Optimization methods for Recurrent Neural Networks training

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Introduction

The model

Definition of RNN

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

$$\boldsymbol{y}^t \triangleq F(\boldsymbol{z}^t) \tag{1}$$

$$\boldsymbol{z}^t \triangleq W^{out} \cdot \boldsymbol{a}^t + \boldsymbol{b}^{out} \tag{2}$$

$$\boldsymbol{a}^t \triangleq W^{rec} \cdot \boldsymbol{h}^{t-1} + W^{in} \cdot \boldsymbol{u}^t + \boldsymbol{b}^{rec} \tag{3}$$

$$\boldsymbol{h}^t \triangleq \sigma(\boldsymbol{a}^t) \tag{4}$$

$$\boldsymbol{h}^0 \triangleq \boldsymbol{0}, \tag{5}$$

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

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

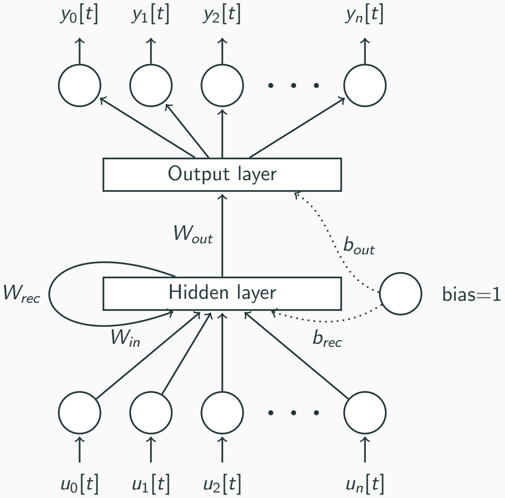

Figure 1: RNN model.

The optimization problem

Given a dataset D:

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

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

$$L_D(\boldsymbol{x}) \triangleq \frac{1}{N} \sum_{i=1}^{N} \sum_{t=1}^{T} L_t(\overline{\boldsymbol{y}}_t^{(i)}, \boldsymbol{y}_t^{(i)}(\boldsymbol{x})), \tag{7}$$

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

$$\min_{\boldsymbol{x}} L_D(\boldsymbol{x}) \tag{8}$$

Some learning examples

- Regression: mean squared error, linear output

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

- Binary classification: hinge loss, linear output

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

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

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

Stochastic gradient descent (SGD)

Algorithm 1: Stochastic gradient descent

Data:

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

$\boldsymbol{x}_0$: candidate solution

m: size of each mini-batch

Result:

$\boldsymbol{x}$: solution

$\boldsymbol{x} \leftarrow \boldsymbol{x}_0$
while *stop criterion* **do**
    $I \leftarrow$ select m training example $\in D$
    $\alpha \leftarrow$ compute learning rate
    $\boldsymbol{x} \leftarrow \boldsymbol{x} - \alpha \sum_{i \in I} \nabla_{\boldsymbol{x}} L(\boldsymbol{x}; \langle \boldsymbol{u}^{(i)}, \boldsymbol{y}^{(i)} \rangle)$
end

Gradient of a RNN

Gradient structure: unfolding

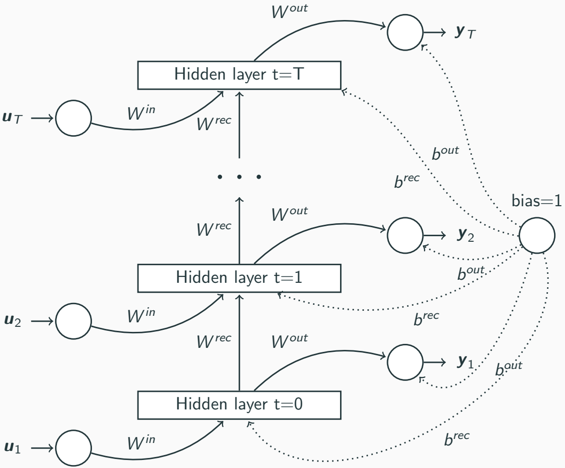

Figure 2: Unfolding of a RNN

Gradient structure: calculus

Consider, for ease of notation, the case where the loss function $L(\bar{\boldsymbol{u}}, \bar{\boldsymbol{y}})$ is defined only on the last step τ. Let $g(\boldsymbol{x}) : \mathbb{R}$ be the function defined by

$$g(\boldsymbol{x}) \triangleq L(F(\boldsymbol{z}^{\tau}(\bar{\boldsymbol{u}}; \boldsymbol{x}), \bar{\boldsymbol{y}}_{\tau})).$$

