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Optimization methods for Recurrent Neural Networks training

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Introduction

Definition of RNN

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

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

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

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

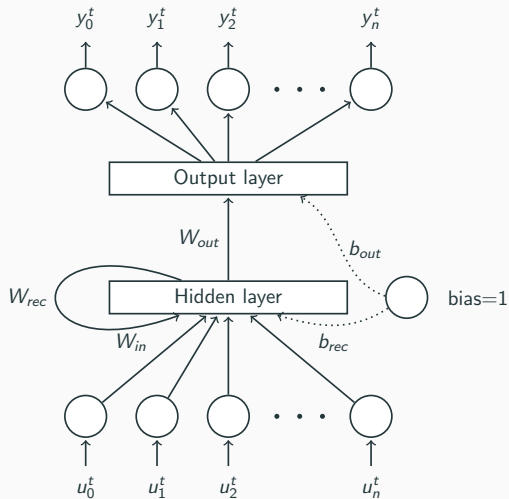
$$\mathbf{h}^t \triangleq \sigma(\mathbf{a}^t) \tag{4}$$

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

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 $\{W^{out}, W^{in}, W^{rec}, \mathbf{b}^{rec}, \mathbf{b}^{out}\}$.

The model



The optimization problem

Given a dataset D :

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

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

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

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

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

- Binary classification: hinge loss, linear output

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

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

$$L(\mathbf{y}, \bar{\mathbf{y}}) = -\frac{1}{M} \sum_{i=1}^M \log(y_i) \cdot \bar{y}_i, \quad F(z_j) = \frac{e^{z_j}}{\sum_{i=1}^M e^{z_i}}. \quad (11)$$

Stochastic gradient descent (SGD)

Algorithm 1: Stochastic gradient descent

Data:

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

\mathbf{x}_0 : candidate solution

m : size of each mini-batch

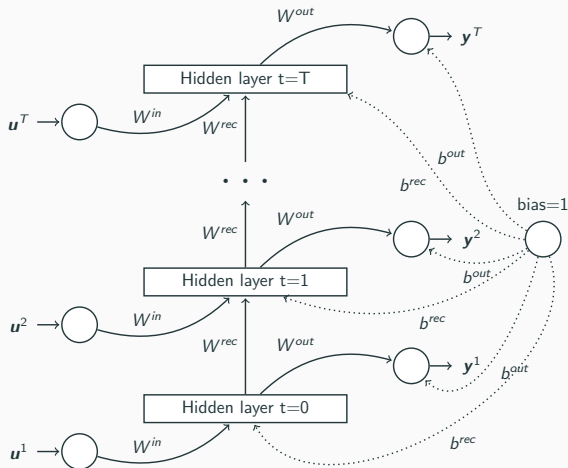
Result:

