# Structure Regularization for Structured Prediction

Xu SUN xusun@pku.edu.cn



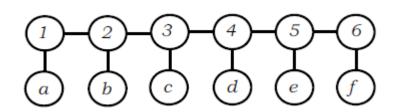
#### **Structured prediction**

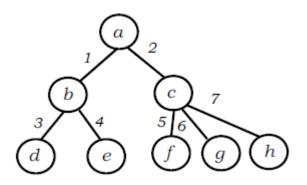
# Structured prediction methods are useful for many areas

- Natural language processing (NLP)
- Vision recognition
- Signal processing
- Bioinformatics
- Speech recognition
- Etc.

#### **Structured prediction**

- For example, many natural language processing (NLP) tasks are structured prediction tasks
  - Parsing
  - SMT
  - POS tagging
  - Word segmentation
  - Named entity recognition
  - Chunking



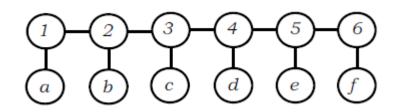


# Given a structured prediction task, is the scale of structure matters?

He PRP reckons **VBZ** DT the JJ current NN account deficit NN will MD VB narrow TO to RB only # # CD 1.8 billion CD IN in September NNP

Or, how about this scale?

structured prediction model (e.g., CRF, HMM, MEMM, or perceptron)

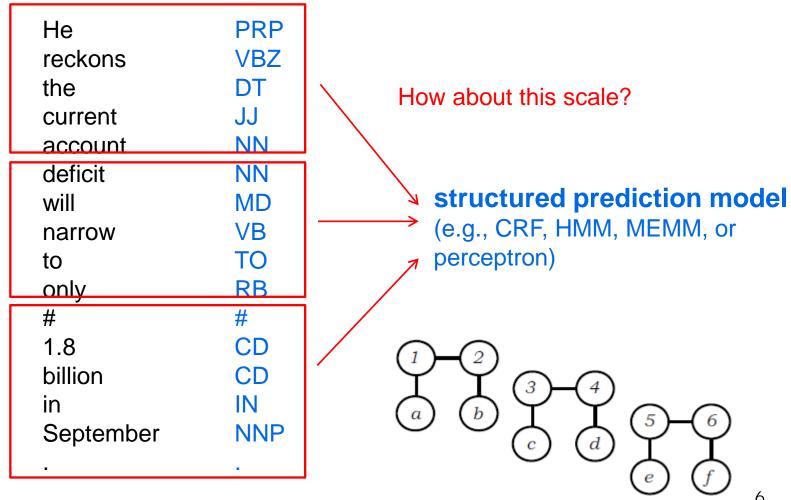


# □ Given a structured prediction task, is the scale of structure matters?

He PRP reckons **VBZ** DT the JJ current NN account deficit NN will MD **VB** narrow TO to RB only # # 1.8 CD billion CD IN in September **NNP** 

5

#### Given a structured prediction task, is the scale of structure matters?



#### □ Sub-question-1

Given a structured prediction task, is the scale of structure matters?

#### **□** Sub-question-2:

- If it matters, which scale is the best?
  - E.g., most of the tasks are based on sentence level, but is it really a good choice?

#### **□** Sub-question-3:

How to find the best scale of complexity in practice?

#### □ Current research trend → using more and more complex structures

- E.g., long distance features, high order dependencies, global information
- This is helpful to some tasks, but also helpless (even harmful) to some other tasks, Why??

#### Our study

- Theoretical analysis:
  - Complex structures is not always good
  - → it can be harmful to generalization ability
  - → we need to find an optimal scale of complexity
- Proposed a solution: structure regularization (SR)

**Theorem 4 (Generalization vs. structure regularization)** Let the structured prediction objective function of G be penalized by structure regularization with factor  $\alpha \in [1, n]$  and  $L_2$  weight regularization with factor  $\lambda$ , and the penalized function has a minimizer f:

$$f = \underset{g \in \mathcal{F}}{\operatorname{argmin}} R_{\alpha,\lambda}(g) = \underset{g \in \mathcal{F}}{\operatorname{argmin}} \left( \frac{1}{mn} \sum_{j=1}^{m\alpha} \mathcal{L}_{\tau}(g, \mathbf{z}'_j) + \frac{\lambda}{2} ||g||_2^2 \right)$$
(8)

