# CS 533: Natural Language Processing <br> Copy Mechanism, Relation-Aware Self-Attention, Hidden Markov Models 

Karl Stratos


Rutgers University

## Review: Conditional Language Models

- Language model (LM) conditioning on $x=\left(x_{1} \ldots x_{T}\right)$

$$
p_{\theta}\left(y_{1} \ldots y_{T^{\prime}} \mid x\right)=\prod_{t^{\prime}=1}^{T^{\prime}+1} p_{\theta}\left(y_{t^{\prime}} \mid x, y_{<t^{\prime}}\right)
$$

- Learnable modules
- Encoder. enc ${ }_{\theta}: \mathcal{V}^{T} \rightarrow \mathbb{R}^{T \times d}$ contextualizes source token embeddings of $x$ (e.g., BiLSTM, Transformer encoder)
- Decoder. dec ${ }_{\theta}: \mathbb{R}^{T \times d} \times \mathcal{V}^{t^{\prime}-1} \rightarrow \mathbb{R}^{V}$ computes logits for next word given source encodings and target history via attention to source encodings (e.g., recurrent, Transformer decoder)
- Encoder-decoder/sequence-to-sequence (seq2seq): Train encoder \& decoder jointly to optimize a function of

$$
p_{\theta}\left(y_{t^{\prime}} \mid x, y_{<t^{\prime}}\right)=\operatorname{softmax}_{y_{t^{\prime}}}\left(\mathbf{d e c}_{\theta}\left(\mathbf{e n c}_{\theta}(x), y_{<t^{\prime}}\right)\right)
$$

## Review: Stepwise Cross-Attention

- Example: RNN decoder with input feeding

- Learns to attend to right source positions, without supervision. Visualization for translating English to French (Bahdanau et al., 2016)
- Transformer decoder (Vaswani et al., 2017): No recurrent or convolutional layers, entirely based on attention with a position-shared feedforward


## The Unknown Word Problem

－Target text may contain rare words like
－Proper names：Lausanne，Cesar，Guilaume，．．．
－Numbers／values：103，95，42，3．141592，3．141593，．．．
－Decoder needs these in target vocab $\mathcal{V}$ to generate at all！
－Note target vocab may be distinct from source vocab $\mathcal{V}_{\text {src }}$ in general（e．g．，translation）
－Brute－force：Include all word types in $\mathcal{V}$ ？Not practical
－By Zipf＇s Law，most words will have extremely low probabilities
－Never enough：Guilaumé？3．141594？Not seen in training data
－Simple／naive approach：Threshold vocab by frequency
－Keep top－$k$（e．g．，$k=100000$ ）most frequent types in $\mathcal{V}$ and replace all other types（＂OOV＂）with special token 〈unk〉 in training
－Problem：Model predicts 〈unk〉 at test time（e．g．，＂〈unk〉 and〈unk〉 have a blue car in 〈unk〉＂）．
－Can be postprocessed，but can we do better？

## Copy Mechanism

- Idea: Unknown target words likely to be copied from source sentence somewhere
- Example: translation (Gulcehre et al., 2016)

- Example: data-to-text generation (Wiseman et al., 2017)

| TEAM | WIN | LOSS | PTS |
| :---: | :---: | :---: | :---: |
| Heat | 11 | 12 | 103 |
| Hawk | 7 | 15 | 95 |

The Atlanta Hawks defeated the Miami Heat, 103-95, at Philips Arena on Wednesday...

