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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 $f : \boldsymbol{\mathcal{X}} \to \boldsymbol{\mathcal{Y}}$.

Central problems in multilabel classification

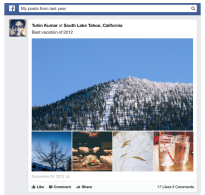
- The size of the output space (searching space) is exponential in the number of microlabels.

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

- 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 [?]
- 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 [**?**, **?**], M^3N [**?**], 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 $(\mathbf{x}, \mathbf{y}) \in \mathcal{X} \times \mathcal{Y}$.
- $\mathbf{x} \in \mathcal{X}$ 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 $\boldsymbol{\phi}(\mathbf{x}, \mathbf{y})$.
- $\mathbf{w}$ 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 $\mathbf{y}' \in \mathcal{Y}$.

Inference problem

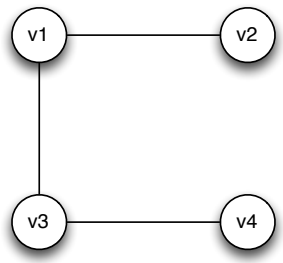
- The prediction $\mathbf{y}_{\mathbf{w}}(\mathbf{x})$ of an input $\mathbf{x}$ is the multilabel $\mathbf{y}$ that maximizes the score function

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

- 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.

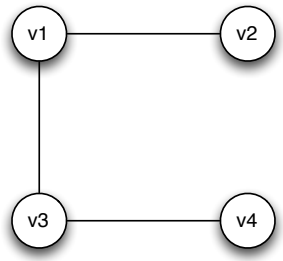


- $\varphi(\mathbf{x}) \in \mathbb{R}^d$ is the input feature map, e.g., bag-of-words of a document.
- $\psi(\mathbf{y}) \in \mathbb{R}^{4|E|}$ is the output feature map which maps the multilabel $\mathbf{y}$ into a collection of edges and labels

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

An example of output feature map

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



- Multilabel $\mathbf{y}$

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

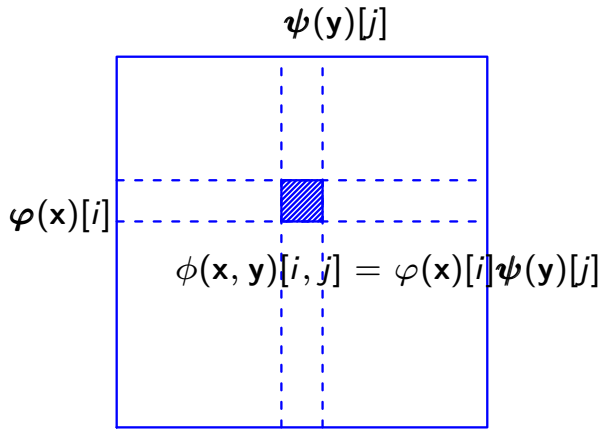
- Output feature map $\boldsymbol{\psi}(\mathbf{y})$

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

Joint feature map

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

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

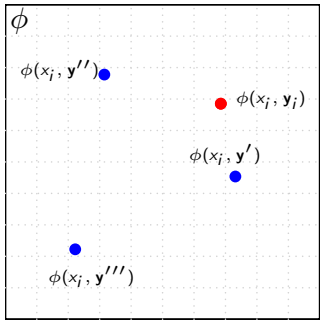


- The score function can be factorized by the output graph G

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

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 ϕ.



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

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

- $\ell(\mathbf{y}, \mathbf{y}_i)$ 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

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

- (**??**) 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 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 $\mu_k \leftarrow \mu_k + \tau(\mu_k^* - \mu_k)$.

Compute duality gap

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

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

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

- $\max_{\mu} g(\mu) \leq \min_{\mathbf{w}} f(\mathbf{w})$, 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 $C^\intercal\nabla g(\mu^t)$.

Bibliography

Argyriou, A., Evgeniou, T., and Pontil, M. (2008).

Convex multi-task feature learning.

Machine Learning, 73(3):243–272.

Bian, W., Xie, B., and Tao, D. (2012).

Corrlog: Correlated logistic models for joint prediction of multiple labels.

Journal of Machine Learning Research - Proceedings Track, pages 109–117.

Cheng, W. and Hüllermeier, E. (2009).

Combining instance-based learning and logistic regression for multilabel classification.

Machine Learning, 76(2-3):211–225.

Esuli, A., Fagni, T., and Sebastiani, F. (2008).

Boosting multi-label hierarchical text categorization.

