Introduction to Neural Networks and Deep Learning

Recurrent Neural Networks

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Outline

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In 1987 Robinson and Fallside [2]

At Cambridge University Engineering Department

- They proposed a new type of neural network based on Linear Control Theory

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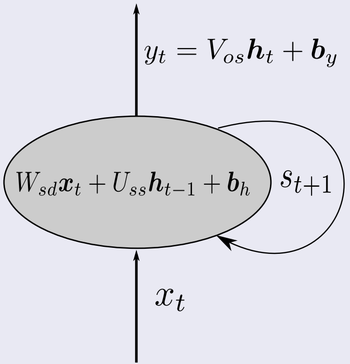
They took the work of Jacobs, 1974 on dynamic nets [1]

$$
\begin{aligned}
s_{t+1} &= As_t + Bx_t \\
y_t &= Cs_t
\end{aligned}
$$

Example of this unit

We have



Furthermore

Jordan Proposed a simple recurrent network

$$\boldsymbol{h}_t = \sigma_h \left(W_{sd} \boldsymbol{x}_t + U_{ss} \boldsymbol{h}_{t-1} + \boldsymbol{b}_h \right)$$

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Where

1. $\boldsymbol{x}_t$ is an input of dimension d.

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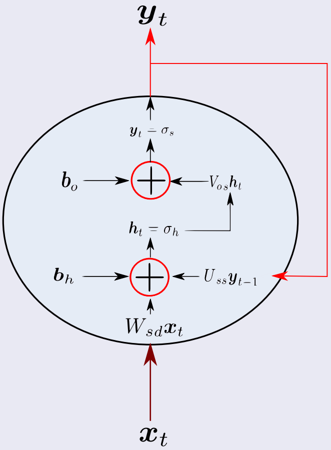
6. σ_h and σ_s are activation functions.

Graphically

We have



What were they used for?

Robinson and Fallside

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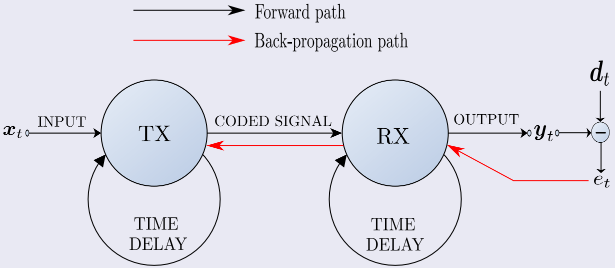
They proposed the following architecture



Outline

Based on the State-Space Model

Basically, a linear system

- Based in a state-determined system model

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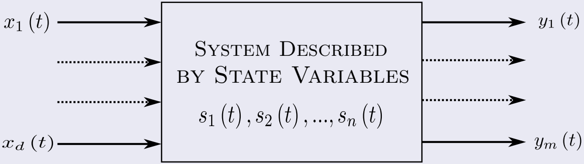
Definition

- A mathematical description of the system in terms of a minimum set of variables $x_i(t)$, $i = 1, ..., n$, together with knowledge of those variables at an initial time t_0 and the system inputs for time $t \geq t_0$, are sufficient to predict the future system state and outputs for all time $t > t_0$.

Therefore

We have a system as a block



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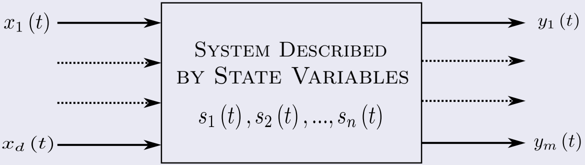

This can be expressed as a state equations

$$
\begin{aligned}
\dot{s}_1 &= f_1(\boldsymbol{x}, \boldsymbol{s}, t) \\
\dot{s}_2 &= f_2(\boldsymbol{x}, \boldsymbol{s}, t) \\
\cdots &= \cdots \\
\dot{s}_n &= f_n(\boldsymbol{x}, \boldsymbol{s}, t)
\end{aligned}
$$

Using Vector Notation

Assuming that we have a linear system and time invariant

- Time-Invariant $\bowtie$ $x(t+\delta)$ directly equates $y(t+\delta)$, for example

$$\alpha x(t+\delta)+\beta=y(t+\delta)$$

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Therefore, using this idea

$$\dot{s}_i = a_{i1}x_1(t)+...+a_{id}x_d(t)+b_{11}s_1(t)+...+b_{1n}s_n(t)$$

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$$\dot{s}_i=a_{i1}x_1(t)+\ldots+a_{id}x_d(t)+b_{11}s_1(t)+\ldots+b_{1n}s_n(t)$$

Or in Matrix form

$$\boldsymbol{y}(t)=A\boldsymbol{x}(t)+B\boldsymbol{s}(t)$$

Then, the discretized version

We introduce an update for the state part

$$
\begin{aligned}
\boldsymbol{y}(t) &= A\boldsymbol{x}(t) + B\boldsymbol{s}(t) \\
\dot{\boldsymbol{s}}(t) &= C\boldsymbol{s}(t)
\end{aligned}
$$

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$$\begin{aligned} \boldsymbol{y}(t) &= A\boldsymbol{x}(t) + B\boldsymbol{s}(t) \\ \dot{\boldsymbol{s}}(t) &= C\boldsymbol{s}(t) \end{aligned}$$

Or our discrete step equations

$$\begin{aligned} \boldsymbol{y}(t) &= A\boldsymbol{x}(t) + B\boldsymbol{s}(t) \\ \boldsymbol{s}(t+1) &= C\boldsymbol{s}(t) \end{aligned}$$

Outline

The Elman Network

In Elman's Equations

$$\boldsymbol{h}_t = \sigma_h \left(W_{sd} \boldsymbol{x}_t + U_{ss} \boldsymbol{h}_{t-1} + \boldsymbol{b}_h \right)$$
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We noticed something different from the linear recurrent system

- The use of activation functions to introduce the concept of non-linearity

Explanation

We have the following

1. The input $\boldsymbol{x}_t$ is coded by W_{sd}

$$W_{sd}\boldsymbol{x}_t$$

2. An state is generated by using the codified version of the input plus a previous state $\boldsymbol{h}_{t-1}$

$$\boldsymbol{h}_t = \sigma_h\left(W_{sd}\boldsymbol{x}_t + U_{ss}\boldsymbol{h}_{t-1} + \boldsymbol{b}_h\right)$$

3. The output is generated using the new state $\boldsymbol{h}_t$

$$\boldsymbol{y}_t = \sigma_y\left(V_{os}\boldsymbol{h}_t + \boldsymbol{b}_y\right)$$

Outline

We need to introduce the concept of cost function

Which as always

- It needs to comply with two properties

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The cost function L must be able to be written as an average

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This allow to apply different optimization techniques as

- Minbatch
- Stochastic Gradient Descent
- etc

Furthermore

Non dependency

- The cost function L must not be dependent on any activation values of a neural network besides the output values.

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If we cannot assure this

- If not Backpropagation becomes too unstable or too complex to solve. For example

$$L = \frac{1}{N}\sum_{t=0}^{N}\left[y_t + h_t - z_t\right]^2$$

  - This gives two entry points to the network.

A List of Cost Functions

The Average Quadratic Cost

$$L = \frac{1}{N}\sum_{t=0}^{N}\left[y_t - z_t\right]^2$$

- Where y_t is the output of the network and z_t is the ground truth of the output.

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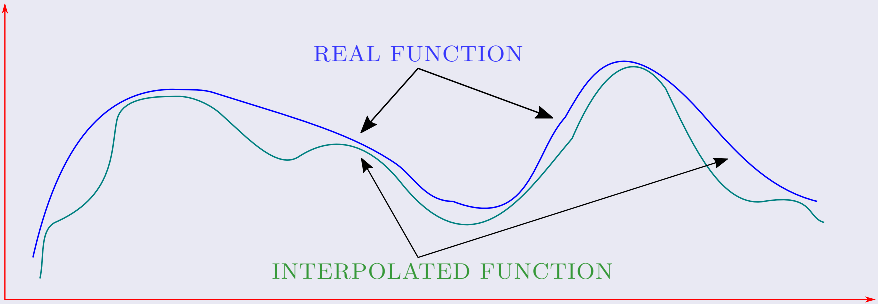
Here, we are interpolating functions



Cross-Entropy Cost

First, the Loss Function

$$L = -\sum_{i=1}^{C} z_i \log\left(y_i\right)$$

- Where y_i is the output and z_i is the ground truth for the class estimation.

Cross-Entropy Cost

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Why $y_i \log(z_i)$?

