

Recurrent neural networks

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The model

Def: RNN

Given an input sequence $\{\mathbf{u}\}_{t=1,\dots,T}$, with $\mathbf{u}_t \in \mathbb{R}^p$, the output sequence of a RNN $\{\mathbf{y}\}_{t=1,\dots,T}$, with $\mathbf{y}_t \in \mathbb{R}^o$, is defined by the following:

$$\mathbf{y}^t \triangleq F(\mathbf{z}^t) \quad (1)$$

$$\mathbf{z}^t \triangleq W^{out} \cdot \mathbf{a}^t + \mathbf{b}^{out} \quad (2)$$

$$\mathbf{a}^t \triangleq W^{rec} \cdot \mathbf{h}^{t-1} + W^{in} \cdot \mathbf{u}^t + \mathbf{b}^{rec} \quad (3)$$

$$\mathbf{h}^t \triangleq \sigma(\mathbf{a}^t) \quad (4)$$

$$\mathbf{h}^0 \triangleq \mathbf{0}, \quad (5)$$

where $\sigma(\cdot) : \mathbb{R} \rightarrow \mathbb{R}$ is a non linear function applied element-wise called **activation function**, $F(\cdot)$ is called **output function**.

The parameters of the net are $\{W^{out}, W^{in}, W^{rec}, \mathbf{b}^{rec}, \mathbf{b}^{out}\}$.

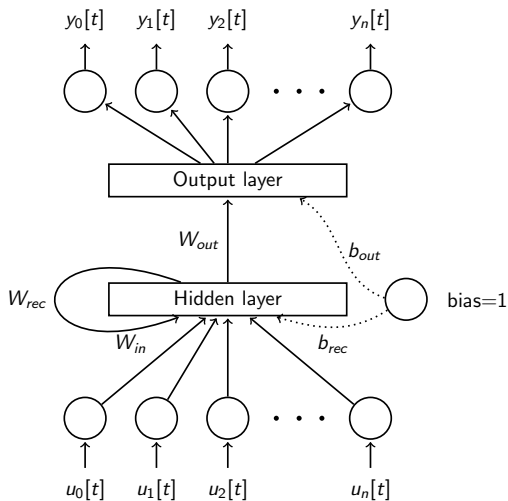


Figure: RNN model.

The optimization problem

Given a dataset D :

$$D \triangleq \{ \{ \bar{\mathbf{u}}^{(i)} \}_{t=1, \dots, T}, \bar{\mathbf{u}}_t^{(i)} \in \mathbb{R}^p, \{ \bar{\mathbf{y}}^{(i)} \}_{t=1, \dots, T}, \bar{\mathbf{y}}_t^{(i)} \in \mathbb{R}^o; i = 1, \dots, N \} \quad (6)$$

we define a loss function $L_D(\mathbf{x})$ over D as

$$L_D(\mathbf{x}) \triangleq \frac{1}{N} \sum_{i=1}^N \sum_{t=1}^T L_t(\bar{\mathbf{y}}_t^{(i)}, \mathbf{y}_t^{(i)}(\mathbf{x})), \quad (7)$$

where $L_t(\cdot, \cdot)$ is an arbitrary loss function for the time step t and \mathbf{x} represents all the parameters of the network. The problem is

$$\min_{\mathbf{x}} L_D(\mathbf{x}) \quad (8)$$

Some learning examples

- ▶ Regression: mean squared error, linear output

$$L(\mathbf{y}, \mathbf{t}) = \frac{1}{M} \sum_{i=1}^M (y_i - t_i)^2, \quad F(\mathbf{y}) = \mathbf{y}. \quad (9)$$

- ▶ Binary classification: hinge loss, linear output

$$L(y, t) = \max(0, 1 - t \cdot y), \quad F(y) = y. \quad (10)$$

- ▶ Multi-way classification: cross entropy loss, softmax output

$$L(\mathbf{y}, \mathbf{t}) = -\frac{1}{M} \sum_{i=1}^M \log(y_i) \cdot t_i, \quad F(y_j) = \frac{e^{y_j}}{\sum_{i=1}^M e^{y_i}}. \quad (11)$$

