,$$

  which is called *inference problem*.
- The inference problem is $\mathcal{NP}$-hard for most joint feature maps on the complete graph.

How to learn w on a complete graph?

- The *margin* of an example $\mathbf{x}_i$ is

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

- $\mathbf{w}$ is solved by *max-margin principle* which aims to maximize $\gamma(\mathbf{x}_i; \mathbf{w}_G)$ over all training example $\mathbf{x}_i, i \in \{1, \cdots, m\}$.
- The inference problem on a complete graph is $\mathcal{NP}$-hardness.
- The parameter space is quadratic in the number of microlabels k.
- We aim to use a joint feature map that allows the inference problem be solved in polynomial time.

Superposition of random trees

- $S(G)$ is a complete set of spanning tree generate from G, $|S(G)| = \ell^{\ell-2}$.
- Recall
  $\phi_G(\mathbf{x},\mathbf{y}) = \{\phi_{G,e}(\mathbf{x},\mathbf{y}_e)\}_{e\in G}, \mathbf{w}_G = \{\mathbf{w}_{G,e}\}_{e\in G}, ||\phi_G(\mathbf{x},\mathbf{y})|| = ||\mathbf{w}_G|| = 1.$
- $\phi_T(\mathbf{x},\mathbf{y}) = \{\phi_e(\mathbf{x},\mathbf{y})\}_{e\in T}$ 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 $T \in S(G)$.
- Rewrite

$$
\begin{aligned}
F(\mathbf{x},\mathbf{y},\mathbf{w}_G) &= \sum_{e\in G}\langle \mathbf{w}_{G,e}, \phi_{G,e}(\mathbf{x},\mathbf{y}_e)\rangle \\
&= \frac{1}{\ell^{\ell-2}} \sum_{T\in S(G)} \sqrt{\frac{\ell}{2}}\langle \mathbf{w}_T, \phi_T(\mathbf{x},\mathbf{y}_e)\rangle \\
&= \frac{1}{n}\sum_{i=1}^{n} a_{T_i}\langle \hat{\mathbf{w}}_{T_i}, \hat{\phi}_{T_i}(\mathbf{x},\mathbf{y}_e)\rangle,
\end{aligned}
$$

$$
||\hat{\phi}_T(\mathbf{x},\mathbf{y})|| = ||\hat{\mathbf{w}}_T|| = 1,\ \frac{1}{n}\sum_{i=1}^{n} a_{T_i}^2 = 1,\ \frac{1}{n}\sum_{i=1}^{n} a_{T_i} \leq 1,\ a_{T_i} \geq 0,\ n = \ell^{\ell-2}.
$$

How many trees?

- If there is a predictor $\mathbf{w}_G$ on complete graph achieves a margin on some training data, with high probability we need n spanning tree predictors $\{\mathbf{w}_{T_i}\}_{i=1}^n$ to achieve a close margin. n is quadratic in terms of ℓ.
- Recall

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

$$||\hat{\phi}_{\mathcal{T}}(\mathbf{x}, \mathbf{y})|| = ||\hat{\mathbf{w}}_{\mathcal{T}}|| = 1, \frac{1}{n}\sum_{i=1}^{n} a_{T_i}^2 = 1, \frac{1}{n}\sum_{i=1}^{n} a_{T_i} \leq 1, a_{T_i} \geq 0, \cancel{n = \ell^{\ell-2}}.$$

Conical combination

- A sample $\mathcal{T} = \{T_1, \cdots, T_n\}$ of n spanning trees drawn from G.
- Normalized feature vectors $\hat{\phi}_{T_i}(\mathbf{x}, \mathbf{y}) = \frac{\phi_{T_i}(\mathbf{x},\mathbf{y})}{||\phi_{T_i}(\mathbf{x},\mathbf{y})||}$, $T_i \in \mathcal{T}$.
- Normalized feature weights $\hat{\mathbf{w}}_{T_i} = \frac{\mathbf{w}_{T_i}}{||\mathbf{w}_{T_i}||}$, $T_i \in \mathcal{T}$.
- Conical combination of spanning trees

$$F(\mathbf{x}, \mathbf{y}, \mathbf{w}_{\mathcal{T}}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} q_i \underbrace{\langle \hat{\mathbf{w}}_{T_i}, \hat{\phi}_{T_i}(\mathbf{x}, \mathbf{y}) \rangle}_{F(\mathbf{x},\mathbf{y},\mathbf{w}_{T_i})}$$

$$\sum_{i=1}^{n} q_i^2 = 1,\ q_i \geq 0,\ \forall i \in \{1, \cdots, n\}.$$

Conical combination (cont.)

