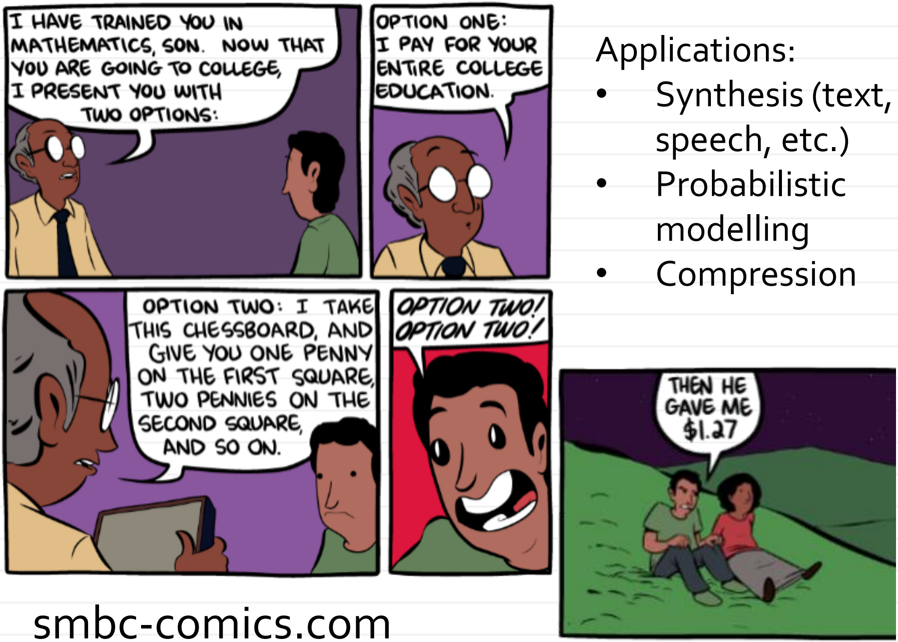
Lecture 10: Deep Sequence Modeling. Recurrent neural networks.

Predictive learning

- Given an element predict *nearby* elements (e.g. next, previous, adjacent, etc.)
- Does not require annotated data ("self-supervised")
- Usually considered as unsupervised, but often works much better than "plain" unsupervised
- Particularly prominent in NLP, but now gaining popularity in many fields

Today's focus: sequence modeling, sequence prediction

Predicting sequences matters



smbc-comics.com

Applications:

- Synthesis (text, speech, etc.)
- Probabilistic modelling
- Compression

Training sequence prediction

*A cat sat on a ma**?***

Inherently probabilistic: need to predict probabilities over alphabet/lexicon

Training sequence prediction

*A cat sat on a ma**?***

Predominantly maximum likelihood learning:

$$\max_\theta \sum_i \log p_\theta(x_t^i \,|\, x_{t-1}^i, x_{t-2}^i, \ldots, x_1^i)$$

Many models go back fixed number of steps:

$$\max_\theta \sum_i \log p_\theta(x_t^i \,|\, \underbrace{x_{t-1}^i, x_{t-2}^i, \ldots, x_{t-N}^i}_{\text{Temporal window}})$$

Fixed window/order architectures

$$p_\theta(x_t^i \,|\, x_{t-1}^i, x_{t-2}^i, \ldots, x_{t-N}^i)$$

- N-grams (with smoothing)
- ConvNets (aka TDNNs)
- Any probabilistic classifier (e.g. decision forest, etc.)

NB: using padding for the special symbol (UNK) we can train model for shorter sequences

Assessing a probabilistic model

1. Train $p_\theta(x_j \mid x_{j-1}, \ldots, x_{j-N})$

2. Evaluate $\prod_{j=1}^{M} p_\theta(x_j \mid x_{j-1}, \ldots, x_{j-N})$
   on a hold-out set (can be a long text)

Common measure (*perplexity)*:

$$\mathrm{PP}(x_1, \ldots, x_M) = \sqrt[M]{\prod_{j=1}^{M} p_\theta(x_j \mid x_{j-1}, \ldots, x_{j-N})}^{\,-1}$$

- log PP = "bits/nats per token"

Probabilistic modeling of long sequences

Assume given $p_\theta(x_t^i \,|\, x_{t-1}^i, x_{t-2}^i, \ldots, x_{t-N}^i)$

$$p(x_M, x_{M-1}, \ldots, x_1) =$$

$$p(x_M \,|\, x_{M-1}, \ldots, x_1) \cdot p(x_{M-1}, x_{M-2}, \ldots, x_1) =$$

$$\prod_{j=2}^{M} p(x_j \,|\, x_{j-1}, \ldots, x_1) \cdot p(x_1) \approx$$

$$\boxed{\prod_{j=1}^{M} p_\theta(x_j \,|\, x_{j-1}, \ldots, x_{j-N})}$$

ML categorical sequence generation

Task: draw a sample sequence with high-probability

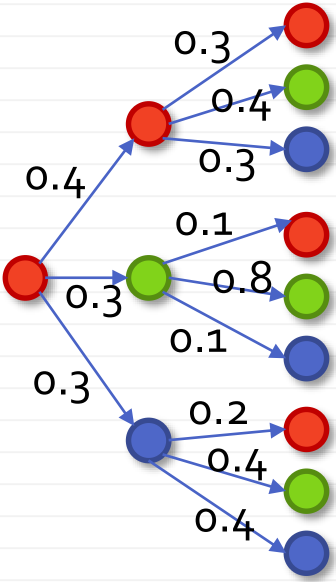
$$\prod_{j=1}^{M} p_\theta(x_j \,|\, x_{j-1}, \ldots, x_{j-N})$$

Option 1: synthesize one-by-one greedily, picking the symbol with highest probability

$$\hat{x}_j = \arg\max_x p_\theta(x \,|\, \hat{x}_{j-1}, \ldots, \hat{x}_{j-N})$$

Option 2: *beam search*

Why greedy synthesis is suboptimal



Toy example: three letters in the alphabet.
Task: synthesize most likely three letter word starting from red.