We compute the gradient as:

$$\begin{aligned} \frac{\partial g}{\partial W^{rec}} &= \frac{\partial g}{\partial \boldsymbol{a}^{\tau}} \cdot \frac{\partial \boldsymbol{a}^{\tau}}{\partial W^{rec}} && (12) \\ &= \nabla L^{T} \cdot J(F) \cdot \frac{\partial \boldsymbol{z}^{\tau}}{\partial \boldsymbol{a}^{\tau}} \cdot \frac{\partial \boldsymbol{a}^{\tau}}{\partial W^{rec}}. && (13) \end{aligned}$$

In matrix notation we have:

$$\frac{\partial \boldsymbol{a}^t}{\partial W^{rec}} = \sum_{k=1}^{t} \frac{\partial \boldsymbol{a}^t}{\partial \boldsymbol{a}^k} \cdot \frac{\partial^+ \boldsymbol{a}^k}{\partial W^{rec}} \tag{14}$$

$$\frac{\partial^+ a^k}{\partial W_j^{rec}} = \begin{bmatrix} h_j^k & 0 & \cdots & \cdots & 0 \\ 0 & h_j^k & \cdots & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & \cdots & h_j^k \end{bmatrix} \tag{15}$$

$$\frac{\partial \boldsymbol{a}^t}{\partial \boldsymbol{a}^k} = \frac{\partial \boldsymbol{a}^t}{\partial \boldsymbol{a}^{k+1}} \cdot diag(\sigma'(\boldsymbol{a}^k)) \cdot W^{rec} \tag{16}$$

$$= \prod_{i=t-1}^{k} diag(\sigma'(\boldsymbol{a}^i)) \cdot W^{rec}. \tag{17}$$

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

Gradient structure: temporal components

Putting all together we obtain:

$$\nabla_{W^{rec}} g = \sum_{k=1}^{\tau} \frac{\partial g}{\partial \boldsymbol{a}^{\tau}} \cdot \frac{\partial \boldsymbol{a}^{\tau}}{\partial \boldsymbol{a}^{k}} \cdot \frac{\partial^{+} \boldsymbol{a}^{k}}{\partial W^{rec}} \tag{18}$$

$$\triangleq \sum_{k=1}^{\tau} \nabla_{W^{rec}} L_{|k}. \tag{19}$$

We refer to $\nabla_{\boldsymbol{x}} g_{|k}$ as the **temporal gradient** for time step k w.r.t. the variable $\boldsymbol{x}$, and it is easy to see that it is the gradient we would compute if we replicated the variable $\boldsymbol{x}$ for each time step and took the derivatives w.r.t. to its k-th replicate.

The vanishing gradient problem

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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Vanishing gradient: an illustration

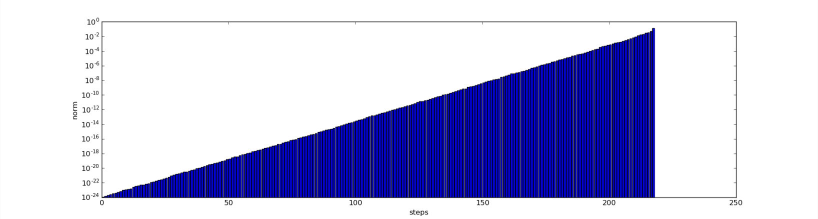


Figure 3: Norm of the temporal gradients at different time steps.