- We can imagine a sequence of class probabilities $y_1, y_2, ..., y_m$ and the likelihood of the data and the model

$$P[data|model] = y_1^{k_1} y_2^{k_2} \cdots y_m^{k_n}$$

Then

Taking the logarithm and multiplying by -1

$$-\log P\left[data|model\right] = -\sum_{i=1}^{C} k_i \log y_i$$

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Then, dividing by the total number of samples

$$-\frac{1}{N}\log P\left[data|model\right] = -\sum_{i=1}^{C} \frac{k_i}{N} \log y_i = -\sum_{i=1}^{C} z_i \log y_i$$

Now, we introduce...

The Kraft–McMillan theorem

- Let each source symbol from the alphabet

$$\mathcal{A} = \{a_1, a_2, ..., a_n\}$$

be encoded into a uniquely decodable code over an alphabet of size r with codeword lengths $\ell_1, \ell_2, ..., \ell_n$. Then

$$\sum_{i=1}^{n} r^{-\ell_1} \leq 1$$

In information theory

The Kraft–McMillan theorem

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It can be seen as representing an implicit probability distribution over $\{x_1, x_2, ..., x_n\}$

$$q(x_i) = (2)^{-\ell_i}$$

- Where ℓ_i is the length of the code for x_i

Now

We have that

- Cross entropy can be interpreted as the expected message-length per datum when a wrong distribution q is assumed while the data actually follows a distribution p.

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The expected message-length under the true distribution p is

$$
\begin{aligned}
E_p[l] &= -E_p\left[\frac{\ln q(x)}{\ln 2}\right] \\
&= -E_p\left[\log_2 q(x)\right] \\
&= -\sum_{x_i} p(x_i) \log_2 q(x) \\
&= H(p, q)
\end{aligned}
$$

Special Case

A special case is the binary class problem, $C = 2$

- Based on the fact that $z_1 + z_2 = 1$ and $y_1 + y_2 = 1$

$$L = -\sum_{i=1}^{2} z_i \log(y_i) = -z_1 \log(y_1) - (1 - z_1)\log(1 - y_1)$$

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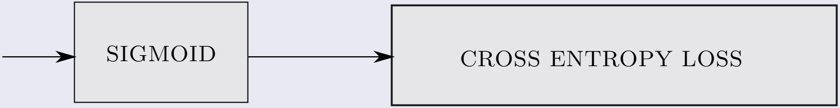
A problem of this

- It could be possible to have a $y_i = 0$

Dealing with this problem

We can use an activation function in front of it



$$y_1 = f\left(v_i\right) = \frac{1}{1+\exp(-v_1)} \quad L = -z_1 \log\left(y_1\right) - \left(1 - z_1\right) \log\left(1 - y_1\right)$$

Another Interpretation

The Loss can be expressed as

$$L = \begin{cases} -\log\left(f\left(y_1\right)\right) & \text{if } z_1 = 1 \\ -\log\left(1 - f\left(y_1\right)\right) & \text{if } z_1 = 0 \end{cases}$$

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Where $z_1 = 1$

- It means that the class $C_i = C_1$ is positive for this sample.

The Gradient of the Binary Cross Entropy

We make a derivative with respect to y_i

$$\frac{\partial L}{\partial y_1} = z_1 \left(f\left(y_1 \right) - 1 \right) + \left(1 - z_1 \right) f\left(y_1 \right)$$

In the case of the Multiclass Problem

We use two things, a softmax

$$f(y_i) = \frac{\exp\{y_i\}}{\sum_{j=1}^{C} \exp\{y_j\}}$$

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As in the multiclass for the Linear Models

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Therefore

- There is only one element of the Target vector z that is not zero, $z_i = z_p$.

We can then simplify

The cost function becomes

$$L=-\sum_{i=1}^{C} z_i \log\left(f\left(y_i\right)\right) = -log\left(\frac{\exp\left\{y_p\right\}}{\sum_{j=1}^{C}\exp\left\{y_p\right\}}\right)$$

Outline

Other Cost Functions

Exponential Cost with hyper-parameter τ

$$L = \tau \exp\left[\frac{1}{\tau}\sum_{i=1}^{N}(y_i - z_i)^2\right]$$

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Hellinger Distance

$$L = \frac{1}{2}\sum_{i=1}^{N}\left(\sqrt{y_i} - \sqrt{z_i}\right)^2$$

- Here the values need to be at the interval $[0, 1]$.

Other Cost Functions

Given Kullback-Leibler Divergence

$$D_{KL}\left(P \parallel Q\right) = \sum_{i} P\left(i\right) \ln \frac{P\left(i\right)}{Q\left(i\right)}$$

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The Final Cost function

$$L = \sum_j \hat{y}_j \log \frac{\hat{y}_j}{y_j^{pred}}$$

Outline

We have the following

Architecture with Quadratic Error

$$\boldsymbol{h}_t = \sigma_h \left(W_{sd}\boldsymbol{x}_t + U_{ss}\boldsymbol{h}_{t-1} + \boldsymbol{b}_h \right)$$

$$\boldsymbol{y}_t = \sigma_y \left(V_{os}\boldsymbol{h}_t + \boldsymbol{b}_y \right)$$

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$$L = \frac{1}{2} \sum_{t=0}^{N} \left[y_t - z_t \right]^2$$

Something Notable

- How do we train something with a recurrence forcing a dependence over time?

Outline

Now, given the dependency over time

We can use the classic unfolding of the network [3, 4] by assuming

- W, U, V, b_h and b_o do not change under the unfolding

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Unfolding?

- Assume that there are not bias correcting terms, only, W, U and V.

Then

Given an observation sequence $\boldsymbol{x} = \{x_1, x_2, ..., x_T\}$

- where $x_i \in \mathbb{R}$, and their corresponding label $y = \{y_1, y_2, ..., y_T\}$

Then

Given an observation sequence $\boldsymbol{x} = \{x_1, x_2, ..., x_T\}$

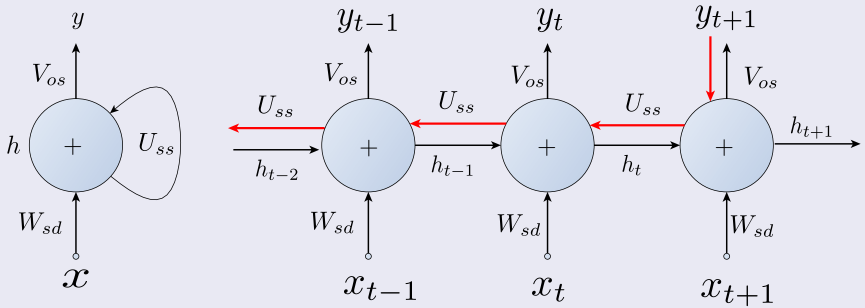
- where $x_i \in \mathbb{R}$, and their corresponding label $y = \{y_1, y_2, ..., y_T\}$

We remove the bias to simplify our derivations

$$
\begin{aligned}
\boldsymbol{h}_t &= \phi_h\left(W_{sd}\boldsymbol{x}_t + U_{ss}\boldsymbol{h}_{t-1}\right)\\
y_t &= \phi_y\left(V_{os}\boldsymbol{h}_t\right)\\
L &= \frac{1}{2}\sum_{t=0}^{T}\left[z_t - y_t\right]^2
\end{aligned}
$$

Unfolding

We can then see the unfolding of the recurrence



Outline

General Chain Rule

General Chain Rule

- When $z = f(x(s,t), y(s,t))$ is the composition of $z = f(x,y)$ and $x = x(s,t)$ and $y = y(s,t)$ then its partial derivatives are given by

$$\frac{\partial z}{\partial s} = \frac{\partial f(x(s,t), y(s,t))}{\partial s} = \frac{\partial f}{\partial x} \times \frac{\partial x}{\partial s} + \frac{\partial f}{\partial y} \times \frac{\partial y}{\partial s}$$
$$\frac{\partial z}{\partial t} = \frac{\partial f(x(s,t), y(s,t))}{\partial t} = \frac{\partial f}{\partial x} \times \frac{\partial x}{\partial t} + \frac{\partial f}{\partial y} \times \frac{\partial y}{\partial t}$$

This allows

To simplify the backpropagation process

$$
\begin{aligned}
\frac{\partial L}{\partial V_{os}} &= \frac{1}{2}\sum_{t=0}^{T}\frac{\partial L}{\partial y_t}\times\frac{\partial y_t}{\partial V_{os}} \\
&= \frac{1}{2}\sum_{t=0}^{T}\frac{\partial L}{\partial y_t}\times\frac{\partial y_t}{\partial net_o}\times\frac{\partial net_o}{\partial V_{os}} \\
&= -\sum_{t=0}^{T}\left[z_t - y_t\right]\times\frac{\partial y_t}{\partial net_o}\times\frac{\partial net_o}{\partial V_{os}}
\end{aligned}
$$

- Where $net_o^t = V_{os}\boldsymbol{h}_t$

Now, we have

We have that

$$\frac{\partial y_t}{\partial net_o} = \begin{pmatrix} \frac{\partial y_{t1}}{\partial net_{o1}} & \frac{\partial y_{t1}}{\partial net_{o2}} & \cdots & \frac{\partial y_{t1}}{\partial net_{oo}} \\ \frac{\partial y_{t2}}{\partial net_{o1}} & \frac{\partial y_{t2}}{\partial net_{o2}} & \cdots & \frac{\partial y_{t2}}{\partial net_{oo}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_{to}}{\partial net_{o1}} & \frac{\partial y_{to}}{\partial net_{o2}} & \cdots & \frac{\partial y_{to}}{\partial net_{oo}} \end{pmatrix}$$

Simplify!!!

