# Recurrent Neural Networks and State Space Models

## Lecture 4

Konstantin Yakovlev [1]

[1]MIPT
Moscow, Russia

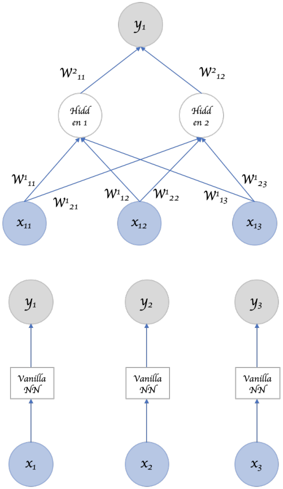
MIPT 2024

# Recap

- Weight initialisation
  - Zero
  - Random
  - Xavier
- Batch Normalization
  - Layer norm
  - Instance norm
  - Group norm
- Convolutions
  - Forward
  - Backward
  - Parameters

# Motivation

**Input**: a sequence of arbitrary length
**Output**: a sequence of arbitrary length
**Proposition**: MLP or CNN will not allow you to get a scalar output given an arbitrary sequence.



# RNN for language modeling

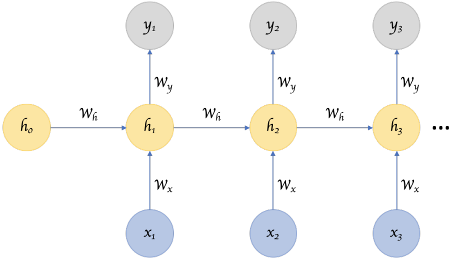
The probability of a sequence of a sequence of $T$ words $(w_1, \dots w_T)$:

$$p(w_1, \dots, w_T) = \prod_{t=1}^{T} p(w_t | w_{<t}),$$

**Notation**

- $\mathbf{x}_t \in \mathbb{R}^d$ input word vector at timestep $t$.
- $\mathbf{W}_x \in \mathbb{R}^{D_h \times d}$ weights matrix used to condition the input word vector $\mathbf{x}_t$.
- $\mathbf{W}_h \in \mathbb{R}^{D_h \times D_h}$ weights matrix used to condition the output of the previous time-step $\mathbf{h}_{t-1}$.
- $\mathbf{h}_{t-1}$ output of the non-linear function at the previous time-step $t - 1$.
- $\sigma(.)$ activation function.
- $y_t = \mathrm{softmax}(\mathbf{W}_y \mathbf{h}_t + \mathbf{b}_y)$ the output probability distribution over the vocabulary; $\mathbf{W}_y \in \mathbb{R}^{|V| \times D_h}$, $\mathbf{b}_y \in \mathbb{R}^{|V|}$.

# Recurrent Neural Network (RNN)



## Architecture

$$
\begin{aligned}
\mathbf{h}_t &= \sigma(\mathbf{W}_x\mathbf{x}_t + \mathbf{W}_h\mathbf{h}_{t-1} + \mathbf{b}_h) \\
\mathbf{z}_t &:= \mathbf{W}_x\mathbf{x}_t + \mathbf{W}_h\mathbf{h}_{t-1} + \mathbf{b}_h \\
\mathbf{h}_t &= \sigma(\mathbf{z}_t) \\
\mathbf{y}_t &= \mathrm{softmax}(\mathbf{W}_y\mathbf{h}_t + \mathbf{b}_y)
\end{aligned}
$$

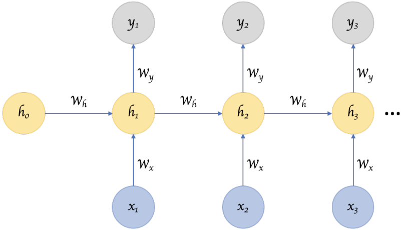
## Criterion

$$
\mathcal{L}(\mathbf{W}, \mathbf{b}) := -\mathbb{E}_{\mathbf{x}} \sum_{t=1}^{T} \underbrace{\sum_{j=1}^{|V|} \mathbb{I}[y_{t,j} = w_t] \log y_{t,j}}_{\mathcal{L}_t(\mathbf{x}_{<t},\mathbf{W},\mathbf{b})} \to \min_{\mathbf{W},\mathbf{b}}
$$

## Problem

$$
\nabla_{\mathbf{W}_h}\mathcal{L} = ?
$$

# RNN backpropagation



**Deriving a gradient w.r.t. $\mathbf{W}_h$**

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_h} = \sum_{t=1}^{T} \frac{\partial \mathcal{L}_t}{\partial \mathbf{W}_h} = \sum_{t=1}^{T} \sum_{k=1}^{t} \frac{\partial \mathcal{L}_t}{\partial \mathbf{h}_t} \frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_k} \frac{\partial \mathbf{h}_k}{\partial \mathbf{W}_h} =$$

$$= \sum_{t=1}^{T} \sum_{k=1}^{t} \frac{\partial \mathcal{L}_t}{\partial \mathbf{h}_t} \left( \prod_{j=k+1}^{t} \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right) \frac{\partial \mathbf{h}_k}{\partial \mathbf{W}_h}.$$

**Vanishing/Exploding gradients**

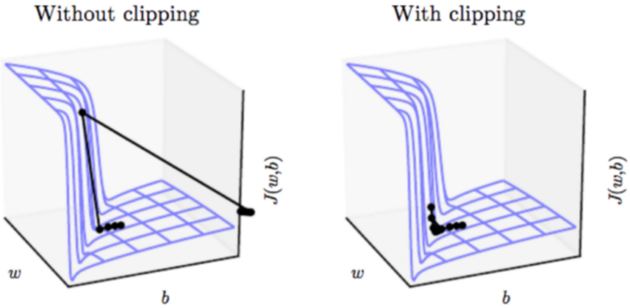
$$\|\frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}}\| \leq \|\mathbf{W}_h\| \cdot \|\mathrm{diag}(\sigma'(\mathbf{z}_{j-1}))\| \leq \|\mathbf{W}_h\| \Rightarrow \| \prod_{j=k+1}^{t} \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \| \leq \|\mathbf{W}_h\|^{t-k}.$$

**Vanishing gradients**: $\|\mathbf{W}_h\| < 1$. **Problem**: dras- tically reducing the learning quality of the model for far-away words.
**Exploding gradients**: $\|\frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}}\| > 1$. **Problem**: if the gradient value grows extremely large, it causes an overflow.

