School of Computer Science
Carnegie Mellon

10-708 Probabilistic Graphical Models

Hybrid Graphical Models and Neural Networks

Readings:
Abdel-Hamid, Deng, Yu, Jiang (2013)

Matt Gormley
Lecture 27
April 20, 2016

Reminders

- HW4: due April 27
- Project presentations: April 29
  - Location: Baker Hall A51
  - Session 1: 8:30 - 12:30 (4 hrs)
  - Lunch break: 12:30 - 1:30 (1 hr)
  - Session 2: 1:30 - 5:00 (3.5 hrs)

Outline

- **Motivation**
- **Hybrid NN + HMM**
  - Model: neural net for emissions
  - Learning: backprop for end-to-end training
  - Experiments: phoneme recognition (Bengio et al., 1992)
- **Background: Recurrent Neural Networks (RNNs)**
  - Bidirectional RNNs
  - Deep Bidirectional RNNs
  - Deep Bidirectional LSTMs
  - Connection to forward-backward algorithm
- **Hybrid RNN + HMM**
  - Model: neural net for emissions
  - Experiments: phoneme recognition (Graves et al., 2013)
- **Hybrid CNN + CRF**
  - Model: neural net for factors
  - Experiments: natural language tasks (Collobert & Weston, 2011)
  - Experiments: pose estimation
- **Tricks of the Trade**

MOTIVATION

	DL	≤ ? ML (e.g., GM)
Empirical goal:	e.g., classification, feature learning	e.g., transfer learning, latent variable inference
Structure:	Graphical	Graphical
Objective:	Something aggregated from local functions	Something aggregated from local functions
Vocabulary:	Neuron, activation/gate function …	Variables, potential function
Algorithm:	A single, unchallenged, inference algorithm -- BP	A major focus of open research, many algorithms, and more to come
Evaluation:	On a black-box score -- end performance	On almost every intermediate quantity
Implementation:	Many untold-tricks	More or less standardized
Experiments:	Massive, real data (GT unknown)	Modest, often simulated data (GT known)

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A slippery slope to mythology?

- How to conclusively determine what an improve in performance could come from:
  - Better model (architecture, activation, loss, size)?
  - Better algorithm (more accurate, faster convergence)?
  - Better training data?
- Current research in DL seem to get everything above mixed by evaluating on a black-box "performance score" that is not directly reflecting
  - Correctness of inference
  - Achievability/usefulness of model
  - Variance due to stochasticity

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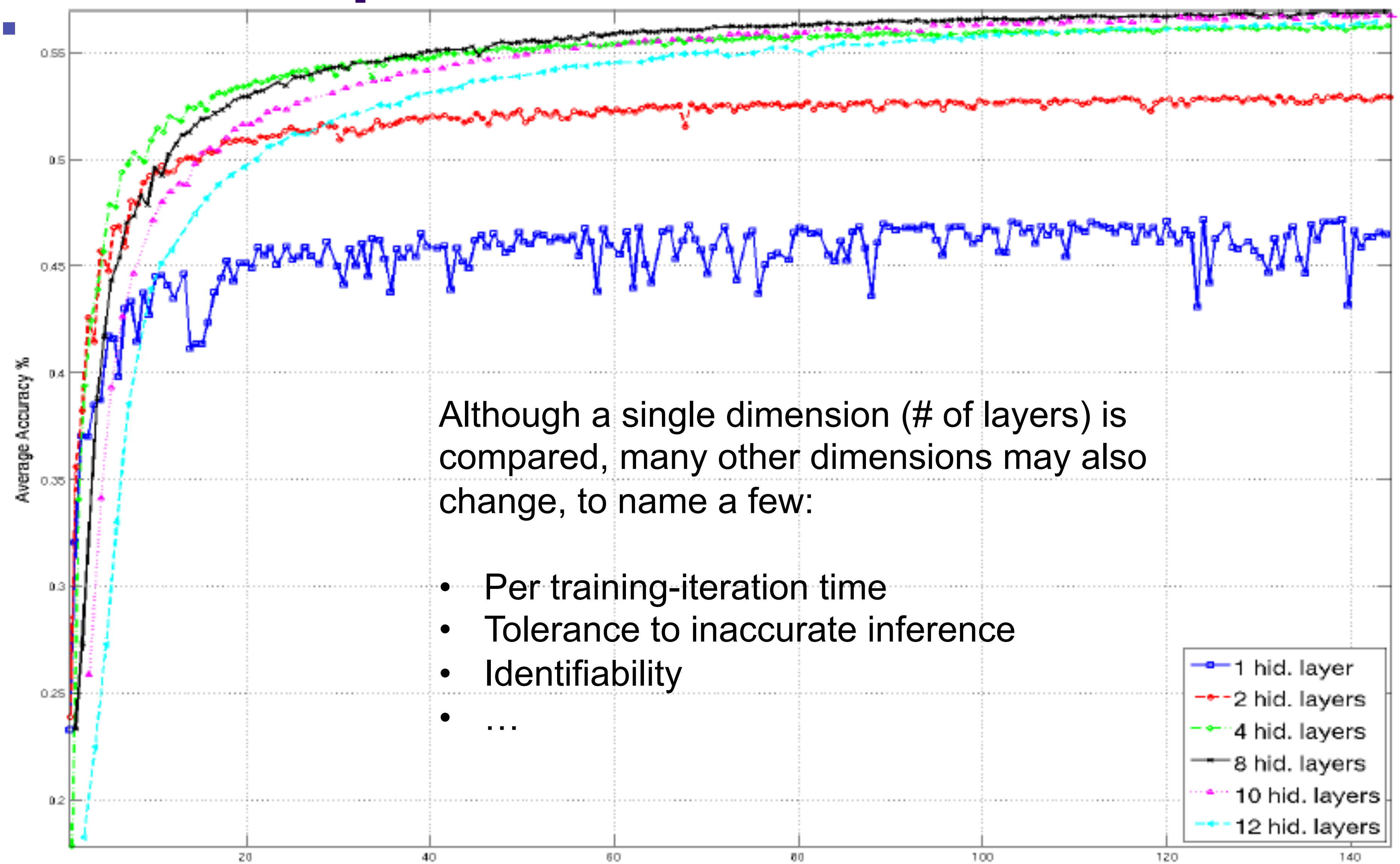
An Example



Although a single dimension (# of layers) is compared, many other dimensions may also change, to name a few:

- Per training-iteration time
- Tolerance to inaccurate inference
- Identifiability
- …

Inference quality

- Training error is the old concept of a classifier with no hidden states, no **inference** is involved, and thus inference accuracy is not an issue
- But a DNN is not just a classifier, some DNNs are not even fully supervised, there are MANY **hidden states**, why their inference quality is not taken seriously?

- In DNN, inference accuracy = visualizing features
  - Study of inference accuracy is badly discouraged
  - Loss/accuracy is not monitored

Conclusion

- In GM: lots of efforts are directed to improving inference accuracy and convergence speed
  - An advanced tutorial would survey dozen's of inference algorithms/ theories, but few use cases on empirical tasks
- In DL: most effort is directed to comparing different architectures and gate functions (based on empirical performance on a downstream task)
  - An advanced tutorial typically consist of a list of all designs of nets, many use cases, but a single name of algorithm: back prop of SGD
- The two fields are similar at the beginning (energy, structure, etc.), and soon diverge to their own signature pipelines
- A convergence might be necessary and fruitful

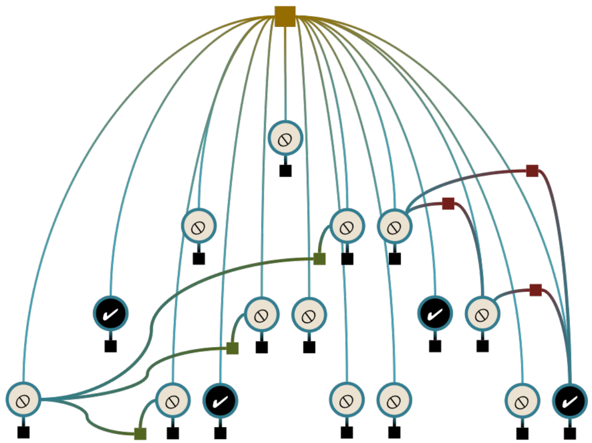
Hybrids of Graphical Models and Neural Networks

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

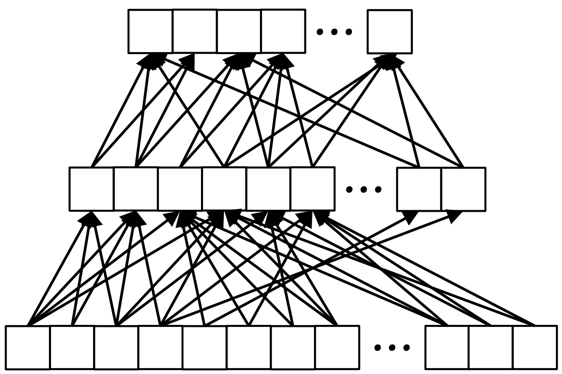
Rather, it is about state-of-the-art collaboration between two complementary techniques.

Motivation:
Hybrid Models

Graphical models let you encode domain knowledge



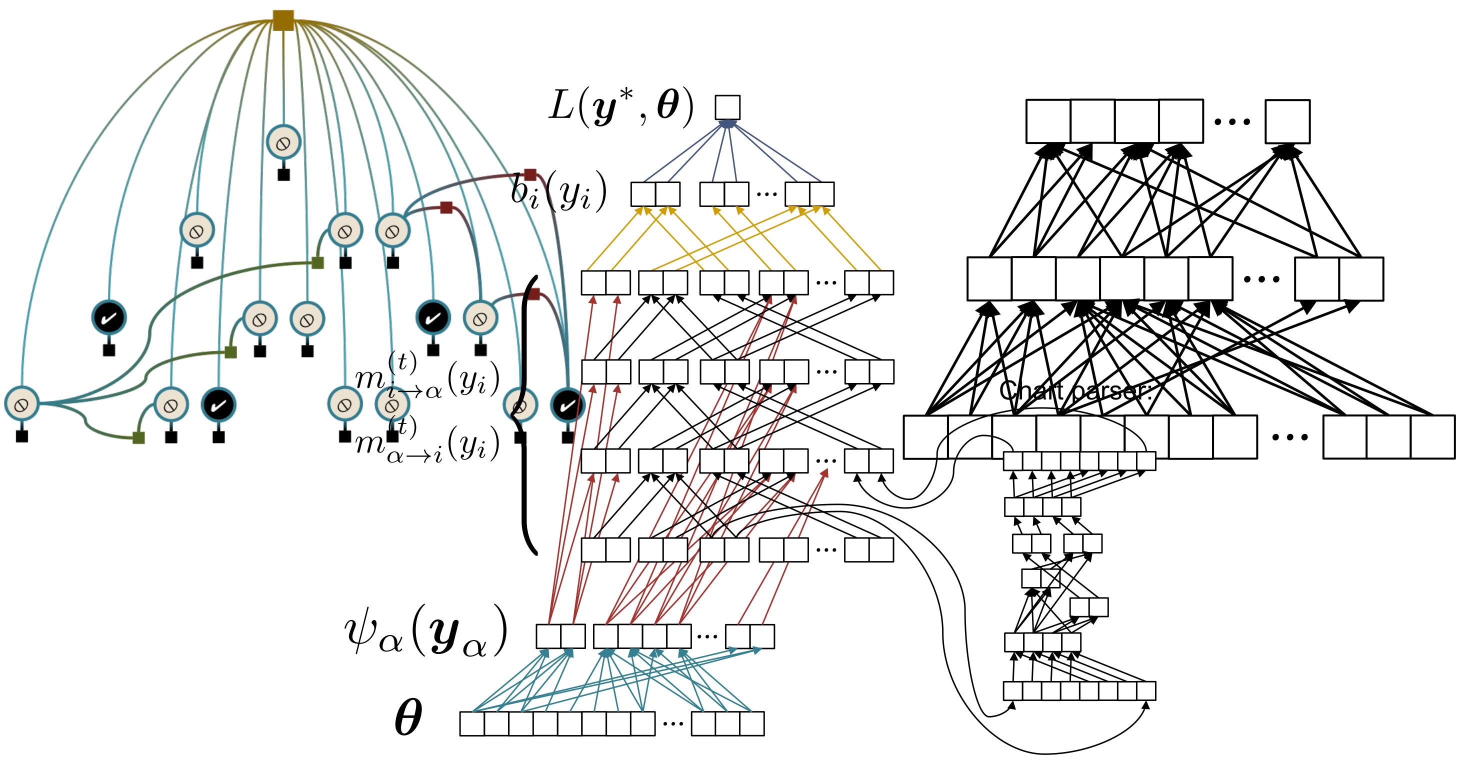
Neural nets are really good at fitting the data discriminatively to make good predictions



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:

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

2. Choose each of these:
   - Decision function

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

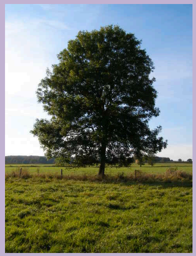
   - Loss function

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

Face

Face

Not a face



Examples: Linear regression, Logistic regression, Neural Network

Examples: Mean-squared error, Cross Entropy

A Recipe for Neural Networks

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2. Choose each of these:

– Decision function

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

– Loss function

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

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)

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

Today's Lecture

- Suppose our decision function is a graphical model!
- We know how to compute marginal probabilities (inference), but how to do make a prediction, **y**?

A Recipe for

Background

1\.

2\. Choose each of these:

- Decision function

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

- Loss function

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

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Recall...

Minimum Bayes Risk Decoding

- Suppose we given a loss function $l(\boldsymbol{y}', \boldsymbol{y})$ and are asked for a single tagging
- How should we choose just one from our probability distribution $p(\boldsymbol{y}|\boldsymbol{x})$?
- A minimum Bayes risk (MBR) decoder $h(\boldsymbol{x})$ returns the variable assignment with minimum **expected** loss under the model's distribution

$$\begin{aligned} h_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \underset{\hat{\boldsymbol{y}}}{\operatorname{argmin}} \ \mathbb{E}_{\boldsymbol{y} \sim p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x})}[\ell(\hat{\boldsymbol{y}}, \boldsymbol{y})] \\ &= \underset{\hat{\boldsymbol{y}}}{\operatorname{argmin}} \ \sum_{\boldsymbol{y}} p_{\boldsymbol{\theta}}(\boldsymbol{y} \mid \boldsymbol{x}) \ell(\hat{\boldsymbol{y}}, \boldsymbol{y}) \end{aligned}$$

Recall...

Minimum Bayes Risk Decoding

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \operatorname*{argmin}_{\hat{\boldsymbol{y}}} \; \mathbb{E}_{\boldsymbol{y} \sim p_{\boldsymbol{\theta}}(\cdot \mid \boldsymbol{x})}[\ell(\hat{\boldsymbol{y}}, \boldsymbol{y})]$$

Consider some example loss functions:

The ***0-1* loss function** returns *1* only if the two assignments are identical and *0* otherwise:

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}) = 1 - \mathbb{I}(\hat{\boldsymbol{y}}, \boldsymbol{y})$$

The MBR decoder is:

$$\begin{aligned} h_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \operatorname*{argmin}_{\hat{\boldsymbol{y}}} \; \sum_{\boldsymbol{y}} p_{\boldsymbol{\theta}}(\boldsymbol{y} \mid \boldsymbol{x})(1 - \mathbb{I}(\hat{\boldsymbol{y}}, \boldsymbol{y})) \\ &= \operatorname*{argmax}_{\hat{\boldsymbol{y}}} \; p_{\boldsymbol{\theta}}(\hat{\boldsymbol{y}} \mid \boldsymbol{x}) \end{aligned}$$

which is exactly the MAP inference problem!

Minimum Bayes Risk Decoding

Recall…

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \underset{\hat{\boldsymbol{y}}}{\text{argmin}} \; \mathbb{E}_{\boldsymbol{y} \sim p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x})}[\ell(\hat{\boldsymbol{y}}, \boldsymbol{y})]$$

Consider some example loss functions:

The **Hamming loss** corresponds to accuracy and returns the number of incorrect variable assignments:

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \sum_{i=1}^{V} (1 - \mathbb{I}(\hat{y}_i, y_i))$$

The MBR decoder is:

$$\hat{y}_i = h_{\boldsymbol{\theta}}(\boldsymbol{x})_i = \underset{\hat{y}_i}{\text{argmax}} \; p_{\boldsymbol{\theta}}(\hat{y}_i \mid \boldsymbol{x})$$

This decomposes across variables and requires the variable marginals.

Today's Lecture

- Suppose our decision function is a graphical model!
- We know how to compute marginal probabilities (inference), but how to do make a prediction, **y**?

- Can we use an MBR decoder as the decision function in this recipe?

A Recipe for

– Decision function

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

– Loss function

4. Train with SGD:

(take small steps opposite the gradient)

$$- \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

A Recipe for Graphical Models

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- **Tricks of the Trade**

HYBRID:
NEURAL NETWORK + HMM

Recall...

Markov Random Field (MRF)

Joint distribution over tags Y_i <u>and</u> words X_i
The individual factors aren't *necessarily* probabilities.