Now, we have that if $i = j$

$$\frac{\partial y_{ti}}{\partial net_{oi}} = \phi_o' \left(net_{oi} \right)$$

Simplify!!!

Now, we have that if $i = j$

$$\frac{\partial y_{ti}}{\partial net_{oi}} = \phi_o' \left(net_{oi}\right)$$

And for the rest, we have $i \neq j$

$$\frac{\partial y_{ti}}{\partial net_{oi}} = 0$$

Finally

We have that

$$\frac{\partial y_t}{\partial net_o} = \begin{pmatrix} \phi_o'(net_{o1}) & 0 & \cdots & 0 \\ 0 & \phi_o'(net_{o2}) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \phi_o'(net_{oo}) \end{pmatrix} = A$$

Now, $\frac{\partial net_o}{\partial V_{os}}$

First we have a component i

$$net_{oi} = \sum_{j=1}^{s} V_{ij} h_j$$

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What happen when we derive with respect to the matrix?

$$\frac{\partial net_o}{\partial V_{os}} = \begin{bmatrix} \frac{\partial net_o}{\partial V_{11}} & \frac{\partial net_o}{\partial V_{12}} & \cdots & \frac{\partial net_o}{\partial V_{1s}} \\ \frac{\partial net_o}{\partial V_{21}} & \frac{\partial net_o}{\partial V_{22}} & \cdots & \frac{\partial net_o}{\partial V_{2s}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial net_o}{\partial V_{o1}} & \frac{\partial net_o}{\partial V_{o2}} & \cdots & \frac{\partial net_o}{\partial V_{os}} \end{bmatrix}$$

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First we have a component i

$$net_{oi} = \sum_{j=1}^{s} V_{ij} h_j$$

What happen when we derive with respect to the matrix?

$$\frac{\partial net_o}{\partial V_{os}} = \begin{bmatrix} \frac{\partial net_o}{\partial V_{11}} & \frac{\partial net_o}{\partial V_{12}} & \cdots & \frac{\partial net_o}{\partial V_{1s}} \\ \frac{\partial net_o}{\partial V_{21}} & \frac{\partial net_o}{\partial V_{22}} & \cdots & \frac{\partial net_o}{\partial V_{2s}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial net_o}{\partial V_{o1}} & \frac{\partial net_o}{\partial V_{o2}} & \cdots & \frac{\partial net_o}{\partial V_{os}} \end{bmatrix}$$

Actually

- A Tensor with three dimensions...

But something quite nice

Each of the components of net_o

- It has the previous structure

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$$net_{oi} = \sum_{k=1}^{s} V_{ik} h_k$$

Then if the V_{jk} does not intervene on it

$$\frac{\partial net_{oi}}{\partial V_{jk}} = 0$$

Additionally if it intervenes

$$\frac{\partial net_{oi}}{\partial V_{jk}} = h_k$$

Therefore

It is possible to collapse the tensor into a 2D Matrix

- Given that the other information is redundant, ad we can rewrite the tensor as

$$F_{ijk} = \frac{\partial net_{oi}}{\partial V_{jk}}$$

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- Given that the other information is redundant, ad we can rewrite the tensor as

$$F_{ijk} = \frac{\partial net_{oi}}{\partial V_{jk}}$$

Then, we have that

$$F_{ijk} = G_{ij} \Leftarrow \text{Better Storage!!!}$$

Therefore, given that a matrix is a tensor also

We have that two tensors, $net^{o \times o}$ and $F^{o \times s \times o}$ [5]

- We will use the contracted product of two tensors which is a generalization of the tensor-vector and tensor-matrix multiplications

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Definition

- Given two tensors $A^{o \times o}$ and $B^{o \times s \times o}$

$$\langle A, B \rangle (k, j) = \sum_{i=1}^{o} A_{i,k} G_{i,j} = A_{i,i} G_{i,j} = \sigma' (net_{oi}) \, h_j$$

Now, the term $\frac{\partial L}{\partial U_{ss}}$

Assuming our change in time step $t \rightarrow t+1$ and given

$$\boldsymbol{h}_t = \phi_h \left(W_{sd} \boldsymbol{x}_t + U_{ss} \boldsymbol{h}_{t-1} \right)$$

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Therefore

- We can think on this as a Markovian Backpropagation

What if we go further

From $t-1 \rightarrow t+1$

$$\frac{\partial L\left(t+1\right)}{\partial U_{ss}} = \frac{\partial L\left(t+1\right)}{\partial y_{t+1}} \times \frac{\partial y_{t+1}}{\partial h_{t+1}} \times \frac{\partial h_{t+1}}{\partial h_t} \times \frac{\partial h_t}{\partial U_{ss}}$$

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However

- How do we calculate $\frac{\partial h_{t+1}}{\partial h_k}$?

We have a proposal

Given the product of functions

$$\frac{\partial h_{t+1}}{\partial h_k} = \frac{\partial h_{k+1}}{\partial h_k} \times \frac{\partial h_{k+2}}{\partial h_{k+1}} \times \cdots \times \frac{\partial h_{t+1}}{\partial h_t}$$

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Here, we know that

$$\frac{\partial h_{i+1}}{\partial h_i} = \frac{\partial h_{i+1}}{\partial net_s} \times \frac{\partial net_s}{\partial h_i}$$

We have that

We have given $\boldsymbol{h}_{i+1} = \phi_h \left(W_{sd} \boldsymbol{x}_i + U_{ss} \boldsymbol{h}_i \right)$ and $net_h = W_{sd} \boldsymbol{x}_i + U_{ss} \boldsymbol{h}_i$

$$\frac{\partial h_{i+1}}{\partial net_s} = \begin{pmatrix} \phi_h' \left(net_{h1} \right) & 0 & \cdots & 0 \\ 0 & \phi_h' \left(net_{h2} \right) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \phi_h' \left(net_{hs} \right) \end{pmatrix} = D_{i+1}$$

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Finally, we have that

$$\frac{\partial net_s}{\partial h_i} = U_{ss}$$

Then

We can aggregate over all the time

$$\frac{\partial L}{\partial U_{ss}} = \sum_{t=0}^{T} \sum_{k=1}^{t} \frac{\partial L\,(t+1)}{\partial y_{t+1}} \times \frac{\partial y_{t+1}}{\partial h_{t+1}} \times \frac{\partial h_{t+1}}{\partial h_k} \times \frac{\partial h_t}{\partial U_{ss}}$$

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Now, we need to derive the L with respect to W_{sd}

$$\frac{\partial L\left(t+1\right)}{\partial W_{sd}} = \frac{\partial L\left(t+1\right)}{\partial h_{t+1}} \times \frac{\partial h_{t+1}}{\partial W_{sd}}$$

Now

Because h_t and x_{t+1}, we need to back propagate to h_t

$$
\begin{aligned}
\frac{\partial L(t+1)}{\partial W_{sd}} &= \frac{\partial L(t+1)}{\partial h_{t+1}} \times \frac{\partial h_{t+1}}{\partial W_{sd}} + \frac{\partial L(t+1)}{\partial h_t} \times \frac{\partial h_t}{\partial W_{sd}} \\
&= \frac{\partial L(t+1)}{\partial h_{t+1}} \times \frac{\partial h_{t+1}}{\partial W_{sd}} + \frac{\partial L(t+1)}{\partial h_{t+1}} \times \frac{\partial h_{t+1}}{\partial h_t} \times \frac{\partial h_t}{\partial W_{sd}}
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Then summing over all the contributions from 0 to T

$$\frac{\partial L(t+1)}{\partial W_{sd}} = \sum_{t=0}^{T} \sum_{k=1}^{t+1} \frac{\partial L(t+1)}{\partial y_{t+1}} \times \frac{\partial y_{t+1}}{\partial h_{t+1}} \times \frac{\partial h_{t+1}}{\partial h_k} \times \frac{\partial h_t}{\partial W_{sd}}$$

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Outline

Vanishing Gradients

We have a problem

$$\frac{\partial h_{k+1}}{\partial h_k} \times \frac{\partial h_{k+2}}{\partial h_{k+1}} \times \cdots \times \frac{\partial h_{t+1}}{\partial h_t}$$

Vanishing Gradients

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$$\frac{\partial h_{k+1}}{\partial h_k} \times \frac{\partial h_{k+2}}{\partial h_{k+1}} \times \cdots \times \frac{\partial h_{t+1}}{\partial h_t}$$

You finish with a vanishing gradient using $\sigma = \frac{1}{1+\exp\{-x\}}$

- This is problematic!!!