# Exploding gradients

**Problem**: if the gradient value grows extremely large, it causes an overflow.
**Solution**: gradient clipping.

```
$\mathbf{g} \leftarrow \frac{\partial \mathcal{L}}{\partial \mathbf{W}}$
if $\|\mathbf{g}\| \geq \text{threshold}$ then
    $\mathbf{g} \leftarrow \frac{\text{threshold}}{\|\mathbf{g}\|}\mathbf{g}$
end if
```



# General overview of solutions

**MLPs and Convolutional Networks**

- Residual connections
- Batch normalisation
- Dropout
- Weight initialization

**RNNs**

- LSTM/GRU architectures
- Layer normalisation
- Dropout
- Weight parametrization

# Weight Parametrization[1]

**Challenge**: gradient explosion/Vanishing
**Solution**: parametrization by unitary matrices Let $\sigma(.) = \mathrm{ReLU}(.)$

$$\|\frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}}\| = \|\mathrm{diag}(\sigma'(\mathbf{z}_{j-1})) \underbrace{\mathbf{W}_h}_{orthogonal} \| = 1$$

Therefore, we avoid exploding gradients.
**Effective parametrization in the complex domain**:

$$\mathbf{W}_h = \mathbf{D}_3\mathbf{R}_2\mathcal{F}^{-1}\mathbf{D}_2\mathbf{\Pi}\mathbf{R}_1\mathcal{F}\mathbf{D}_1,$$

- $\mathbf{D}$ – diagonal matrix, $\mathbf{D}_{jj} = e^{iw_j}$
- $\mathbf{R} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^*}{\|\mathbf{v}\|^2}$ – refection matrix
- $\mathbf{\Pi}$ – fixed radnom index permutation matrix
- $\mathcal{F}$ – Fourier transform

Interestingly, $\mathbf{D}, \mathbf{R}, \mathbf{\Pi}$ requires $\mathcal{O}(D_h)$ computations, while $\mathcal{F}$ requires $\mathcal{O}(D_h \log D_h)$. Vanilla RNN requires $\mathcal{O}(D_h^2)$ computation.
**Activation function**:

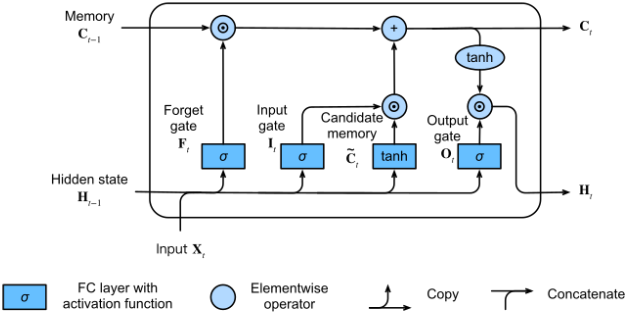
$$\sigma(z) = \mathrm{ReLU}(|z| + b)\frac{z}{|z|}.$$

[1] Arjovsky M., Shah A., Bengio Y. Unitary evolution recurrent neural networks, 2016

# Long-Short-Term Memory network[2]

**Challenge**: RNN poorly models long-term dependencies
**Solution**: introduce a memorization mechanism

$$
\begin{aligned}
\mathbf{i}_t &= \sigma(\mathbf{W}^i_x \mathbf{x}_t + \mathbf{W}^i_h \mathbf{h}_{t-1} + \mathbf{b}_i) \\
\mathbf{f}_t &= \sigma(\mathbf{W}^f_x \mathbf{x}_t + \mathbf{W}^f_h \mathbf{h}_{t-1} + \mathbf{b}_f) \\
\mathbf{o}_t &= \sigma(\mathbf{W}^o_x \mathbf{x}_t + \mathbf{W}^o_h \mathbf{h}_{t-1} + \mathbf{b}_o) \\
\tilde{\mathbf{c}}_t &= \tanh(\mathbf{W}^c_x \mathbf{x}_t + \mathbf{W}^c_h \mathbf{h}_{t-1} + \mathbf{b}_c) \\
\mathbf{c}_t &= \mathbf{f}_t \circ \mathbf{c}_{t-1} + \mathbf{i}_t \circ \tilde{\mathbf{c}}_t \\
\mathbf{h}_t &= \mathbf{o}_t \circ \tanh(\mathbf{c}_t)
\end{aligned}
$$



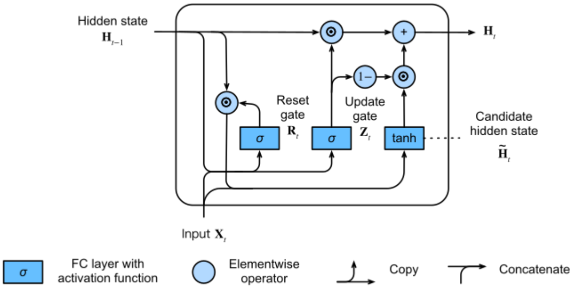
where $\mathbf{i}_i$ – input gate, $\mathbf{f}_i$ – forget gate, $\mathbf{o}_i$ – output gate, $\tilde{\mathbf{c}}_t$ – new memory cell, $\mathbf{c}_t$ – final memory cell
**Note**: Initialize $\mathbf{b}_f \gg 1$, $\mathbf{b}_i \gg 1$.

[2] Hochreiter S., Schmidhuber J. Long Short-Term Memory, 1997

# Gated Recurrent Units[3]

**Architecture**:

$$
\begin{aligned}
\mathbf{u}_t &= \sigma(\mathbf{W}_x^u \mathbf{x}_t + \mathbf{W}_h^u \mathbf{h}_{t-1} + \mathbf{b}_u) \\
\mathbf{r}_t &= \sigma(\mathbf{W}_x^r \mathbf{x}_t + \mathbf{W}_h^r \mathbf{h}_{t-1} + \mathbf{b}_r) \\
\tilde{\mathbf{h}}_t &= \tanh(\mathbf{r}_t \circ \mathbf{W}_h \mathbf{h}_{t-1} + \mathbf{W}_x \mathbf{x}_{t-1}) \\
\mathbf{h}_t &= (1 - \mathbf{u}_t) \circ \tilde{\mathbf{h}}_t + \mathbf{u}_t \circ \mathbf{h}_{t-1}
\end{aligned}
$$



- $\mathbf{u}_t$ – update gate
- $\mathbf{r}_t$ – reset gate
- $\tilde{\mathbf{h}}_t$ – new memory

**Note**: initialize $\mathbf{b}_u \gg 1$, $\mathbf{b}_r \gg 1$.

[3] Cho et al. On the Properties of Neural Machine Translation: Encoder–Decoder Approaches, 2014

# Layer Normalization[4]

**Challenge**: batch normalization can not be applied to the case when the minibatches have to be small.
**Solution**: introduce layer normalization. Define $\mathrm{LN} : \mathbb{R}^D \to \mathbb{R}^D$, with two parameters $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{R}^D$.

$$\mathrm{LN}(\mathbf{z}; \boldsymbol{\alpha}, \boldsymbol{\beta})_i = \frac{z_i - \mu}{\sigma}\alpha_i + \beta_i, \ \ i = \overline{1, D},$$

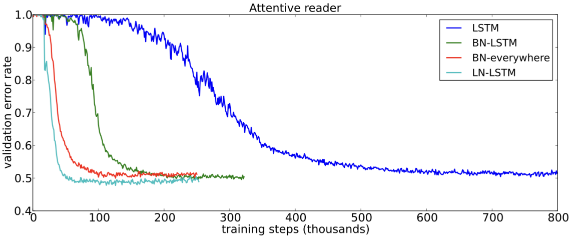
$$\mu = \frac{1}{D}\sum_{i=1}^{D} z_i, \quad \sigma = \sqrt{\frac{1}{D}\sum_{i=1}^{D}(z_i - \mu)^2}.$$

**LSTM with layer normalization**:

$$\begin{pmatrix} \mathbf{f}_t \\ \mathbf{i}_t \\ \mathbf{o}_t \\ \mathbf{g}_t \end{pmatrix} = \mathrm{LN}(\mathbf{W}_h\mathbf{h}_{t-1}; \boldsymbol{\alpha}_1, \boldsymbol{\beta}_1) + \mathrm{LN}(\mathbf{W}_x\mathbf{x}_t; \boldsymbol{\alpha}_2, \boldsymbol{\beta}_2) + \mathbf{b}$$

$$\mathbf{c}_t = \sigma(\mathbf{f}_t) \circ \mathbf{c}_{t-1} + \sigma(\mathbf{i}_t) \circ \tanh(\mathbf{g}_t)$$

$$\mathbf{h}_t = \sigma(\mathbf{o}_t) \circ \tanh(\mathrm{LN}(\mathbf{c}_t; \boldsymbol{\alpha}_3, \boldsymbol{\beta}_3))$$

