Sequence Processing

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Overview

Recurrent neural networks

- Elman-RNN
- Long Short Term Memory
- Gated recurrent Units
- Orthogonal networks

Applications

Neural Attention and Transformers

Code snippets

Motivation

- Thus far we have never integrated information over time.
- We want the ability to create internal memory.
- Consider the sentence: I live in Paris. I speak ...
- ... French.
- Clearly it is likely for someone in Paris to speak French.
- Memory should help networks taking Paris into account when deciding what language is spoken.

Recurrent neural networks

Motivation

- Recurrent neural networks are often considered the goto choice for sequences.
- Chapter ten in [GBC16], for example, bears the title "Sequence Modeling: Recurrent and Recursive Nets".

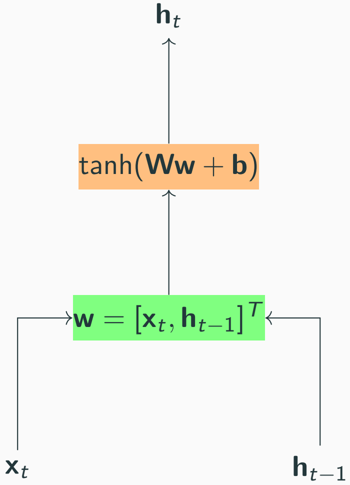
Elman-recurrent neural networks

A simple solution is to add a state to the network and feed this state recurrently back into the network [Elm90],

$$\overline{\mathbf{h}_t} = \mathbf{W}_h \mathbf{h}_t + \mathbf{W}_x \mathbf{x}_t + \mathbf{b}, \tag{1}$$

$$\mathbf{h}_{t+1} = f(\overline{\mathbf{h}_t}). \tag{2}$$

Elman-recurrent neural networks



$\mathbf{h}_t$
$\tanh(\mathbf{W}\mathbf{w} + \mathbf{b})$
$\mathbf{w} = [\mathbf{x}_t, \mathbf{h}_{t-1}]^T$
$\mathbf{x}_t$
$\mathbf{h}_{t-1}$

Unrolling in Time

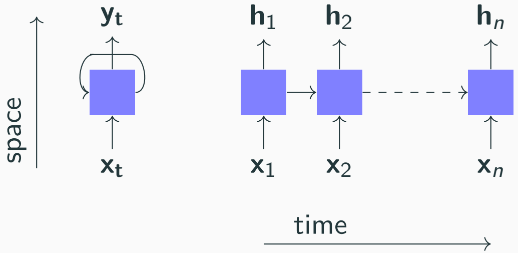


Figure: The rolled (left) cell can be unrolled (right) by considering all inputs it saw during the current gradient computation iteration.

Stability of recurrent connections

For an intuition. Consider a linear network without activations or inputs.

$$\mathbf{h}_{t+1} = \mathbf{W}_h \mathbf{h}_t \tag{3}$$

The evolution of the **h**-sequence is guided by it's largest eigenvalue. If an eigenvalue larger than one exists. The state explodes. If all eigenvalues are smaller than one the state vanishes [GBC16].

Long Short Term Memory (LSTM)

