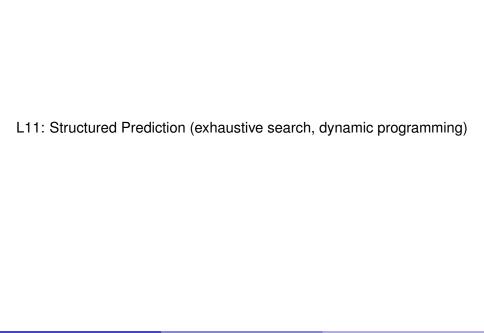
Machine Learning

A. G. Schwing & M. Telgarsky

University of Illinois at Urbana-Champaign, 2018



• Getting to know structured prediction

- Getting to know structured prediction
- Understanding basic structured inference algorithms

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Reading material:

- Getting to know structured prediction
- Understanding basic structured inference algorithms

Reading material:

 D. Koller and N. Friedman; Probabilistic Graphical Models: Principles and Techniques;

$$\min_{\boldsymbol{w}} \frac{C}{2} \|\boldsymbol{w}\|_2^2 + \sum_{i \in \mathcal{D}} \epsilon \ln \sum_{\hat{y}} \exp \frac{L(y^{(i)}, \hat{y}) + F(\boldsymbol{w}, x^{(i)}, \hat{y})}{\epsilon} - F(\boldsymbol{w}, x^{(i)}, y^{(i)})$$

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Attention:

Scoring function

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Attention:

• Scoring function $F(\mathbf{w}, x^{(i)}, y^{(i)})$

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- Scoring function $F(\mathbf{w}, x^{(i)}, y^{(i)})$
- Loss function

$$\min_{\boldsymbol{w}} \frac{C}{2} \|\boldsymbol{w}\|_2^2 + \sum_{i \in \mathcal{D}} \epsilon \ln \sum_{\hat{y}} \exp \frac{L(\boldsymbol{y}^{(i)}, \hat{\boldsymbol{y}}) + F(\boldsymbol{w}, \boldsymbol{x}^{(i)}, \hat{\boldsymbol{y}})}{\epsilon} - F(\boldsymbol{w}, \boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})$$

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- Loss function (log-loss, hinge-loss)

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How to get to

Logistic regression

$$\min_{\boldsymbol{w}} \frac{C}{2} \|\boldsymbol{w}\|_2^2 + \sum_{i \in \mathcal{D}} \epsilon \ln \sum_{\hat{y}} \exp \frac{L(\boldsymbol{y}^{(i)}, \hat{\boldsymbol{y}}) + F(\boldsymbol{w}, \boldsymbol{x}^{(i)}, \hat{\boldsymbol{y}})}{\epsilon} - F(\boldsymbol{w}, \boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})$$

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- Logistic regression
- Binary SVM

$$\min_{\boldsymbol{w}} \frac{C}{2} \|\boldsymbol{w}\|_2^2 + \sum_{i \in \mathcal{D}} \epsilon \ln \sum_{\hat{y}} \exp \frac{L(\boldsymbol{y}^{(i)}, \hat{\boldsymbol{y}}) + F(\boldsymbol{w}, \boldsymbol{x}^{(i)}, \hat{\boldsymbol{y}})}{\epsilon} - F(\boldsymbol{w}, \boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})$$

Attention:

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- Logistic regression
- Binary SVM
- Multiclass regression

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- Logistic regression
- Binary SVM
- Multiclass regression
- Multiclass SVM
- Deep Learning

$$y^* = \arg\max_{\hat{y}} F(\mathbf{w}, x, \hat{y})$$

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How to solve it?

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How to solve it?

Exhaustive search over all classes (easy for binary/few classes)





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Correlations not taken into account



Correlations not taken into account

Correlations taken into account

 Formulate it as prediction of all four letter words (multiclass prediction):

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$$y \in \mathcal{Y} = \{1, \dots, 26^4\}$$

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Problem:

 Formulate it as prediction of all four letter words (multiclass prediction):

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• Problem: Really large output space

Example: Disparity map estimation

How big is the output space?

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How big is the output space?





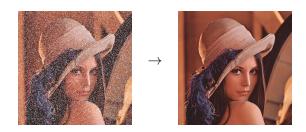


Image

Independent Prediction Structured Prediction

Example: De-noising

Example: De-noising



Example: De-noising



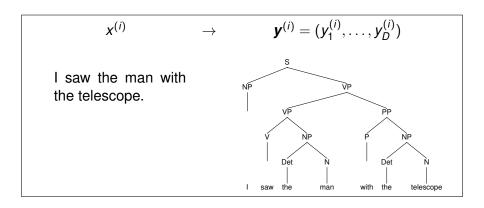
Predictions from neighboring pixel are useful.

$$oldsymbol{x}^{(i)} \qquad
ightarrow \, oldsymbol{y}^{(i)} = (y_1^{(i)}, \ldots, y_D^{(i)})$$

• Image segmentation (estimate a labeling)

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- Image segmentation (estimate a labeling)
- Sentence parsing (estimate a parse tree)



