

# Structured output prediction for multilabel classification

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#### Multilabel classification

- Multilabel classification is an important research field in machine learning.
- ▶ Input variable  $\mathbf{x} \in \mathcal{X}$  is in d dimensional input space  $\mathcal{X} = \mathbb{R}^d$ .
- ▶ Output variable  $\mathbf{y} = (y_1, \dots, y_l) \in \mathcal{Y}$  is a binary vector consist of l binary variables  $y_j \in \{+1, -1\}$ .
- **y** is called a multilabel,  $y_j$  is called a microlabel.
- Output space is composed by a Cartesian product of / sets

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

For example, in document classification, a document x can be classified as "news", "movie", and "science"

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

▶ The goal is to find a mapping function  $f \in \mathcal{H}$  that predicts the best values of an output given an input  $f : \mathcal{X} \to \mathcal{Y}$ .



### Central problems in multilabel classification

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

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

- 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.



$$\mathbf{y} = (\underbrace{+1}, \underbrace{-1}, \underbrace{+1}, \underbrace{-1}, \underbrace{+1}, \underbrace{-1}, \underbrace{-1}, \underbrace{-1})$$
Ted Alice David Mark Alex Zoe 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.



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

Drug discovery, a drug can be effective for multiple symptoms.



$$\mathbf{y} = (\underbrace{+1}_{\text{heart stroke blood fever digest liver swelling}}, \underbrace{+1}_{\text{heart stroke blood fever digest liver swelling}})$$

### 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<sup>3</sup>N [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
- Structured output learning with known output graph
- Structured output learning with unknown output graph
- Future work
- Experimental results

#### **Preliminaries**

- ▶ Training examples come in pairs  $(x, y) \in \mathcal{X} \times \mathcal{Y}$ .
- $ightharpoonup x \in \mathcal{X}$  is an arbitrary input space.
- $ightharpoonup \mathcal{Y}$  is an output space of a collection of  $\ell$ -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  $y_i \in \{-1, +1\}$ .
- ▶ We are given a set of m training examples  $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^m$ .
- **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  $F(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{w}, \phi(\mathbf{x}, \mathbf{y}) \rangle$ .
- w makes sure example x with correct multilabel y achieves higher score than with any other incorrect multilabel  $\mathbf{y}' \in \mathcal{Y}$ .



### Inference problem

▶ The prediction  $y_w(x)$  of an input x is the multilabel y that maximizes the score function

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

- Search space  $|\mathbf{\mathcal{Y}}| = 2^{\ell}$  is exponential in size.
- ▶ (1) is called *inference* problem which is 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  $\phi$  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.



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

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

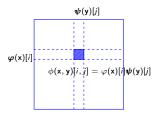
• Output feature map  $\psi(y)$ 

$$\psi(\mathbf{y}) = (\underbrace{0}_{--}, \underbrace{0}_{-+}, \underbrace{1}_{+-}, \underbrace{0}_{+-}, \underbrace{0}_{-+}, \underbrace{0}_{-+}, \underbrace{1}_{+-}, \underbrace{0}_{+-}, \underbrace{0}_{-+}, \underbrace{1}_{+-}, \underbrace{1}_{+-}$$

### Joint feature map

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

$$oldsymbol{\phi}(\mathsf{x},\mathsf{y}) = (oldsymbol{\phi}_e(\mathsf{x},\mathsf{y}))_{e \in E} = (oldsymbol{arphi}(\mathsf{x}) \otimes oldsymbol{\psi}_e(\mathsf{y}_e))_{e \in E}.$$



▶ The score function can be factorized by the output graph *G* 

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

### **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  $\phi$ .



- ► The model is max-margin conditional random field MMCRF [Rousu et al., 2007, Su et al., 2010].
- The primal optimization problem is defined as

$$\min_{\mathbf{w}, \xi_k} \quad \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{k=1}^m \xi_k$$
 (2)

$$\begin{aligned} \textbf{s.t.} \quad & \langle \textbf{w}, \boldsymbol{\phi}(\textbf{x}_k, \textbf{y}_k) \rangle - \langle \textbf{w}, \boldsymbol{\phi}(\textbf{x}_k, \textbf{y}) \rangle \geq \ell(\textbf{y}_k, \textbf{y}) - \xi_k, \\ & \xi_k \geq 0, \forall \ \textbf{y} \in \boldsymbol{\mathcal{Y}}, k \in \{1, \dots, m\}. \end{aligned}$$

 $\triangleright$   $\ell(y, y_i)$  scales the margin according to the multilabel y.

# Marginal-dual optimization

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

$$\max_{\alpha \geq 0} \quad \alpha^{\mathsf{T}} \ell - \frac{1}{2} \alpha^{\mathsf{T}} K \alpha$$

$$\mathbf{s.t.} \quad \sum_{\mathbf{y} \in \mathcal{Y}} \alpha(i, \mathbf{y}) \leq C, \ \forall i \in \{1, \cdots, m\}.$$
(3)

- (3) is also challenging due to the exponential number of dual variables.
- We use edge marginals to replace the dual variables [Taskar et al., 2004]

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

▶ The margin-dual optimization problem is

$$\max_{\mu \in \mathcal{M}} \quad \mu^{\mathsf{T}} \ell - \frac{1}{2} \mu^{\mathsf{T}} K \mu. \tag{4}$$

▶ The number of marginal-dual variable is  $m \times 4|E|$ .