Given

Given the commutativity of the product

- You could put together the derivative of the sigmoid's

$$f\left(x\right)=\frac{ds\left(x\right)}{dx}=\frac{e^{-x}}{\left(1+e^{-x}\right)^{2}}$$

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$$f(x) = \frac{ds(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2}$$

Therefore, deriving again

$$\frac{df(x)}{dx} = -\frac{e^{-x}}{(1+e^{-x})^2} + \frac{2(e^{-x})^2}{(1+e^{-x})^3}$$

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After making $\frac{df(x)}{dx} = 0$

- We have the maximum is at $x = 0$

Therefore

The maximum for the derivative of the sigmoid

- $f(0) = 0.25$

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Therefore, Given a **Deep** Network

- We could finish with

$$\lim_{k\to\infty}\left(\frac{ds(x)}{dx}\right)^k = \lim_{k\to\infty}(0.25)^k \to 0$$

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The maximum for the derivative of the sigmoid

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$$\lim_{k \to \infty} \left(\frac{ds(x)}{dx} \right)^k = \lim_{k \to \infty} (0.25)^k \to 0$$

A Vanishing Derivative or Vanishing Gradient

- Making quite difficult to do train a deeper network using this activation function for Deep Learning and even in Shallow Learning

For the case of vanishing gradient, we have that

Rearranging terms in $\frac{\partial h_{k+1}}{\partial h_k} \times \frac{\partial h_{k+2}}{\partial h_{k+1}} \times \cdots \times \frac{\partial h_{t+1}}{\partial h_t}$

- We have

$$\left[\prod_{k=0}^{T} \frac{\partial h_{k+1}}{\partial net_s}\right] [U_{ss}]^{T+1}$$

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Then, given the sigmoid

$$\prod_{k=0}^{T} \frac{\partial h_{k+1}}{\partial net_s} = \begin{bmatrix} \prod_{k=0}^{T} \phi_h'\left(net_{h1}^{k}\right) & 0 & \cdots & 0 \\ 0 & \prod_{k=0}^{T} \phi_h'\left(net_{h2}^{k}\right) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \prod_{k=0}^{T} \phi_h'\left(net_{hs}^{k}\right) \end{bmatrix}$$

It is clear

That you have the phenomena of vanishing gradient

- Do we have a way to fixing this?

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That you have the phenomena of vanishing gradient

- Do we have a way to fixing this?

Yes

- The use of new activation functions.

For example, the ReLu activation function

The need to introduce a new function

$$f(x) = x^{+} = \max(0, x)$$

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$$f(x) = x^{+} = \max(0, x)$$

It is called ReLu or Rectifier

With a smooth approximation (Softplus function)

$$f(x) = \frac{\ln\left(1 + e^{kx}\right)}{k}$$

Outline

However

Here the gradient can explode

- Thus, the need to control the gradient...

However

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- Thus, the need to control the gradient...

Therefore, we will use the following analysis [6]

- "The Emergence of Spectral Universality in Deep Networks" by Jeffrey Pennington, Samuel S. Schoenholz, Surya Ganguli

We have

The following dynamic

$$\boldsymbol{h}_t = \phi_h\left(s_t\right),\ \boldsymbol{s}_t = W_{sd}\boldsymbol{x}_t + U_{ss}\boldsymbol{h}_{t-1} + b_h$$

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$$\boldsymbol{h}_t = \phi_h\left(s_t\right),\ \boldsymbol{s}_t = W_{sd}\boldsymbol{x}_t + U_{ss}\boldsymbol{h}_{t-1} + b_h$$

Then, we have the following Jacobian

$$J = \frac{\partial h_T}{\partial h_0} = \prod_{t=1}^{L} D_t U_{SS}$$

Here, we have

Where as we saw it D_t is a diagonal matrix

- With entries $D^t_{ij} = \phi'\left(s^l_i\right)\delta_{ij}$
  - Here δ_{ij} is the Kronecker delta function

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It is closely related to the backpropagation operator

- Mapping output errors to weight matrices at a given layer,
  - in the sense that if the former is well-conditioned, then the latter tends to be well-conditioned for all weight layers.

Actually

Given this matrix J

- We have that if we can analyze the set of eigenvalues (Spectrum)

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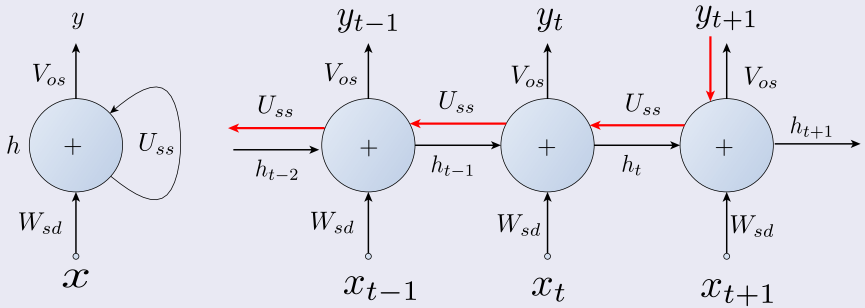
We can try to get a way

- To stabilize our training

A Trick

A RNN can be seen as a deep neural network



Remember the structure of the layer

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Therefore, we have that

$$s_{it} = \sum_j W_{ij}x_j^t + \sum_k U_{ik}h_k^{t-1} + b_i$$

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Therefore, we have that

$$s_{it} = \sum_j W_{ij}x_j^t + \sum_k U_{ik}h_k^{t-1} + b_i$$

We assume the following about the temporal layer weights

$$[U_{ss}, W_{sd}] \sim N\left(0, \frac{\sigma_w^2}{N}\right), b_h \sim N\left(0, \sigma_b^2\right)$$

- Here $N = s$ the state dimension.

Outline

Therefore, we have

In [7, 8]

- In these works, it has been shown that the propagation of a distribution through the N multiple layers, when N is large:
  - It tends to a Gaussian Distribution

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  - It tends to a Gaussian Distribution

With Zero Mean and Variance q^t

$$q^t = Var\left[q^{t-1}|\sigma_w, \sigma_b\right] = \sigma_w^2 \frac{1}{\sqrt{2\pi}} \int \phi_z \left(\sqrt{q^{t-1}} z\right)^2 \exp^{-\frac{z^2}{2}} dz + \sigma_b^2$$

- where σ_w and σ_b are standard deviations for $[W_{sd}, U_{ss}]$ and b_h respectively.
- With no correlation between the weights.

How is this possible?

We know the basic feedforward works as with the following propagation

$$x^t = \underset{\text{Act Function}}{\phi}\left(W^l \boldsymbol{x}^{t-1} + \boldsymbol{b}^t\right) \text{ for } t = 1, ..., D$$

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- Force the network to start to go from random to a more deterministic behavior

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- Force the network to start to go from random to a more deterministic behavior

For this we assume that the weights $W^l_{i,j}$ come from a Gaussian $N\left(0, \frac{\sigma_w^2}{N_{t-1}}\right)$

- Thus for N_t neurons at layer t in our case the unfolding:

$$d^2_{NE}\left(\boldsymbol{h}, 0\right) = q^t \approx \frac{1}{N_t}\sum_{i=1}^{N_t}\left(h_i^t - 0\right)^2 \approx Var\left(h^t\right)$$

Basically

The second central moment

- AKA THE VARIANCE!

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- AKA THE VARIANCE!

In a similar way

$$\boldsymbol{b}^t \sim N\left(0, \sigma_b^2 I\right)$$

The Gaussian always the Gaussian!!!

The Gaussian always the Gaussian!!!

Something Notable

- We can say q^t converges to a Zero Mean Gaussina since

$$h_i^t = \boldsymbol{w}_i^t \cdot \phi\left(\boldsymbol{h}^{t-1}\right) + b_i^t$$

  - It is a weighted sum of a larger number of uncorrelated random variables.
  - And Gaussian distributed because of that

How!!?? From Bayesian Casuality

Given a path in $G = (V, E)$

There are the edges connecting $[X_1, X_2, ..., X_k]$.

How!!?? From Bayesian Casuality

Given a path in $G = (V, E)$

There are the edges connecting $[X_1, X_2, ..., X_k]$.

Therefore

Given the directed edge $X \rightarrow Y$, we say the tail of the edge is at X and the head of the edge is Y.

Basic Classifications of Meetings

Head-to-Tail

A path $X \to Y \to Z$ is a **head-to-tail meeting**, the edges meet head-to-tail at Y, and Y is a head-to-tail node on the path.

