

Recurrent Neural Networks

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Outline

- Why RNNs?
- Gradient troubles.
- LSTMs
- Practical training tips
- Non-sequential data
- Discussion & controversies (why RNNs pt. 2)

WHY RNNS?

Supervised learning

Neural nets excel at implementing functions

$$f: \mathbb{R}^n \rightarrow \mathbb{R}^m$$

Crucial modeling assumption: n, m are known and fixed.

Variable sized data

- Classify if text is grammatical.
- Generate a sentence.
- Forecast demand for a product based on sales history
- Translation: map this sequence of English words to French ones
- Speech recognition: map this sequence of speech to characters.

Text generation

Generate a sentence

(or equivalently)

Learn a function that assigns probabilities to sentences.

Formally:

Let x_1, x_2, \dots, x_T be the words of the sentence.

We want: $p(x_1, x_2, x_3, \dots, x_T)$.

Text generation solutions

$$\begin{aligned} p(x_1, x_2, x_3, \dots, x_T) &= \\ p(x_1)p(x_2|x_1) \dots p(x_T|x_1, \dots, x_{T-1}) &= \\ \prod_{t=1}^T p(x_t|x_1, \dots, x_{t-1}) \end{aligned}$$

Now we need to learn $p(x_t|x_1, \dots, x_{t-1})$!

Learning $p(x_t | x_1, \dots, x_{t-1}) \dots$

1. Assume distant past doesn't matter,
$$p(x_t | x_1, \dots, x_{t-1}) \approx p(x_t | x_{t-n+1}, \dots, x_{t-1})$$

These are called “n-gram text models”

Learning $p(x_t | x_1, \dots, x_{t-1}) \dots$

2. Simply reduce x_1, \dots, x_{t-1} to a fixed-size representation

Can take weighted average of word embeddings

This is nicely developed in Attention is All You Need paper.

Learning $p(x_t | x_1, \dots, x_{t-1}) \dots$

3. Introduce a hidden (i.e. not directly observed) state h_t .

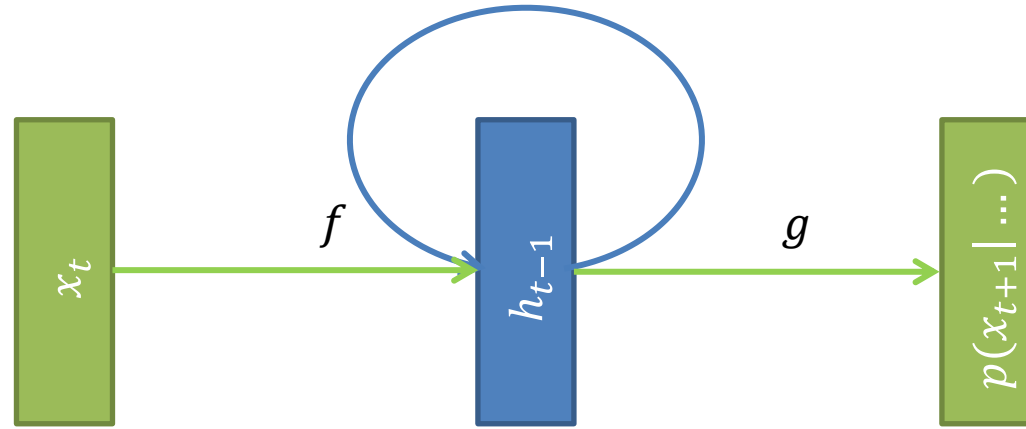
h_t summarizes x_1, \dots, x_{t-1} .

Compute h_t using this recurrence:

$$h_t = f(h_{t-1}, x_t)$$

$$p(x_{t+1} | x_1, \dots, x_t) = g(h_t)$$

RNNs are networks with state



$$h_t = f(h_{t-1}, x_t)$$
$$p(x_{t+1} | x_1, \dots, x_t) = g(h_t)$$

f, g are implemented as feedforward neural nets.

RNN Example

Input: a sequence of bits 1,0,1,0,0,1

Output: the parity

Solution:

The hidden state will be just 1 bit – parity so far:

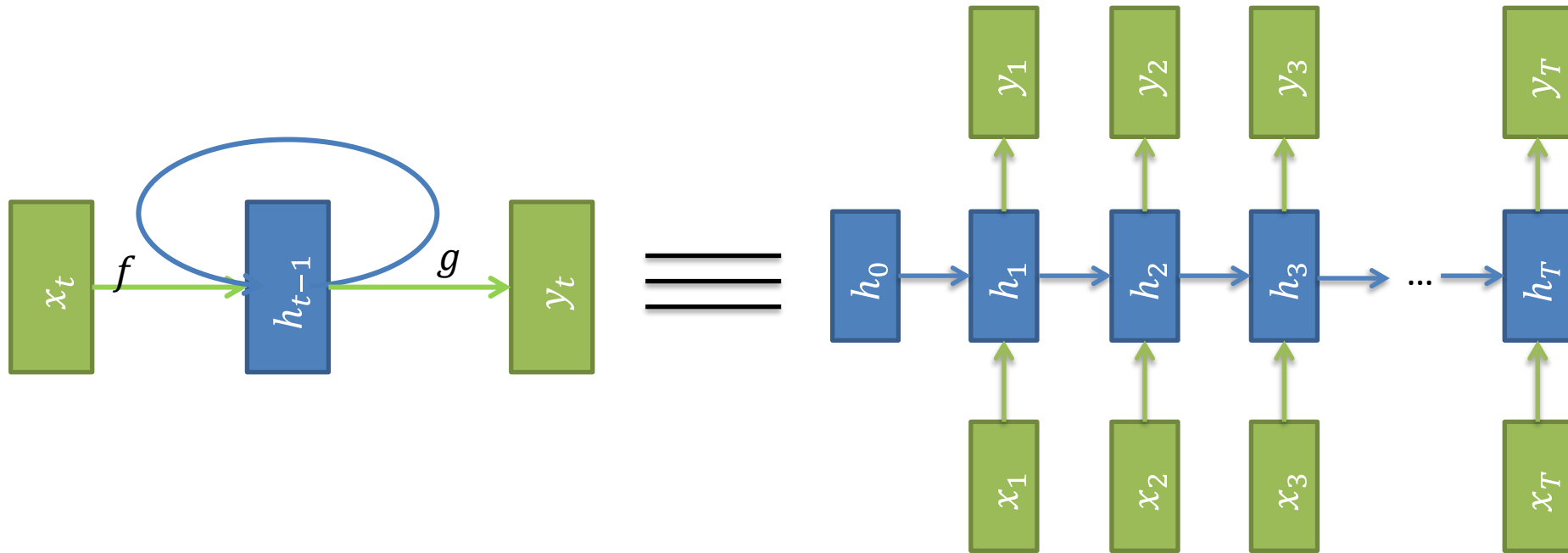
$$h_0 = 0$$

$$h_t = XOR(h_{t-1}, x_t)$$

$$y_T = h_T$$

RNNs are dynamical systems

Time is discrete, we can unroll:

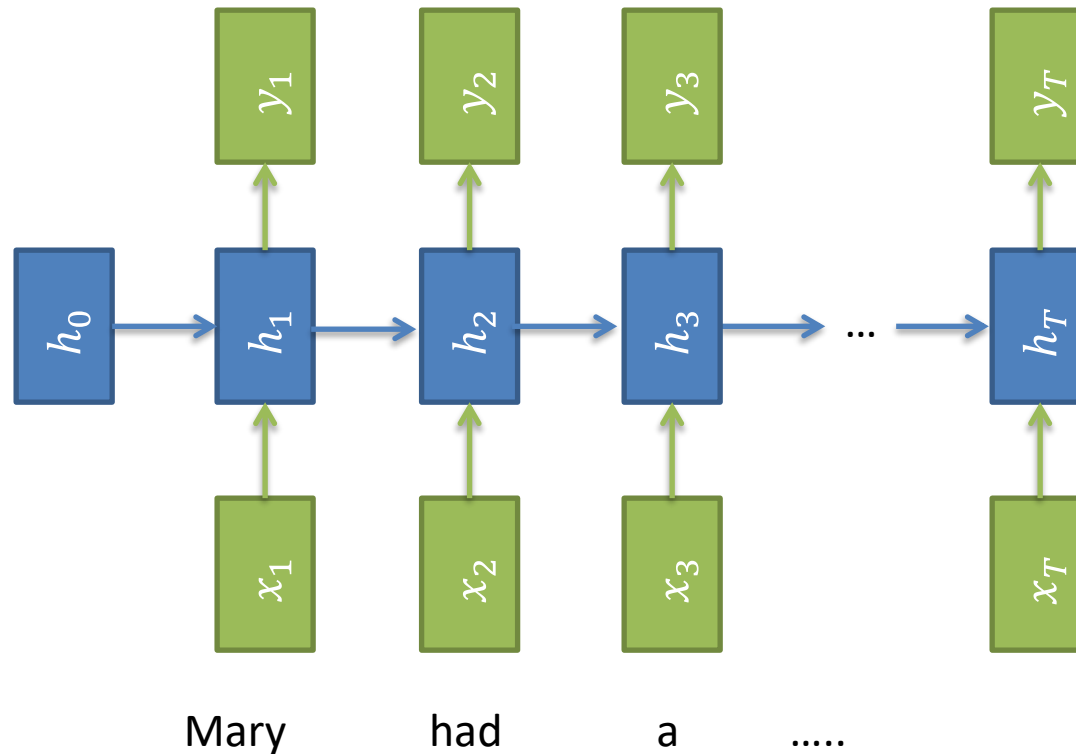


Thus the RNN is a very deep network, with same “arrows” computing the same function!

RNNs transform sequences

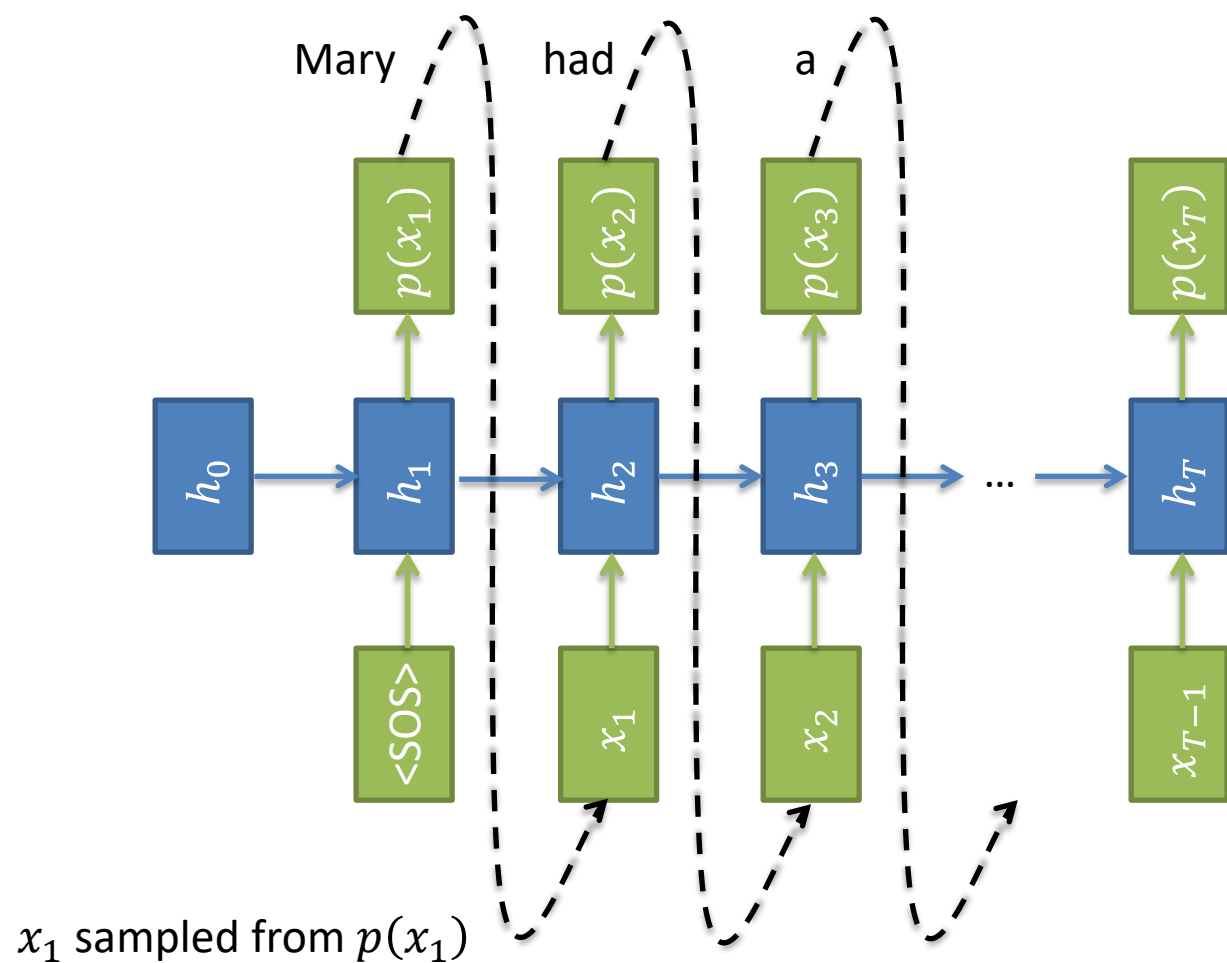
Transform a sequence x_1, x_2, \dots, x_T into y_1, y_2, \dots, y_T :