Greedy solution: 

Best solution: 

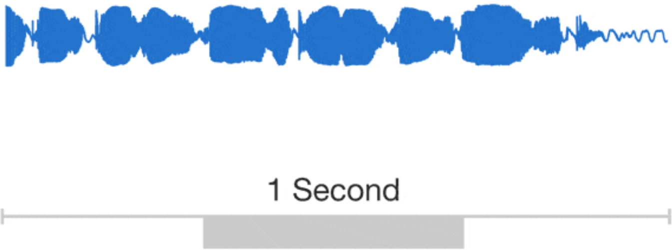
Beam search

The c??????

$$\prod_{j=1}^{M} p_\theta(x_j \,|\, x_{j-1}, \ldots, x_{j-N})$$

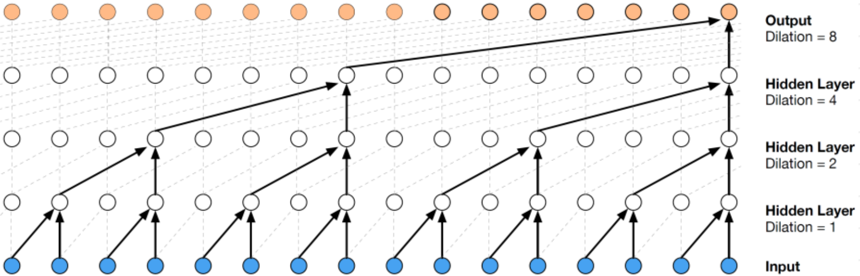
The ca?????	The cat????	The cat????
	The cap????	
The co?????	The cor????	The cap????
	The col????	
The ch?????	The cha????	The cor????
	The cho????	

WaveNet: real-valued sequence modeling



- Generating raw waveforms at 16 kHz (very uncommon)

WaveNet: dilated ConvNet



- Repeated pattern of dilations:

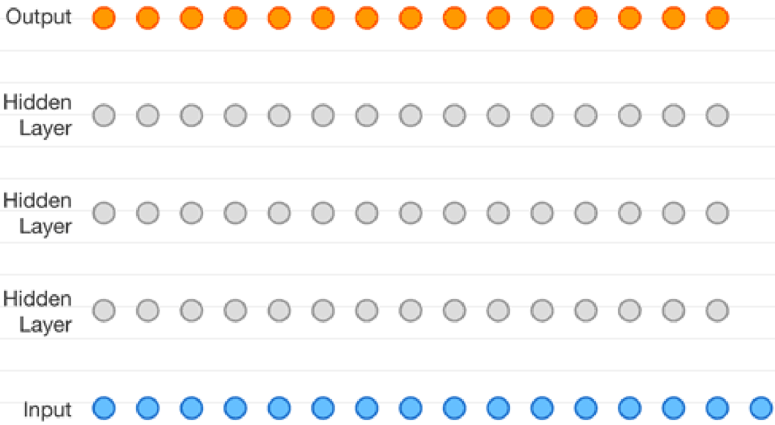
  1,2,...512,1,2,...512,...
- Gated (bilinear) non-linearity:

$$\mathbf{z} = \tanh\left(W_{f,k} * \mathbf{x}\right) \odot \sigma\left(W_{g,k} * \mathbf{x}\right)$$

- There are also skip connections

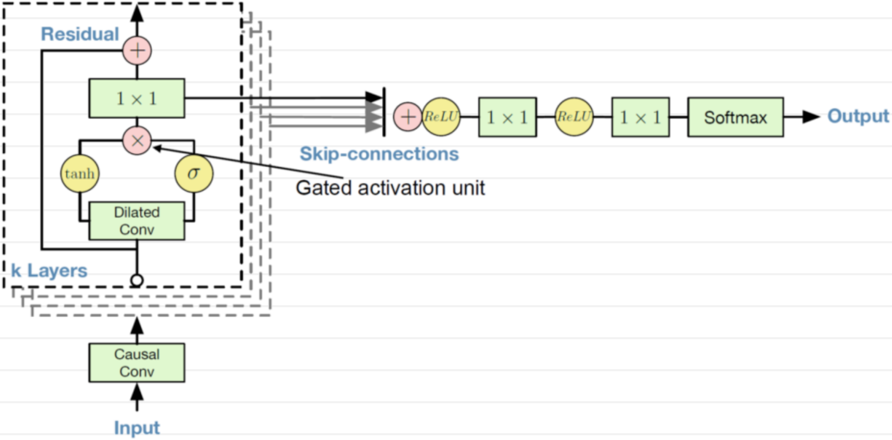
[van der Oord et al, 2016]

Synthesis with casual dilated ConvNet



[van der Oord et al, 2016]

Details of the ConvBlock



[van der Oord et al, 2016]

WaveNet: speech results

- Trained on 24.6 hours of speech
- Receptive field is 0.24 seconds
- Conditioned on the speaker ID