- Approaches: Data pre-processing, attention-based
- Non-copy approaches
- Subword tokenization (e.g., BPE): No "unknown" words, but sequences longer and may also benefit from copy mechanism
- Scaling softmax to accommodate bigger $\mathcal{V}$ (e.g., hierarchical softmax, sampling-based methods)


## Data Pre－Processing Approach（Luong et al．，2015）

－Original data：Apply an unsupervised aligner to get alignments
－The ecotax portico in Pont－de－Buis
－Le portique écotaxe de Pont－de－Buis
－Conventional pre－processing

- The 〈unk〉 portico in 〈unk〉
- Le 〈unk〉 〈unk〉 de 〈unk〉
－Copyable Model pre－processing
－The $\langle\text { unk }\rangle_{1}$ portico in $\langle\text { unk }\rangle_{2}$
－Le $\langle u n k\rangle_{0}\langle u n k\rangle_{1}$ de $\langle u n k\rangle_{2}$
－Positional All Model pre－processing
－The $\langle u n k\rangle$ portico in 〈unk〉
－Le $p_{0}\langle$ unk $\rangle p_{-1}\langle\mathrm{unk}\rangle p_{1}$ de $p_{0}\langle\mathrm{unk}\rangle p_{-1}$
－Positional Unknown Model pre－processing
－The 〈unk〉 portico in 〈unk〉
－Le $\langle\text { unk }\rangle_{1}\langle\text { unk }\rangle_{-1}$ de $\langle u n k\rangle_{1}$


## Attention-Based Approaches

- Data pre-processing approach: Simple and effective (1-2 points improvement over strong NMT baselines)
- Limitations
- Requires an external word aligner in the pipeline
- Fixed-size window ( $\langle\mathrm{unk}\rangle_{-7} \ldots\langle\mathrm{unk}\rangle_{7}$ ), can't handle copy from far away in source sequence
- Idea: Make the model learn when and what to copy without supervision, by attention
- Pointer networks (Vinyals et al., 2015): Only what to copy
- CopyNet (Gu et al., 2016): Both when and what to copy, applied on summarization
- Concurrent work by Gulcehre et al., 2016: Different modeling details, applied on both translation and summarization
- When to copy: Modeled by a "switching network" (learned jointly)


## Conditional LM with a Copy Mechanism

- Single training example now consists of

$$
x=\left(x_{1} \ldots x_{T}\right) \quad y=\left(y_{1} \ldots y_{T^{\prime}}\right) \quad z=\left(z_{1} \ldots z_{T^{\prime}}\right)
$$

where $z_{t^{\prime}} \in\{0,1\}$ is 1 iff $y_{t^{\prime}}$ is copied from $x$

- Assume for now that $z$ is observed
- Just decide to set $z_{t^{\prime}}=1$ if $y_{t^{\prime}}$ appears in $x$ somewhere.
- Conditional LM with a copy mechanism

$$
p_{\theta}(y, z \mid x)=\prod_{t^{\prime}=1}^{T^{\prime}+1} p_{\theta}\left(y_{t^{\prime}}, z_{t^{\prime}} \mid x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)
$$

- Further decomposition by the chain rule

$$
p_{\theta}\left(y_{t}, z_{t^{\prime}} \mid x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)=\underbrace{p_{\theta}\left(z_{t^{\prime}} \mid x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)}_{\text {"switching network" }} \times p_{\theta}\left(y_{t^{\prime}} \mid x, y_{<t^{\prime}}, z_{\leq t^{\prime}}\right)
$$

## Parameterization

- Switching network

$$
\begin{aligned}
& p_{\theta}\left(1 \mid x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)=\sigma\left(f_{\theta}\left(x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)\right) \\
& p_{\theta}\left(0 \mid x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)=1-\sigma\left(f_{\theta}\left(x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)\right)
\end{aligned}
$$

$f_{\theta}\left(x, y_{<t^{\prime}}, z_{<t^{\prime}}\right) \in \mathbb{R}$ computed from current state (e.g., $h_{t}$ if RNN, current embedding if Transformer)

- If $z_{t^{\prime}}=1$, "dynamic LM" with vocab $\{w \in x\}$

$$
p_{\theta}\left(y_{t^{\prime}}=w \mid x, y_{<t^{\prime}}, z_{\leq t^{\prime}}\right)=\sum_{t=1: x_{t}=w}^{T} \underbrace{A_{t, t^{\prime}}^{\theta}}_{\text {attention from } t^{\prime} \text {-t target to } t \text {-th source }}
$$