$p(\text{had}|\text{Mary})$ $p(\text{a}|\dots)$ $p(\text{little}|\dots)$



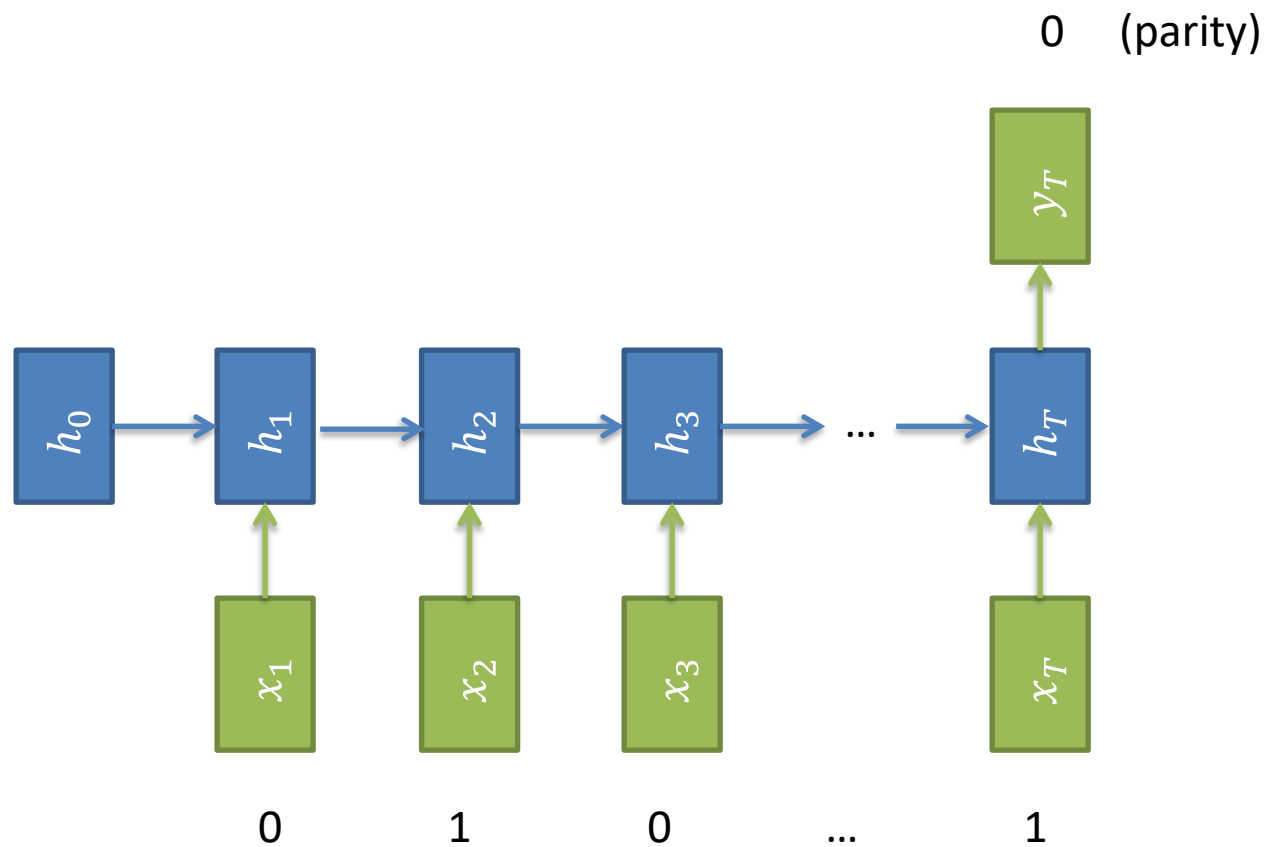
RNNs generate sequences

Generate a sequence (scan)



RNNs summarize sequences

Summarize a sequence (fold):



**RNN TRAINING,
GRADIENT TROUBLE!**

Training RNNs

In principle very easy:

1. Unroll in time
2. Apply the backpropagation algorithm to get gradients with respect to parameters
3. Train as usual

In practice:

Gradient computation can be numerically unstable.
Getting good gradients is difficult.

A linear dynamical system

$$h_t = w \cdot h_{t-1} = w^t h_0$$

When:

1. $w > 1$ it diverges: $\lim_{t \rightarrow \infty} h_t = \text{sign}(h_0) \cdot \infty$
2. $w = 1$ it is constant $\lim_{t \rightarrow \infty} h_t = h_0$
3. $-1 < w < 1$ it decays to 0: $\lim_{t \rightarrow \infty} h_t = 0$
4. $w = -1$ flips between $\pm h_0$
5. $w < -1$ diverges, changes sign at each step

A multidimensional linear dyn. system

$$h_t \in \mathbb{R}^n, W \in \mathbb{R}^{n \times n}$$

$$h_t = W h_{t-1}$$

Compute the eigen-decomposition of W :

$$W = Q \Lambda Q^{-1} = Q \begin{bmatrix} \lambda_{11} & & \\ & \ddots & \\ & & \lambda_{nn} \end{bmatrix} Q^{-1}$$

Then

$$\begin{aligned} h_t &= W h_{t-1} = W^t h_0 = Q \Lambda^t Q^{-1} h_0 = \\ &= Q \begin{bmatrix} \lambda_{11}^t & & \\ & \ddots & \\ & & \lambda_{nn}^t \end{bmatrix} Q^{-1} h_0 \end{aligned}$$

A multidimensional dyn. system cont.

$$h_t = Wh_{t-1} = W^t h_0 = Q\Lambda^t Q^{-1} h_0$$

If largest eigenvalue has norm:

1. $|\lambda_1| > 1$, system diverges
2. $|\lambda_1| = 1$, system is stable or oscillates
3. $|\lambda_1| < 1$, system decays to 0

This is similar to the scalar case.

A nonlinear dynamical system

$$h_t = \tanh(w \cdot h_{t-1})$$

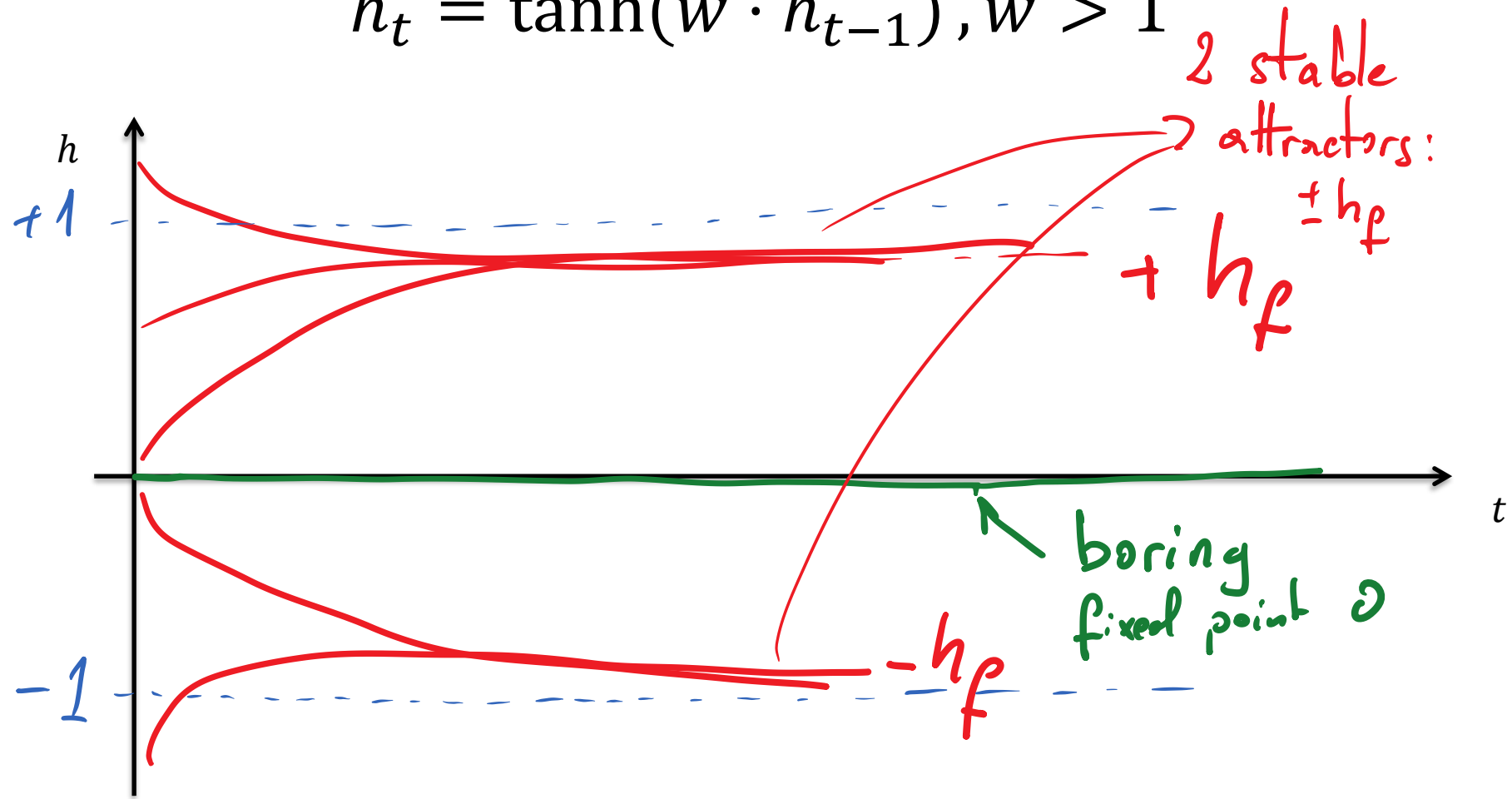
Output is bounded (can't diverge!)

If $w > 1$ has 3 fixed points: $0, \pm h_f$. Starting the iteration from $h_0 \neq 0$ it ends at $\pm h_f$ (effectively remembers the sign).

If $w \leq 1$ has one fixed point: 0

A nonlinear dynamical system

$$h_t = \tanh(w \cdot h_{t-1}), w > 1$$



Gradients in RNNs

Recall RNN equations:

$$h_t = f(h_{t-1}, x_t; \theta)$$

$$y_t = g(h_t)$$

Assume supervision only at the last step:

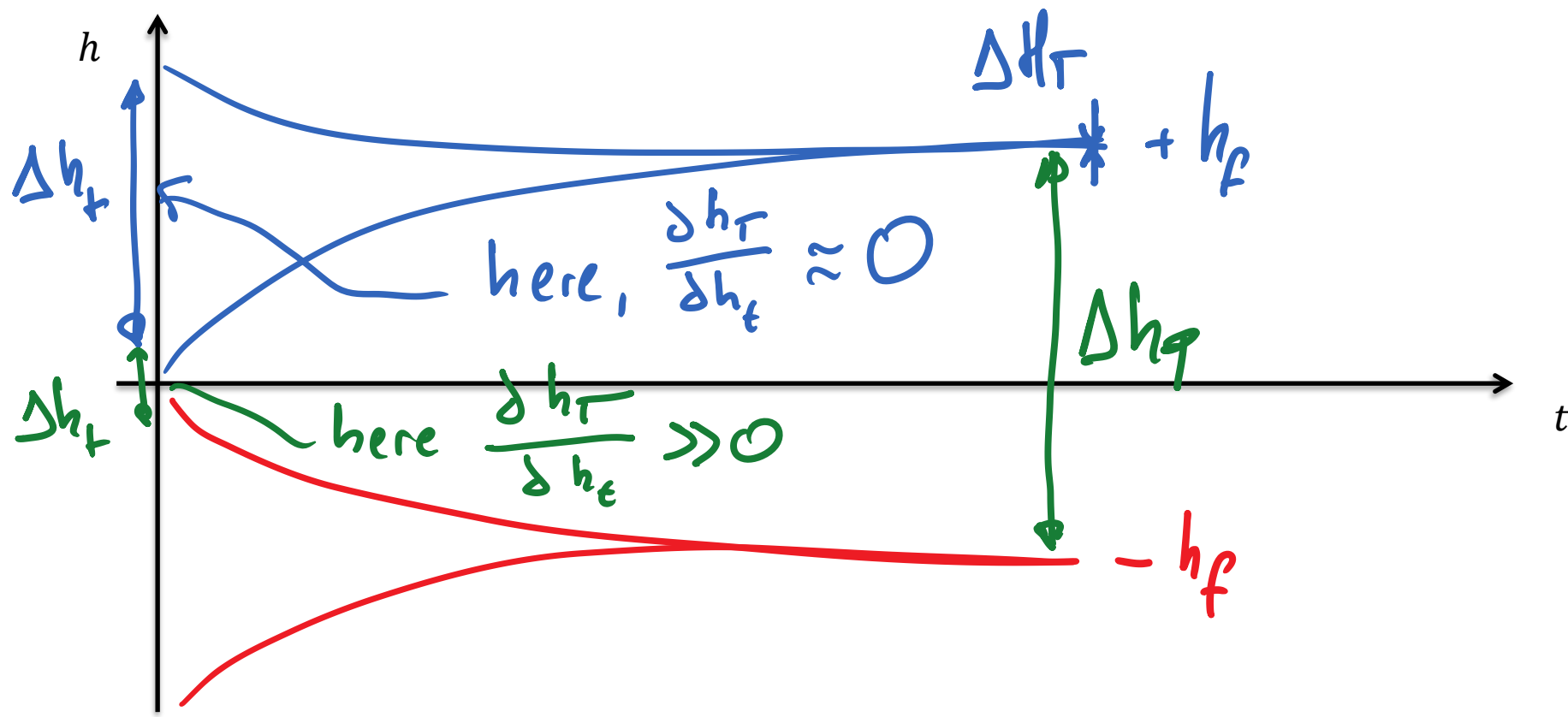
$$L = e(y_T)$$

The gradient is

$$\frac{\partial L}{\partial \theta} = \sum_t \frac{\partial L}{\partial h_T} \frac{\partial \mathbf{h}_T}{\partial \mathbf{h}_t} \frac{\partial h_t}{\partial \theta}$$

Trouble with $\frac{\partial h_T}{\partial h_t} \approx \frac{\Delta h_T}{\Delta h_t}$

$\frac{\partial h_T}{\partial h_t}$ measures how much h_T changes when h_t changes.



Another look at $\frac{\partial h_T}{\partial h_t}$

Let:

$$h_t = \tanh(w \cdot h_{t-1})$$

Then:

$$\frac{\partial h_t}{\partial h_0} = \frac{\partial h_t}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial h_{t-2}} \frac{\partial h_{t-2}}{\partial h_{t-3}} \cdots \frac{\partial h_1}{\partial h_0}$$

$$\frac{\partial h_{i+1}}{\partial h_i} = \tanh'(wh_t) w$$

$$\frac{\partial h_t}{\partial h_0} = \prod_{i=0}^{t-1} \tanh'(wh_i) w = w^t \prod_{i=0}^{t-1} \tanh'(wh_i)$$

Backward phase is linear!

Vanishing gradient

If $\frac{\partial h_T}{\partial h_t} = 0$ the network forgets all information from time t when it reaches time T .

This makes it impossible to discover correlations between inputs at distant time steps.

This is a modeling problem.