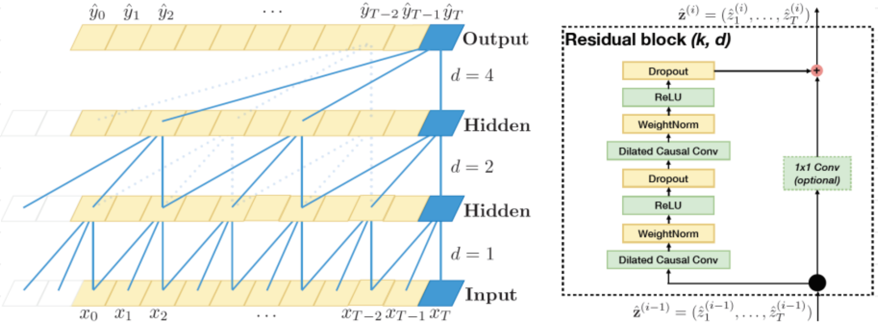
[van der Oord et al, 2016]

WaveNet: piano results

- Trained on 60 hours of piano (from YouTube)

[van der Oord et al, 2016]

Similar ConvNet for sequence modeling



[Bai et al. 2018]

ConvNets vs RNNs

Sequence Modeling Task	Model Size (≈)	Models			
		LSTM	GRU	RNN	**TCN**
Seq. MNIST (accuracy^h)	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$^\ell$)	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$^\ell$)	13M	**78.93**	92.48	114.50	89.21
Word-level Wiki-103 (perplexity)	-	48.4	-	-	**45.19**
Word-level LAMBADA (perplexity)	-	4186	-	14725	**1279**
Char-level PTB (bpc$^\ell$)	3M	1.41	1.42	1.52	**1.35**
Char-level text8 (bpc)	5M	1.52	1.56	1.69	**1.45**

[Bai et al. 2018]

Picking a probabilistic model

- N-grams
- CNNs (aka TDNNs)
- Any probabilistic classifier

Common problem: picking size of the window

- Avoiding overfitting
- To work on instances of different length
- To track long-range behavior

Probabilistic modeling of long sequences

$$p(x_M, x_{M-1}, \ldots, x_1) =$$

$$p(x_M \,|\, x_{M-1}, \ldots, x_1) \cdot p(x_{M-1}, x_{M-2}, \ldots, x_1) =$$

$$\prod_{j=2}^{M} p(x_j \,|\, x_{j-1}, \ldots, x_1) \cdot p(x_1) \approx$$

$$\boxed{\prod_{j=1}^{M} p_\theta(x_j \,|\, h_{j-1})}$$

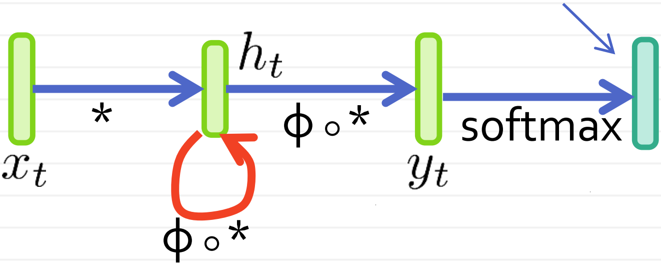
"context variable"

$$h_{j-1} = F(x_{j-1}, h_{j-2})$$

Let us use a simple network here!

Recurrent neural network (RNN)

$$p_\theta(x_t^i \mid x_{t-1}^i, x_{t-2}^i, \ldots, x_1)$$



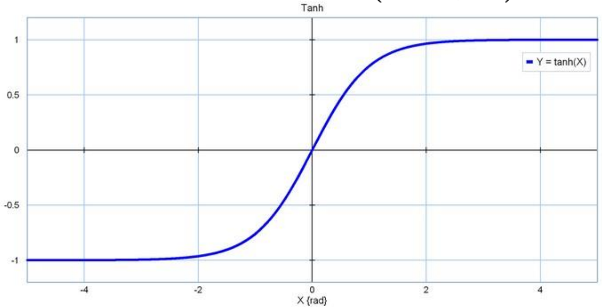
$$h_t = W\phi(h_{t-1}) + W_x x_t$$

$$y_t = W_y\phi(h_t)$$

NB: I omit bias terms but they can be useful!

