

#### 10-418/10-618 Machine Learning for Structured Data

MACHINE LEARNING DEPARTMENT

Machine Learning Department School of Computer Science Carnegie Mellon University

## **Course Overview**

+

# What is Structured Prediction?

Matt Gormley Lecture 1 Aug. 29, 2022

## WHAT IS STRUCTURED PREDICTION?

### Structured Prediction

 The focus of most Intro ML courses is classification

- Given observations:  $\mathbf{x} = (x_1, x_2, ..., x_K)$
- Predict a (binary) label: y
- Many real-world problems require structured prediction
  - Given observations:  $\mathbf{x} = (x_1, x_2, ..., x_K)$
  - Predict a structure:  $y = (y_1, y_2, ..., y_J)$
- Some classification problems benefit from latent structure

### Structured Prediction

#### **Classification / Regression**

- Input can be semistructured data
- Output is a single number (integer / real)
- 3. In linear models, features can be arbitrary combinations of [input, output] pair
- 4. Output space is small
- 5. Inference is trivial

#### **Structured Prediction**

- Input can be semi-structured data
- Output is a sequence of numbers representing a structure
- 3. In linear models, features can be arbitrary combinations of [input, output] pair
- Output space may be exponentially large in the input space
- Inference problems are NP-hard or #P-hard in general and often require approximations

## Structured Prediction Examples

### [Human Language Technologies]

Task	Input	Output	
Speech Recognition	40 haf   dh   ih   s   w   uh   z   iy   z   iy   f   ao   r   ah   s   haf   ao   ao   ao   ao   ao   ao   ao	This was easy for us.	
Syntactic Parsing	time flies like an arrow	time flies like an arrow	
Semantic Parsing	Send a text to Alice that I'll be late	<pre>txt(recipient = Alice,   msg = "I'll be late")</pre>	
Machine Translation	WHERE IS THE TRAIN STATION?	¿DONDE ESTA LA ESTACION DE TRENES?	

## Structured Prediction Training Dataset: Part-of-Speech (POS) Tagging

Data:  $\mathcal{D} = \{oldsymbol{x}^{(n)}, oldsymbol{y}^{(n)}\}_{n=1}^N$ 

Sample 1:	n	v flies	p like	an	$\begin{array}{c c}  & y \\ \hline  & x \\ \end{array}$	
Sample 2:	n	n	like	an	$\begin{array}{c c} & & \\ & & \\ \hline & & \\ & & \\ \end{array}$	
Sample 3:	n	fly	with	heir	$ \begin{array}{c c}                                    $	
Sample 4:	with	n	you	will	$\begin{array}{c c} & & \\ & &$	

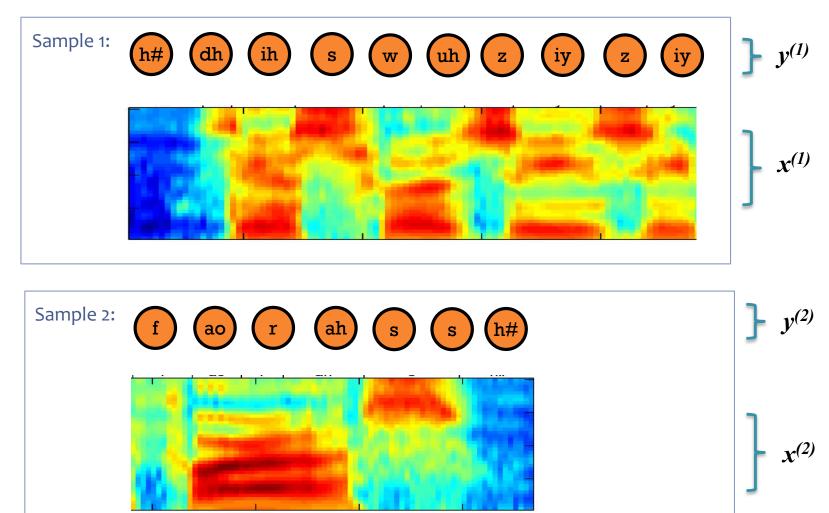
## Structured Prediction Training Dataset: Handwriting Recognition

Data:  $\mathcal{D} = \{oldsymbol{x}^{(n)}, oldsymbol{y}^{(n)}\}_{n=1}^N$ 

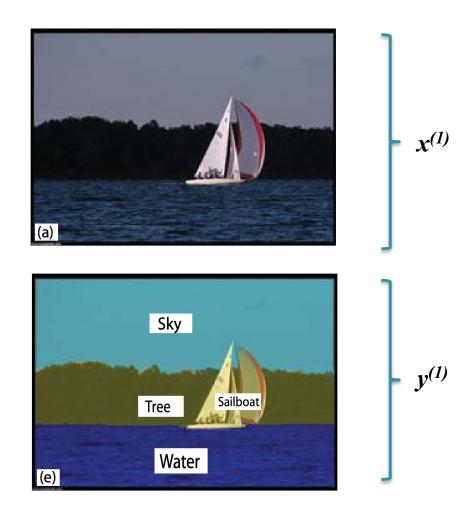


## Structured Prediction Training Dataset: Phoneme (Speech) Recognition

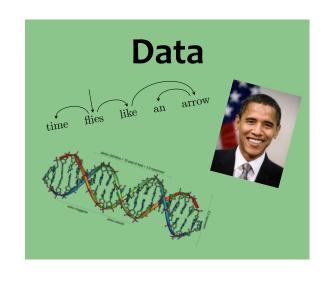
Data:  $\mathcal{D} = \{oldsymbol{x}^{(n)}, oldsymbol{y}^{(n)}\}_{n=1}^N$ 

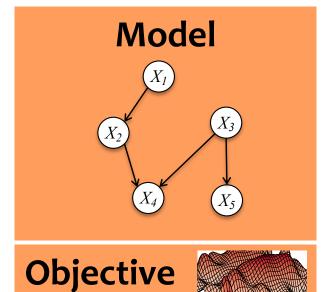


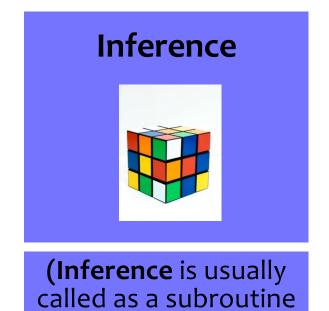
## Structured Prediction Training Dataset: Scene Understanding



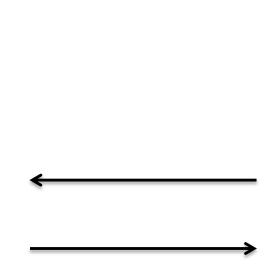
## Structured Prediction

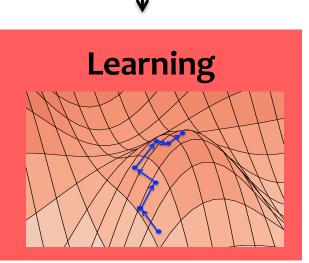






in learning)





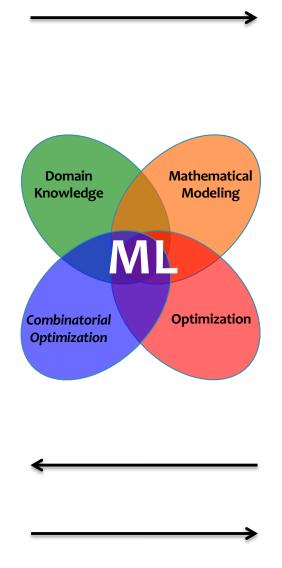
### Structured Prediction

The data inspires
the structures
we want to
predict

**Inference** finds

{best structure, marginals, partition function} for a new observation

(Inference is usually called as a subroutine in learning)



Our **model**defines a score
for each structure

It also tells us what to optimize

Learning tunes the parameters of the model

## DECOMPOSING A STRUCTURE INTO PARTS

- Many real-world problems require structured prediction
  - Given observations:

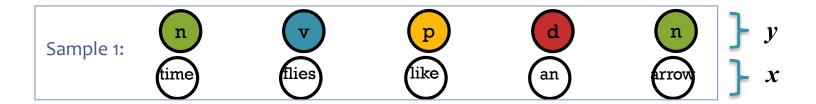
$$x = (x_1, x_2, ..., x_K)$$

- Given observations: 
$$x = (x_1, x_2, ..., x_K)$$
  
- Predict a structure:  $y = (y_1, y_2, ..., y_J)$ 

- The most important idea in structured prediction:
  - Do NOT treat the output structure v as a single monolithic piece of data
  - Instead, divide that structure into its pieces

- Why divide a structure into its pieces?
  - amenable to efficient inference
  - enable natural parameter sharing during learning
  - easier definition of fine-grained loss functions
  - clearer depiction of model's uncertainty
  - easier specification of **interactions** between the parts
  - (may) lead to natural definition of a search problem
- A key step in formulating a task as a structured prediction

#### **Example 1: Part-of-speech Tagging**

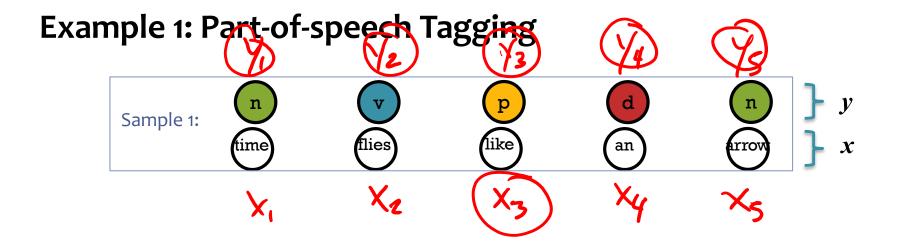


#### **Question:**

How would you decompose the structure *y* into parts?

- A. How many variables would you need to represent said decomposition?
- B. What values could each variable take?

