10-708 Probabilistic Graphical Models

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Learning MRFs & CRFs

+

Neural Potential Functions

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Lecture 7
Feb. 22, 2021

Q&A

Q: What are the subsets in Question 4 of HW1?
Is the question even asking what you meant to ask?

A: The subset notation in Q4 follows I-map notation (e.g. page 60, of Koller & Friedman textbook). Alas, we never introduced this notation in class and, as such, the whole question was not asking what we wanted.

Since this was our mistake, we'll figure out someway to even the playing field on Q4. I'll post more detail on Piazza after class…

Reminders

- Homework 1: PGM Representation
  - Out: Mon, Feb. 15
  - Due: Mon, Feb. 22 at 11:59pm
- Homework 2: Exact inference and supervised learning (CRF+RNN)
  - Out: Mon, Feb. 22
  - Due: Mon, Mar. 08 at 11:59pm

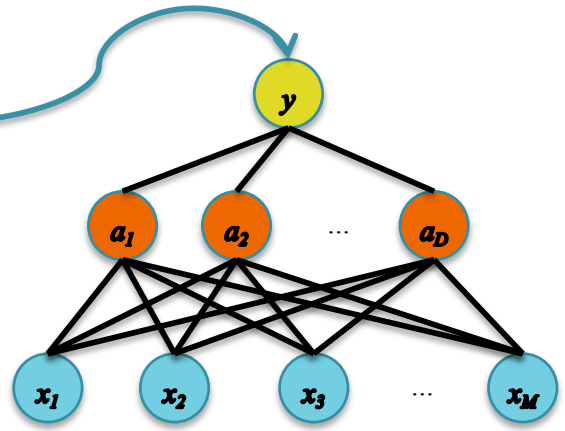
MRF LEARNING (LOG-LINEAR CASE)

Options for MLE of MRFs

- **Setting I:** $\psi_C(\boldsymbol{x}_C) = \theta_{C,\boldsymbol{x}_C}$
  A. MLE by inspection (Decomposable Models)
  B. Iterative Proportional Fitting (IPF)

- **Setting II:** $\psi_C(\boldsymbol{x}_C) = \exp(\boldsymbol{\theta} \cdot \boldsymbol{f}(\boldsymbol{x}_C))$
  C. Generalized Iterative Scaling
  D. Gradient-based Methods

- **Setting III:** $\psi_C(\boldsymbol{x}_C) =$
  E. Gradient-based Methods



Title Here

Whiteboard

- log-linear MRF model (i.e. with feature based potentials)
- log-linear MRF derivatives
- log-linear MRF training with SGD

LOG-LINEAR PARAMETERIZATION OF CONDITIONAL RANDOM FIELD

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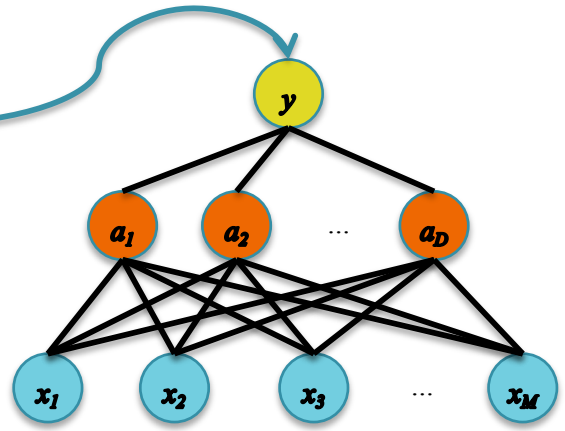
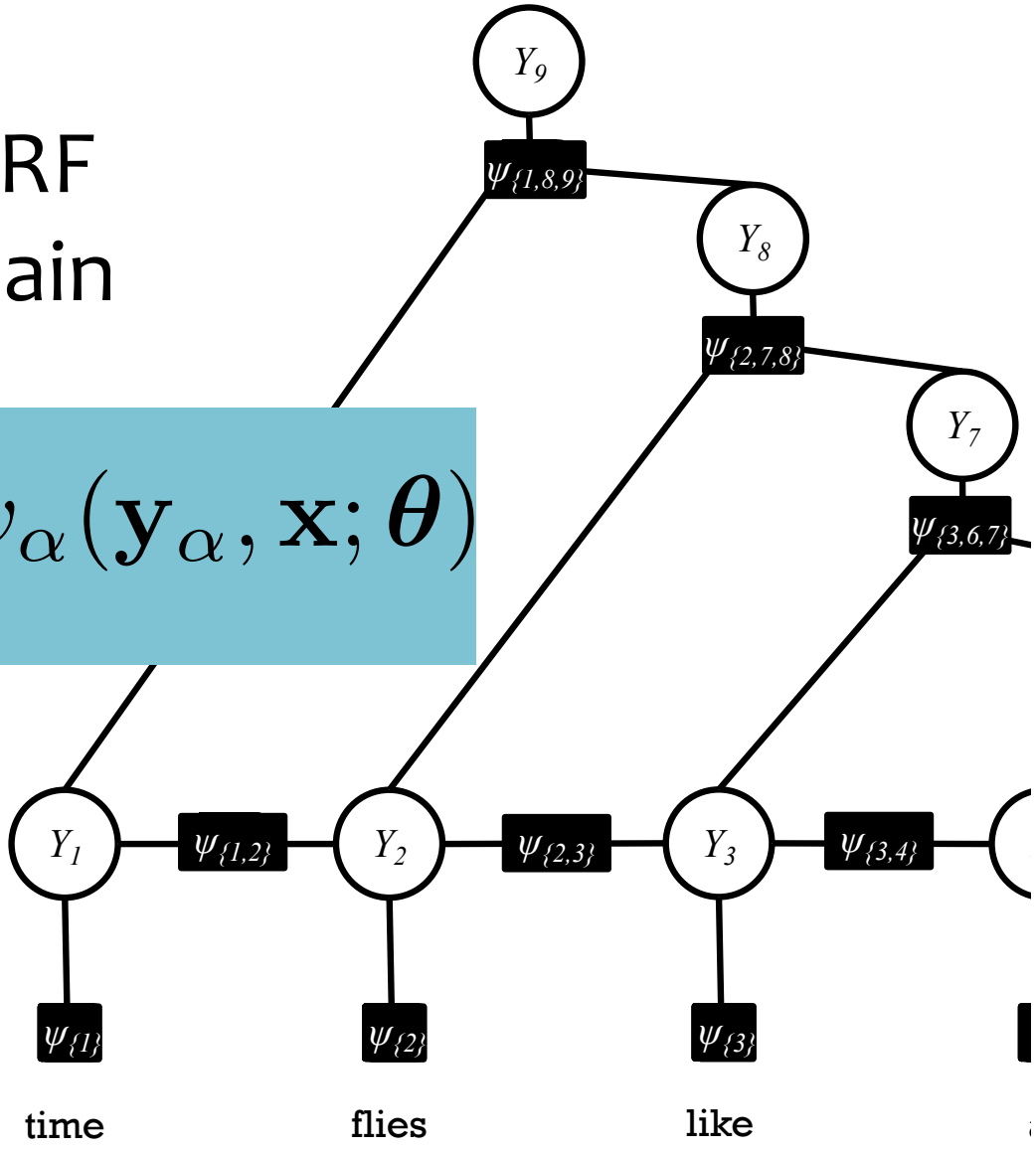