Most popular non-linearity for RNNs

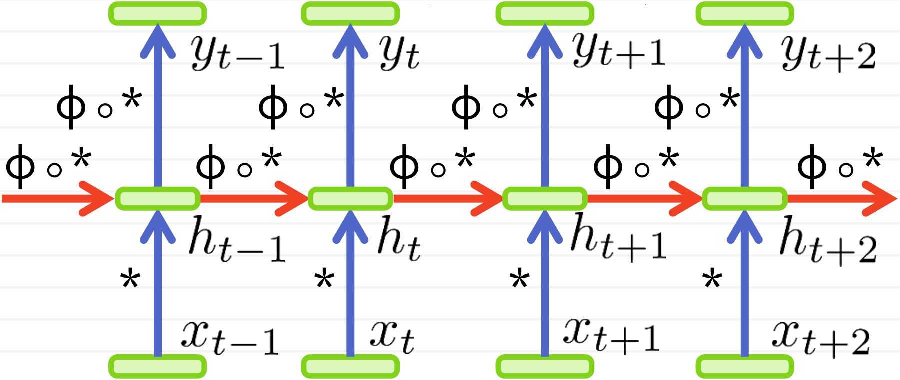
$$\tanh x : \mathbb{R} \to (-1; 1)$$



$$[\tanh x]' = 1 - \tanh^2 x$$

$$|[\tanh x]'| \leq 1$$

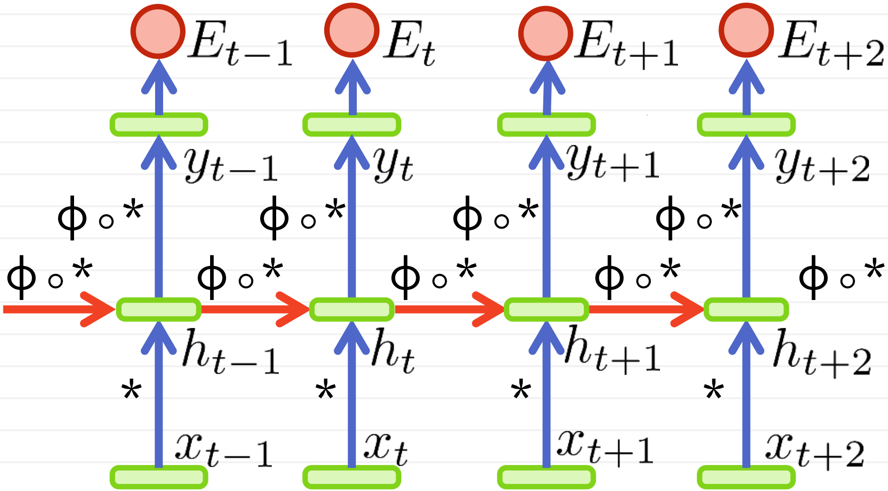
Unwrapping RNN



$$h_t = W\phi(h_{t-1}) + W_x x_t$$

$$y_t = W_y \phi(h_t)$$

Training RNN



$$h_t = W\phi(h_{t-1}) + W_x x_t \qquad y_t = W_y \phi(h_t)$$

Training RNN

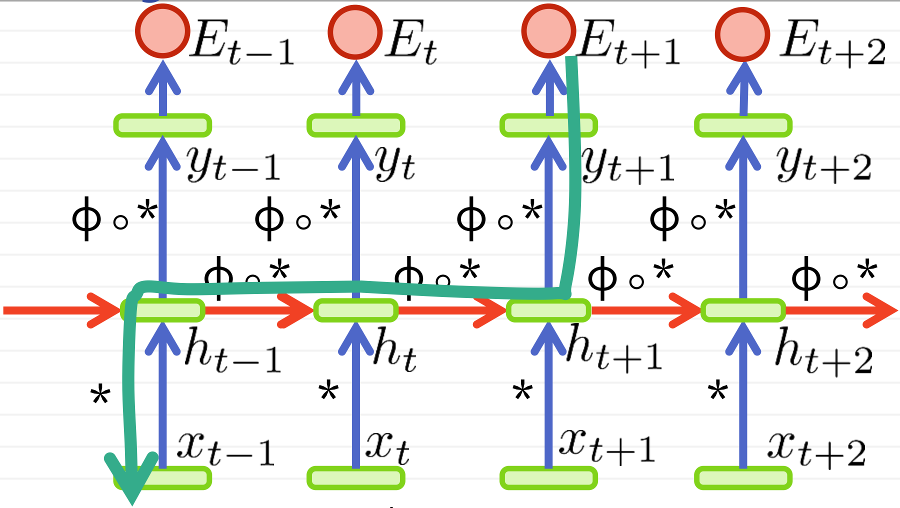
$$h_t = W\phi(h_{t-1}) + W_x x_t$$

$$y_t = W_y \phi(h_t)$$

$$E = \sum_{t=1}^{S} E_t \qquad \frac{dE}{dW} = \sum_{t=1}^{S} \frac{dE_t}{dW}$$

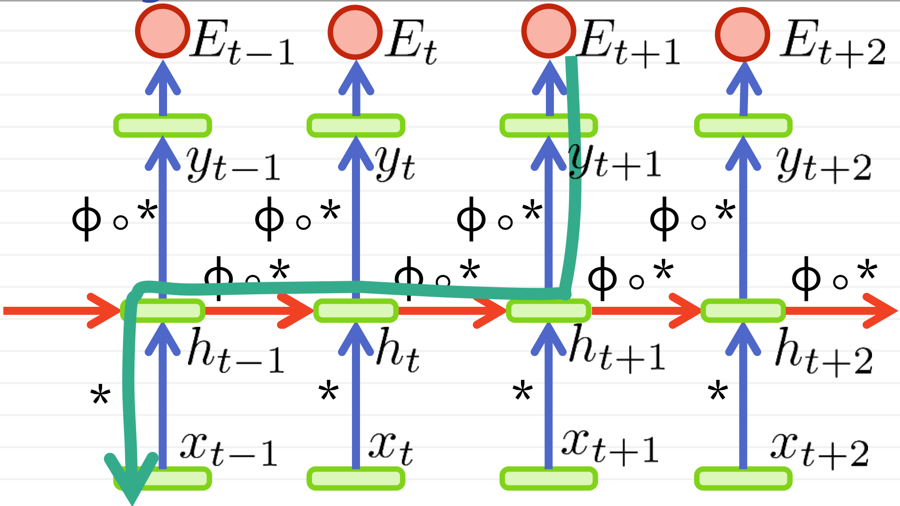
$$\frac{\partial E_t}{\partial W} = \sum_{k=1}^{t} \frac{\partial E_t}{\partial y_t} \frac{\partial y_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial h_k}{\partial W}$$

