Scaling Hidden Markov Models

April 28, 2021

Latent Variables Models in NLP

- ▶ NLP benchmarks are dominated by fully observed models
 - Transformers
 - Previously, Recurrent Neural Networks

We instead explore latent variable models

Latent Variable Models: Motivation

- ▶ LVMs posit a generative process involving unseen variables
- Maintain uncertainty over latent representations, rather than just output correlations

- Often improves interpretability and controllability
- ▶ Bottlenecked by the computational complexity of inference

Research Question

To what extent is the performance of tractable latent variable models limited by scale and choices in parameterization?

This work: Scale hidden Markov models (HMMs) on language modeling using techniques drawn from recent advances in neural networks

Language Modeling

How now, brown _____

- Given the words seen so far, predict the next word
- ► Language requires modeling long-range phenomena

Hidden Markov Models in NLP

► Simplest latent variable models for time series data

- Are thought to be very poor language models
- We show they are better than previously thought, once scaled

Background: Hidden Markov Models

Hidden Markov Models (HMMs)

- Classical models for unsupervised per-word tag induction
 - Part-of-speech induction
 - Word alignment for translation
- Admits tractable exact inference
 - Strong conditional independence assumptions
 - Finite set of discrete latent states

Hidden Markov Models (HMMs)

For times t, model states $z_t \in [Z]$, and tokens $x_t \in [X]$,



This yields the joint distribution

$$p(x,z) = \prod_{t} p(x_t \mid z_t) p(z_t \mid z_{t-1})$$

with

start state
$$p(z_1),$$
 transitions $p(z_t \mid z_{t-1}),$ and emissions $p(x_t \mid z_t)$

represented as vectors and matrices

Inference

Given observed $x = (x_1, \dots, x_T)$ We wish to maximize

$$p(x) = \sum_{z_1} \cdots \sum_{z_T} p(x, z) = \alpha_1^\top \Lambda_2 \Lambda_3 \cdots \Lambda_T \mathbf{1},$$

where we have the

start,
$$[\alpha_1]_{z_1} = p(x_1 \mid z_1)p(z_1),$$
 and transition operators,
$$[\Lambda_t]_{z_{t-1},z_t} = p(x_t \mid z_t)p(z_t \mid z_{t-1})$$

The result of each matvec gives the alphas of the forward algorithm, i.e. $\alpha_3 = \alpha_1 \Lambda_2 \Lambda_3$ has entries corresponding to $p(z_3, x_{1:3})$

Requires $O(TZ^2)$ operations in total!

Inference

$$p(x) = \alpha_1^{\top} \Lambda_2 \cdots \Lambda_T \mathbf{1}$$



- ► Each node corresponds to a state
- Each edge to an entry in the transition operator matrix

Scaling HMMs

Lessons from Large Neural Language Models

Large models perform better but are ...

1. Slow to train

2. Prone to overfitting

We must overcome these issues when scaling HMMs

3 Techniques for Training Large HMMs

- Compact neural parameterization
 - **†** Generalization
- State dropout
 - **↑** Speed **↑** Generalization
- ▶ Block-sparse emission constraints
 - **♦** Speed
- ▶ Will cover a fourth in the second part of this talk

Technique 1: Neural Parameterization

▶ The transition and emission matrices have Z^2 and ZX entries

 Causes the number of parameters to explode as the state size increases

We instead use a low-dimensional decomposition of all conditional distributions that greatly reduces the number of parameters

Neural Parameterization: Softmax

For both the transition and emission matrices, we use a softmax parameterization, which assumes a nonlinear D-dimensional decomposition

with embeddings $U \in \mathbb{R}^{Z \times D}$, $V \in \mathbb{R}^{Z \times D}$ or $\mathbb{R}^{X \times D}$

▶ Can further parameterize U or $V = MLP(E_u)$

Technique 2: State Dropout

 Dropout is a common technique for regularizing neural networks

- Reduces a network's reliance on a particular neuron
- Extend dropout to the states of an HMM
 - ► Encourage broad utilization of all states

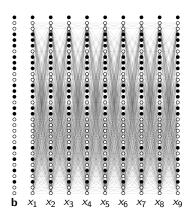
State Dropout

- ightharpoonup At each batch, sample dropout mask $\mathbf{b} \in \{0,1\}^Z$
- Compute distributional parameters by indexing into embeddings U, V

$$\left(\mathbf{b} \circ \boxed{U_{\mathsf{trans}}} \right) imes \left(\mathbf{b} \circ \boxed{V_{\mathsf{trans}}} \right)^{ op} \left(\mathbf{b} \circ \boxed{U_{\mathsf{emit}}} \right) imes \boxed{V_{\mathsf{emit}}}^{ op}$$