General CRF

The topology of the graphical model for a CRF doesn't have to be a chain

$$p_{\boldsymbol{\theta}}(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{x})} \prod_{\alpha} \psi_{\alpha}(\mathbf{y}_{\alpha}, \mathbf{x}; \boldsymbol{\theta})$$



Log-linear CRF Parameterization

$$p_{\boldsymbol{\theta}}(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{x})} \prod_{\alpha} \psi_{\alpha}(\mathbf{y}_{\alpha}, \mathbf{x}; \boldsymbol{\theta})$$

Define each potential function in terms of a fixed set of feature functions:

$$\psi_{\alpha}(\mathbf{y}_{\alpha}, \mathbf{x}; \boldsymbol{\theta}) = \exp(\boldsymbol{\theta} \cdot \mathbf{f}_{\alpha}(\mathbf{y}_{\alpha}, \mathbf{x}))$$

Predicted variables

Observed variables

Log-linear CRF Parameterization

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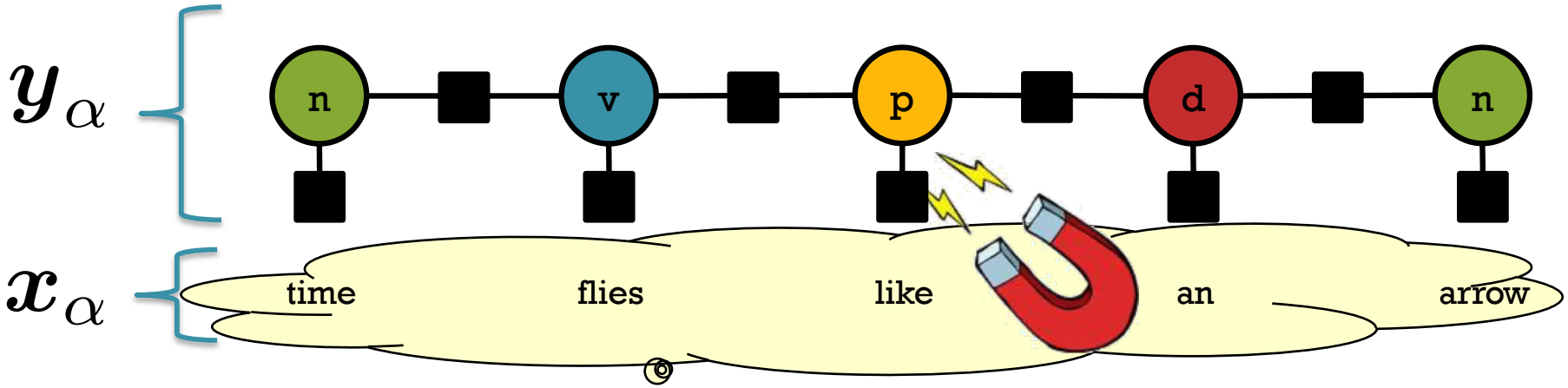

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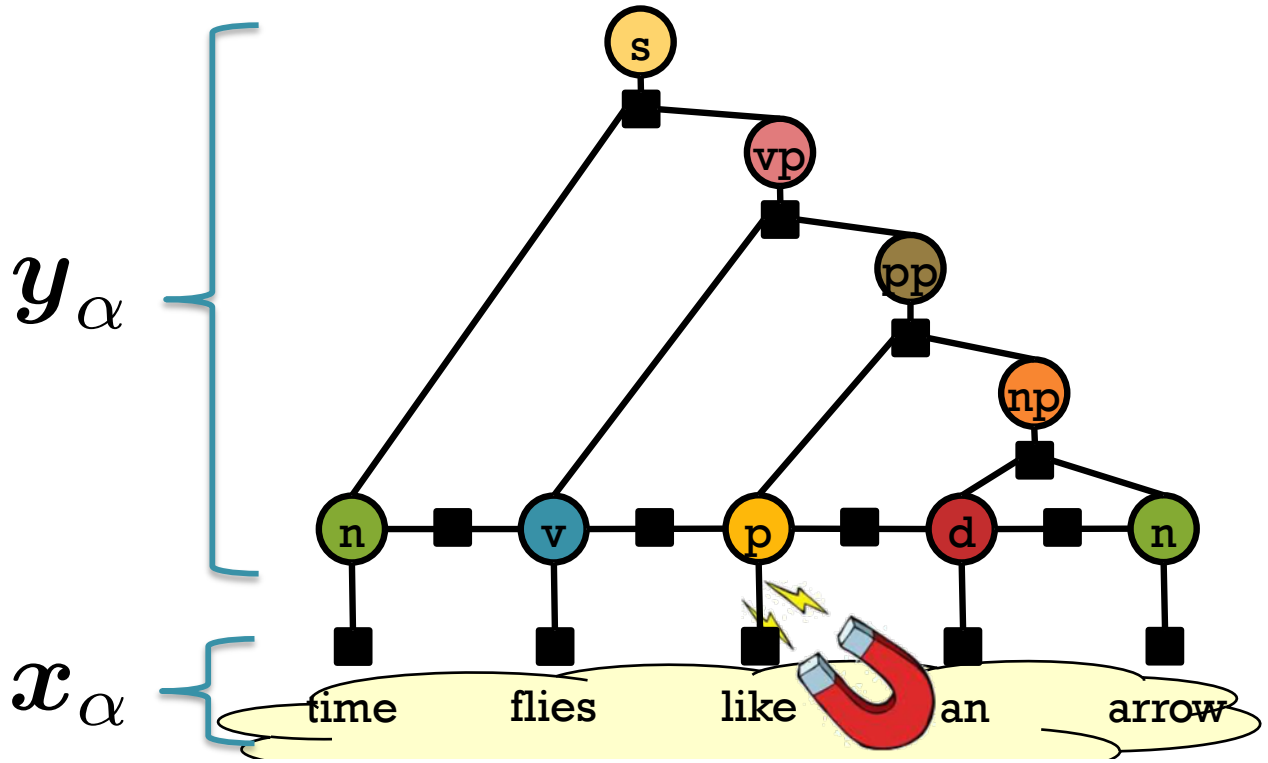
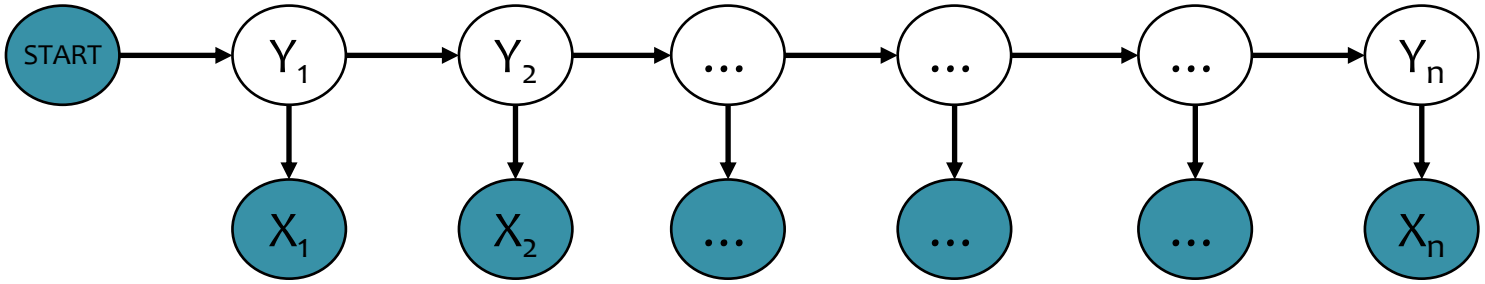