Training RNN



$$\frac{\partial E_t}{\partial W} = \sum_{k=1}^{t} \frac{\partial E_t}{\partial y_t} \frac{\partial y_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial h_k}{\partial W}$$

Training RNN



In practice: unwrapping for a finite number of time-steps (or training on bounded length sequences)

Training RNN

$$\frac{\partial E_t}{\partial W} = \sum_{k=1}^{t} \frac{\partial E_t}{\partial y_t} \frac{\partial y_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial h_k}{\partial W}$$

$$\frac{\partial h_t}{\partial h_k} = \prod_{i=k+1}^{t} \frac{\partial h_i}{\partial h_{i-1}} = \prod_{i=k+1}^{t} W^T \mathrm{diag}(\phi'(h_{i-1}))$$

$$\left\| \frac{\partial h_i}{\partial h_{i-1}} \right\|_2 \leq \|W\|_2 L_\phi = \sigma_{max} L_\phi$$

$$\left\| \frac{\partial h_i}{\partial h_k} \right\|_2 \leq (\sigma_{max} L_\phi)^{t-k}$$

Challenges with training RNN

$$\frac{\partial E_t}{\partial W} = \sum_{k=1}^{t} \frac{\partial E_t}{\partial y_t} \frac{\partial y_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial h_k}{\partial W}$$

$$\left\| \frac{\partial h_i}{\partial h_k} \right\|_2 \leq (\sigma_{max} L_\phi)^{t-k}$$

$$\sigma_{\max} L_\phi < 1$$

vanishing gradient:
network ignores
long links

$$\sigma_{\max} L_\phi > 1$$

exploding gradient:
learning quickly
“explodes”

LayerNorm

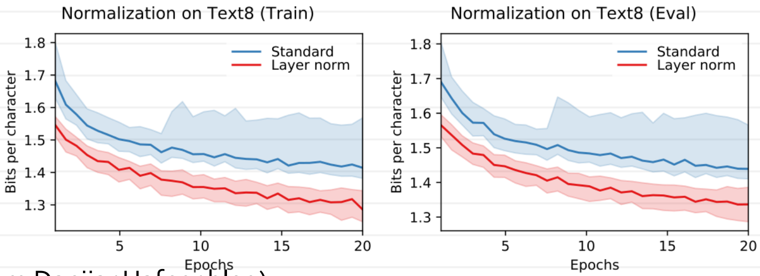
- Further improves the situation with vanishing/exploding gradients
- Often used in NLP instead of batchnorm

[Ba et al. ICLR16]

a is the input, **g** and **b** are learnable

$$\mu^t = \frac{1}{H}\sum_{i=1}^{H} a_i^t \qquad \sigma^t = \sqrt{\frac{1}{H}\sum_{i=1}^{H}\left(a_i^t - \mu^t\right)^2}$$

$$\mathbf{h}^t = \tanh\left(\frac{\mathbf{g}}{\sigma^t}\odot\left(\mathbf{a}^t - \mu^t\right) + \mathbf{b}\right)$$

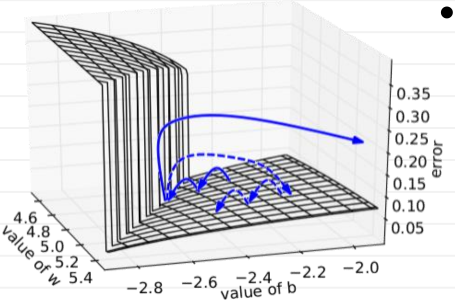


(graph from Danijar Hafner blog)

Gradient clipping

Algorithm 1 Pseudo-code for norm clipping

$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$
if $\|\hat{\mathbf{g}}\| \geq threshold$ **then**
  $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}}$
end if



- Simple trick handles gradient explosion (provided that the "valley" is wide)

[Pascanu et al. 2013]

Handling vanishing gradient

$$\frac{\partial E_t}{\partial W} = \sum_{k=1}^{t} \frac{\partial E_t}{\partial y_t} \frac{\partial y_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial h_k}{\partial W}$$

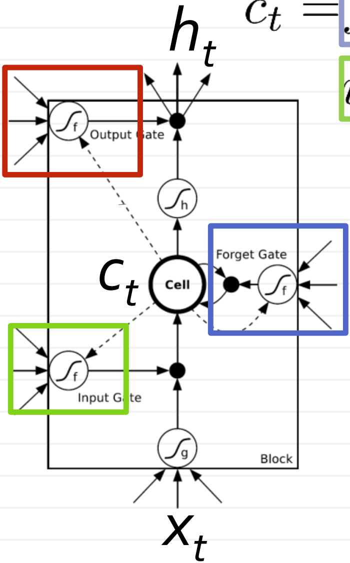
$$\sigma_{\max} L_\phi < 1$$

- Even if the gradient does not vanish totally, the information stored in low-energy subspaces will not be propagated
- Idea: we need mechanism to ensure long-term propagation.

