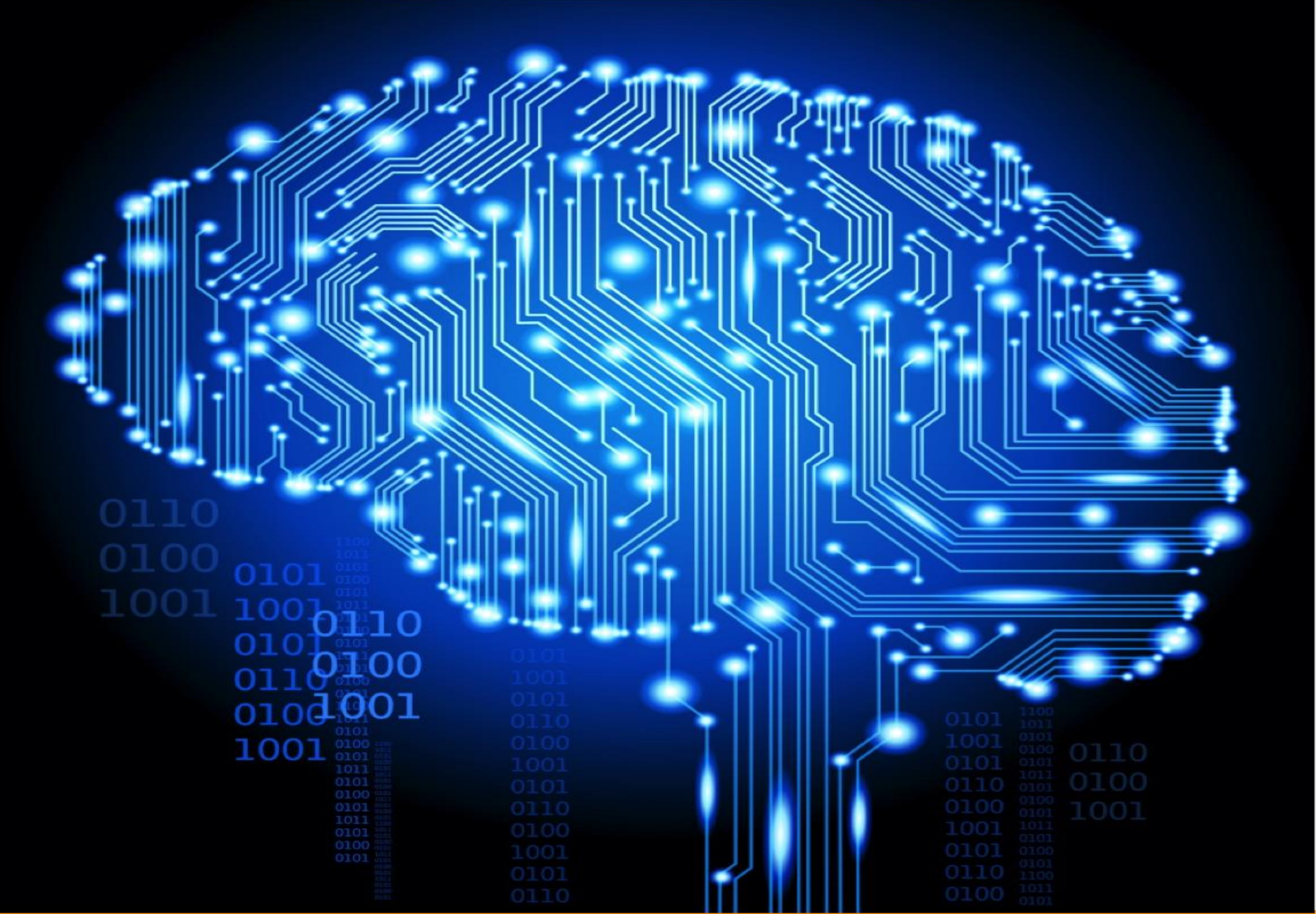


Lecture 6: Recurrent & Graph Neural Networks

Efstratios Gavves

Lecture overview

- Sequential data
- Recurrent Neural Networks
- Backpropagation through time
- Exploding and vanishing gradients
- LSTMs and variants
- Encoder-Decoder Architectures
- Graph Neural Networks

Sequence data

Sequence applications

Example of sequential data

- Videos
- Other?

Example of sequential data

- Videos
- Other?
- Time series data
  - Stock exchange
  - Biological measurements
  - Climate measurements
  - Market analysis
- Speech/Music
- User behavior in websites
- .....

Applications

- Machine translation
- Image captioning
- Question answering
- Video generation
- Speech synthesis
- Speech recognition

A sequence of probabilities

- Sequence → Chain rule of probabilities

$$p(x) = \prod_i p(x_i | x_1, \ldots, x_{i-1})$$

- For instance, let's model that "`This is the best course!`"

$$p(\texttt{This is the best course!}) =$$
$$= p(\texttt{This}) \cdot$$
$$p(\texttt{is}|\texttt{This}) \cdot$$
$$p(\texttt{the}|\texttt{This is}) \cdot \ldots \cdot$$
$$p(\texttt{!}|\texttt{This is the best course})$$

What is the problem with sequences?

- ???

What is the problem with sequences?

- Sequences might be of arbitrary or even infinite lengths
- Infinite parameters?

What is the problem with sequences?