Conditional Random Fields (CRFs) for time series data

LINEAR-CHAIN CRFS

Shortcomings of Hidden Markov Models

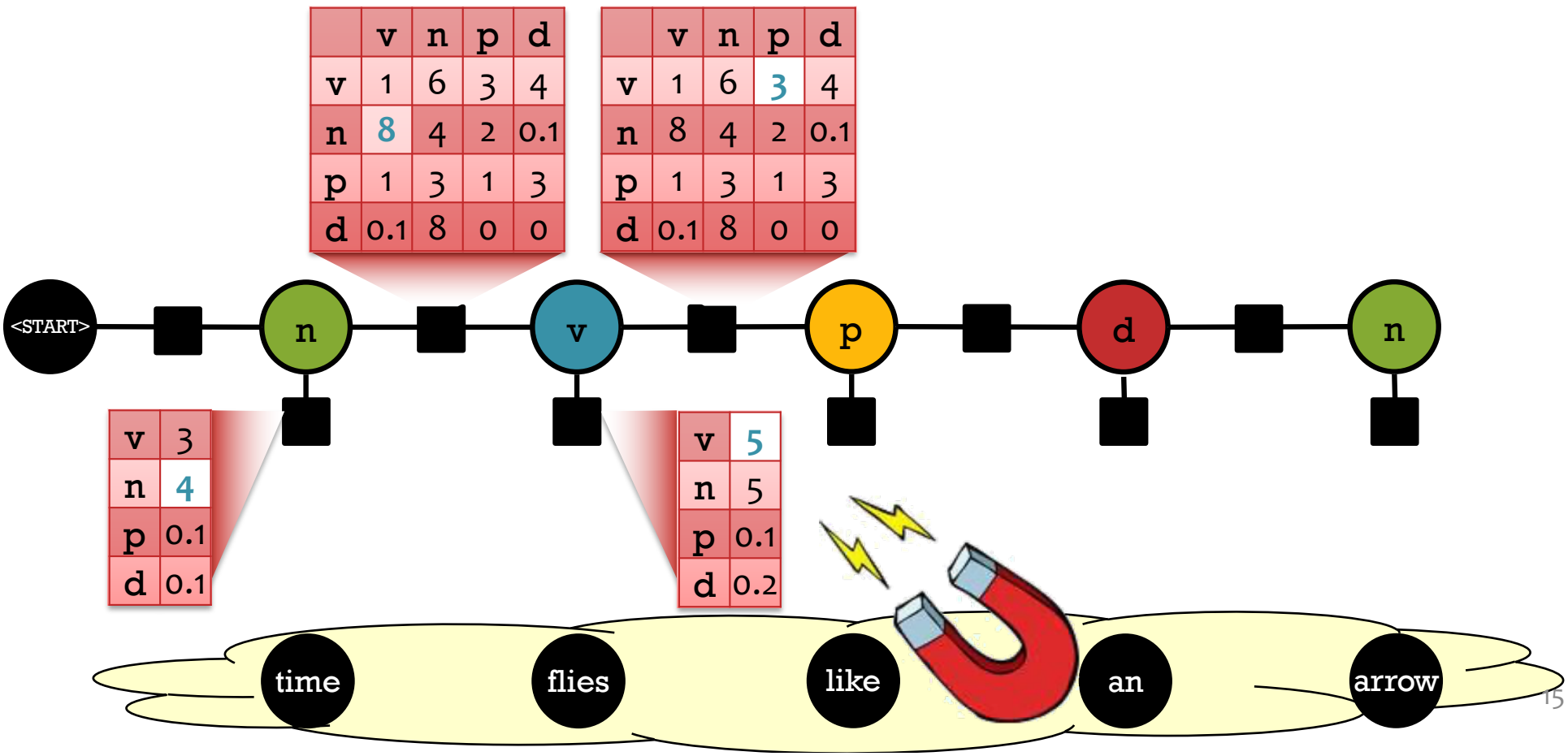


- HMM models capture dependences between each state and only its corresponding observation
  - NLP example: In a sentence segmentation task, each segmental state may depend not just on a single word (and the adjacent segmental stages), but also on the (non-local) features of the whole line such as line length, indentation, amount of white space, etc.
- Mismatch between learning objective function and prediction objective function
  - HMM learns a joint distribution of states and observations P(**Y**, **X**), but in a prediction task, we need the conditional probability P(**Y**|**X**)

Conditional Random Field (CRF)