Long Short-term Memory: cell update

$$c_t = \boxed{f_t \odot} c_{t-1} +$$
$$\boxed{i_t \odot} \phi(W_x x_t + W h_{t-1} + b)$$

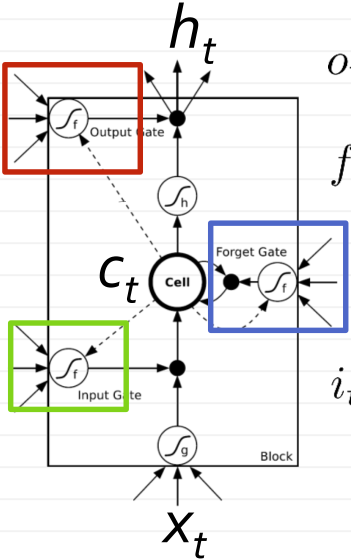
$$h_t = \boxed{o_t \odot} \phi(c_t)$$



LSTM RNN

[Graves 12]
[Hochreiter & Schmidhuber 97]

Long Short-term Memory: gate activations



$$o_t = \sigma(W_{xo}x_t + W_{ho}h_{t-1} + b_o)$$

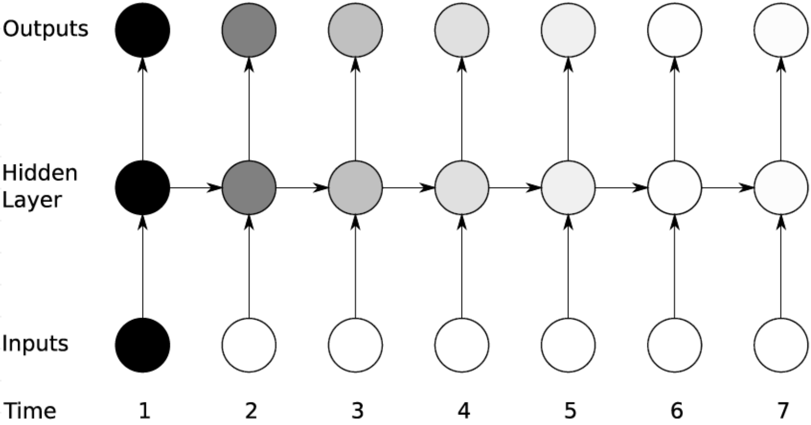
$$f_t = \sigma(W_{xf}x_t + W_{hf}h_{t-1} + b_f)$$

$$i_t = \sigma(W_{xi}x_t + W_{hi}h_{t-1} + b_i)$$

LSTM RNN

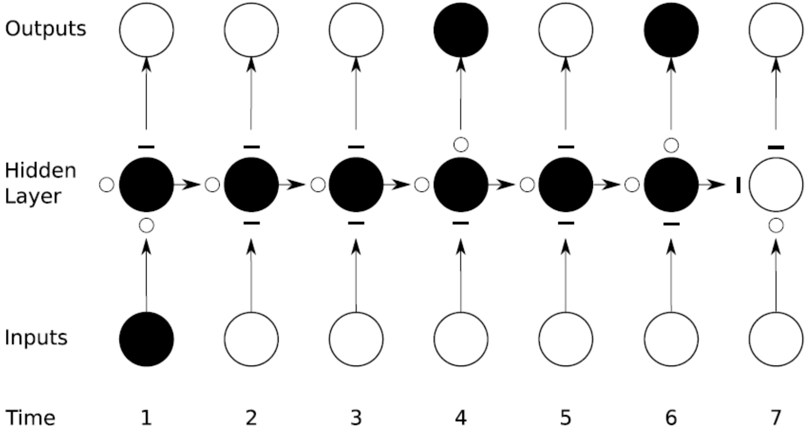
[Graves 12]
[Hochreiter & Schmidhuber 97]

Vanishing gradient visualization



The influence of an input unit quickly vanishes with time [Graves 12]

Long Short-term Memory



O = gate open

▬ = gate closed

[Graves 12]

[Hochreiter & Schmidhuber 97]

Recap: RNN-LSTM as a probabilistic model

$$p(x_t | x_1 \dots x_{t-1}) = ?$$

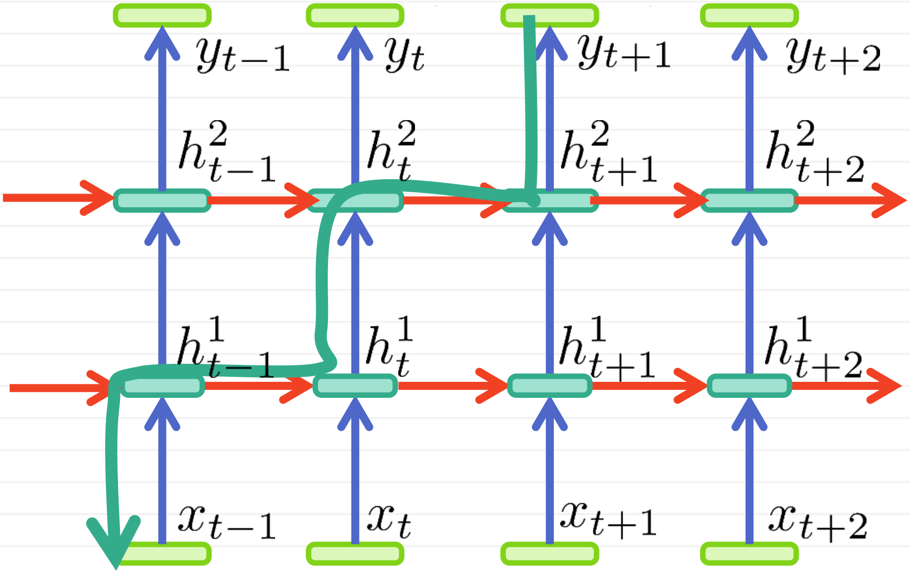
$$h_t = \mathrm{LSTM}(x_{t-1}, h_{t-1})$$

$$y_t = W_y h_t$$

$$p_t^i = \frac{\exp(y_t^i)}{\sum_k \exp(y_t^k)} = p(i | x_1, \dots x_{t-1})$$

$$x_t \sim \{p_t^i\}$$

Multi-layer RNNs



Computer generated "Linux kernel code"