Exploding gradient

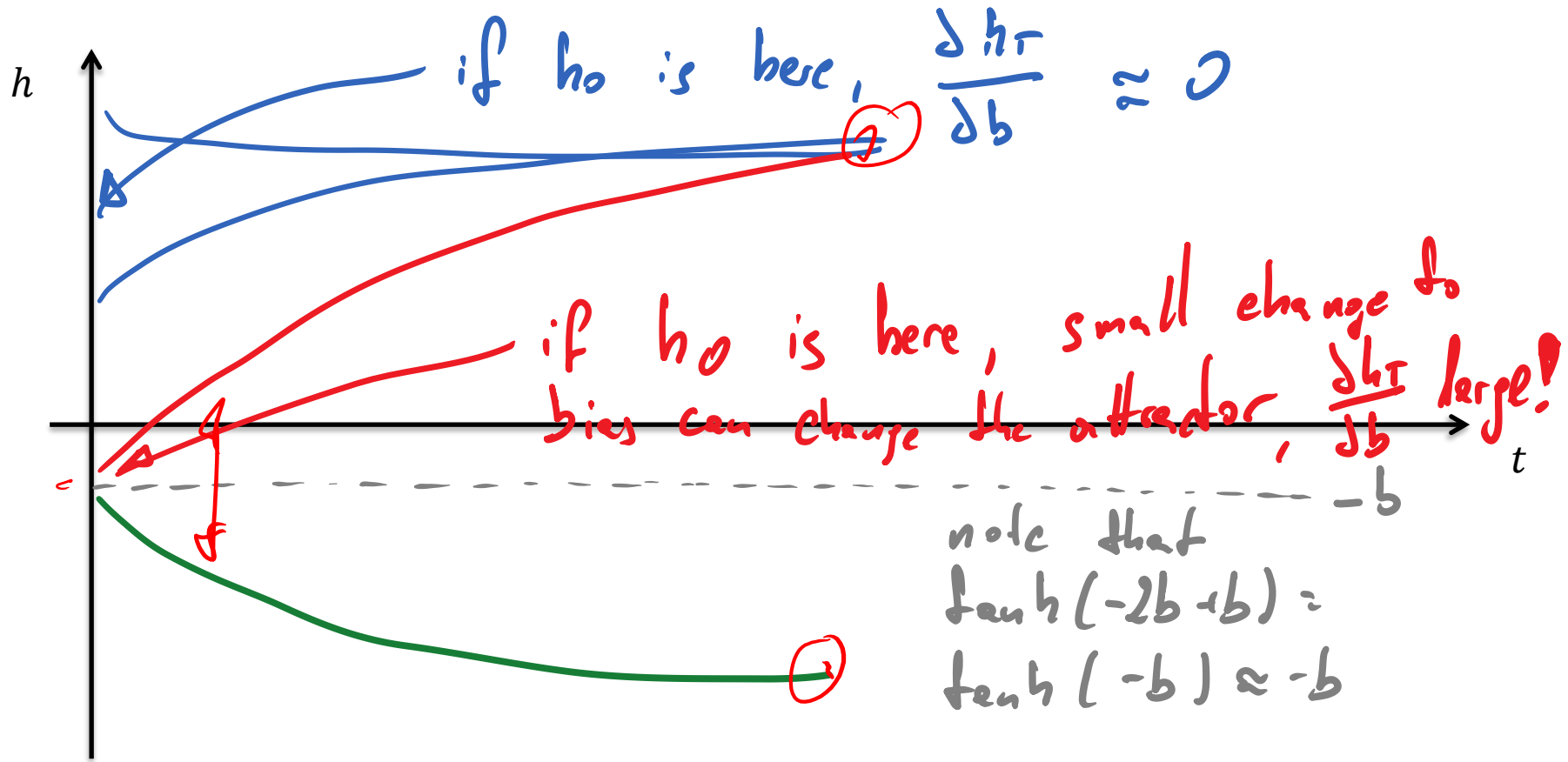
When $\frac{\partial h_T}{\partial h_t}$ is large $\frac{\partial \text{Loss}}{\partial \theta}$ will be large too.

Making a gradient step $\theta \leftarrow \alpha \frac{\partial \text{Loss}}{\partial \theta}$ can drastically change the network, or even destroy it.

This is not a problem of information flow, but of training stability!

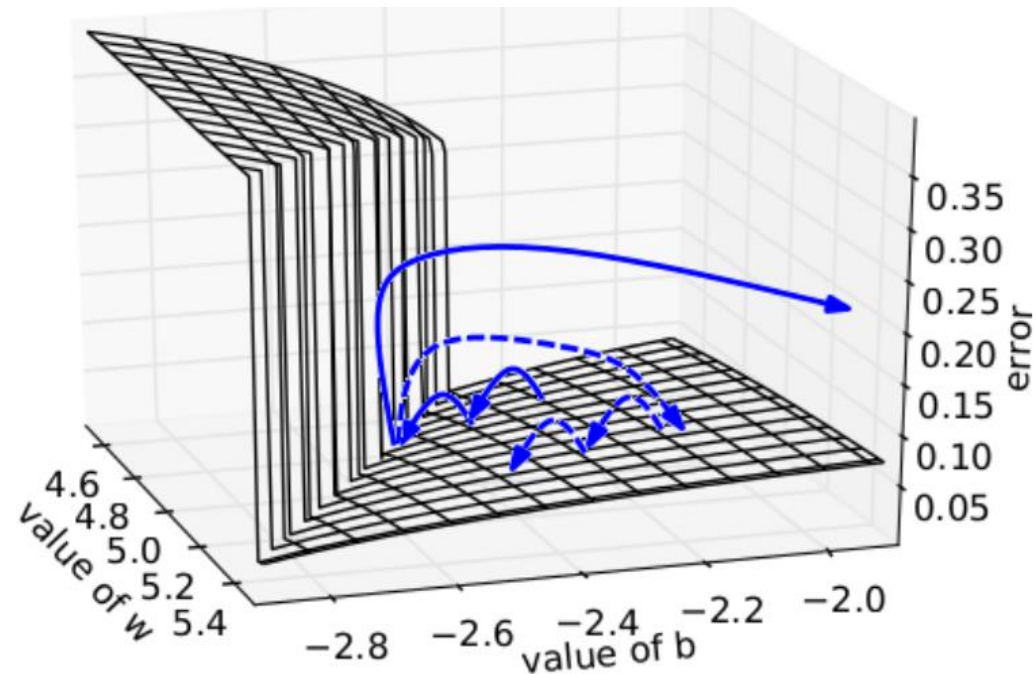
Exploding gradient intuition #1

$$h_t = \tanh(2h_{t-1} + b)$$



Exploding gradient intuition #2

$$\begin{aligned}h_0 &= \sigma(0.5) \\h_t &= \sigma(wh_{t-1} + b) \\L &= (h_{50} - 0.7)^2\end{aligned}$$



Summary: trouble with $\frac{\partial h_T}{\partial h_t}$

RNNs are difficult to train because:

$\frac{\partial h_T}{\partial h_t}$ can be 0 – vanishing gradient

$\frac{\partial h_T}{\partial h_t}$ can be ∞ – exploding gradient

With both phenomena governed by the spectral norm of the weight matrix (norm of the largest eigenvalue, magnitude of w in the scalar case).

Exploding gradient solution

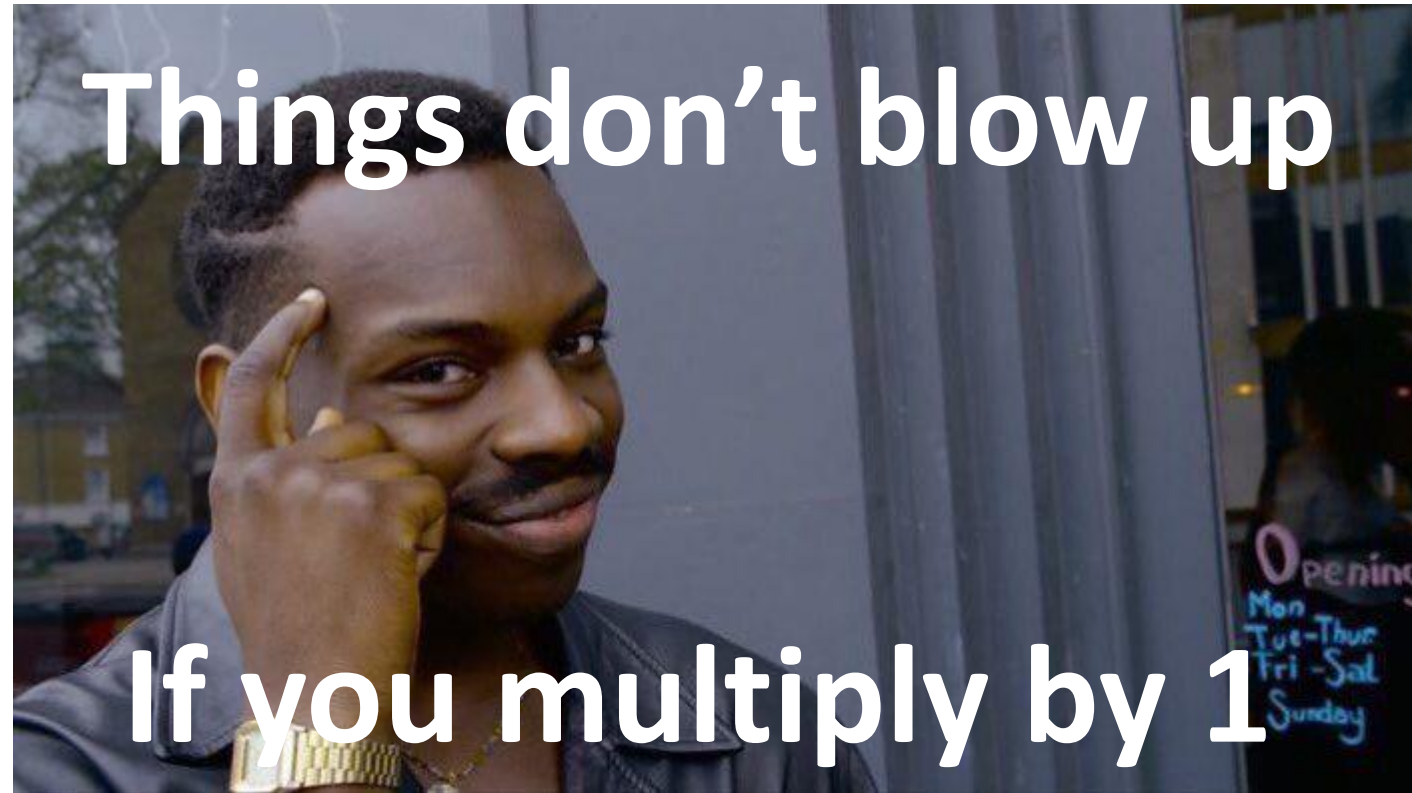
Don't do large steps.

Pick a gradient norm threshold and scale down all larger gradients.

This prevents the model from doing a large learning update and destroying itself.

VANISHING GRADIENT SOLUTION: LSTM

LSTM



LSTM intuitions

Recall the scalar case

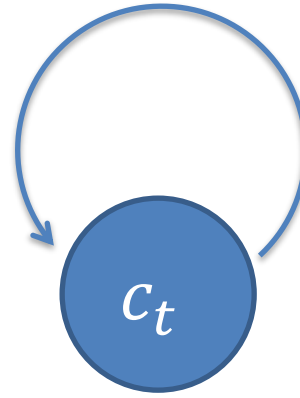
$$h_t = wh_{t-1}$$

It maximally preserves information when $w = 1$

The LSTM introduces a memory cell c_t that will keep information forever:

$$c_t = 1 \cdot c_{t-1}$$

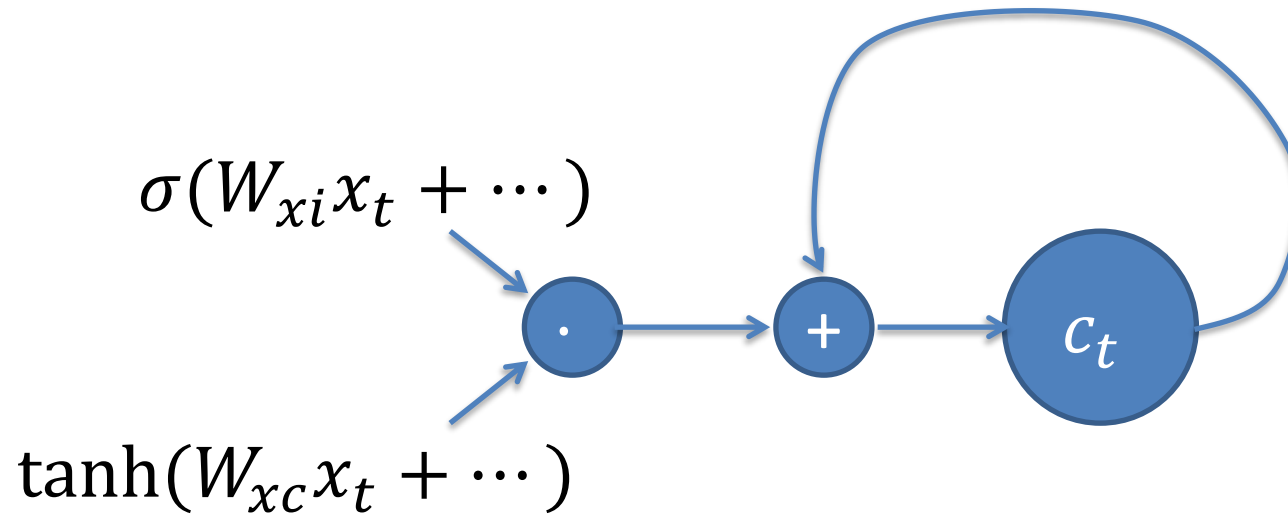
Memory cell



Memory cell preserves information

$$c_t = c_{t-1}$$
$$\frac{\partial c_T}{\partial c_t} = 1$$

Gates



Gates selectively load information into the memory cell:

$$i_t = \sigma(W_{xi}x_t + \dots)$$
$$c_t = c_{t-1} + i_t \cdot \tanh(W_{xc}x_t + \dots)$$