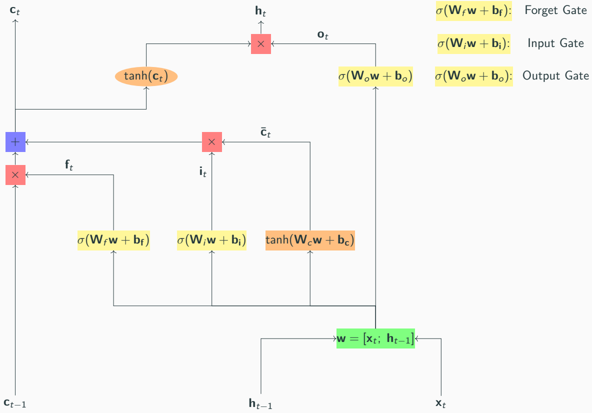

$\mathbf{c}_t$
$\mathbf{h}_t$
$\sigma(\mathbf{W}_f\mathbf{w} + \mathbf{b_f})$: Forget Gate
$\times$
$\mathbf{o}_t$
$\sigma(\mathbf{W}_i\mathbf{w} + \mathbf{b_i})$: Input Gate
$\tanh(\mathbf{c}_t)$
$\sigma(\mathbf{W}_o\mathbf{w} + \mathbf{b}_o)$
$\sigma(\mathbf{W}_o\mathbf{w} + \mathbf{b}_o)$: Output Gate
$+$
$\times$
$\bar{\mathbf{c}}_t$
$\times$
$\mathbf{f}_t$
$\mathbf{i}_t$
$\sigma(\mathbf{W}_f\mathbf{w} + \mathbf{b_f})$
$\sigma(\mathbf{W}_i\mathbf{w} + \mathbf{b_i})$
$\tanh(\mathbf{W}_c\mathbf{w} + \mathbf{b_c})$
$\mathbf{w} = [\mathbf{x}_t;\ \mathbf{h}_{t-1}]$
$\mathbf{c}_{t-1}$
$\mathbf{h}_{t-1}$
$\mathbf{x}_t$

Figure: An LSTM cell as described in[HS97; Gre+16].

Long Short Term Memory (LSTM)

Like a differentiable memory chip [Gra12] LSTM-memory can store n_h numbers. Gates govern all changes to the cell state. Gate and state equations are defined as [HS97; Gre+16]

$$\mathbf{z}_t = \tanh(\mathbf{W}_z \mathbf{x}_t + \mathbf{R}_z \mathbf{h}_{t-1} + \mathbf{b}_z), , \tag{4}$$

$$\mathbf{i}_t = \sigma(\mathbf{W}_i \mathbf{x}_t + \mathbf{R}_i \mathbf{h}_{t-1} + \mathbf{p}_i \odot \mathbf{c}_{t-1} + \mathbf{b}_i), \tag{5}$$

$$\mathbf{f}_t = \sigma(\mathbf{W}_f \mathbf{x}_t + \mathbf{R}_f \mathbf{h}_{t-1} + \mathbf{p}_f \odot \mathbf{c}_{t-1} + \mathbf{b}_f), \tag{6}$$

$$\mathbf{c}_t = \mathbf{z}_t \odot \mathbf{i}_t + \mathbf{c}_{t-1} \odot \mathbf{f}_t, \tag{7}$$

$$\mathbf{o}_t = \sigma(\mathbf{W}_o \mathbf{x}_t + \mathbf{R}_o \mathbf{h}_{t-1} + \mathbf{p}_o \odot \mathbf{c}_t + \mathbf{b}_o), \tag{8}$$

$$\mathbf{h}_t = \tanh(\mathbf{c}_t) \odot \mathbf{o}_t. \tag{9}$$

Potential new states $\mathbf{z}_t$ are called block input. $\mathbf{i}$ is called the input gate. The forget gate is $\mathbf{f}$ and $\mathbf{o}$ denotes the output gate. $\mathbf{p} \in \mathbb{R}^{n_h}$ are peephole weights, $\mathbf{W} \in \mathbb{R}^{n_i \times n_h}$ denotes input, $\mathbf{R} \in \mathbb{R}^{n_o \times n_h}$ are the recurrent matrices. $\odot$ indicates element-wise products.

Long Short Term Memory (LSTM)