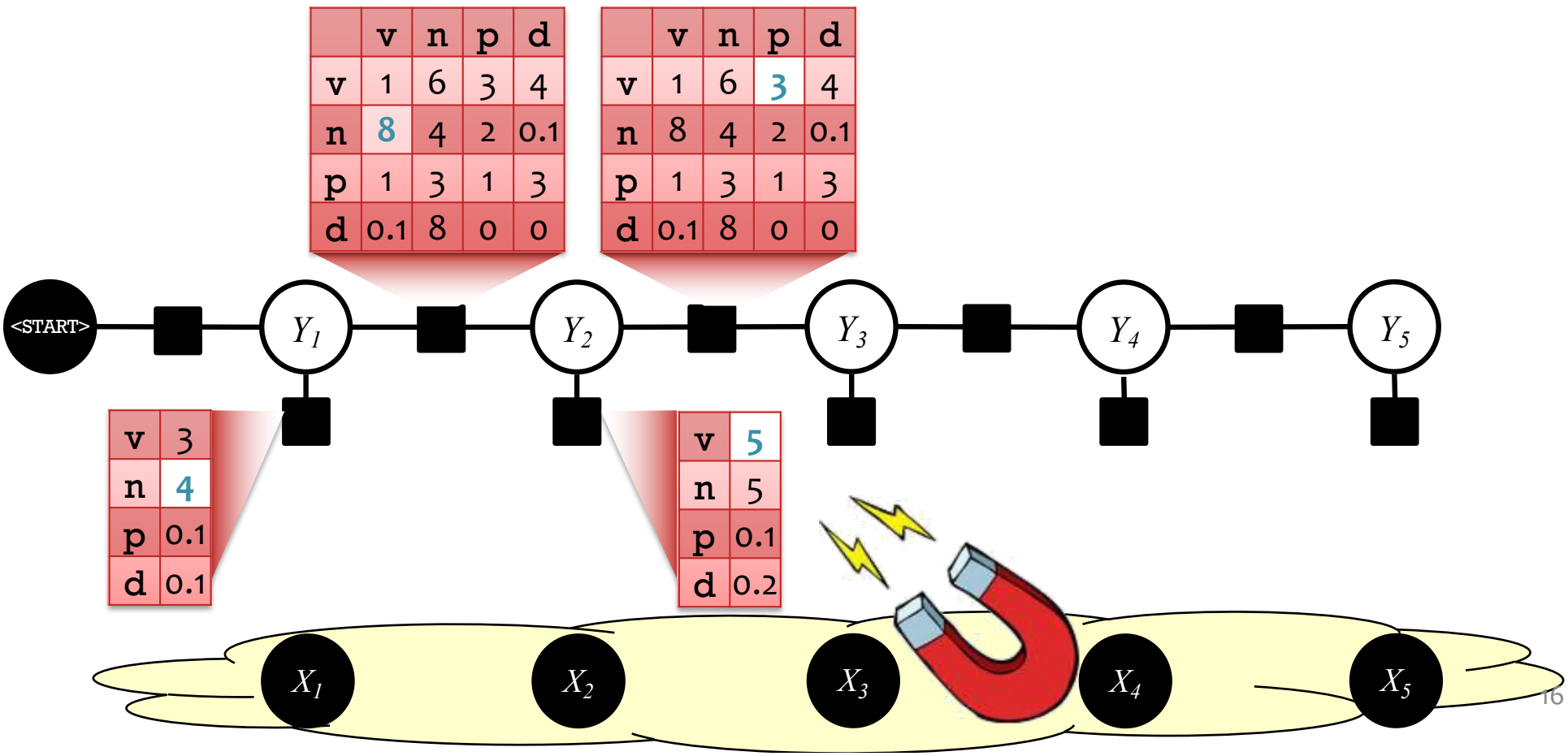
Conditional distribution over tags X_i given words w_i.
The factors and Z are now specific to the sentence w.

$$p(\text{n, v, p, d, n} \mid \text{time, flies, like, an, arrow}) = \frac{1}{Z}(4 * 8 * 5 * 3 * \ldots)$$



Conditional Random Field (CRF)

Recall: Shaded nodes in a graphical model are **observed**

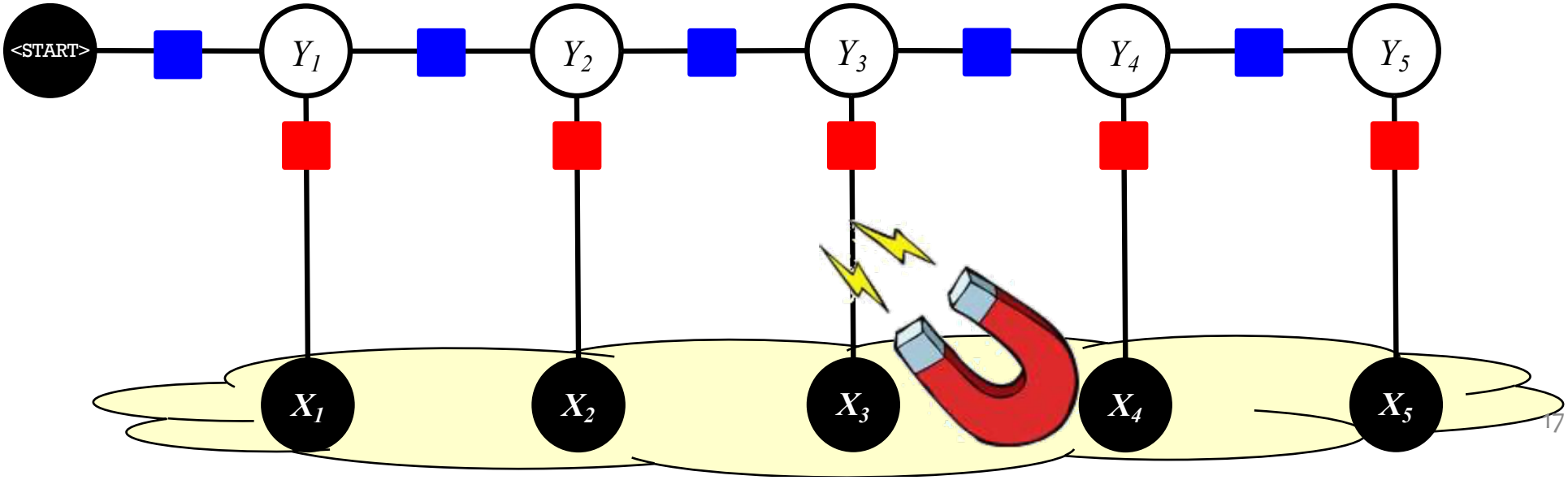


Conditional Random Field (CRF)

This **linear-chain CRF** is just **like an HMM,** except that its factors are **not** necessarily probability distributions

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{x})} \prod_{k=1}^{K} \psi_{\text{em}}(y_k, x_k)\psi_{\text{tr}}(y_k, y_{k-1})$$

$$= \frac{1}{Z(\mathbf{x})} \prod_{k=1}^{K} \exp(\boldsymbol{\theta} \cdot \mathbf{f}_{\text{em}}(y_k, x_k))\exp(\boldsymbol{\theta} \cdot \mathbf{f}_{\text{tr}}(y_k, y_{k-1}))$$



Exercise

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{x})} \prod_{k=1}^{K} \psi_{\text{em}}(y_k, x_k)\psi_{\text{tr}}(y_k, y_{k-1})$$

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Select All That Apply: Which model does the above distribution share the most in common with?