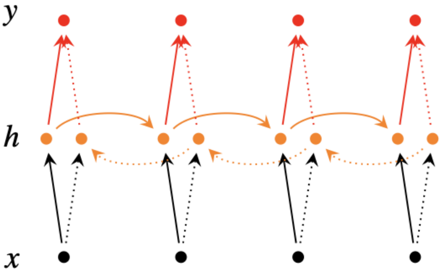


[4] Ba, Jimmy et al. Layer Normalization, 2016

# Deep Bidirectional RNNs

**Challenge**: Consider the part-of-speech tagging task: $p(\mathbf{y}_{1:n}|\mathbf{x}_{1:n}) = \prod_{i=1}^{n} p(y_i|\mathbf{x}_{1:n})$. A vanilla RNN can not be conditioned on $\mathbf{x}_{i:n}$.
**Solution**: introduce a Bidirectional recurrent neural network (BRNN).

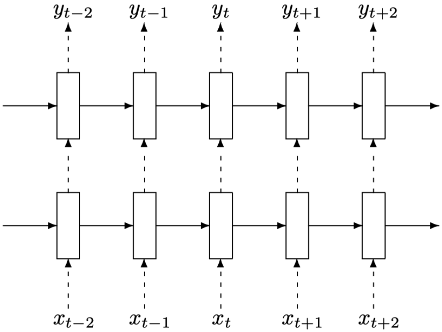
$$\vec{\mathbf{h}}_t = \sigma(\vec{\mathbf{W}}_x \mathbf{x}_t + \vec{\mathbf{W}}_h \mathbf{h}_{t-1} + \vec{\mathbf{b}})$$
$$\overleftarrow{\mathbf{h}}_t = \sigma(\overleftarrow{\mathbf{W}}_x \mathbf{x}_t + \overleftarrow{\mathbf{W}}_h \mathbf{h}_{t+1} + \overleftarrow{\mathbf{b}})$$
$$\mathbf{y}_t = \mathrm{softmax}(\mathbf{W}_y[\vec{\mathbf{h}}_t, \overleftarrow{\mathbf{h}}_t] + \mathbf{b}_y)$$

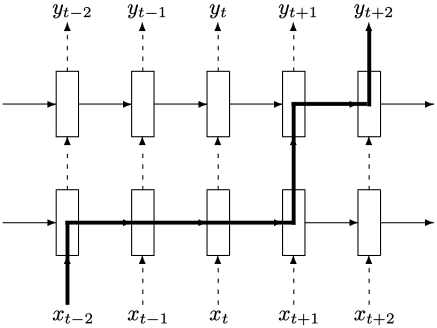


**Extension**: multi-layered BRNNs.

# Naive dropout [5]

**Idea**: apply the dropout operator only to the non-recurrent connections.

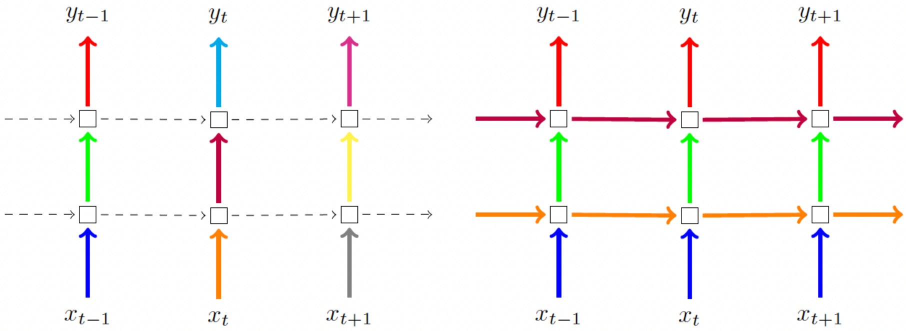




| Model | Training set | Validation set |
|---|---|---|
| Non-regularized LSTM | 71.6 | 68.9 |
| Regularized LSTM | 69.4 | **70.5** |

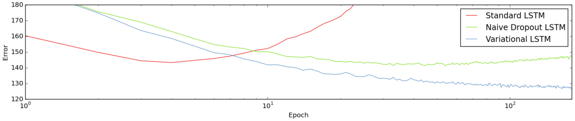
[5] Zaremba W. et al. Recurrent neural network regularization, 2014

# Variational Dropout[6]



(a) Naive dropout RNN

(b) Variational RNN



[6] Gal Y. et al. A Theoretically Grounded Application of Dropout in Recurrent Neural Networks, 2016

# Variational dropout: theoretical explanation

**Approximate Variational Inference in Bayesian Neural Networks**: Let $q(\mathbf{w})$ be ana approximating variational distribution:

$$\mathrm{KL}(q(\mathbf{w})||p(\mathbf{w}|\mathbf{X},\mathbf{Y})) \propto$$

$$-\sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{w})} \log p(\mathbf{y}_i|\mathbf{f}(\mathbf{x}_i,\mathbf{w})) + \mathrm{KL}(q(\mathbf{w})||p(\mathbf{w})) \to \min_q$$

**Variational Inference with RNNs**:

$$\mathbf{w} = [\mathbf{m}_k]_{k=1}^{K} = [\mathbf{W}_h, \mathbf{W}_x, \mathbf{W}_y, \mathbf{b}_h, \mathbf{b}_y].$$

**Approximating posterior distribution**:

$$q(\mathbf{w}) = \prod_{k=1}^{K} q(\mathbf{w}_k),$$

$$q(\mathbf{w}_k) = p\mathcal{N}(\mathbf{w}_k|\mathbf{0},\sigma^2\mathbf{I}) + (1-p)\mathcal{N}(\mathbf{w}_k|\mathbf{m}_k,\sigma^2\mathbf{I})$$

**Interpretation**: Evaluating the model output $\mathbf{f}(\mathbf{x}_i,\hat{\mathbf{w}})$ with a sample $\hat{\mathbf{w}} \sim q(\mathbf{w})$ corresponds to randomly masking rows in each weight matrix during the forward pass if $\sigma$ is small enough.

**Predictive distribution**:

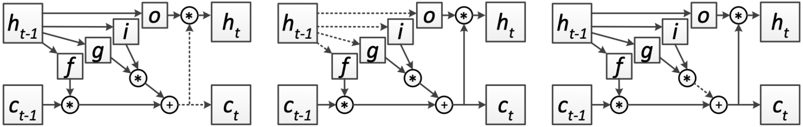
$$p(\mathbf{y}^*|\mathbf{x}^*,\mathbf{X},\mathbf{Y}) \approx \mathbb{E}_{q(\mathbf{w})} p(\mathbf{y}^*|\mathbf{x}^*,\mathbf{w}) \approx$$

$$\frac{1}{K}\sum_{j=1}^{J} p(\mathbf{y}^*|\mathbf{x}^*,\hat{\mathbf{w}}_j), \quad \hat{\mathbf{w}}_j \sim q(\mathbf{w}).$$

We perform dropout at test time and average results (MC dropout).