(a) Unnormalized transition logits (b) Unnormalized emission logits

State Dropout: Inference



- Shaded nodes depict dropped states
- Ignore dropped states during inference

Technique 3: Block-Sparse Emission Constraints

Reduce cost of marginalization by enforcing structure

Only allow each word to be emit by a subset of states

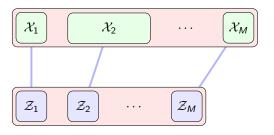
 Cost of inference is quadratic in the size of the largest subset due to sparsity

(maybe show how this affects Λ_t ? ie multiply masked emission column with A)

Block-Sparse Emission Constraints: Alignment

Start with a joint partitioning of both states and wards

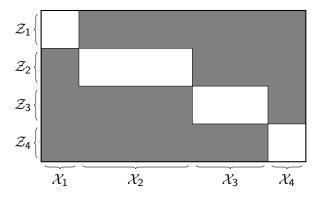
Indices $m \in [M]$ State partitions \mathcal{Z}_m Word partitions \mathcal{X}_m



Block-Sparse Emission Constraints

Given the unnormalized emission logits,

- Mask out unaligned state-word entries
- Normalize rows across words in aligned partition



Block-Sparse Emissions: Inference

Given each word x_t , only the states in the correct group can occur



Method Recap

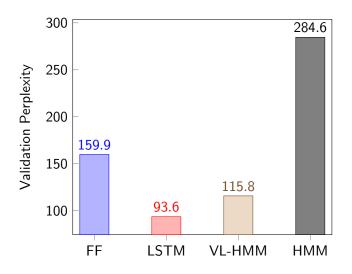
- Compact neural parameterization
 - **Generalization**
- State dropout
 - **↑** Speed **↑** Generalization
- ▶ Block-sparse emission constraints
 - **♦** Speed
- ► A fourth after experiments



Experiments

- Language modeling on Penn Treebank
- Baselines
 - Feedforward 5-gram model
 - 2-layer LSTM
 - A 900 state HMM (Buys et al 2018)
- Model
 - ▶ 2¹⁵ (32k) state very large HMM (VL-HMM)
 - M = 128 groups (256 states per type), obtained via Brown Clustering
 - Dropout rate of 0.5 during training

Results on PTB Validation Data



State Size Ablation



Validation perplexity on PTB by state size ($\lambda = 0.5$ and M = 128)

Other Ablations

Model	Param	Train	Val
VL-HMM (2 ¹⁴)	7.2M	115	134
- neural param	423M	119	169
- state dropout	7.2M	88	157

Discussion

Greatly scaled the state size of HMMs

Performance improved with increasing state size

- Still a large gap between RNNs and HMMs
- ▶ Does the emission sparsity constraint improve computation complexity at the price of accuracy?

Speeding up HMMs with Low-Rank

Decompositions

Fast Inference with Low-Rank Decompositions

► The previous approach relied a pre-specified emission sparsity constraint

► Can we scale inference with a weaker constraint?

Exploit structure in the transition matrix to speed up inference

Inference

Start by unpacking inference to reveal the most expensive step

$$p(x) = \alpha_1^{\top} \Lambda_2 \Lambda_3 \cdots \Lambda_T \mathbf{1}$$

with

start,
$$[\alpha_1]_{z_1} = p(x_1 \mid z_1)p(z_1),$$
 and transition operators,
$$[\Lambda_t]_{z_{t-1},z_t} = p(x_t \mid z_t)p(z_t \mid z_{t-1})$$

Inference

Decompose transition operators into transition matrix A and emission matrix O

$$\begin{aligned} p(x) &= \alpha_1^\top \Lambda_2 \cdot \Lambda_T \mathbf{1} \\ &= \alpha_1^\top (A \operatorname{diag}([O]_{\cdot, x_2})) \cdots \Lambda_T \mathbf{1} \\ &= \alpha_1^\top A \operatorname{diag}([O]_{\cdot, x_2}) \cdots A \operatorname{diag}([O]_{\cdot, x_T}) \mathbf{1} \end{aligned}$$

where the most expensive steps are the matrix-vector products $\alpha_t^{\top} A$, which take $O(Z^2)$ computation

Fast Matrix-Vector Products

- ▶ Goal is to reduce the naive matvec complexity of $O(Z^2)$
- Various methods
 - Sparsity (nnz entries)
 - ► Fast Fourier Transform (Z log Z)
 - ► Low-Rank decomposition (ZR)

► We utilize low-rank decompositions

Low-Rank Factorization

Factor transition matrix $A \in [0,1]Z \times Z$ into product of matrices $U, V \in \mathbb{R}^{Z \times R}$

$$\boxed{\alpha^\top} \times \boxed{A} = \boxed{\alpha^\top} \times \boxed{U} \times \boxed{V^\top}$$

resulting in two matrix-vector products of cost O(ZR) each

- ► Constraint: Entries of A must be nonnegative
- Solution: Use a nonnegative matrix factorization (NMF)

$$A = \phi(U)\phi(V)^{\top},$$

with
$$\phi: \mathbb{R}^{\textit{Z} \times \textit{R}} \rightarrow \mathbb{R}_{+}^{\textit{Z} \times \textit{R}}$$