**Answer:** 



#### **Question:**

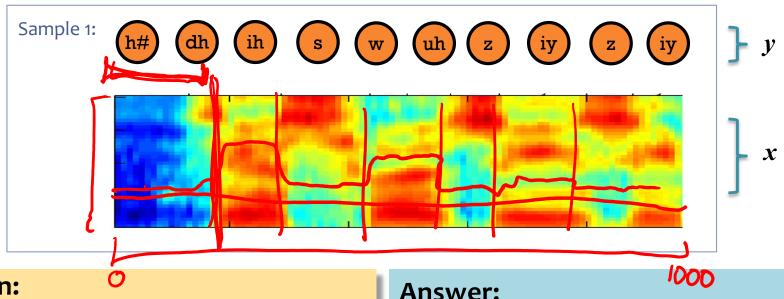
How would you decompose the structure *y* into parts?

- A. How many variables would you need to represent said decomposition?
- B. What values could each variable take?

#### **Answer:**

- A. For each word in the sentence create one tag variable, e.g. the t'th word x<sub>t</sub> has a tag variable y<sub>t</sub>.
- B. Each tag variable y<sub>t</sub> ranges over the set of possible part-of-speech tags {a, d, n, p, v, ...}

#### **Example 2: Phoneme Recognition**

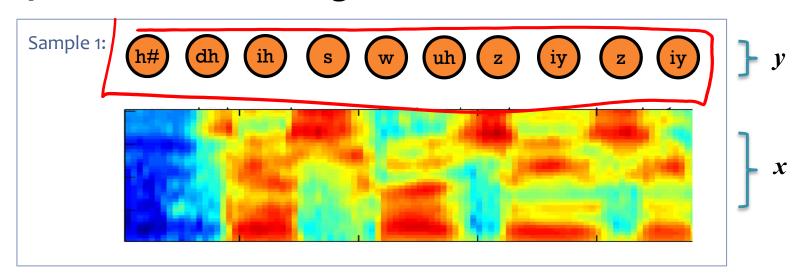


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#### **Example 2: Phoneme Recognition**



#### **Question:**

How would you decompose the structure *y* into parts?

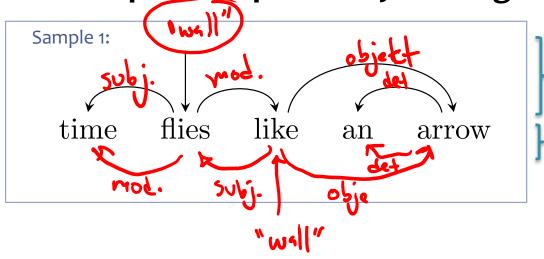
- A. How many variables would you need to represent said decomposition?
- B. What values could each variable take?

#### **Answer:**

- A. Assume the speech signal consists of T segments of 10 milliseconds each, then create T phoneme variables y<sub>1</sub>, y<sub>2</sub>, ..., y<sub>T</sub>
- B. Each phoneme variable y<sub>t</sub> can be a phoneme {dh, h#, ih, iy, ...} or the special symbol "—" meaning "no phoneme"

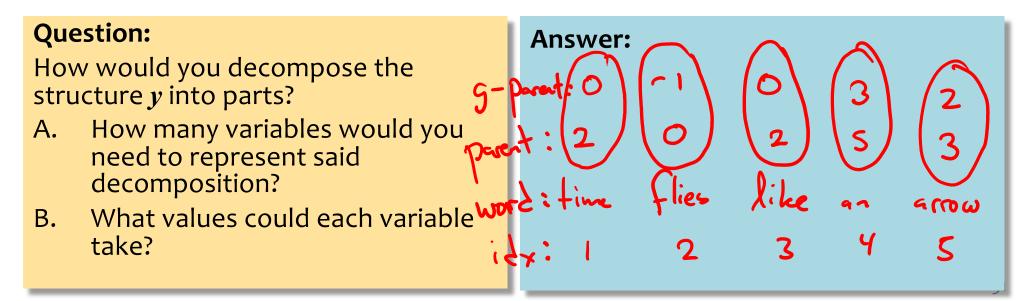
y

**Example 3: Dependency Parsing** 



Definition of a Dependency Parse:

- Each word must have exactly one parent
- The parent must be another word in the sentence OR the "wall"
- 3. Exactly one word must have the "wall" as its parent
- 4. The resulting directed graph must be acyclic

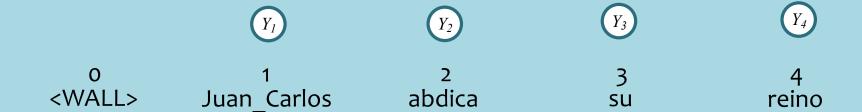


#### **Example 3: Dependency Parsing**

#### **Answer:**

Solution #1: (most obvious solution)

- A. Have one variable for each word in the sentence
- B. Each variable can take on an integer indicating which word is its parent

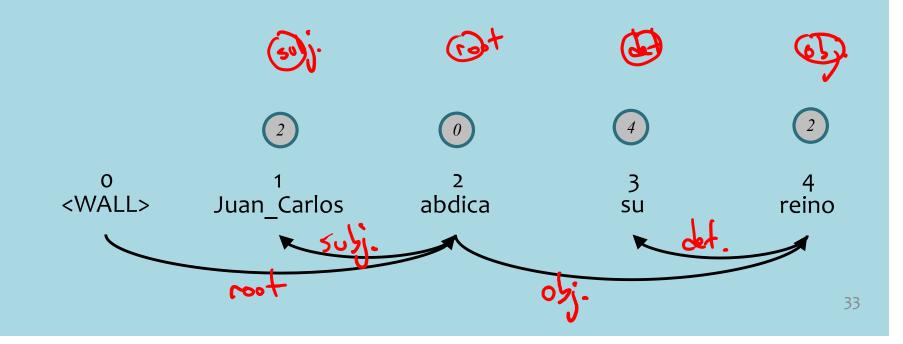


#### **Example 3: Dependency Parsing**

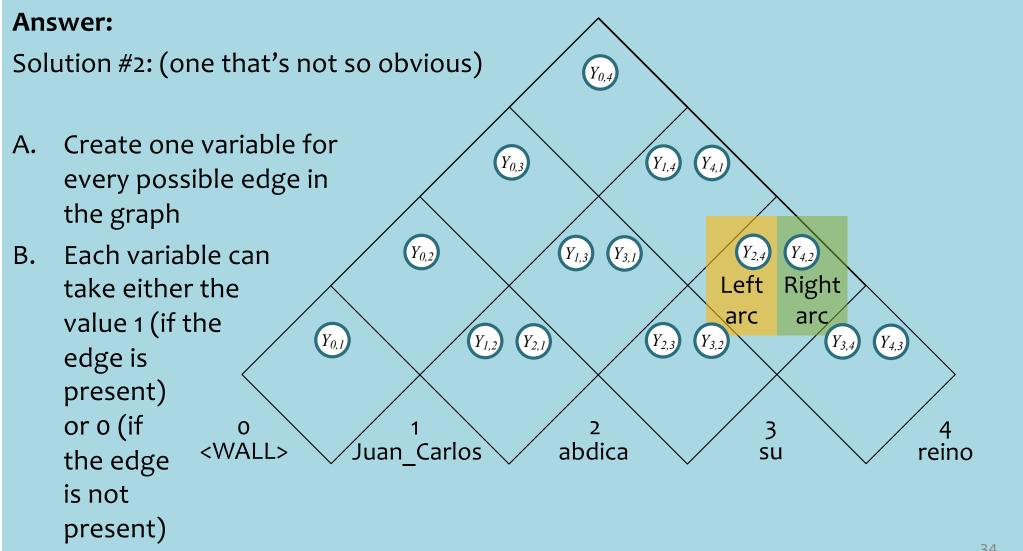
#### **Answer:**

Solution #1: (most obvious solution)

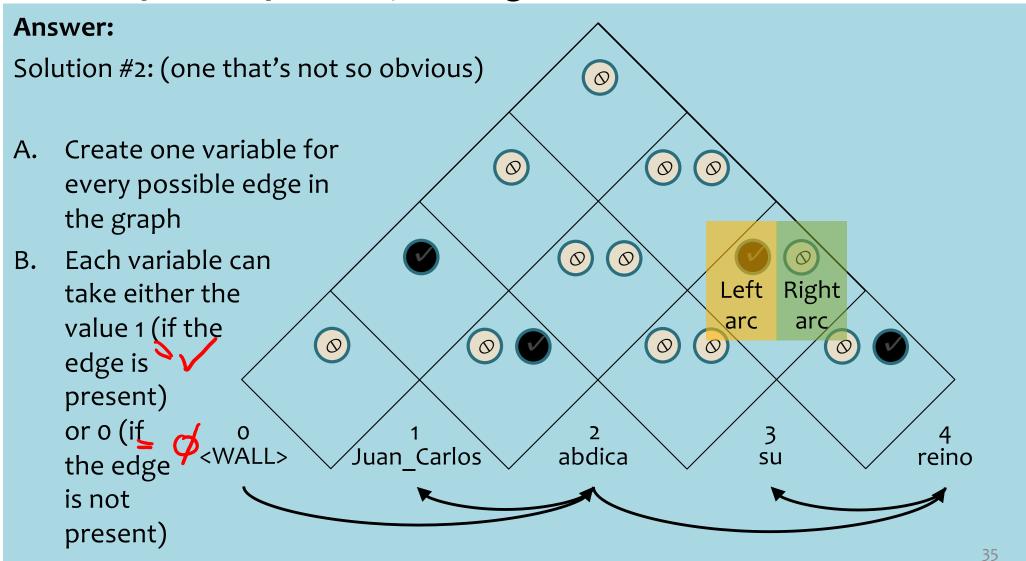
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**Example 3: Dependency Parsing** 



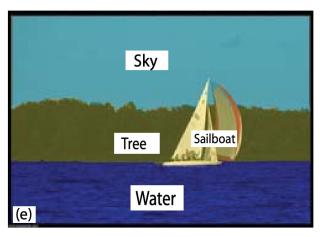
**Example 3: Dependency Parsing** 



#### **Example 4: Scene Understanding**







#### **Question:**

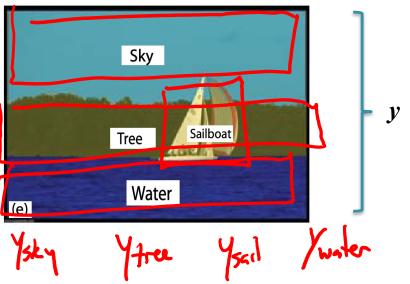
How would you decompose the structure *y* into parts?