\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    $\mathbf{x} \leftarrow \mathbf{x} - \alpha \sum_{i \in I} \nabla_{\mathbf{x}} L(\mathbf{x}; \bar{\mathbf{u}}^{(i)}, \bar{\mathbf{y}}^{(i)})$ 
6 end
```

Gradient of a RNN

Gradient structure: unfolding



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

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

We compute the gradient as:

$$\frac{\partial g}{\partial W^{rec}} = \frac{\partial g}{\partial \mathbf{a}^\tau} \cdot \frac{\partial \mathbf{a}^\tau}{\partial W^{rec}} \quad (12)$$

$$= \nabla L^\tau \cdot J(F) \cdot \frac{\partial \mathbf{z}^\tau}{\partial \mathbf{a}^\tau} \cdot \frac{\partial \mathbf{a}^\tau}{\partial W^{rec}}. \quad (13)$$

In matrix notation we have:

$$\frac{\partial \mathbf{a}^t}{\partial W^{rec}} = \sum_{k=1}^t \frac{\partial \mathbf{a}^t}{\partial \mathbf{a}^k} \cdot \frac{\partial^+ \mathbf{a}^k}{\partial W^{rec}} \quad (14)$$

$$\frac{\partial^+ \mathbf{a}^k}{\partial W_j^{rec}} = \begin{bmatrix} h_j^k & 0 & \dots & \dots & 0 \\ 0 & h_j^k & \dots & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \dots & \dots & h_j^k \end{bmatrix} \quad (15)$$

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

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

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

Gradient structure: temporal components

Putting all together:

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

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

We refer to $\nabla_{\mathbf{x}} g_{|k}$ as the **temporal gradient** for time step k w.r.t. the variable \mathbf{x} .

It is the gradient we would compute if we replicated the variable \mathbf{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.

A pathological problem example

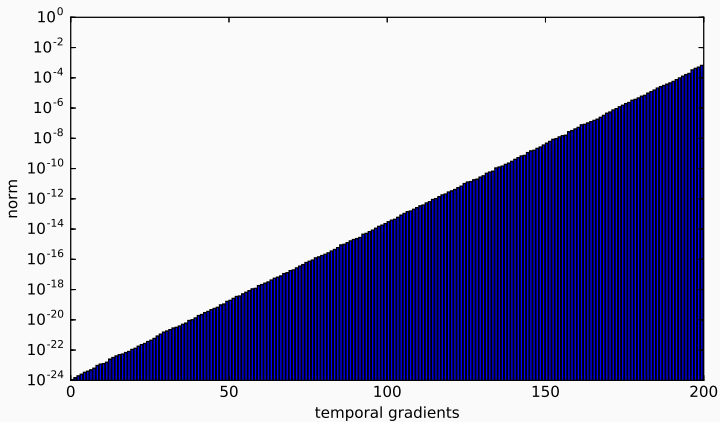
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Vanishing gradient: an illustration



Vanishing gradient: a sufficient condition

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

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

$$W^{\text{rec}} = S \cdot D \cdot V^T \quad (21)$$

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:

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

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

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

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

A new SGD approach for training RNNs

The matrix W^{rec} is **scaled** to have a desired spectral radius.

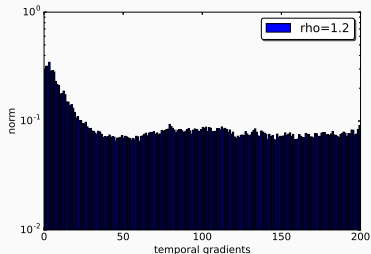
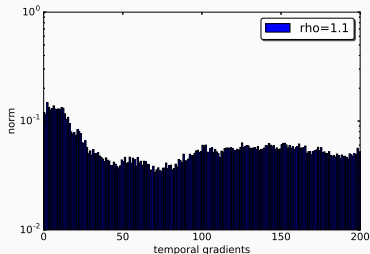
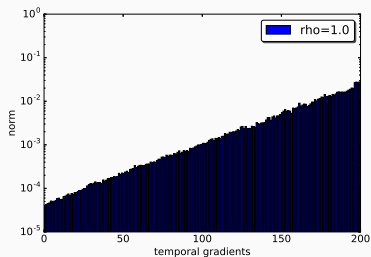
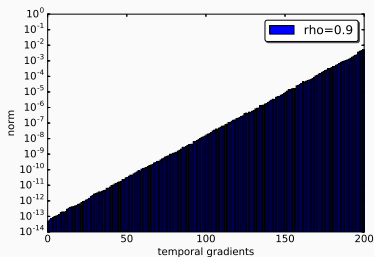
Algorithm 2: Recurrent weight matrix initialization scheme

Data:

ρ = desired spectral radius

- 1 $W_{rec} \sim \mathcal{N}(0, \sigma^2)$
 - 2 $r \leftarrow \text{spectral_radius}(W_{rec})$
 - 3 $W_{rec} \leftarrow \frac{\rho}{r} \cdot W_{rec}$
 - 4 **return** W_{rec}
-

The effect of initialization on the temporal gradients



The effect of initialization on the rate of success

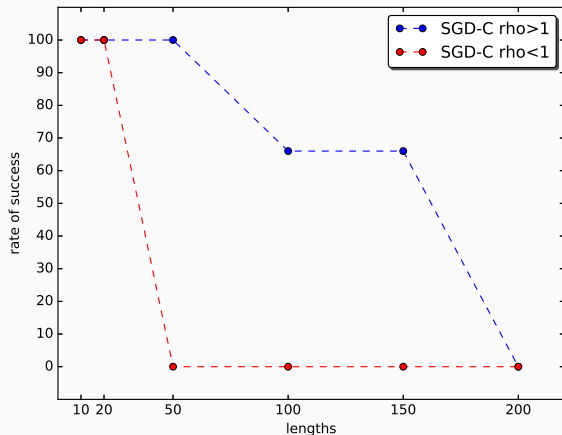


Figure 1: Rate of success for the temporal order task.

A different descent direction

Combine the temporal gradients to obtain a descent direction which does not suffer from the vanishing gradient problem.

- Normalize the temporal gradients:

$$s_t(\mathbf{x}) = \frac{\nabla L_t(\mathbf{x})}{\|\nabla L_t(\mathbf{x})\|}. \quad (25)$$

- Combine the normalized gradients in a convex way:

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

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

- Introduce the gradient norm:

$$d(\mathbf{x}) = -\|\nabla L(\mathbf{x})\| \frac{s(\mathbf{x})}{\|s(\mathbf{x})\|}. \quad (27)$$

Algorithm 3: RNN training

Data:

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

m : size of each mini-batch

μ : constant learning rate

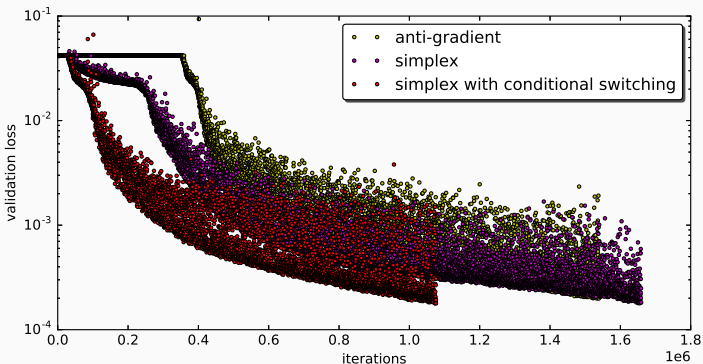
τ : gradient clipping threshold

ρ : initial spectral radius

ψ threshold for the direction norm