- Sequences might be of arbitrary or even infinite lengths
- Infinite parameters?
- No, better share and reuse parameters
- RecurrentModel(`I think, therefore, I am.` | θ)

  can be reused also for

  RecurrentModel(`Everything is repeated in circles. History is a Master because it teaches that it doesn’t exist. It is the permutations that matter`| θ)
- For a ConvNet that is not straightforward
- Why?

What is the problem with sequences?

- Sequences might be of arbitrary or even infinite lengths
- Infinite parameters?
- No, better share and reuse parameters
- RecurrentModel(`I think, therefore, I am.` | θ)

  can be reused also for

  RecurrentModel(`Everything is repeated in circles. History is a Master because it teaches that it doesn’t exist. It is the permutations that matter`| θ)
- For a ConvNet that is not straightforward
- Why? Fixed dimensionalities

Some properties of sequences?

Some properties of sequences

- Data inside a sequence are non identically, independently distributed (IID)
  - The next “word” depends on the previous “words”
  - Ideally on all of them
- We need context, and we need memory!

- **Big question:** How to model context and memory ?

I am Bond , James Bond

McGuire
Bond
tired
am
!

Properties of sequences

- Data inside a sequence are non identically, independently distributed (IID)
  - The next “word” depends on the previous “words”
  - Ideally on all of them
- We need context, and we need memory!

- **Big question:** How to model context and memory ?

McGuire

Bond

I am Bond , James Bond tired

am

!

One-hot vectors

- A vector with all zeros except for the active dimension
- 12 words in a sequence → 12 One-hot vectors
- After the one-hot vectors apply an embedding
  - Word2Vec, GloVE

Vocabulary	One-hot vectors							
I	I	1	I	0	I	0	I	0
am	am	0	am	1	am	0	am	0
Bond	Bond	0	Bond	0	Bond	1	Bond	0
James	James	0	James	0	James	0	James	1
tired	tired	0	tired	0	tired	0	tired	0
,	,	0	,	0	,	0	,	0
McGuire	McGuire	0	McGuire	0	McGuire	0	McGuire	0
!	!	0	!	0	!	0	!	0

Why not indices instead of one-hot vectors?

One-hot representation OR? Index representation

$$x_{t=1,2,3,4} = \begin{array}{cccc} I & am & James & McGuire \\ \end{array}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

I am James McGuire

$$x_{"I"} = 1$$
$$x_{"am"} = 2$$
$$x_{"James"} = 4$$
$$x_{"McGuire"} = 7$$

Why not indices instead of one-hot vectors?

One-hot representation OR? Index representation

$$
x_{t=1,2,3,4} = \begin{array}{cccc} I & am & James & McGuire \end{array}
$$

$$
x_{t=1,2,3,4} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}
$$

I am James McGuire

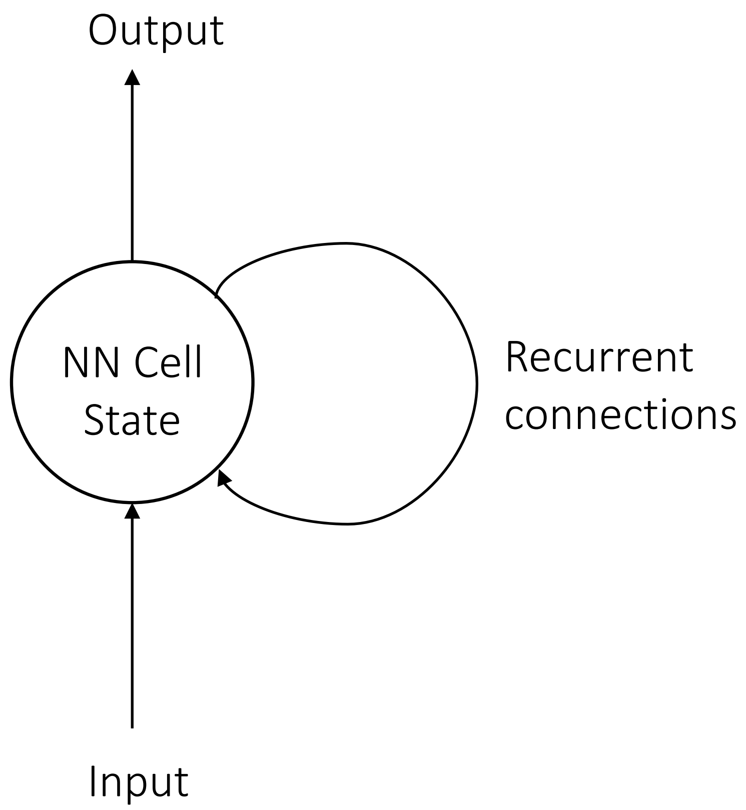
$$x_{"I"} = 1$$
$$x_{"am"} = 2$$
$$x_{"James"} = 4$$
$$x_{"McGuire"} = 7$$

$$\ell_2(x_{am}, x_{McQuire}) = \sqrt{2}$$
$$=$$
$$\ell_2(x_I, x_{am}) = \sqrt{2}$$

$$\ell_2(x_{am}, x_{McQuire}) = (7-2)^2 = 5$$
$$\neq$$
$$\ell_2(x_I, x_{am}) = (2-1)^2 = 1$$