Stochastic gradient descent (SGD)

Algorithm 1: Stochastic gradient descent

Data:

$D = \{\langle \mathbf{u}^{(i)}, \mathbf{y}^{(i)} \rangle\}$: training set

\mathbf{x}_0 : candidate solution

m : size of each mini-batch

Result:

\mathbf{x} : solution

```
1  $\mathbf{x} \leftarrow \mathbf{x}_0$ 
2 while stop criterion do
3    $I \leftarrow$  select  $m$  training example  $\in D$ 
4    $\alpha \leftarrow$  compute learning rate
5    $\mathbf{x} \leftarrow \mathbf{x} - \alpha \sum_{i \in I} \nabla_{\mathbf{x}} L(\mathbf{x}; \langle \mathbf{u}^{(i)}, \mathbf{y}^{(i)} \rangle)$ 
6 end
```

Convergence of SGD

- ▶ Nemirovski (2009)[4]: proof of convergence in the convex case
- ▶ there are no theoretical guarantees in the non-convex case
- ▶ in practice it always works: SGD is the standard framework in most of neural networks applications.

A pathological problem example

An input sequence:

marker	0	1	0	...	0	1	0	0
value	0.3	0.7	0.1	...	0.2	0.4	0.6	0.9

The predicted output should be the sum of the two one-marked positions (1.1).

Why is this a difficult problem?

Because of its long time dependencies.

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Gradient

Let $L_t(\bar{\mathbf{u}}, \bar{\mathbf{y}})$ the loss function for the time step t and $g_t(\mathbf{x}) : \mathbb{R}$ be the function defined by

$$g_t(\mathbf{x}) \triangleq L_t(F(\mathbf{z}^t(\bar{\mathbf{u}}; \mathbf{x}), \bar{\mathbf{y}}_t))$$

and

$$g(\mathbf{x}) \triangleq \sum_{t=1}^T g_t(\mathbf{x})$$

$$\frac{\partial g}{\partial W_{rec}} = \sum_{t=1}^T \nabla L_t^T \cdot J(F) \cdot \frac{\partial \mathbf{z}^t}{\partial \mathbf{a}^t} \cdot \frac{\partial \mathbf{a}^t}{\partial W_{rec}} \quad (12)$$

$$= \sum_{t=1}^T \frac{\partial g_t}{\partial \mathbf{a}^t} \cdot \frac{\partial \mathbf{a}^t}{\partial W_{rec}} \quad (13)$$

Let's consider a single output unit u , and a weight w_{lj} , we have

$$\frac{\partial a_u^t}{\partial w_{lj}} = \sum_{k=1}^t \frac{\partial a_u^t}{\partial a_l^k} \cdot \frac{\partial a_l^k}{\partial w_{lj}} \quad (14)$$

$$= \sum_{k=1}^t \delta_{lu}^{tk} \cdot \phi_j^{t-1} \quad (15)$$

where

$$\delta_{lu}^{tk} \triangleq \frac{\partial a_u^t}{\partial a_l^k} \quad (16)$$

Let $P(l)$ be the set of parents of neuron l , defined as the set of parents in the unfolded network.

$$\delta_{lu}^{tk} = \sum_{h \in P(l)} \delta_{hu}^{tk} \cdot \sigma'(a_h^{t-1}) \cdot w_{hl} \quad (17)$$

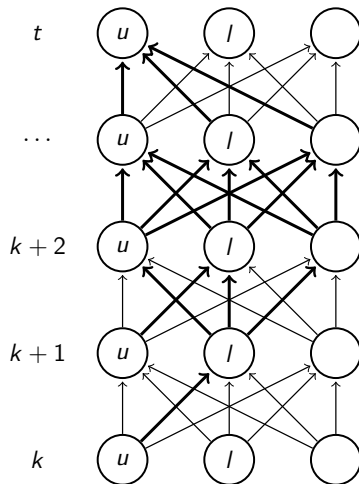


Figure: Nodes involved in $\frac{\partial a_u^t}{\partial a_l^k}$.