Assume the point-wise loss  $\ell_{\tau}$  is convex and differentiable, and is bounded by  $\ell_{\tau}(f, \mathbf{z}, k) \leq \gamma$ . Assume  $f(\mathbf{x}, k)$  is  $\rho$ -admissible. Let a local feature value be bounded by v such that  $\mathbf{x}_{(k,q)} \leq v$  for  $q \in \{1, \ldots, d\}$ . Then, for any  $\delta \in (0,1)$ , with probability at least  $1 - \delta$  over the random draw of the training set S, the generalization risk R(f) is bounded by

$$\underbrace{R(f)} \leq \underbrace{R_e(f)} + \underbrace{\frac{2d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \left(\frac{(4m-2)d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \gamma\right)\sqrt{\frac{\ln\delta^{-1}}{2m}}} \tag{9}$$

Expected risk (risk on test data)

Empirical risk (risk on training data)

Overfitting risk (risk of overfitting from training data to test data)

**Theorem 4 (Generalization vs. structure regularization)** Let the structured prediction objective function of G be penalized by structure regularization with factor  $\alpha \in [1, n]$  and  $L_2$  weight regularization with factor  $\lambda$ , and the penalized function has a minimizer f:

$$f = \underset{g \in \mathcal{F}}{\operatorname{argmin}} R_{\alpha,\lambda}(g) = \underset{g \in \mathcal{F}}{\operatorname{argmin}} \left( \frac{1}{mn} \sum_{j=1}^{m\alpha} \mathcal{L}_{\tau}(g, \mathbf{z}'_j) + \frac{\lambda}{2} ||g||_2^2 \right)$$
(8)

Assume the point-wise loss  $\ell_{\tau}$  is convex and differentiable, and is bounded by  $\ell_{\tau}(f, \mathbf{z}, k) \leq \gamma$ . Assume  $f(\mathbf{x}, k)$  is  $\rho$ -admissible. Let a local feature value be bounded by v such that  $\mathbf{x}_{(k,q)} \leq v$  for  $q \in \{1, \ldots, d\}$ . Then, for any  $\delta \in (0,1)$ , with probability at least  $1 - \delta$  over the random draw of the training set S, the generalization risk R(f) is bounded by

$$R(f) \le R_e(f) + \frac{2d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \left(\frac{(4m-2)d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \gamma\right) \sqrt{\frac{\ln \delta^{-1}}{2m}}$$
(9)

# Complexity of structure (nodes of a training sample with structured dependencies)

→ Complex structure leads to higher overfitting risk

**Theorem 4 (Generalization vs. structure regularization)** Let the structured prediction objective function of G be penalized by structure regularization with factor  $\alpha \in [1, n]$  and  $L_2$  weight regularization with factor  $\lambda$ , and the penalized function has a minimizer f:

$$f = \underset{g \in \mathcal{F}}{\operatorname{argmin}} R_{\alpha,\lambda}(g) = \underset{g \in \mathcal{F}}{\operatorname{argmin}} \left( \frac{1}{mn} \sum_{j=1}^{m\alpha} \mathcal{L}_{\tau}(g, \mathbf{z}'_j) + \frac{\lambda}{2} ||g||_2^2 \right)$$
(8)

Assume the point-wise loss  $\ell_{\tau}$  is convex and differentiable, and is bounded by  $\ell_{\tau}(f, \mathbf{z}, k) \leq \gamma$ . Assume  $f(\mathbf{x}, k)$  is  $\rho$ -admissible. Let a local feature value be bounded by v such that  $\mathbf{x}_{(k,q)} \leq v$  for  $q \in \{1, \ldots, d\}$ . Then, for any  $\delta \in (0,1)$ , with probability at least  $1 - \delta$  over the random draw of the training set S, the generalization risk R(f) is bounded by

$$R(f) \le R_e(f) + \frac{2d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \left(\frac{(4m-2)d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \gamma\right) \sqrt{\frac{\ln\delta^{-1}}{2m}}$$
(9)

## Strength of structure regularization (strength of decomposition)

→ Stronger SR leads to reduction of overfitting risk

**Theorem 4 (Generalization vs. structure regularization)** Let the structured prediction objective function of G be penalized by structure regularization with factor  $\alpha \in [1, n]$  and  $L_2$  weight regularization with factor  $\lambda$ , and the penalized function has a minimizer f:

$$f = \underset{g \in \mathcal{F}}{\operatorname{argmin}} R_{\alpha,\lambda}(g) = \underset{g \in \mathcal{F}}{\operatorname{argmin}} \left( \frac{1}{mn} \sum_{j=1}^{m\alpha} \mathcal{L}_{\tau}(g, \mathbf{z}'_j) + \frac{\lambda}{2} ||g||_2^2 \right)$$
(8)