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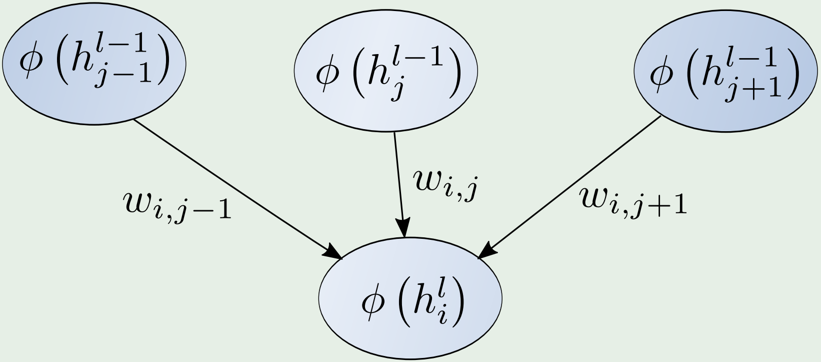
Head-to-Head

A path $X \to Y \leftarrow Z$ is a **head-to-head meeting**, the edges meet head-to-head at Y, and Y is a head-to-head node on the path.

Examples

Actually Head-to-Head



Blocking Information $\approx$ Conditional Independence

Definition 2.2

Let $G = (V, E)$ be a DAG, $A \subseteq V$, X and Y be distinct nodes in $V - A$, and ρ be a path between X and Y .

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Let $G = (V, E)$ be a DAG, $A \subseteq V$, X and Y be distinct nodes in $V - A$, and ρ be a path between X and Y .
Then ρ is **blocked** by A if one of the following holds:

1. There is a node $Z \in A$ on the path ρ, and the edges incident to Z on ρ meet head-to-tail at Z.
2. There is a node $Z \in A$ on the path ρ, and the edges incident to Z on ρ, meet tail-to-tail at Z.
3. There is a node Z, such that Z and all of Z's descendent's are not in A, on the chain ρ, and the edges incident to Z on ρ meet head-to-head at Z.

Thus

We can use the following idea

$$
\begin{aligned}
q^t =& \frac{1}{N_t}\sum_{i=1}^{N_t}\left[\boldsymbol{w}_i^t\phi\left(h^{t-1}\right)+b_i^t\right]^2\\
=& \frac{1}{N_t}\sum_{i=1}^{N_l}\left[\left(\boldsymbol{w}_i^t\phi\left(h^{t-1}\right)\right)^2+b_i^t\boldsymbol{w}_i^t\phi\left(h^{t-1}\right)+\left(b_i^t\right)^2\right]\\
=& \frac{1}{N_t}\sum_{i=1}^{N_l}\left[\left(\boldsymbol{w}_i^t\phi\left(h^{t-1}\right)\right)^2+\left(b_i^t\right)^2\right]+b_i^t\left[\underbrace{\frac{1}{N_t}\sum_{i=1}^{N_l}\boldsymbol{w}_i^t\phi\left(h^{t-1}\right)}_{0}\right]
\end{aligned}
$$

Therefore

Something Notable

$$q^t = \frac{1}{N_t} \sum_{i=1}^{N_t} \left[\left(\boldsymbol{w}_i^l \phi \left(h^{t-1} \right) \right)^2 + \left(b_i^t \right)^2 \right]$$

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Thus, we have that

$$q^t = \frac{1}{N_t} \sum_{i=1}^{N_t} \left[\left(\sum_{j=1}^{N_{t-1}} \boldsymbol{w}_{ij}^l \phi \left(h_j^{t-1} \right) \right)^2 + \left(b_i^t \right)^2 \right]$$

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$$\left(\sum_{j=1}^{N_{t-1}} \boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\right)^2=\sum_{j=1}^{N_{t-1}}\left[\boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\right]^2+\sum_{j,k=1,k\neq j}^{N_{t-1}}\boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\boldsymbol{w}_{ik}^{l}\phi\left(h_k^{t-1}\right)$$

Thus, we have that

Something Notable

$$\left(\sum_{j=1}^{N_{t-1}} \boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\right)^2 = \sum_{j=1}^{N_{t-1}}\left[\boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\right]^2 + \sum_{j,k=1,k\neq j}^{N_{t-1}} \boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\boldsymbol{w}_{ik}^{l}\phi\left(h_k^{t-1}\right)$$

But given the Gaussian $N\left(0, \frac{\sigma_w^2}{N_{t-1}}\right)$ and no correlation at weights

- $\frac{1}{N_t}\sum_{i=1}^{N_t} \boldsymbol{w}_{ij}^{l}\boldsymbol{w}_{ik}^{l} = 0$

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Something Notable

$$\left(\sum_{j=1}^{N_{t-1}} \boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\right)^2 = \sum_{j=1}^{N_{t-1}}\left[\boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\right]^2 + \sum_{j,k=1,k\neq j}^{N_{t-1}} \boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\boldsymbol{w}_{ik}^{l}\phi\left(h_k^{t-1}\right)$$

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Therefore

$$\frac{1}{N_t}\sum_{i=1}^{N_t}\sum_{j=1}^{N_{t-1}}\left[\boldsymbol{w}_{ij}^{l}\phi\left(h_j^{t-1}\right)\right]^2 = \sigma_w^2\frac{1}{N_{t-1}}\sum_{j=1}^{N_{t-1}}\left[\phi\left(h_j^{t-1}\right)\right]^2$$

Therefore

Here, we can say that $h_j^{t-1} \approx \sqrt{q^{t-1}}$

$$q^t \approx \rho_w^2 \frac{1}{\sqrt{2\pi}} \int \phi_z \left(\sqrt{q^{t-1}} z \right)^2 \exp^{-\frac{z^2}{2}} dz + \rho_b^2$$

Therefore

We have an initial condition

$$q^1 = \frac{\sigma_w^2}{N} \sum_{i=1}^{N} \left(x_i^0 \right)^2 + \sigma_b^2$$

We have two conditions

We have that if $q^1 = q^*$

- Then, the dynamics start at the fixed point and the distribution of D_t is independent of t.

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Even, when $q^1 \neq q^*$

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Therefore

- As such, when L is large, it is often a good approximation to assume that $q^1 = q^*$ for all t when computing the spectrum of J

Outline

Now, assume that

Now, consider the evolution of a single input through the network x_{it}

- Since the weights and biases are independent with zero mean

$$E\left[s_{it}\right] = 0$$

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$$E\left[s_{it}\right]=0$$

The second moment of the Gaussian random variable (Actually the Covariance)

$$E\left[s_{it}s_{jt}\right]=q^{t}\delta_{ij}$$

Where the second moment

Of a Gaussian Distribution is

$$\int_{-\infty}^{\infty} s^2 \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{(s-\mu)}{2\sigma^2}\right\} ds$$

Here we have

Here q^t is the variance of the pre-activations in the t^{th} layer due to an input $\boldsymbol{x}_t$

$$q^t = \frac{\sigma_w^2}{\sqrt{2\pi}} \int \phi_h^2\left(\sqrt{q^{t-1}}\boldsymbol{s}_{it-1}\right) \exp\left\{-\frac{1}{2}\boldsymbol{s}_{it}^2\right\} d\boldsymbol{s}_{it} + \sigma_b^2$$

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They describe the pass through the recursion of the RNN

- For any choice of σ_w^2 and σ_b^2 and a bounded ϕ_h the previous equation converges to a specific fix point.

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They describe the pass through the recursion of the RNN

- For any choice of σ_w^2 and σ_b^2 and a bounded ϕ_h the previous equation converges to a specific fix point.

This recursion has a fixed point

$$q^* = \frac{\sigma_w^2}{\sqrt{2\pi}} \int \phi_h^2 \left(\sqrt{q^*} \boldsymbol{s}_{it-1} \right) \exp\left\{ -\frac{1}{2} \boldsymbol{s}_{it}^2 \right\} d\boldsymbol{s}_{it} + \sigma_b^2$$

A Fixed Point

Definition

- In mathematics, a fixed point of a function is an element of the function's domain that is mapped to itself by the function.

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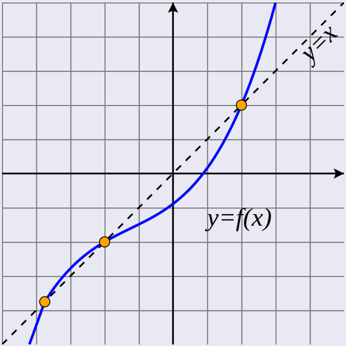
Example



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Not only that

- $q^1 \neq q^*$ a few layers is often sufficient to approximately converge to a fixed point.

So when t is large

- So it is a good approximation to assume $q^t = q^*$.

