Aalto University
School of Science
and Technology

Max-Margin Learning with A Random Sample of Spanning Trees

Hongyu Su

Helsinki Institute for Information Technology HIIT
Department of Computer Science
Aalto University

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Multilabel classification

- Multilabel classification is an important research field in machine learning.
  - For example, a document can be classified as "science", "genomics", and "drug discovery".
  - Each input variable $\mathbf{x} \in \boldsymbol{\mathcal{X}}$ is associated with multiple output variables $\mathbf{y} \in \boldsymbol{\mathcal{Y}}, \boldsymbol{\mathcal{Y}} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_l, \mathcal{Y}_i = \{+1, -1\}$.
  - The goal is to find a mapping function that predicts the best values of an output given an input $f \in \mathcal{H} : \boldsymbol{\mathcal{X}} \rightarrow \boldsymbol{\mathcal{Y}}$.
- The central problems of multilabel classification:
  - The size of the output space $\boldsymbol{\mathcal{Y}}$ is exponential in the number of microlabels.
  - The dependency of microlabels needs to be exploited to improve the prediction performance.

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, $\mathrm{M}^3\mathrm{N}$, 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

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

  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

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

- $\mathbf{w}$ 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

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

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

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

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

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

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

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

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

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

- This is equivalent to

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

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

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

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

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

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

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

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

Fast Inference 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 $\hat{\phi}_{T_i}(\mathbf{x}, \mathbf{y}) = \frac{\phi_{T_i}(\mathbf{x},\mathbf{y})}{||\phi_{T_i}(\mathbf{x},\mathbf{y})||}$, $T_i \in \mathcal{T}$.
- Conical 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

$$\begin{aligned}
\min_{\xi,\gamma,\mathbf{q},\mathcal{W}} \quad & \frac{1}{2\gamma^2} + \frac{C}{\gamma}\sum_{k=1}^{m}\xi_k \\
\textbf{s.t.} \quad & \frac{1}{n}\sum_{i=1}^{n} q_i \langle \hat{\mathbf{w}}_{T_i}, \hat{\phi}_{T_i}(\mathbf{x}_k,\mathbf{y}_k)\rangle - \max_{\mathbf{y}\in\boldsymbol{\mathcal{Y}}} \frac{1}{n}\sum_{i=1}^{n} q_i \langle \hat{\mathbf{w}}_{T_i}, \hat{\phi}_{T_i}(\mathbf{x}_k,\mathbf{y})\rangle \\
& \geq \gamma - \xi_k, \xi_k \geq 0, \forall k \in \{1,\cdots,m\}, \sum_{i=1}^{n} q_i = 1, q_i \geq 0, \forall i \in \{1,\cdots,n\}.
\end{aligned}$$

- This is equivalent to

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

Convex combination (cont.)

- This can be expressed equivalently as

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

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.
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