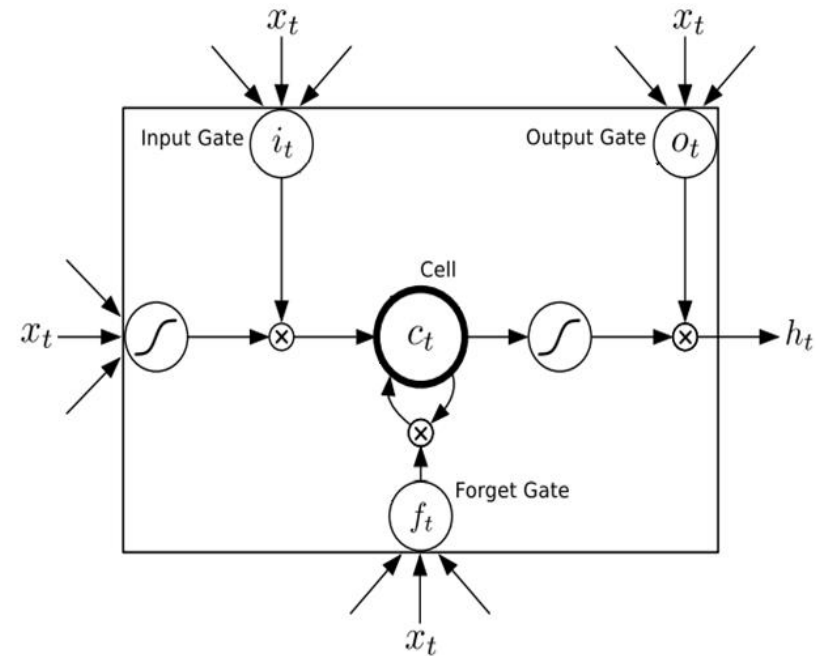
LSTM: the details

Hidden state is a pair of:

- c_t information in the cell, hidden from the rest of the network
- h_t information extracted from the cell into the network

Update equations:

$$\begin{aligned}i_t &= \sigma(W_{xi}x_t + W_{hi}h_{t-1} + b_i) \\f_t &= \sigma(W_{xf}x_t + W_{hf}h_{t-1} + b_f) \\o_t &= \sigma(W_{xo}x_t + W_{ho}h_{t-1} + b_o) \\c_t &= i_t \tanh(W_{xc}x_t + W_{hc}h_{t-1} + b_c) \\&\quad + f_t c_{t-1} \\h_t &= o_t \tanh c_t\end{aligned}$$



LSTM in action

Cell sensitive to position in line:

The sole importance of the crossing of the Berezina lies in the fact that it plainly and indubitably proved the fallacy of all the plans for cutting off the enemy's retreat and the soundness of the only possible line of action--the one Kutuzov and the general mass of the army demanded--namely, simply to follow the enemy up. The French crowd fled at a continually increasing speed and all its energy was directed to reaching its goal. It fled like a wounded animal and it was impossible to block its path. This was shown not so much by the arrangements it made for crossing as by what took place at the bridges. When the bridges broke down, unarmed soldiers, people from Moscow and women with children who were with the French transport, all--carried on by vis inertiae--pressed forward into boats and into the ice-covered water and did not, surrender.

Cell that turns on inside quotes:

"You mean to imply that I have nothing to eat out of.... On the contrary, I can supply you with everything even if you want to give dinner parties," warmly replied Chichagov, who tried by every word he spoke to prove his own rectitude and therefore imagined Kutuzov to be animated by the same desire.

Kutuzov, shrugging his shoulders, replied with his subtle penetrating smile: "I meant merely to say what I said."

Cell that robustly activates inside if statements:

```
static int __dequeue_signal(struct sigpending *pending, sigset_t *mask,
                           siginfo_t *info)
{
    int sig = next_signal(pending, mask);
    if (sig) {
        if (current->notifier) {
            if (sigismember(current->notifier_mask, sig)) {
                if (!(current->notifier)(current->notifier_data)) {
                    clear_thread_flag(TIF_SIGPENDING);
                    return 0;
                }
            }
        }
        collect_signal(sig, pending, info);
    }
    return sig;
}
```

A large portion of cells are not easily interpretable. Here is a typical example:

```
/* Unpack a filter field's string representation from user-space
 * buffer. */
char *audit_unpack_string(void **bufp, size_t *remain, size_t len)
{
    char *str;
    if (!*bufp || (len == 0) || (len > *remain))
        return ERR_PTR(-EINVAL);
    /* Of the currently implemented string fields, PATH_MAX
     * defines the longest valid length.
     */
```

Cell that turns on inside comments and quotes:

```
/* Duplicate LSM field information. The lsm_rule is opaque, so
 * re-initialized. */
static inline int audit_dupe_lsm_field(struct audit_field *df,
                                       struct audit_field *sf)
{
    int ret = 0;
    char *lsm_str;
    /* Our own copy of lsm_str */
    lsm_str = kstrdup(sf->lsm_str, GFP_KERNEL);
    if (unlikely(!lsm_str))
        return -ENOMEM;
    df->lsm_str = lsm_str;
    /* Our own (refreshed) copy of lsm_rule */
    ret = security_audit_rule_init(df->type, df->op, df->lsm_str,
                                   (void **)&df->lsm_rule);
    /* Keep currently invalid fields around in case they
     * become valid after a policy reload. */
    if (ret == -EINVAL) {
        pr_warn("audit rule for LSM '%s' is invalid\n",
                df->lsm_str);
        ret = 0;
    }
    return ret;
}
```

Cell that is sensitive to the depth of an expression:

```
#ifdef CONFIG_AUDITSYSCALL
static inline int audit_match_class_bits(int class, u32 *mask)
{
    int i;
    if (classes[class]) {
        for (i = 0; i < AUDIT_BITMASK_SIZE; i++)
            if (mask[i] & classes[class][i])
                return 0;
    }
    return 1;
}
```

Cell that might be helpful in predicting a new line. Note that it only turns on for some "j":

```
char *audit_unpack_string(void **bufp, size_t *remain, size_t len)
{
    char *str;
    if (!*bufp || (len == 0) || (len > *remain))
        return ERR_PTR(-EINVAL);
    /* Of the currently implemented string fields, PATH_MAX
     * defines the longest valid length.
     */
    if (len > PATH_MAX)
        return ERR_PTR(-ENAMETOOLONG);
    str = kmalloc(len + 1, GFP_KERNEL);
    if (unlikely(!str))
        return ERR_PTR(-ENOMEM);
    memcpy(str, *bufp, len);
    str[len] = 0;
    *bufp += len;
    *remain -= len;
    return str;
}
```

LSTM fixes vanishing gradient

- With input gate closed, and forget gate opened, LSTM preserves information in the memory cell - gradients flow into distant time steps.
- The gates decouple the decision **if** information should be stored from **what** information should be stored.

LSTM variant: peephole connections

Peephole connections allow the gates to “peep” into the cell value:

$$\begin{aligned}i_t &= \sigma(W_{xi}x_t + W_{hi}h_{t-1} + \mathbf{W}_{ci}\mathbf{c}_{t-1} + b_i) \\f_t &= \sigma(W_{xf}x_t + W_{hf}h_{t-1} + \mathbf{W}_{cf}\mathbf{c}_{t-1} + b_f) \\c_t &= f_t c_{t-1} + i_t \tanh(W_{xc}x_t + W_{hc}h_{t-1} + b_c) \\o_t &= \sigma(W_{xo}x_t + W_{ho}h_{t-1} + \mathbf{W}_{co}\mathbf{c}_t + b_o) \\h_t &= o_t \tanh c_t\end{aligned}$$

LSTM Variant: projection

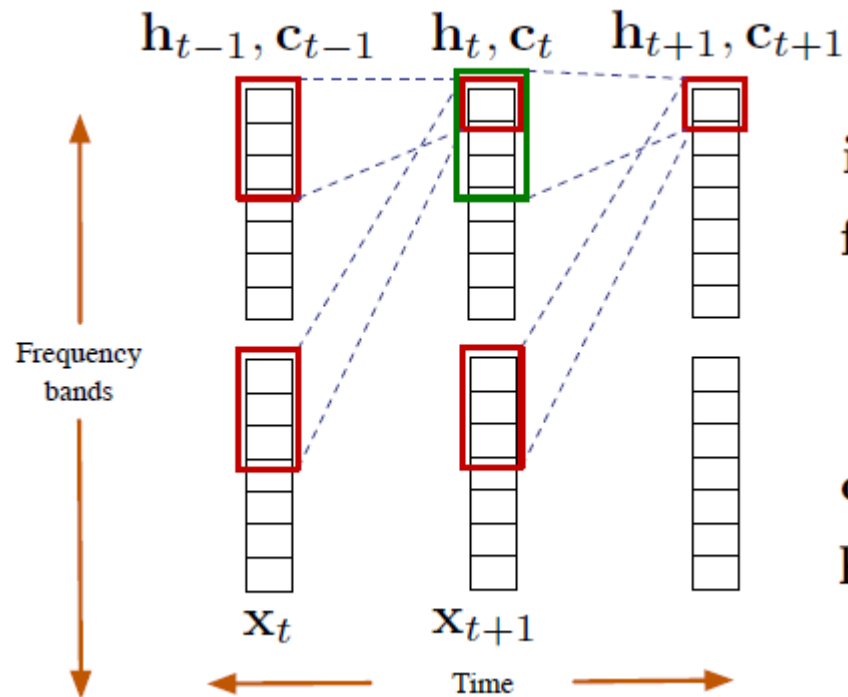
Projections reduce the number of parameters and computations: for N LSTM units we need $O(N^2)$ parameters and flops.

With projections we only need $O(2NP)$, which is beneficial when $P \ll N$:

$$\begin{aligned}i_t &= \sigma(W_{xi}x_t + W_{hi}h_{t-1} + W_{ci}c_{t-1} + b_i) \\f_t &= \sigma(W_{xf}x_t + W_{hf}h_{t-1} + W_{cf}c_{t-1} + b_f) \\c_t &= f_t c_{t-1} + i_t \tanh(W_{xc}x_t + W_{hc}h_{t-1} + b_c) \\o_t &= \sigma(W_{xo}x_t + W_{ho}h_{t-1} + W_{co}c_t + b_o) \\h'_t &= o_t \tanh c_t \\ \mathbf{h}_t &= \mathbf{W}_p \mathbf{h}'_t\end{aligned}$$

LSTM variant: ConvLSTM

Replace matrix multiplications with convolutions!
Both are linear operations.



$$\mathbf{i}_t = \sigma(\mathbf{W}_{xi} * \mathbf{x}_t + \mathbf{W}_{hi} * \mathbf{h}_{t-1} + \mathbf{b}_i)$$

$$\mathbf{f}_t = \sigma(\mathbf{W}_{xf} * \mathbf{x}_t + \mathbf{W}_{hf} * \mathbf{h}_{t-1} + \mathbf{b}_f)$$

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} +$$

$$+ \mathbf{i}_t \odot \tanh(\mathbf{W}_{xc} * \mathbf{x}_t + \mathbf{W}_{hc} * \mathbf{h}_{t-1} + \mathbf{b}_c)$$

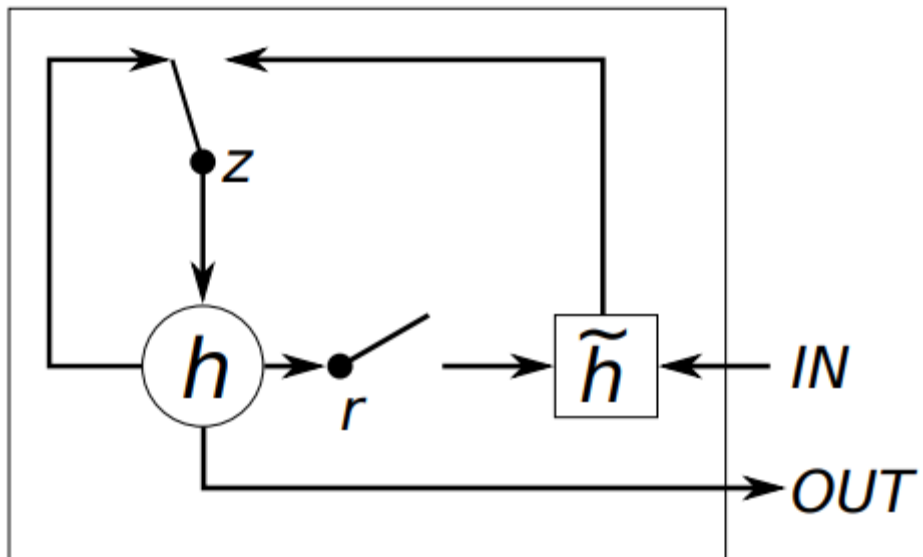
$$\mathbf{o}_t = \sigma(\mathbf{W}_{xo} * \mathbf{x}_t + \mathbf{W}_{ho} * \mathbf{h}_{t-1} + \mathbf{b}_o)$$

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

The GRU cell – an LSTM alternative

The GRU is similar to the LSTM, but:

- uses only two gates: reset (r) and update (z)
- Doesn't have a separate c_t from h_t .



$$r_t^j = \sigma (W_r \mathbf{x}_t + U_r \mathbf{h}_{t-1})^j$$

$$\tilde{h}_t^j = \tanh (W \mathbf{x}_t + U (\mathbf{r}_t \odot \mathbf{h}_{t-1}))^j$$

$$z_t^j = \sigma (W_z \mathbf{x}_t + U_z \mathbf{h}_{t-1})^j$$

$$h_t^j = (1 - z_t^j) h_{t-1}^j + z_t^j \tilde{h}_t^j$$

Echo state networks

You have no gradient problems

If you don't train you weights!



Echo state networks

Dynamics:

$$h_t = (1 - a)h_{t-1} + a \tanh(W_h h_{t-1} + W_x x_t)$$

$$y_t = W_y h_t$$

Algorithm:

Repeat until it works:

- Initialize W_x randomly
- Initialize W_h randomly, scale to have largest eigenvalue ≈ 1
- Fit W_y , can use the matrix pseudo-inverse formula

Each “training” run is very fast, can sample thousands of configurations.

Unitary Evolution RNN

What if

$$h_t = \sigma(W h_{t-1} + U x_t)$$

But W is unitary (all complex eigenvalues have norm 1)?

Then we have no exponential explosion/decay!

How to ensure W is unitary?