A. Hidden Markov Model
B. Bernoulli Naïve Bayes
C. Gaussian Naïve Bayes
D. Logistic Regression

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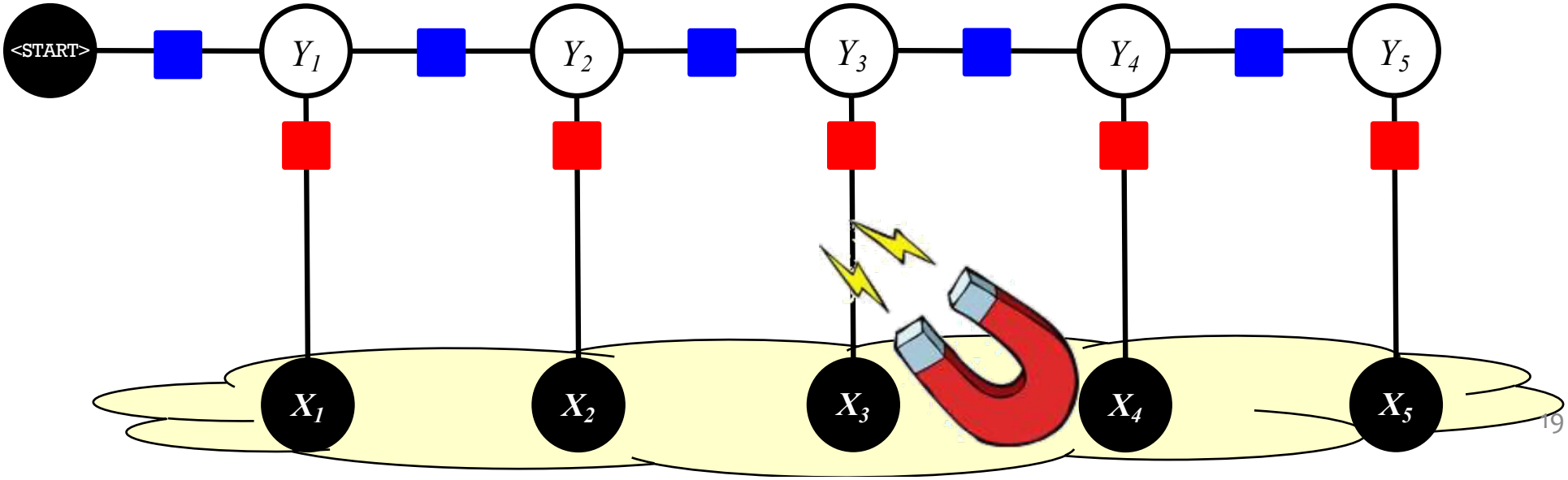
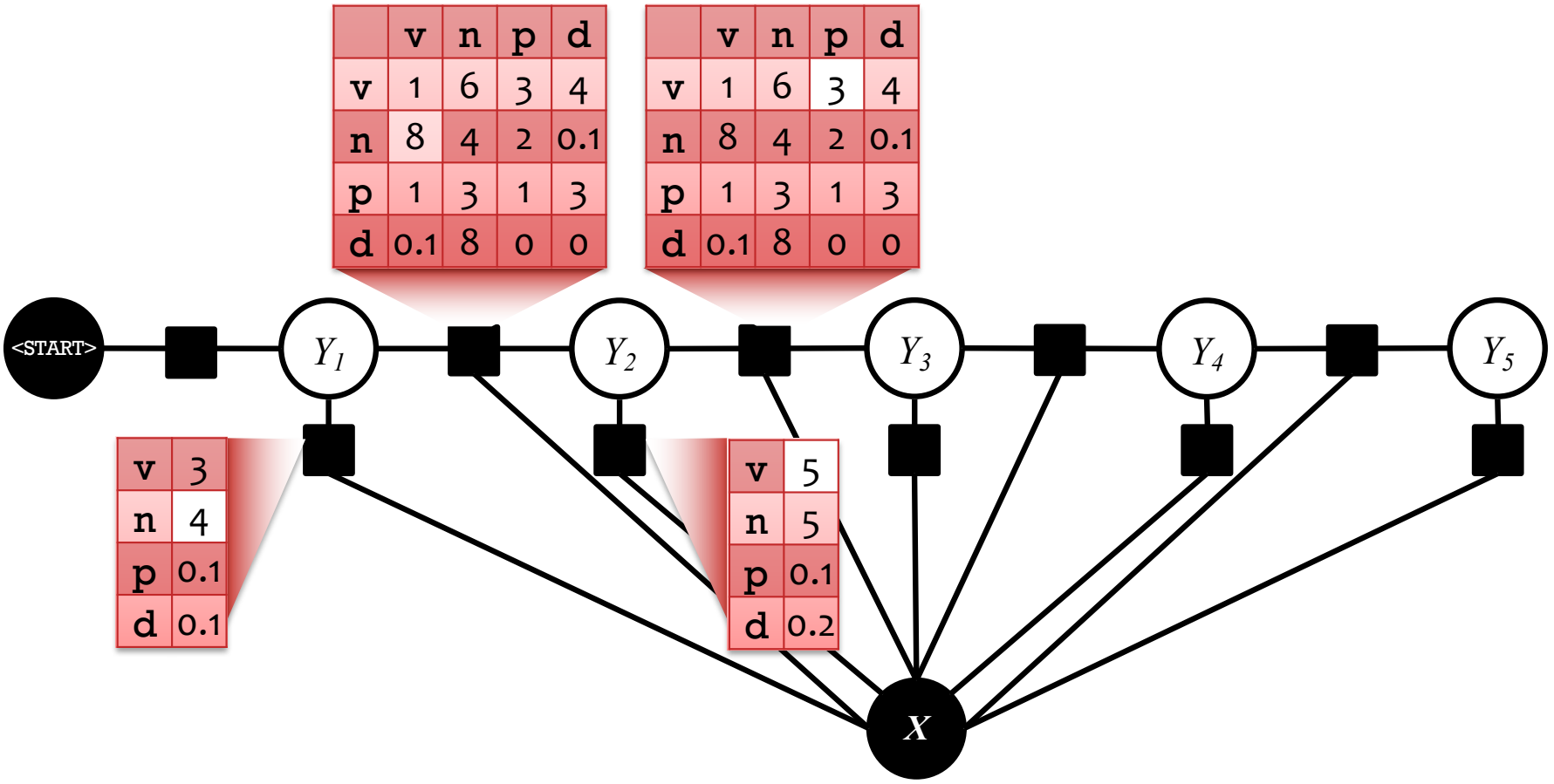