- If $z_{t^{\prime}}=0, \operatorname{vocab} \mathcal{V}$

$$
p_{\theta}\left(y_{t^{\prime}}=w \mid x, y_{<t^{\prime}}, z_{\leq t^{\prime}}\right)=\underbrace{p_{\theta}\left(y_{t^{\prime}}=w \mid x, y_{<t^{\prime}}\right)}_{\text {usual next word probability }}
$$

## Supervised vs Unsupervised Loss

- Supervised training: Maximize $\log p_{\theta}(y, z \mid x)$ in training data
- Inference: At each step $t^{\prime}$, consider all

$$
\begin{array}{ll}
p_{\theta}\left(w, 1 \mid x, y_{<t^{\prime}}, z_{<t^{\prime}}\right) & \forall w \in \mathcal{V} \\
p_{\theta}\left(w, 0 \mid x, y_{<t^{\prime}}, z_{<t^{\prime}}\right) & \forall w \in x
\end{array}
$$

- Unsupervised training: Maximize $\log p_{\theta}(y \mid x)$ in training data

$$
\begin{aligned}
p_{\theta}\left(y_{t^{\prime}} \mid x, y_{<t^{\prime}}\right) & =\sum_{z \in\{0,1\}} p_{\theta}\left(y_{t^{\prime}}, z \mid x, y_{<t^{\prime}}\right) \\
& =\sigma\left(f_{\theta}\left(x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)\right)\left(\sum_{t=1: x_{t}=y_{t^{\prime}}}^{T} A_{t, t^{\prime}}^{\theta}\right)+ \\
& \left(1-\sigma\left(f_{\theta}\left(x, y_{<t^{\prime}}, z_{<t^{\prime}}\right)\right)\right) p_{\theta}\left(y_{t^{\prime}}=w \mid x, y_{<t^{\prime}}\right)
\end{aligned}
$$

Switching network $f_{\theta}$ trained without supervision, inference remains the same

## Illustration



Image credit: See et al. (2017)

## Self-Attention as a Fully Connected Directed Graph

- Self-attention viewed as a fully connected directed graph
- Natural generalization: Incorporate edge types in the model

- Example edge types: Relative positions, relation between table cells (e.g., cell-column, cell-row)


## Relation-Aware Self-Attention (Shaw et al., 2018)

- Extra parameters in the multi-head attention module
- $b_{\tau}^{K} \in \mathbb{R}^{d / H}$ for every relation type $\tau$
- $b_{\tau}^{V} \in \mathbb{R}^{d / H}$ for every relation type $\tau$
- Self-attention weight from $x_{t^{\prime}}$ to $x_{t}$ with relation $\tau_{t^{\prime}, t}$ under head $h$

$$
l_{t^{\prime}, t}^{h}=\frac{q_{t^{\prime}}^{h} \cdot\left(k_{t}^{h}+b_{\tau_{t^{\prime}, t}}^{K}\right)}{d / H}
$$

Probabilities: $\left(\alpha_{t^{\prime}, 1}^{h} \ldots \alpha_{t^{\prime}, T}^{h}\right)=\operatorname{softmax}\left(l_{t^{\prime}, 1}^{h} \ldots l_{t^{\prime}, T}^{h}\right)$

- Answer value

$$
a_{t^{\prime}}^{h}=\sum_{t=1}^{T} \alpha_{t, t^{\prime}}^{h}\left(v_{t}^{h}+b_{\tau_{t^{\prime}, t}}^{V}\right)
$$

- Relation bias is shared across all heads. Efficient batch computation still possible by construction