Recurrent Neural Networks

Backprop through time



Memory

- Memory is a mechanism that learns a representation of the past
- At timestep t project all previous information $1, \dots, t$ onto a latent space c_t
  - Memory controlled by a neural network h_θ with shared parameters θ
- Then, at timestep $t+1$ re-use the parameters θ and the previous c_t

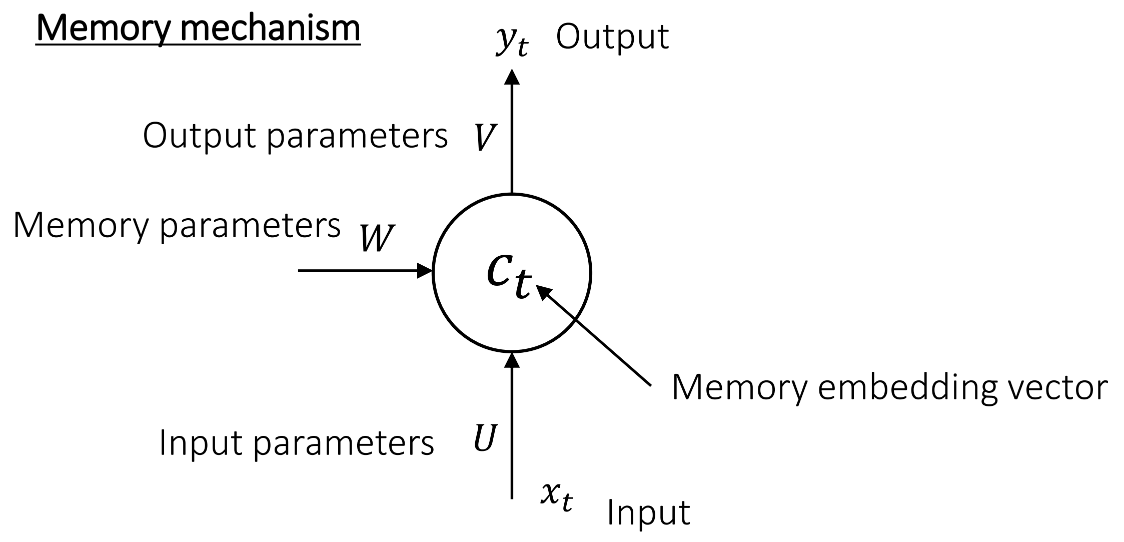
$$c_{t+1} = h_\theta(x_{t+1}, c_t)$$

$$\dots$$

$$c_{t+1} = h_\theta(x_{t+1}, h_\theta(x_t, h_\theta(x_{t-1}, \dots h_\theta(x_1, c_0))))$$

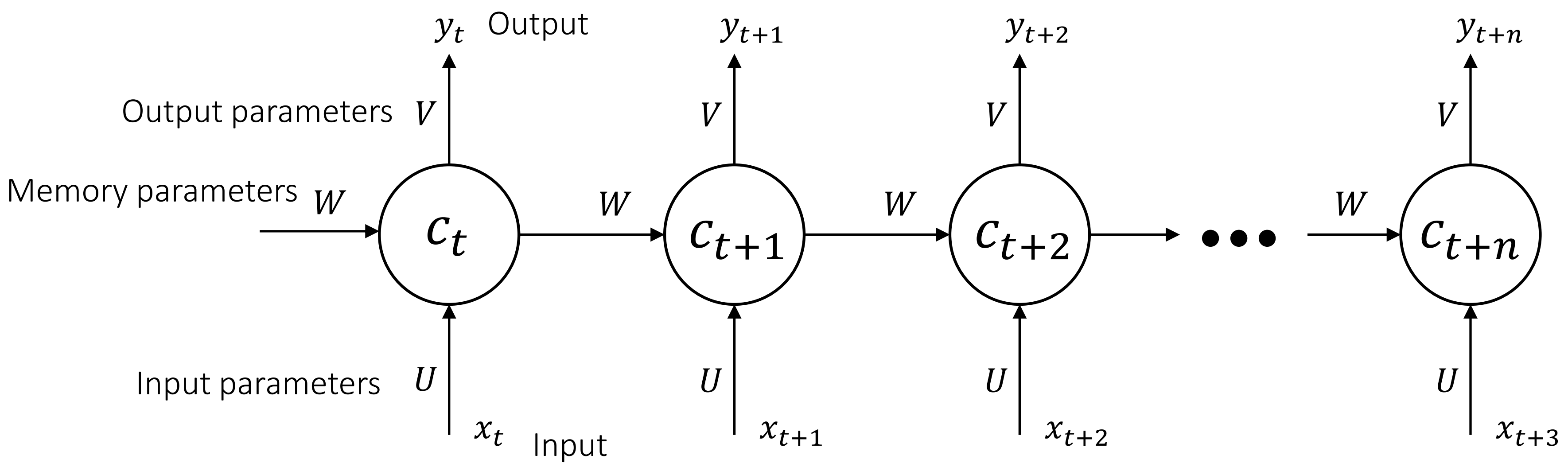
A graphical representation of memory

- In the simplest case, what are the Inputs/Outputs of our system
- Sequence inputs → we model them with parameters U
- Sequence outputs → we model them with parameters V
- Memory I/O → we model it with parameters W