Conditional Random Field (CRF)

- That is the **vector** X
- Because it's observed, we can condition on it for free
- Conditioning is how we converted from the MRF to the CRF (i.e. when taking a slice of the emission factors)



Conditional Random Field (CRF)

- This is the **standard** linear-chain CRF definition
- It permits rich, overlapping features of the vector $\boldsymbol{X}$

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{x})} \prod_{k=1}^{K} \psi_{\text{em}}(y_k, \mathbf{x}) \psi_{\text{tr}}(y_k, y_{k-1}, \mathbf{x})$$

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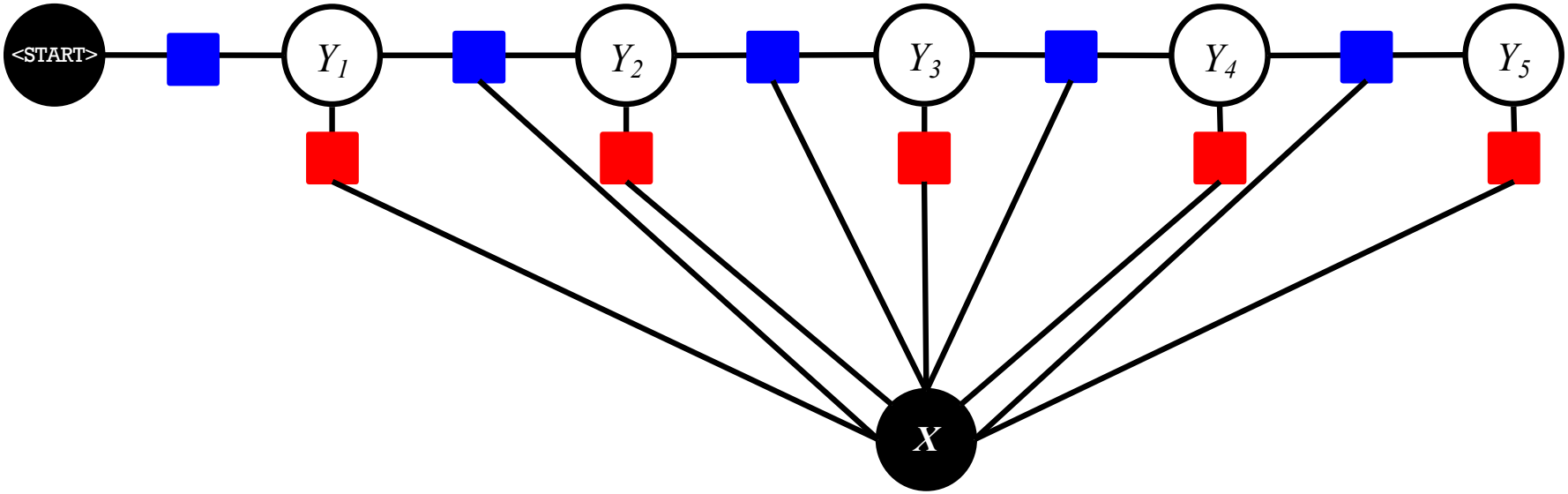

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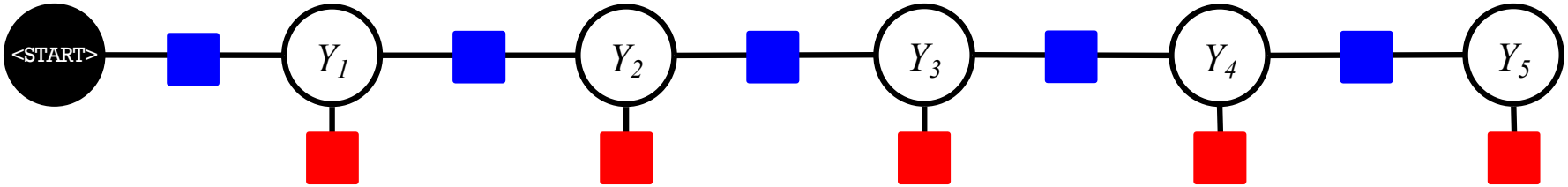

Visual Notation: Usually we draw a CRF **without** showing the variable corresponding to $\boldsymbol{X}$

CRF LEARNING (LOG-LINEAR CASE)

Title Here

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- log-linear CRF model (i.e. with feature based potentials)
- log-linear CRF derivatives
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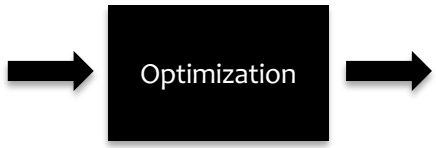
Recipe for Gradient-based Learning

1. Write down the objective function
2. Compute the partial derivatives of the objective (i.e. gradient, and maybe Hessian)
3. Feed objective function and derivatives into black box

4. Retrieve optimal parameters from black box

Optimization Algorithms

What is the black box?



- Newton's method
- Hessian-free / Quasi-Newton methods
  - Conjugate gradient
  - L-BFGS
- Stochastic gradient methods
  - Stochastic gradient descent (SGD)
  - SGD with momentum
  - Adam

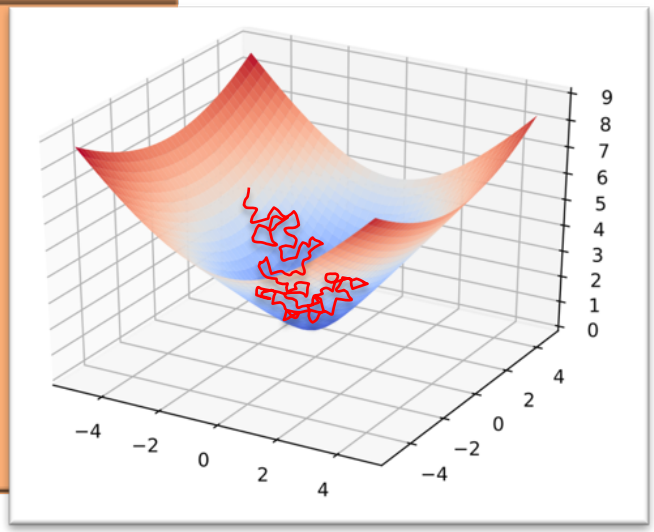
Stochastic Gradient Descent (SGD)

Assume we have an objective that decomposes additively:

$$\text{Let } J(\boldsymbol{\theta}) = \sum_{i=1}^{N} J^{(i)}(\boldsymbol{\theta})$$

