

Newton update in L₂-norm random tree approximation

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Preliminaries

- $ightharpoonup \mathcal{X}$ is an arbitrary input space, $\mathbf{x} \in \mathcal{X}$.
- $ightharpoonup \mathcal{Y}$ is an output space of a set of ℓ -dimensional *multilabels*

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

- y_i is a microlabel and $y_i \in \{1, \dots, r_i\}, r_i \in \mathbb{Z}$.
- ▶ For example, multilabel binary classification $y_i \in \{-1, +1\}$.
- ▶ Training examples are sampled from $(x, y) \in \mathcal{X} \times \mathcal{Y}$.
- **Each** example (x, y) is mapped into a joint feature space $\phi(x, y)$.
- **w** is the weight vector in the joint feature space.
- ▶ Define a linear score function $F(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{w}, \phi(\mathbf{x}, \mathbf{y}) \rangle$.
- ▶ The prediction $y_w(x)$ of an input x is the multilabel y that maximizes the score function

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

 (1) is called *inference* problem which is NP-hard for most output feature maps.



Markov network

- We assume that the output feature map ϕ is a potential function on a Markov network G = (E, V).
- ▶ *G* is a complete graph with $|V| = \ell$ nodes and $|E| = \frac{\ell(\ell-1)}{2}$ undirected edges.
- $ightharpoonup \varphi(x)$ is the input feature map, e.g., bag-of-words feature of an example x.
- $lackbox{}\psi(y)$ is the output feature map which is a collection of edges and labels

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

lacktriangle The joint feature is the Kronecker product of $oldsymbol{arphi}({ t x})$ and $oldsymbol{\psi}({ t y})$

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

The score function is

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



Inference in terms of all spanning trees

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

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

- ▶ For a complete graph, there are $\ell^{\ell-2}$ unique spanning trees.
- We can write $F(\mathbf{w}, \mathbf{x}, \mathbf{y})$ as a conic combination of all spanning trees

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

- ▶ U(G) is the uniform distribution over $\ell^{\ell-2}$ spanning trees.
- ▶ There is a exponential dependency on the number of spanning trees.

A sample of spanning trees

▶ Instead of using all spanning trees, we can just use *n* spanning trees

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

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 $\mathbf{x} \in \mathcal{X}$ is associated with multiple output variables $\mathbf{y} \in \mathcal{Y}, \mathcal{Y} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_l, \mathcal{Y}_i = \{+1, -1\}.$
 - ▶ The goal is to find a mapping function that predicts the best values of an output given an input $f \in \mathcal{H} : \mathcal{X} \to \mathcal{Y}$.
- ► The central problems of multilabel classification:
 - The size of the output space 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, M³N, 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 $(\mathcal{NP}\text{-hard}).$

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

$$\begin{split} & \Gamma_{\textit{G}}(\textbf{y}) = \{\Gamma_{e}(\textbf{y}_{e})\}_{e \in \textit{G}}, \\ & \Gamma_{e}(\textbf{y}_{e}) = [\textbf{1}_{\textbf{y}_{e}==00}, \textbf{1}_{\textbf{y}_{e}==01}, \textbf{1}_{\textbf{y}_{e}==10}, \textbf{1}_{\textbf{y}_{e}==11}] \end{split}$$

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

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

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.)

- w ensures an input x_i with a correct multilabel y_i achieves a higher score than with any incorrect multilabel y ∈ Y.
- ▶ The predicted output y(x) for a given input x is computed by

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

which is called inference problem.

 \blacktriangleright The inference problem is $\mathcal{NP}\text{-hard}$ 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

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

- **w** is solved by *max-margin principle* which aims to maximize $\gamma(\mathbf{x}_i; \mathbf{w}_G)$ over all training example $\mathbf{x}_i, i \in \{1, \dots, m\}$.
- lacktriangle The inference problem on a complete graph is \mathcal{NP} -hardness.
- ightharpoonup 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

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

$$||\hat{\phi}_{T}(\mathbf{x},\mathbf{y})|| = ||\hat{\mathbf{w}}_{T}|| = 1, \frac{1}{n} \sum_{i=1}^{n} a_{T_{i}}^{2} = 1, \frac{1}{n} \sum_{i=1}^{n} a_{T_{i}} \leq 1, \ a_{T_{i}} \geq 0, \ \text{ sector}.$$

Conical combination

- ▶ A sample $\mathcal{T} = \{T_1, \dots, T_n\}$ 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

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

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

Conical combination (cont.)

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

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

This is equivalent to

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

Inference Problem

▶ The inference problem of RTA is defined as finding the multilabel $y_{\mathcal{T}}(x)$ that maximizes the sum of scores over a collection of trees

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

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

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

▶ There is no guarantee that there exists a tree $T_t \in \mathcal{T}$ in which the maximizer of $F_{\mathcal{T}_t}$ 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 $\Theta(KI)$ 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 × K multilabels in Θ(nKI) time

$$\mathcal{Y}_{\mathcal{T},\kappa} = \mathcal{Y}_{\mathcal{T}_1,\kappa} \cup \cdots \mathcal{Y}_{\mathcal{T}_n,\kappa}.$$

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

$$F(\mathbf{x}, \mathbf{y}, \mathbf{w}_{T}) = \frac{1}{n} \sum_{i=1}^{n} q_{i} \langle \hat{\mathbf{w}}_{T_{i}}, \hat{\phi}_{T_{i}}(\mathbf{x}, \mathbf{y}) \rangle$$
$$\sum_{i=1}^{n} q_{i} = 1, \ q_{i} \geq 0, \ \forall i \in \{1, \cdots, n\}.$$

Convex combination (cont.)

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

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

This is equivalent to

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

Convex combination (cont.)

This can be expressed equivalently as

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

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.