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

	v	n	p	d
v	1	6	3	4
n	8	4	2	0.1
p	1	3	1	3
d	0.1	8	0	0

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v	1	6	3	4
n	8	4	2	0.1
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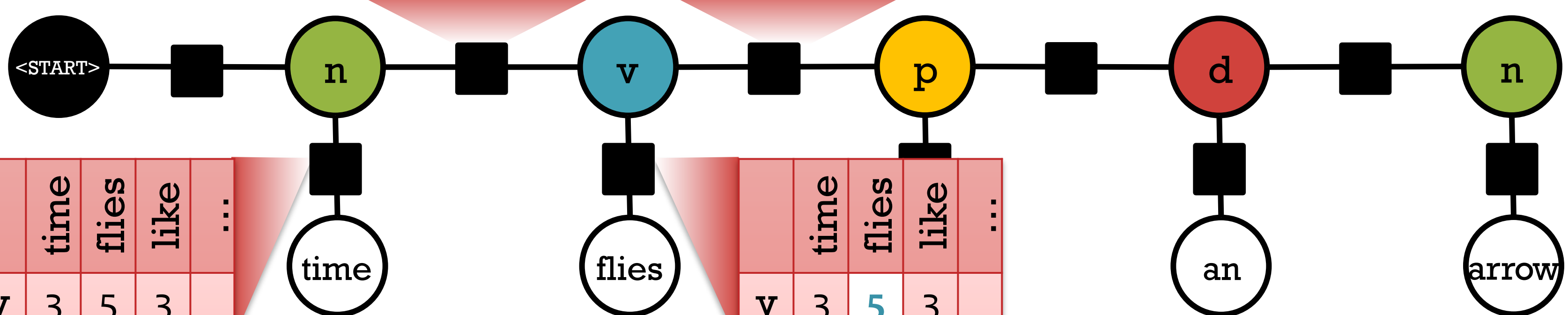


	time	flies	like	…
v	3	5	3	
n	4	5	2	
p	0.1	0.1	3	
d	0.1	0.2	0.1	

	time	flies	like	…
v	3	5	3	
n	4	5	2	
p	0.1	0.1	3	
d	0.1	0.2	0.1	

Recall…

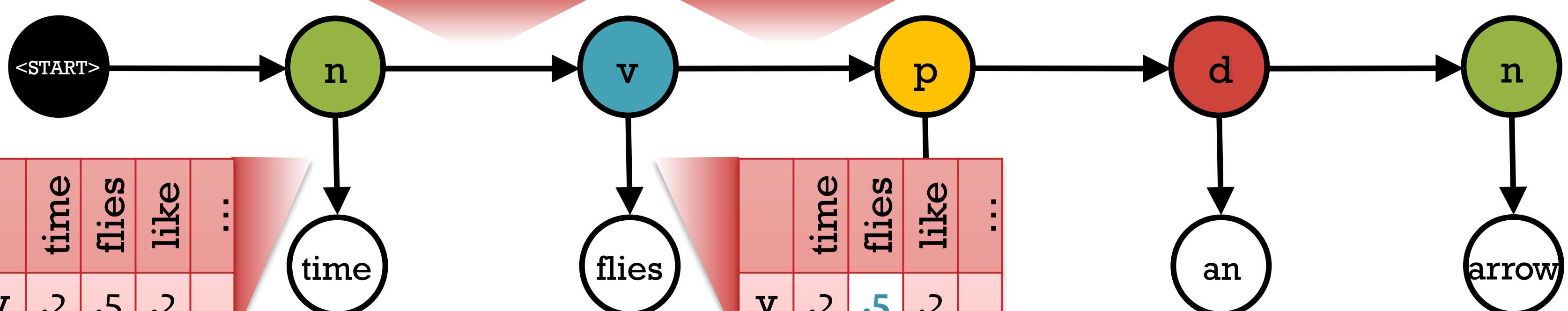
Hidden Markov Model

But sometimes we *choose* to make them probabilities.
Constrain each row of a factor to sum to one. Now $Z = 1$.

$$p(\text{n, v, p, d, n, time, flies, like, an, arrow}) = \cancel{\frac{1}{Z}}(.3 * .8 * .2 * .5 * \ldots)$$

	v	n	p	d
v	.1	.4	.2	.3
n	.8	.1	.1	0
p	.2	.3	.2	.3
d	.2	.8	0	0

	v	n	p	d
v	.1	.4	.2	.3
n	.8	.1	.1	0
p	.2	.3	.2	.3
d	.2	.8	0	0



	time	flies	like	…
v	.2	.5	.2	
n	.3	.4	.2	
p	.1	.1	.3	
d	.1	.2	.1	

	time	flies	like	…
v	.2	.5	.2	
n	.3	.4	.2	
p	.1	.1	.3	
d	.1	.2	.1	

Hybrid: NN + HMM

(Bengio et al., 1992)

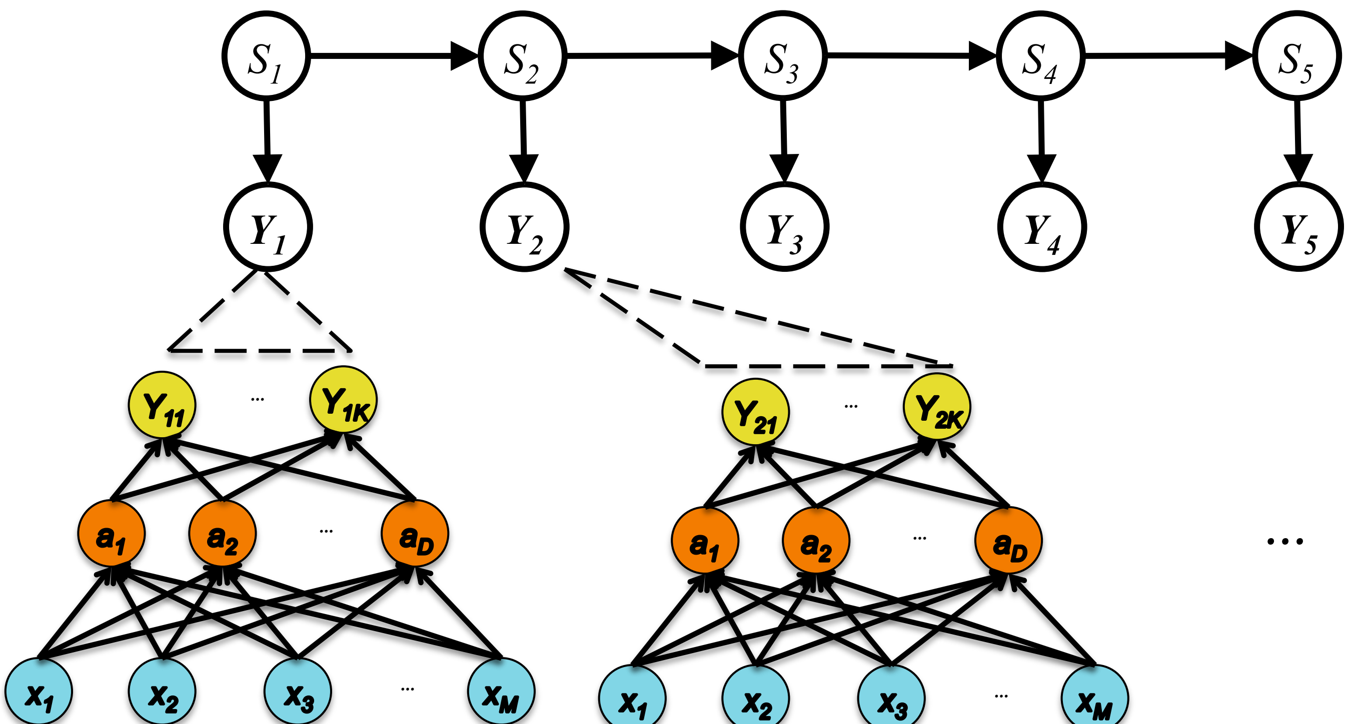
Discrete HMM state: $S_t \in \{/p/, /t/, /k/, /b/, /d/, \ldots, /g/\}$

Continuous HMM emission: $Y_t \in \mathcal{R}^K$

HMM: $p(\mathbf{Y}, \mathbf{S}) = \prod_{t=1}^{T} p(Y_t | S_t) p(S_t | S_{t-1})$

Gaussian emission:

$$p(Y_t | S_t = i) = b_{i,t} = \sum_k \frac{Z_k}{((2\pi)^n \mid \Sigma_k \mid)^{1/2}} \exp(-\frac{1}{2}(Y_t - \mu_k)\Sigma_k^{-1}(Y_t - \mu_k)^T)$$



Hybrid: NN + HMM

(Bengio et al., 1992)

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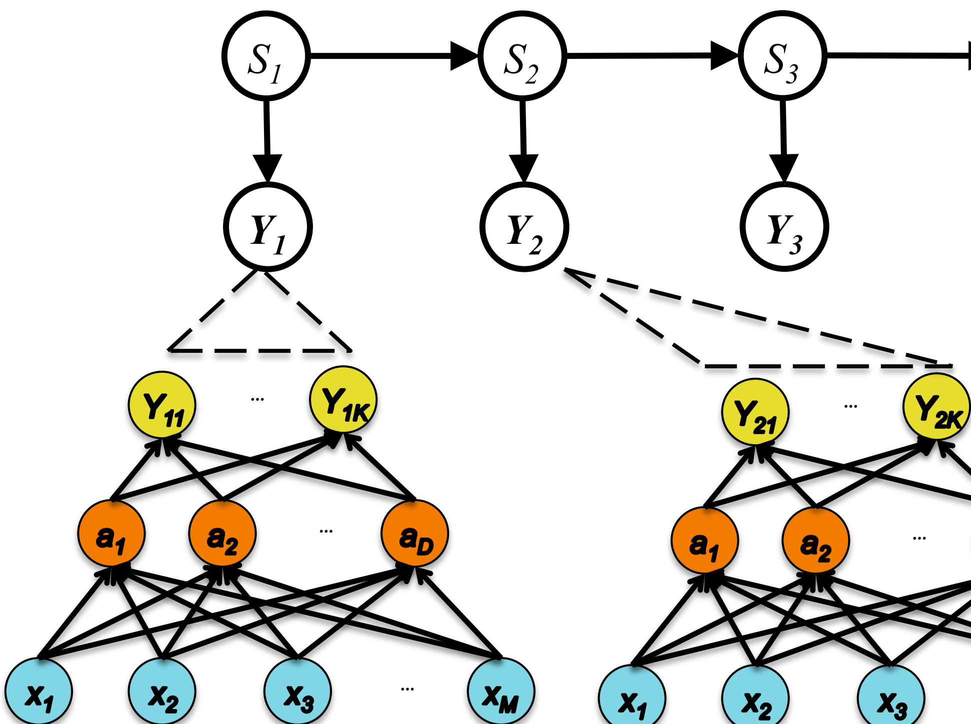
Continuous HMM emission: $Y_t \in \mathcal{R}^K$

HMM: $p(\mathbf{Y}, \mathbf{S}) = \prod_{t=1}^{T} p(Y_t|S_t) p(S_t|S_{t-1})$

$$p(Y_t|S_t = i) = b_{i,t} = \sum_k \frac{Z_k}{((2\pi)^n \mid \Sigma_k \mid)^{1/2}} e$$

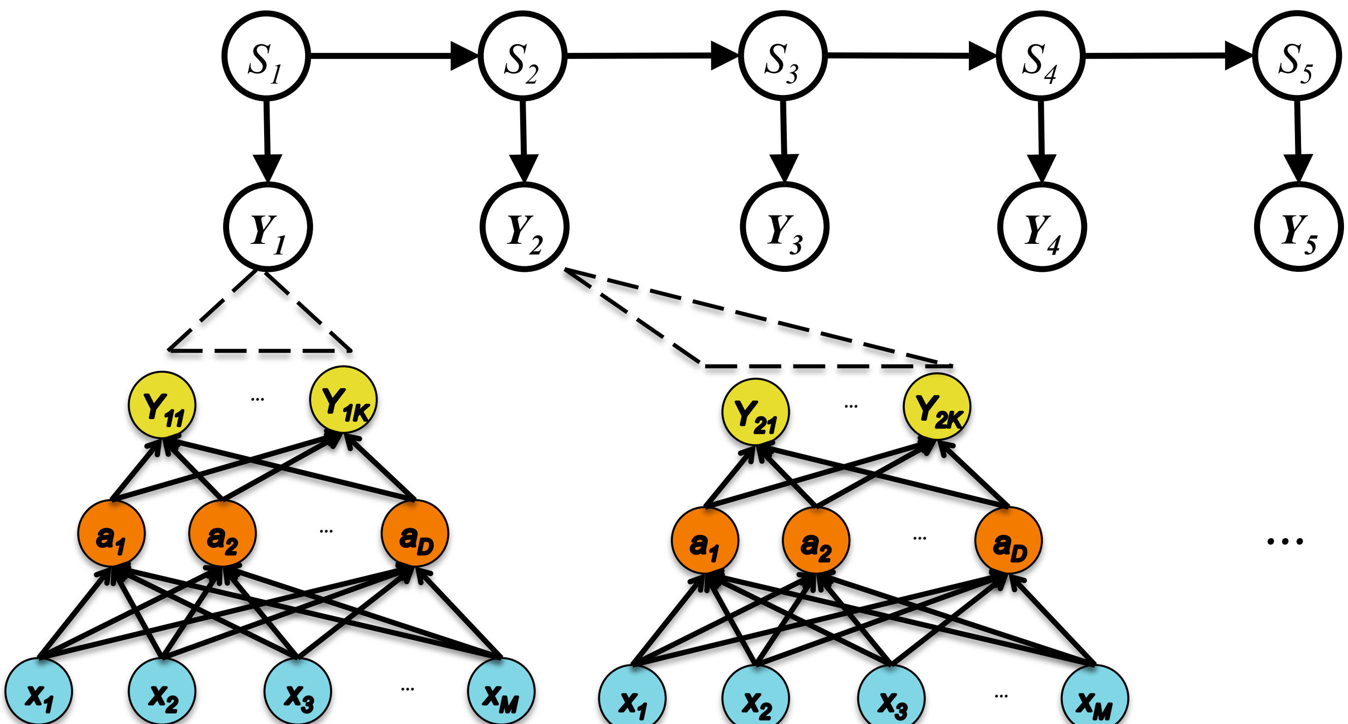


Lots of oddities to this picture:

- **Clashing visual notations** (graphical model vs. neural net)
- HMM generates data **top-down**, NN generates **bottom-up** and they meet in the middle.
- The “observations” of the HMM are not actually observed (i.e. x’s appear in NN only)

So what are we missing?

Hybrid: NN + HMM



$$a_{i,j} = p(S_t = i | S_{t-1} = j)$$
$$b_{i,t} = p(Y_t | S_t = i)$$

Hybrid: NN + HMM

Forward-backward algorithm: a "feed-forward" algorithm for computing alpha-beta probabilities.

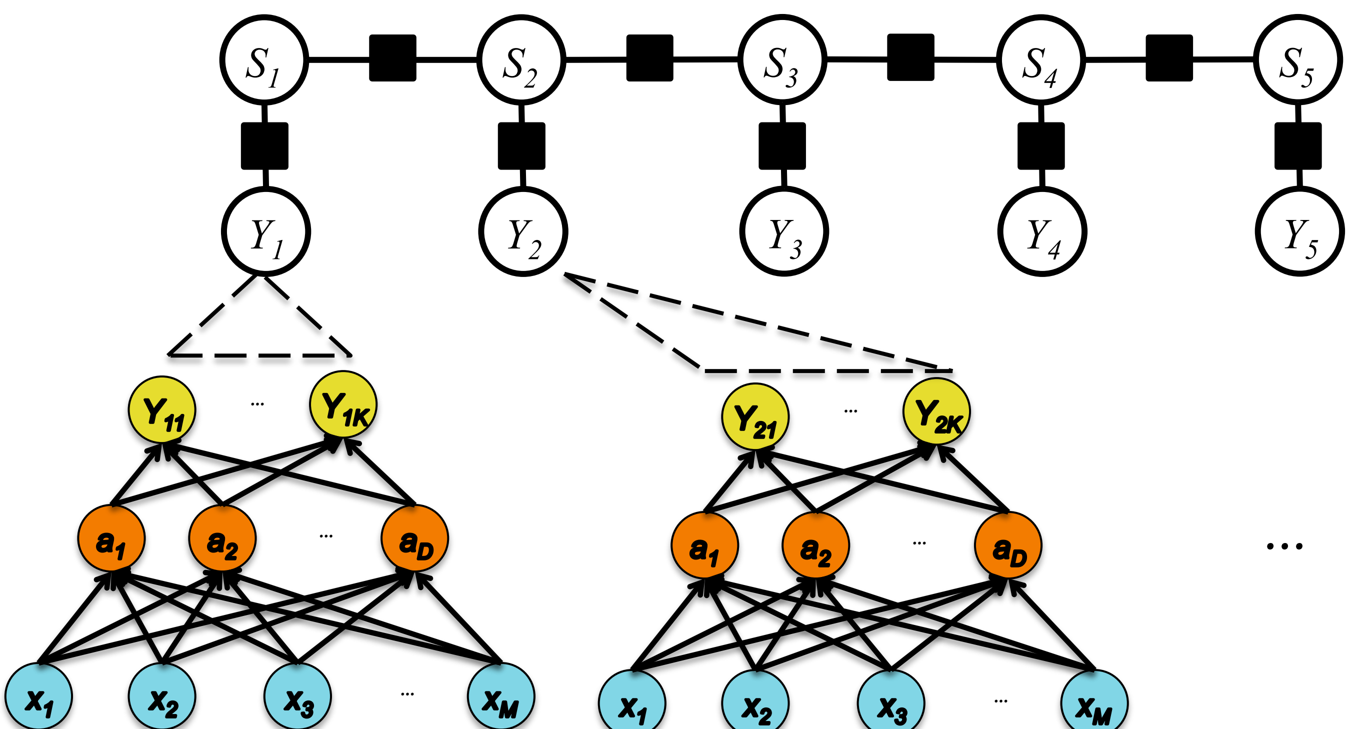
$$\alpha_{i,t} = P(Y_1^t \text{ and } S_t = i \mid model) = b_{i,t} \sum_j a_{ji} \alpha_{j,t-1}$$

$$\beta_{i,t} = P(Y_{t+1}^T \mid S_t = i \text{ and } model) = \sum_j a_{ij} b_{j,t+1} \beta_{j,t+1}$$

$$\gamma_{i,t} = P(S_t = i \mid Y_1^t \text{ and } model) = \alpha_{i,t} \, \beta_{i,t}$$

Log-likelihood: a "feed-forward" objective function.

$$\log p(\mathbf{S}, \mathbf{Y}) = \alpha_{\text{END},T}$$



A Recipe for Graphical Models

Decision / Loss Function for Hybrid NN + HMM

1. Given training data:

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

Forward-backward algorithm: a "feed-forward" algorithm for computing alpha-beta probabilities.

$$\alpha_{i,t} = P(Y_1^t \text{ and } S_t = i \mid model) = b_{i,t} \sum_j a_{ji} \alpha_{j,t-1}$$

$$\beta_{i,t} = P(Y_{t+1}^T \mid S_t = i \text{ and } model) = \sum_j a_{ij} b_{j,t+1} \beta_{j,t+1}$$

$$\gamma_{i,t} = P(S_t = i \mid Y_1^t \text{ and } model) = \alpha_{i,t} \beta_{i,t}$$

2. Choose each of these:
   - Decision function

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

   - Loss function

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

Log-likelihood: a "feed-forward" objective function.

$$\log p(\mathbf{S}, \mathbf{Y}) = \alpha_{\mathsf{END},T}$$

nt)

$$- \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

How do we compute the gradient?