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- What values could each variable take?

#### **Answer:**

#### **Example 4: Scene Understanding**





#### **Question:**

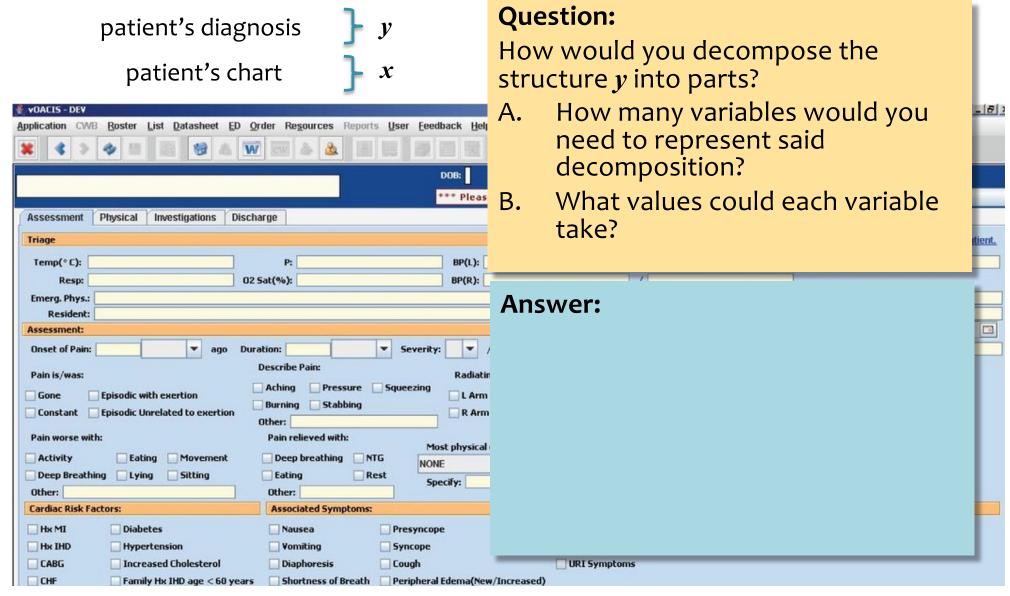
How would you decompose the structure *y* into parts?

- A. How many variables would you need to represent said decomposition?
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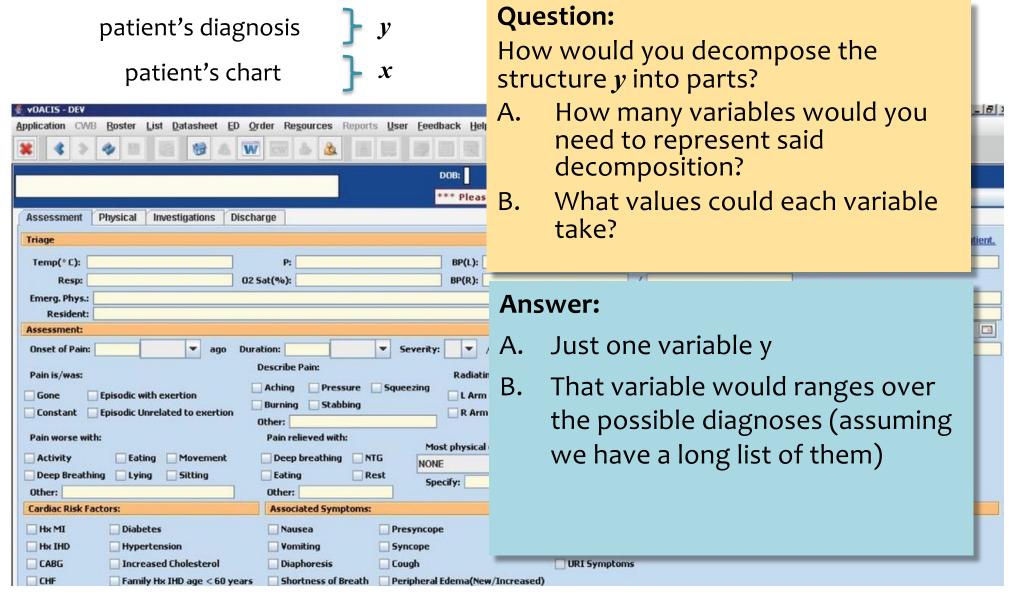
#### **Answer:**

- A. One output variable  $y_{i,j}$  for each of pixel  $x_{i,i}$
- B. The value of each y<sub>i,j</sub> would be one of the possible labels, e.g. {sailboat, sky, tree, water, mountain, ...}

Example 5: Medical Diagnosis



Example 5: Medical Diagnosis

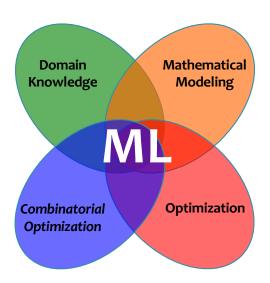


#### Takeaways from these examples

- 1. The structure often provides an obvious decomposition (e.g. POS tagging)
- Dealing with variable size structures can be tricky (e.g. phoneme recognition)
- There are often many ways to decomposition the structure (e.g. dependency parsing)
- Sometimes the less obvious decomposition may be the "simpler" one (e.g. scene understanding)
- 5. Don't confuse structure in the input for structure in the output (e.g. medical diagnosis)

### Structured Prediction

The data inspires
the structures
we want to
predict



Our **model**defines a score
for each structure

It also tells us what to optimize

**Inference** finds

{best structure, marginals, partition function} for a new observation

(Inference is usually called as a subroutine in learning)

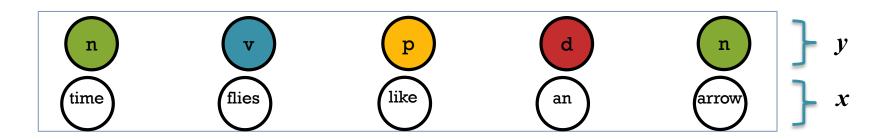
Learning tunes the parameters of the model

(without any math!)

### WHAT IS A MODEL?

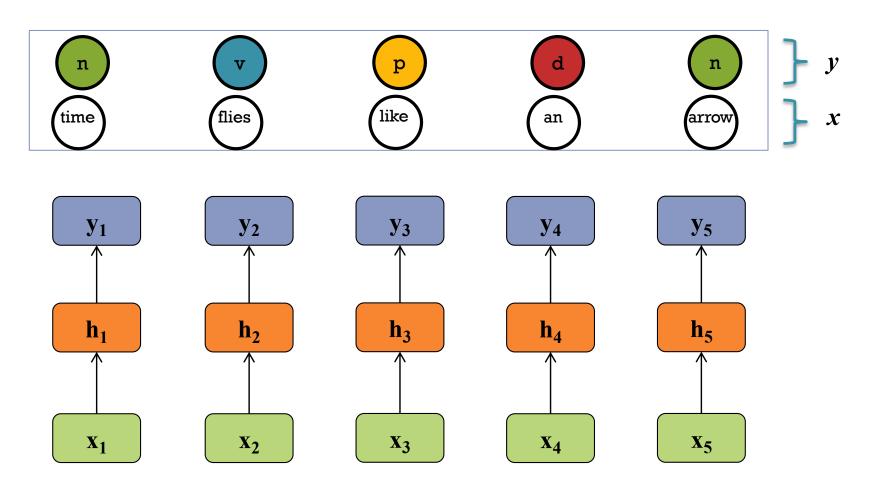
## A Not-very-interesting Model

**Question:** How could we apply a standard feed-forward neural network (MLP) that expects a **fixed size input/output** to a prediction task with **variable length input/output**?



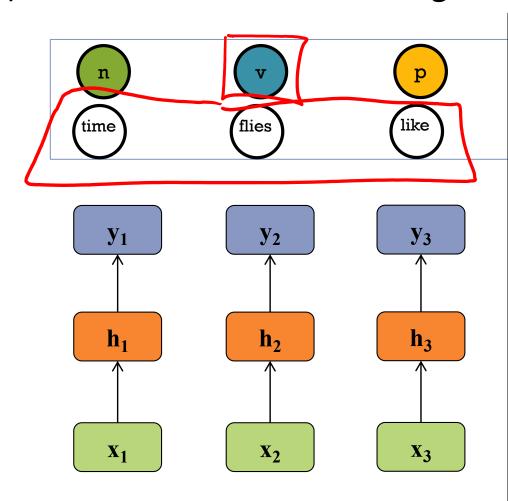
## A Not-very-interesting Model

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## A Not-very-interesting Model

**Question:** How could we apply a standard feed-forward neural network (MLP) that expects a **fixed size input/output** to a prediction task with **variable length input/output**?



**Q:** Why is this model not-very-interesting?

**A:** Because it only considers the interaction between the current word x<sub>t</sub> and the current tag y<sub>t</sub>

In other words, it makes an independent classification decision for each tag.

For part-of-speech tagging, we know that verbs are much more likely to follow nouns. But this model CANNOT learn that.

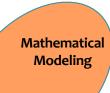
## Joint Modeling

After we come up with a way to decompose our structure into variables, what comes next?