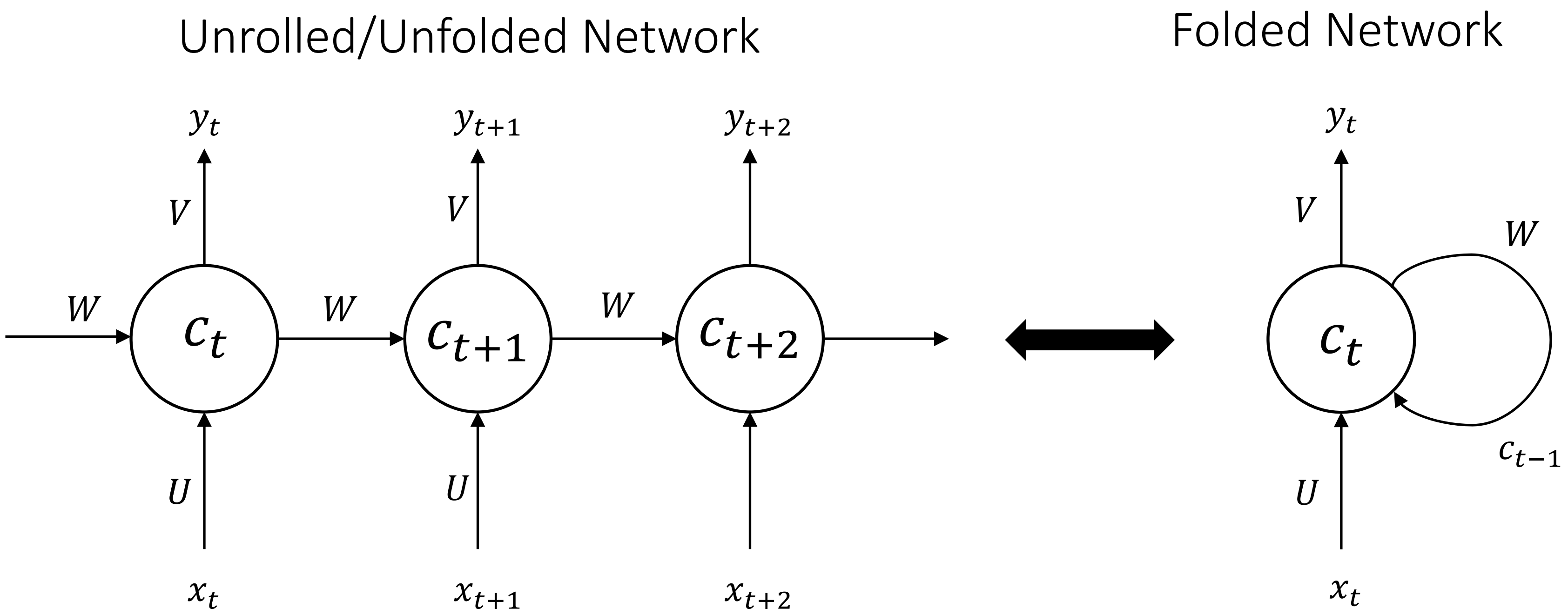


A graphical representation of memory

- In the simplest case, what are the Inputs/Outputs of our system
- Sequence inputs → we model them with parameters U
- Sequence outputs → we model them with parameters V
- Memory I/O → we model it with parameters W



Folding the memory



Recurrent Neural Networks - RNNs

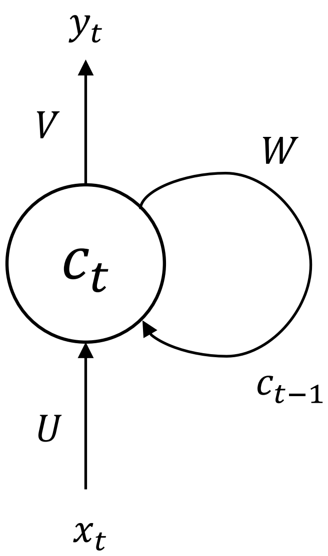
- Basically, two equations

$$c_t = \tanh(U\,x_t + W c_{t-1})$$
$$y_t = \mathrm{softmax}(V\,c_t)$$

- And a loss function

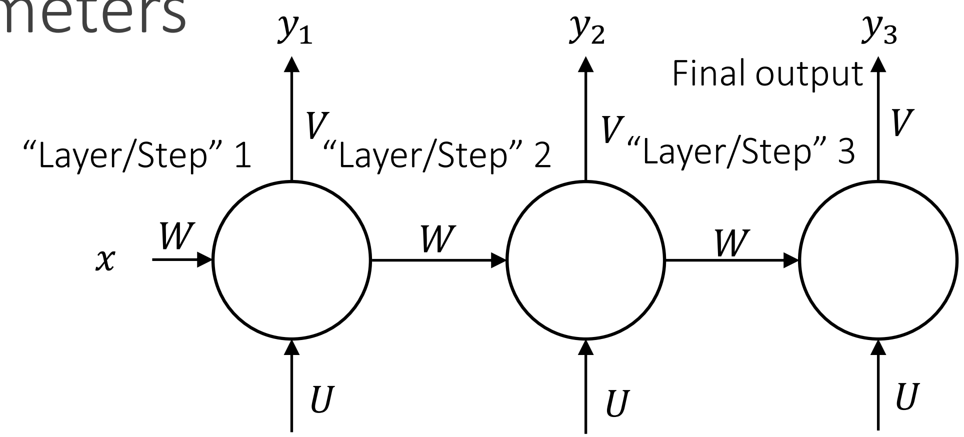
$$\mathcal{L} = \sum_t \mathcal{L}_t(y_t, y_t^*)$$
$$= \sum_t y_t^* \log y_t$$