Vanishing gradient: a sufficient condition

$$\frac{\partial \boldsymbol{a}^t}{\partial \boldsymbol{a}^k} = \prod_{i=t-1}^{k} diag(\sigma'(\boldsymbol{a}^i)) \cdot W^{rec}. \tag{20}$$

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

$$W^{rec} = S \cdot D \cdot V^T \tag{21}$$

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

$$\frac{\partial \boldsymbol{a}^t}{\partial \boldsymbol{a}^k} = \prod_{i=t-1}^{k} diag(\sigma'(\boldsymbol{a}^i)) \cdot S \cdot D \cdot V^T \tag{22}$$

Since U and V are orthogonal matrix, hence

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

and

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

we get

$$\left\|\frac{\partial \boldsymbol{a}^t}{\partial \boldsymbol{a}^k}\right\|_2 = \left\|(\prod_{i=t-1}^{k} diag(\sigma'(\boldsymbol{a}^i)) \cdot S \cdot D \cdot V^T)\right\|_2 \tag{23}$$

$$\leq (\sigma'_{max} \cdot \mu_{max})^{t-k-1} \tag{24}$$

A new SGD approach for training RNNs

Initialization

Motivated by the bounds for the vanishing gradient on the singular values of the recurrent matrix we explored an initialization scheme which **scales the spectral radius** of such matrix.

Algorithm 2: Recurrent weight matrix initialization scheme

Data:

$\rho =$ desired spectral radius

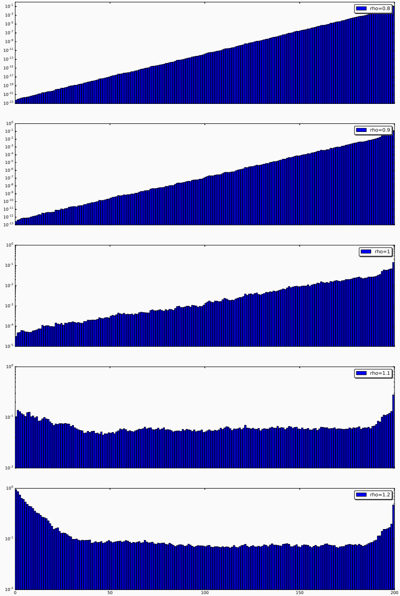
$W_{rec} \sim \mathcal{N}(0, \sigma^2)$

$r \leftarrow \text{spectral\_radius}(W_{rec})$

$W_{rec} \leftarrow \frac{\rho}{r} \cdot W_{rec}$

return W_{rec}

Effect of initialization on the temporal gradients



Effect of initialization on the rate of success

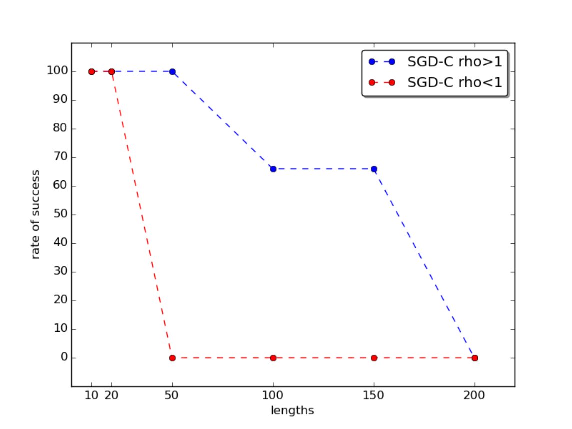


Figure 5: Rate of success (mean of 3 runs) for the temporal order task for various lengths with SGD modified with gradient clipping. In blue and red the results when W_{rec} is initialized with spectral radius bigger and smaller than one respectively.