- We can define a joint model over those variables
- The joint model defines a score for each possible structure allowed by our decomposition
- The model should give high scores to "good" structures and low scores to "bad" structures
  - in probability terms: high scores for likely structures and low scores for unlikely structures
  - "likely structures" could be defined as those appearing in your training dataset
- (Hopefully, the joint model is also able to capture interesting interactions between pairs, triples, quadruples, ... of variables)

# How do we write down a joint model?

(Factor Graphs)

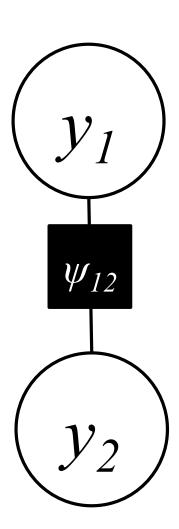


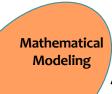
## An Abstraction for Modeling

#### **Factor Graph**

(bipartite graph)

- variables (circles)
- factors (squares)



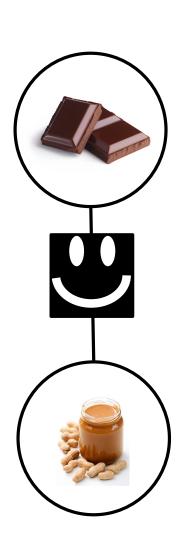


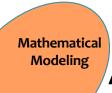
#### **Factor Graph**

(bipartite graph)

- variables (circles)
- factors (squares)

Factors have local opinions



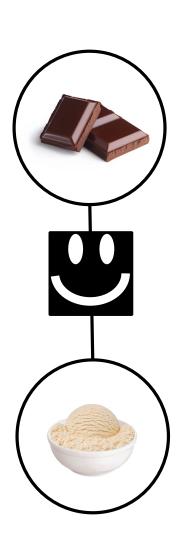


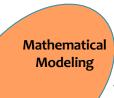
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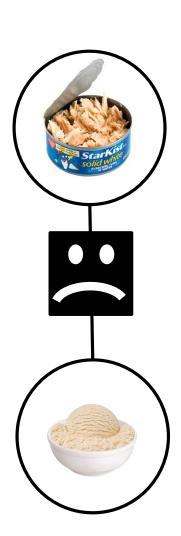


#### **Factor Graph**

(bipartite graph)

- variables (circles)
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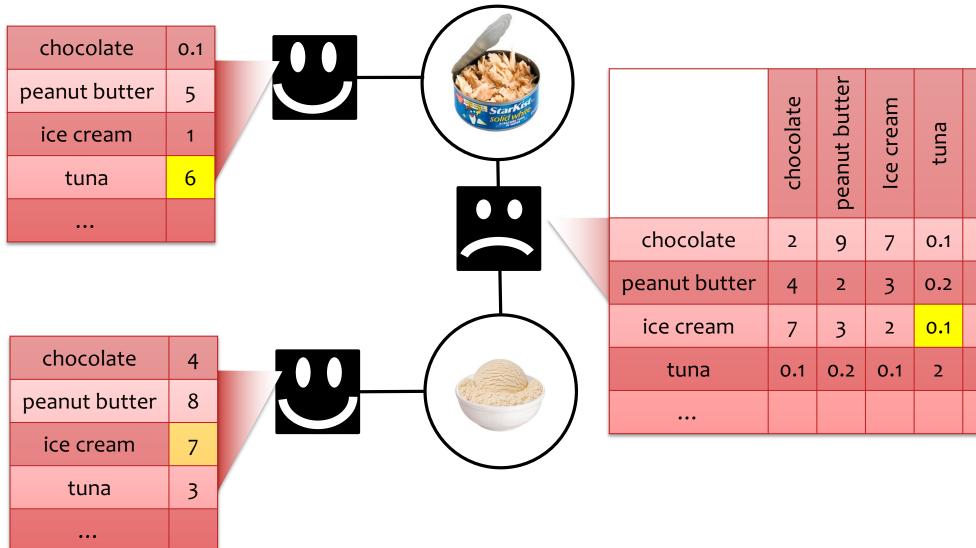
Factors have local opinions



Mathematical Modeling

## An Abstraction for Modeling

P(tuna, ice cream) = ?

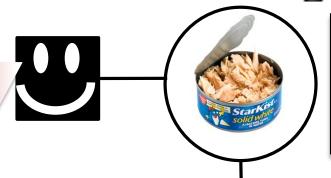


Mathematical Modeling

## An Abstraction for Modeling

 $P(\text{tuna, ice cream}) = \frac{1}{Z} (6 * 7 * 0.1)$ 

chocolate	0.1	
peanut butter	5	
ice cream	1	
tuna	6	
•••		



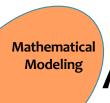
Uh-oh! The probabilities of
the various assignments sum
up to $Z > 1$ .

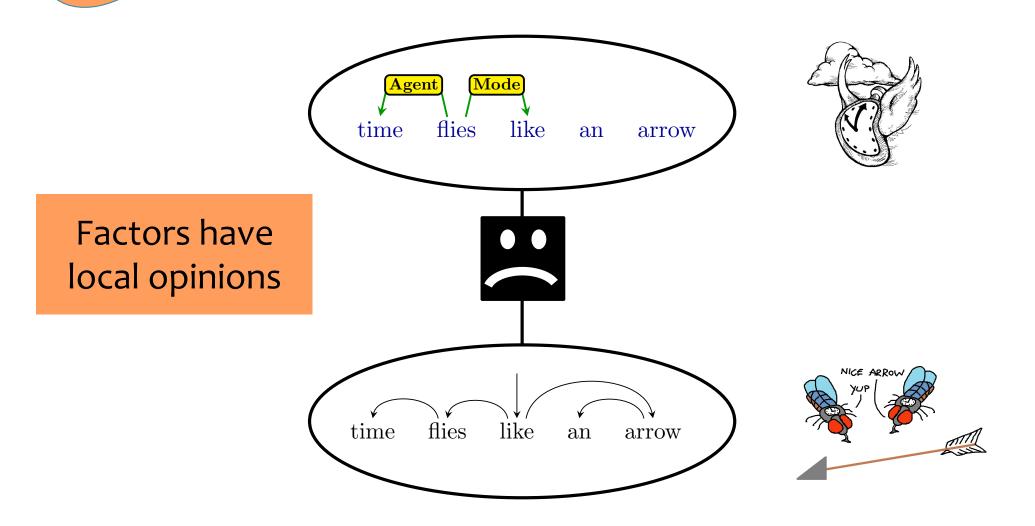
So divide them all by Z.

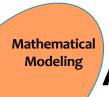
chocolate	4
peanut butter	8
ice cream	7
tuna	3

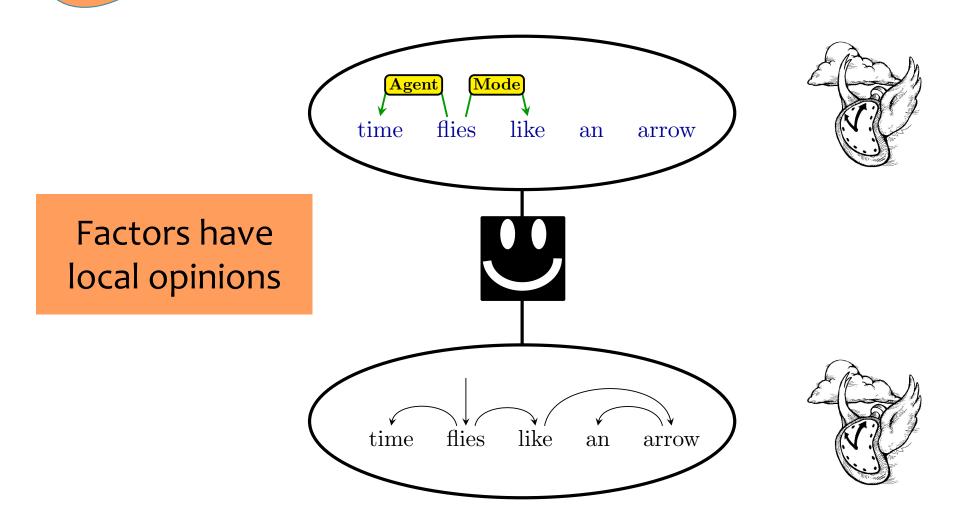
	cho	peanu	Ice	tı	
chocolate	2	9	7	0.1	
peanut butter	4	2	3	0.2	
ice cream	7	3	2	0.1	
tuna	0.1	0.2	0.1	2	

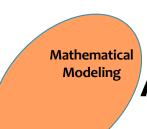
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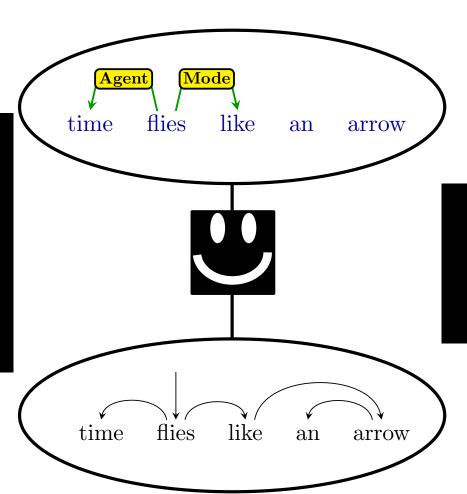








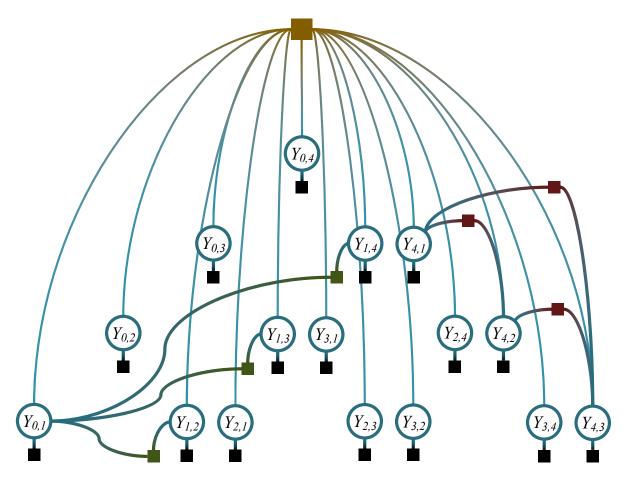
The domains of these variables is exponential in the length of the sentence!