assuming the cross-entropy loss function

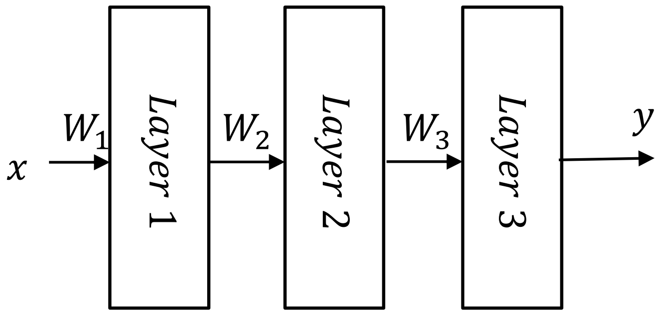


RNNs vs MLPs

- Is there a big difference?
- Instead of layers → Steps
- Outputs at every step → MLP outputs in every layer possible
- Main difference: Instead of layer-specific parameters → Layer-shared parameters



3-gram Unrolled Recurrent Network



3-layer Neural Network

Hmm, layers share parameters ?!?

- How is the training done? Does Backprop remain the same?

Hmm, layers share parameters ?!?

- How is the training done? Does Backprop remain the same?
- Basically, chain rule
  - So, again the same concept
- Yet, a bit more tricky this time, as the gradients survive over time

Backpropagation through time

$$c_t = \tanh(U\,x_t + W c_{t-1})$$
$$y_t = \text{softmax}(V\,c_t)$$
$$\mathcal{L} = \sum_t y_t^* \log y_t$$

- Let's say we focus on the third timestep loss

$$\frac{\partial \mathcal{L}}{\partial V} = \cdots$$
$$\frac{\partial \mathcal{L}}{\partial W} = \cdots$$
$$\frac{\partial \mathcal{L}}{\partial U} = \cdots$$

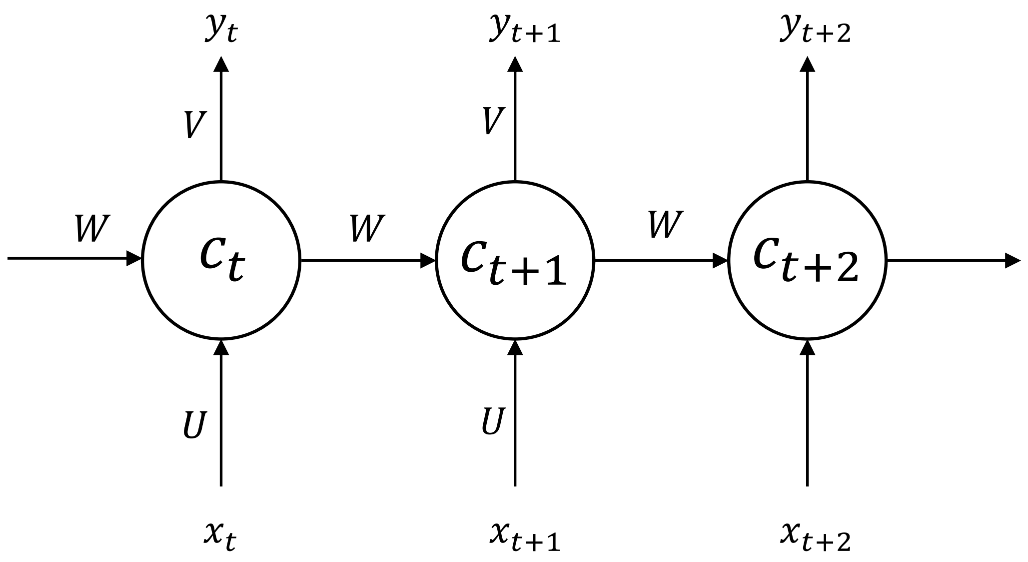
Backpropagation through time: $\partial \mathcal{L}_t / \partial V$

- Expanding the chain rule

$$\frac{\partial \mathcal{L}_t}{\partial V} = \frac{\partial \mathcal{L}_t}{\partial y_{t_k}} \frac{\partial y_{t_k}}{\partial c_{t_l}} \frac{\partial c_{t_l}}{\partial V_{ij}} = \cdots$$
$$= \cdots = (y_t - y_t^*) \otimes c_t$$

- All terms depend only on the current timestep t
- Then, we should sum up all the gradients for all time steps

$$\frac{\partial \mathcal{L}}{\partial V} = \sum_t \frac{\partial \mathcal{L}_t}{\partial V}$$



Backpropagation through time: $\partial \mathcal{L}_t / \partial W$

$$c_t = \tanh(U\, x_t + W c_{t-1})$$
$$y_t = \mathrm{softmax}(V\, c_t)$$

- Expanding with the chain rule

$$\frac{\partial \mathcal{L}_t}{\partial W} = \frac{\partial \mathcal{L}_t}{\partial y_t} \frac{\partial y_t}{\partial c_t} \frac{\partial c_t}{\partial W}$$

