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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

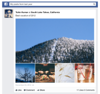
- The size of the output space (searching space) is exponential in the number of microlabels.

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

- 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 [?]
- Problem transformation
  - Model the multilabel classification as a collection of single-label classification problems and solve each problem independently.
  - For example, ML-KNN [?], CC [?, ?], IBLR [?].
- Algorithm adaptation
  - Modify the single-label classification algorithm for multilabel classification problems.
  - For example, ADABOOST.MH [?, ?], CORRLOG [?], MTL [?].
- 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 [**?**].
- Hierarchical classification
  - The output graph is a rooted tree or a DAG defining different levels of granularities.
  - For example, SSVM [**?**, **?**].
- Graph labeling
  - The output graph takes a more general form (e.g., a tree, a chain).
  - For example, CRF [**?**, **?**], $\mathrm{M}^3\mathrm{N}$ [**?**], MMCRF [**?**, **?**], SPIN [**?**].
- 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 [**?**].
  - MMCRF to work with general output graph structures [**?**].
- Structured output prediction models working with unknown output graph.
  - MVE to combine multiple structured output predictors with ensemble [**?**].
  - AMM and MAM to aggregate the inference results from multiple structured output predictors [**?**, **?**].
  - RTA to perform joint learning and inference over a collection of random spanning trees [**?**].
- 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 $(\mathbf{x}, \mathbf{y}) \in \boldsymbol{\mathcal{X}} \times \boldsymbol{\mathcal{Y}}$.
- $\mathbf{x} \in \boldsymbol{\mathcal{X}}$ 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

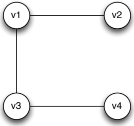
- The prediction $\mathbf{y}_{\mathbf{w}}(\mathbf{x})$ of an input $\mathbf{x}$ is the multilabel $\mathbf{y}$ that maximizes the score function

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

- Search space $|\mathcal{Y}| = 2^{\ell}$ is exponential in size.
- (**??**) 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.

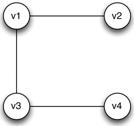


- $\varphi(\mathbf{x}) \in \mathbb{R}^d$ is the input feature map, e.g., bag-of-words of a document.
- $\boldsymbol{\psi}(\mathbf{y}) \in \mathbb{R}^{4|E|}$ is the output feature map which maps the multilabel $\mathbf{y}$ into a collection of edges and labels

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

An example of output feature map

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



- Multilabel $\mathbf{y}$

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

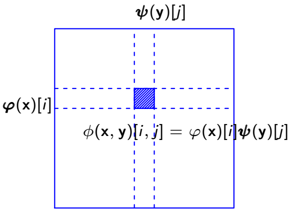
- Output feature map $\boldsymbol{\psi}(\mathbf{y})$

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

Joint feature map

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

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

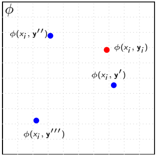


- The score function can be factorized by the output graph G

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

Optimization problem

- To learn parameter $\mathbf{w}$, 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 $\boldsymbol{\phi}$.



- The model is max-margin conditional random field MMCRF [?, ?].
- The primal optimization problem is defined as

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

- $\ell(\mathbf{y}, \mathbf{y}_i)$ scales the margin according to the multilabel $\mathbf{y}$.

Marginal-dual optimization

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

$$\max_{\alpha \geq 0} \quad \alpha^{\intercal}\ell - \frac{1}{2}\alpha^{\intercal}K\alpha \tag{3}$$
$$\textbf{s.t.} \quad \sum_{\mathbf{y}\in\mathcal{Y}} \alpha(i,\mathbf{y}) \leq C, \forall i \in \{1,\cdots,m\}.$$

- (**??**) is also challenging due to the exponential number of dual variables.
- We use edge marginals to replace the dual variables [**?**]

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

- 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

- (**??**) 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

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

- (**??**) is an instantiation of MAP problem
  - G is tree, exact inference with polynomial time algorithm, e.g, dynamic programming in [**?**]
  - G is general graph, approximate inference, e.g. loopy belief propagation in [**?**]
- 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)

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

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

Compute duality gap

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

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

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

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

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

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

So far in slides

- We have been working with multilabel classification problems in general.
- We assume label correlation is described an output graph given *apriori*.
- We develop structured output prediction model utilizing the output graph.
  - Tree, the inference problem can be solved exactly with a polynomial time algorithm, e.g., dynamic programming.
  - General graph, the inference problem is $\mathcal{NP}$-hard and can be solved with approximation algorithm, e.g., loopy belief propagation.
- 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 $\boldsymbol{\phi}$ 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.
- G models all pairwise correlations.
- $\boldsymbol{\varphi}(\mathbf{x})$ is the input feature map, e.g., bag-of-words feature of an example $\mathbf{x}$.
- $\boldsymbol{\psi}(\mathbf{y})$ is the output feature map which is a collection of edges and labels

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

- 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 complete graph G

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

Inference in terms of all spanning trees

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

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

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

- 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

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

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

- $U(G)$ 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 $F_{\mathcal{T}}(\mathbf{w},\mathbf{x},\mathbf{y})$ [?].

Random spanning tree approximation RTA

- The optimization problem of RTA is defined as [?]