Information Retrieval, 11(4):287–313.

Bibliography (cont.)

Lafferty, J. D., McCallum, A., and Pereira, F. C. N. (2001).

Conditional random fields: Probabilistic models for segmenting and labeling sequence data.

In *Proceedings of the 8th International Conference on Machine Learning (ICML 2001)*, pages 282–289. Morgan Kaufmann Publishers Inc.

Marchand, M., Su, H., Morvant, E., Rousu, J., and Shawe-Taylor, J. (2014).

Multilabel structured output learning with random spanning trees of max-margin markov networks.

In *Advances in Neural Information Processing System NIPS2014*, page to appear.

Read, J., Pfahringer, B., Holmes, G., and Frank, E. (2009).

Classifier chains for multi-label classification.

In Buntine, W., Grobelnik, M., Mladenić, D., and Shawe-Taylor, J., editors, *Machine Learning and Knowledge Discovery in Databases*, volume 5782, pages 254–269. Springer Berlin Heidelberg.

Bibliography (cont.)

Read, J., Pfahringer, B., Holmes, G., and Frank, E. (2011).

Classifier chains for multi-label classification.

Machine Learning, 85(3):333–359.

Rousu, J., Saunders, C., Szedmak, S., and Shawe-Taylor, J. (2007).

Efficient algorithms for max-margin structured classification.

Predicting Structured Data, pages 105–129.

Schapire, R. and Singer, Y. (1999).

Improved boosting algorithms using confidence-rated predictions.

Machine Learning, 37(3):297–336.

Su, H. (2015).

Multilabel Classification through Structured Output Learning - Methods and Applications.

PhD thesis, Department of Information and Computer Science, Aalto University.

Bibliography (cont.)

Su, H., Gionis, A., and Rousu, J. (2014).

Structured prediction of network response.

In *Proceedings, 31th International Conference on Machine Learning ICML2014*, volume 32 of *Journal of Machine Learning Research WCP*, pages 442–450.

Su, H., Heinonen, M., and Rousu, J. (2010).

Structured output prediction of anti-cancer drug activity.

In *Proceedings, 5th IAPR International Conference on Pattern Recognition in Bioinformatics (PRIB2010)*, volume 6282 of *Lecture Note in Computer Science*, pages 38–49.

Su, H. and Rousu, J. (2011).

Multi-task drug bioactivity classification with graph labeling ensembles.

In *Proceedings, 6th IAPR International Conference on Pattern Recognition in Bioinformatics (PRIB2011)*, volume 7035 of *Lecture Note in Computer Science*, pages 157–167.

Bibliography (cont.)

Su, H. and Rousu, J. (2013).

Multilabel classification through random graph ensembles.

In *Proceedings, 5th Asian Conference on Machine Learning (ACML2013)*, volume 29 of *Journal of Machine Learning Research WCP*, pages 404–418.

Su, H. and Rousu, J. (2015).

Multilabel classification through random graph ensembles.

Machine Learning, 99(2):231–256.

Taskar, B., Abbeel, P., and Koller, D. (2002).

Discriminative probabilistic models for relational data.

In *Proceedings of the Eighteenth Conference on Uncertainty in Artificial Intelligence (UAI 2002)*, pages 485–492, San Francisco, CA, USA. Morgan Kaufmann Publishers Inc.

Bibliography (cont.)

Taskar, B., Guestrin, C., and Koller, D. (2004).

Max-margin markov networks.

In Thrun, S., Saul, L., and Schölkopf, B., editors, *Advances in Neural Information Processing Systems 16*, pages 25–32. MIT Press.

Tsochantaridis, I., Hofmann, T., Joachims, T., and Altun, Y. (2004).

Support vector machine learning for interdependent and structured output spaces.

In *Proceedings of the 21th International Conference on Machine Learning (ICML 2004)*, pages 823–830. ACM.

Tsochantaridis, I., Joachims, T., Hofmann, T., and Altun, Y. (2005).

Large margin methods for structured and interdependent output variables.

Journal of Machine Learning Research, 6:1453–1484.

Bibliography (cont.)

Tsoumakas, G., Katakis, I., and Vlahavas, I. (2010).

Mining multi-label data.

In Maimon, O. and Rokach, L., editors, *Data Mining and Knowledge Discovery Handbook*, pages 667–685. Springer US.

Zhang, M. and Zhou, Z. (2007).

Ml-knn: A lazy learning approach to multi-label learning.

Pattern Recognition, 40:2007.