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- Image segmentation (estimate a labeling)
- Sentence parsing (estimate a parse tree)
- Protein folding (estimate a protein structure)
- Stereo vision (estimate a disparity map)

$$\mathbf{x}^{(i)}$$
 \rightarrow $\mathbf{y}^{(i)} = (\mathbf{y}_1^{(i)}, \dots, \mathbf{y}_D^{(i)})$

• "Standard" Prediction: output $y \in \mathcal{Y}$ is a scalar number

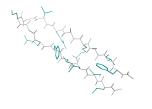
$$\mathcal{Y} = \{1, \dots, K\}$$
 or $\mathcal{Y} = \mathbb{R}$

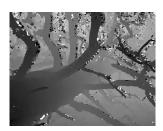
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• "Structured" Prediction: output **y** is a structured output:





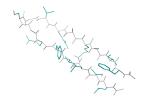


• "Standard" Prediction: output $y \in \mathcal{Y}$ is a scalar number

$$\mathcal{Y} = \{1, \dots, K\}$$
 or $\mathcal{Y} = \mathbb{R}$

• "Structured" Prediction: output **y** is a structured output:







We can transition between both formulations. K possibly really large.

$$y = (y_1, ..., y_D)$$
 $y_d \in \{1, ..., K\}$

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Inference/Prediction:

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$$\mathbf{y}^* = \arg\max_{\hat{\mathbf{y}}} F(\mathbf{w}, x, \hat{\mathbf{y}}) =$$

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How many possibilities do we have to store and explore?

$$y = (y_1, ..., y_D)$$
 $y_d \in \{1, ..., K\}$

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How many possibilities do we have to store and explore?

$$K^D$$

That's a problem. What can we do?

lf

$$F(\boldsymbol{w}, x, \hat{y}_1, \dots, \hat{y}_D) = \sum_{d=1}^{D} f_d(\boldsymbol{w}, x, \hat{y}_d)$$

$$\max_{\hat{\mathbf{y}}} F(\mathbf{w}, x, \hat{y}_1, \dots, \hat{y}_D) = \max_{\hat{\mathbf{y}}} \sum_{d=1}^{D} f_d(\mathbf{w}, x, \hat{y}_d) =$$

Ιf

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Why not predict every variable y_d from $\mathbf{y} = (y_1, \dots, y_D)$ separately?

If

$$F(\mathbf{w}, x, \hat{y}_1, \dots, \hat{y}_D) = \sum_{d=1}^{D} f_d(\mathbf{w}, x, \hat{y}_d)$$

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Why not predict every variable y_d from $\mathbf{y} = (y_1, \dots, y_D)$ separately?

Correlations not explicitly taken into account

Score function decomposes less trivially:

$$F(\boldsymbol{w}, x, y_1, \dots, y_D) = \sum_{r \in \mathcal{R}} f_r(\boldsymbol{w}, x, \boldsymbol{y}_r)$$

Restriction set $r \subseteq \{1, ..., D\}$ Set of all restrictions: \mathcal{R} Score function decomposes less trivially:

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Restriction set $r \subseteq \{1, \dots, D\}$

Set of all restrictions: R

Example: $r = \{1, 2\}$

$$f_{\{1,2\}}(\mathbf{y}_{\{1,2\}}) = f_{\{1,2\}}(y_1, y_2) = [f_{\{1,2\}}(1,1), f_{\{1,2\}}(1,2), \ldots]$$

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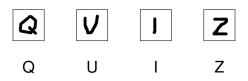
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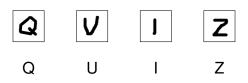
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Q	0	8.0	0.2	0.1	0.1
U		٠			
I Z	:				
Z					
V					



Example:

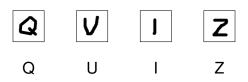
$$F(\mathbf{w}, x, y_1, \dots, y_4) = f_1(\mathbf{w}, x, y_1) + f_2(\mathbf{w}, x, y_2) + f_3(\mathbf{w}, x, y_3) + f_4(\mathbf{w}, x, y_4) + f_{1,2}(\mathbf{w}, x, y_1, y_2) + f_{2,3}(\mathbf{w}, x, y_2, y_3) + f_{3,4}(\mathbf{w}, x, y_3, y_4)$$



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How many function values need to be stored if $y_d \in \{1, ..., 26\} \ \forall d$?



Example:

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How many function values need to be stored if $y_d \in \{1, \dots, 26\} \ \forall d$?