## Applications of Relation-Aware Self-Attention

- Relative position encoding (Shaw et al., 2018)
- Original Transformer: Add constant (or learnable) absolute position embeddings at input vectors
- Now: For some $k$ (e.g., $k=8$ ), use $2 k+1$ relation types representing local distances
- Tokens beyond window clipped to $k$ or $-k$
- Can entirely replace additive position embeddings, even modest improvement
- Value bias $b_{\tau}^{V}$ found unnecessary given key bias $b_{\tau}^{T}$ (for MT)
- Relation between tokens in structured input (Müller et al., 2019)
- Task: question answering from a table (represented as a flat sequence of words)
- Idea: Distinguish relations between table cells, row header, column header, question, etc.



## Sequence Labeling/Tagging

- Switching gears, we'll consider the sequence labeling (aka. tagging) problem.
- Task: Given sentence $x_{1} \ldots x_{T} \in \mathcal{V}$, output a correct label sequence $y_{1} \ldots y_{T} \in \mathcal{Y}$
- Many applications: part-of-speech tagging, named-entity recognition
- This is a structured prediction problem: Output space is $\mathcal{Y}^{T}$ possible label sequences
- Why not just frame it as seq2seq?
- Seq2seq needs a lot of data, and is typically very challenging to train well (lots of engineering efforts)
- In contrast, we can exploit conditional independence assumptions to derive exact and effective algorithms
- In tagging, exact inference called "Viterbi", exact marginalization called "forward". Both dynamic programming


## Example: Part-Of-Speech (POS) Tagging

- Task. Given a sentence, output a sequence of POS tags.
- Ambiguity. A word can have many possible POS tags.

$$
\begin{aligned}
& \text { the/DT man/NN saw/VBD the/DT cut/NN } \\
& \text { the/DT saw/NN cut/VBD the/DT man/NN }
\end{aligned}
$$

- Evaluation. Per-position accuracy (can consider others, like sentence-level accuracy)
- Definition of POS tags in Penn Treebank (English)


Other definitions: universal tagset (12 tags, language agnostic)

## Example: Named-Entity Recognition (NER)

- Task. Given a sentence, identify and label all spans that are "named entities"

- Reduction to tagging. "Linearize" labeled spans into a label sequence using "BIO" scheme

```
John/B-PER Smith/I-PER works/O at/O New/B-ORG
York/I-ORG Times/I-ORG
```

Number of tagging labels: $2 \times$ number of entity types +1

| West | B-MISC |  |
| :--- | :--- | :--- |
| Indian | I-MISC |  |
| all-rounder | 0 |  |
| Phil | B-PER |  |
| Simmons | I-PER |  |
| took | 0 |  |
| four | 0 |  |
| for | 0 |  |
| 38 | 0 |  |
| on | 0 |  |
| Friday | 0 |  |
| as | 0 |  |
| Leicestershire | B-ORG |  |
| beat $\quad 0$ |  |  |
| Somerset <br> by$\quad 0$ | B-ORG |  |

CoNLL 2003 dataset, 4 entity
types (PER, ORG, LOC, MISC)

## NER Evaluation

- Most words are tagged as O (not an entity), so accuracy is meaningless (vacuously high by predicting O always)
- Better metric: precision/recall/F1
- Per-entity F1 score (harmonic mean of precision and recall)

$$
\begin{aligned}
F_{1}(e) & =\frac{2 p(e) r(e)}{p(e)+r(e)} \\
p(e) & =\frac{t p(e)}{t p(e)+f p(e)} \times 100 \quad r(e)=\frac{t p(e)}{t p(e)+f n(e)} \times 100
\end{aligned}
$$

- Global F1 score: Single performance number

$$
\begin{aligned}
F_{1} & =\frac{2 p r}{p+r} \\
p & =\frac{t p}{t p+f p} \times 100 \quad r=\frac{t p}{t p+f n} \times 100
\end{aligned}
$$