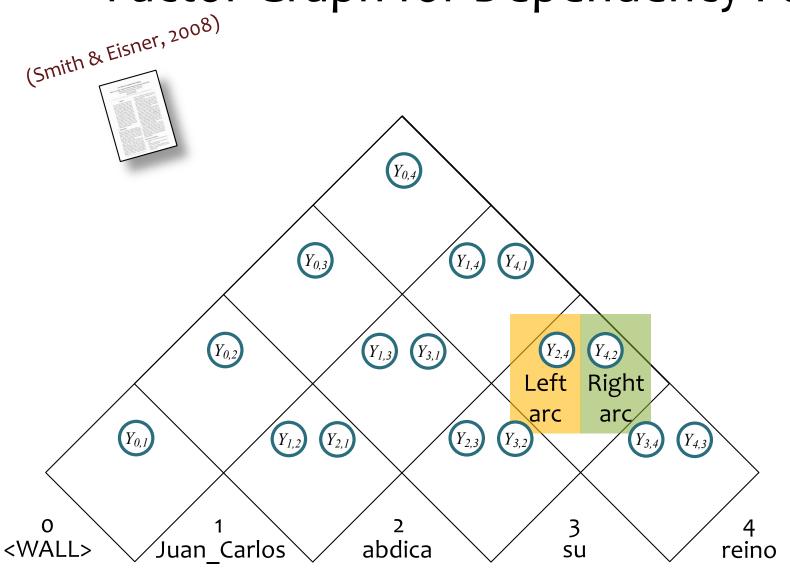


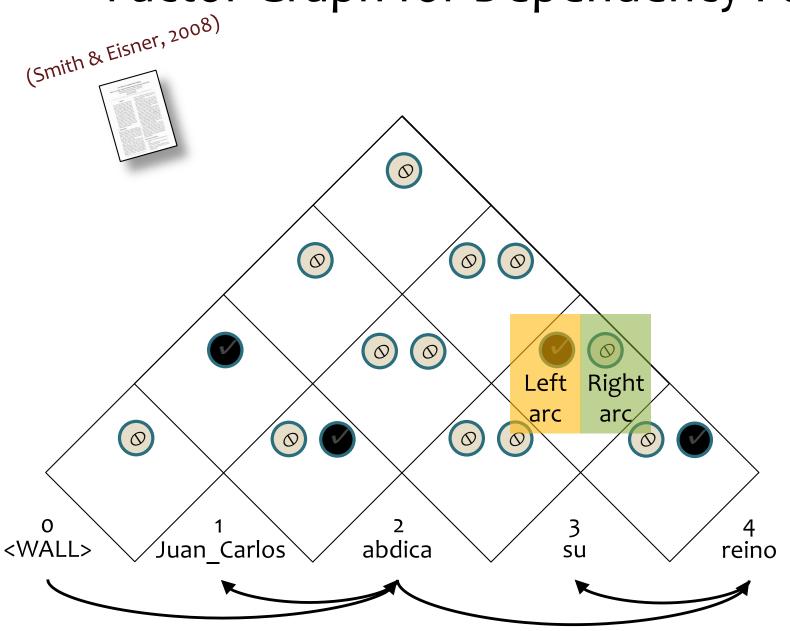
This factor would be massive

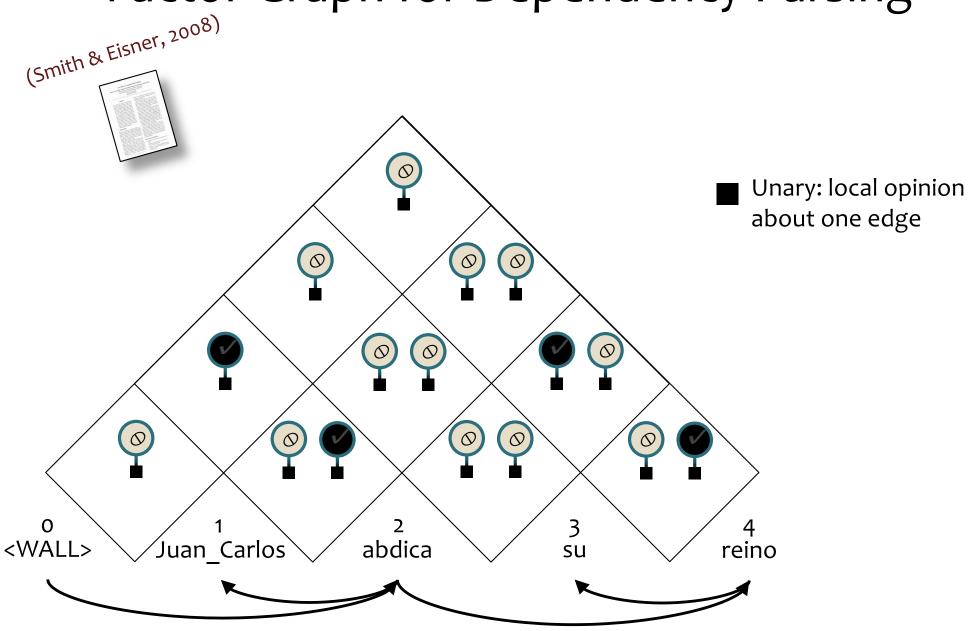
That's why decomposing into many small variables is so important

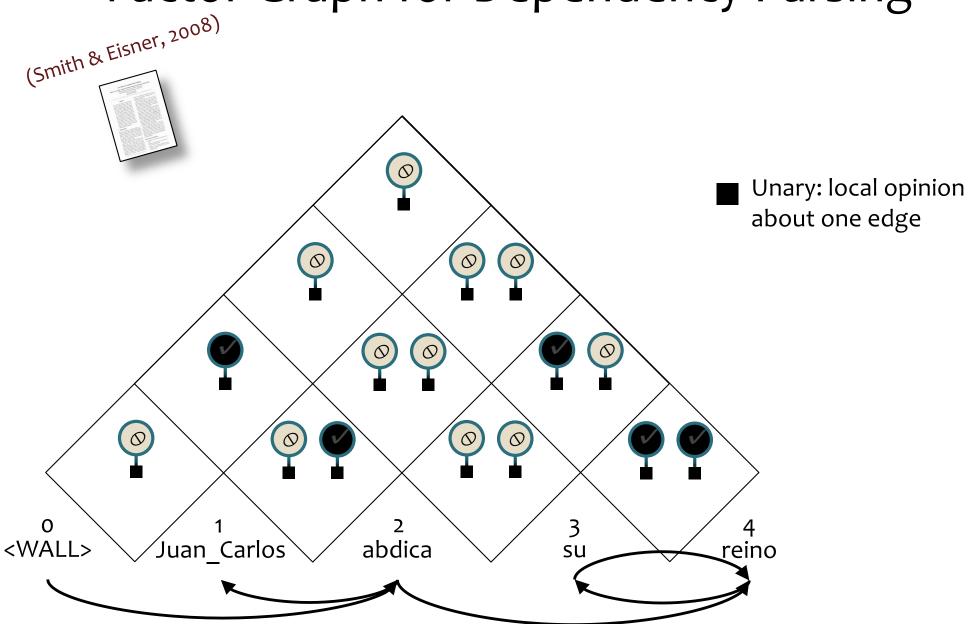
## **EXAMPLE: FACTOR GRAPH FOR DEPENDENCY PARSING**