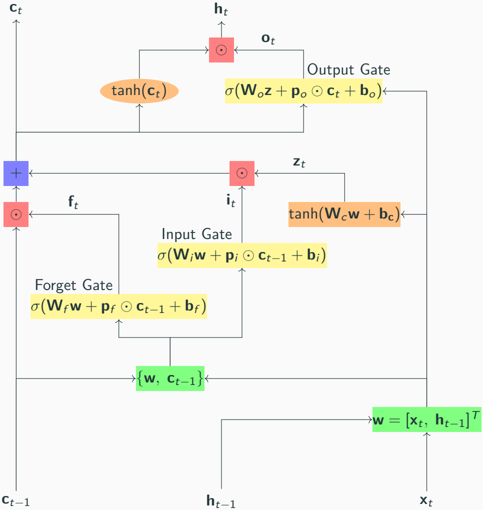

$\mathbf{c}_t$
$\mathbf{h}_t$
$\odot$
$\mathbf{o}_t$
Output Gate
$\tanh(\mathbf{c}_t)$
$\sigma(\mathbf{W}_o\mathbf{z} + \mathbf{p}_o \odot \mathbf{c}_t + \mathbf{b}_o)$
$+$
$\odot$
$\mathbf{z}_t$
$\odot$
$\mathbf{f}_t$
$\mathbf{i}_t$
$\tanh(\mathbf{W}_c\mathbf{w} + \mathbf{b_c})$
Input Gate
$\sigma(\mathbf{W}_i\mathbf{w} + \mathbf{p}_i \odot \mathbf{c}_{t-1} + \mathbf{b}_i)$
Forget Gate
$\sigma(\mathbf{W}_f\mathbf{w} + \mathbf{p}_f \odot \mathbf{c}_{t-1} + \mathbf{b}_f)$
$\{\mathbf{w},\ \mathbf{c}_{t-1}\}$
$\mathbf{w} = [\mathbf{x}_t,\ \mathbf{h}_{t-1}]^T$
$\mathbf{c}_{t-1}$
$\mathbf{h}_{t-1}$
$\mathbf{x}_t$

Figure: An LSTM-cell with peephole connections as described in [HS97; Gre+16]

Gated recurrent Units

$$\mathbf{r}_t = \sigma(\mathbf{W}_r\mathbf{h}_{t-1} + \mathbf{V}_r\mathbf{x}_t + \mathbf{b}_r), \tag{10}$$

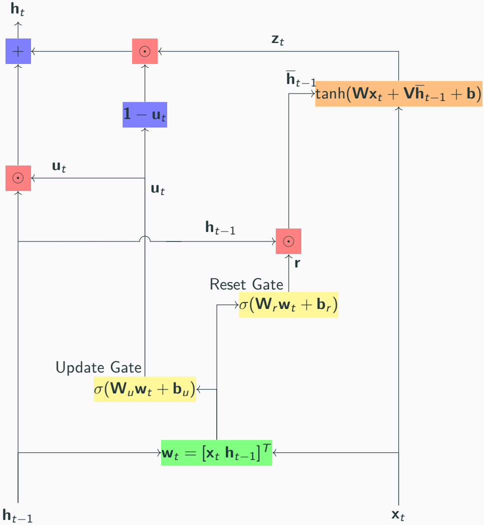
$$\mathbf{u}_t = \sigma(\mathbf{W}_u\mathbf{h}_{t-1} + \mathbf{V}_u\mathbf{x}_t + \mathbf{b}_u) \tag{11}$$

$$\mathbf{z}_t = \tanh(\mathbf{W}(\mathbf{r}_t \odot \mathbf{h}_{t-1}) + \mathbf{V}\mathbf{x}_t + \mathbf{b}), \tag{12}$$

$$\mathbf{h}_t = \mathbf{u}_t \odot \mathbf{z}_t + (1 - \mathbf{u}_t) \odot \mathbf{h}_{t-1}. \tag{13}$$

$\mathbf{h}_t \in \mathbb{R}^{n_h}$ denotes the cell state and output at time t. The block input is called $\mathbf{z}_t \in \mathbb{R}^{n_h}$. The reset $\mathbf{r} \in \mathbb{R}^{n_h}$ and update gates $\mathbf{u} \in \mathbb{R}^{n_h}$ take care of memory management. $\mathbf{W} \in \mathbb{R}^{n_i \times n_h}$ denote input matrices, $\mathbf{V} \in \mathbb{R}^{n_h \times n_h}$ is used for recurrent weight matrices.