A different descent direction

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 gradients:

$$s_t(\boldsymbol{x}) = \frac{\nabla L_{|t}(\boldsymbol{x})}{\left\|\nabla L_{|t}(\boldsymbol{x})\right\|}. \tag{25}$$

- Combine the normalized gradients in a convex way:

$$s(\boldsymbol{x}) = \sum_{t=1}^{T} \beta_t \cdot s_t(\boldsymbol{x}). \tag{26}$$

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

- Introduce the gradient norm:

$$d(\boldsymbol{x}) = -\left\|\nabla L(\boldsymbol{x})\right\| \frac{s(\boldsymbol{x})}{\|s(\boldsymbol{x})\|}. \tag{27}$$

Algorithm 3: RNN training

Data:

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

m: size of each mini-batch

μ: constant learning rate

τ: gradient clipping threshold

ρ: initial spectral radius

ψ threshold for the direction norm

$W_{rec}, W_{in}, W_{out} \sim \mathcal{N}(0, \sigma^2)$

$\boldsymbol{b}_{out}, \boldsymbol{b}_{rec} \leftarrow 0$

$r \leftarrow \text{spectral\_radius}(W_{rec})$

$W_{rec} \leftarrow \frac{\rho}{r} \cdot W_{rec}$

$\theta_0 = [W_{rec}, W_{in}, W_{out}, \boldsymbol{b}_{out}, \boldsymbol{b}_{rec}]$

while *stop criterion* **do**

  $I \leftarrow$ sample m training example $\in D$

  $\{\nabla_\theta L_{|t}\}_{t=1}^{T} \leftarrow \text{compute\_temporal\_gradients}(\theta_k, I)$

  $\boldsymbol{d}_k \leftarrow \text{simplex\_combination}(\{\nabla_\theta L_{|t}\})$

  if $\|\nabla_\theta L(\theta_k)\|_2 > \psi$ **then**

    $\boldsymbol{d}_k \leftarrow \nabla_\theta L(\theta_k)$

  end

  $$\alpha_k = \begin{cases} \mu & \text{if } \|\boldsymbol{d}_k\|_2 \leq \tau \\ \frac{\mu \cdot \tau}{\|\boldsymbol{d}_k\|_2} & \text{otherwise} \end{cases}$$

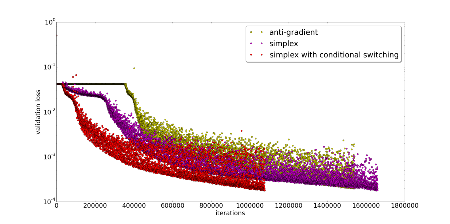
  $\theta_{k+1} \leftarrow \theta_k + \alpha_k \boldsymbol{d}_k$

  $k \leftarrow k + 1$

end

return θ_k

Effect of the simplex direction



(a) Loss (in log scale) for the addition task during training

	anti-gradient	simplex with conditional switching
addition	1807466	**1630666**
temporal order	2164800	**1010000**

(b) Number of iterations

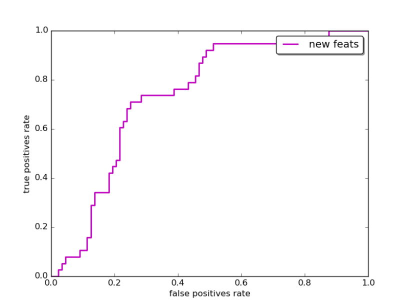
Figure 6: Comparison between SGD using as descent direction the anti-gradient, the simplex direction and the simplex direction with conditional switching.

A real case: Lupus disease prediction

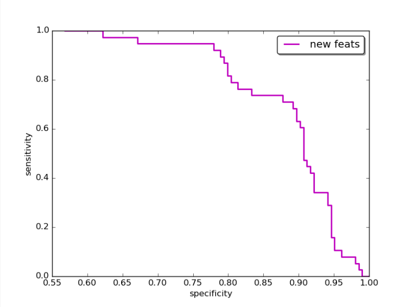
An example of patience record

	Visit 0	Visit 1	Visit 2	Visit 3	Visit 4
age	44.23	44.63	44.77	44.98	45.58
MyasteniaGravis	0	0	0	0	0
arthritis	1	0	1	1	0
c3level	119	96	85.42	76	76
c4level	9	7	6	6	6
hematological	0	0	6	6	6
skinrash	0	0	0	0	0
sledai2kInferred	12	2	2	2	0
...					
SDI	0	0	0	0	**1**

Numerical results for the lupus disease prediction



(a)



(b)

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