## Generative Probabilistic Tagger

- Model defines a joint distribution $p_{\theta}\left(x_{1} \ldots x_{T}, y_{1} \ldots y_{T}\right)$ over any pairs of sentence and a label sequence.
- Can generate $x_{1} \ldots x_{T}$, although we will not use the tagger for generation
- By the chain rule

$$
\begin{aligned}
& p_{\theta}\left(x_{1} \ldots x_{T}, y_{1} \ldots y_{T}\right) \\
& =p_{\theta}\left(y_{1} \mid y_{0}\right) \times p_{\theta}\left(x_{1} \mid y_{0} y_{1}\right) \times p_{\theta}\left(y_{2} \mid x_{1}, y_{0} y_{1}\right) \times p_{\theta}\left(x_{2} \mid x_{1}, y_{0} y_{1} y_{2}\right) \\
& \cdots \times p_{\theta}\left(y_{T} \mid x_{<T}, y_{<T}\right) \times p_{\theta}\left(x_{T} \mid x_{<T}, y_{\leq T}\right) \times p_{\theta}\left(y_{*} \mid x_{\leq T}, y_{\leq T}\right)
\end{aligned}
$$

Thus only need to model transition probabilities $p_{\theta}\left(y_{t} \mid x_{<t}, y_{<t}\right)$ and emission probabilities $p_{\theta}\left(x_{t} \mid x_{<t}, y_{\leq t}\right)$


## Marginalization and Inference

- Two central calculations in structured prediction
- Marginalization. What is the marginal probability of $x_{1} \ldots x_{T}$ under the model?

$$
\sum_{y_{1} \ldots y_{T} \in \mathcal{Y}^{T}} p_{\theta}\left(x_{1} \ldots x_{T}, y_{1} \ldots y_{T}\right)
$$

- Inference. Given $x_{1} \ldots x_{T}$, what is the most probable $y_{1} \ldots y_{T} \in \mathcal{Y}^{T}$ under the model?

$$
\begin{aligned}
& \underset{y_{1} \ldots y_{T} \in \mathcal{Y}^{T}}{\arg \max } p_{\theta}\left(y_{1} \ldots y_{T} \mid x_{1} \ldots x_{T}\right) \\
& =\underset{y_{1} \ldots y_{T} \in \mathcal{Y}^{T}}{\arg \max } p_{\theta}\left(x_{1} \ldots x_{T}, y_{1} \ldots y_{T}\right)
\end{aligned}
$$

- Generally intractable, that is we must exhaustively enumerate $|\mathcal{Y}|^{T}$ tag sequences (exponential in length).


## (First-Order) Markov Assumption

- We define the model as

$$
\begin{aligned}
& p_{\theta}\left(y_{t} \mid x_{<t}, y_{<t}\right)=p_{\theta}\left(y_{t} \mid x_{<t}, y_{t-1}\right) \\
& p_{\theta}\left(x_{t} \mid x_{<t}, y_{\leq t}\right)=p_{\theta}\left(x_{t} \mid x_{<t}, y_{t}\right)
\end{aligned}
$$

- Transition probability: Current label conditionally independent of all past labels given only previous label
- Emission probability: Current word conditionally independent of all past labels given only current label

- Is this a reasonable assumption for tagging? (Note that even if the assumption is false we can still use this model on any data.)
- But now marginalization and inference can be done exactly in time linear (rather than exponential) in sequence length.