Gated recurrent units


$\mathbf{h}_t$
$+$
$\odot$
$\mathbf{z}_t$
$\overline{\mathbf{h}}_{t-1}$
$\tanh(\mathbf{W}\mathbf{x}_t + \mathbf{V}\overline{\mathbf{h}}_{t-1} + \mathbf{b})$
$\mathbf{1} - \mathbf{u}_t$
$\mathbf{u}_t$
$\odot$
$\mathbf{u}_t$
$\mathbf{h}_{t-1}$
$\odot$
$\mathbf{r}$
Reset Gate
$\sigma(\mathbf{W}_r\mathbf{w}_t + \mathbf{b}_r)$
Update Gate
$\sigma(\mathbf{W}_u\mathbf{w}_t + \mathbf{b}_u)$
$\mathbf{w}_t = [\mathbf{x}_t\ \mathbf{h}_{t-1}]^T$
$\mathbf{h}_{t-1}$
$\mathbf{x}_t$

Stiefel Manifold Weight Updates [Wisdom2016]

$$\mathbf{h}_t = \mathrm{ReLU}(\mathbf{W}_h \mathbf{h}_t + \mathbf{W}_x \mathbf{x}_t + \mathbf{b}) \tag{14}$$

$$\mathbf{W}_{k+1} = (\mathbf{I} + \frac{\lambda}{2}\mathbf{A}_k)^{-1}(\mathbf{I} - \frac{\lambda}{2}\mathbf{A}_k)\mathbf{W}_k, \tag{15}$$

$$\text{where} \qquad \mathbf{A} = \mathbf{W}\overline{\nabla_{\mathbf{w}} F}^T - \overline{\mathbf{W}}^T \nabla_{\mathbf{w}} F. \tag{16}$$

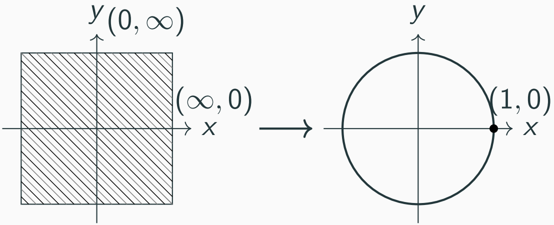


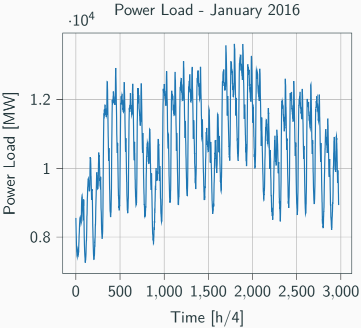
Figure: Fix the optimized matrix eigenvalues onto the unit circle.

Summary

- LSTM works like a differentiable memory chip.
- When in doubt, use LSTM.

Applications

Time-series forecasting



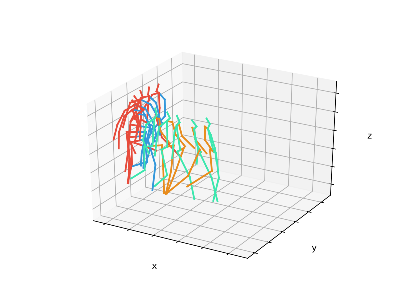
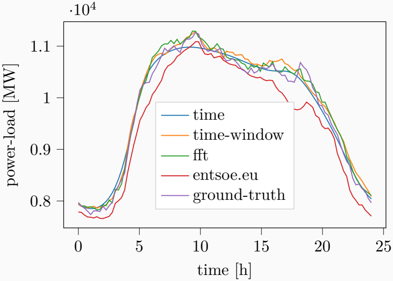
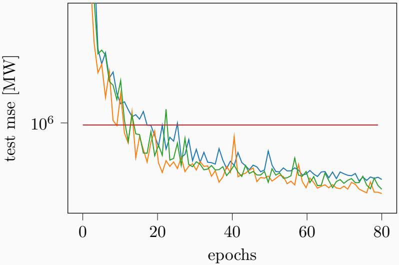


Figure: Monovariate power-load and multivariate motion-capture time series data.

Day-ahead power-load

Day-ahead power load forecasting using European Network of Transmission system operators for electricity data: [WGY20]





Language Processing

One hot encoding for letters. A possible encoding looks for all characters in a dataset. The number of occurring characters determines the length of every one-hot character vector. A system that accepts text and produces text, therefore, maps one-hot encoded sequences onto each other.

Neural Keyboard

Given a sequence of input letters or words LSTM, for example, can model the probability of the next letter or word.

$$p_n(y_i|y_1, y_2, \dots, y_{i-1} = LSTM(y_{i-1}, c_{i-1}, h_{i-1}) \tag{17}$$

This could, for example, help users type.