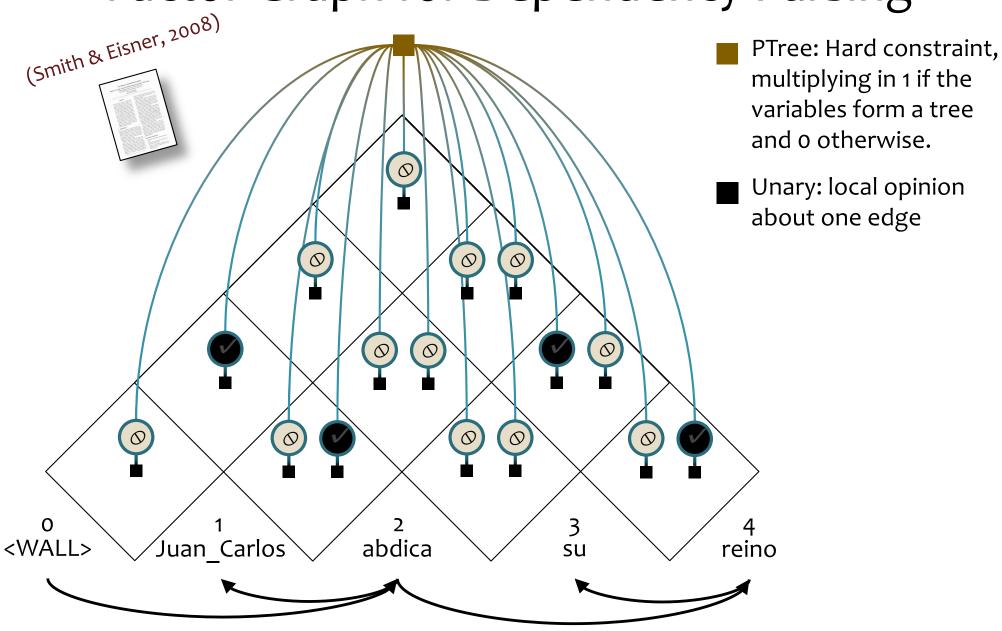


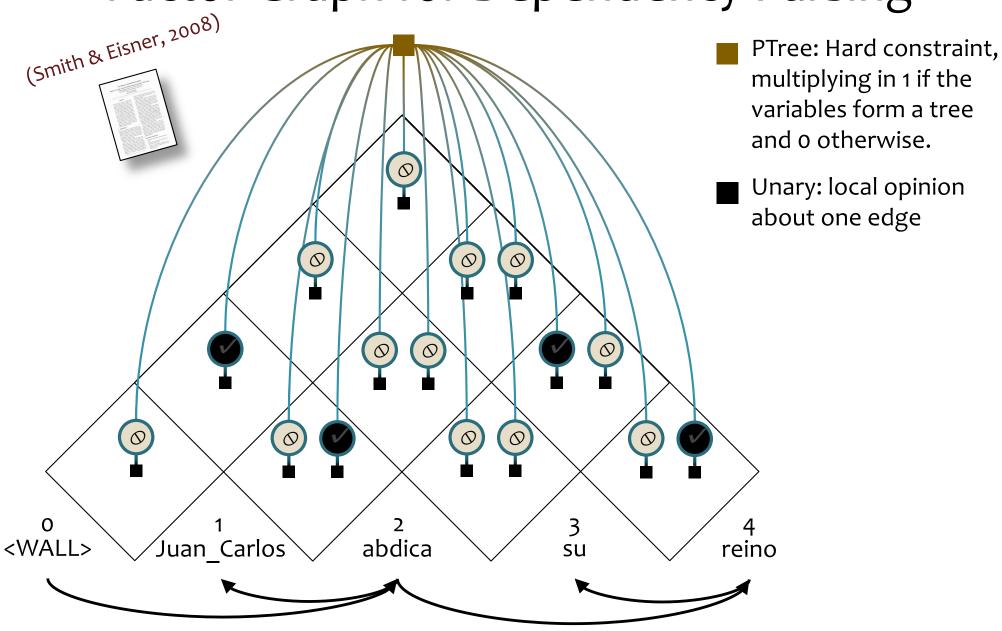


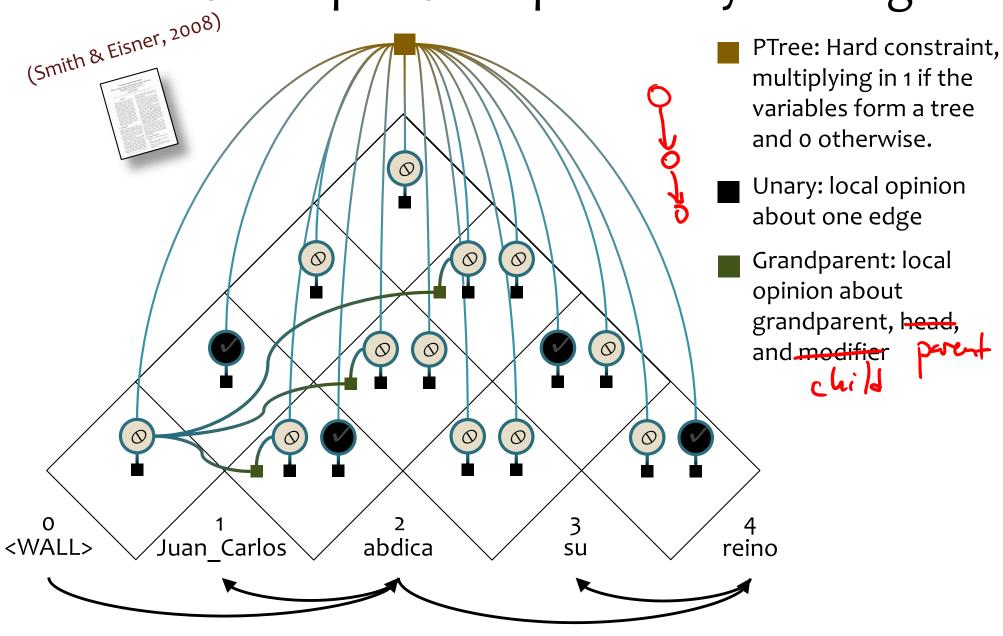


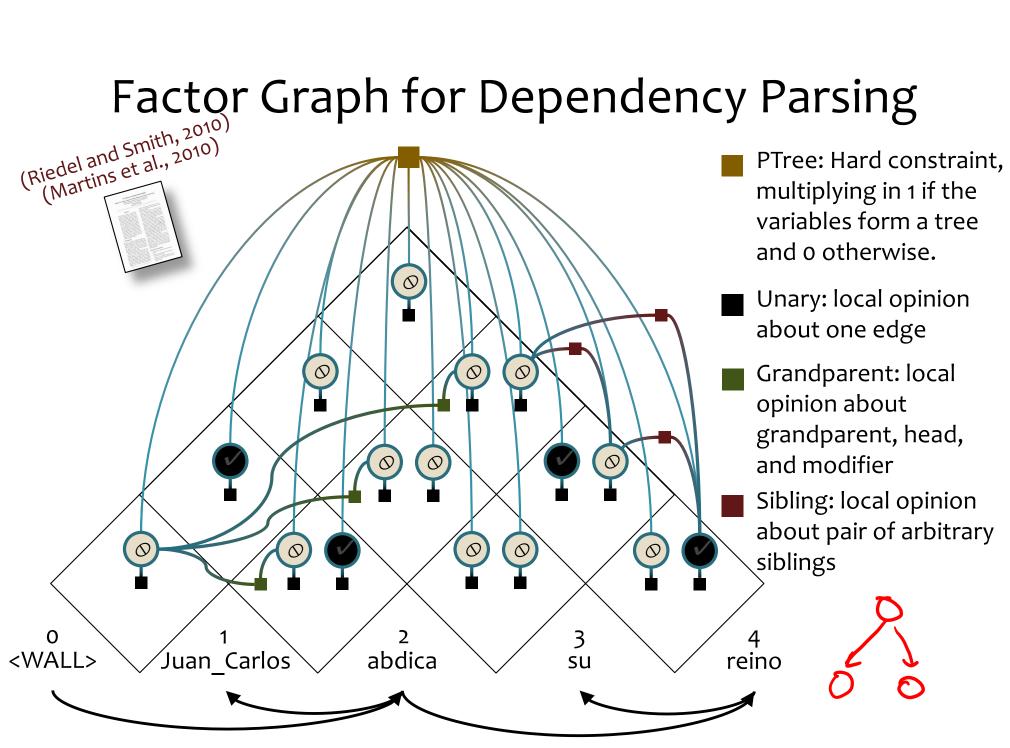


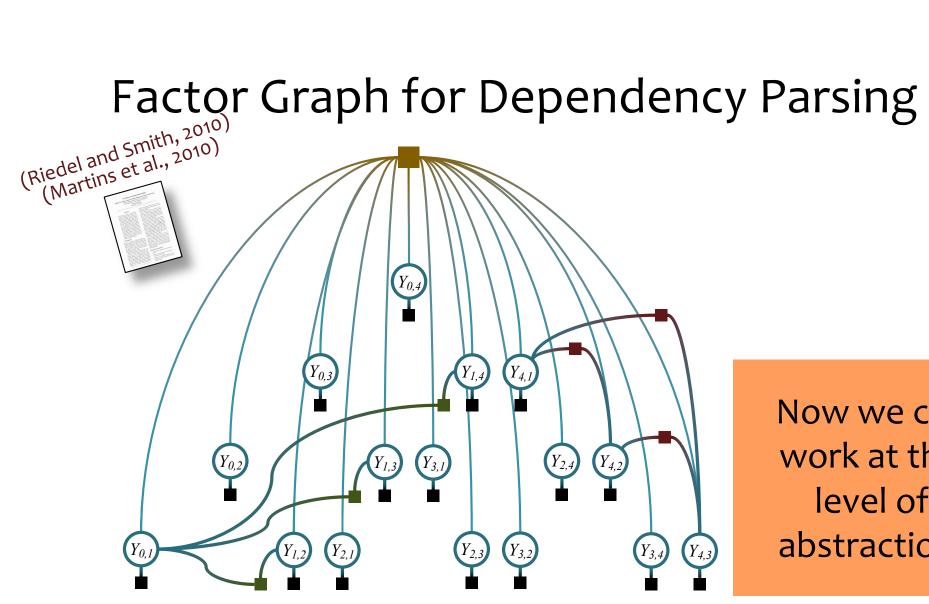












Now we can work at this level of abstraction.

$$p_{\theta}(\boldsymbol{y}) = \frac{1}{Z} \prod_{\alpha} \psi_{\alpha}(\boldsymbol{y}_{\alpha})$$

#### **VARIABLES AND INTERACTIONS**

## Joint Modeling

#### When do we add factors?

In order to determine which subsets of variables should have factors between them, we need to think about which variable **interactions** we want to model.

If we expect there to be an interesting interaction between some collection of variables, then we should add a factor to express an opinion about it

## Scene Understanding

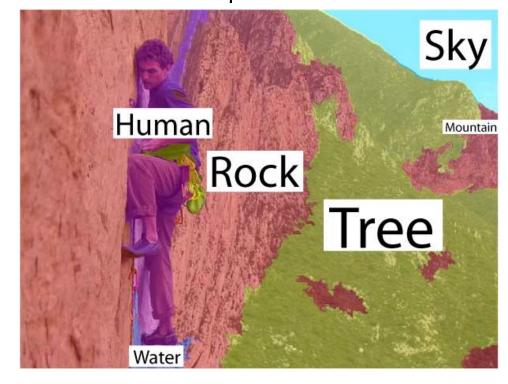
#### Variables:

- boundaries of image regions
- tags of regions

#### Interactions:

- semanticplausibility ofnearby tags
- continuity of tags
   across visually
   similar regions (i.e.
   patches)

Labels with top-down information



(Li et al., 2009)

## Scene Understanding

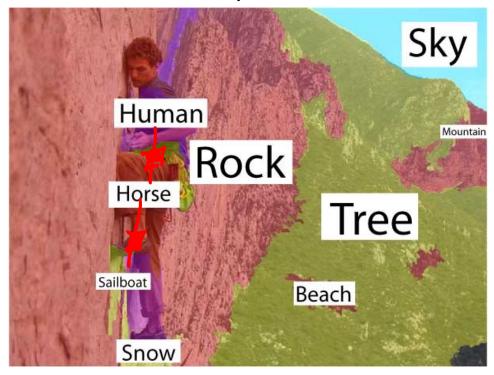
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Labels without top-down information



(Li et al., 2009)

## Word Alignment / Phrase Extraction

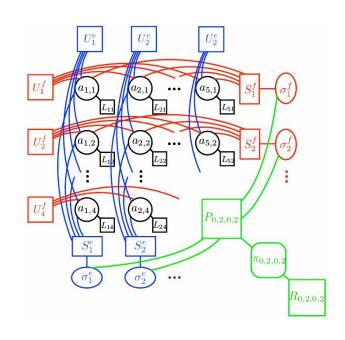
#### Variables (boolean):

For each (Chinese phrase, English phrase) pair, are they linked?