# Recurrent Dropout without Memory Loss[7]

**Challenge**: information loss in memory cells of LSTMs when applying recurrent dropout
**Solution**: a novel dropout mechanism $\mathbf{c}_t = \mathbf{f}_t \circ \mathbf{c}_{t-1} + \mathbf{i}_t \circ d(\tilde{\mathbf{c}}_t)$



(a) Moon et al., 2015 (b) Gal, 2015 (c) Ours

| Dropout rate | Sampling | Moon et al. (2015) | | Gal (2015) | | Ours | |
|---|---|---|---|---|---|---|---|
| | | Valid | Test | Valid | Test | Valid | Test |
| 0.0 | – | 130.0 | 125.2 | 130.0 | 125.2 | 130.0 | 125.2 |
| 0.25 | per-step | **113.0** | **108.7** | 119.8 | 114.2 | 106.1 | 100.0 |
| 0.5 | per-step | 124.0 | 116.5 | **118.3** | **112.5** | 102.8 | 98.0 |
| 0.25 | per-sequence | 121.0 | 113.0 | 120.5 | 114.0 | 106.3 | 100.7 |
| 0.5 | per-sequence | 137.7 | 126.2 | 125.2 | 117.9 | **103.2** | **96.8** |

[7] Semeniuta S. et al. Recurrent Dropout without Memory Loss, 2016

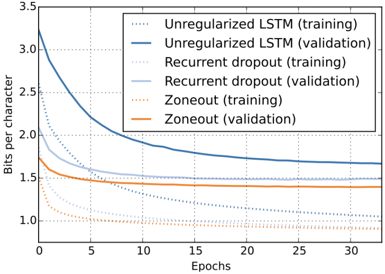
# Zoneout[8]

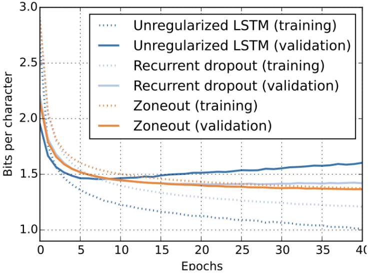
**Challenge**: the repeated application of the same transition operator can make the dynamics of an RNN sensitive to minor perturbations in the hidden state

**Solution**: regularize transition dynamics

$$\mathbf{c}_t = d_t^c \circ \mathbf{c}_{t-1} + (1 - d_t^c) \circ (\mathbf{f}_t \circ \mathbf{c}_{t-1} + \mathbf{i}_t \circ \tilde{\mathbf{c}}_t),$$

$$\mathbf{h}_t = d_t^h \circ \mathbf{h}_{t-1} + (1 - d_t^h) \circ (\mathbf{o}_t \circ \tanh(\mathbf{c}_t))$$





[8] Krueger D. et al. ZONEOUT: Regularizing RNNs by Randomly Preserving Hidden Activations, 2017

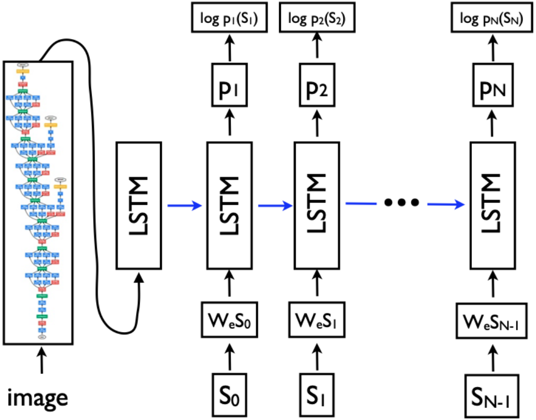
# Application: Image Captioning[9]

**Training**:

$$-\sum_{(I,S)\in\mathfrak{D}} \log p(s_t|s_{<t}, I) \to \min_{\mathbf{W},\mathbf{b}}$$

**Inference**: generate a sentence given an image

- Sampling: $\hat{s}_t \sim p(s_t|s_{<t}, I)$
- Beam Search: iteratively consider the set of the $k$ best sentences up to time $t$ as candidates to generate sentences of size $t+1$, and keep only the resulting best $k$ of them



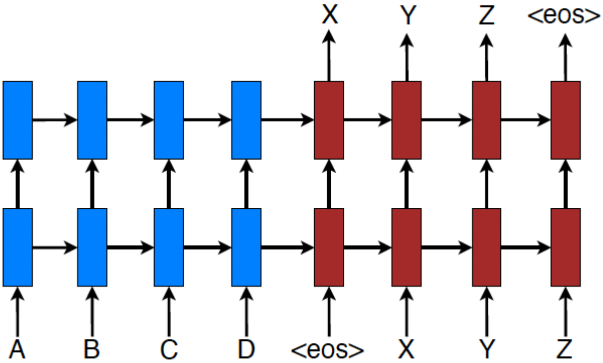
[9] Vinyals O. et al. Show and Tell: A Neural Image Caption Generator, 2015

# Application: Neural Machine Translation[10]

**Architecture**

An encoder computes a representation $\mathbf{s}$ for each source sentence and an autoregressive decoder.

$$\log p(\mathbf{y}|\mathbf{x}) = \sum_{i=1}^{|\mathbf{y}|} \log p(y_i|\mathbf{y}_{<i}, \mathbf{s})$$



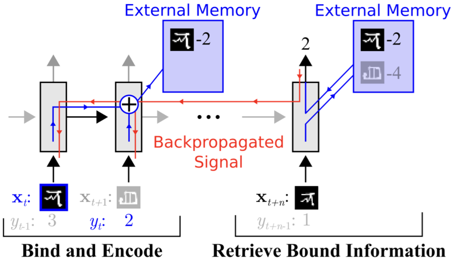
[10] Luong, et al. Addressing the Rare Word Problem in Neural Machine Translation, 2015

# Application: Black-Box Meta Learning[11]

Consider a "few-shot learning" task
**Challenge**: fine-tuning is prone to poor learning
**Solution**: Memory-Augmented Neural Networks

$$\text{Supervised learning}: \quad f: x \mapsto y,$$
$$\text{Supervised meta-learning}: \quad f: (\mathfrak{D}_{\text{train}}, x) \mapsto y.$$

$$\boldsymbol{\theta}^* = \arg\min_{\theta} \mathbb{E}_{\mathfrak{D}} \sum_{t=1}^{|\mathfrak{D}|} \log \underbrace{p_{\boldsymbol{\theta}}}_{\text{RNN}} (y_t | \mathbf{x}_t, \mathfrak{D}_{1:t-1}).$$