Assume the point-wise loss  $\ell_{\tau}$  is convex and differentiable, and is bounded by  $\ell_{\tau}(f, \mathbf{z}, k) \leq \gamma$ . Assume  $f(\mathbf{x}, k)$  is  $\rho$ -admissible. Let a local feature value be bounded by v such that  $\mathbf{x}_{(k,q)} \leq v$  for  $q \in \{1, \ldots, d\}$ . Then, for any  $\delta \in (0,1)$ , with probability at least  $1 - \delta$  over the random draw of the training set S, the generalization risk R(f) is bounded by

$$R(f) \le R_e(f) + \frac{2d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \left(\frac{(4m-2)d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \gamma\right) \sqrt{\frac{\ln\delta^{-1}}{2m}}$$
(9)

#### **Number of training samples**

→ More training samples leads to reduction of overfitting risk

**Theorem 4 (Generalization vs. structure regularization)** Let the structured prediction objective function of G be penalized by structure regularization with factor  $\alpha \in [1, n]$  and  $L_2$  weight regularization with factor  $\lambda$ , and the penalized function has a minimizer f:

$$f = \underset{g \in \mathcal{F}}{\operatorname{argmin}} R_{\alpha,\lambda}(g) = \underset{g \in \mathcal{F}}{\operatorname{argmin}} \left( \frac{1}{mn} \sum_{j=1}^{m\alpha} \mathcal{L}_{\tau}(g, \mathbf{z}'_j) + \frac{\lambda}{2} ||g||_2^2 \right)$$
(8)

Assume the point-wise loss  $\ell_{\tau}$  is convex and differentiable, and is bounded by  $\ell_{\tau}(f, \mathbf{z}, k) \leq \gamma$ . Assume  $f(\mathbf{x}, k)$  is  $\rho$ -admissible. Let a local feature value be bounded by v such that  $\mathbf{x}_{(k,q)} \leq v$  for  $q \in \{1, \ldots, d\}$ . Then, for any  $\delta \in (0,1)$ , with probability at least  $1 - \delta$  over the random draw of the training set S, the generalization risk R(f) is bounded by

$$R(f) \le R_e(f) + \frac{2d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \left(\frac{(4m-2)d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \gamma\right) \sqrt{\frac{\ln\delta^{-1}}{2m}}$$
(9)

#### ✓ Conclusions from our analysis:

- 1. Complex structure → low empirical risk & high overfitting risk
- 2. Simple structure → high empirical risk & low overfitting risk
- 3. Need a balanced complexity of structures

**Theorem 4 (Generalization vs. structure regularization)** Let the structured prediction objective function of G be penalized by structure regularization with factor  $\alpha \in [1, n]$  and  $L_2$  weight regularization with factor  $\lambda$ , and the penalized function has a minimizer f:

$$f = \underset{g \in \mathcal{F}}{\operatorname{argmin}} R_{\alpha,\lambda}(g) = \underset{g \in \mathcal{F}}{\operatorname{argmin}} \left( \frac{1}{mn} \sum_{j=1}^{m\alpha} \mathcal{L}_{\tau}(g, \mathbf{z}'_j) + \frac{\lambda}{2} ||g||_2^2 \right)$$
(8)

Assume the point-wise loss  $\ell_{\tau}$  is convex and differentiable, and is bounded by  $\ell_{\tau}(f, \mathbf{z}, k) \leq \gamma$ . Assume  $f(\mathbf{x}, k)$  is  $\rho$ -admissible. Let a local feature value be bounded by v such that  $\mathbf{x}_{(k,q)} \leq v$  for  $q \in \{1, \ldots, d\}$ . Then, for any  $\delta \in (0,1)$ , with probability at least  $1 - \delta$  over the random draw of the training set S, the generalization risk R(f) is bounded by

$$R(f) \le R_e(f) + \frac{2d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \left(\frac{(4m-2)d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \gamma\right) \sqrt{\frac{\ln\delta^{-1}}{2m}}$$
(9)

- ☐ In other words, more intuitively:
  - Too complex structure → high accuracy on training + very easy to overfit → low accuracy on testing
  - 2. Too simple structure → very low accuracy on training + not easy to overfit → low accuracy on testing