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

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

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

- The marginal-dual form is given by

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

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

- 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

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

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

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

- 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 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

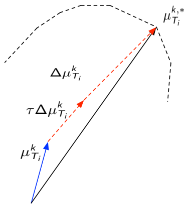
$$\mathcal{Y}_{T_t,K} = \{\mathbf{y}_{T_t,1}, \cdots, \mathbf{y}_{T_t,K}\}.$$

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

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

- 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

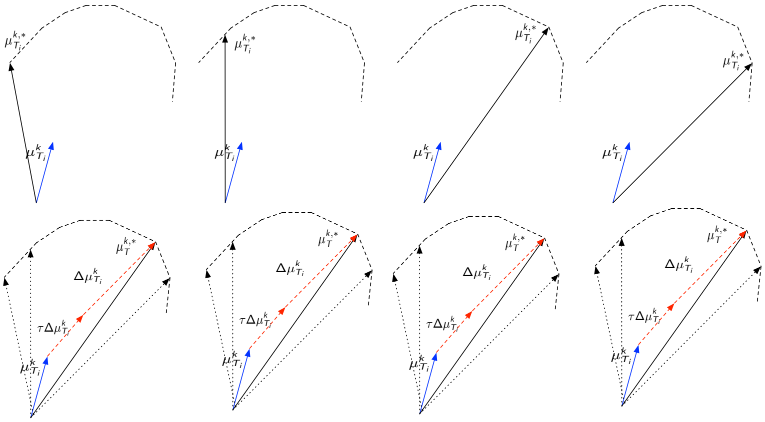


- Line search gives the optimal feasible solution as a stationary point (τ)

$$\begin{aligned} \max_{\tau} \quad & f(\mu_{T_i}^k + \tau\Delta\mu_{T_i}^k) \\ \textbf{s.t.} \quad & 0 \leq \tau \leq 1. \end{aligned} \tag{7}$$

- $\tau = 0$ 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

$$\begin{aligned} \max_{\tau} \quad & \sum_{i=1}^{n} f(\mu_{T_i}^{k} + \tau \Delta \mu_{T_i}^{k}) \\ \textbf{s.t.} \quad & 0 \leq \tau \leq 1. \end{aligned}$$

- 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

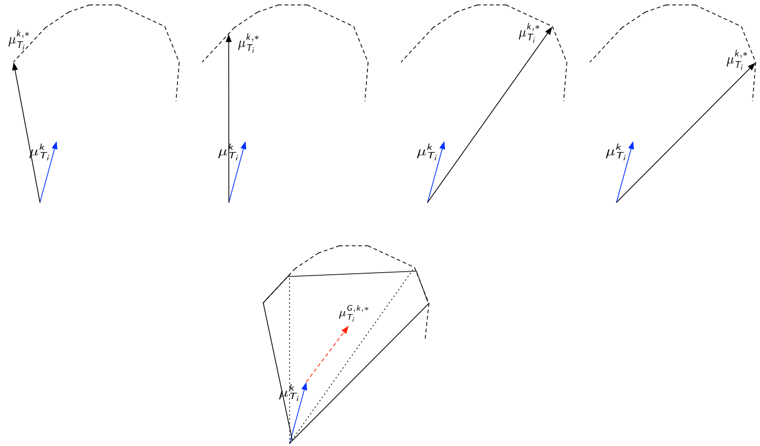
$$\mu_{T}^{k,*} \notin \mu_{T_i}^{k,*}{}_{i=1}^{n}.$$

  2. κ-best inference algorithm

$$(\mu_{T_i}^{k,*_h})_{h=1}^{\kappa} = \operatorname*{\mathbf{argmax}}_{\mu \in \mathcal{M}} \mu^{\intercal} g_{T_i}^{k}, \ \forall i$$

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

Update with multiple directions



Newton method to compute τ

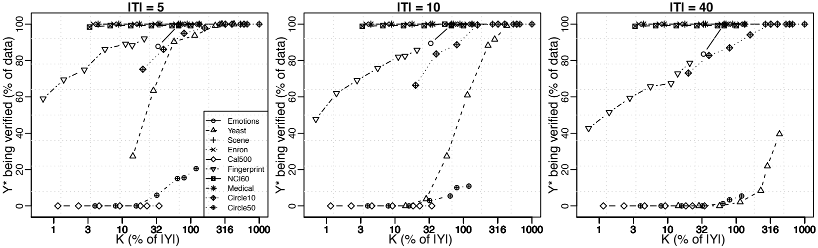
- We want to find τ that maximize the objective function given the update

$$\max_{\tau} \quad f(\mu^{G,k} + \Delta\mu^{G,k+1})$$
$$\textbf{s.t.} \quad 0 \leq \tau_i \leq 1, \sum_{i=1}^{n} \tau_i \leq 1, \forall i.$$

- 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.

Performance of the 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

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*

Figure : Prediction performance of each algorithm in terms of microlabel loss and 0/1 loss. The best performing algorithm is highlighted with boldface, the second best is in italic

Conclusion

- Structured output prediction in multilabel classification problems.
- Utilize label correlation described by an output graph to make accuracy predictions.
- We focus on the problems where the output graph is unknown.
- We model the complete pairwise correlation with an complete graph.
- We approach the $\mathcal{NP}$-hard inference problem on the complete graph by a collection of its spanning trees.
- The proposed model has better performance on multilabel benchmark datasets.
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