**Retrieving a memory**: Given a key $\mathbf{k}_t = f(\mathbf{x}_t)$

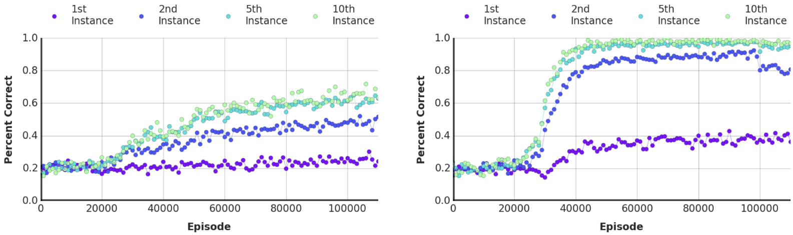
$$\mathbf{w}_t^{\text{read}}(i) = \frac{\exp(\text{sim}(\mathbf{k}_t, \mathbf{M}_t(i)))}{\sum_j \exp(\text{sim}(\mathbf{k}_t, \mathbf{M}_t(j)))}, \quad \mathbf{k}_t \in \mathbb{R}^d,$$

$$\mathbf{r}_t = \sum_i \mathbf{w}_t^{\text{read}}(i) \mathbf{M}_t(i), \quad \mathbf{M}_t \in \mathbb{R}^{m \times d}.$$

$$\mathbf{w}_t^{\text{usage}} = \gamma \mathbf{w}_{t-1}^{\text{usage}} + \mathbf{w}_t^{\text{read}} + \mathbf{w}_t^{\text{write}},$$
$$\mathbf{w}_t^{\text{write}} = \alpha \mathbf{w}_{t-1}^{\text{read}} + (1-\alpha)\mathbf{w}_{t-1}^{\text{least-used}},$$
$$\mathbf{w}_t^{\text{least-used}}(i) = \begin{cases} 0, & \mathbf{w}_t^{\text{usage}}(i) > \text{bottom}_n(\mathbf{w}_t^{\text{usage}}) \\ 1, & \text{otherwise} \end{cases}$$
$$\mathbf{M}_t(i) = \mathbf{M}_{t-1}(i) + \mathbf{w}_t^{\text{write}}(i)\mathbf{k}_t$$

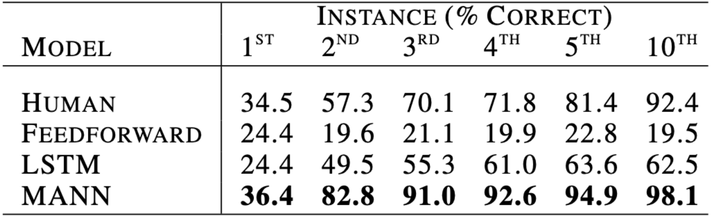
[11] Santoro A. et. al, One-shot Learning with Memory-Augmented Neural Networks, 2016

# Memory-Augmented Neural Network: evaluation



(a) LSTM, five random classes/episode, one-hot vector labels

(b) MANN, five random classes/episode, one-hot vector labels



| Model | Instance (% Correct) 1st | 2nd | 3rd | 4th | 5th | 10th |
|---|---|---|---|---|---|---|
| Human | 34.5 | 57.3 | 70.1 | 71.8 | 81.4 | 92.4 |
| Feedforward | 24.4 | 19.6 | 21.1 | 19.9 | 22.8 | 19.5 |
| LSTM | 24.4 | 49.5 | 55.3 | 61.0 | 63.6 | 62.5 |
| MANN | **36.4** | **82.8** | **91.0** | **92.6** | **94.9** | **98.1** |

**Experimental setup**: few-shot classification tasks of Ominiglot images.

**Results**: The proposed MANN architecture substantially outperforms the baselines: feedforward RNN, LSTM, and human.

# HyperNetworks[12]

**Idea**: the normalization policy is fixed (ex. Layer Normalization). The learnable policy would give an increase in prediction accuracy.
**Solution**: adaptive weight generation with a hypernetwork.

$$\mathbf{h}_t = \sigma(\mathbf{d}_h(\mathbf{z}_h) \odot \mathbf{W}_h \mathbf{h}_{t-1} + \mathbf{d}_x(\mathbf{x}_t) \odot \mathbf{W}_x \mathbf{x}_t + \mathbf{b}(\mathbf{z}_b)),$$

$$\mathbf{d}_h(\mathbf{z}_h) = \mathbf{W}_{hz}\mathbf{z}_h, \quad \mathbf{d}_x(\mathbf{z}_x) = \mathbf{W}_{xz}\mathbf{z}_x,$$

$$\mathbf{b}(\mathbf{z}_b) = \mathbf{W}_{bz}\mathbf{z}_b + \mathbf{b}_0,$$

$$\hat{\mathbf{x}}_t = [\mathbf{h}_{t-1}, \mathbf{x}_t],$$

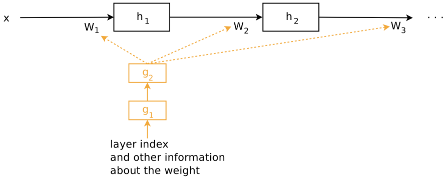
$$\hat{\mathbf{h}}_t = \sigma(\hat{\mathbf{W}}_h \hat{\mathbf{h}}_{t-1} + \hat{\mathbf{W}}_x \hat{\mathbf{x}}_{t-1} + \hat{\mathbf{b}}),$$

$$\mathbf{z}_h = \hat{\mathbf{W}}_{hh}\hat{\mathbf{h}}_{t-1} + \hat{\mathbf{b}}_{hh},$$

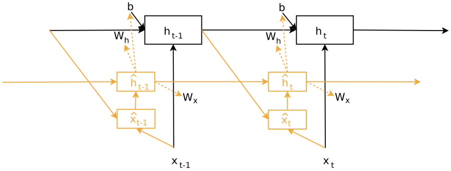
$$\mathbf{z}_x = \hat{\mathbf{W}}_{hx}\hat{\mathbf{h}}_{t-1} + \hat{\mathbf{b}}_{hx},$$

$$\mathbf{z}_b = \hat{\mathbf{W}}_{hb}\hat{\mathbf{h}}_{t-1}.$$

## General overview



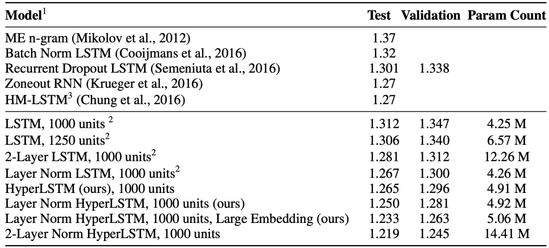
## HyperRNNs architecture



[12] Ha D. et. al, HyperNetworks, 2016

# HyperNetworks: evaluation

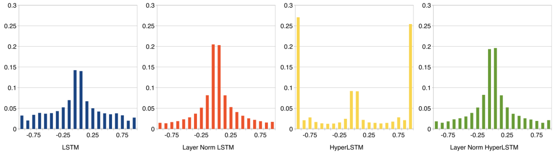
## Evaluation on Penn Treebank



| Model[1] | Test | Validation | Param Count |
|---|---|---|---|
| ME n-gram (Mikolov et al., 2012) | 1.37 | | |
| Batch Norm LSTM (Cooijmans et al., 2016) | 1.32 | | |
| Recurrent Dropout LSTM (Semeniuta et al., 2016) | 1.301 | 1.338 | |
| Zoneout RNN (Krueger et al., 2016) | 1.27 | | |
| HM-LSTM[3] (Chung et al., 2016) | 1.27 | | |
| LSTM, 1000 units [2] | 1.312 | 1.347 | 4.25 M |
| LSTM, 1250 units[2] | 1.306 | 1.340 | 6.57 M |
| 2-Layer LSTM, 1000 units[2] | 1.281 | 1.312 | 12.26 M |
| Layer Norm LSTM, 1000 units[2] | 1.267 | 1.300 | 4.26 M |
| HyperLSTM (ours), 1000 units | 1.265 | 1.296 | 4.91 M |
| Layer Norm HyperLSTM, 1000 units (ours) | 1.250 | 1.281 | 4.92 M |
| Layer Norm HyperLSTM, 1000 units, Large Embedding (ours) | 1.233 | 1.263 | 5.06 M |
| 2-Layer Norm HyperLSTM, 1000 units | 1.219 | 1.245 | 14.41 M |

Layer Norm HyperLSTM significantly outperforms Layer Norm LSTM.