```
1  $W_{rec}, W_{in}, W_{out} \sim \mathcal{N}(0, \sigma^2)$ 
2  $\mathbf{b}_{out}, \mathbf{b}_{rec} \leftarrow 0$ 
3  $r \leftarrow \text{spectral\_radius}(W_{rec})$ 
4  $W_{rec} \leftarrow \frac{\rho}{r} \cdot W_{rec}$ 
5  $\theta_0 = [W_{rec}, W_{in}, W_{out}, \mathbf{b}_{out}, \mathbf{b}_{rec}]$ 
6 while stop criterion do
7    $I \leftarrow$  sample  $m$  training example  $\in D$ 
8    $\{\nabla_{\theta} L_t\}_{t=1}^T \leftarrow \text{compute\_temporal\_gradients}(\theta_k, I)$ 
9    $\mathbf{d}_k \leftarrow \text{simplex\_combination}(\{\nabla_{\theta} L_t\})$ 
10  if  $\|\nabla_{\theta} L(\theta_k)\|_2 > \psi$  then
11     $\mathbf{d}_k \leftarrow \nabla_{\theta} L(\theta_k)$ 
12  end
13   $\alpha_k = \begin{cases} \mu & \text{if } \|\mathbf{d}_k\|_2 \leq \tau \\ \frac{\mu \cdot \tau}{\|\mathbf{d}_k\|_2} & \text{otherwise} \end{cases}$ 
14   $\theta_{k+1} \leftarrow \theta_k + \alpha_k \mathbf{d}_k$ 
15   $k \leftarrow k + 1$ 
16 end
17 return  $\theta_k$ 
```

Effect of the simplex direction



(a) Loss for the addition task during training.

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

(b) Average number of iterations to converge.

A case study: Lupus disease prediction

Lupus disease prediction

The **goal** is to predict whether a patient will develop the lupus disease in the near future given its medical history.

Dataset:

- ▶ Gathered by the “Lupus Clinic”, Reumatologia, Università Sapienza, Rome.
- ▶ Patients have a different number of visits.
- ▶ Visits are not equally spaced over time.
- ▶ Small dataset (~ 100 negatives, 40 positives).

An example of a record of a patient

	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

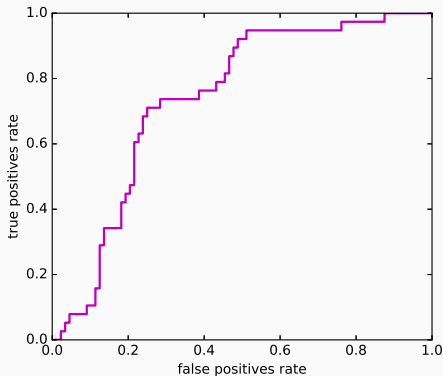


Figure 2: ROC curve. AUC score is 0.74

- ▶ Results considered promising by medical experts.
- ▶ Improvable when more data will be available.