Conclusion

- RNNs are versatile and suitable for many different sentence processing tasks.
- But, there's more!

Example: Machine Translation

[BCB15] used RNN for the task of machine translation.

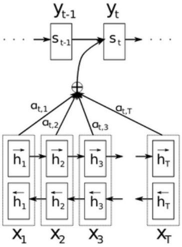
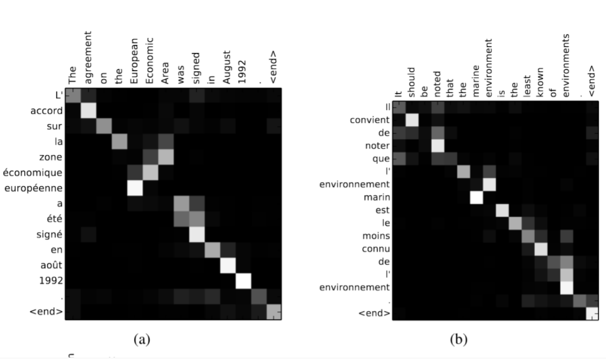


Figure 1: The graphical illustration of the proposed model trying to generate the t-th target word y_t given a source sentence $(x_1, x_2, \ldots, x_T)$.

Figure: An RNN-based translation system. Figure from [BCB15].

Neural attention in machine translation

Attention weights group related inputs together, allowing a decoder to find a suitable translation.

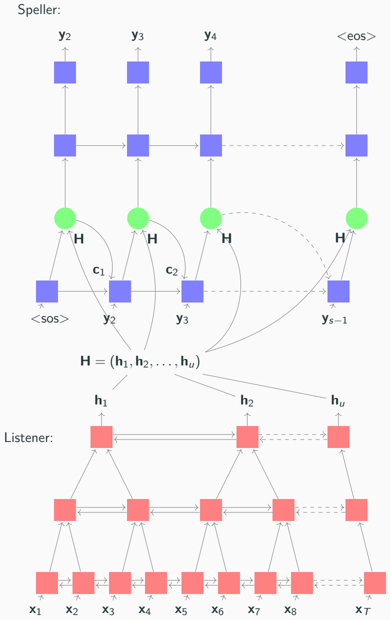


(a)

(b)

Figure: Attention plots as observed by [BCB15].

Speech Processing [Cha+15]



Attention weights

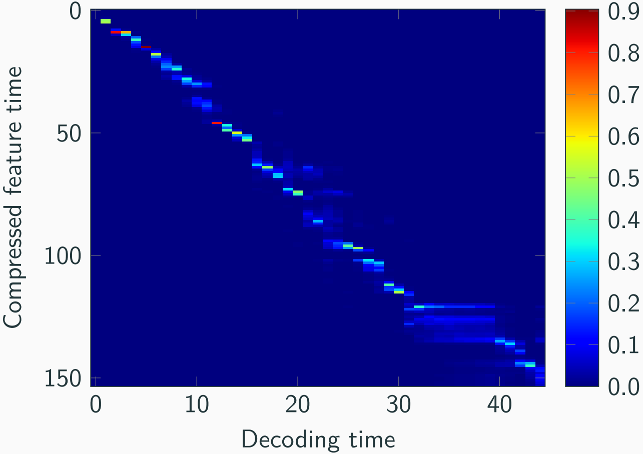


Figure: Attention weights for the speech processing example. On a TIMIT-recording.

Neural Attention and Transformers

Bahadanau attention

Proposed in [BCB15],

$$\mathbf{c}_i = \sum_{j=i}^{T_x} \alpha_{ij} \mathbf{h}_j \tag{18}$$

The idea is to find new αs for every decoding time step i. These are computed using a softmax

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{T_x} \exp(e_{ik})} \tag{19}$$

if the alignment model outputs $e_{ij} = a(s_{i-1}, h_j)$. Finally, a denotes a feedforward network function of the decoder state $\mathbf{s}_{i-1}$ and annotation $\mathbf{h}_j$.