Recall…

Training

Backpropagation

Backpropagation is just repeated application of the **chain rule** from Calculus 101.

Graphical Model and Log-likelihood

Neural Network

$$\boldsymbol{y} = g(\boldsymbol{u}) \text{ and } \boldsymbol{u} = h(\boldsymbol{x}).$$

How to compute these partial derivatives?

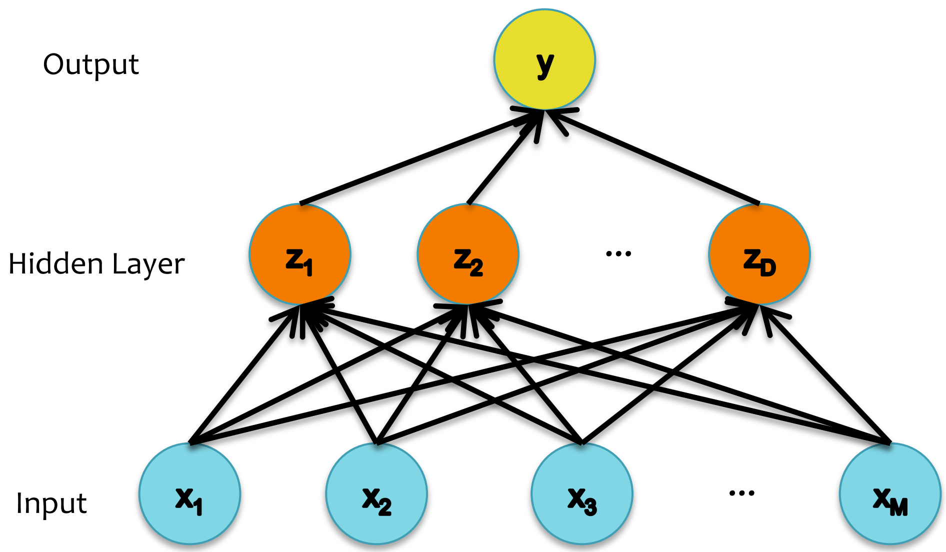
Chain Rule:

$$\frac{dy_i}{dx_k} = \sum_{j=1}^{J} \frac{dy_i}{du_j}\frac{du_j}{dx_k}, \quad \forall i, k$$

Recall...

Training Backpropagation

What does this picture actually mean?



(F) Loss
$J = \frac{1}{2}(y - y^{(d)})^2$

↑

(E) Output (sigmoid)
$y = \frac{1}{1+\exp(b)}$

↑

(D) Output (linear)
$b = \sum_{j=0}^{D} \beta_j z_j$

↑

(C) Hidden (sigmoid)
$z_j = \frac{1}{1+\exp(a_j)}, \ \forall j$

↑

(B) Hidden (linear)
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

↑

(A) Input
Given $x_i, \ \forall i$

Recall...

Training Backpropagation

Case 2:
Neural
Network

Forward

$$J = y^* \log q + (1 - y^*) \log(1 - q)$$

$$q = \frac{1}{1 + \exp(-b)}$$

$$b = \sum_{j=0}^{D} \beta_j z_j$$

$$z_j = \frac{1}{1 + \exp(-a_j)}$$

$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$$

Backward

$$\frac{dJ}{dq} = \frac{y^*}{q} + \frac{(1 - y^*)}{q - 1}$$

$$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(b)}{(\exp(b) + 1)^2}$$

$$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$$

$$\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$$

$$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(a_j)}{(\exp(a_j) + 1)^2}$$

$$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$$

$$\frac{dJ}{dx_i} = \frac{dJ}{da_j}\frac{da_j}{dx_i}, \quad \frac{da_j}{dx_i} = \sum_{j=0}^{D} \alpha_{ji}$$

Hybrid: NN + HMM

Computing the Gradient: $\nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$

Forward computation

$$\log p(\mathbf{S}, \mathbf{Y}) = \alpha_{\text{END},T}$$

$$\alpha_{i,t} = \ldots \text{(forward prob)}$$

$$\beta_{i,t} = \ldots \text{(backward prop)}$$

$$\gamma_{i,t} = \ldots \text{(marginals)}$$

$$a_{i,j} = \ldots \text{(transitions)}$$

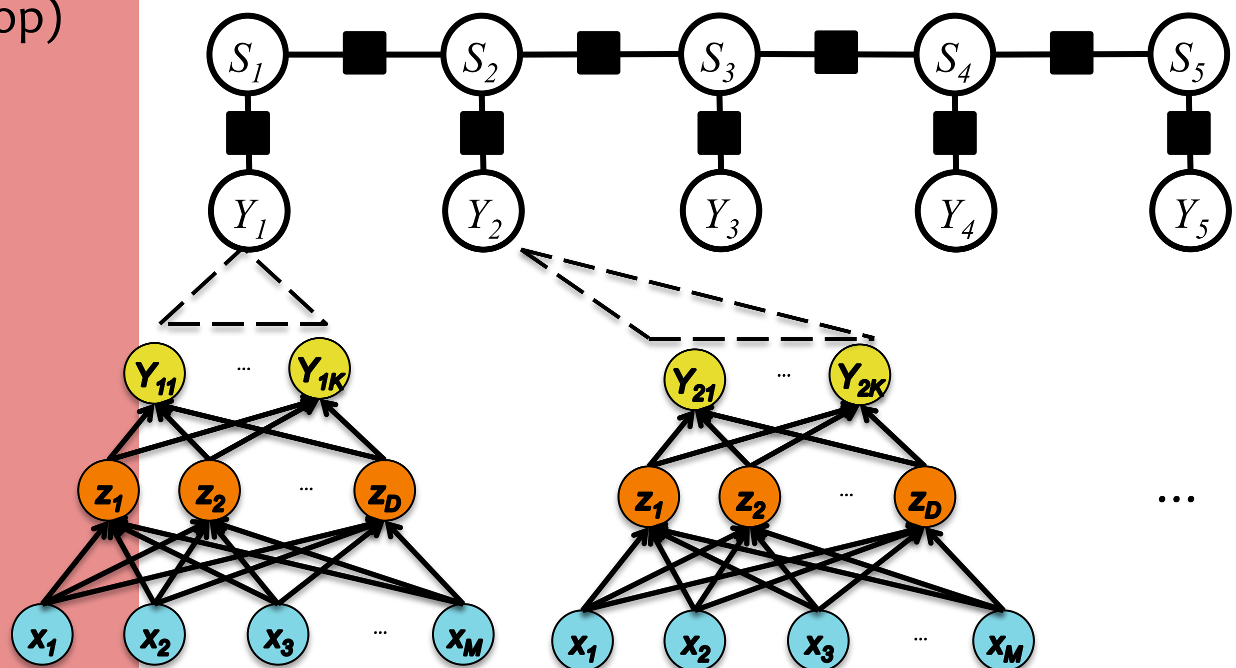
$$b_{i,t} = \ldots \text{(emissions)}$$

$$y_{tk} = \frac{1}{1 + \exp(-b)}$$

$$b = \sum_{j=0}^{D} \beta_j z_j$$

$$z_j = \frac{1}{1 + \exp(-a_j)}$$

$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$$



Hybrid: NN + HMM

Computing the Gradient: $\nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$

Forward computation

$$J = \log p(\mathbf{S}, \mathbf{Y}) = \alpha_{\text{END},T}$$

$\alpha_{i,t} = \ldots$ (forward prob)

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$$y_{tk} = \frac{1}{1 + \exp(-b)}$$

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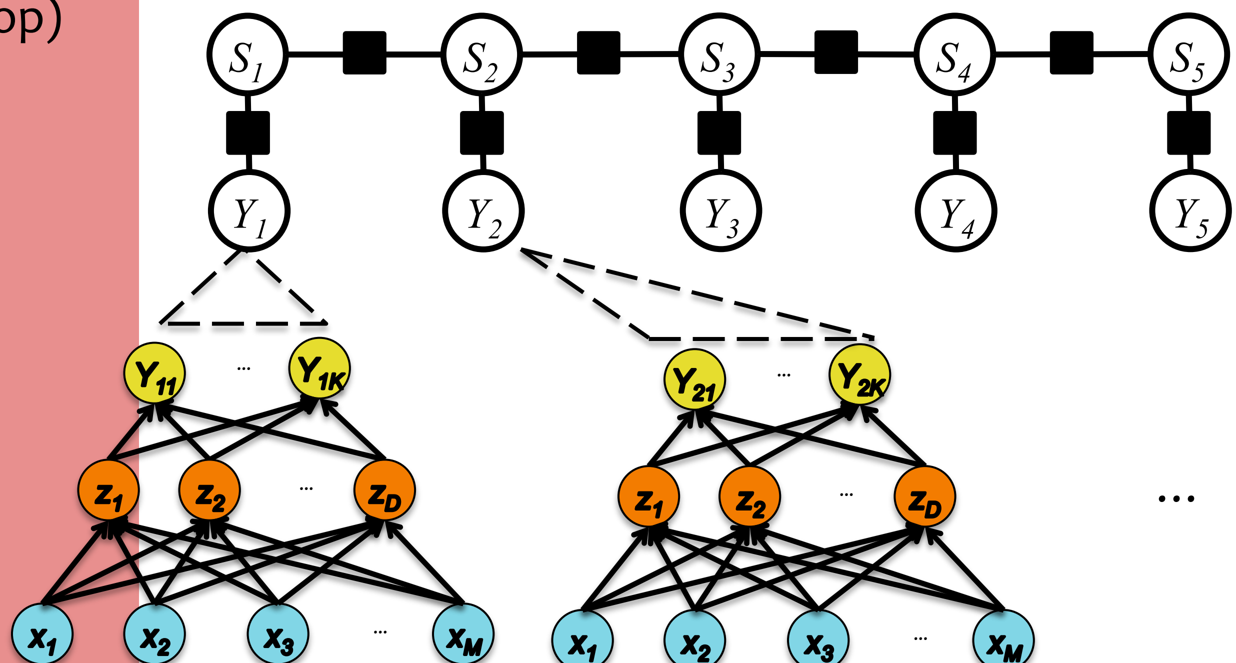

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Computing the Gradient: $\nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$

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$$J = \log p(\mathbf{S}, \mathbf{Y}) = \alpha_{\text{END},T}$$

$$\alpha_{i,t} = \ldots \text{(forward prob)}$$

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$$y_{tk} = \frac{1}{1 + \exp(-b)}$$

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Backward computation

$$\frac{dJ}{db_{i,t}} = \frac{\partial \alpha_{F_{model},T}}{\partial \alpha_{i,t}} \frac{\partial \alpha_{i,t}}{\partial b_{i,t}} = \left(\sum_j \frac{\partial \alpha_{j,t+1}}{\partial \alpha_{i,t}} \frac{\partial L_{model}}{\partial \alpha_{j,t+1}}\right)\left(\sum_j a_{ji} \alpha_{j,t-1}\right)$$

$$= \left(\sum_j b_{j,t+1} a_{ji} \frac{\partial \alpha_{F_{model},T}}{\partial \alpha_{j,t+1}}\right)\left(\sum_j a_{ji} \alpha_{j,t-1}\right) = \beta_{i,t} \frac{\alpha_{i,t}}{b_{i,t}} = \frac{\gamma_{i,t}}{b_{i,t}}$$

Hybrid: NN + HMM

Computing the Gradient: $\nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$

Forward computation

$$J = \log p(\mathbf{S}, \mathbf{Y}) = \alpha_{\text{END},T}$$

$$\alpha_{i,t} = \ldots \text{(forward prob)}$$

$$\beta_{i,t} = \ldots \text{(backward prop)}$$

$$\gamma_{i,t} = \ldots \text{(marginals)}$$

$$a_{i,j} = \ldots \text{(transitions)}$$

$$b_{i,t} = \ldots \text{(emissions)}$$

$$y_{tk} = \frac{1}{1 + \exp(-b)}$$

$$b = \sum_{j=0}^{D} \beta_j z_j$$

$$z_j = \frac{1}{1 + \exp(-a_j)}$$

$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$$

Backward computation

$$\frac{dJ}{db_{i,t}} = \frac{\gamma_{i,t}}{b_{i,t}}$$

$$\frac{dJ}{dy_{t,k}} = \sum_{b_{i,t}} \frac{dJ}{db_{i,t}} \frac{db_{i,t}}{dy_{t,k}}$$

$$\frac{\partial b_{i,t}}{\partial Y_{jt}} = \sum_k \frac{Z_k}{((2\pi)^n \mid \Sigma_k \mid)^{1/2}} \left(\sum_l d_{k,lj}(\mu_{kl} - Y_{lt})\right) \exp\left(-\frac{1}{2}(Y_t - \mu_k)\Sigma_k^{-1}(Y_t - \mu_k)^T\right)$$

$$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(b)}{(\exp(b)+1)^2}$$

$$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$$

$$\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$$

$$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(a_j)}{(\exp(a_j)+1)^2}$$

$$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$$

Hybrid: NN + HMM

Computing the Gradient: $\nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$

Forward computation

$$J = \log p(\mathbf{S}, \mathbf{Y}) = \alpha_{\text{END},T}$$

$\alpha_{i,t} = \ldots$ (forward prob)

$\beta_{i,t} = \ldots$ (backward prop)

$\gamma_{i,t} = \ldots$ (marginals)

The derivative of the log-likelihood with respect to the neural network parameters!

$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$$

Backward computation

$$\frac{dJ}{db_{i,t}} = \frac{\gamma_{i,t}}{b_{i,t}}$$

$$\frac{dJ}{dy_{t,k}} = \sum_{b_{i,t}} \frac{dJ}{db_{i,t}} \frac{db_{i,t}}{dy_{t,k}}$$

$$\frac{\partial b_{i,t}}{\partial Y_{jt}} = \sum_k \frac{Z_k}{((2\pi)^n \mid \Sigma_k \mid)^{1/2}} (\sum_l d_{k,lj}(\mu_{kl} - Y_{lt})) \exp(-\frac{1}{2}(Y_t - \mu_k)\Sigma_k^{-1}(Y_t - \mu_k)^T)$$

$$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(b)}{(\exp(b)+1)^2}$$

$$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$$

$$\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$$

$$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(a_j)}{(\exp(a_j)+1)^2}$$

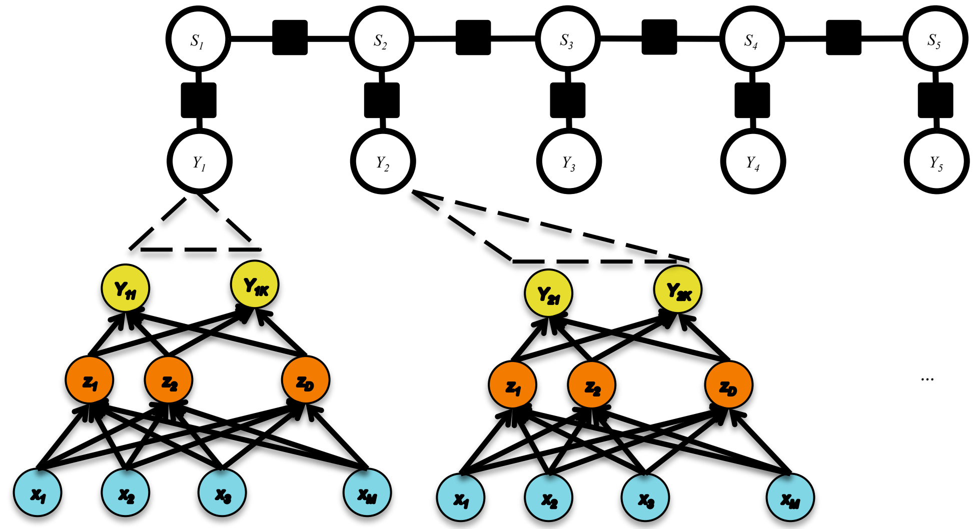
$$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$$