## The normalized histogram plots of the hidden states



The normalization policy of HyperLSTM appears to be doing something very different from statistical normalization.

# Mixture-of-Experts Layer[13]

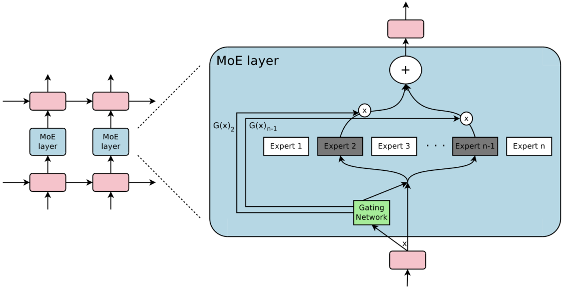
**Challenge**: an increase in model capacity is accompanied by an increase in computational cost.

**Solution**: Sparsely-Gated Mixture-of-Experts Layer (MoE).

**Mixture-of-Experts layer**

$$y = \sum_{i=1}^{n} \underbrace{G(x)_i}_{\text{gating network}} \cdot \underbrace{E_i(x)}_{\text{expert network}}$$

## General overview



**Noisy Top-k Gating Network**

$$\text{topk}(\mathbf{v}) = \begin{cases} v_i, & v_i \in \max_k(\mathbf{v}), \\ -\infty, & \text{otherwise} \end{cases}$$

$$\mathbf{G}(\mathbf{x}) = \text{softmax}(\text{topk}(\mathbf{x}\mathbf{W}_g + \text{softplus}(\mathbf{x}\mathbf{W}_{\text{noise}})\epsilon)),$$

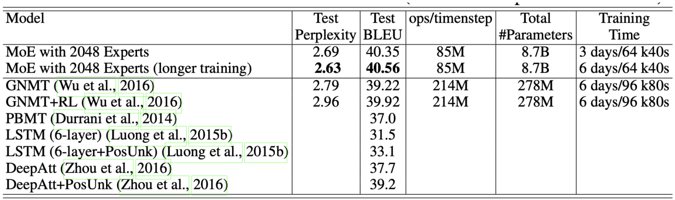
$$\epsilon \sim \mathcal{N}(\mathbf{0}_n, \mathbf{I}_n).$$

The noise term helps with load balancing.

[13] Shazeer N. et. al, Outrageously Large Neural Networks: The Sparsely-Gated Mixture-of-Experts Layer, 2017

# Mixture-of-Experts: evaluation

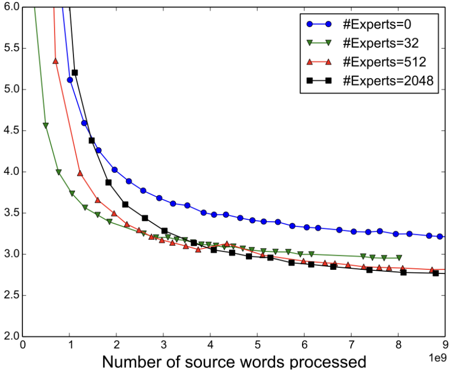
## Machine translation WMT14(En-Fr)



| Model | Test Perplexity | Test BLEU | ops/timenstep | Total #Parameters | Training Time |
|---|---|---|---|---|---|
| MoE with 2048 Experts | 2.69 | 40.35 | 85M | 8.7B | 3 days/64 k40s |
| MoE with 2048 Experts (longer training) | **2.63** | **40.56** | 85M | 8.7B | 6 days/64 k40s |
| GNMT (Wu et al., 2016) | 2.79 | 39.22 | 214M | 278M | 6 days/96 k80s |
| GNMT+RL (Wu et al., 2016) | 2.96 | 39.92 | 214M | 278M | 6 days/96 k80s |
| PBMT (Durrani et al., 2014) | | 37.0 | | | |
| LSTM (6-layer) (Luong et al., 2015b) | | 31.5 | | | |
| LSTM (6-layer+PosUnk) (Luong et al., 2015b) | | 33.1 | | | |
| DeepAtt (Zhou et al., 2016) | | 37.7 | | | |
| DeepAtt+PosUnk (Zhou et al., 2016) | | 39.2 | | | |

Each MoE layer contains 2048 feed-forward experts. There is a significant gain in BLEU score on top of the strong baselines.

## Perplexity on WMT14(En-Fr)



As we increased the number of experts to approach 2048, the test perplexity of our model continued to improve.

# Softmax Bottleneck[14]

### Language Modeling with Softmax

$$p(x_t|c) = \mathrm{softmax}(\mathbf{h}_c^\top \mathbf{E}_w),$$

$$c = x_{<t}, \quad \mathbf{E}_w \in \mathbb{R}^{d\times|\mathcal{V}|},$$

$$\mathbf{H}_\theta = \begin{pmatrix} \mathbf{h}_{c_1}^\top \\ \dots \\ \mathbf{h}_{c_N}^\top \end{pmatrix}, \quad \mathbf{W}_\theta = \begin{pmatrix} \mathbf{w}_1^\top \\ \dots \\ \mathbf{w}_{|\mathcal{V}|}^\top \end{pmatrix},$$

$$\mathbf{A} = \| \log \pi(x_j|c_i) \|, \quad i = \overline{1, N}, j = \overline{1, |\mathcal{V}|},$$

where $\{c_i\}_{i=1}^N$ are all possible context in the natural language and $\pi(.|.)$ is data distribution.

### Matrix factorization problem

$$\mathbf{H}_\theta \mathbf{W}_\theta^\top = \mathbf{A}', \quad \mathbf{A}' = \mathbf{A} + \underbrace{\mathrm{diag}(\boldsymbol{\lambda})}_{N\times N} \mathbf{1}_N \mathbf{1}_{|\mathcal{V}|}^\top.$$

**Proposition (Softmax Bottleneck)**: if $d < \mathrm{rank}(A) - 1$ for any $\theta$, there exists a context $c$ such that $\pi(.|c) \neq p(.|c)$. **Solution: Mixture of Softmaxes**

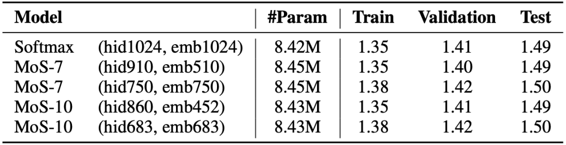
$$p(x_t|c) = \sum_{k=1}^{K} \pi(c)_k \mathrm{softmax}(\mathbf{h}_{c,k}^\top \mathbf{E}_w),$$

$$\sum_{k=1}^{k} \pi(c)_k = 1, \quad \hat{\mathbf{A}} = \underbrace{\log(\sum_{k=1}^{K} \mathbf{\Pi}_k \exp(\mathbf{H}_{\theta,k} \mathbf{W}_\theta^\top))}_{\text{high-rank}}.$$

[14] Yang Z. et. al, Breaking the Softmax Bottleneck: A High-Rank RNN Language Model, 2018