In matrix notation we have:

$$\frac{\partial \mathbf{a}^t}{\partial W^{rec}} = \sum_{k=1}^t \frac{\partial \mathbf{a}^t}{\partial \mathbf{a}^k} \cdot \frac{\partial^+ \mathbf{a}^k}{\partial W^{rec}} \quad (18)$$

$$\frac{\partial^+ \mathbf{a}^k}{\partial W_j^{rec}} = \begin{bmatrix} \phi_j^k & 0 & \dots & \dots & 0 \\ 0 & \phi_j^k & \dots & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \dots & \dots & \phi_j^k \end{bmatrix} \quad (19)$$

$$\frac{\partial \mathbf{a}^t}{\partial \mathbf{a}^k} = \frac{\partial \mathbf{a}^t}{\partial \mathbf{a}^{k+1}} \cdot \text{diag}(\sigma'(\mathbf{a}^k)) \cdot W^{rec} \quad (20)$$

$$= \prod_{i=t-1}^k \text{diag}(\sigma'(\mathbf{a}^i)) \cdot W^{rec}. \quad (21)$$

The derivatives with respect to the other variables are computed in a similar fashion.

Vanishing gradient: a sufficient condition

$$\frac{\partial \mathbf{a}^t}{\partial \mathbf{a}^k} = \prod_{i=t-1}^k \text{diag}(\sigma'(\mathbf{a}^i)) \cdot W^{\text{rec}}. \quad (22)$$

Taking the singular value decomposition of W^{rec} :

$$W^{\text{rec}} = S \cdot D \cdot V^T \quad (23)$$

where S, V^T are squared orthogonal matrices and $D \triangleq \text{diag}(\mu_1, \mu_2, \dots, \mu_r)$ is the diagonal matrix containing the singular values of W^{rec} . Hence:

$$\frac{\partial \mathbf{a}^t}{\partial \mathbf{a}^k} = \prod_{i=t-1}^k \text{diag}(\sigma'(\mathbf{a}^i)) \cdot S \cdot D \cdot V^T \quad (24)$$

Since U and V are orthogonal matrix, hence

$$\|U\|_2 = \|V^T\|_2 = 1,$$

and

$$\|diag(\lambda_1, \lambda_2, \dots, \lambda_r)\|_2 = \lambda_{max},$$

we get

$$\left\| \frac{\partial \mathbf{a}^t}{\partial \mathbf{a}^k} \right\|_2 = \left\| \left(\prod_{i=t-1}^k diag(\sigma'(\mathbf{a}^i)) \cdot S \cdot D \cdot V^T \right) \right\|_2 \quad (25)$$

$$\leq (\sigma'_{max} \cdot \mu_{max})^{t-k-1} \quad (26)$$

Existent solutions

- ▶ Long short-term memory (LSTM). Hochreiter, Schmidhuber (1997)[1]
 - ▶ the network structure is modified with specialized "memory cells"
 - ▶ a truncated version of back-propagation is employed (but works also without it)
- ▶ Hessian-Free optimization (HF). Martens (2010) [3]
 - ▶ a second order method
 - ▶ a "cheap" approximation of the Hessian is employed
 - ▶ the quadratic sub-problem is solved through conjugate gradient + structural damping
- ▶ Pascanu, Bengio (2013) [5]
 - ▶ a first order method
 - ▶ uses a penalty to deal with the vanishing gradient problem