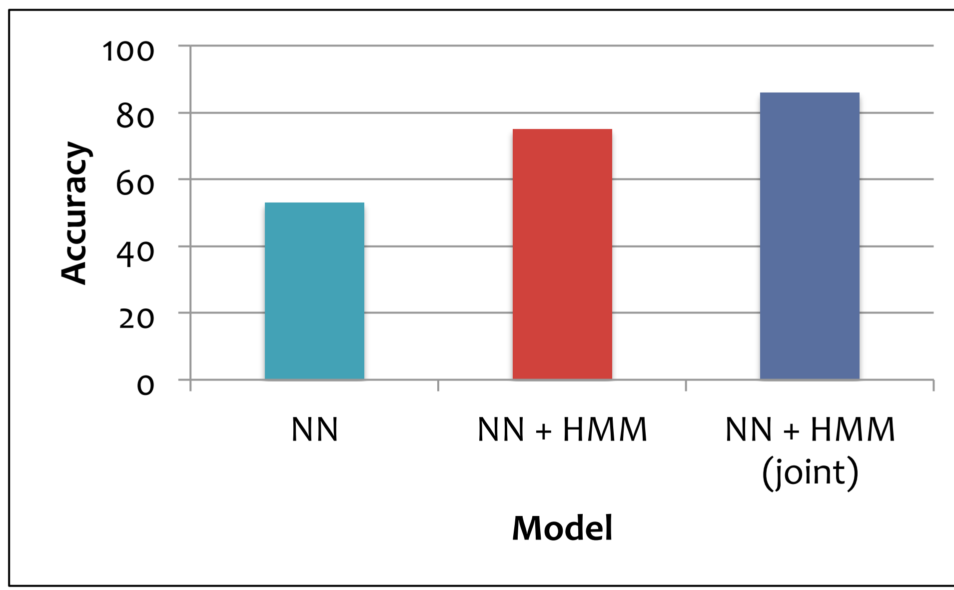
(Bengio et al., 1992)

Hybrid: NN + HMM

Experimental Setup:

- **Task:** Phoneme Recognition (aka. speaker independent recognition of plosive sounds)
- **Eight output labels:**
  - /p/, /t/, /k/, /b/, /d/, /g/, /dx/, /all other phonemes/
  - These are the HMM hidden states
- **Metric:** Accuracy
- **3 Models:**
  1. NN only
  2. NN + HMM (trained independently)
  3. NN + HMM (jointly trained)





Outline

- **Motivation**
- **Hybrid NN + HMM**
  - Model: neural net for emissions
  - Learning: backprop for end-to-end training
  - Experiments: phoneme recognition (Bengio et al., 1992)
- **Background: Recurrent Neural Networks (RNNs)**
  - Bidirectional RNNs
  - Deep Bidirectional RNNs
  - Deep Bidirectional LSTMs
  - Connection to forward-backward algorithm
- **Hybrid RNN + HMM**
  - Model: neural net for emissions
  - Experiments: phoneme recognition (Graves et al., 2013)
- **Hybrid CNN + CRF**
  - Model: neural net for factors
  - Experiments: natural language tasks (Collobert & Weston, 2011)
  - Experiments: pose estimation
- **Tricks of the Trade**

BACKGROUND: RECURRENT NEURAL NETWORKS

Recurrent Neural Networks (RNNs)

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\mathbf{h} = (h_1, h_2, \ldots, h_T), h_i \in \mathcal{R}^J$

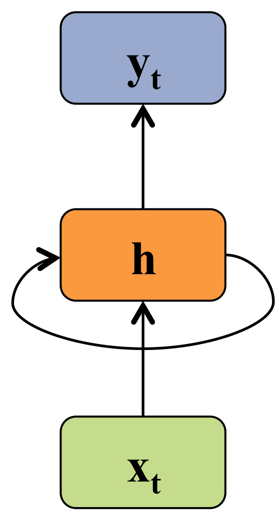
outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Definition of the RNN:

$$h_t = \mathcal{H}\left(W_{xh}x_t + W_{hh}h_{t-1} + b_h\right)$$

$$y_t = W_{hy}h_t + b_y$$



Recurrent Neural Networks (RNNs)

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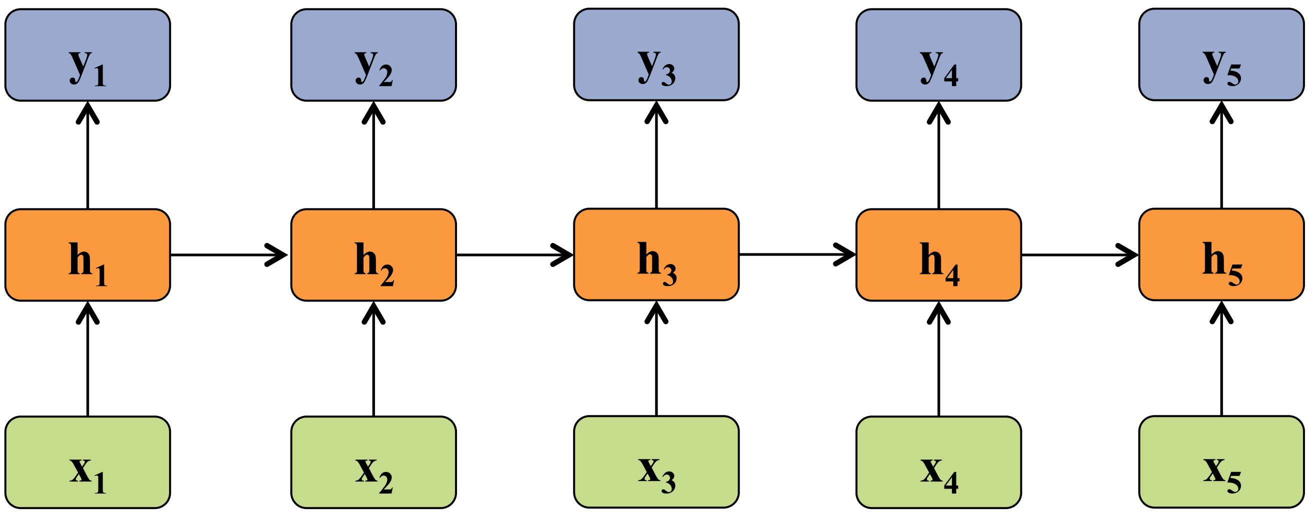

Recurrent Neural Networks (RNNs)

$$\text{inputs: } \mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$$

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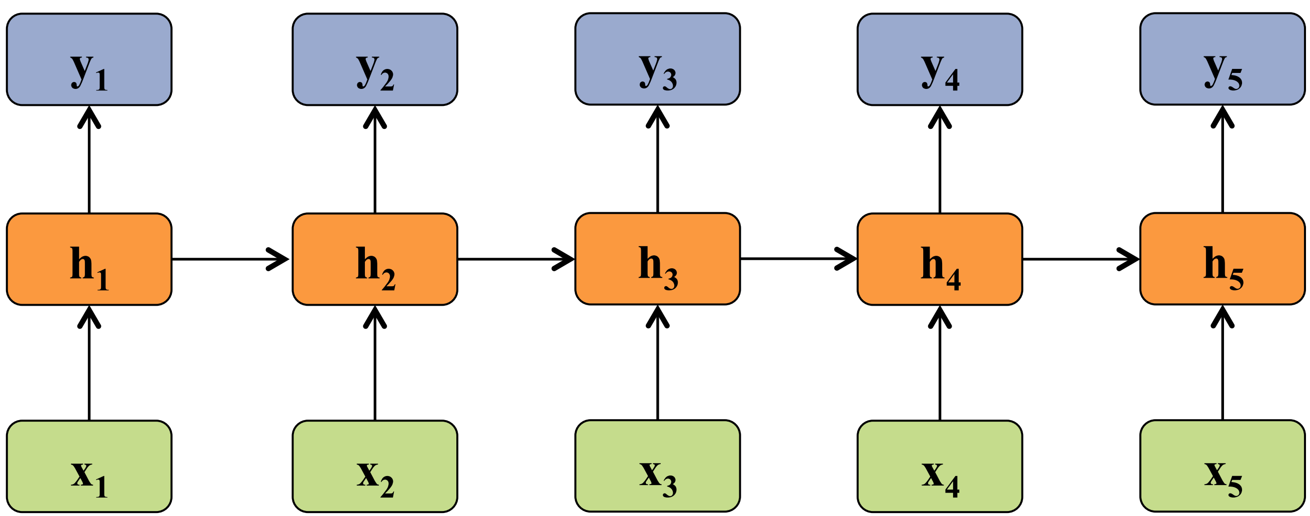
Definition of the RNN:

$$h_t = \mathcal{H}\left(W_{xh}x_t + W_{hh}h_{t-1} + b_h\right)$$

$$y_t = W_{hy}h_t + b_y$$



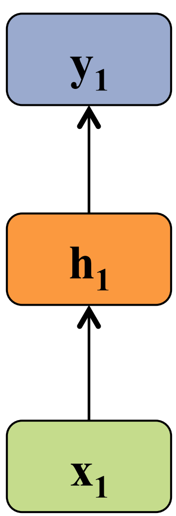
Recurrent Neural Networks (RNNs)

$$\begin{aligned} \text{inputs: } & \mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I \\ \text{hidden units: } & \mathbf{h} = (h_1, h_2, \ldots, h_T), h_i \in \mathcal{R}^J \\ \text{outputs: } & \mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K \\ \text{nonlinearity: } & \mathcal{H} \end{aligned}$$

Definition of the RNN:

$$h_t = \mathcal{H}\left(W_{xh} x_t + W_{hh} h_{t-1} + b_h\right)$$

$$y_t = W_{hy} h_t + b_y$$



- If $T=1$, then we have a standard feed-forward **neural net with one hidden layer**
- All of the deep nets from last lecture (DNN, DBN, DBM) required **fixed size inputs/ outputs**

Recurrent Neural Networks (RNNs)

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\mathbf{h} = (h_1, h_2, \ldots, h_T), h_i \in \mathcal{R}^J$

outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

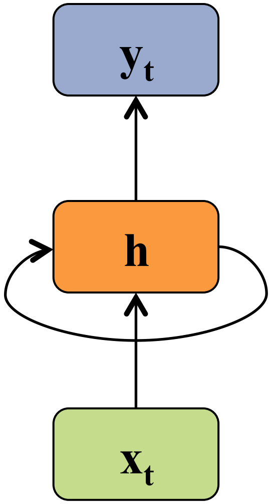
nonlinearity: $\mathcal{H}$

Definition of the RNN:

$$h_t = \mathcal{H}\left(W_{xh}x_t + W_{hh}h_{t-1} + b_h\right)$$

$$y_t = W_{hy}h_t + b_y$$

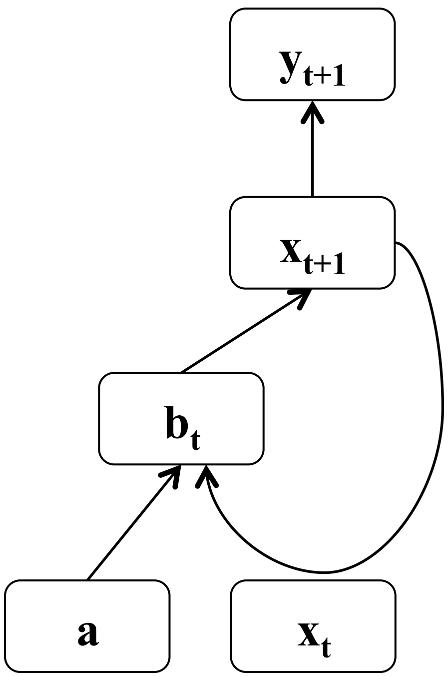
- By unrolling the RNN through time, we can **share parameters** and accommodate **arbitrary length** input/output pairs
- Applications: **time-series data** such as sentences, speech, stock-market, signal data, etc.



Background: Backprop through time

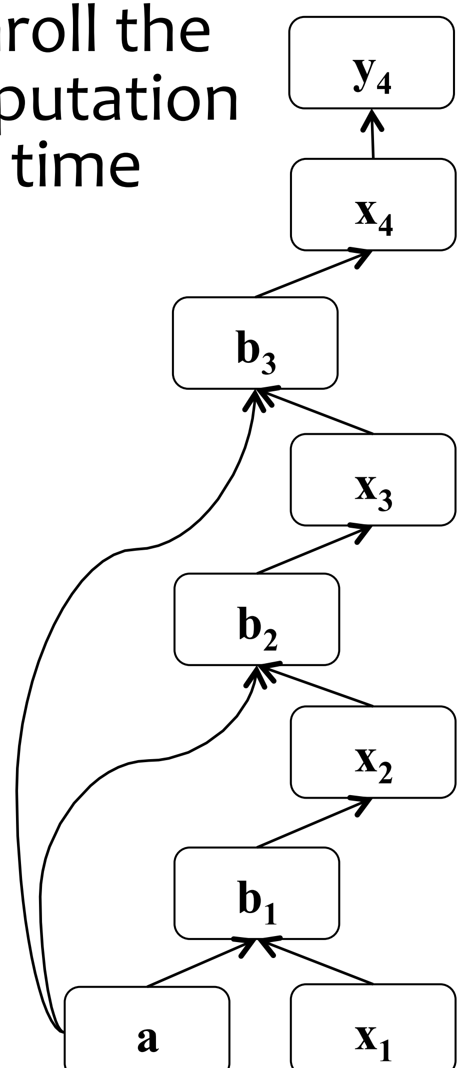
(Robinson & Fallside, 1987)
(Werbos, 1988)
(Mozer, 1995)

Recurrent neural network:



BPTT:

1. Unroll the computation over time



2. Run backprop through the resulting feed-forward network

Bidirectional RNN

$$\text{inputs: } \mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$$

$$\text{hidden units: } \overrightarrow{\mathbf{h}} \text{ and } \overleftarrow{\mathbf{h}}$$

$$\text{outputs: } \mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$$

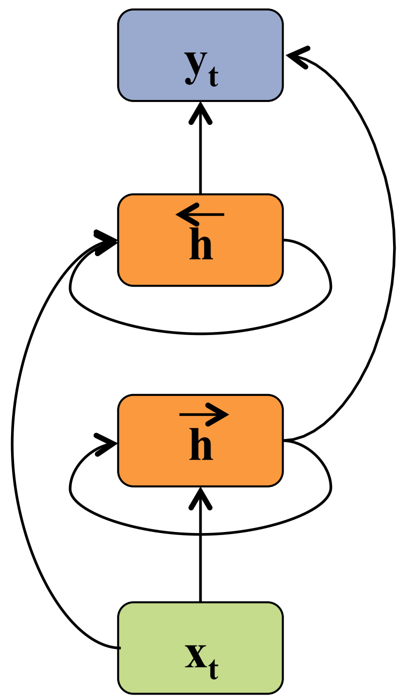
$$\text{nonlinearity: } \mathcal{H}$$

Recursive Definition:

$$\overrightarrow{h}_t = \mathcal{H}\left(W_{x\overrightarrow{h}} x_t + W_{\overrightarrow{h}\overrightarrow{h}} \overrightarrow{h}_{t-1} + b_{\overrightarrow{h}}\right)$$

$$\overleftarrow{h}_t = \mathcal{H}\left(W_{x\overleftarrow{h}} x_t + W_{\overleftarrow{h}\overleftarrow{h}} \overleftarrow{h}_{t+1} + b_{\overleftarrow{h}}\right)$$

$$y_t = W_{\overrightarrow{h}y} \overrightarrow{h}_t + W_{\overleftarrow{h}y} \overleftarrow{h}_t + b_y$$



Bidirectional RNN

inputs: $\mathbf{x} = (x_1, x_2, \dots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\overrightarrow{\mathbf{h}}$ and $\overleftarrow{\mathbf{h}}$

outputs: $\mathbf{y} = (y_1, y_2, \dots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Recursive Definition:

$$\overrightarrow{h}_t = \mathcal{H}\left(W_{x\overrightarrow{h}} x_t + W_{\overrightarrow{h}\overrightarrow{h}} \overrightarrow{h}_{t-1} + b_{\overrightarrow{h}}\right)$$

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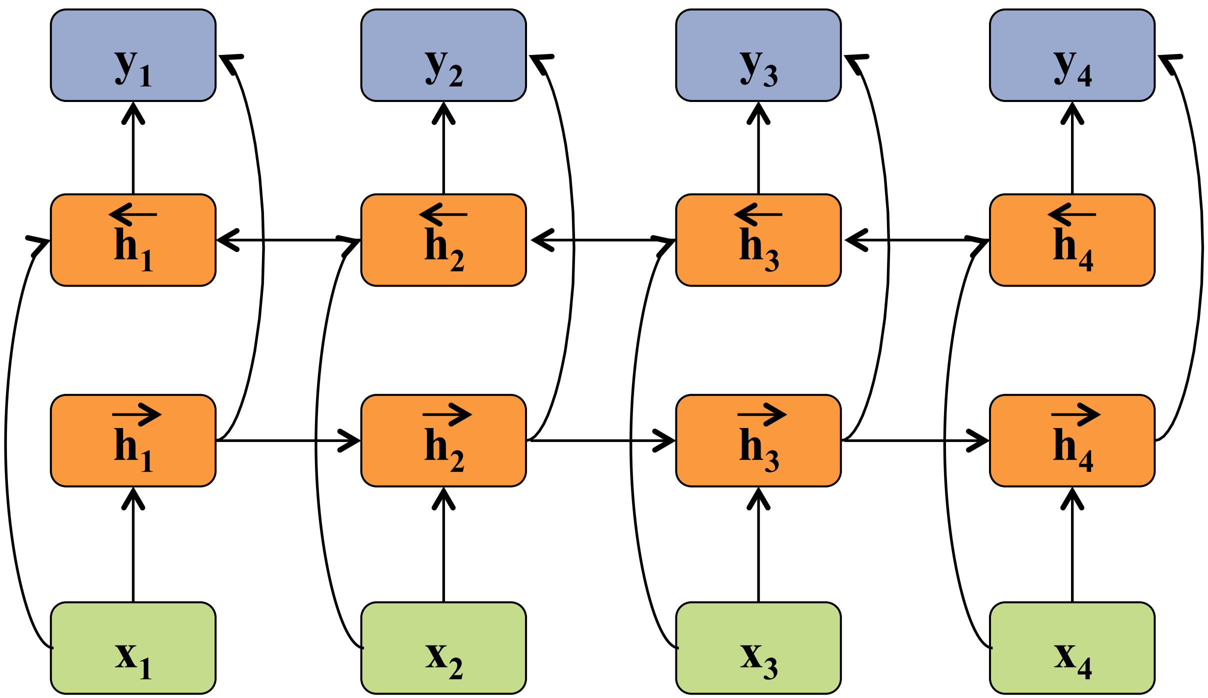