Farlier: 26^4 v.s. now: $3 \cdot 26^2 (+4 \cdot 26)$

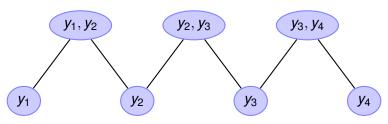
Visualization of the decomposition:

$$F(\mathbf{w}, x, y_1, \dots, y_4) = f_1(\mathbf{w}, x, y_1) + f_2(\mathbf{w}, x, y_2) + f_3(\mathbf{w}, x, y_3) + f_4(\mathbf{w}, x, y_4) + f_{1,2}(\mathbf{w}, x, y_1, y_2) + f_{2,3}(\mathbf{w}, x, y_2, y_3) + f_{3,4}(\mathbf{w}, x, y_3, y_4)$$

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+ $f_{1,2}(\mathbf{w}, x, y_1, y_2) + f_{2,3}(\mathbf{w}, x, y_2, y_3) + f_{3,4}(\mathbf{w}, x, y_3, y_4)$



Edges denote subset relationship

• Predicting every variable separately:

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Markov random field with only unary variables

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Markov random field with only unary variables

• Multi-variate prediction:

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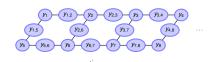






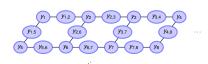








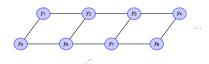




$$F(\boldsymbol{w}, x, \boldsymbol{y}) = \sum_{d=1}^{D} f_d(\boldsymbol{w}, x, y_d) + \sum_{i,j} f_{i,j}(\boldsymbol{w}, x, y_i, y_j)$$



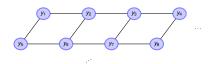




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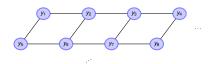


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- Unary term:
- Pairwise term:





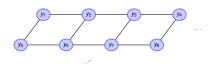


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- Unary term: image evidence
- Pairwise term:





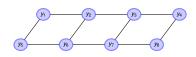


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- Unary term: image evidence
- Pairwise term: smoothness prior



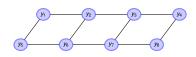




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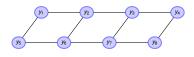


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- Unary term:
- Pairwise term:





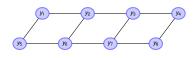


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- Pairwise term:







$$F(\boldsymbol{w}, x, \boldsymbol{y}) = \sum_{d=1}^{D} f_d(\boldsymbol{w}, x, y_d) + \sum_{i,j} f_{i,j}(\boldsymbol{w}, x, y_i, y_j)$$

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- Pairwise term: smoothness prior

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Some inference algorithms:

Exhaustive search

$$\mathbf{y}^* = \arg\max_{\hat{\mathbf{y}}} \sum_r f_r(\mathbf{w}, x, \hat{\mathbf{y}}_r)$$

- Exhaustive search
- Dynamic programming

$$\mathbf{y}^* = \arg\max_{\hat{\mathbf{y}}} \sum_r f_r(\mathbf{w}, x, \hat{\mathbf{y}}_r)$$

- Exhaustive search
- Dynamic programming
- Integer linear program

$$\mathbf{y}^* = \arg\max_{\hat{\mathbf{y}}} \sum_r f_r(\mathbf{w}, x, \hat{\mathbf{y}}_r)$$

- Exhaustive search
- Dynamic programming
- Integer linear program
- Linear programming relaxation

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- Exhaustive search
- Dynamic programming
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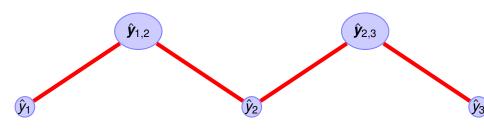
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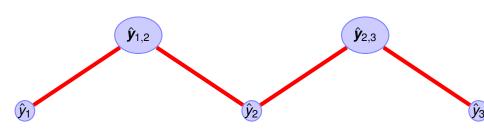
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- Advantage: very simple to implement
- **Disadvantage:** very slow for reasonably sized problems: K^D

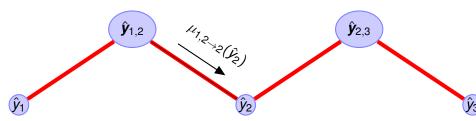


$$\max_{\hat{\boldsymbol{y}}} F(\boldsymbol{w}, x, \hat{\boldsymbol{y}}) = \max_{\hat{y}_1, \hat{y}_2, \hat{y}_3} \left(f_3(\hat{y}_3) + f_{2,3}(\hat{y}_2, \hat{y}_3) + f_2(\hat{y}_2) + f_1(\hat{y}_1) + f_{1,2}(\hat{y}_1, \hat{y}_2) \right)$$



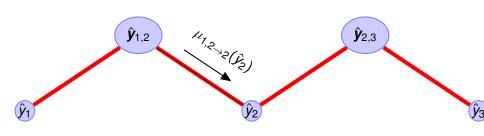
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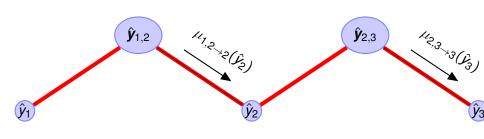
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A. G. Schwing & M. Telgarsky (Uofl)

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What to do for general loopy graphs?

- Integer Linear Programs
- Linear Programming relaxations
- Dynamic programming extensions (message passing)
- Graph cut algorithms

• Why structured output spaces?

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- Inference algorithms for structured output spaces?

Important topics of this lecture

- Getting to know structured prediction
- Understood some inference algorithms

Up next:

More inference algorithms for structured output spaces