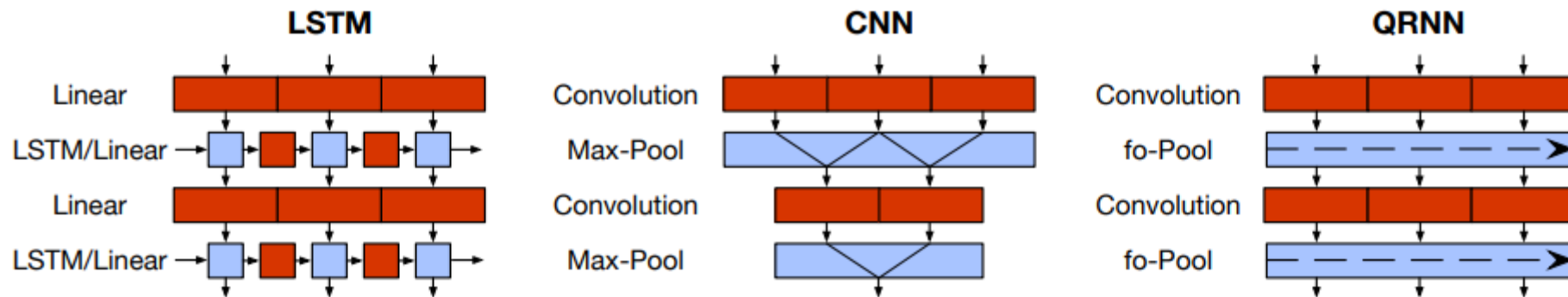
Let:
$$W = D_3 R_2 \mathcal{F}^{-1} D_2 \Pi R_1 \mathcal{F} D_1$$

- D , a diagonal matrix with $D_{j,j} = e^{i w_j}$, with parameters $w_j \in \mathbb{R}$,
- $R = I - 2 \frac{v v^*}{\|v\|^2}$, a reflection matrix in the complex vector $v \in \mathbb{C}^n$,
- Π , a fixed random index permutation matrix, and
- \mathcal{F} and \mathcal{F}^{-1} , the Fourier and inverse Fourier transforms.

QuasiRNNs

RNNs are inherently sequential.

How much can we parallelize?



$$\mathbf{Z} = \tanh(\mathbf{W}_z * \mathbf{X})$$

$$\mathbf{F} = \sigma(\mathbf{W}_f * \mathbf{X})$$

$$\mathbf{O} = \sigma(\mathbf{W}_o * \mathbf{X}),$$

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + (1 - \mathbf{f}_t) \odot \mathbf{z}_t$$

$$\mathbf{h}_t = \mathbf{o}_t \odot \mathbf{c}_t.$$

No-nonlinearity RNN

Model uses a different weight matrix for each input symbol:

$$\mathbf{h}_t = \mathbf{W}_{\mathbf{x}_t} \mathbf{h}_{t-1} + \mathbf{b}_{\mathbf{x}_t}$$

$$p(\mathbf{x}_{t+1}) = \text{softmax}(\mathbf{l}_t)$$

$$\mathbf{l}_t = \mathbf{W}_{ro} \mathbf{h}_t + \mathbf{b}_{ro}$$

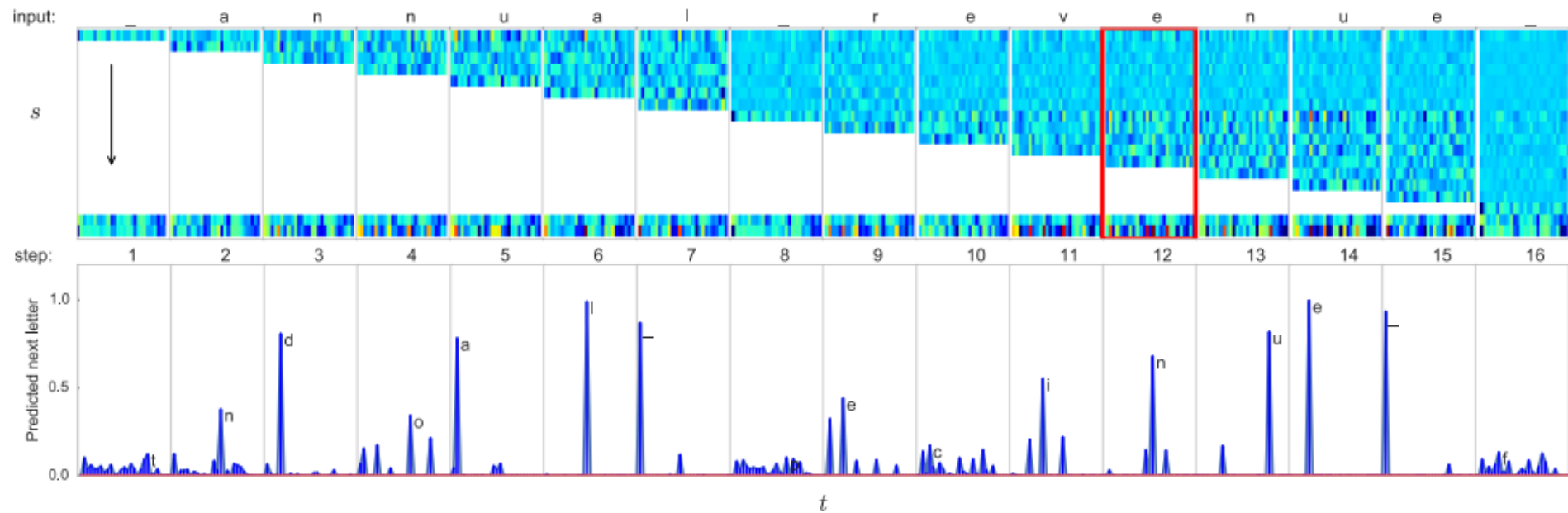
We can decompose an output at time t into contributions from previous time states:

$$\mathbf{l}_t = \mathbf{b}_{ro} + \sum_{s=0}^t \kappa_s^t$$

$$\kappa_s^t = \mathbf{W}_{ro} \left(\prod_{s'=s+1}^t \mathbf{W}_{\mathbf{x}_{s'}} \right) \mathbf{b}_{\mathbf{x}_s}$$

No-nonlinearity RNN

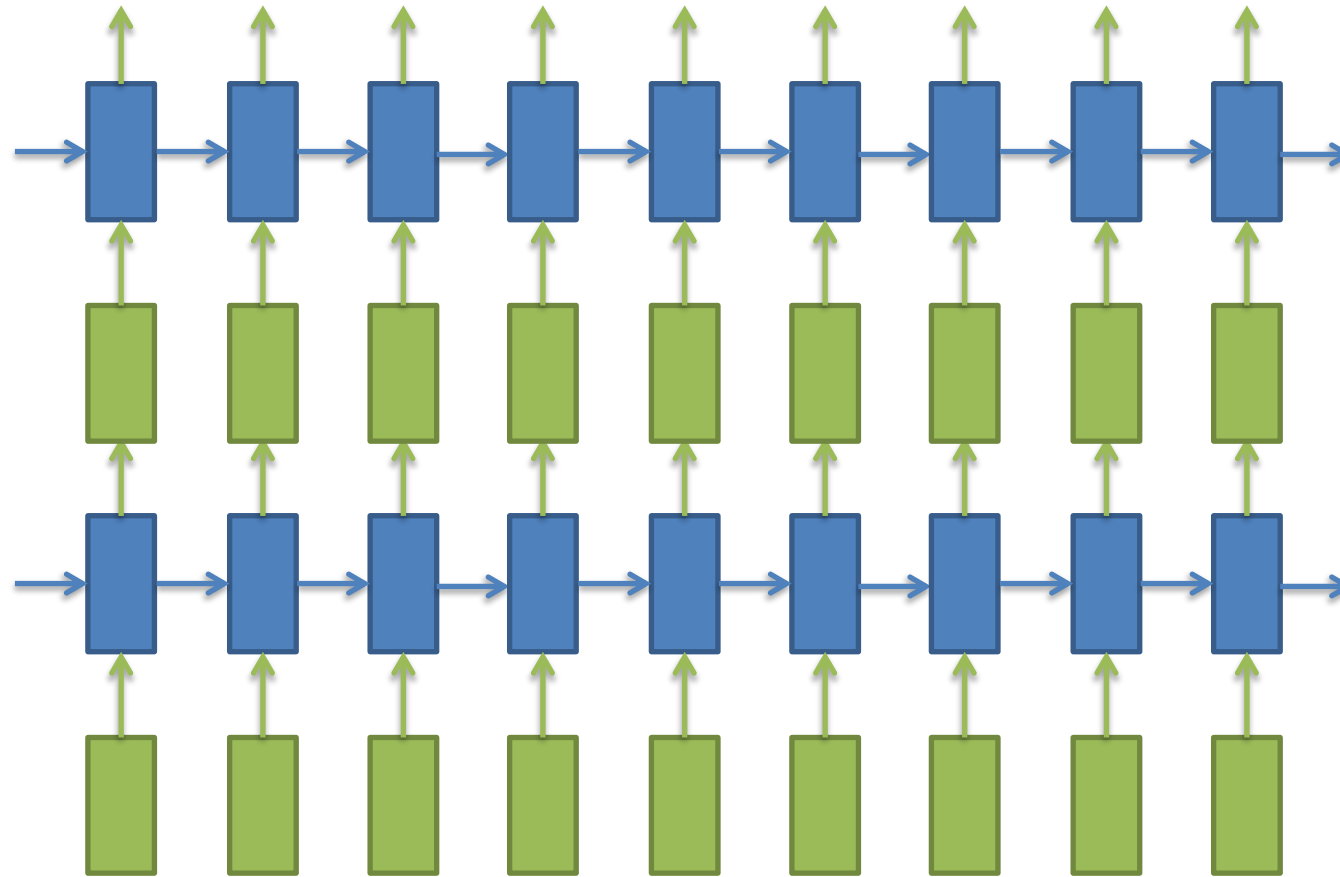
Visualization of contributions from past timesteps:



RNNS – PRACTICAL ASPECTS

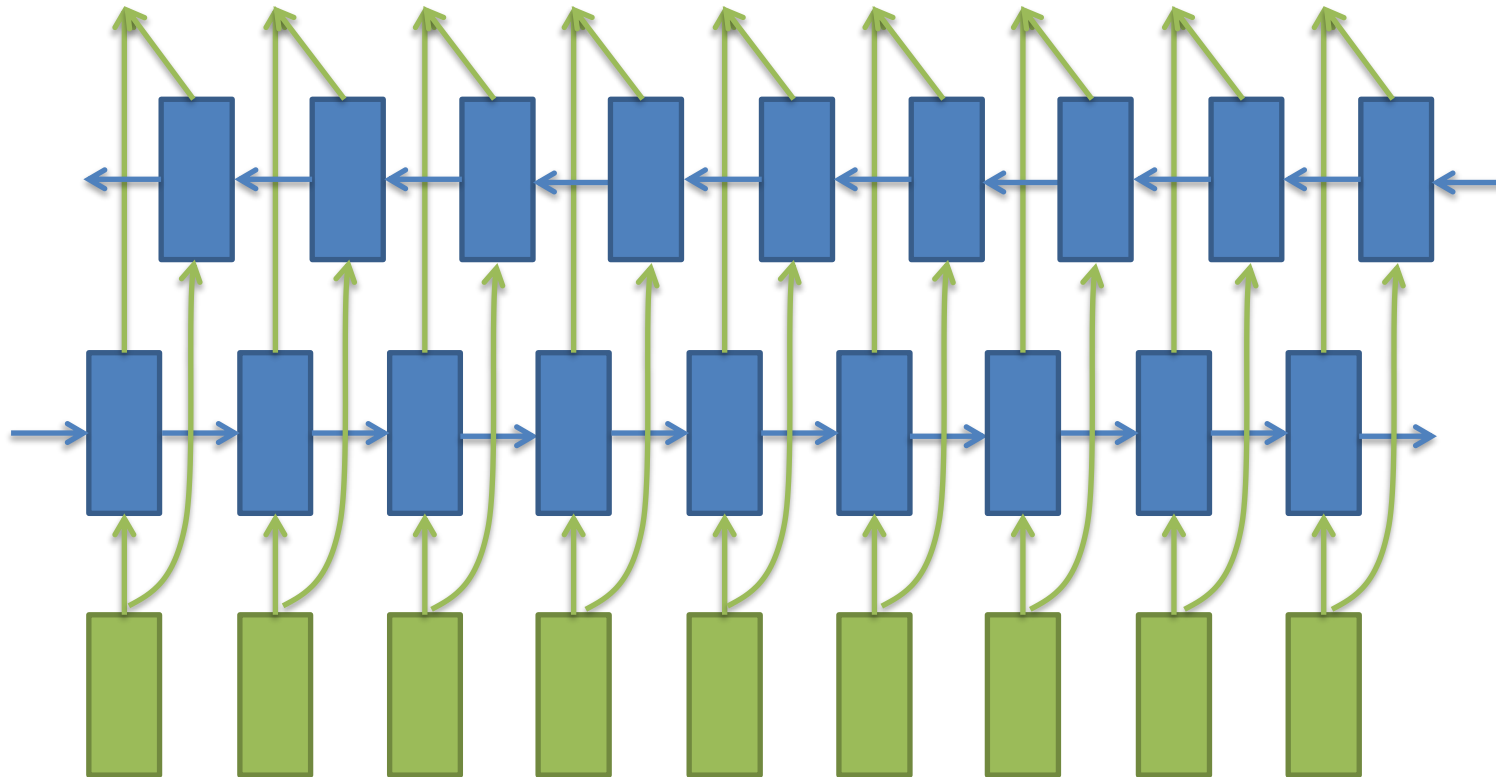
Stacking RNNs

You can create a deep RNN by stacking



Bidirectional RNNs

Concatenate two RNNs: one going forward in time, one back in time.



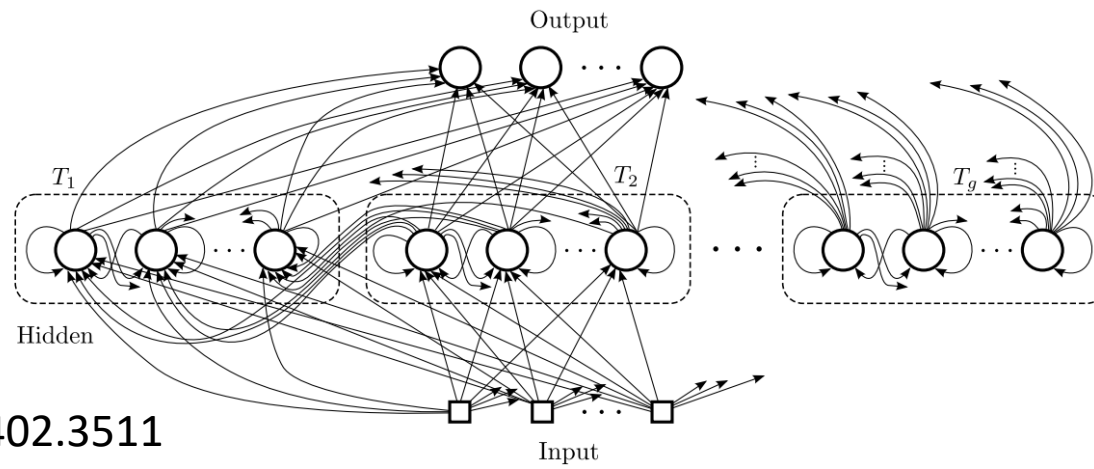
Schuster, M. and Paliwal, K.K., 1997. Bidirectional recurrent neural networks. *IEEE Transactions on Signal Processing*, 45(11), pp.2673-2681.