© Andrej Karpathy:

```
static void do_command(struct seq_file *m, void *v)
{
  int column = 32 << (cmd[2] & 0x80);
  if (state)
    cmd = (int)(int_state ^ (in_8(&ch->ch_flags) & Cmd) ? 2 : 1);
  else
    seq = 1;
  for (i = 0; i < 16; i++) {
    if (k & (1 << 1))
      pipe = (in_use & UMXTHREAD_UNCCA) +
        ((count & 0x00000000fffffff8) & 0x000000f) << 8;
    if (count == 0)
      sub(pid, ppc_md.kexec_handle, 0x20000000);
    pipe_set_bytes(i, 0);
  }
  /* Free our user pages pointer to place camera if all dash */
  subsystem_info = &of_changes[PAGE_SIZE];
  rek_controls(offset, idx, &soffset);
  /* Now we want to deliberately put it to device */
  control_check_polarity(&context, val, 0);
  for (i = 0; i < COUNTER; i++)
    seq_puts(s, "policy ");
}
```

More fun: 1) http://karpathy.github.io/2015/05/21/rnn-effectiveness/ 2) your assignment

Interpretable LSTM Cells

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;
}
```

[Karpathy et al. ICLR16]

Interpretable LSTM Cells

Cell that turns on inside comments and quotes:

[Karpathy et al. ICLR16]

Interpretable LSTM Cells

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;
}
```

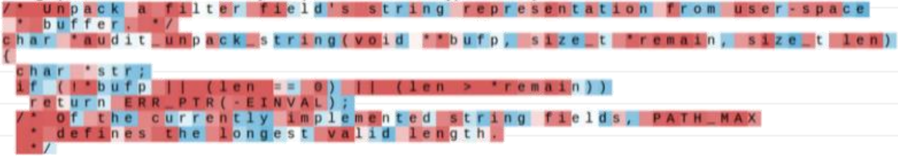
Cell that might be helpful in predicting a new line. Note that it only turns on for some ")":

```
char *audit_unpack_string(void **bufp, size_t *remain, si
{
  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;
}
```

[Karpathy et al. ICLR16]

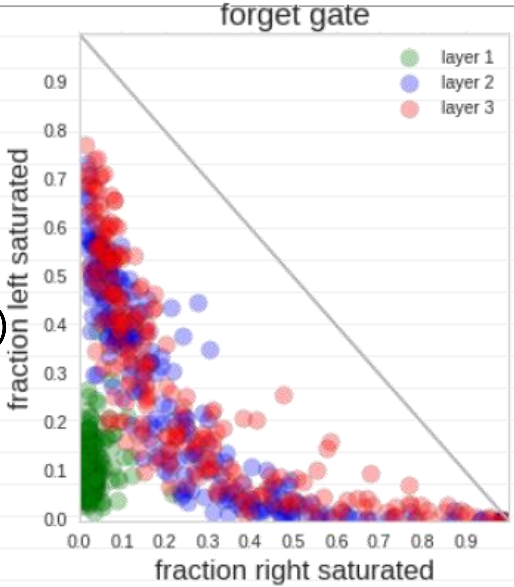
Non-interpretable LSTM Cells

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



[Karpathy et al. ICLR16]

Interpretable LSTM Cells



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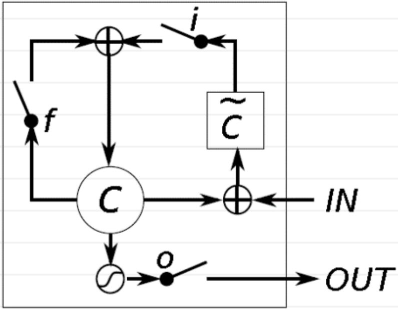
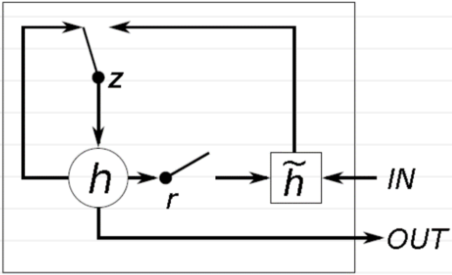
[Karpathy et al. ICLR16]

Gated Recurrent Units (GRU)



(a) Long Short-Term Memory



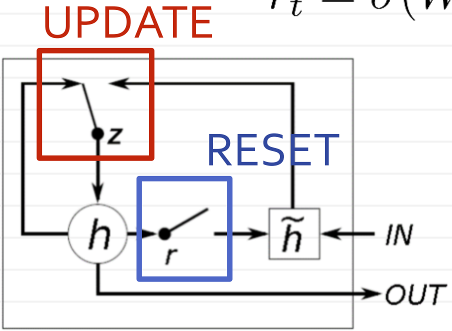
(b) Gated Recurrent Unit

[Cho et al. 14]
[Chung et al. 14]

Gated Recurrent Units (GRU)