Additionally

The independence of the weights and biases implies

- The covariance between different pre-activations in the same layer will be given by

$$E\left[z_{it;a}z_{jt;b}\right] = q^{t}_{ab}\delta_{ij}$$

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The independence of the weights and biases implies

- The covariance between different pre-activations in the same layer will be given by

$$E\left[z_{it;a}z_{jt;b}\right] = q_{ab}^{t}\delta_{ij}$$

Therefore

$$q_{ab}^{t} = \sigma_{w}^{2}\int\phi_{h}\left(u_{1}\right)\sigma_{h}\left(u_{2}\right)Dz_{1}Dz_{2} + \rho_{b}^{2}$$

- Where $Dz = \frac{1}{\sqrt{2\pi}}\int\exp\left\{-\frac{1}{2}s^{2}\right\}ds$
- $u_{1} = \sqrt{q_{aa}^{t-1}}$
- $u_{2} = \sqrt{q_{bb}^{t-1}}\left[c_{ab}^{t-1}s_{1} + \sqrt{1-\left(c_{ab}^{t-1}\right)^{2}}z_{2}\right]$
- $c_{ab}^{t} = \frac{q_{ab}^{t}}{\sqrt{q_{aa}^{t}q_{bb}^{t}}}$

Therefore

Therefore, we can look at the variance of the Jacobian Matrix elements

$$\chi = \frac{1}{N}\left\langle Tr\left[\left(D_t U_{SS}\right)^T D_t U_{SS}\right]\right\rangle = \sigma_w^2 \int \left[\sigma_h'\left(\sqrt{q^*}\boldsymbol{s}_{it}\right)\right]^2 \exp\left\{-\frac{1}{2}\boldsymbol{s}_{it}^2\right\} d\boldsymbol{s}_{it}$$

Then

$\chi\left(\rho_w, \rho_b\right)$

- It separates $\left(\rho_w, \rho_b\right)$ plane into two regions.

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When $\chi > 1$

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When $\chi > 1$

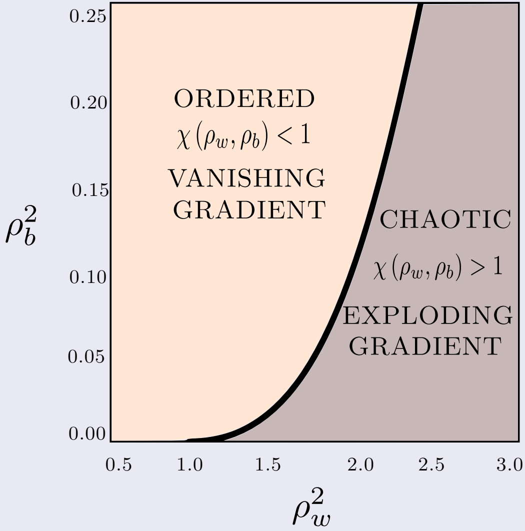
- Forward signal propagation expands and folds space in a chaotic manner and gradients explode

When $\chi < 1$

- Forward signal propagation contracts in an ordered manner and gradients exponentially vanishes

This Regions establish the stability of the network

We have the following



Therefore

It is clear that

- When we choose same $\rho_b = \rho_w$ we have a convergence of the network

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Having other values

- It requires a careful choosing of the values

Outline

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Although, the Vanishing and Exploding Gradients

- They are a problem for the RNN's

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Although, the Vanishing and Exploding Gradients

- They are a problem for the RNN's

If we use the full BPTT

- We confront limitations on the amount of Memory and Hardware available

Thus a popular strategy

- It is the Truncated BPTT [9, 10]

Therefore

They proposed using a truncation on the BPTT

- To solve the problem with the Vanishing and Exploding Gradient

Therefore

They proposed using a truncation on the BPTT

- To solve the problem with the Vanishing and Exploding Gradient

What is Truncated BPTT?

- In general, this should be regarded as a heuristic technique for simplifying the computation.
  - Which it is a good approximation true gradient

The Algorithm

Truncated BPTT

1. for $t = 1$ to T do:
2. Run the RNN for one step, computing h_t and y_t
3. if t divides k_1 then
4. Run BPTT from t to $t - k_2$

The Algorithm

Truncated BPTT

1. for $t = 1$ to T do:
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Something Notable

1. It was first used by Elman [11]
2. Also Mikolov et al. [12] used the TBPTT to train RNN on word-level language modeling.

Outline

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Initialization of the Hidden State

This is the classic problem in RNN

- How to initialize the h_s hidden state?

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- How to initialize the h_s hidden state?

There are two main mehtods

1. Initialize h_s to the zero vector.
2. Adaptive noisy initialization of h_s
3. Find the steady state

The Simplest One

We can simply initialize h_s

- To a zero state

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We can simply initialize h_s

- To a zero state

Quite simple and easy to apply

- However do we have something better?

Adaptive noisy initialization

It is proposed by Zimmermann et al. [13]

- They proposed to use the residual error once the back-propagation was done for $\boldsymbol{h}_0$

Adaptive noisy initialization

It is proposed by Zimmermann et al. [13]

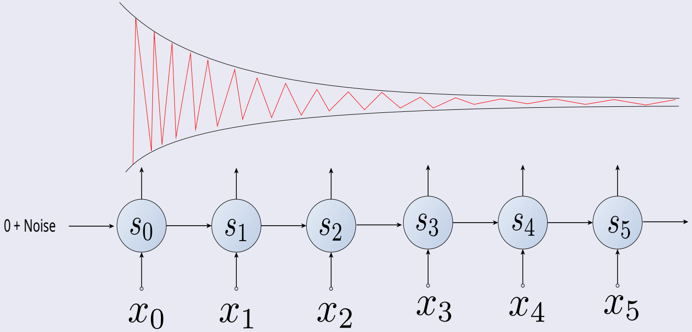
- They proposed to use the residual error once the back-propagation was done for $\boldsymbol{h}_0$

This is done

- By disturbing $\boldsymbol{h}_0$ with a noise term Θ which follows the distribution of the residual error.

Adaptive Noise

The network tries to stabilize the output



Example of this initializations

Source https://r2rt.com/non-zero-initial-states-for-recurrent-neural-networks.html

What about the Weight Parameters?

We could simply initialize them to zero

- Denger Will Robinson!!!

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A simple example with the following feed-forward architecture

$$
\begin{aligned}
\boldsymbol{w} &= \sigma_1\left(W_{hi}\boldsymbol{x}\right) \\
\boldsymbol{y} &= \sigma_2\left(W_{oh}\boldsymbol{w}\right) \\
L &= \frac{1}{2}\left[\boldsymbol{y}-\boldsymbol{z}\right]^2
\end{aligned}
$$

Therefore

We have by back-propagation

$$\Delta W_{ho} = \left[\sigma_2'\left(W_{oh}\sigma_1\left(W_{hi}\boldsymbol{x}_1\right)\right) - \boldsymbol{z}\right]\sigma_2'\left(W_{oh}\sigma_1\left(W_{hi}\boldsymbol{x}\right)\right)W_{oh}\sigma_1'\left(W_{hi}\boldsymbol{x}\right)\boldsymbol{x}$$

Therefore

We have by back-propagation

$$\Delta W_{ho} = \left[\sigma_2'\left(W_{oh}\sigma_1\left(W_{hi}\boldsymbol{x}_1\right)\right) - \boldsymbol{z}\right]\sigma_2'\left(W_{oh}\sigma_1\left(W_{hi}\boldsymbol{x}\right)\right)W_{oh}\sigma_1'\left(W_{hi}\boldsymbol{x}\right)\boldsymbol{x}$$

Therefore

$$\Delta W_{ho} = 0$$

Therefore

Not a good idea

- What else we can do?

Therefore

Not a good idea

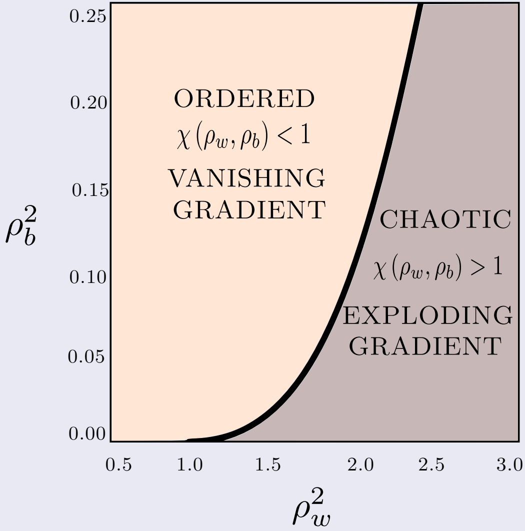
- What else we can do?

We have heuristics as the Gaussian initialization

$$w_{ij} \sim N\left(0, \sigma^2\right)$$

Do you remember?