## Forward Algorithm for Exact Marginalization

- Now no need to consider all $|\mathcal{Y}|^{T}$ candidates because of the Markov assumptions
- This is a dynamic programming (DP) algorithm. Given $x_{1} \ldots x_{T}$, the DP table we fill out is $\pi \in \mathbb{R}^{T \times|\mathcal{Y}|}$ where

$$
\pi(t, y)=\sum_{y_{1} \ldots y_{t} \in \mathcal{Y}^{t}: y_{t}=y} p_{\theta}\left(x_{1} \ldots x_{t}, y_{1} \ldots y_{t}\right)
$$

- Output $\sum_{y \in \mathcal{Y}} \pi(T, y) \times p_{\theta}\left(y_{*} \mid x_{\leq T}, y\right)$ as the marginal probability of $x_{1} \ldots x_{T}$
- We will see that computing each $\pi(t, y)$ will only take $O(|\mathcal{Y}|)$ time, hence the total runtime is $O\left(T|\mathcal{Y}|^{2}\right)$.
- Base case is easy: Compute for all $y \in \mathcal{Y}$

$$
\pi(1, y)=p_{\theta}\left(y \mid y_{0}\right) \times p_{\theta}\left(x_{1} \mid y\right)
$$

## Forward Algorithm: Main Body $(t>1)$

$$
\begin{aligned}
\pi\left(t, y^{\prime}\right) & =\sum_{y_{\leq t}: y_{t}=y^{\prime}} p_{\theta}\left(x_{\leq t}, y_{\leq t}\right) \\
& =\sum_{y<t} p_{\theta}\left(x_{\leq t}, y_{<t} y^{\prime}\right) \\
& =\sum_{y<t} p_{\theta}\left(x_{<t}, y_{<t}\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y_{<t}\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y_{<t}, y^{\prime}\right)
\end{aligned}
$$

## Forward Algorithm: Main Body $(t>1)$

$$
\begin{aligned}
\pi\left(t, y^{\prime}\right) & =\sum_{y_{\leq t}: y_{t}=y^{\prime}} p_{\theta}\left(x_{\leq t}, y_{\leq t}\right) \\
& =\sum_{y<t} p_{\theta}\left(x_{\leq t}, y_{<t} y^{\prime}\right) \\
& =\sum_{y<t} p_{\theta}\left(x_{<t}, y_{<t}\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y_{<t}\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y_{<t}, y^{\prime}\right) \\
& \stackrel{*}{=} \sum_{y<t} p_{\theta}\left(x_{<t}, y_{<t}\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y_{t-1}\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right)
\end{aligned}
$$

## Forward Algorithm: Main Body $(t>1)$

$$
\begin{aligned}
\pi\left(t, y^{\prime}\right) & =\sum_{y_{\leq t}: y_{t}=y^{\prime}} p_{\theta}\left(x_{\leq t}, y_{\leq t}\right) \\
& =\sum_{y<t} p_{\theta}\left(x_{\leq t}, y_{<t} y^{\prime}\right) \\
& =\sum_{y<t} p_{\theta}\left(x_{<t}, y_{<t}\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y_{<t}\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y_{<t}, y^{\prime}\right) \\
& \stackrel{*}{=} \sum_{y<t} p_{\theta}\left(x_{<t}, y_{<t}\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y_{t-1}\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right) \\
& =\sum_{y} \sum_{y<t-1} p_{\theta}\left(x_{<t}, y_{<t-1} y\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right)
\end{aligned}
$$

## Forward Algorithm: Main Body $(t>1)$

$$
\begin{aligned}
\pi\left(t, y^{\prime}\right) & =\sum_{y_{\leq t}: y_{t}=y^{\prime}} p_{\theta}\left(x_{\leq t}, y_{\leq t}\right) \\
& =\sum_{y_{<t}} p_{\theta}\left(x_{\leq t}, y_{<t} y^{\prime}\right) \\
& =\sum_{y<t} p_{\theta}\left(x_{<t}, y_{<t}\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y_{<t}\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y_{<t}, y^{\prime}\right) \\
& \stackrel{*}{=} \sum_{y<t} p_{\theta}\left(x_{<t}, y_{<t}\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y_{t-1}\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right) \\
& =\sum_{y} \sum_{y<t-1} p_{\theta}\left(x_{<t}, y_{<t-1} y\right) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right) \\
& =\sum_{y} \underbrace{\pi(t-1, y)}_{\text {already computed }} \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right)
\end{aligned}
$$