Clockwork RNN

Units operate at different frequencies.

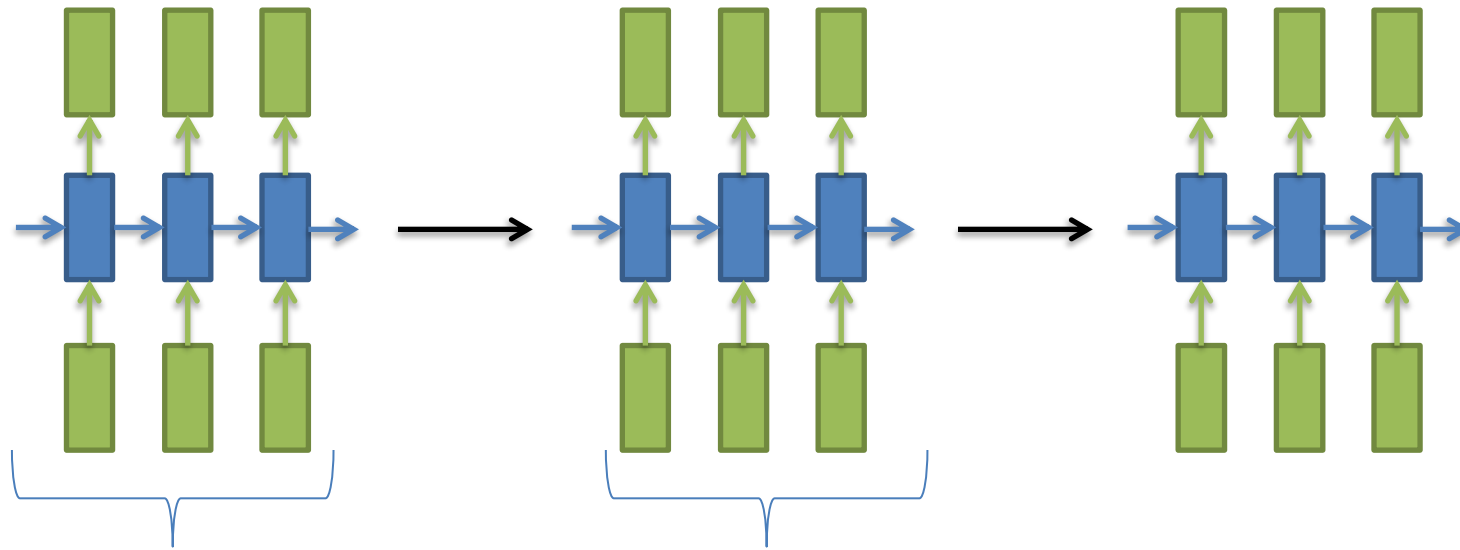
Slower neurons feed data to faster ones, but not vice versa.

The diagram illustrates the update equation for the hidden state $y_H^{(t)}$ at time t . On the left, a vertical vector $y_H^{(t)}$ is shown with a 'period' axis ranging from 1 to 16, where the period doubles for each step (1, 2, 4, 8, 16). The equation is:
$$y_H^{(t)} = f\left(W_H \cdot y_H^{(t-1)} + W_I \cdot x_t \right)$$
 The weight matrix W_H is a 16x16 matrix with a lower triangular structure of shaded blocks, indicating that slower units (higher period) feed into faster units (lower period). The input weight matrix W_I is a 16x4 matrix with shaded blocks in the top half, indicating that inputs feed into slower units.



Truncated BPTT

Sometimes, it is not necessary to unroll the RNN until the very beginning.



1. Unroll for K steps,
do fprob, bprop,
update weights

2. Copy the hidden state

3. Start from saved state, unroll
do fprob & bprop & update

4. Copy the hidden state, repeat

Dynamic evaluation

Train on test set during eval:

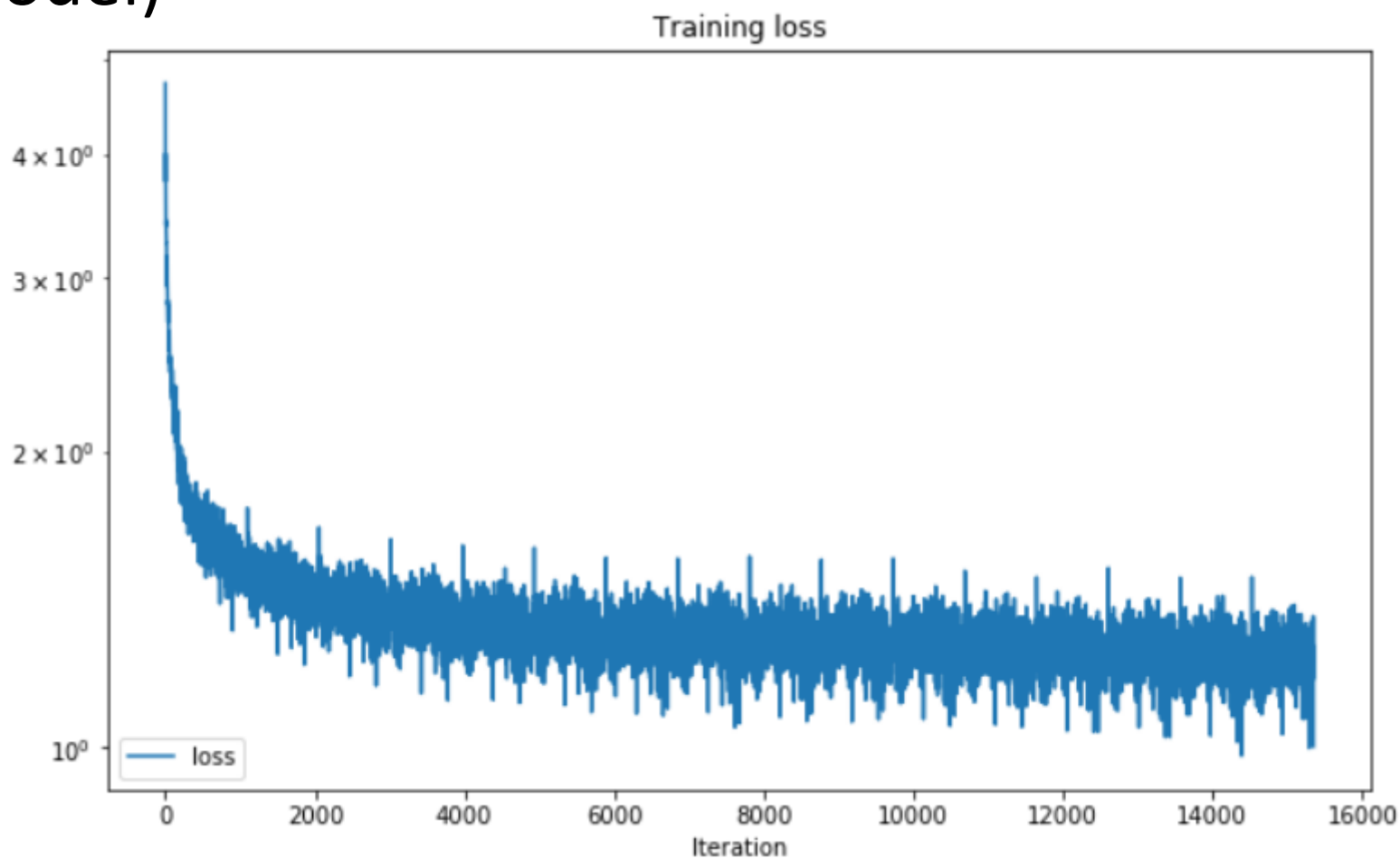
- For language modeling, we get implicit feedback during evaluation – at each step we make a prediction and get the correct answer
- We can use this for training (nb. we become dependent on test set ordering)
- Used by A. Graves for Hutter Prize Wikipedia experiments.

Practical aspects of RNN training

1. Use as much supervision as possible
when intermediate targets are available, use them!
2. Use curriculum learning
start with shortest examples, then do longer ones.
3. Monitor your gradients.
4. Use gradient clipping
aim to clip a few % of all steps.
5. Play with echo-state-like or orthogonal initialization
It works well for LSTMs & GRUs too

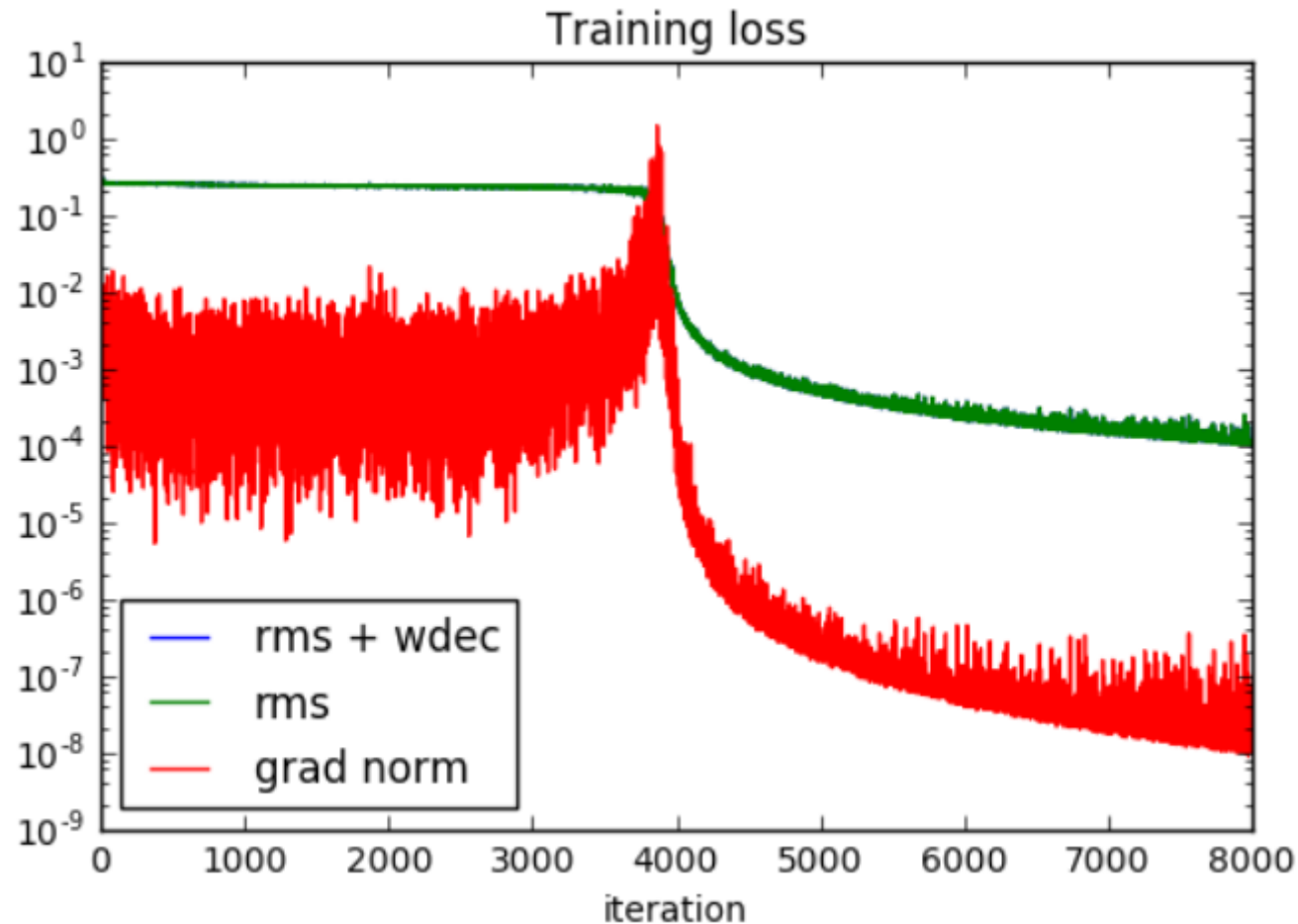
What to expect during RNN training?

Task with frequent supervision (e.g. language model)



What to expect during RNN training?

Task with distant supervision (parity)



Batch norm for RNNs?

Recall batch normalization:

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\dots m}\}$;
Parameters to be learned: γ, β
Output: $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \quad // \text{ mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 \quad // \text{ mini-batch variance}$$

$$\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \quad // \text{ normalize}$$

$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) \quad // \text{ scale and shift}$$

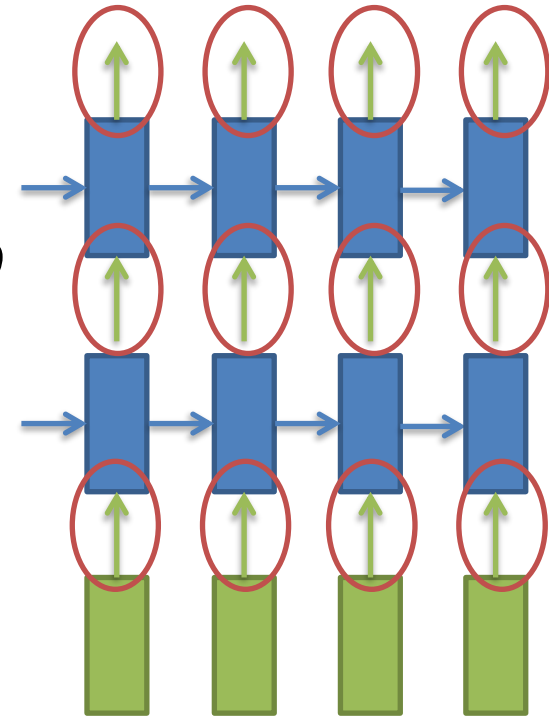
Easy BN for RNNs

Apply to the “vertical” arrows only:

$$\begin{pmatrix} f_t \\ i_t \\ o_t \\ g_t \end{pmatrix} = W_h h_{t-1} + \mathbf{BN}(W_x x_t; \gamma) + b$$

$$c_t = \sigma(f_t) c_{t-1} + \sigma(i_t) \odot \tanh(g_t)$$

$$h_t = \sigma(o_t) \odot \tanh(c_t)$$



Full BN for RNNs

Can also apply BN to recurrent connections:

$$\begin{pmatrix} f_t \\ i_t \\ o_t \\ g_t \end{pmatrix} = \mathbf{BN}(W_h h_{t-1}, \gamma_h) + \mathbf{BN}(W_x x_t; \gamma_x) + b$$
$$c_t = \sigma(f_t) c_{t-1} + \sigma(i_t) \odot \tanh(g_t)$$
$$h_t = \sigma(o_t) \odot \tanh(\mathbf{BN}(c_t; \gamma_c, \beta_c))$$

But:

1. Need to use separate batch norms for hiddens, inputs and cell values.
2. Need to use per-timestep statistics (γ are the same, but mean and variance are per time step)

LayerNorm (arxiv.org/abs/1607.06450) works too and is somewhat easier to use, as it stores no stats.