We have the following



Furthermore

We have heuristics

- For Relu — We multiply the randomly generated values of W by:

$$\sqrt{\frac{2}{size^{l-1}}}$$

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Other common one

$$\sqrt{\frac{2}{size^{l-1}+size^{l}}}$$

Outline

History of LSTM

They were introduced by

- LSTM was proposed in 1997 by Sepp Hochreiter and Jürgen Schmidhuber [14]

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Properties

- In 1999, Felix Gers and his advisor Jürgen Schmidhuber and Fred Cummins introduced the forget gate (also called "keep gate") into LSTM architecture.
  - It enables the LSTM to reset its own state

Long Short Term Memory (LSTM)

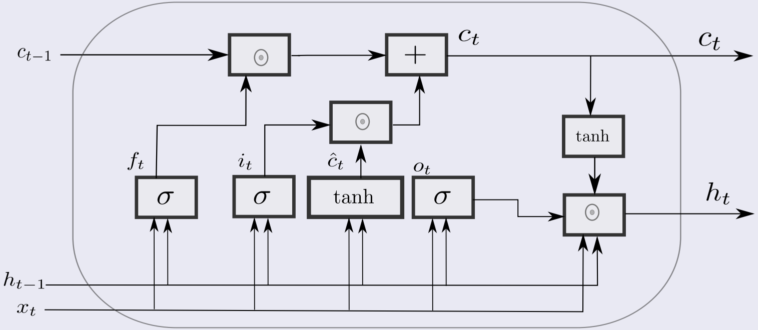
We have the following Architecture (Component wise product $\odot$)

$$
\begin{aligned}
\boldsymbol{f}_t &= \text{sig}\left[W_f \boldsymbol{x}_t + U_f \boldsymbol{h}_{t-1} + \boldsymbol{b}_f\right] \text{ (Forget Gate)} \\
\boldsymbol{i}_t &= \text{sig}\left[W_i \boldsymbol{x}_t + U_i \boldsymbol{h}_{t-1} + \boldsymbol{b}_i\right] \text{ (Input/Update Gate)} \\
\boldsymbol{o}_t &= \text{sig}\left[W_o \boldsymbol{x}_t + U_o \boldsymbol{h}_{t-1} + \boldsymbol{b}_o\right] \text{ (Output Gate)} \\
\hat{\boldsymbol{c}}_t &= \tanh\left[W_c \boldsymbol{x}_t + U_c \boldsymbol{h}_{t-1} + \boldsymbol{b}_c\right] \text{ (Intermediate Cell Gate)} \\
\boldsymbol{c}_t &= \boldsymbol{f}_t \odot \boldsymbol{c}_{t-1} + \boldsymbol{i}_t \odot \hat{\boldsymbol{c}}_t \text{ (Cell State Gate)} \\
\boldsymbol{h}_t &= \boldsymbol{o}_t \odot \tanh\left(\boldsymbol{c}_t\right) \text{ (Hidden State)}
\end{aligned}
$$

- Where σ is a sigmoid function.

Graphically

We have that



Here, Sepp Hochreiter and Jürgen Schmidhuber [14, 15] say

In the RNN

$$\boldsymbol{h}_t = \sigma_h\left(W_{sd}\boldsymbol{x}_t + U_{ss}\boldsymbol{h}_{t-1}\right)$$

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$$\begin{aligned} \boldsymbol{c}_t &= \boldsymbol{f}_t \odot \boldsymbol{c}_{t-1} + \boldsymbol{i}_t \odot \hat{\boldsymbol{c}}_t \text{ (Cell State Gate)} \\ \boldsymbol{h}_t &= \boldsymbol{o}_t \odot \tanh\left(\boldsymbol{c}_t\right) \end{aligned}$$

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You need the forget term, the input term ant the intermediate cell

- To update the state

You can see

Something Notable

- The cell keeps track of the dependencies between the elements in the input sequence and the state

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Something Notable

- The cell keeps track of the dependencies between the elements in the input sequence and the state

The input gate

- It is in charge of how much of the input flows into the cell gate

$$\boldsymbol{i}_t = \sigma\left[W_i \boldsymbol{x}_t + U_i \boldsymbol{h}_{t-1} + \boldsymbol{b}_i\right]$$

What is the meaning?

We have that

- The sigmoid layer decides what values to update

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- The sigmoid layer decides what values to update

They impact the term $\boldsymbol{i}_t \odot \hat{\boldsymbol{c}}_t$

- Making possible to decide how to control the cell intermediate values

Now

The forget gate

- How much of the previous cell gate time value remains in the cell at time t

$$\boldsymbol{f}_t = \sigma\left[W_f \boldsymbol{x}_t + U_f \boldsymbol{h}_{t-1} + \boldsymbol{b}_f\right]$$

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Actually

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Actually

- It uses previous state and input

Then the sigmoid actually can be interpreted as

- Sigmoid: value 0 and 1 – “completely forget” vs. “completely keep”

Furthermore

The output gate

- It controls the extent to which the value in the cell is used to compute the actual state

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Thus a type of control

- Between the previous cell state and the new cell state

Finally

We have the update of the cell as

$$\boldsymbol{c}_t = \boldsymbol{f}_t \odot \boldsymbol{c}_{t-1} + \boldsymbol{i}_t \odot \hat{\boldsymbol{c}}_t$$

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Basically

- Apply forget operation to previous internal cell state.
- Add new candidate values, scaled by how much we decided to update

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$$\boldsymbol{c}_t = \boldsymbol{f}_t \odot \boldsymbol{c}_{t-1} + \boldsymbol{i}_t \odot \hat{\boldsymbol{c}}_t$$

Basically

- Apply forget operation to previous internal cell state.
- Add new candidate values, scaled by how much we decided to update

We can see as

- Drop old information and add new information about subject's gender.

Outline

Thus at the output layer and update state

We have

$$
\begin{aligned}
\boldsymbol{o}_t =& \sigma\left[W_o \boldsymbol{x}_t + U_o \boldsymbol{h}_{t-1} + \boldsymbol{b}_o\right] \text{ (Output Gate)} \\
\boldsymbol{h}_t =& \boldsymbol{o}_t \odot \tanh\left(\boldsymbol{c}_t\right) \text{ (Hidden State)}
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Therefore, we have that

- Sigmoid layer: decide what linear combination of state/input to output

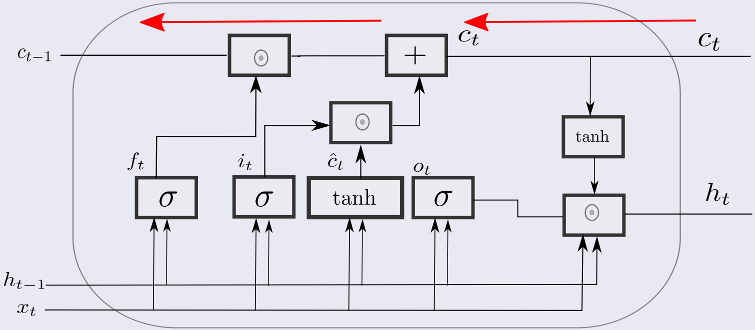
Additionally, we have that the tanh squashes the values between -1 and 1

- The output is used to filter a version of cell state!!!

Something nice about LSTM

Quite nice

- Backpropagation from c_t to c_{t-1} requires only elementwise multiplication!



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Achievements

LSTM achieved record results in natural language text compression

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Finally

- Won the ICDAR handwriting competition (2009)

Right now

Something Notable

- As of 2016, major technology companies including Google, Apple, and Microsoft were using LSTM as fundamental components in new products.

Outline

History

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Something Notable

- The GRU is like a long short-term memory (LSTM) with forget gate...
  - but has fewer parameters than LSTM, as it lacks an output gate

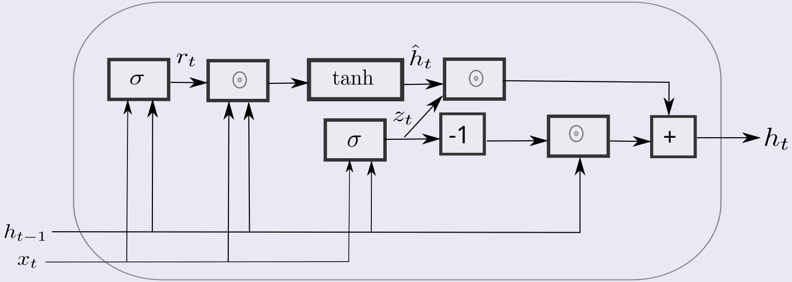
Gated Recurrent Units

Architecture

$$
\begin{aligned}
\boldsymbol{z}_t =& \sigma\left[W_z \boldsymbol{x}_t + U_z \boldsymbol{h}_{t-1} + \boldsymbol{b}_z\right] \text{ (Update Gate)} \\
\boldsymbol{r}_t =& \sigma\left[W_r \boldsymbol{x}_t + U_r \boldsymbol{h}_{t-1} + \boldsymbol{b}_r\right] \text{ (Reset Gate)} \\
\hat{\boldsymbol{h}}_t =& \tanh\left[W_h \boldsymbol{x}_t + U_h \boldsymbol{r}_t \odot \boldsymbol{h}_{t-1} + \boldsymbol{b}_h\right] \\
\boldsymbol{h}_t =& (1 - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1} + \boldsymbol{z}_t \odot \hat{\boldsymbol{h}}_t
\end{aligned}
$$