## Viterbi Algorithm for Exact Inference

- Same idea: No need to consider all $|\mathcal{Y}|^{T}$ candidates because of the Markov assumptions
- Given $x_{1} \ldots x_{T}$, the DP table we fill out is $\pi \in \mathbb{R}^{T \times|\mathcal{Y}|}$ where

$$
\pi(t, y)=\max _{y_{1} \ldots y_{t} \in \mathcal{Y}^{t}: y_{t}=y} p_{\theta}\left(x_{1} \ldots x_{t}, y_{1} \ldots y_{t}\right)
$$

- Exactly the same as forward if we switch sum with max

$$
\begin{aligned}
\pi(1, y) & =p_{\theta}\left(y \mid y_{0}\right) \times p_{\theta}\left(x_{1} \mid y\right) \\
\pi\left(t, y^{\prime}\right) & =\max _{y} \pi(t-1, y) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right)
\end{aligned}
$$

- But this only gives us the joint probability of $x_{1} \ldots x_{T}$ and its most likely tag sequence. How do we extract the actual tag sequence?


## Backtracking for Viterbi

- Keep an additional chart to record the path:

$$
\beta\left(t, y^{\prime}\right)=\underset{y \in \mathcal{Y}}{\arg \max } \pi(t-1, y) \times p_{\theta}\left(y^{\prime} \mid x_{<t}, y\right) \times p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right)
$$

for $t=2 \ldots T$.

- After running Viterbi, we can "backtrack"

$$
\begin{gathered}
y_{T}^{*}=\underset{y \in \mathcal{Y}}{\arg \max } \pi(T, y) \times p_{\theta}\left(y_{*} \mid x_{\leq T}, y\right) \\
y_{T-1}^{*}=\beta\left(T, y_{T}^{*}\right) \\
\vdots \\
y_{1}^{*}=\beta\left(2, y_{2}^{*}\right)
\end{gathered}
$$

$$
\text { and return } y_{1}^{*} \ldots y_{T}^{*}
$$

## Other Details

- In practice, we always operate in log space for numerical stability. The DP tables will store log probabilities, e.g., in forward

$$
\begin{aligned}
\pi(1, y)=\log p_{\theta}\left(y \mid y_{0}\right) & +\log p_{\theta}\left(x_{1} \mid y\right) \\
\pi\left(t, y^{\prime}\right)=\underset{y}{\operatorname{logsumexp}}( & \left(\pi(t-1, y)+\log p_{\theta}\left(y^{\prime} \mid x_{<t}, y\right)\right. \\
& \left.+\log p_{\theta}\left(x_{t} \mid x_{<t}, y^{\prime}\right)\right)
\end{aligned}
$$

where $\operatorname{logsumexp}_{y} f(y)=\log \sum_{y} \exp (f(y))$ is the usual numerically stable calculation for log space

- Debugging. Debugging is crucial, the first DP implementation is almost certainly incorrect.
- Construct a small model randomly (e.g., with $|\mathcal{Y}|=5$ )
- Generate a short sequence (e.g., $x_{1} \ldots x_{7}$ ) and compute marginalization and inference exactly by brute-force
- Check if the output of forward/Viterbi matches with brute-force


## The Hidden Markov Model

- Further Markov assumption on observation generation yields hidden Markov model (HMM)

$$
\begin{aligned}
& p_{\theta}\left(y_{t} \mid x_{<t}, y_{<t}\right)=t_{\theta}\left(y_{t} \mid y_{t-1}\right) \\
& p_{\theta}\left(x_{t} \mid x_{<t}, y_{\leq t}\right)=o_{\theta}\left(x_{t} \mid y_{t}\right)
\end{aligned}
$$