# Softmax Bottleneck: evaluation

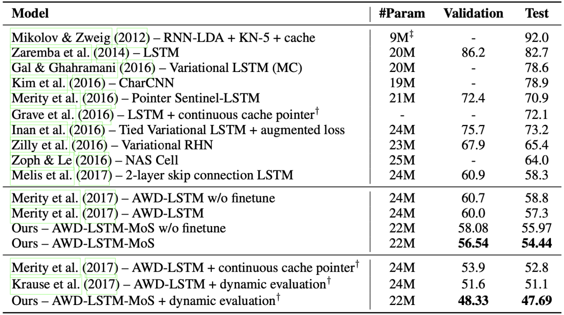
## Character-level Language Modeling



| Model | | #Param | Train | Validation | Test |
|---|---|---|---|---|---|
| Softmax | (hid1024, emb1024) | 8.42M | 1.35 | 1.41 | 1.49 |
| MoS-7 | (hid910, emb510) | 8.45M | 1.35 | 1.40 | 1.49 |
| MoS-7 | (hid750, emb750) | 8.45M | 1.38 | 1.42 | 1.50 |
| MoS-10 | (hid860, emb452) | 8.43M | 1.35 | 1.41 | 1.49 |
| MoS-10 | (hid683, emb683) | 8.43M | 1.38 | 1.42 | 1.50 |

The models performs on par with each other, indicating that the softmax bottleteck problem diminishes when $\mathrm{rank}(A)$ is relatively small.

## Language modeling on Penn Treebank



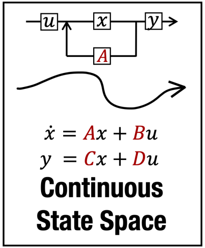
| Model | #Param | Validation | Test |
|---|---|---|---|
| Mikolov & Zweig (2012) – RNN-LDA + KN-5 + cache | 9M$^{\ddagger}$ | - | 92.0 |
| Zaremba et al. (2014) – LSTM | 20M | 86.2 | 82.7 |
| Gal & Ghahramani (2016) – Variational LSTM (MC) | 20M | - | 78.6 |
| Kim et al. (2016) – CharCNN | 19M | - | 78.9 |
| Merity et al. (2016) – Pointer Sentinel-LSTM | 21M | 72.4 | 70.9 |
| Grave et al. (2016) – LSTM + continuous cache pointer$^{\dagger}$ | - | - | 72.1 |
| Inan et al. (2016) – Tied Variational LSTM + augmented loss | 24M | 75.7 | 73.2 |
| Zilly et al. (2016) – Variational RHN | 23M | 67.9 | 65.4 |
| Zoph & Le (2016) – NAS Cell | 25M | - | 64.0 |
| Melis et al. (2017) – 2-layer skip connection LSTM | 24M | 60.9 | 58.3 |
| Merity et al. (2017) – AWD-LSTM w/o finetune | 24M | 60.7 | 58.8 |
| Merity et al. (2017) – AWD-LSTM | 24M | 60.0 | 57.3 |
| Ours – AWD-LSTM-MoS w/o finetune | 22M | 58.08 | 55.97 |
| Ours – AWD-LSTM-MoS | 22M | **56.54** | **54.44** |
| Merity et al. (2017) – AWD-LSTM + continuous cache pointer$^{\dagger}$ | 24M | 53.9 | 52.8 |
| Krause et al. (2017) – AWD-LSTM + dynamic evaluation$^{\dagger}$ | 24M | 51.6 | 51.1 |
| Ours – AWD-LSTM-MoS + dynamic evaluation$^{\dagger}$ | 22M | **48.33** | **47.69** |

The proposed approach outperforms the baselines by a huge margin.

# The Challenges of Continuous Time Series[15]

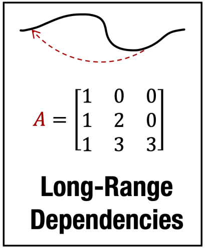
**Difficult challenges**:

- Handle information across long distances
- Understand the continuous nature of the data (insensitivity to the resolution)
- Be very efficient, at both training and inference time



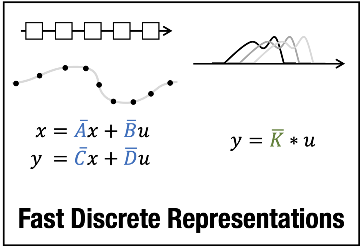
$$\dot{x} = Ax + Bu$$
$$y = Cx + Du$$

**Continuous State Space**



$$A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1 & 3 & 3 \end{bmatrix}$$

**Long-Range Dependencies**



$$x = \bar{A}x + \bar{B}u$$
$$y = \bar{C}x + \bar{D}u$$

$$y = \bar{K} * u$$

**Fast Discrete Representations**

[15] Structured State Spaces for Sequence Modeling (S4)

# Three Paradigms for Time Series[16]

**Recurrence**

- ✓ Efficient inference (constant-time state updates)
- × Slow to train (lack of parallelizability)
- × Vanishing/exploding gradient problem for long sequences

**Convolutions**

- ✓ Efficient training (parallelizable)
- × Slow in online or autoregressive settings (has to recompute over entire input for every new datapoint)
- × Fixed context size

**Continuous-time**

- ✓ Automatically handles irregularly-sampled data
- ✓ Mathematically tractable to analyze
- × Extremely slow at both training and inference

[16] Structured State Spaces: A Brief Survey of Related Models

# The State Space Sequence Model[17]

**Definition** ((Linear Time Invariant) State Space Model). Given an input signal $u(t) \in \mathbb{R}^M$, an output signal $y(t) \in \mathbb{R}^M$, and a latent state $x(t) \in \mathbb{R}^N$:

$$
\begin{aligned}
x'(t) &= \underbrace{\mathbf{A}}_{N\times N} x(t) + \underbrace{\mathbf{B}}_{N\times M} u(t) \\
y(t) &= \underbrace{\mathbf{C}}_{M\times N} x(t)
\end{aligned}
$$

Or, equivalently, $y = \mathrm{SSM}(\mathbf{A}, \mathbf{B}, \mathbf{C})(u)$.

**Discretization**. Given a stepsize parameter $\Delta \in \mathbb{R}_{++}$. Then, using the Euler's method,

$$
\begin{aligned}
x_k &= x_{k-1} + \Delta(\mathbf{A}x_{x-1} + \mathbf{B}u_k) \\
&= \underbrace{(\mathbf{I} + \Delta\mathbf{A})}_{\overline{\mathbf{A}}} x_{k-1} + \underbrace{(\Delta\mathbf{B})}_{\overline{\mathbf{B}}} u_k
\end{aligned}
$$

**The convolutional representation (Efficient Training)**. Assume that $x_{-1} = \mathbf{0}$.

$$
\begin{aligned}
x_k &= \overline{\mathbf{A}}^k\overline{\mathbf{B}}u_0 + \overline{\mathbf{A}}^{k-1}\overline{\mathbf{B}}u_1 + \ldots + \overline{\mathbf{B}}u_k, \\
y_k &= \mathbf{C}\overline{\mathbf{A}}^k\overline{\mathbf{B}}u_0 + \mathbf{C}\overline{\mathbf{A}}^{k-1}\overline{\mathbf{B}}u_1 + \ldots + \mathbf{C}\overline{\mathbf{B}}u_k, \\
y &= u * \overline{\mathbf{K}}, \quad \overline{\mathbf{K}} = (\mathbf{C}\overline{\mathbf{B}}, \ldots, \mathbf{C}\overline{\mathbf{A}}^k\overline{\mathbf{B}}, \ldots)
\end{aligned}
$$

**Definition**. We call $\overline{\mathbf{K}}$ by a State Space Kernel (SSK).

[17] Albert Gu, Modeling sequences with structured state spaces

# The State Space Sequence Model

**Convolution Complexities**. For a sequence of length $L$ and a Kernel of length $K$:

- A naive convolution has complexity $O(LK)$
- an FFT-convolution has complexity $O((L+K)\log(L+K))$.