How to regularize an RNN

L2 penalty/Weight decay is bad:

- Scaling a weight matrix scales its eigenvalues.
- Small weight matrices with small eigenvalues will lead to fast information decay!

Weight noise

We want low-precision weights, not small weights.

Add noise to weights!

For all weights w :

$\text{noise_w} = \text{random.normal()} * 0.02$ (or 0.05)

$w += \text{noise_w}$

Do fprop, do backprop

For all weights w :

$w -= \text{noise_w}$

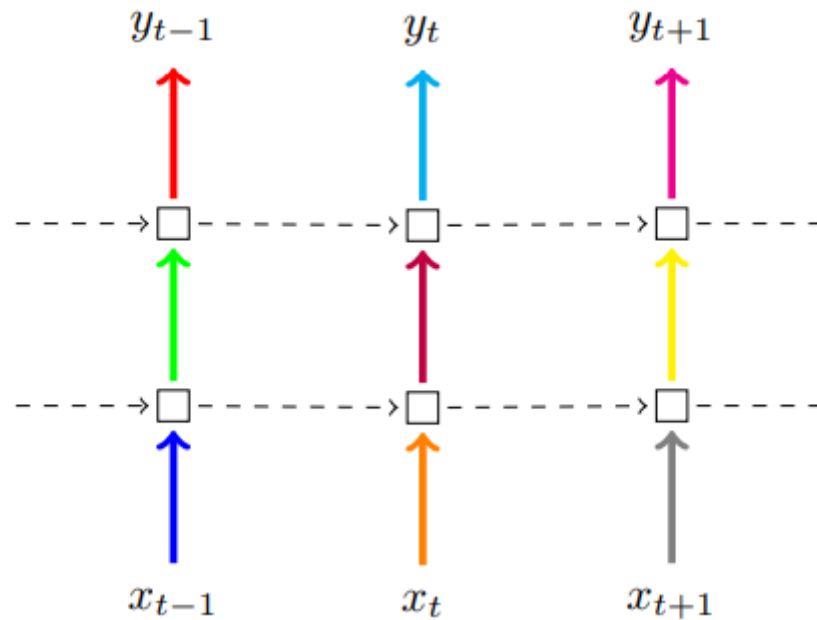
Apply gradients.

More principled: A. Graves “Practical variational inference for neural networks”

Recurrent dropout

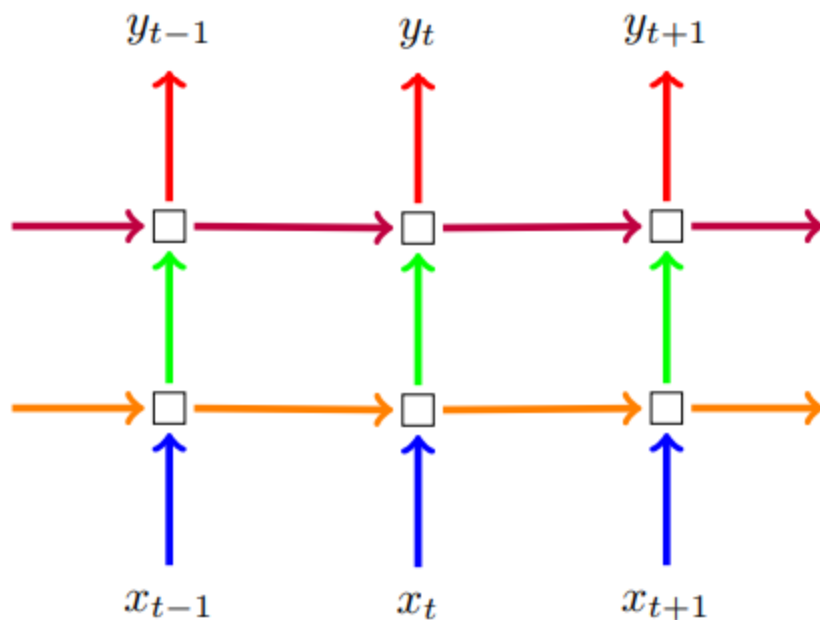
Simplest approach (Zaremba)

Dropout only to the “vertical” arrows



Better dropout

Apply the same dropout mask across all time steps (Gal's dropout)



Zoneout

Randomly keep past values for h_t or c_t :

$$c_t = d_t^c \odot c_{t-1} + (1 - d_t^c) \odot (f_t \odot c_{t-1} + i_t \odot g_t)$$

$$h_t = d_t^h \odot h_{t-1} + (1 - d_t^h) \odot (o_t \odot \tanh(f_t \odot c_{t-1} + i_t \odot g_t))$$

Seems to work best with probability of keeping c s larger than that of keeping h s.

Teacher forcing

At training time, the net sees only correct data.

Input: Mary had a little lamb

$p(\text{Mary})$

$p(\text{had} | \text{Mary})$

$p(\text{a} | \text{Mary had})$

$p(\text{little} | \text{Mary had a})...$

At generation time:

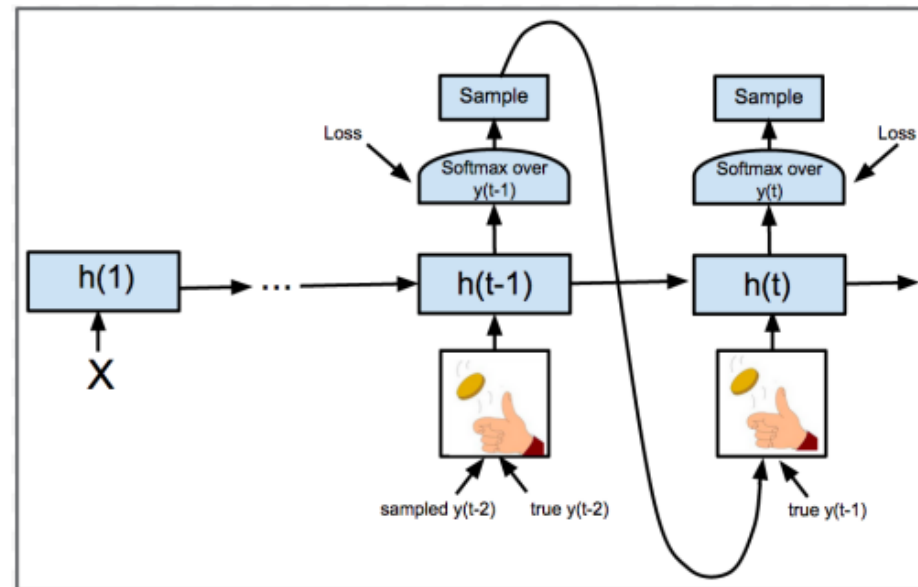
$p(?) \rightarrow$ sampled Mary

$p(? | \text{Mary}) \rightarrow$ sampled cucumber

$p(? | \text{Mary cucumber}) \rightarrow$ panic!!!!

Scheduled sampling

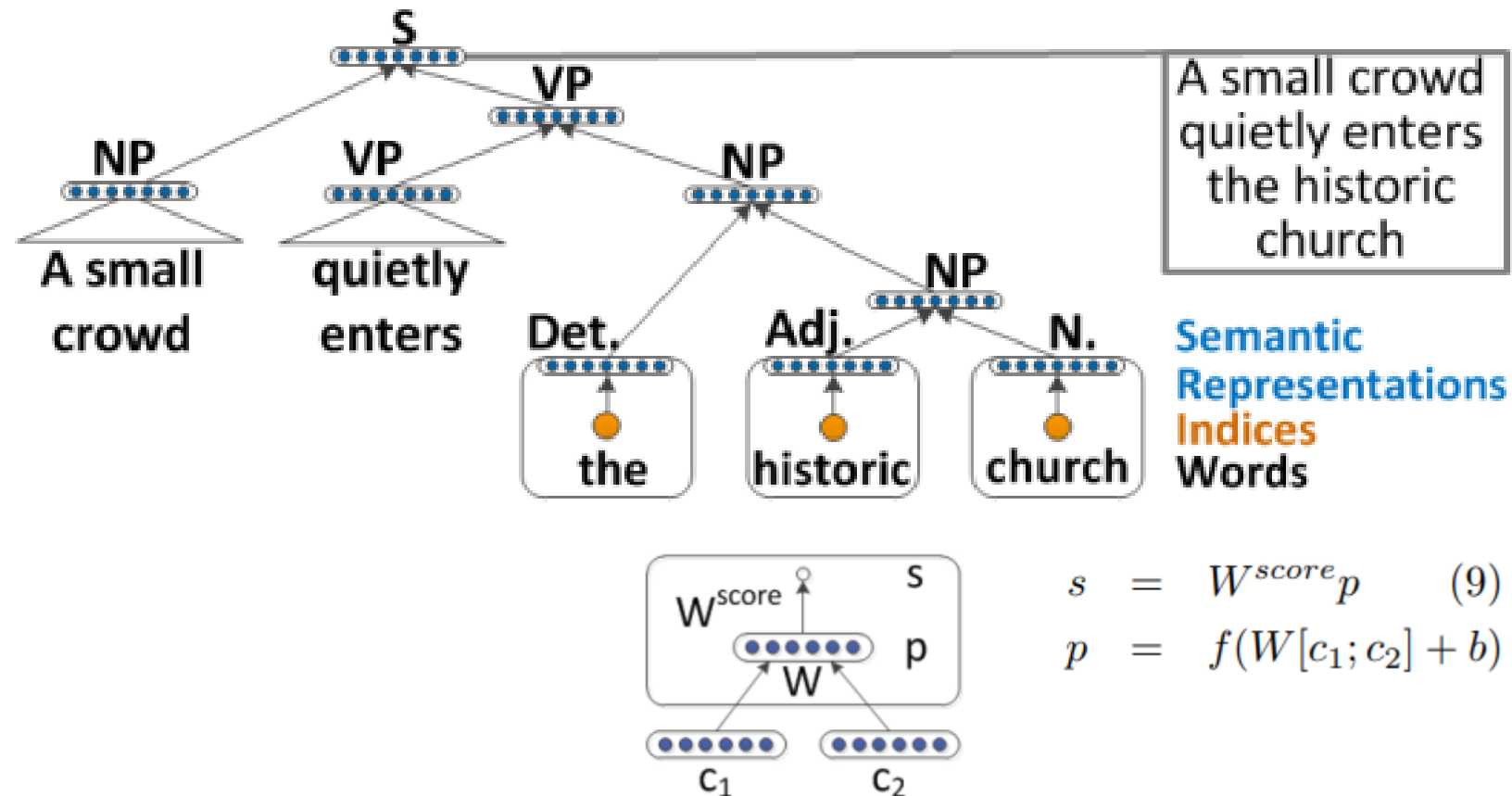
Pragmatic solution to teacher forcing:
Allow mistakes during training, too.



BEYOND SEQUENCES

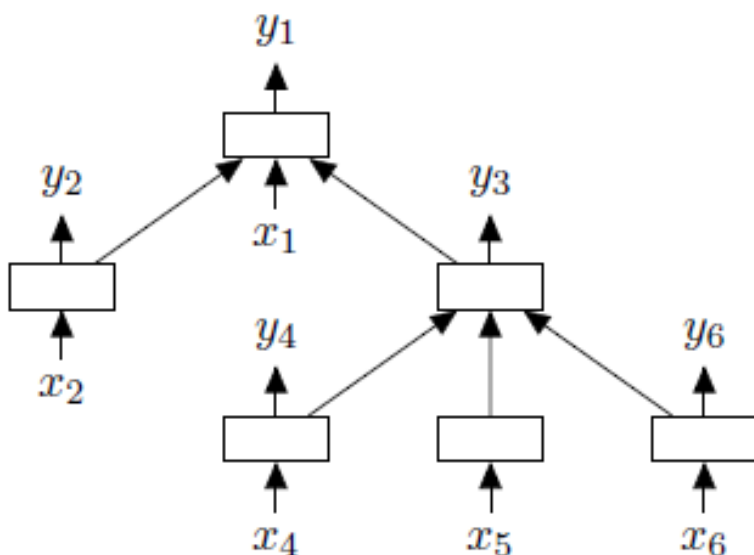
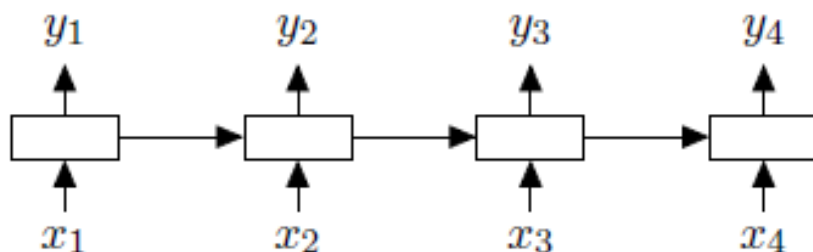
Recursive Neural Networks

Neural Network operating on binary trees



Tree LSTM

Extend LSTM form sequences to trees: need to aggregate all incoming nodes $C(j)$.