# **Conditional gradient optimization**

▶ (4) is optimized by conditional gradient decent which optimizes  $\mu_k$  that corresponds to a single example while keeps others  $(\mu_j, j \neq k)$  fixed

$$\max_{\mu_k \in \mathcal{M}} \quad \mu_k^{\mathsf{T}} \ell_k - \frac{1}{2} \sum_j \mu_k^{\mathsf{T}} K \mu_j, \, \forall k.$$

- Current gradient of  $\mu_k$  is given by  $g_i = \ell_i \sum_i K \mu_i$ .
- Compute a feasible solution  $\mu_k^*$  as an update direction

$$\mu_k^* = \underset{\mu_k \in \mathcal{M}}{\operatorname{argmax}} \, \mu_k^{\mathsf{T}} g_k = \underset{\mu_k \in \mathcal{M}}{\operatorname{argmax}} \, \sum_{e} \mu(k, e)^{\mathsf{T}} g(k, e). \tag{5}$$

- ▶ (5) is an instantiation of MAP problem
  - G is tree, exact inference with polynomial time algorithm, e.g, dynamic programming in [Rousu et al., 2007]
  - ► G is general graph, approximate inference, e.g. loopy belief propagation in [Su et al., 2010]
- ▶ Perform the update via exact line search  $\mu_k \leftarrow \mu_k + \tau(\mu_k^* \mu_k)$ .

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#### **Exact line search**

Line search gives the optimal feasible solution as a stationary point  $(\tau)$ 

$$\max_{\tau} \quad g(\mu_k + \tau \Delta \mu_k)$$
s.t.  $0 < \tau < 1$ .

- $\tau = 0$  corresponds to no update.
- Feasible maximum update is achieved at  $\tau = 1$ .
- The cost of computing (6) is significantly smaller than the cost of computing (5).

### Compute duality gap

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

$$f(\mathbf{w}) = \frac{1}{2}||\mathbf{w}||^2 + C\sum_{k=1}^m (\ell_k - \langle \mathbf{w}, \Delta \phi(\mathbf{x}_k, \mathbf{y}_k) \rangle)$$
$$g(\mu) = \sum_{k=1}^m \mu_k \ell_k - \frac{1}{2}\sum_{k=1}^m \sum_{j=1}^m \mu_k K^{\Delta \phi}(\mathbf{x}_k, \mathbf{y}_k; \mathbf{x}_j, \mathbf{y}_j) \mu_j$$

- ▶  $\max_{\mu} g(\mu) \leq \min_{\mathbf{w}} f(\mathbf{w})$ , gap is minimized at optimal.
- ▶ Duality gap at  $\mu^t$

$$f(\mathbf{w}^{t}) - g(\mu^{t}) = C\left(\ell - K^{\Delta \phi} \mu^{t}\right) - \mu^{t} \left(\ell - K^{\Delta \phi} \mu^{t}\right)$$
$$= C^{\mathsf{T}} \nabla g(\mu^{t}) - \mu^{t\mathsf{T}} \nabla g(\mu^{t})$$

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



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#### So far

- We work with multilabel classification problems in general.
- In addition, we assume there is an output graph given apriori.
- We develop structured output prediction method which model the label correlations with an output graph.
- If the output graph is tree-like, the inference problem can be solved exactly with a polynomial time algorithm, e.g., dynamic programming.
- If the output graph is a general graph structure, the inference problem is  $\mathcal{NP}$ -hardand can be solved with approximation algorithm, e.g., loopy belief propagation.
- The next question is 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.
  - $\blacktriangleright$  Solve the  $\mathcal{NP}\text{-hardinference}$  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  $\phi$  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.
- ightharpoonup arphi(x) is the input feature map, e.g., bag-of-words feature of an example x.
- ullet  $\psi(y)$  is the output feature map which is a collection of edges and labels

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

ightharpoonup The joint feature is the Kronecker product of arphi(x) and  $\psi(y)$ 

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

▶ The score function can be factorized by the complete graph *G* 

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



### Inference in terms of all spanning trees

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

$$y_{w}(x) = \mathop{argmax}_{y \in \mathcal{Y}} F(w, x, y) = \mathop{argmax}_{y \in \mathcal{Y}} \sum_{e \in E} \langle w_{e}, \phi_{e}(x, y_{e}) \rangle.$$

- ▶ 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

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

- ▶ 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  $\ell$ .

### A sample of n spanning trees

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

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

When

$$n \geq \frac{\ell^2}{\epsilon^2} \left( \frac{1}{16} + \frac{1}{2} \ln \frac{8\sqrt{n}}{\delta} \right),$$

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  $F_{\mathcal{T}}(\mathbf{w}, \mathbf{x}, \mathbf{y})$  [Marchand et al., 2014].

# Random spanning tree approximation RTA

▶ The optimization problem of RTA is defined as [Marchand et al., 2014]

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

#### Inference Problem for a collection of trees

▶ 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  $\Theta(\ell)$  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  $\Theta(K\ell)$  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 in  $\Theta(nK\ell)$  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  $\mathcal{Y}_{\mathcal{T},K}$ .





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