Graphically, we have the architecture

GRU Architecture



Main Observations

There is a gate used to combine the state $\boldsymbol{h}_{t-1}$,

- The $\boldsymbol{z}_t$ gate that basically uses the information of the input and the previous state to decide how to update

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$$\boldsymbol{h}_t = (1 - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1} + \boldsymbol{z}_t \odot \hat{\boldsymbol{h}}_t$$

The intermediate step $\hat{\boldsymbol{h}}_t$

- A bounded version of the possible state $\boldsymbol{h}_t$

Next

We have that a reset gate

$$\boldsymbol{r}_t = \sigma\left[W_r \boldsymbol{x}_t + U_r \boldsymbol{h}_{t-1} + \boldsymbol{b}_r\right]$$

- To update

$$\hat{\boldsymbol{h}}_t = \tanh\left[W_h \boldsymbol{x}_t + U_h \boldsymbol{r}_t \odot \boldsymbol{h}_{t-1} + \boldsymbol{b}_h\right]$$

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LSTM can perform unbounded counting[16]

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  - It simulates a counting machine used for theoretical CS

Denny Britz, Anna Goldie, Minh-Thang Luong, Quoc Le of Google Brain

- LSTM cells consistently outperform GRU cells in "the first large-scale analysis of architecture variations for Neural Machine Translation."

Outline

Given that we want to do sequence modeling

Stock Options

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Stock Options

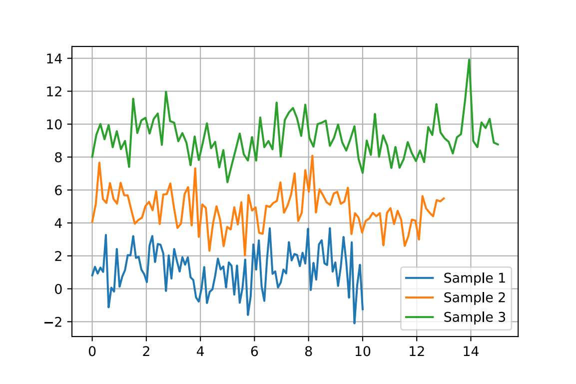
Predict next phrase

- Question: If I am a man ?
  - Prediction: you are homo sapiens

What do we have in this sequences of data?

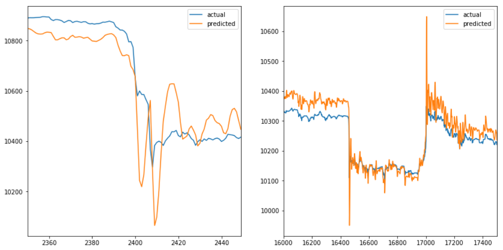
Sequences have different lengths

- We need to handle variable-length sequences



Furthermore

We need to track long-term dependencies



Not only that

Maintain information about order

- “We have a mother living in Yucatan, Mexico”

Not only that

Maintain information about order

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Share parameters across the sequence

- Do you remember the state $\boldsymbol{h}_t$?

However

There is a need to increase their power

- Given the amounts of data we have right know

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This is based in the following idea [19]

- Hypothesis, hierarchical model can be exponentially more efficient at representing some functions than a shallow one.

In the case of RNN's

Certain Transitions are not Deep

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They are

- Hidden-to-hidden $\boldsymbol{h}_{t-1} \to \boldsymbol{h}_t$
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Meaning

- They are all shallow in the sense that there exists no intermediate, nonlinear hidden layer.

Outline

Bengio et al. [20]

Gave the following Hypothesis

- In sampling algorithms (Markov Chains and MCMC techniques) suffer from a fundamental problem
  - Given unconnected or weakly connected regions of distributions

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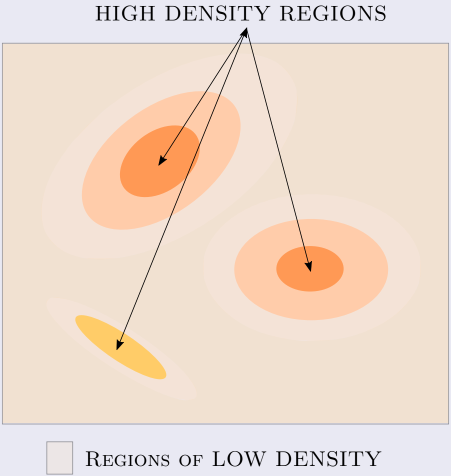
This means that we have a slow mixing of samples

- In order to represent distributions

Example

A Big Problem



The Main Problem

We have that

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Why?

- Jumping around in the MCMC method is quite slow and scarce

Implications in Learning Algorithms

Given that some form of sampling is at the core of many learning algorithms

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However as the model improves

- its corresponding distribution sharpens and mixing becomes slower

Basically

We have slow downs on the learning in shallow models

Outline

Therefore

We need to build deeper structures to reach more capabilities

- For example the vector representation of documents

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We need to build deeper structures to reach more capabilities

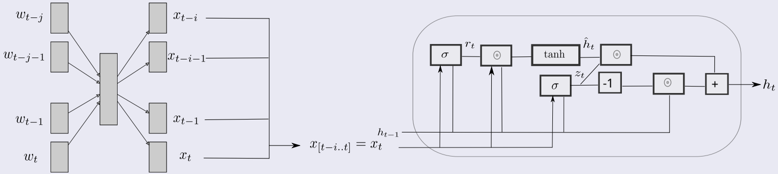
- For example the vector representation of documents

Here a extra layer of representation can be used for doing representation

- For Example, Mikolov et al. [21]

Basically a shallow network before the main architecture

An Encoder Layer before a GRU



The equations

They will look like

$$
\begin{aligned}
w_{t'}^{encoded} =& \sigma\left[Aw_t + b_{w_t}\right] \\
x_t =& \sigma\left[Bw_{t'}^{encoded} + b_{x_t}\right] \\
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Deep Transition Architectures

In a deep transition RNN (DT-RNN)

- At each time step the next state is computed by the sequential application of multiple transition layers.

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With a Caveat

- The hidden state output is used as the input state on the next one

For example, at the encoder phase

For the i^{th} source word in the forward direction, we have $\boldsymbol{h}_i = \boldsymbol{h}_{i,L_s}$

$$\boldsymbol{h}_{i,1} = GRU_1\left(\boldsymbol{x}_1, \boldsymbol{h}_{i-1,L_s}\right)$$
$$\boldsymbol{h}_{i,k} = GRU_k\left(0, \boldsymbol{h}_{i,k-1}\right) \text{ for } 1 < k \leq L_s$$

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The sequence word is reversed and you have a backward state then

$$C \equiv \left[\overrightarrow{\boldsymbol{h}}_{i,L_s}, \overleftarrow{\boldsymbol{h}}_{i,L_s}\right]$$

Then

Decoder phase uses the outputs from the previous GRU and something called attention (We will look at this latter)

$$\boldsymbol{s}_{j,1} = GRU_1\left(\boldsymbol{y}_{j-1}, \boldsymbol{s}_{j-1}, L_t\right)$$
$$\boldsymbol{s}_{j,2} = GRU_2\left(ATT, \boldsymbol{s}_{j-1}, L_t\right)$$
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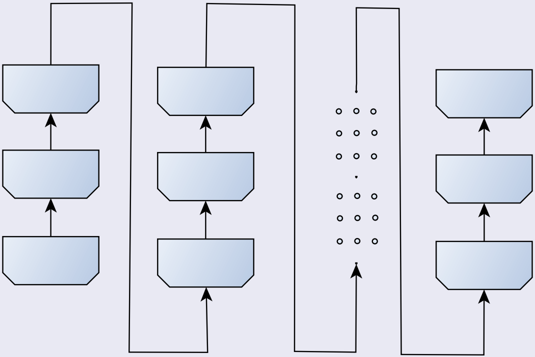
Then, the target word state $s_j \equiv s_{j,L_t}$

- It is used by a feed-forward neural network to predict the current target network

Deep Transition Decoder

We have the following depiction of the architecture



Outline

There are many other examples

Basically

- We are far from the classic methods as
  1. Autoregressive integrated moving average (ARMA)
  2. Auto Regressive Integrated Moving Average (ARIMA)
  3. etc

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Basically

- We are far from the classic methods as
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  3. etc

These RNN architectures are taking the prediction of time series

- To another level!!!

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