Proper structure → good accuracy on training + not easy to overfit → high accuracy on testing

**Theorem 4 (Generalization vs. structure regularization)** Let the structured prediction objective function of G be penalized by structure regularization with factor  $\alpha \in [1, n]$  and  $L_2$  weight regularization with factor  $\lambda$ , and the penalized function has a minimizer f:

$$f = \underset{g \in \mathcal{F}}{\operatorname{argmin}} R_{\alpha,\lambda}(g) = \underset{g \in \mathcal{F}}{\operatorname{argmin}} \left( \frac{1}{mn} \sum_{j=1}^{m\alpha} \mathcal{L}_{\tau}(g, \mathbf{z}'_j) + \frac{\lambda}{2} ||g||_2^2 \right)$$
(8)

Assume the point-wise loss  $\ell_{\tau}$  is convex and differentiable, and is bounded by  $\ell_{\tau}(f, \mathbf{z}, k) \leq \gamma$ . Assume  $f(\mathbf{x}, k)$  is  $\rho$ -admissible. Let a local feature value be bounded by v such that  $\mathbf{x}_{(k,q)} \leq v$  for  $q \in \{1, \ldots, d\}$ . Then, for any  $\delta \in (0,1)$ , with probability at least  $1 - \delta$  over the random draw of the training set S, the generalization risk R(f) is bounded by

$$R(f) \le R_e(f) + \frac{2d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \left(\frac{(4m-2)d\tau^2 \rho^2 v^2 n^2}{m\lambda\alpha} + \gamma\right) \sqrt{\frac{\ln\delta^{-1}}{2m}}$$
(9)

- 1. Simple structure → low overfitting risk & high empirical risk
- 2. Complex structure → high overfitting risk & low empirical risk
- 3. Need a balanced complexity of structures

Some intuition in the proof (as in the full version paper):

- 1) The decomposition can improve stability
- 2) Better stability leads to better generalization (less overfitting)

#### **Theoretical analysis: Learning speed**

**Proposition 5** (Convergence rates vs. structure regularization) With the aforementioned assumptions, let the SGD training have a learning rate defined as  $\eta = \frac{c\epsilon\beta\alpha^2}{q\kappa^2n^2}$ , where  $\epsilon > 0$  is a convergence tolerance value and  $\beta \in (0,1]$ . Let t be a integer satisfying

$$t \ge \frac{q\kappa^2 n^2 \log (qa_0/\epsilon)}{\epsilon \beta c^2 \alpha^2} \tag{15}$$

where n and  $\alpha \in [1, n]$  is like before, and  $a_0$  is the initial distance which depends on the initialization of the weights  $\mathbf{w}_0$  and the minimizer  $\mathbf{w}^*$ , i.e.,  $a_0 = ||\mathbf{w}_0 - \mathbf{w}^*||^2$ . Then, after t updates of  $\mathbf{w}$  it converges to  $\mathbb{E}[g(\mathbf{w}_t) - g(\mathbf{w}^*)] \leq \epsilon$ .

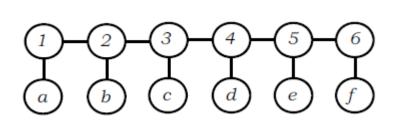
#### ■ SR also with faster speed

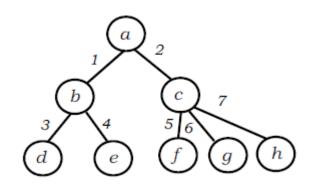
(a by-product of simpler structures)

✓ using structure regularization can quadratically accelerate the convergence rate

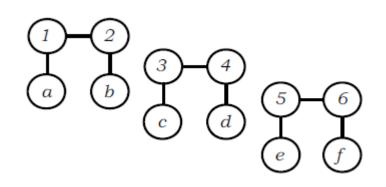
#### Illustration

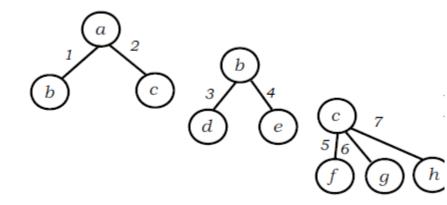
#### Complex structures (high complexity)