Algorithm 2 Stochastic Gradient Descent (SGD)

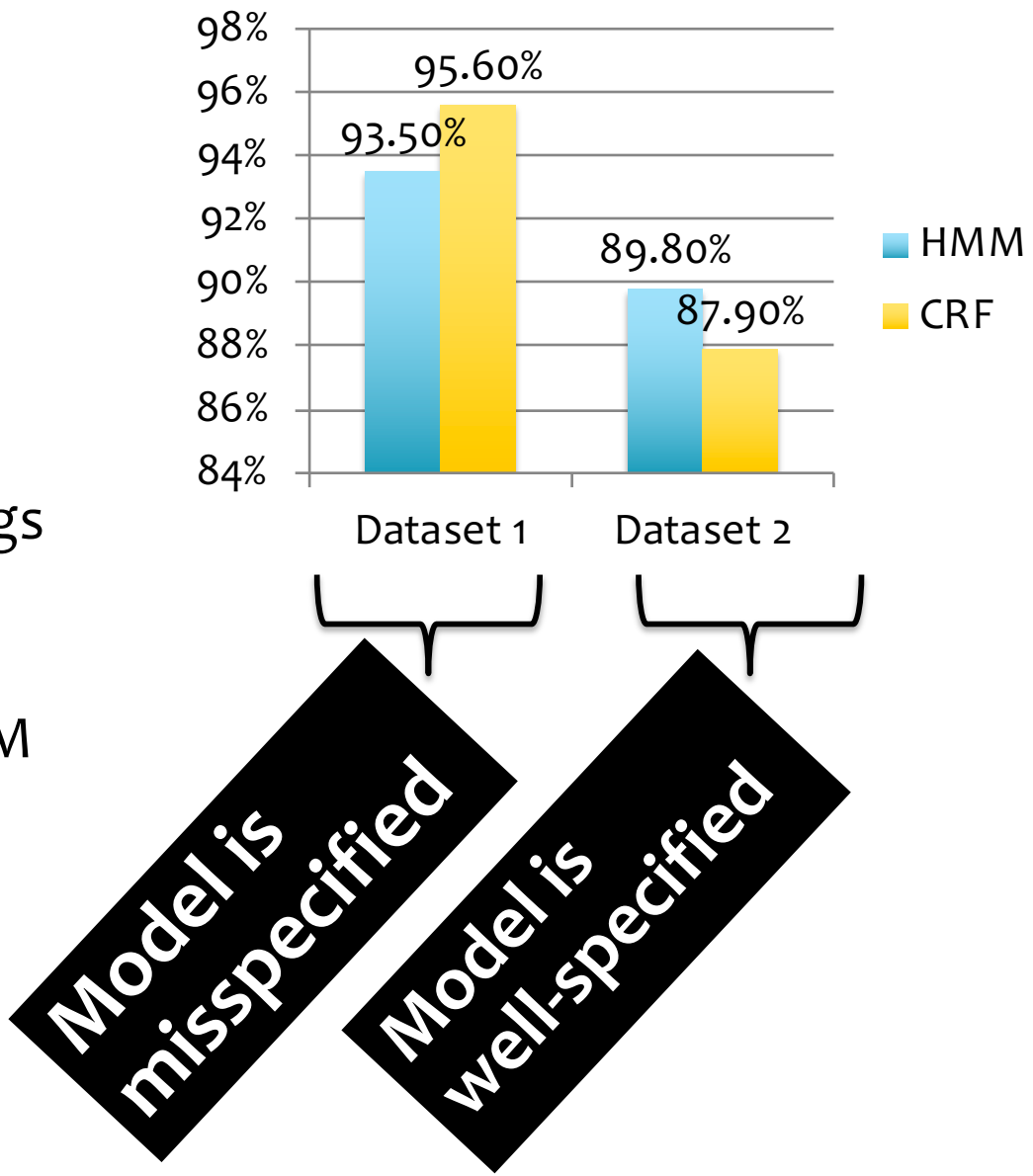
1: **procedure** SGD($\mathcal{D}, \boldsymbol{\theta}^{(0)}$)
2: $\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
3: $\quad$ **while** not converged **do**
4: $\quad\quad i \sim \text{Uniform}(\{1, 2, \ldots, N\})$
5: $\quad\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta})$
6: $\quad$ **return** $\boldsymbol{\theta}$



Generative vs. Discriminative

Liang & Jordan (ICML 2008) compares **HMM** and **CRF** with **identical features**

- Dataset 1: (Real)
  - WSJ Penn Treebank (38K train, 5.5K test)
  - 45 part-of-speech tags
- Dataset 2: (Artificial)
  - Synthetic data generated from HMM learned on Dataset 1 (1K train, 1K test)
- Evaluation Metric: Accuracy



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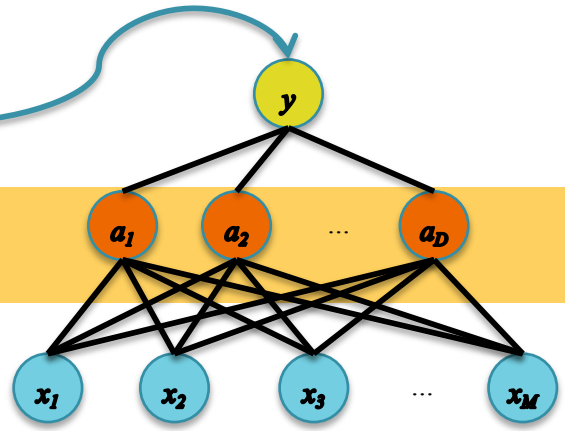


NEURAL POTENTIAL FUNCTIONS

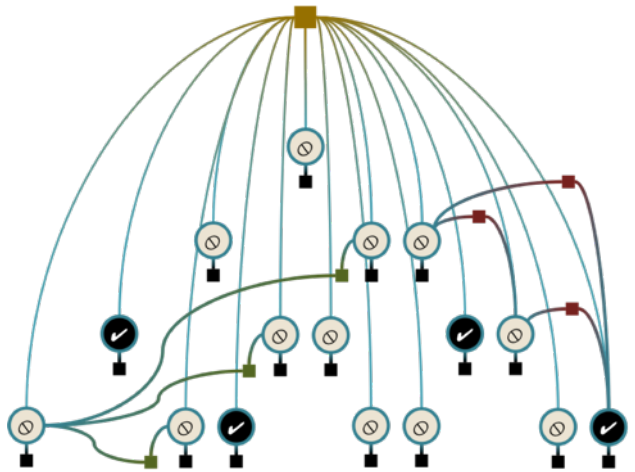
Hybrids of Graphical Models and Neural Networks

This lecture is not about a convergence of the two fields.