$$\tilde{h}_j = \sum_{k \in C(j)} h_k,$$

$$i_j = \sigma \left(W^{(i)} x_j + U^{(i)} \tilde{h}_j + b^{(i)} \right),$$

$$f_{jk} = \sigma \left(W^{(f)} x_j + U^{(f)} h_k + b^{(f)} \right),$$

$$o_j = \sigma \left(W^{(o)} x_j + U^{(o)} \tilde{h}_j + b^{(o)} \right),$$

$$u_j = \tanh \left(W^{(u)} x_j + U^{(u)} \tilde{h}_j + b^{(u)} \right),$$

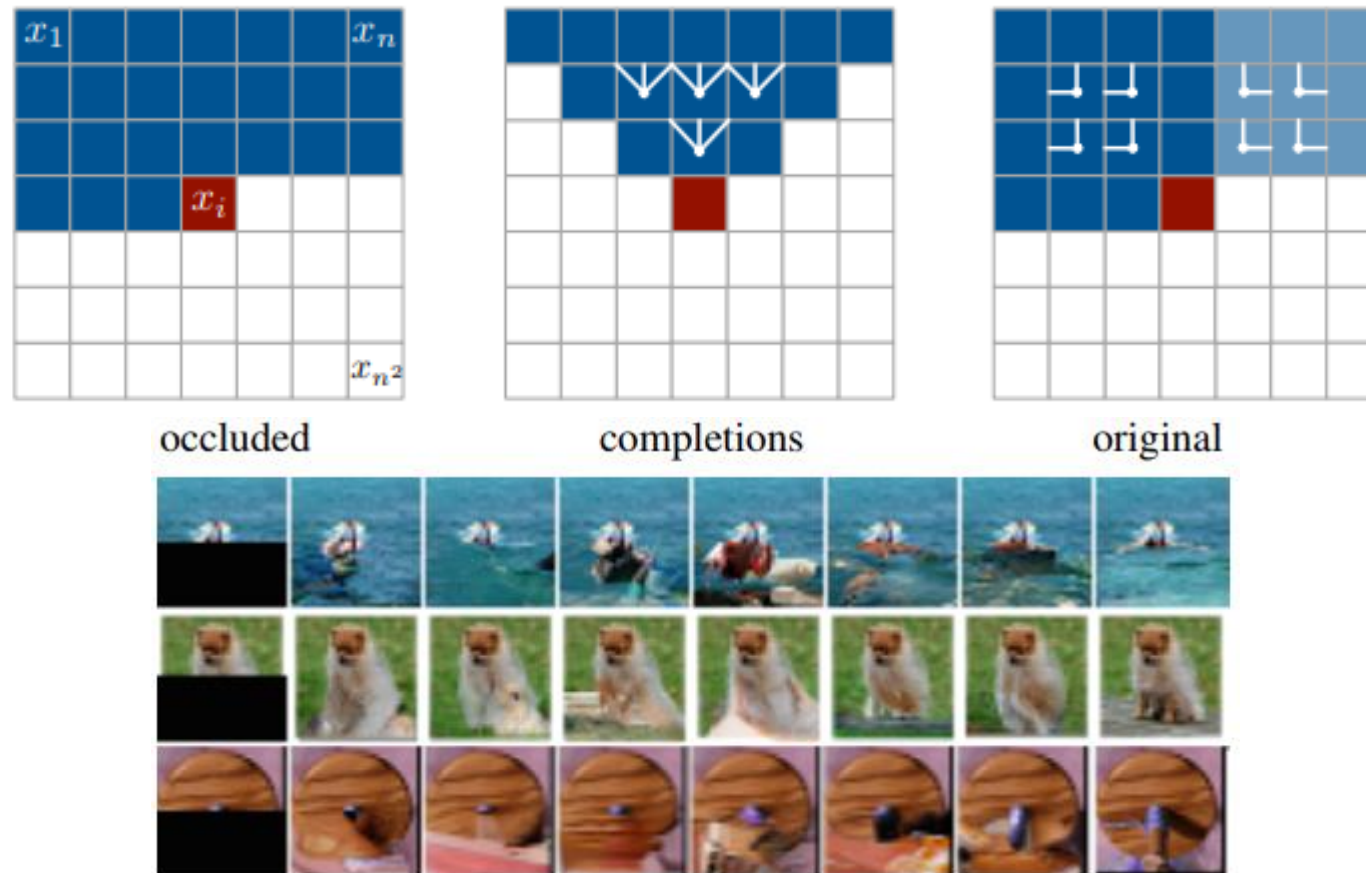
$$c_j = i_j \odot u_j + \sum_{k \in C(j)} f_{jk} \odot c_k,$$

$$h_j = o_j \odot \tanh(c_j),$$

Pixel RNN

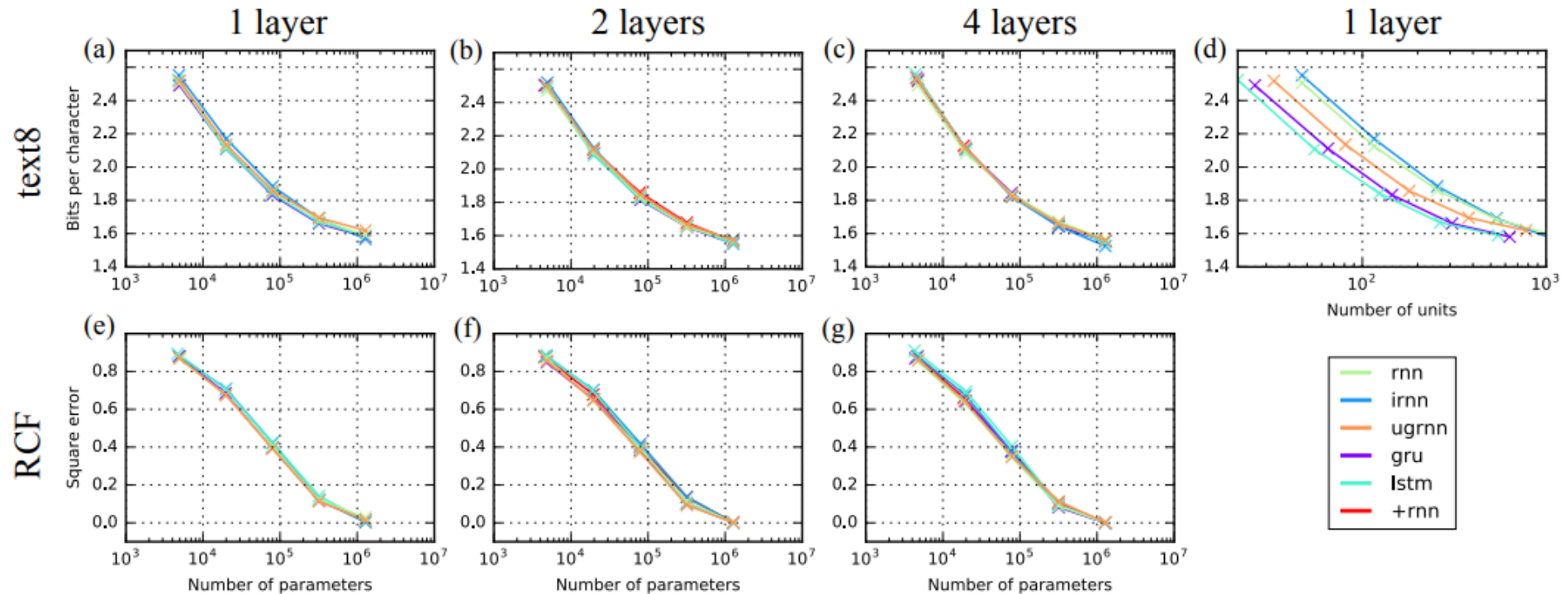
Generate images pixel by pixel.

Generate pixels row-wise – condition only on pixels higher/to the left



DISCUSSIONS AND CONTROVERSIES

Are all RNNs created equal?



All RNN architectures reach same performance*

All models store about 5 bits/parameter.

* When you can afford the search for good hyper-parameters, and have enough data to not need regularization.

Are all RNNs created equal?

On practical tasks the gated RNNs are typically better.

Cell	newstest2013	Params
LSTM	22.22 \pm 0.08 (22.33)	68.95M
GRU	21.78 \pm 0.05 (21.83)	66.32M
Vanilla-Dec	15.38 \pm 0.28 (15.73)	63.18M

Table 2: BLEU scores on newstest2013, varying the type of encoder and decoder cell.

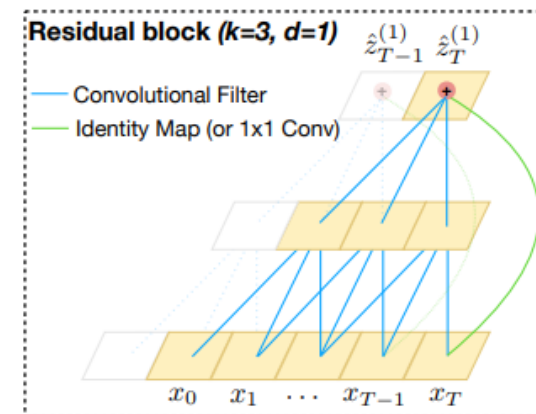
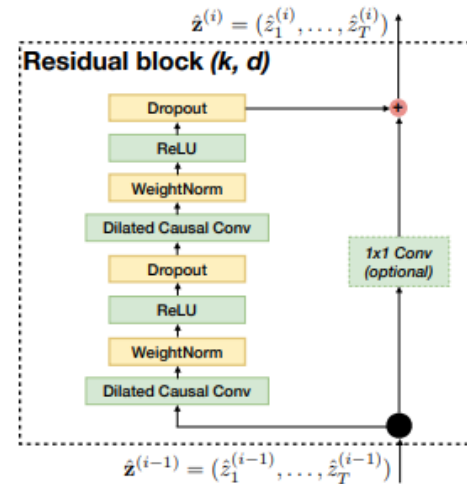
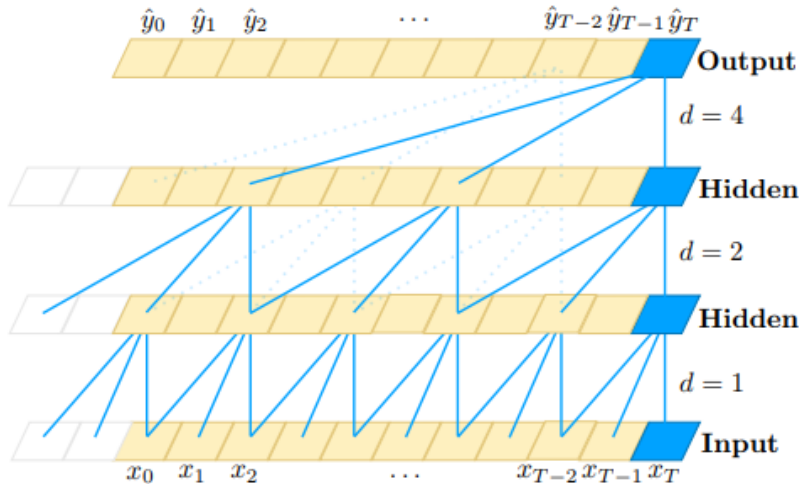
Maybe this is because tuning vanilla RNNs is expensive.

Sidenote: Baidu used vanilla RNNs in deep speech to make inference cheap.

TCN: do we need RNNs at all?

Autoregressive models with truncated history give good results, e.g. the Wavenet.

The TCN architecture is similar:



TCN Results

Sequence Modeling Task	Model Size (\approx)	Models			
		LSTM	GRU	RNN	TCN
Seq. MNIST (accuracy ^{<i>h</i>})	70K	87.2	96.2	21.5	99.0
Permuted MNIST (accuracy)	70K	85.7	87.3	25.3	97.2
Adding problem $T=600$ (loss ^{ℓ})	70K	0.164	5.3e-5	0.177	5.8e-5
Copy memory $T=1000$ (loss)	16K	0.0204	0.0197	0.0202	3.5e-5
Music JSB Chorales (loss)	300K	8.45	8.43	8.91	8.10
Music Nottingham (loss)	1M	3.29	3.46	4.05	3.07
Word-level PTB (perplexity ^{ℓ})	13M	78.93	92.48	114.50	88.68
Word-level Wiki-103 (perplexity)	-	48.4	-	-	45.19
Word-level LAMBADA (perplexity)	-	4186	-	14725	1279
Char-level PTB (bpc ^{ℓ})	3M	1.36	1.37	1.48	1.31
Char-level text8 (bpc)	5M	1.50	1.53	1.69	1.45

TCN results, SOTA?

TCN vs. SoTA RESULTS					
Task	TCN Result	Size	SoTA	Size	Model
Seq. MNIST (acc.)	99.0	21K	99.0	21K	Dilated GRU (Chang et al., 2017)
P-MNIST (acc.)	97.2	42K	95.9	42K	Zoneout (Krueger et al., 2017)
Adding Prob. 600 (loss)	5.8e-5	70K	5.3e-5	70K	Regularized GRU
Copy Memory 1000 (loss)	3.5e-5	70K	0.011	70K	EURNN (Jing et al., 2017)
JSB Chorales (loss)	8.10	300K	3.47	-	DBN+LSTM (Vohra et al., 2015)
Nottingham (loss)	3.07	1M	1.32	-	DBN+LSTM (Vohra et al., 2015)
Word PTB (ppl)	88.68	13M	47.7	22M	AWD-LSTM-MoS + Dynamic Eval. (Yang et al., 2018)
Word Wiki-103 (ppl)	45.19	148M	40.4	>300M	Neural Cache Model (Large) (Grave et al., 2017)
Word LAMBADA (ppl)	1279	56M	138	>100M	Neural Cache Model (Large) (Grave et al., 2017)
Char PTB (bpc)	1.31	3M	1.22	14M	2-LayerNorm HyperLSTM (Ha et al., 2017)
Char text8 (bpc)	1.45	4.6M	1.29	>12M	HM-LSTM (Chung et al., 2016)

Stability: do we need RNNs at all?

J. Miller, M. Hardt: arxiv.org/abs/1805.10369

A system is $\lambda < 1$ contractive if

$$\|\phi_w(h, x) - \phi_w(h', x)\| \leq \lambda \|h - h'\|$$

The difference of one step outputs is smaller than the difference of the hidden states.

Proposition (Informal version of Proposition 1). *Assuming the system ϕ is λ -contractive and under additional Lipschitz assumptions, we show if $k \geq O(\log(1/(1 - \lambda)\epsilon))$, then the difference in predictions between the recurrent and truncated model is negligible, $\|y_t - y_t^k\| \leq \epsilon$.*

Note: if the LSTM has a forget gate, it will never be fully open, the LSTM is contractive!

Conclusions

What RNNs have brought to DL?

1. Hidden state and recurrence 😊
2. Gating units
Highway networks, Wavenet etc. all use gates despite being feed-forward.
Gates decouple **if** from **what**.
3. Training hacks, Gradient clipping.
It allows stable training with larger learning rates, and helps feedforward net training too.

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