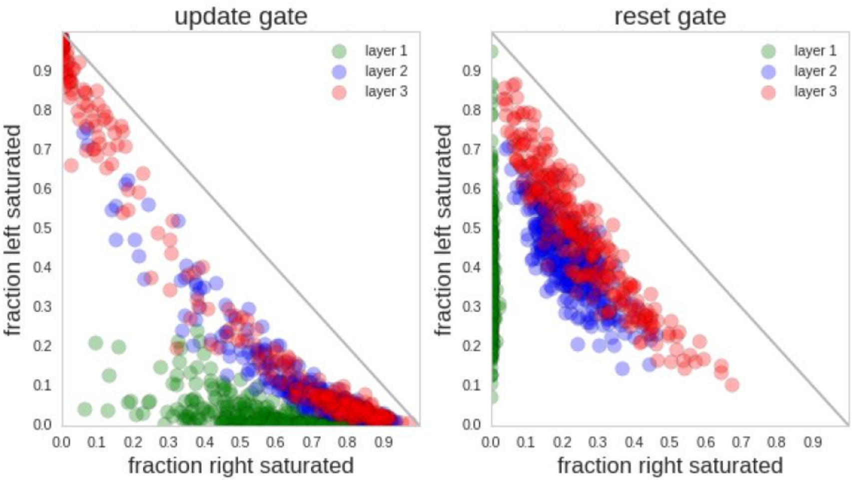
$$h_t = (1 - z_t) \odot h_{t-1} +$$
$$z_t \odot \phi(W_x x_t + W \; r_t \odot h_{t-1} + b)$$

$$z_t = \sigma(W_{xz} x_t + W_{hz} h_{t-1} + b_z)$$
$$r_t = \sigma(W_{xr} x_t + W_{hr} h_{t-1} + z_r)$$



[Cho et al. 14]
[Chung et al. 14]

GRU gate statistics



[Karpathy et al. ICLR16]

Plain vs LSTM vs GRU

Success at predicting next characters in the test sequence (cross-entropy loss) [Karpathy et al. ICLR16]:

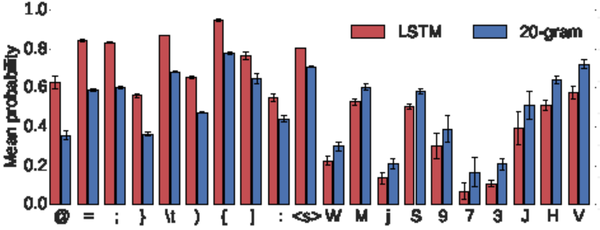
	LSTM			RNN			GRU		
Layers	1	2	3	1	2	3	1	2	3
Size	War and Peace Dataset								
64	1.449	1.442	1.540	1.446	1.401	1.396	1.398	**1.373**	1.472
128	1.277	1.227	1.279	1.417	1.286	1.277	1.230	**1.226**	1.253
256	1.189	**1.137**	1.141	1.342	1.256	1.239	1.198	1.164	1.138
512	1.161	1.092	1.082	-	-	-	1.170	1.201	**1.077**
	Linux Kernel Dataset								
64	1.355	**1.331**	1.366	1.407	1.371	1.383	1.335	1.298	1.357
128	1.149	1.128	1.177	1.241	**1.120**	1.220	1.154	1.125	1.150
256	1.026	**0.972**	0.998	1.171	1.116	1.116	1.039	0.991	1.026
512	0.952	0.840	0.846	-	-	-	0.943	0.861	**0.829**

Model \ n	1	2	3	4	5	6	7	8	9	20
	War and Peace Dataset									
n-gram	2.399	1.928	1.521	1.314	1.232	1.203	**1.194**	1.194	1.194	1.195
n-NN	2.399	1.931	1.553	1.451	1.339	**1.321**	-	-	-	-
	Linux Kernel Dataset									
n-gram	2.702	1.954	1.440	1.213	1.097	1.027	0.982	0.953	0.933	**0.889**
n-NN	2.707	1.974	1.505	1.395	**1.256**	1.376	-	-	-	-

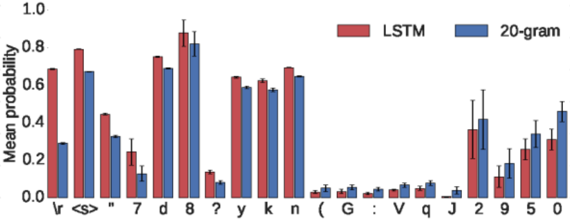
RNN success cases

Success at predicting next characters in the test sequence (cross-entropy loss) [Karpathy et al. ICLR16]:

Linux kernel:

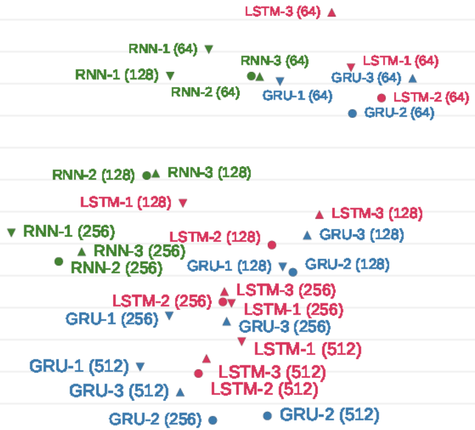


War and peace:



Plain vs LSTM vs GRU

Model similarity (t-SNE embedding of character probabilities):



[Karpathy et al. ICLR16]

Recap and outlook

- Sequence prediction
- ConvNets and Recurrent nets are SOA in wide variety of domains (NLP, speech/signal, bioinformatics)
- Gating in RNN makes its memory longer
- Sequence prediction extends to other tasks (fixed->seq, seq->fixed, seq->seq, fixed->fixed) – *next lecture*

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