Transformers

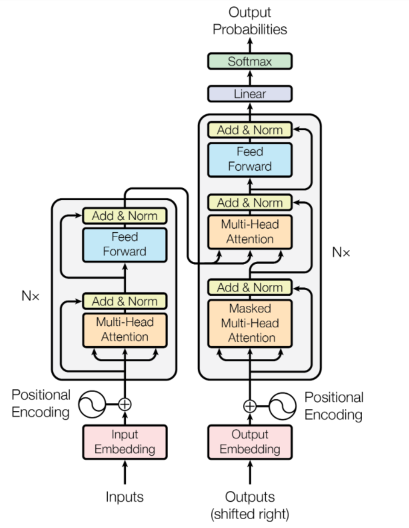


Figure: The transformer architecture as shown in [Vas+17]

Transformers

[Vas+17] defines dot product attention as,

$$\mathbf{C} = \sigma_s(\frac{\mathbf{QK}^T}{\sqrt{d_k}})\mathbf{V} \tag{20}$$

With context $\mathbf{C} \in \mathbb{R}^{t,d_k}$, queries $\mathbf{Q} \in \mathbb{R}^{t,d_k}$, keys $\mathbf{K} \in \mathbb{R}^{t,d_k}$, and values $\mathbf{V} \in \mathbb{R}^{t,d_k}$. σ_s denots the softmax.

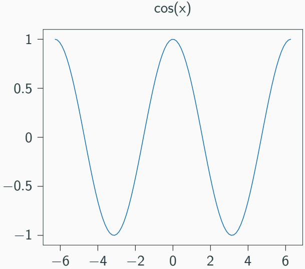
Matrix multiplication and dot products

We can express matrix multiplication as dot products.

$$\mathbf{QK} = \begin{pmatrix} \mathbf{q}_{1,1 \ldots d_k} \cdot \mathbf{k}_{1 \ldots d_k,1} & \mathbf{q}_{1,1 \ldots d_k} \cdot \mathbf{k}_{1 \ldots d_k,2} & \cdots \\ \mathbf{q}_{2,1 \ldots d_k} \cdot \mathbf{k}_{1 \ldots d_k,1} & \mathbf{q}_{2,1 \ldots d_k} \cdot \mathbf{k}_{1 \ldots d_k,2} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \qquad (21)$$

Alternatively the dot product of two vectors can be written as:

$$\mathbf{q} \cdot \mathbf{k} = |\mathbf{q}||\mathbf{k}|cos(\theta) \qquad (22)$$



Denoising Diffusion Probabilistic Models

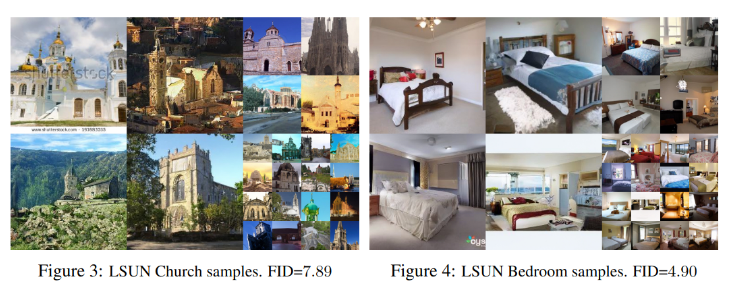


Figure 3: LSUN Church samples. FID=7.89

Figure 4: LSUN Bedroom samples. FID=4.90

Figure: Diffusion models rely on a combination of unets and self attention [HJA20].

Conclusion

- Transformers dominate large parts of modern deep learning.
- Their versatility comes at the cost of an enourmous data hunger.
- CNN and RNN are still often the better choice on smaller data-sets.
- In today's exercise you can choose to train a generative RNN or a generative transformer.

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[Vas+17] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. "Attention is all you need." In: *Advances in neural information processing systems* 30 (2017).

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[WGY20] Moritz Wolter, Juergen Gall, and Angela Yao. "Sequence Prediction using Spectral RNNs." In: *29th International Conference on Artificial Neural Networks*. 2020.

Code snippets

Sequence coding with dictionaries

```
for int_seq in sequences:
char_seq = []
for int_char in int_seq:
    char_seq.append(
      inv_vocab[int(int_char)])
res.append(char_seq)
```