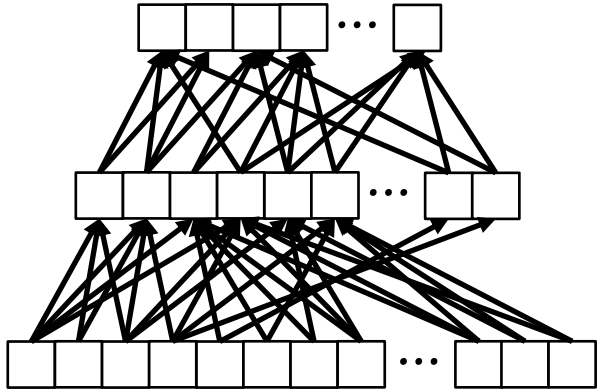
Rather, it is about state-of-the-art collaboration between two complementary techniques.

Motivation:
Hybrid Models

Graphical models let you encode domain knowledge



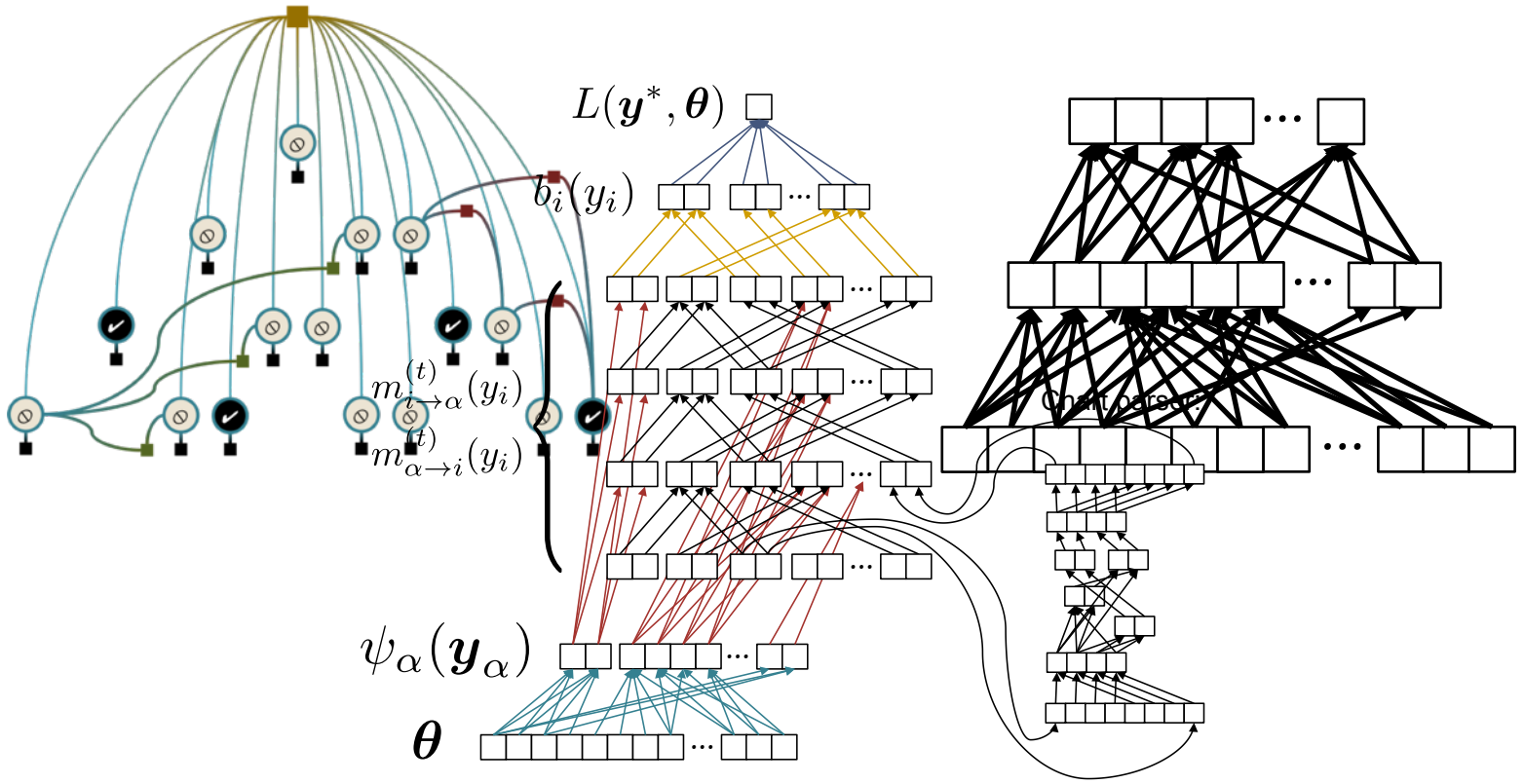
Neural nets are really good at fitting the data discriminatively to make good predictions



Could we define a neural net that incorporates domain knowledge?

Motivation:
Hybrid Models

Key idea: Use a NN to learn features for a GM, then train the entire model by backprop



A Recipe for Neural Networks

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^{N}$$

Face *Face* *Not a face*

2. Choose each of these:
   - Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

   - Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

Examples: Linear regression, Logistic regression, Neural Network

Examples: Mean-squared error, Cross Entropy

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3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:

(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

BACKPROPAGATION AND BELIEF PROPAGATION

Whiteboard:

- CRF w/LSTM potentials
- Gradient of MRF/CRF log-likelihood with respect to log potentials
- Gradient of MRF/CRF log-likelihood with respect to potentials
- Backprop with MRF/CRF log-likelihood as a loss function

Factor Derivatives

Log-probability:

$$\log p(\mathbf{y}) = \left[\sum_{\alpha} \log \psi_\alpha(\mathbf{y}_\alpha)\right] - \log \sum_{\mathbf{y}' \in \mathcal{Y}} \prod_{\alpha} \psi_\alpha(\mathbf{y}'_\alpha) \quad (1)$$

Derivatives:

$$\frac{\partial \log p(\mathbf{y})}{\partial \log \psi_\alpha(\mathbf{y}'_\alpha)} = \mathbb{1}(\mathbf{y}_\alpha = \mathbf{y}'_\alpha) - p(\mathbf{y}'_\alpha) \quad (2)$$

$$\frac{\partial \log p(\mathbf{y})}{\partial \psi_\alpha(\mathbf{y}'_\alpha)} = \frac{\mathbb{1}(\mathbf{y}_\alpha = \mathbf{y}'_\alpha) - p(\mathbf{y}'_\alpha)}{\psi_\alpha(\mathbf{y}'_\alpha)} \quad (3)$$