Method Recap

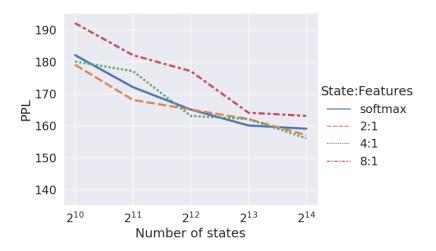
- ▶ Target key $O(Z^2)$ matvec step in inference
- ▶ Use NMF to reduce cost to O(ZR)
- ▶ How small can R be relative to Z without sacrificing accuracy?



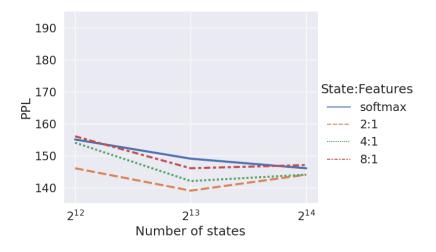
Experiments

- ► Language modeling on PTB
- ▶ Feature map $\phi(U) = \exp(UW)$, with learned $W \in \mathbb{R}^{R \times R}$
- ► No sparsity constraints

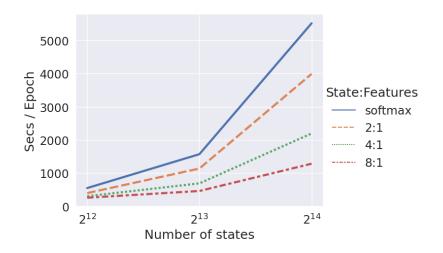
Scaling on PTB (Validation)



Further Scaling on PTB with Dropout (Validation)



Speed Comparison



Conclusion (TODO)

- ▶ Hopeful that HMMs can be competitive language models
- Introduced 4 techniques for tackling speed and overfitting
- Future work will extend to other discrete latent variable models

EOS

Citations

Generalized Softmax

Softmax

$$p(z_t \mid z_{t-1}) = \frac{\exp(\mathbf{u}_{z_{t-1}}^{\top} \mathbf{v}_{z_t})}{\sum_{z} \exp(\mathbf{u}_{z_{t-1}}^{\top} \mathbf{v}_{z})}$$

Generalized Softmax

$$p(z_t \mid z_{t-1}) = \frac{K(\mathbf{u}, \mathbf{v})}{\sum_z K(\mathbf{u}, \mathbf{v}_z)} = \frac{\phi(\mathbf{u})^\top \phi(\mathbf{v})}{\sum_z \phi(\mathbf{u})^\top \phi(\mathbf{v}_z)},$$

for positive kernel $K: \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}_+$ and feature map $\phi: \mathbb{R}^D \to \mathbb{R}^R$

Generalized Softmax: Inference

▶ The key $O(Z^2)$ step in the forward algorithm:

$$p(z_t \mid x_{< t}) = \sum_{z_{t-1}} p(z_t \mid z_{t-1}) p(z_{t-1} \mid x_{< t})$$

In matrix form,

$$oldsymbol{\gamma}_t = \underbrace{lpha_{t-1}}_{\mathbb{R}^Z} \underbrace{igwedge_{\mathbb{R}^{Z imes Z}}}_{\mathbb{R}^{Z imes Z}},$$

where we have the probability of the

current state,
$$[\gamma_t]_{z_t} = p(z_t \mid x_{< t}),$$
 last state,
$$[\alpha_{t-1}]_{z_{t-1}} = p(z_{t-1} \mid x_{< t}),$$
 transition probability,
$$[\Lambda]_{z_{t-1},z_t} = p(z_t \mid z_{t-1})$$

Generalized Softmax: Inference

Use generalized softmax in transition distribution

$$[\Lambda]_{z_{t-1},z_t} = \rho(z_t \mid z_{t-1}) \propto \phi(\mathbf{u}_{z_{t-1}})^\top \phi(\mathbf{v}_{z_t})$$

► Allows us to apply associative property of matrix multiplication

$$\begin{split} \gamma_t &= \alpha_{t-1} \Lambda \\ &= \alpha_{t-1} (\operatorname{diag}(d) \phi(U) \phi(V)^\top) \\ &= \underbrace{(\alpha_{t-1} \circ d)}_{\mathbb{R}^Z} \underbrace{\phi(U)}_{\mathbb{R}^{Z \times f}} \underbrace{\phi(V)}_{\mathbb{R}^{f \times Z}}^\top, \end{split}$$

with stacked embeddings $\phi(U), \phi(V) = [\phi(\mathbf{v}_1), \dots, \phi(\mathbf{v}_Z)]$ and normalizing constants d

► Takes *O*(*Zf*) time from left to right!