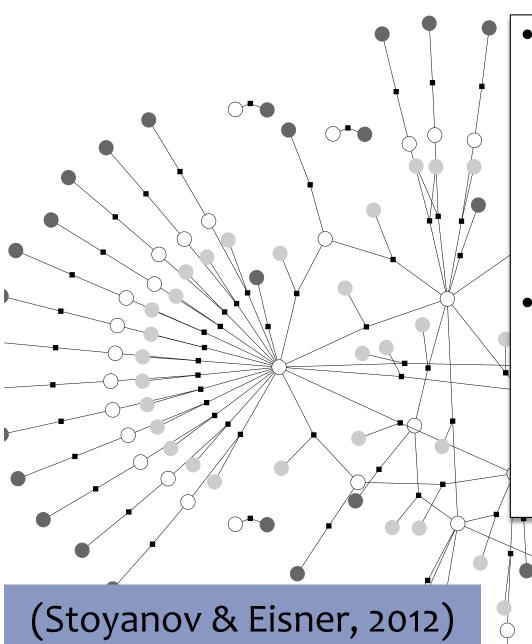
# 

#### Interactions:

- Word fertilities
- Few "jumps" (discontinuities)
- Syntactic reorderings
- "ITG contraint" on alignment
- Phrases are disjoint (?)



## Congressional Voting



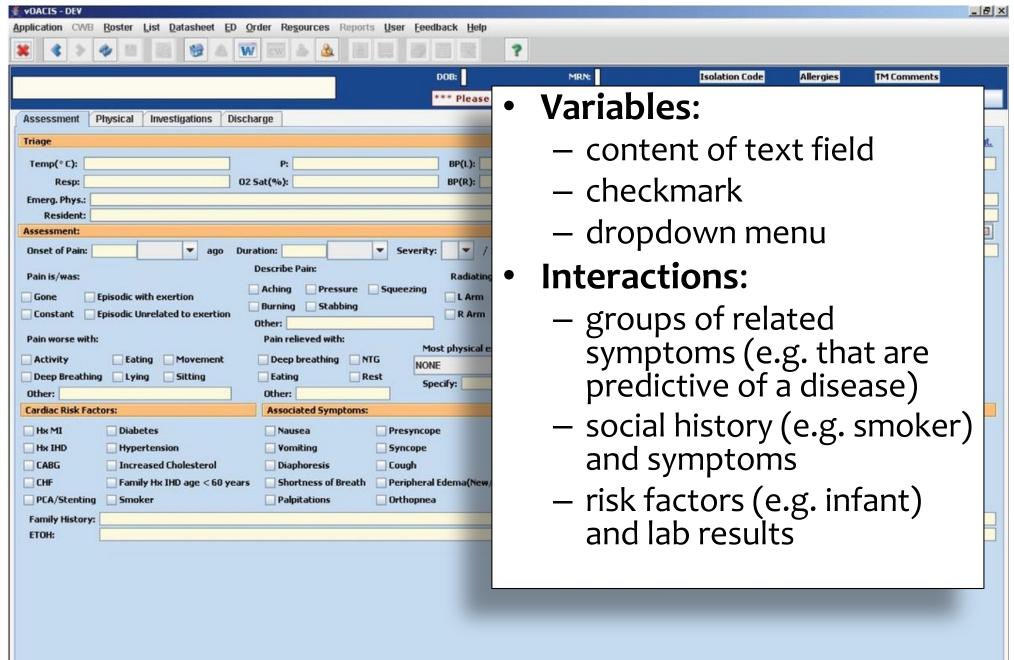
#### • Variables:

- Representative's vote
- Text of all speeches of a representative
- Local contexts of references between two representatives

#### • Interactions:

- Words used by representative and their vote
- Pairs of representatives and their local context

## Medical Diagnosis



(we'll talk about this in a later lecture...)

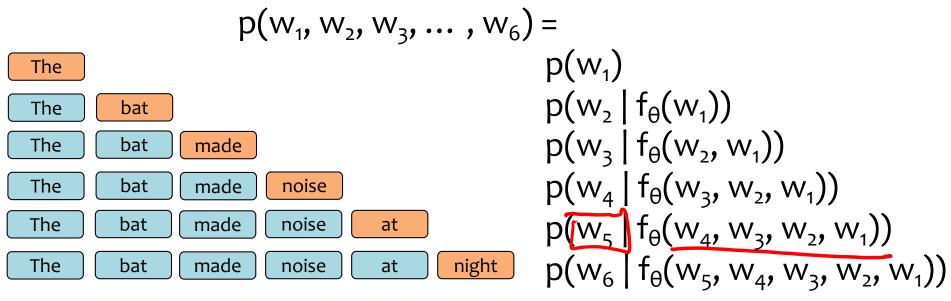
## EXAMPLE: RECURRENT NEURAL NETWORK LANGUAGE MODEL

# What if I want to model EVERY possible interaction?

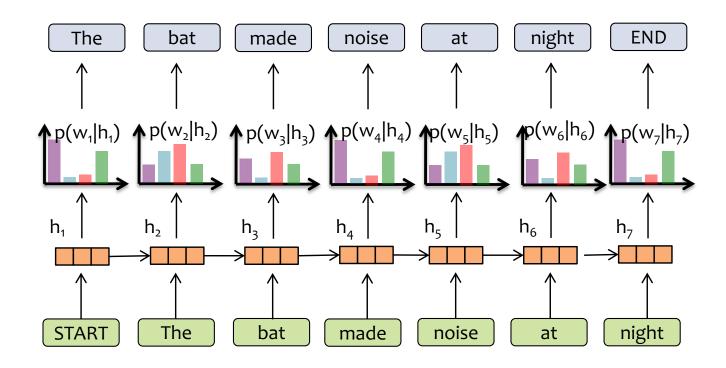
... or at least the interactions of the current variable with all those that came before it...

(RNN-LMs)

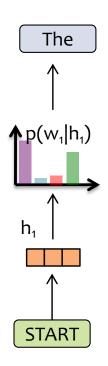
RNN Language Model: 
$$p(w_1, w_2, \dots, w_T) = \prod_{t=1}^T p(w_t \mid f_{\boldsymbol{\theta}}(w_{t-1}, \dots, w_1))$$



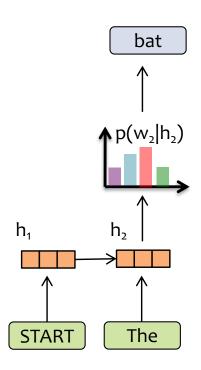
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- (2) define distribution  $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$  that conditions on the vector



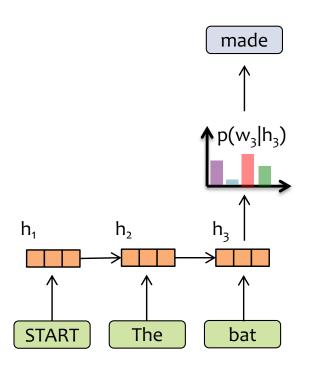
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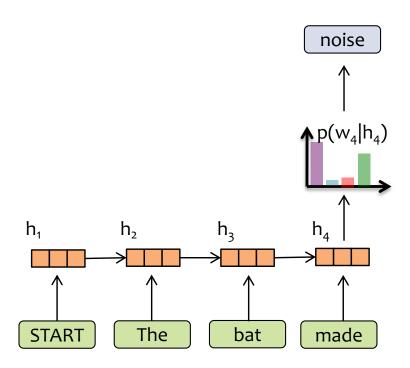
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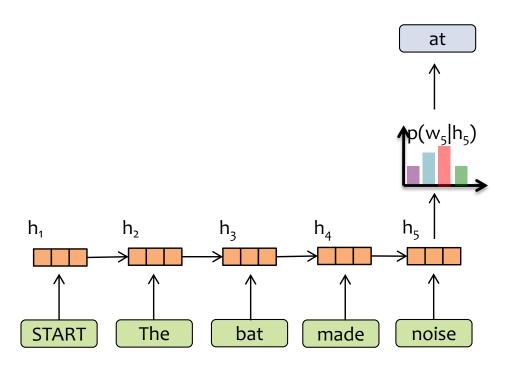
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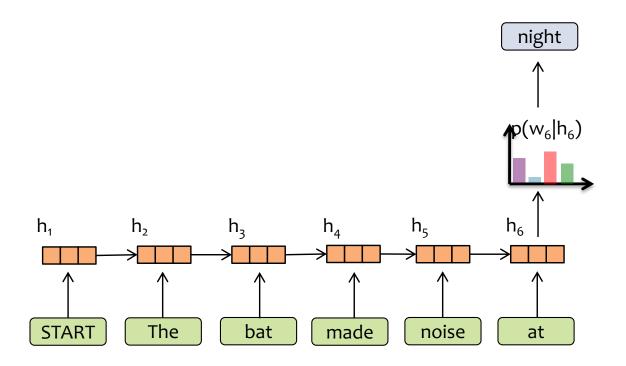
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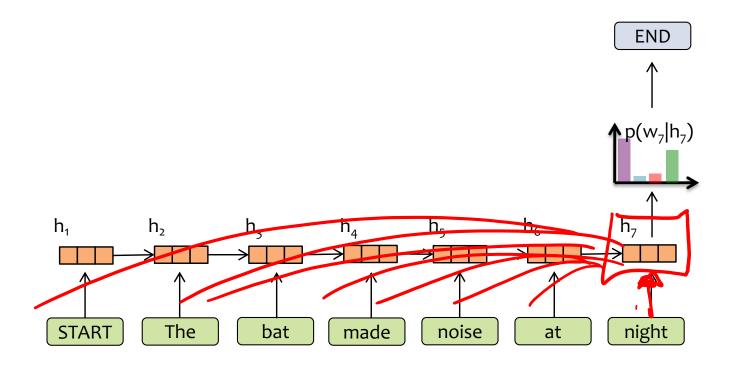