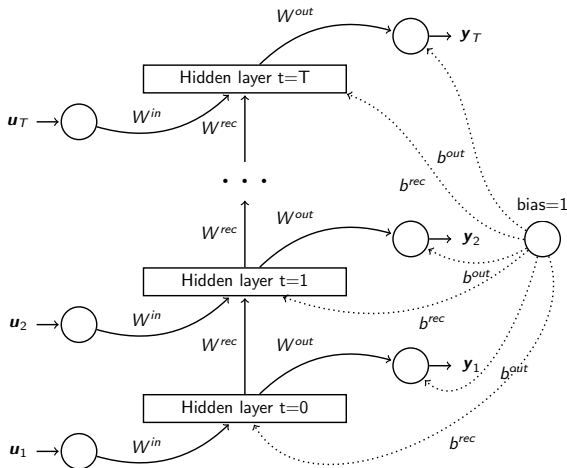
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Understanding the gradient structure: unfolding



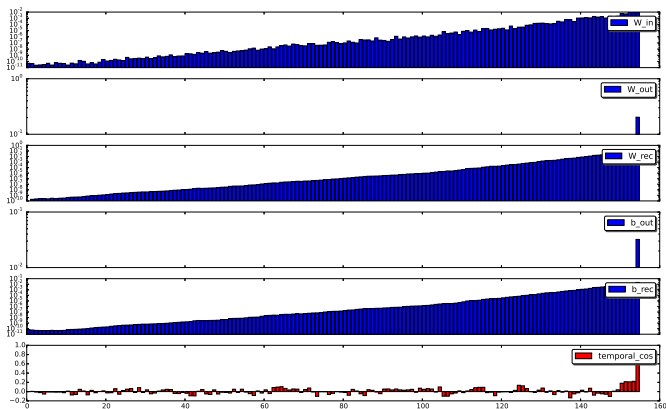
Understanding the gradient structure

It's easy to see that

$$\nabla L(\mathbf{x}) = \sum_{t=1}^T \nabla L_{|t}(\mathbf{x}), \quad (27)$$

where $\nabla L_{|t}$ is the gradient computed imagining to replicate all the variables for each time step and taking the derivatives w.r.t. the variables for step t

Temporal gradient norms: an illustration



A new proposal

The idea is to use the structure of the gradient to compute a "descent" direction which does not suffer from the vanishing problem.

- normalize the temporal components:

$$g_t(\mathbf{x}) = \frac{\nabla L_{|t}(\mathbf{x})}{\|\nabla L_{|t}(\mathbf{x})\|}. \quad (28)$$

- combine the normalized gradients in a simplex:

$$g(\mathbf{x}) = \sum_{t=1}^T \beta_t \cdot g_t(\mathbf{x}). \quad (29)$$

with $\sum_{t=1}^T \beta_t = 1, \beta_t > 0$ (randomly picked at each iteration).

- exploit the gradient norm:

$$d(\mathbf{x}) = \|\nabla L(\mathbf{x})\| \frac{g(\mathbf{x})}{\|g(\mathbf{x})\|}. \quad (30)$$

Open Issues: Initialization

- ▶ Some tasks, like the XOR one, are still "unresolved" (even for the other approaches). They cannot be solved with most of the seeds used for the initialization
- ▶ it seems to be an **initialization** matter

Popular strategies for initialization are:

- ▶ "small random weights", usually drawn from gaussian or uniform distribution with zero mean (Pascanu).
- ▶ sparse initialization: only some weights are actually sampled from a distribution, the other are set to zero (HF).
- ▶ ESN-like initialization[2].

Open Issues: Learning rate

- ▶ the **learning rate** is usually tuned by hand, there is no convergence theory for SGD in the non convex case
- ▶ a **gradient clipping** technique is often employed:

Algorithm 2: Gradient clipping

```
1  $\mathbf{g} \leftarrow \nabla_{\mathbf{x}} L$   
2 if  $\|\mathbf{g}\| \geq \textit{threshold}$  then  
3    $\mathbf{g} \leftarrow \frac{\textit{threshold}}{\|\mathbf{g}\|} \mathbf{g}$   
4 end
```

- ▶ some **momentum** or **averaging** technique often yield better convergence time, again tuned by hand

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