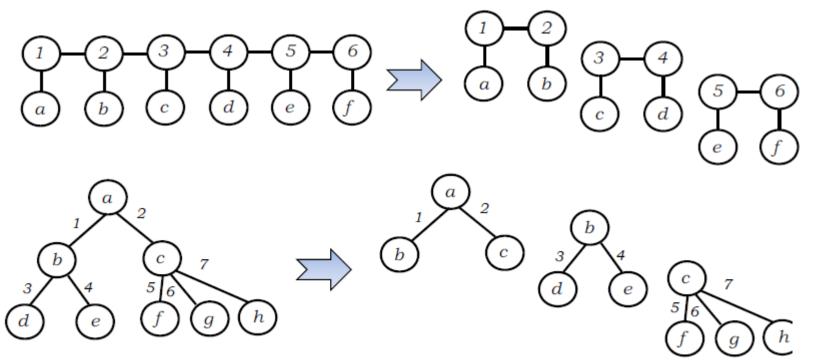


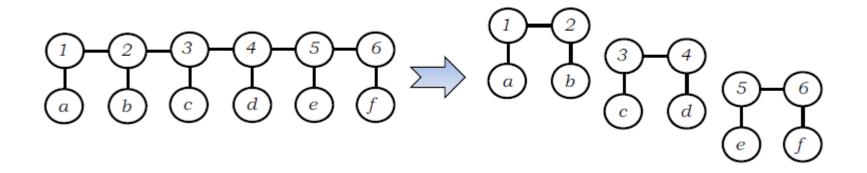
#### □ Simple structures (low complexity)





- We propose structure regularization (SR) to find good complexity
  - Simply split the structures!
  - Can (almost) be seen as a preprocessing step of the training data

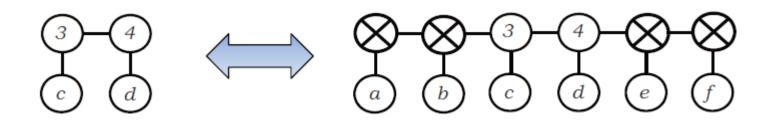


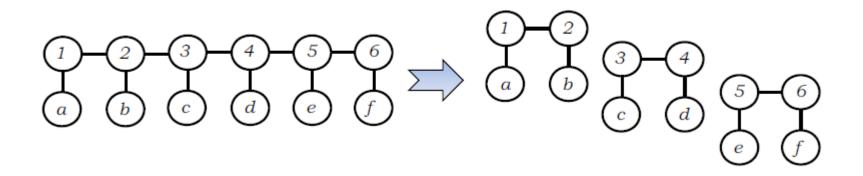


■ Will the split causes feature loss? – loss of long distance features?

#### No loss of any (long distance) features

- → We can first extract features, then split the structures
- → Or, by simply copying observations to mini-samples, i.e., the split is only on tag-structures, like this:





#### Is structure regularization also required for test data?

No, no use of SR for testing data (in current implementation & experiments)

- → Like other regularization methods, SR is only for the training
- →i.e., No SR on the test stage (no decomposition of test samples)!

#### Structure & weight regularization

1: **Input**: model weights  $\boldsymbol{w}$ , training set S, structure regularization strength  $\alpha$ 

$$R_{\alpha,\lambda}(G_S) \triangleq R_{\alpha}(G_S) + N_{\lambda}(G_S)$$

```
Algorithm 1 Training with structure regularization
```

```
2: repeat
          S' \leftarrow \emptyset
 3:
         for i = 1 \rightarrow m do
 4:
               Randomly decompose z_i \in S into mini-samples N_{\alpha}(z_i) = \{z_{(i,1)}, \dots, z_{(i,\alpha)}\}
 5:
               S' \leftarrow S' \cup N_{\alpha}(\boldsymbol{z}_i)
 6:
          end for
 7:
          for i=1 \rightarrow |S'| do
 8:
               Sample z' uniformly at random from S', with gradient \nabla g_{z'}(w)
 9:
               \boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \nabla g_{\boldsymbol{z}'}(\boldsymbol{w})
10:
          end for
11:
                                        The implementation is very simple
     until Convergence
13: return w
```