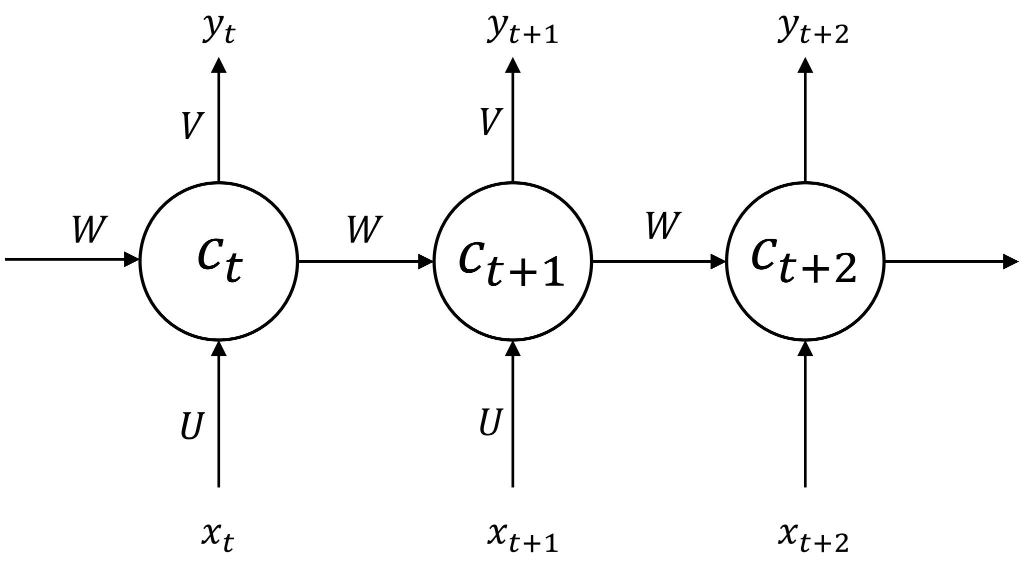
- However, c_t itself depends on c_{t-1} → $\frac{\partial c_t}{\partial W}$ depends also on c_{t-1} → The current dependency of c_t to W is recurrent
  - And continuing till we reach $c_{-1} = [0]$
- So, in the end we have

$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{k=0}^{t} \frac{\partial \mathcal{L}_t}{\partial y_t} \frac{\partial y_t}{\partial c_t} \frac{\partial c_t}{\partial c_k} \frac{\partial c_k}{\partial W}$$

- The gradient $\frac{\partial c_t}{\partial c_k}$ itself is subject to the chain rule

$$\frac{\partial c_t}{\partial c_k} = \frac{\partial c_t}{\partial c_{t-1}} \frac{\partial c_{t-1}}{\partial c_{t-2}} \cdots \frac{\partial c_{k+1}}{\partial c_k} = \prod_{j=k+1}^{t} \frac{\partial c_j}{\partial c_{j-1}}$$

- Then, we should sum up all the gradients for all time steps

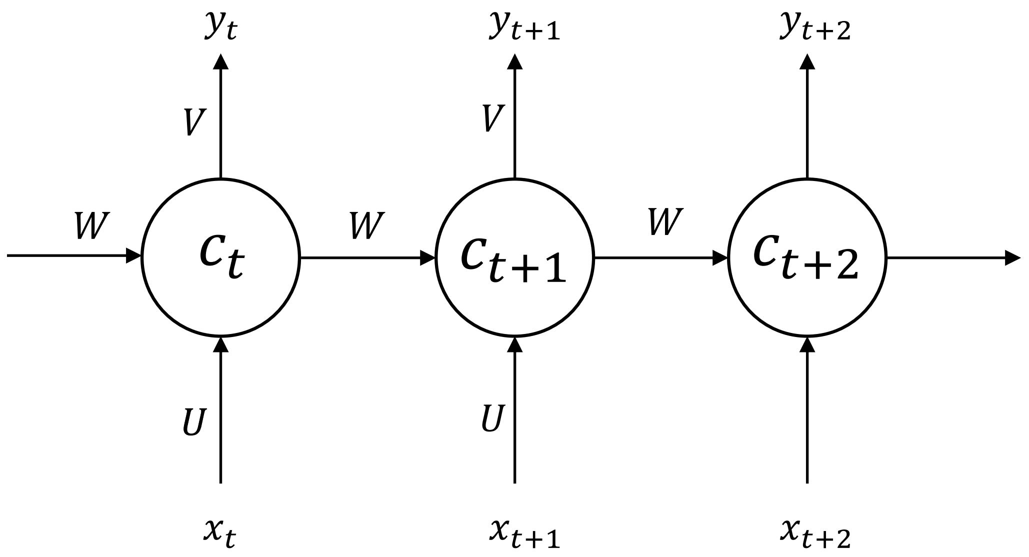


Backpropagation through time: $\partial \mathcal{L}_t / \partial U$

- For parameter matrix U a similar process

$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{k=0}^{t} \frac{\partial \mathcal{L}_t}{\partial y_t} \frac{\partial y_t}{\partial c_t} \frac{\partial c_t}{\partial c_k} \frac{\partial c_k}{\partial W}$$