Bidirectional RNN

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\overrightarrow{\mathbf{h}}$ and $\overleftarrow{\mathbf{h}}$

outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Recursive Definition:

$$\overrightarrow{h}_t = \mathcal{H}\left(W_{x\overrightarrow{h}} x_t + W_{\overrightarrow{h}\overrightarrow{h}} \overrightarrow{h}_{t-1} + b_{\overrightarrow{h}}\right)$$

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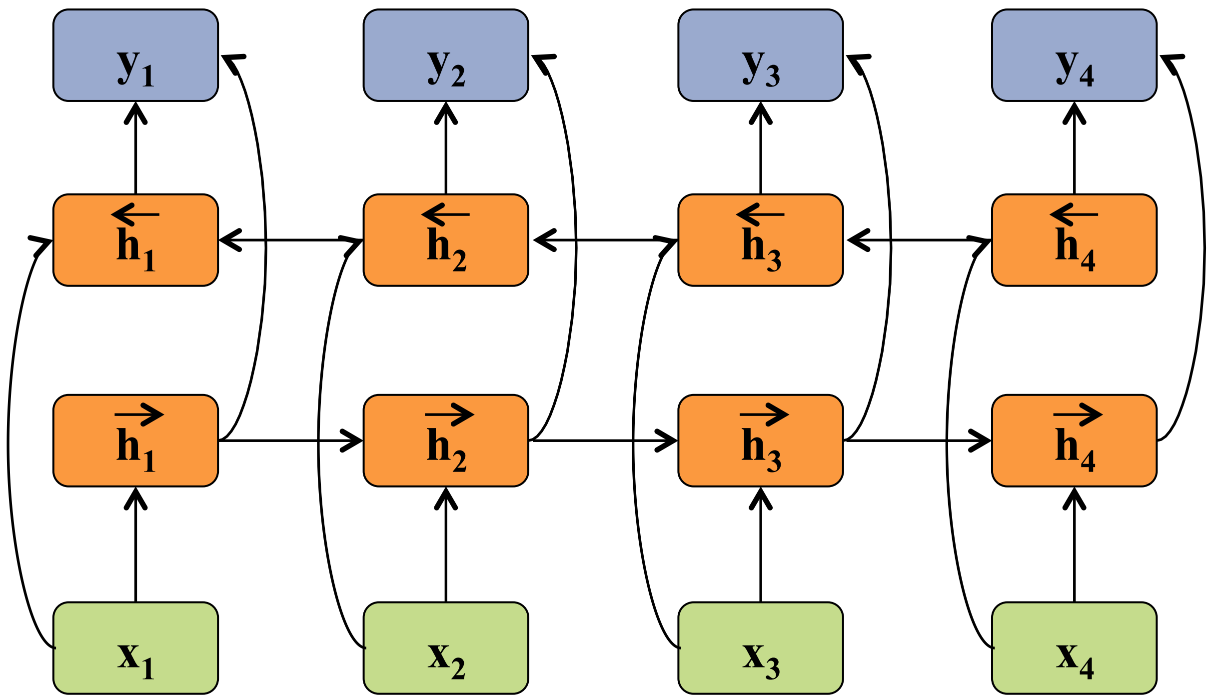
$$y_t = W_{\overrightarrow{h}y} \overrightarrow{h}_t + W_{\overleftarrow{h}y} \overleftarrow{h}_t + b_y$$



Bidirectional RNN

inputs: $\mathbf{x} = (x_1, x_2, \dots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\overrightarrow{\mathbf{h}}$ and $\overleftarrow{\mathbf{h}}$

outputs: $\mathbf{y} = (y_1, y_2, \dots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Recursive Definition:

$$\overrightarrow{h}_t = \mathcal{H}\left(W_{x\overrightarrow{h}} x_t + W_{\overrightarrow{h}\overrightarrow{h}} \overrightarrow{h}_{t-1} + b_{\overrightarrow{h}}\right)$$

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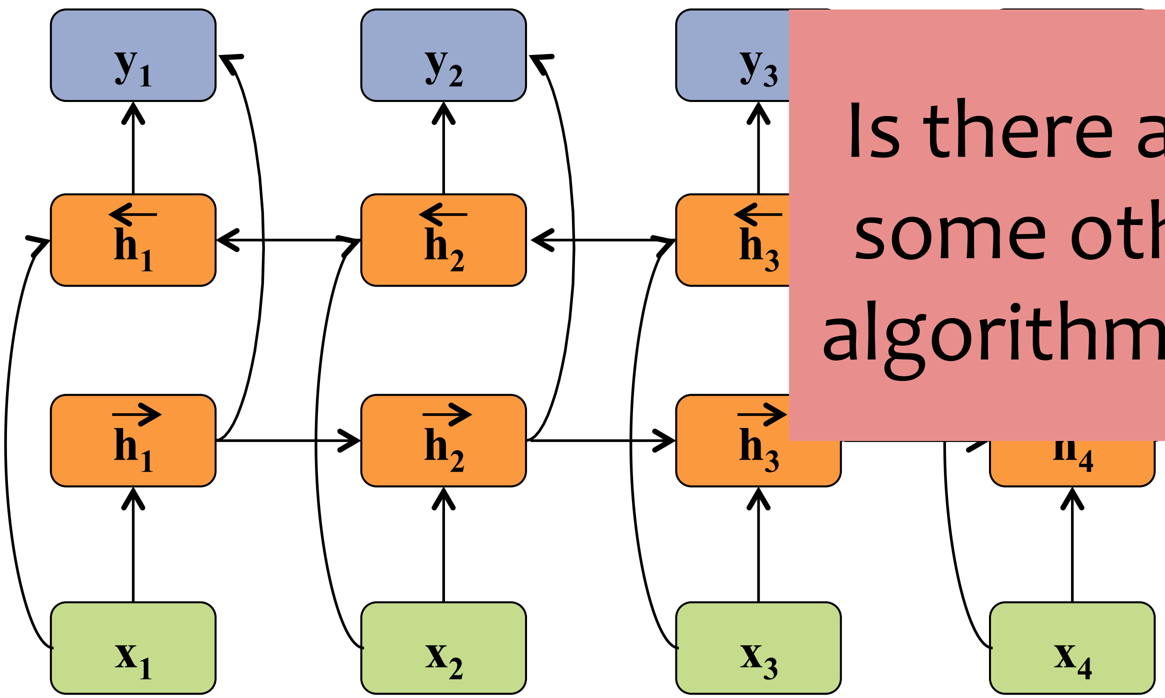
$$y_t = W_{\overrightarrow{h}y} \overrightarrow{h}_t + W_{\overleftarrow{h}y} \overleftarrow{h}_t + b_y$$



Is there an analogy to some other recursive algorithm(s) we know?

Deep RNNs

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Recursive Definition:

$$h_t^n = \mathcal{H}\left(W_{h^{n-1}h^n} h_t^{n-1} + W_{h^n h^n} h_{t-1}^n + b_h^n\right)$$

$$y_t = W_{h^N y} h_t^N + b_y$$

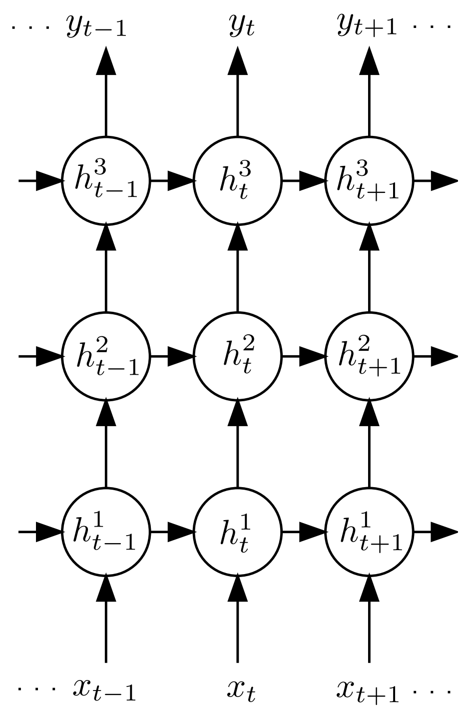


Figure from (Graves et al., 2013)

Deep Bidirectional RNNs

$$\text{inputs: } \mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$$

$$\text{outputs: } \mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$$

$$\text{nonlinearity: } \mathcal{H}$$

- Notice that the upper level hidden units have input from **two previous layers** (i.e. wider input)
- Likewise for the output layer
- What analogy can we draw to DNNs, DBNs, DBMs?

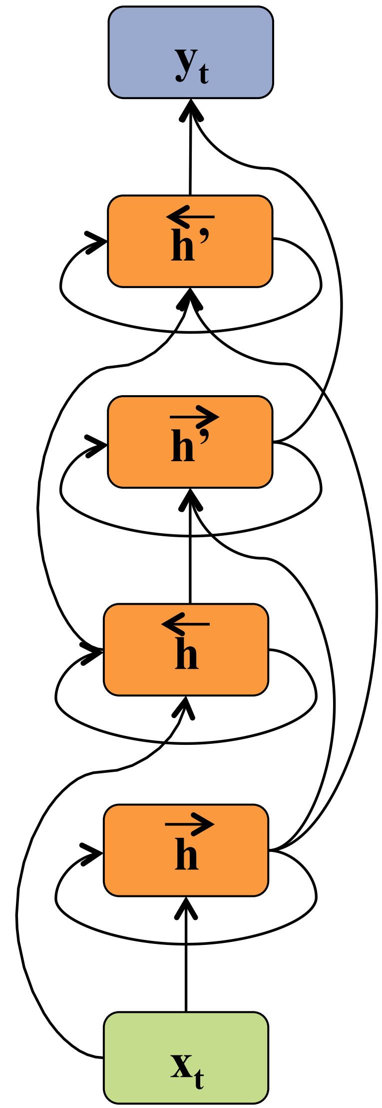
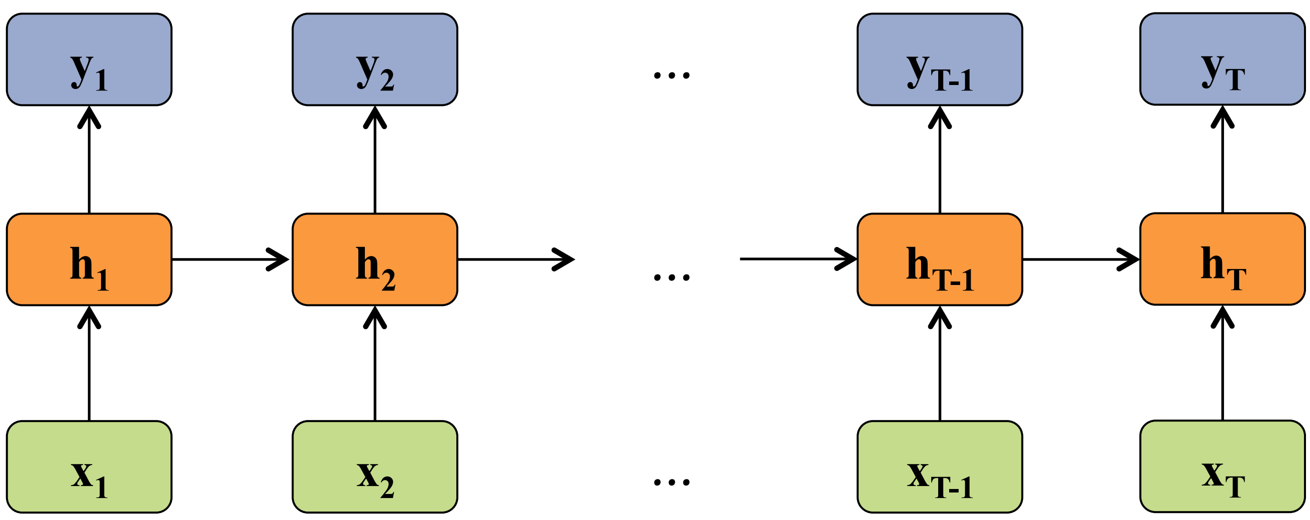


Figure from (Graves et al., 2013)

Long Short-Term Memory (LSTM)

Motivation:

- Standard RNNs have trouble learning long distance dependencies
- LSTMs combat this issue



Long Short-Term Memory (LSTM)

Motivation:

- Vanishing gradient problem for Standard RNNs
- Figure shows sensitivity (darker = more sensitive) to the input at time t=1

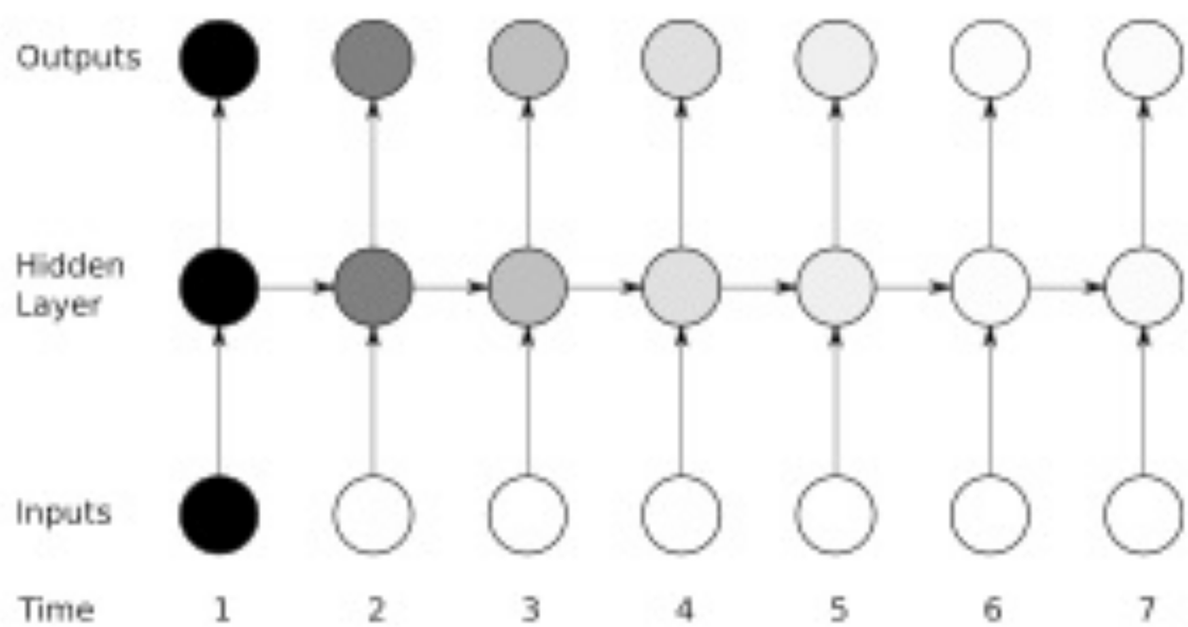


Figure from (Graves, 2012)

Long Short-Term Memory (LSTM)

Motivation:

- LSTM units have a rich internal structure
- The various "gates" determine the propagation of information and can choose to "remember" or "forget" information