- To solve $\{\mathbf{w}_{T_i}\}_{T_i \in \mathcal{T}}$, we need to work on the optimization problem

$$\min_{\xi,\gamma,\mathbf{q},\mathcal{W}} \quad \frac{1}{2\gamma^2} + \frac{C}{\gamma}\sum_{k=1}^{m}\xi_k$$

$$\text{s.t.} \quad \frac{1}{\sqrt{n}}\sum_{i=1}^{n} q_i \langle \hat{\mathbf{w}}_{T_i}, \hat{\phi}_{T_i}(\mathbf{x}_k,\mathbf{y}_k)\rangle - \max_{\mathbf{y}\in\boldsymbol{\mathcal{Y}}} \frac{1}{\sqrt{n}}\sum_{i=1}^{n} q_i \langle \hat{\mathbf{w}}_{T_i}, \hat{\phi}_{T_i}(\mathbf{x}_k,\mathbf{y})\rangle$$

$$\geq \gamma - \xi_k, \xi_k \geq 0, \forall k \in \{1,\cdots,m\}, \sum_{i=1}^{n} q_i^2 = 1, q_i \geq 0, \forall i \in \{1,\cdots,n\}.$$

- This is equivalent to

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

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

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

Inference Problem

- 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

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

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

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

- 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 Over 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 $\Theta(Kl)$ 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 in $\Theta(nKl)$ time

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

- For now, we assume the best scoring multilabel of a collection of trees exists in the list $\mathcal{Y}_{\mathcal{T},K}$.
- We proved that with a high probability $\mathbf{y}_{\mathcal{T}}$ will appear in $\mathcal{Y}_{\mathcal{T},K}$.
- We can identify $\mathbf{y}_{\mathcal{T}}$ from $\mathcal{Y}_{\mathcal{T},K}$.

Convex combination

- A sample $\mathcal{T}$ of n spanning trees drawn from G.
- Normalized feature weights $\hat{\mathbf{w}}_{T_i} = \frac{\mathbf{w}_{T_i}}{||\mathbf{w}_{T_i}||}$, $T_i \in \mathcal{T}$.
- Normalized feature vectors $\hat{\phi}_{T_i}(\mathbf{x}, \mathbf{y}) = \frac{\phi_{T_i}(\mathbf{x},\mathbf{y})}{||\phi_{T_i}(\mathbf{x},\mathbf{y})||}$, $T_i \in \mathcal{T}$.
- Convex combination of spanning trees

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

$$\sum_{i=1}^{n} q_i = 1,\ q_i \geq 0,\ \forall i \in \{1, \cdots, n\}.$$

Convex combination (cont.)

- To solve $\{\mathbf{w}_{T_i}\}_{T_i \in \mathcal{T}}$, we need to work on the optimization problem

$$\min_{\xi,\gamma,\mathbf{q},\mathcal{W}} \quad \frac{1}{2\gamma^2} + \frac{C}{\gamma}\sum_{k=1}^{m}\xi_k$$

$$\text{s.t.} \quad \frac{1}{n}\sum_{i=1}^{n} q_i\langle \hat{\mathbf{w}}_{T_i}, \hat{\phi}_{T_i}(\mathbf{x}_k,\mathbf{y}_k)\rangle - \max_{\mathbf{y}\in\mathcal{Y}}\frac{1}{n}\sum_{i=1}^{n} q_i\langle \hat{\mathbf{w}}_{T_i}, \hat{\phi}_{T_i}(\mathbf{x}_k,\mathbf{y})\rangle$$

$$\geq \gamma - \xi_k, \xi_k \geq 0, \forall k \in \{1,\cdots,m\}, \sum_{i=1}^{n} q_i = 1, q_i \geq 0, \forall i \in \{1,\cdots,n\}.$$

- This is equivalent to

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

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

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

Convex combination (cont.)

- This can be expressed equivalently as

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

Conclusions

- We show that if there is a learner $\mathbf{w}_G$ defined on a complete graph achieves a margin on some training data, then with a random collection of spanning tree learners $\{\mathbf{w}_{T_i}\}_{i=1}^{n}$ we can achieve a similar margin with high probability. Besides, n is polynomial in k.
- We propose two methods to combine the random collection of trees, namely, convex combination and conical combination.

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