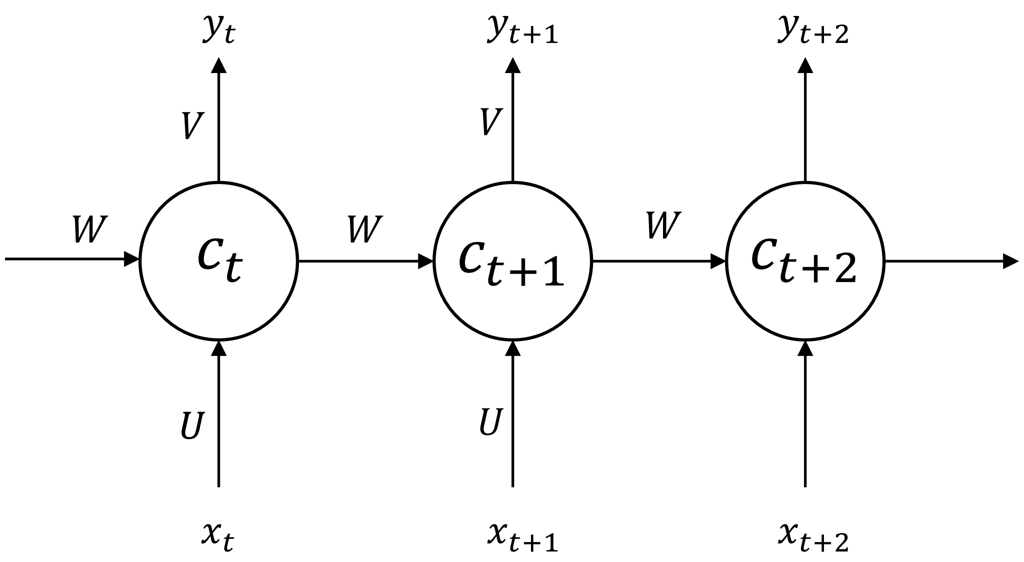
$$c_t = \tanh(U\, x_t + W c_{t-1})$$
$$y_t = \text{softmax}(V\, c_t)$$



Trading off Weight Update Frequency & Gradient Accuracy

- At time t we use current weights w_t to compute states c_t and outputs y_t
- Then, we use the states and outputs to backprop and get w_{t+1}
- Then, at $t+1$ we use w_{t+1} and the current state c_t to y_{t+1} and c_{t+1}
- Then we update the weights again with y_{t+1}.
  - The problem is y_{t+1} was computed with c_t in mind, which in turns depends on the old weights w_t, not the current ones w_{t+1}. So, the new gradients are only an estimate
  - Getting worse and worse, the more we backprop through time