#### Some advantages

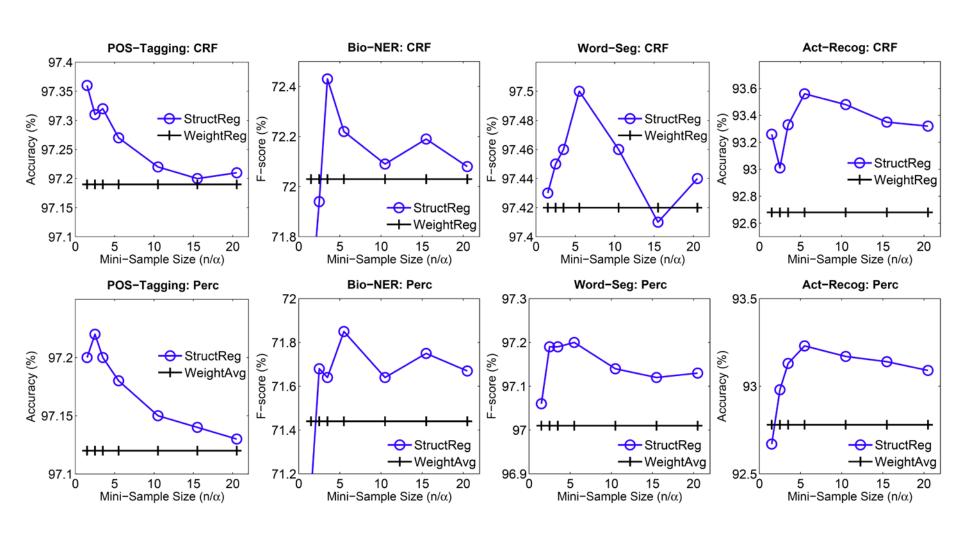
If the original obj. function is convex, can still keep the convexity of the objective function

- No conflict with the weight regularization
  - E.g, L2, and/or L1 regularization

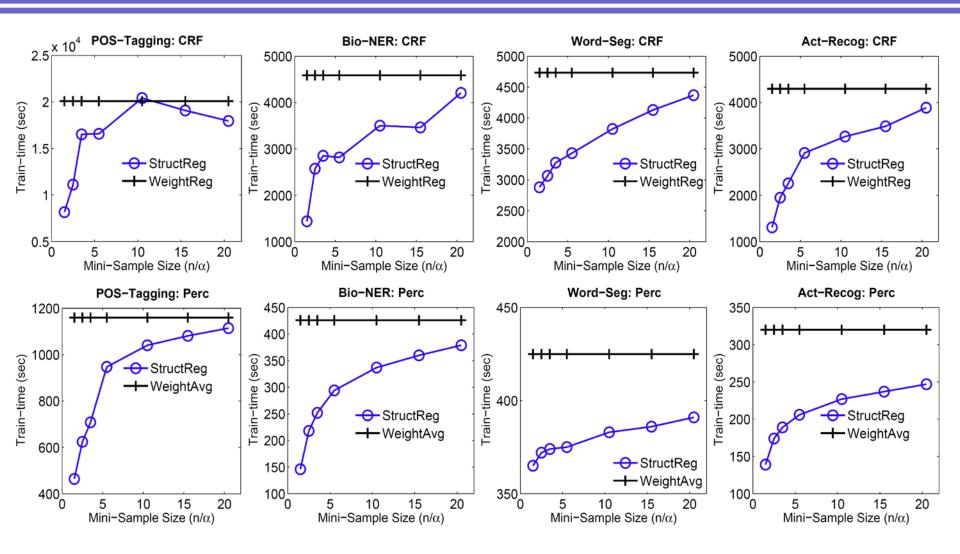
- □ General purpose and model-independent (because act like a preprocessing step)
  - E.g., can be used for different types of models, including CRFs, perceptrons, & neural networks

#### **Experiments-1: accuracy**

#### State-of-the-art scores on competitive tasks



#### **Experiments-2: Learning speed**



#### □ Also with faster speed

(a by-product of simpler structures)

#### **Conclusions**

#### Question: Is structure complexity matters in structured prediction?

- Theoretical analysis to the question
  - 1) Yes it matters
  - 2) High complexity of structures → high overfitting risk
  - 3) Low complexity → high empirical risk
  - 4) We need to find an optimal complexity of structures

#### Proposed a solution

- Split the original structure to find the optimal complexity
- Better accuracies in real tasks, & faster (a by-product)

#### This work is published at NIPS 2014:

Xu Sun. Structure Regularization for Structured Prediction. In Advances in Neural Information Processing Systems (NIPS). 2402-2410. 2014

### Thanks for your attention!

Plz email xusun@pku.edu.cn if any question.

Source code is available upon request.