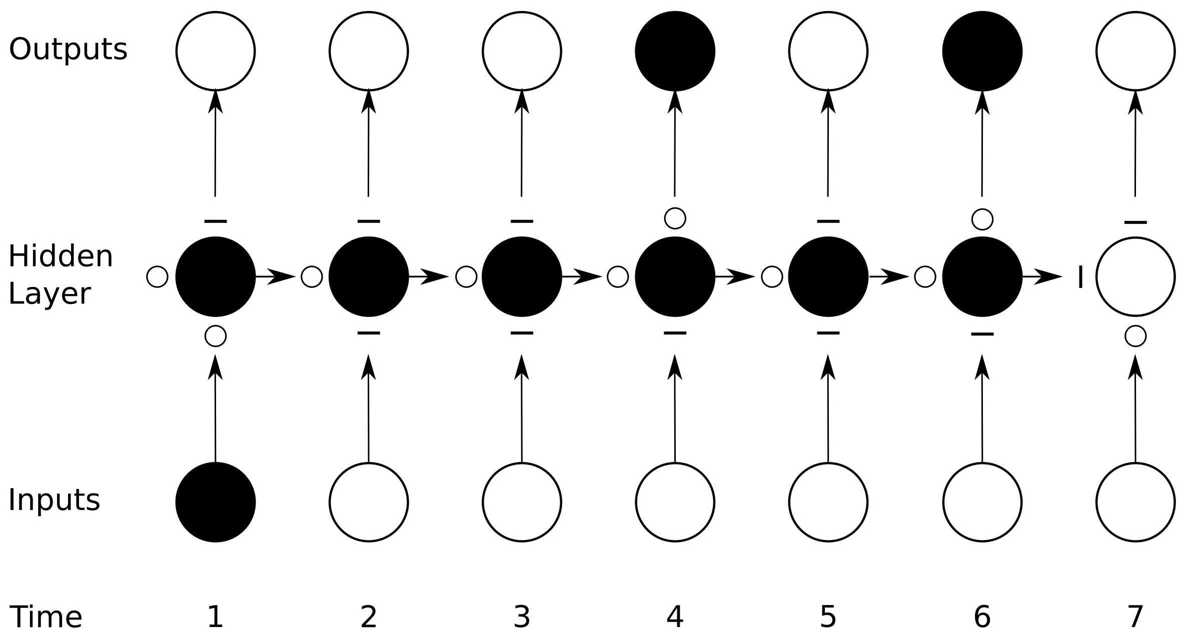
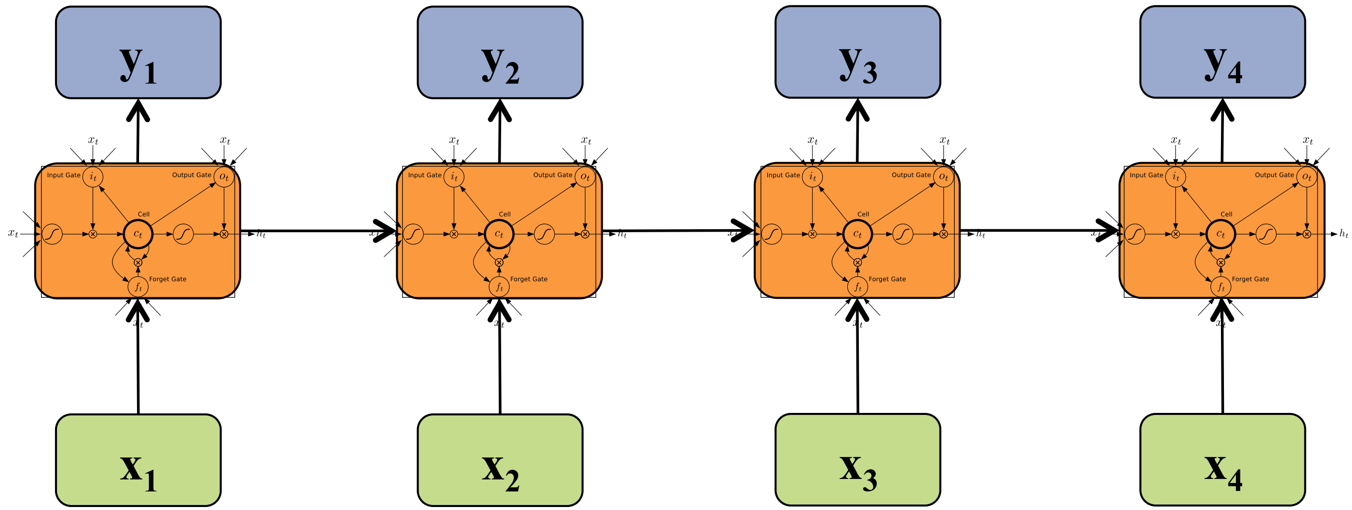


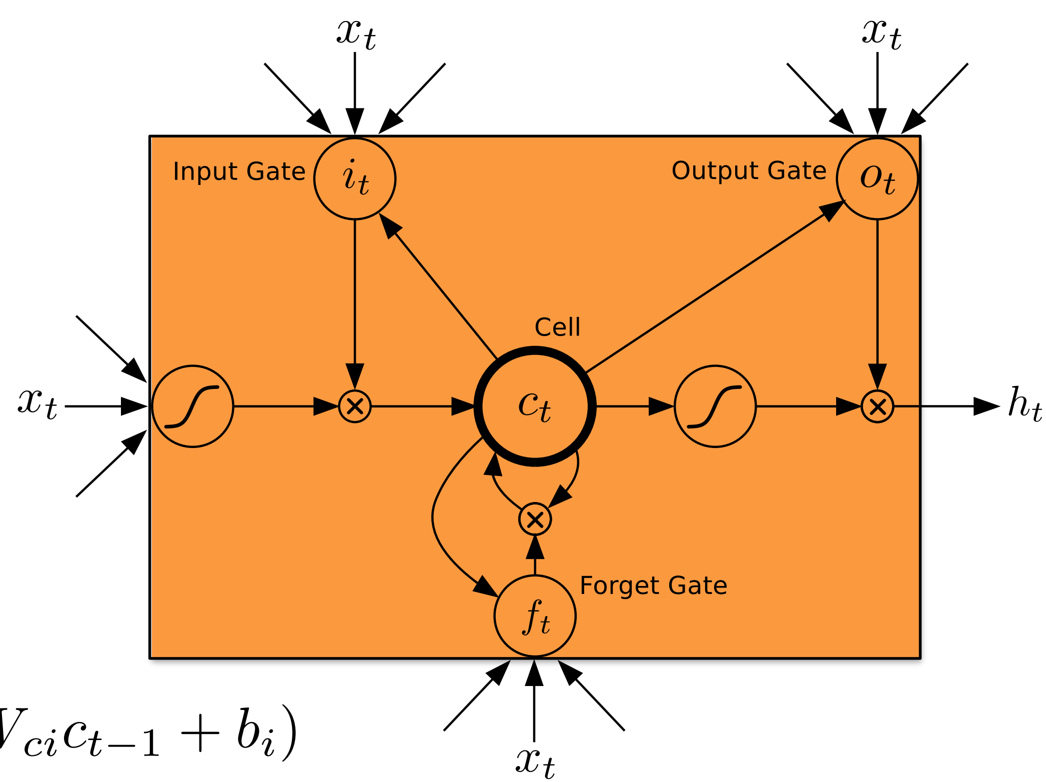
Figure from (Graves, 2012)

Long Short-Term Memory (LSTM)



Long Short-Term Memory (LSTM)

- **Input gate:** masks out the standard RNN inputs
- **Forget gate:** masks out the previous cell
- **Cell:** stores the input/ forget mixture
- **Output gate:** masks out the values of the next hidden



$$i_t = \sigma\left(W_{xi}x_t + W_{hi}h_{t-1} + W_{ci}c_{t-1} + b_i\right)$$

$$f_t = \sigma\left(W_{xf}x_t + W_{hf}h_{t-1} + W_{cf}c_{t-1} + b_f\right)$$

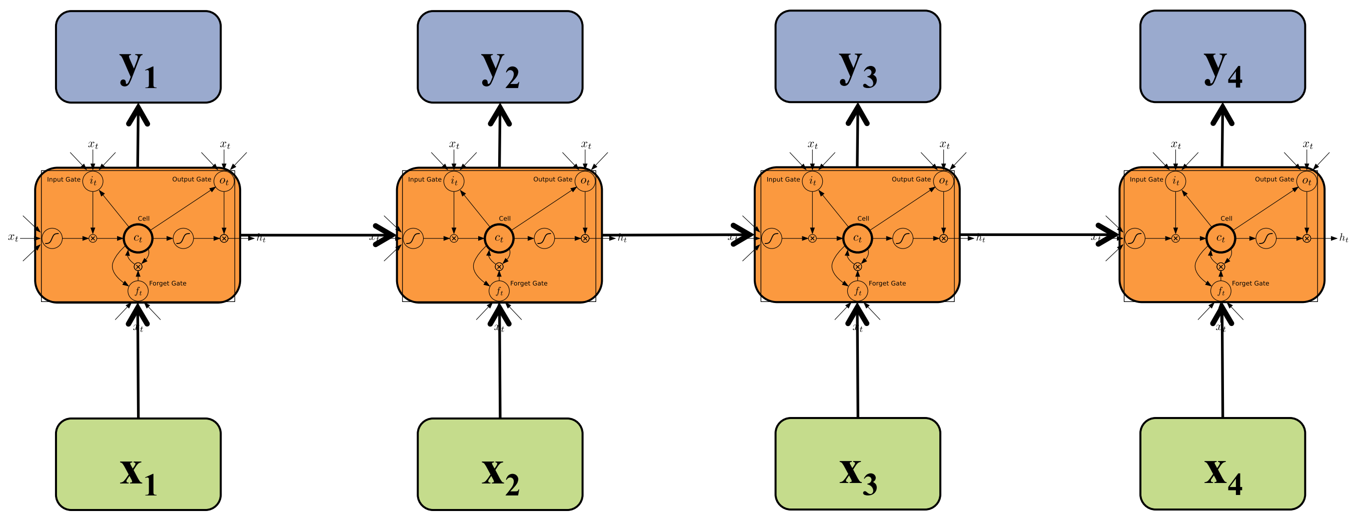
$$c_t = f_t c_{t-1} + i_t \tanh\left(W_{xc}x_t + W_{hc}h_{t-1} + b_c\right)$$

$$o_t = \sigma\left(W_{xo}x_t + W_{ho}h_{t-1} + W_{co}c_t + b_o\right)$$

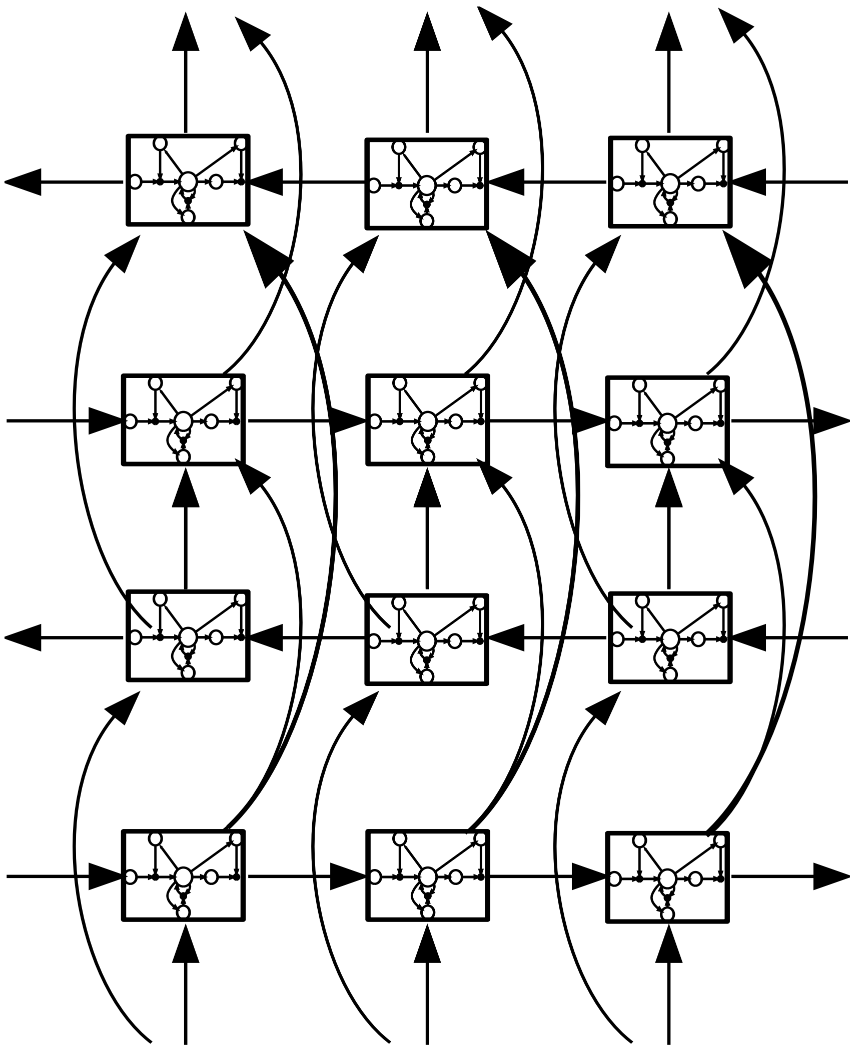
$$h_t = o_t \tanh(c_t)$$

Figure from (Graves et al., 2013)

Long Short-Term Memory (LSTM)



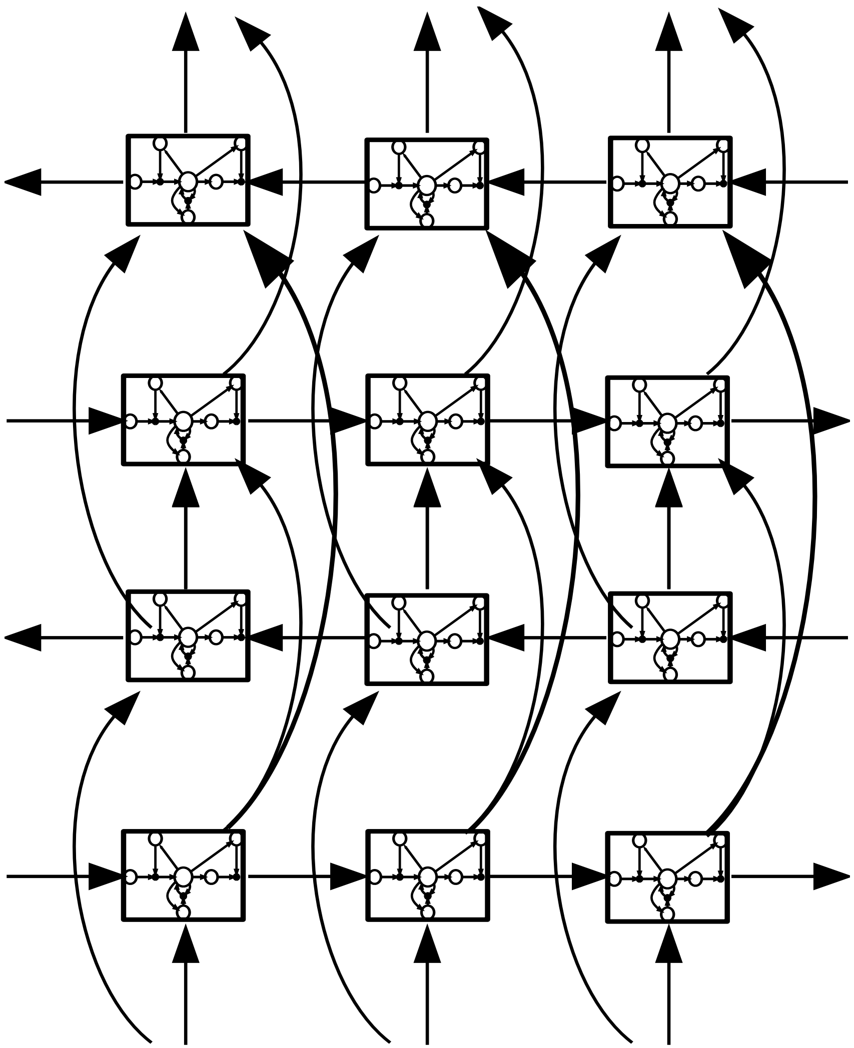
Deep Bidirectional LSTM (DBLSTM)



- Figure: input/output layers not shown
- **Same general topology** as a Deep Bidirectional RNN, but with **LSTM units** in the hidden layers
- No additional **representational power** over DBRNN, but **easier to learn** in practice

Figure from (Graves et al., 2013)

Deep Bidirectional LSTM (DBLSTM)



How important is this particular architecture?

Jozefowicz et al. (2015) **evaluated 10,000 different LSTM-like architectures** and found several variants that worked just as well on several tasks.

Figure from (Graves et al., 2013)

Outline

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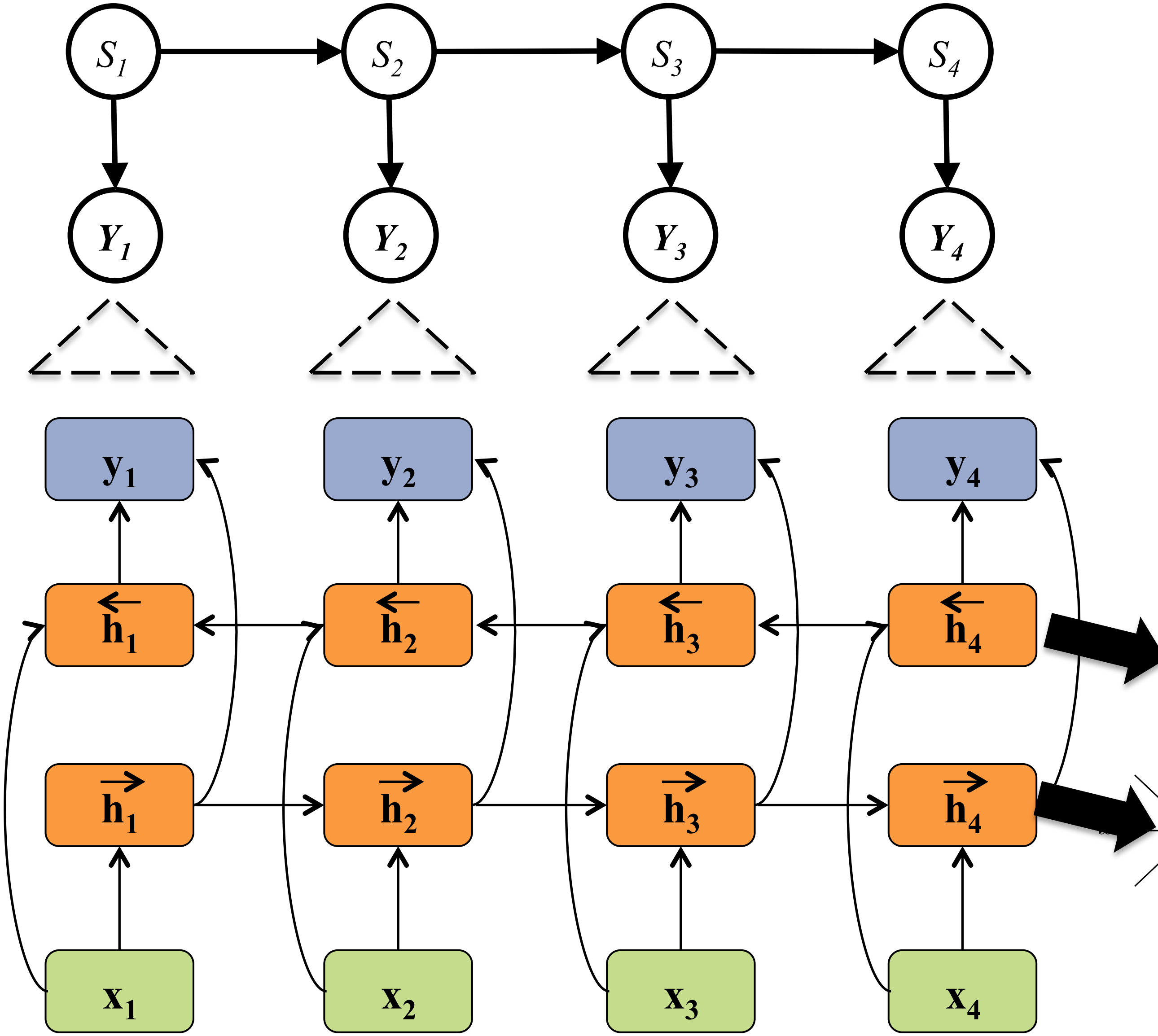
  - Experiments: pose estimation
- **Tricks of the Trade**