- Simplest form of labeled sequence generation


$$
p_{\theta}\left(x_{1} \ldots x_{T}, y_{1} \ldots y_{T}\right)=\prod_{t=1}^{T} \underbrace{t_{\theta}\left(y_{t} \mid y_{t-1}\right)}_{\text {transition prob }} \times \underbrace{o_{\theta}\left(x_{t} \mid y_{t}\right)}_{\text {emission prob }} \times t_{\theta}\left(y_{*} \mid y_{T}\right)
$$

- Central model in NLP and machine learning: Tagging English text with a probabilistic model (Merialdo, 1994)
- Underlying tag sequence often unobserved (hence "hidden")


## Forward Algorithm for HMMs in Matrix Form

- Organize HMM probabilities in matrix form
- Emission matrix: $O \in \mathbb{R}^{|\mathcal{V}| \times|\mathcal{Y}|}$ where $O_{x, y}=o_{\theta}(x \mid y)$
- Transition matrix: $T \in \mathbb{R}^{|\mathcal{Y}| \times|\mathcal{Y}|}$ where $T_{y^{\prime}, y}=t_{\theta}\left(y^{\prime} \mid y\right)$
- Forward algorithm

$$
p_{\theta}\left(x_{1} \ldots x_{T}\right)=\underbrace{\tau_{\infty}^{\top}}_{1 \times|\mathcal{Y}|} \underbrace{\operatorname{diag}\left(O_{x_{T}}\right)}_{|\mathcal{Y}| \times|\mathcal{Y}|} \underbrace{T}_{|\mathcal{Y}| \times|\mathcal{Y}|} \cdots \underbrace{\operatorname{diag}\left(O_{x_{1}}\right)}_{|\mathcal{Y}| \times|\mathcal{Y}|} \underbrace{\tau_{0}}_{|\mathcal{Y}| \times 1}
$$

$O_{x} \in \mathbb{R}^{|\mathcal{Y}|}$ is row $x$ of $O,\left[\tau_{0}\right]_{y}=t_{\theta}\left(y \mid y_{0}\right),\left[\tau_{\infty}\right]_{y}=t_{\theta}\left(y_{*} \mid y\right)$

- Compact/insightful view of stepwise marginalization in dynamic programming as matrix-matrix product

$$
\sum_{y \in \mathcal{Y}} \pi(t-1, y) \times t_{\theta}\left(y^{\prime} \mid y\right) \times o_{\theta}\left(x_{t} \mid y^{\prime}\right)
$$

## Learning HMMs

- Supervised. If $y_{1} \ldots y_{T}$ observed, just maximize

$$
\log p_{\theta}\left(x_{1} \ldots x_{T}, y_{1} \ldots y_{T}\right)=\sum_{t=1}^{T} \log t_{\theta}\left(y_{t} \mid y_{t-1}\right)+\log o_{\theta}\left(x_{t} \mid y_{t}\right)
$$

Pre-neural: Parameters are raw probabilities, closed-form MLE by constrained optimization

$$
t\left(y^{\prime} \mid y\right)=\frac{\operatorname{count}\left(y, y^{\prime}\right)}{\sum_{y^{\prime} \in \mathcal{Y}} \operatorname{count}\left(y, y^{\prime}\right)} \quad o(x \mid y)=\frac{\operatorname{count}(x, y)}{\sum_{x \in \mathcal{V}} \operatorname{count}(x, y)}
$$

(i.e., "training" means counting word/tag bigrams off of labeled sequences). If parametric, can do gradient ascent

- Unsupervised. If $y_{1} \ldots y_{T}$ unobserved, can still maximize marginal probability of $x_{1} \ldots x_{T}$

$$
\log p_{\theta}\left(x_{1} \ldots x_{T}\right)=\log \underbrace{\sum_{y_{1} \ldots y_{T}} p_{\theta}\left(x_{1} \ldots x_{T}, y_{1} \ldots y_{T}\right)}_{\text {computable with forward alg. }}
$$