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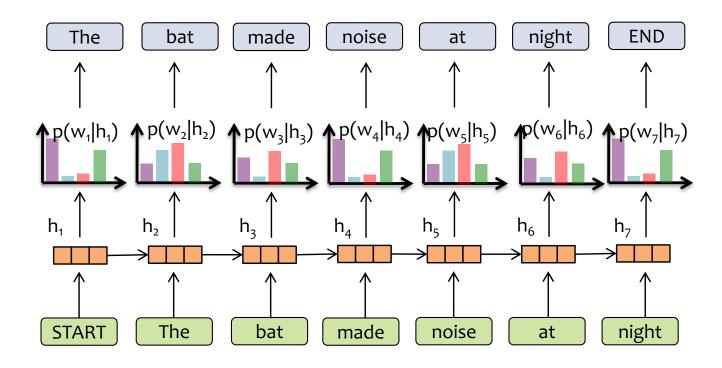
## RNN Language Model



#### **Key Idea:**

- (1) convert all previous words to a fixed length vector
- (2) define distribution  $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$  that conditions on the vector  $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$

# RNN Language Model

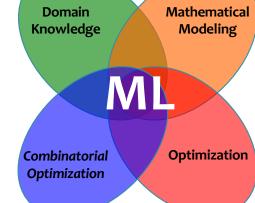


$$p(w_1, w_2, w_3, ..., w_T) = p(w_1 | h_1) p(w_2 | h_2) ... p(w_2 | h_T)$$

## A PREVIEW OF INFERENCE

## Structured Prediction

The data inspires
the structures
we want to
predict



Our **model**defines a score
for each structure

It also tells us what to optimize

**Inference** finds

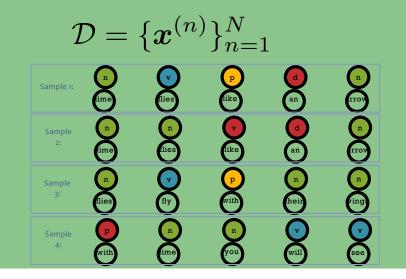
{best structure, marginals, partition function} for a new observation

(Inference is usually called as a subroutine in learning)

Learning tunes the parameters of the model

## Structured Prediction

#### 1. Data



#### 2. Model

$$p(\boldsymbol{x}\mid\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \prod_{C\in\mathcal{C}} \psi_C(\boldsymbol{x}_C)$$

#### 3. Objective

$$\ell(\theta; \mathcal{D}) = \sum_{n=1}^{N} \log p(\boldsymbol{x}^{(n)} \mid \boldsymbol{\theta})$$

#### 5. Inference

1. Marginal Inference

$$p(\boldsymbol{x}_C) = \sum_{\boldsymbol{x}': \boldsymbol{x}_C' = \boldsymbol{x}_C} p(\boldsymbol{x}' \mid \boldsymbol{\theta})$$

2. Partition Function

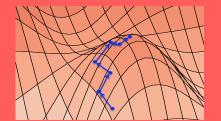
$$Z(\boldsymbol{\theta}) = \sum \prod \psi_C(\boldsymbol{x}_C)$$

3. MAP Inference

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{argmax}} p(\boldsymbol{x} \mid \boldsymbol{\theta})$$

#### 4. Learning

$$\boldsymbol{\theta}^* = \operatorname*{argmax}_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}; \mathcal{D})$$



## 5. Inference

#### 1. Marginal Inference (#P-Hard)

Compute marginals of variables and cliques

$$p(x_i) = \sum_{\boldsymbol{x}': x_i' = x_i} p(\boldsymbol{x}' \mid \boldsymbol{\theta}) \qquad \qquad p(\boldsymbol{x}_C) = \sum_{\boldsymbol{x}': \boldsymbol{x}_C' = \boldsymbol{x}_C} p(\boldsymbol{x}' \mid \boldsymbol{\theta})$$

#### 2. Partition Function (#P-Hard)

Compute the normalization constant

$$Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C)$$

# 3. MAP Inference (NP-Hard)

Compute variable assignment with highest probability

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{argmax}} p(\boldsymbol{x} \mid \boldsymbol{\theta})$$

#### 4. Sampling (cf. convergence, variance)

Draw a sample variable assignment

$$\mathbf{x} \sim p(\cdot|\boldsymbol{\theta})$$

## Q&A

**Q:** But in **deep learning** we don't need to solve these inference problems, right?

**A:** Wrong... it's not that we don't *need* to solve them, it's that we often can't!

#### Questions you could ask your RNN-LM or seq2seq model:

- X 1. What is the probability of the 7<sup>th</sup> token being 'zebra' (marginal inference)
- X 2. For an unnormalized model, what is the normalization constant? (partition function)
- X 3. What is the most probable output sequence? (MAP inference)
- ✓ 4. Give me 10 samples from the distribution.

# Topics (Part I)

- Search-Based Structured Prediction
  - Reductions to Binary Classification
  - Learning to Search
  - RNN-LMs
  - seq2seq models
- Graphical Model Representation
  - Directed GMs vs.
     Undirected GMs vs.
     Factor Graphs
  - Bayesian Networks vs.
     Markov Random Fields vs.
     Conditional Random Fields

- Graphical Model Learning
  - Fully observed Bayesian Network learning
  - Fully observed MRF learning
  - Fully observed CRF learning
  - Parameterization of a GM
  - Neural potential functions

#### Exact Inference

- Three inference problems:
  - (1) marginals
  - (2) partition function
  - (3) most probably assignment
- Variable Elimination
- Belief Propagation (sumproduct and max-product)

# Topics (Part II)

- Learning for Structure Prediction
  - Structured Perceptron
  - Structured SVM
  - Neural network potentials
- (Approximate) MAP Inference
  - MAP Inference via MILP
  - MAP Inference via LP relaxation
- Approximate Inference by Sampling
  - Monte Carlo Methods
  - Gibbs Sampling
  - Metropolis-Hastings
  - Markov Chains and MCMC

- Parameter Estimation
  - Bayesian inference
  - Topic Modeling
- Approximate Inference by Optimization
  - Variational Inference
  - Mean Field Variational Inference
  - Coordinate Ascent V.I. (CAVI)
  - Variational EM
  - Variational Bayes
- Bayesian Nonparametrics
  - Dirichlet Process
  - DP Mixture Model
- Deep Generative Models
  - Variational Autoencoders

## **SYLLABUS HIGHLIGHTS**

# Syllabus Highlights

The syllabus is located on the course webpage:

http://418.mlcourse.org http://618.mlcourse.org



The course policies are required reading.

# Syllabus Highlights

- **Grading 418:** 60% homework, 15% midterm, 20% final, 5% participation
- **Grading 618:** 55% homework, 15% midterm, 15% final, 5% participation, 10% project
- Midterm Exam: in-class exam, Fri, Oct. 14
- Final Exam: final exam week, date/time TBD by registrar
- **Homework:** ~6 assignments
  - 8 grace days for homework assignments
  - Late submissions: 75% day 1, 50% day 2,
     25% day 3
  - No submissions accepted after 3 days w/o extension
  - Extension requests: for emergency situations, see syllabus
- Recitations: Fridays, same time/place as lecture (optional, interactive sessions)

- Readings: required, online PDFs, recommended for after lecture
- Technologies:
  - Piazza (discussion),
  - Gradescope (homework),
  - Google Forms (polls),
  - Zoom (livestream),
  - Panopto (video recordings)
- Academic Integrity:
  - Collaboration encouraged, but must be documented
  - Solutions must always be written independently
  - No re-use of found code / past assignments
  - Severe penalties (i.e., failure)
- Office Hours: posted on Google Calendar on "Office Hours" page

### Lectures

- You should ask lots of questions
  - Interrupting (by raising a hand, turning on your video, and waiting to be called on) to ask your question is strongly encouraged
  - Use the chat to ask questions in real time (TAs will be monitoring the chat and will either answer or interrupt the instructor)
  - Asking questions later on Piazza is also great
- When I ask a question...
  - I want you to answer
  - Even if you don't answer, think it through as though I'm about to call on you
- Interaction improves learning (both in-class and at my office hours)

## Homework

There will be 6 homework assignments during the semester. The assignments will consist of both conceptual and programming problems.

	Main Topic	Implementation	Application Area	Туре
HW1	PyTorch Primer	MLP for Sequence Tagging	NLP	written + programming
HW2	Learning to Search	seq2seq + Dagger	speech recognition	written + programming
HW3	Marginal inference and MLE	RNN + Tree CRF	NLP	written + programming
HW4	MCMC	word embeddings + Gibbs sampler	topic modeling	written + programming
HW5	Variational Inference	mean field for cyclic CRF	computer vision	written + programming
HW6	Advanced Topics	NA		written

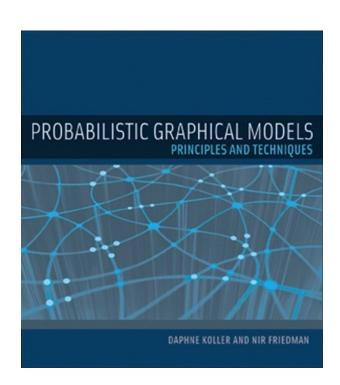
# Mini-Project (10-618 only)

#### Goals:

- Explore a learning / inference technique of your choosing
- Application and dataset will be provided (in the style of a Kaggle competition)
- Deeper understanding of methods in real-world application
- Work in teams of 2 students

## **Textbooks**

You are not required to read a textbook, but Koller & Friedman is a thorough reference text that includes a lot of the topics we cover.



## Prerequisites

## What they are:

- Introductory machine learning.
   (i.e. 10-301, 10-315, 10-601, 10-701)
- Significant experience programming in a general programming language.
  - The homework will require you to use Python,
     so you will need to be proficient in Python.
- 3. College-level probability, calculus, linear algebra, and discrete mathematics.

# Q&A