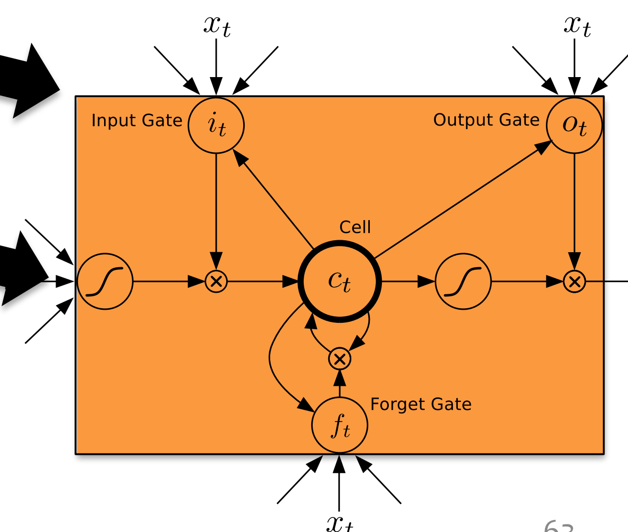
HYBRID:
RNN + HMM

Hybrid: RNN + HMM

(Graves et al., 2013)

- Graves et al. (2013) uses a Deep Bidirectional LSTM
- Each hidden unit is an LSTM
- Deep ➔ More than two layers



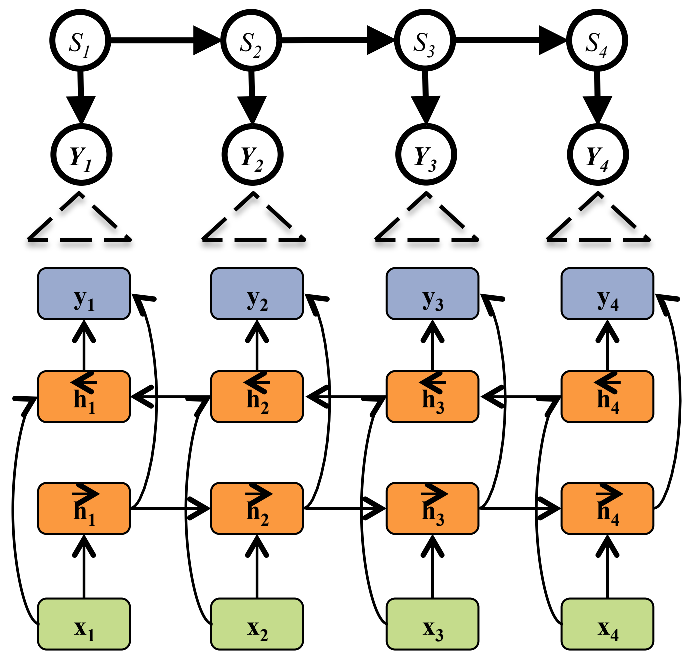


Hybrid: RNN + HMM

(Graves et al., 2013)

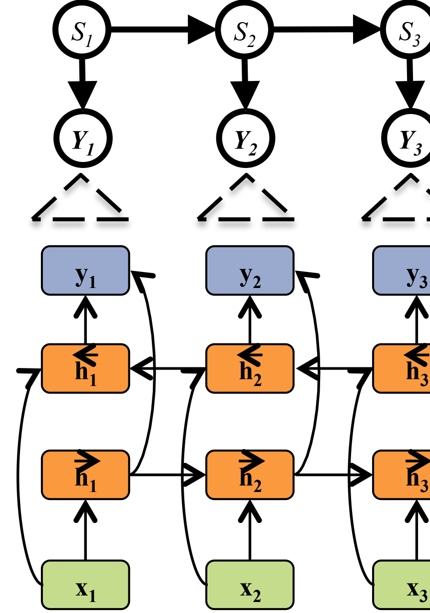
The model, inference, and learning can be **analogous** to our NN + HMM hybrid

- **Objective:** log-likelihood
- **Model:** HMM/Gaussian emissions
- **Inference:** forward-backward algorithm
- **Learning:** SGD with gradient by backpropagation



(Graves et al., 2013)

Hybrid: RNN + HMM



Experimental Setup:

- **Task:** Phoneme Recognition
- **Dataset:** TIMIT
- **Metric:** Phoneme Error Rate
- **Two classes of models:**
  1. Neural Net only
  2. NN + HMM hybrids

TRAINING METHOD	TEST PER
CTC	21.57 ± 0.25
CTC (NOISE)	18.63 ± 0.16
TRANSDUCER	$\mathbf{18.07 \pm 0.24}$

1. Neural Net only

NETWORK	DEV PER TEST PER
DBRNN	19.91 ± 0.22 21.92 ± 0.35
DBLSTM	17.44 ± 0.156 19.34 ± 0.15
DBLSTM (NOISE)	16.11 ± 0.15 $\mathbf{17.99 \pm 0.13}$

2. NN + HMM hybrids

Outline

- **Motivation**
- **Hybrid NN + HMM**
  - Model: neural net for emissions
  - Learning: backprop for end-to-end training
  - Experiments: phoneme recognition (Bengio et al., 1992)
- **Background: Recurrent Neural Networks (RNNs)**
  - Bidirectional RNNs
  - Deep Bidirectional RNNs
  - Deep Bidirectional LSTMs
  - Connection to forward-backward algorithm
- **Hybrid RNN + HMM**
  - Model: neural net for emissions
  - Experiments: phoneme recognition (Graves et al., 2013)
- **Hybrid CNN + CRF**
  - Model: neural net for factors
  - Experiments: natural language tasks (Collobert & Weston, 2011)
  - Experiments: pose estimation
- **Tricks of the Trade**

HYBRID:
CNN + CRF

Recall…

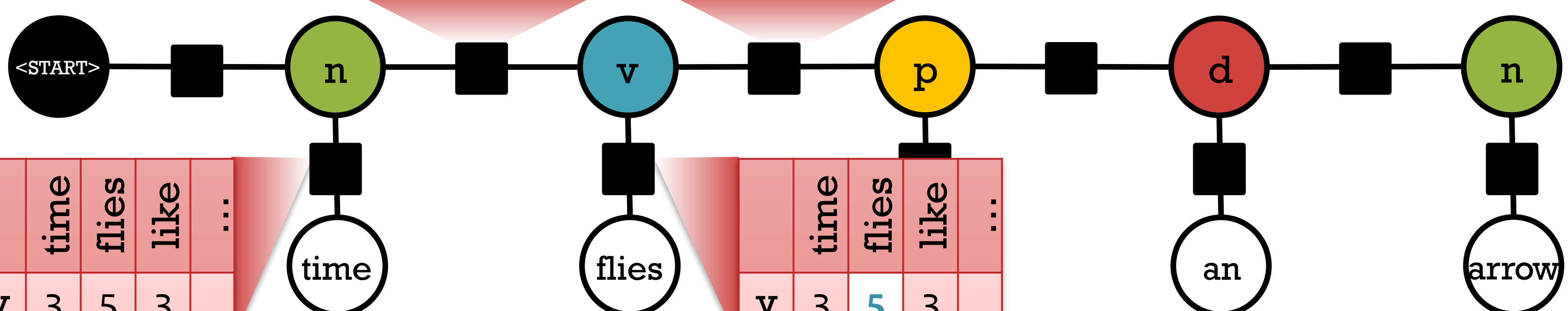
Markov Random Field (MRF)

Joint distribution over tags Y_i <u>and</u> words X_i

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

	v	n	p	d
v	1	6	3	4
n	8	4	2	0.1
p	1	3	1	3
d	0.1	8	0	0

	v	n	p	d
v	1	6	3	4
n	8	4	2	0.1
p	1	3	1	3
d	0.1	8	0	0



	time	flies	like	…
v	3	5	3	
n	4	5	2	
p	0.1	0.1	3	
d	0.1	0.2	0.1	

	time	flies	like	…
v	3	5	3	
n	4	5	2	
p	0.1	0.1	3	
d	0.1	0.2	0.1	

Recall...

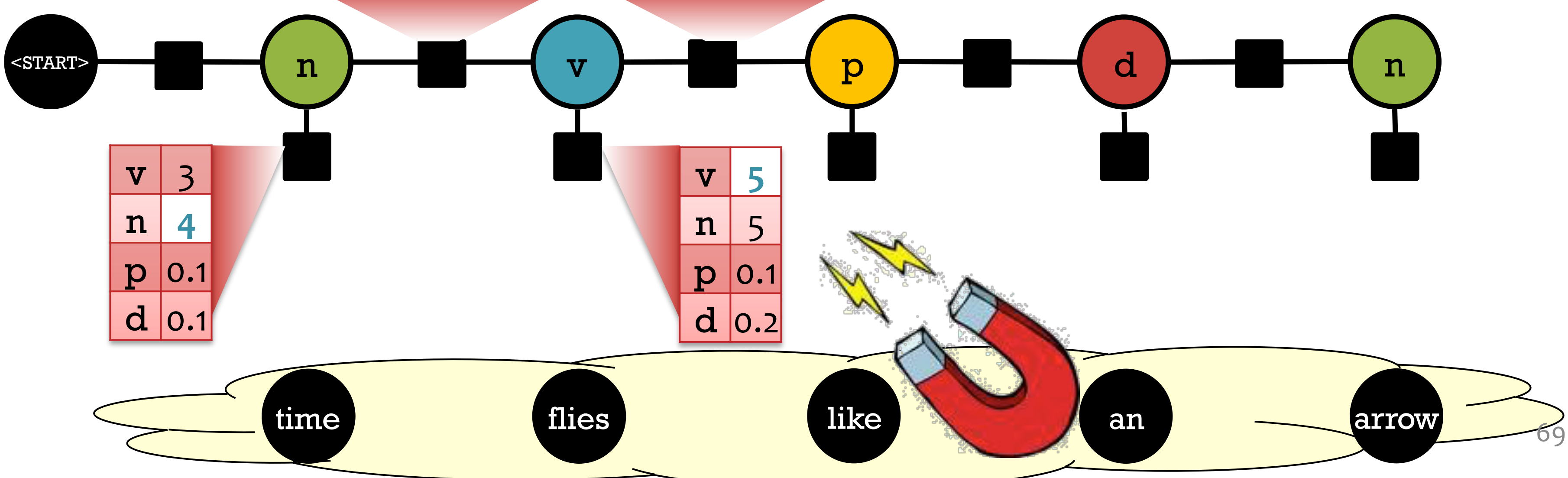
Conditional Random Field (CRF)

Conditional distribution over tags Y_i <u>given</u> words x_i.
The factors and Z are now specific to the sentence $\boldsymbol{x}$.

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

	v	n	p	d
v	1	6	3	4
n	8	4	2	0.1
p	1	3	1	3
d	0.1	8	0	0

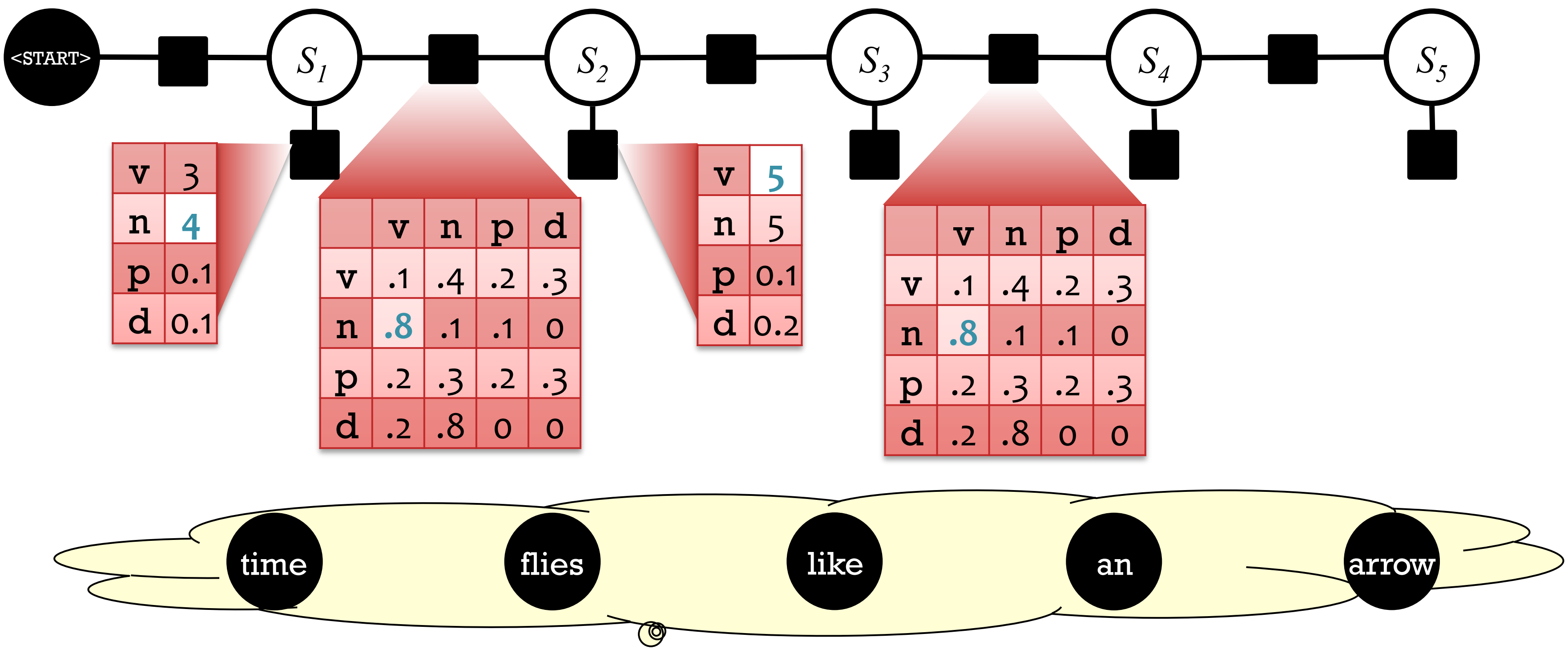
	v	n	p	d
v	1	6	3	4
n	8	4	2	0.1
p	1	3	1	3
d	0.1	8	0	0



v	3
n	4
p	0.1
d	0.1

v	5
n	5
p	0.1
d	0.2

Hybrid: Neural Net + CRF



v	3
n	4
p	0.1
d	0.1

	v	n	p	d
v	.1	.4	.2	.3
n	.8	.1	.1	0
p	.2	.3	.2	.3
d	.2	.8	0	0

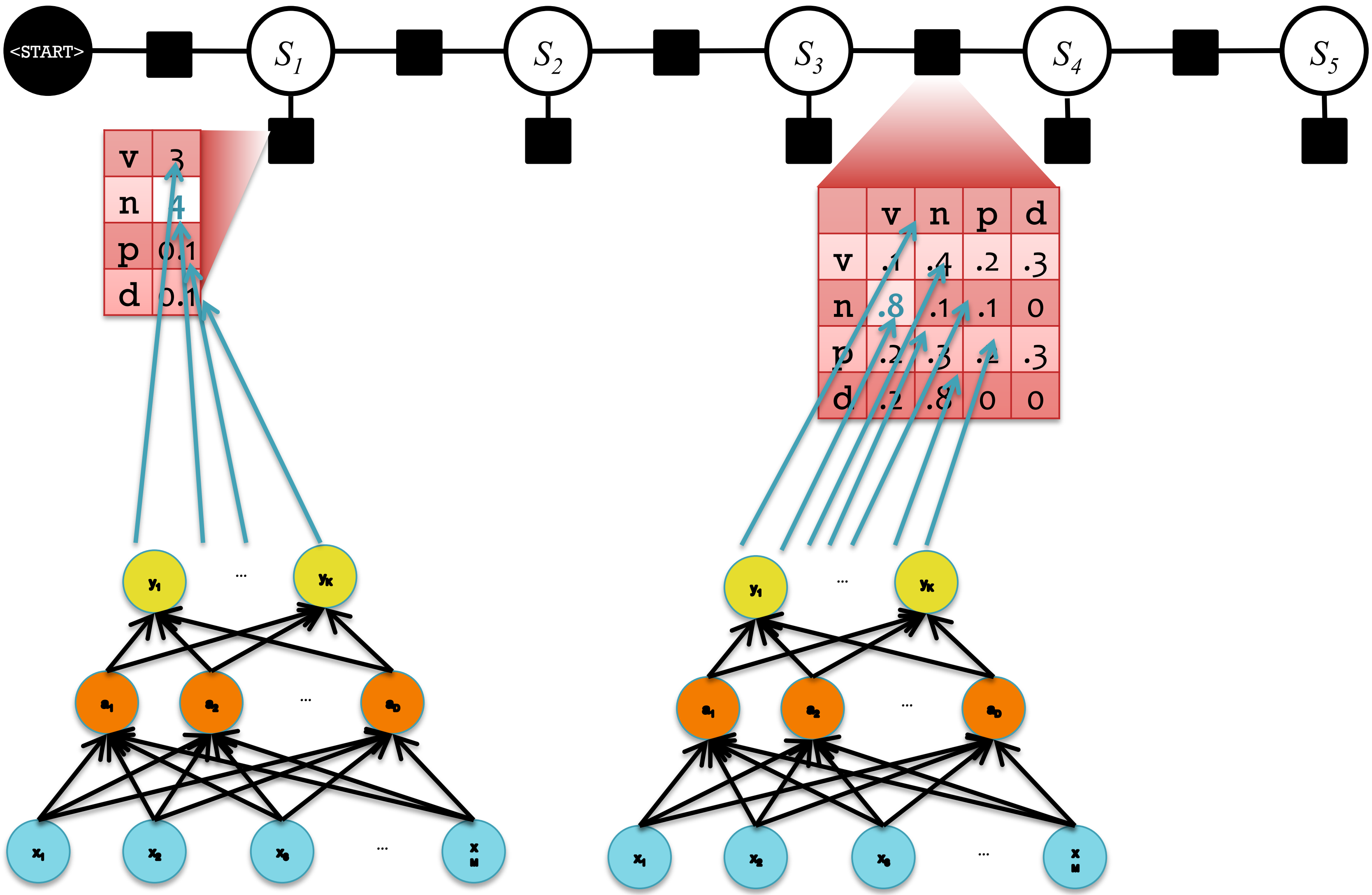
v	5
n	5
p	0.1
d	0.2

	v	n	p	d
v	.1	.4	.2	.3
n	.8	.1	.1	0
p	.2	.3	.2	.3
d	.2	.8	0	0

- In a standard CRF, each of the factor cells is a parameter (e.g. transition or emission)
- In the hybrid model, these values are computed by a neural network with its own parameters