**Note**: the statement is true for an instantiated $\overline{\mathbf{K}}$, however, generating it can be highly non-trivial.

### Lemma (Gating Mechanism of RNNs)

*A gated recurrence*

$$x_t = (1-\sigma(z))x_{t-1} + \sigma(z)u_t,$$

*where $z$ is an arbitrary real number, can be viewed as the Backward-Euler discretization of a linear ODE $x'(t) = -x(t) + u(t)$.*

### Proof.

First, write down the discretization $x_t - x_{t-1} = \exp(z)(-x_t + u_t)$. Hence, we get the recurrence, setting $\Delta = \exp(z)$. □

# Computational Difficulty of SSM

**Challenge** (Convolutional mode computation). The SSM has optimal convolutional mode if the SSK can be computed in $\tilde{O}(L+N)$.

**Proposition** (Naive computation). Suppose that $\mathbf{B} \in \mathbb{R}^{N\times 1}$. Then, for a general matrix $\overline{\mathbf{A}}$ it takes $O(LN^2)$ to compute

$$\overline{\mathbf{K}} = (\overline{\mathbf{B}}, \dots, \overline{\mathbf{A}}^{L-1}\overline{\mathbf{B}}) \in \mathbb{R}^{N\times L}.$$

**Challenge** (Recurrent mode computation). The SSM has optimal recurrent mode if its Matrix-Vector Multiplication can be comuted in $O(N)$.

**S4D: Diagonal SSM**. If **A** is diagonal, computing the SSK becomes simple ($\mathbf{B} \in \mathbb{R}^{N\times 1}$, $\mathbf{C} \in \mathbb{R}^{1\times N}$):

$$\overline{\mathbf{K}} =$$

$$[\overline{\mathbf{B}}_0\mathbf{C}_0, \dots, \overline{\mathbf{B}}_{N-1}\mathbf{C}_{N-1}] \begin{pmatrix} 1 & \overline{\mathbf{A}}_0 & \dots & \overline{\mathbf{A}}_0^{L-1} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \overline{\mathbf{A}}_{N-1} & \dots & \overline{\mathbf{A}}_{N-1}^{L-1} \end{pmatrix}$$

**Note**: Vandermonde are well-studied and the convolution can be implemented in $\tilde{O}(N+L)$ time and $O(N+L)$ space.

# Sequence Model Complexities

| | Convolution | Recurrence | S4 |
|---|---|---|---|
| Parameters | $LH$ | $\underline{H^2}$ | $\underline{H^2}$ |
| Training | $\underline{\tilde{L}H(B+H)}$ | $BLH^2$ | $\underline{B\tilde{L}H + BH\tilde{H}}$ |
| Space | $BLH$ | $BLH$ | $BLH$ |
| Parallel | ✓ | × | ✓ |
| Inference | $LH^2$ | $\underline{H^2}$ | $\underline{H^2}$ |

Table: Complexity of various sequence models in terms of sequence length (L), batch size (B), and hidden dimension (H);

# HIPPO: Continuous Memory with Optimal Polynomial Projections

**Research Question**: How can SSMs be instantiated to be able to model long-range dependencies?

**HIPPO Problem Setup**: Given an input function $f(t) \in \mathbb{R}$. As for the quality of an approximation, introduce an inner product

$$\langle f, g \rangle_\mu = \int_0^\infty f(x)g(x)d\mu(x),$$

So the corresponding norm $\|f\|_{L_2(\mu)} = \langle f, f \rangle^{1/2}$. Given an orthogonal basis $\{g_n\}_{n=1}^N$. The task is to seek for $g^{(t)} \in \mathcal{G} := \operatorname{lin}(g_1, \dots, g_N)$ that minimizes $\|f_{\leq t} - g^{(t)}\|_{L^2(\mu_t)}$ for $\mu_t$ supported on $(-\infty, t]$.

Additionally, we get an expression for the optimal coefficients $c_n^{(t)} = \langle f_{\leq t}, g_n \rangle_{\mu^{(t)}}$.

**Example**: HIPPO-LegS (Scaled Legendre measures). Let $\mu^{(t)} := \frac{1}{t}\mathbf{1}_{[0,t]}$ and

$$g_n(x; t) := (2n+1)^{1/2} P_n(2x/t - 1),$$

where $P_n$ are the basic Legendre polynomials.

## Theorem

$$c'(t) = -\frac{1}{t}\mathbf{A}c(t) + \frac{1}{t}\mathbf{B}f(t), \ \mathbf{B}_n = (2n+1)^{1/2},$$

$$\mathbf{A}_{nk} = \begin{cases} (2n+1)^{1/2}(2k+1)^{1/2}, & n > k \\ n+1, & n = k \\ 0, & n < k \end{cases}$$

# HIPPO: effectiveness and efficiency

**Remark**: Matrix-Vector multiplication with HIPPO-LegS matrix can be computed in $O(N)$ operations.

### Theorem

*Let $f : \mathbb{R}_+ \to \mathbb{R}$ be a differentiable function and let $g^{(t)}$ be its projection at time $t$ by HIPPO-LegS with maximum polynomial degree $N-1$. If $f$ has order-$k$ bounded derivatives then*

$$\|f_{\le t} - g^{(t)}\|_{L_2(\mu^{(t)})} = O(t^k N^{-k+1/2}).$$

**Empirical Evaluation** on Character Trajectory classification on out-of-distribution timescales.

| Model | Sampling Rate Change | | Missing Values + Timestamps | |
|---|---|---|---|---|
| | 100Hz → 200Hz | 200Hz → 100Hz | Upscale | Downscale |
| LSTM [86] | 31.9 | 28.2 | 24.4 | 34.9 |
| GRU [31] | 25.4 | 64.6 | 28.2 | 27.3 |
| GRU-D [23] | 23.1 | 25.5 | 05.5 | 07.7 |
| ODE-RNN [176] | 41.8 | 31.5 | 04.3 | 07.7 |
| NCDE [107] | 44.7 | 11.3 | 63.9 | 69.7 |
| LMU [218] | 06.0 | 13.1 | 39.3 | 67.8 |
| **HIPPO-LegS** | **88.8** | **90.1** | **94.5** | **94.9** |

**Evaluation** on a toy function approximation.

| Method | MSE | Speed (elements / s) |
|---|---|---|
| LSTM | 0.25 | 35,000 |
| HIPPO-LegS | 0.02 | 470,000 |

# Summary

- RNN for Language modeling
- RNN backpropagation and related issues
- LSTM and GRU networks
- Layer Normalization and dropout mechanisms
- Applications: Neural Nachine Translation, Image Captioning, Black-Box Meta Learning
- HyperNetworks
- Mixture-of-Experts Layer
- Softmax Bottleneck
- State Space Models: S4D and HIPPO