Hybrid: Neural Net + CRF

Forward computation



(Collobert & Weston, 2011)

Hybrid: CNN + CRF

- For **computer vision,** Convolutional Neural Networks are in **2-dimensions**
- For **natural language,** the CNN is **1-dimensional**

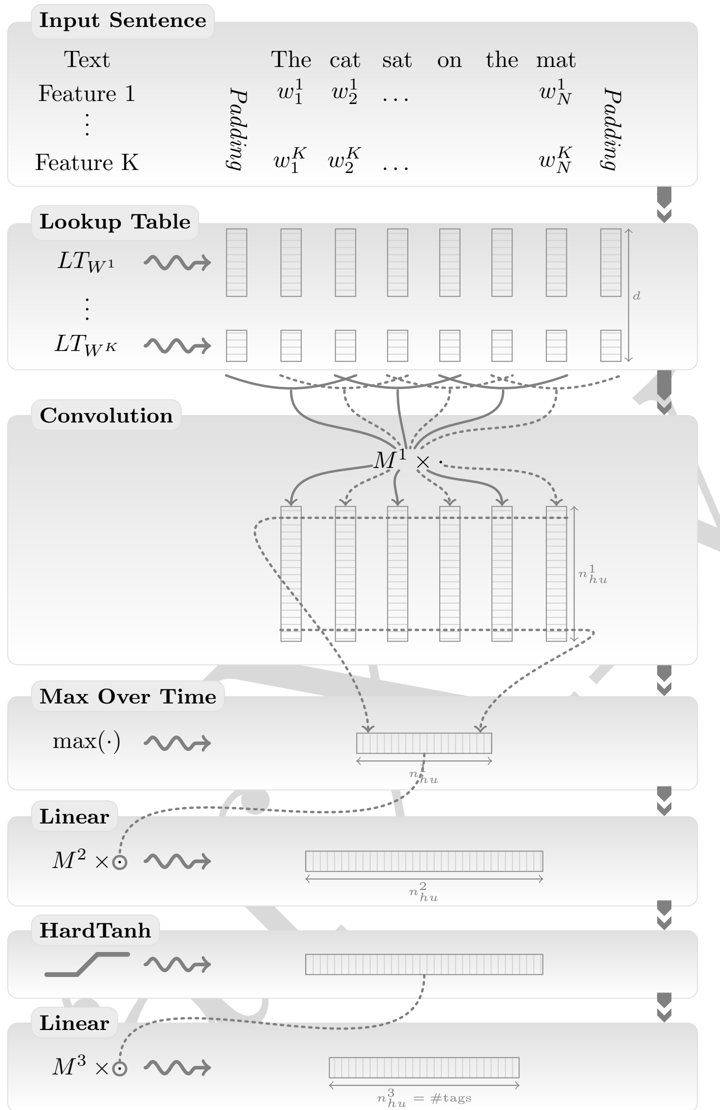


Figure from (Collobert & Weston, 2011)

(Collobert & Weston, 2011)

Hybrid: CNN + CRF

"NN + SLL"

- Model: Convolutional Neural Network (CNN) with **linear-chain CRF**
- Training objective: maximize **sentence-level likelihood** (SLL)

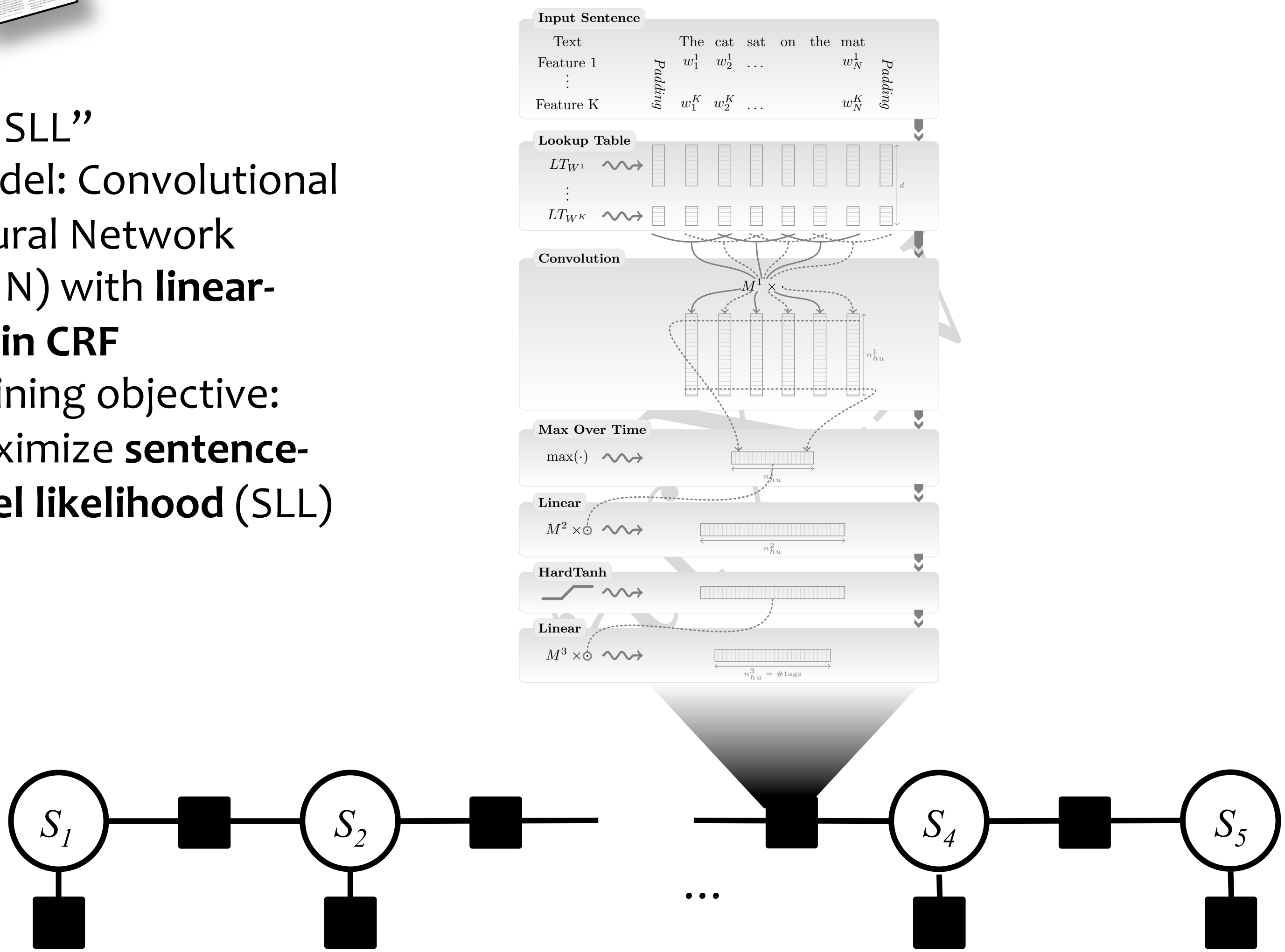
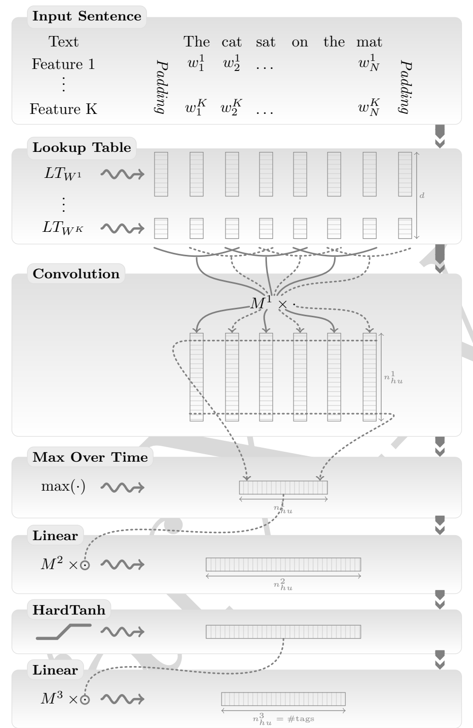


Figure from (Collobert & Weston, 2011)

Hybrid: CNN + CRF

"NN + WLL"

- Model: Convolutional Neural Network (CNN) with **logistic regression**
- Training objective: maximize **word-level likelihood** (WLL)



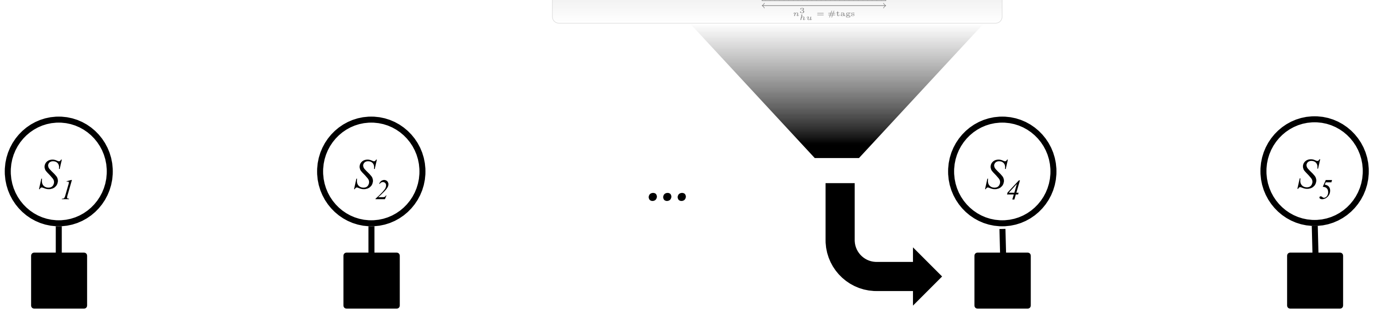


Figure from (Collobert & Weston, 2011)

(Collobert & Weston, 2011)

Hybrid: CNN + CRF

Experimental Setup:

- **Tasks:**
  - Part-of-speech tagging (POS),
  - Noun-phrase and Verb-phrase Chunking,
  - Named-entity recognition (NER)
  - Semantic Role Labeling (SRL)
- **Datasets / Metrics:** Standard setups from NLP literature (higher PWA/F1 is better)
- **Models:**
  - Benchmark systems are typical – non-neural network systems
  - NN+WLL: hybrid CNN with logistic regression
  - NN+SLL: hybrid CNN with linear-chain CRF

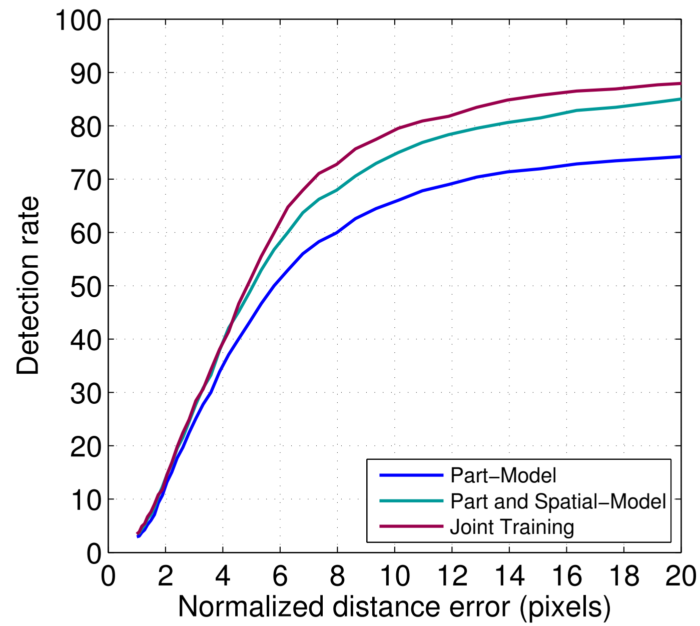
Approach	**POS** (PWA)	**Chunking** (F1)	**NER** (F1)	**SRL** (F1)
Benchmark Systems	97.24	94.29	89.31	77.92
NN+WLL	96.31	89.13	79.53	55.40
NN+SLL	96.37	90.33	81.47	70.99

(Thompson et al., 2014)

Hybrid: CNN + MRF

Experimental Setup:

- **Task:** pose estimation
- **Model:** Deep CNN + MRF



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TRICKS OF THE TRADE

Backprop in Practice

Y LeCun
MA Ranzato

- Use ReLU non-linearities (tanh and logistic are falling out of favor)
- Use cross-entropy loss for classification
- Use Stochastic Gradient Descent on minibatches
- Shuffle the training samples
- Normalize the input variables (zero mean, unit variance)
- Schedule to decrease the learning rate
- Use a bit of L1 or L2 regularization on the weights (or a combination)
  - But it's best to turn it on after a couple of epochs
- Use "dropout" for regularization
  - Hinton et al 2012 http://arxiv.org/abs/1207.0580
- Lots more in [LeCun et al. "Efficient Backprop" 1998]
- Lots, lots more in "Neural Networks, Tricks of the Trade" (2012 edition) edited by G. Montavon, G. B. Orr, and K-R Müller (Springer)

Deep Learning Tricks of the Trade

- Y. Bengio (2012), "Practical Recommendations for Gradient-Based Training of Deep Architectures"

  - Unsupervised pre-training
  - Stochastic gradient descent and setting learning rates
  - Main hyper-parameters
    - Learning rate schedule & early stopping
    - Minibatches
    - Parameter initialization
    - Number of hidden units
    - L1 or L2 weight decay
    - Sparsity regularization
  - Debugging → use finite difference gradient checks
  - How to efficiently search for hyper-parameter configurations

Slide from Socher, MLSS 2014

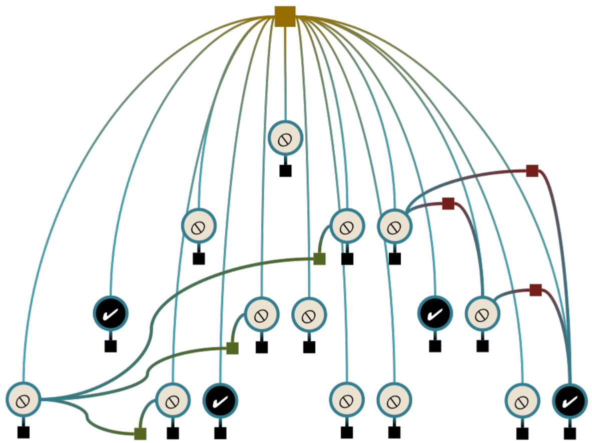
Tricks of the Trade

- **Lots of them:**
  - Pre-training helps (but isn't always necessary)
  - Train with adaptive gradient variants of SGD (e.g. AdaGrad, AdaDelta)
  - Use max-margin loss function (i.e. hinge loss) – though only sub-differentiable it often gives better results
  - …
- A few years back, they were considered "**poorly documented**" and "requiring great expertise"
- Now there are lots of **good tutorials** that describe (very important) specific implementation details
- Many of them **also apply to training graphical models**!

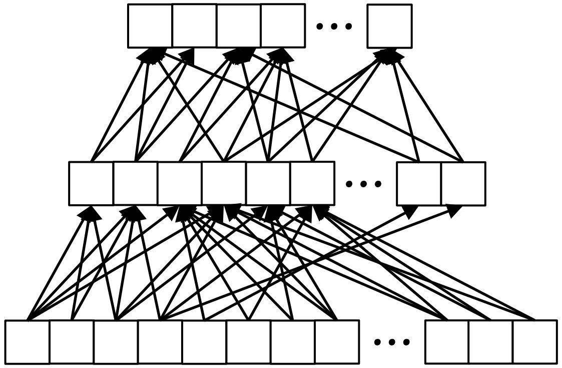
SUMMARY

Summary:
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?

Summary:
Hybrid Models

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