$$c_t = \tanh(U\, x_t + W c_{t-1})$$
$$y_t = \mathrm{softmax}(V\, c_t)$$

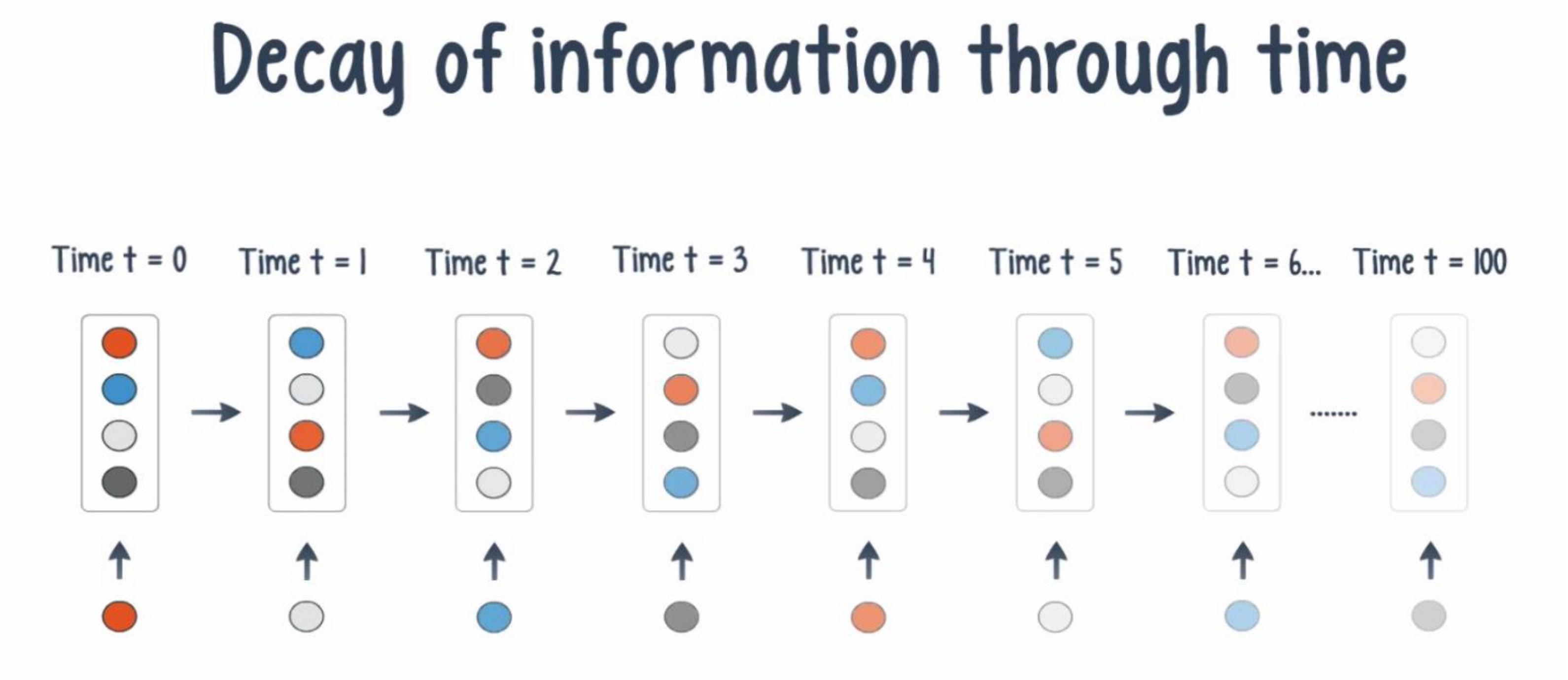


Potential solutions

- Do fewer updates
  - That might slow down training

- We can also make sure we do not backprop through more steps than our frequency of updates
  - But then we do not compute the full gradients
  - Bias again → not really gaining much

Vanishing gradients
Exploding gradients
Truncated backprop



An alternative formulation of an RNN

- Easier for mathematical analysis, and doesn't change the mechanics of the recurrent neural network

$$c_t = W \cdot \tanh(c_{t-1}) + U \cdot x_t + b$$
$$\mathcal{L} = \sum_t \mathcal{L}_t(c_t)$$
$$\theta = \{W, U, b\}$$

What is the problem

- As we just saw, the gradient $\frac{\partial c_t}{\partial c_k}$ itself is subject to the chain rule

$$\frac{\partial c_t}{\partial c_k} = \frac{\partial c_t}{\partial c_{t-1}} \frac{\partial c_{t-1}}{\partial c_{t-2}} \dots \frac{\partial c_{k+1}}{\partial c_k} = \prod_{j=k+1}^{t} \frac{\partial c_j}{\partial c_{j-1}}$$

- Product of ever expanding Jacobians
  - Ever expanding because we multiply more and more for longer dependencies

Let's look again the gradients

- Minimize the total loss over all time steps

$$\arg\min_{\theta} \sum_{t} \mathcal{L}_t(c_{t,\theta})$$

$$\frac{\partial \mathcal{L}_t}{\partial W} = \cdots$$

Let's look again the gradients

- Minimize the total loss over all time steps

$$\arg\min_{\theta} \sum_{t} \mathcal{L}_t(c_{t,\theta})$$

$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{\tau=1}^{t} \frac{\partial \mathcal{L}_t}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \frac{\partial c_\tau}{\partial W}$$

$$\frac{\partial \mathcal{L}}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} = \underbrace{\frac{\partial \mathcal{L}}{\partial \mathrm{c_t}} \cdot \frac{\partial c_t}{\partial \mathrm{c_{t-1}}} \cdot \frac{\partial c_{t-1}}{\partial \mathrm{c_{t-2}}}}_{t \ll \tau \;\rightarrow\; \text{short-term factors}} \cdot \underbrace{\ldots \cdot \frac{\partial c_{\tau+1}}{\partial \mathrm{c_\tau}}}_{t \gg \tau \;\rightarrow\; \text{long-term factors}}$$

Let's look again the gradients

- Minimize the total loss over all time steps

$$\arg\min_{\theta} \sum_{t} \mathcal{L}_t(c_{t,\theta})$$

$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{\tau=1}^{t} \frac{\partial \mathcal{L}_t}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \frac{\partial c_\tau}{\partial W}$$

$$\frac{\partial \mathcal{L}}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} = \frac{\partial \mathcal{L}}{\partial c_t} \cdot \frac{\partial c_t}{\partial c_{t-1}} \cdot \frac{\partial c_{t-1}}{\partial c_{t-2}} \cdot \ldots \cdot \frac{\partial c_{\tau+1}}{\partial c_\tau}$$

$$\left\| \frac{\partial c_{t+1}}{\partial c_t} \right\| \leq \|W^T\| \cdot \|diag(\sigma'(c_t))\|$$

Let's look again the gradients

$$\left\|\frac{\partial c_{t+1}}{\partial \mathrm{c_t}}\right\| \leq \|W^T\| \cdot \|diag(\sigma'(c_t))\|$$

- If we assume that the norm of the weight W is bounded
  - Spectral radius (max eigenvalue) is smaller than an arbitrary small number $\lambda_1 < \frac{1}{\gamma}$

- And if we assume that the non linearity is bounded

$$\|diag(\sigma'(c_t))\| < \gamma$$
$$\Rightarrow$$
$$\left\|\frac{\partial c_{t+1}}{\partial \mathrm{c_t}}\right\| < \frac{1}{\gamma}\gamma < 1$$

Let's look again the gradients

- Minimize the total loss over all time steps

$$\arg\min_{\theta} \sum_t \mathcal{L}_t(c_{t,\theta})$$

$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{\tau=1}^{\mathrm{t}} \frac{\partial \mathcal{L}_t}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \frac{\partial c_\tau}{\partial W}$$

$$\frac{\partial \mathcal{L}}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} = \underbrace{\frac{\partial \mathcal{L}}{\partial \mathrm{c_t}} \cdot \frac{\partial c_t}{\partial \mathrm{c_{t-1}}} \cdot \frac{\partial c_{t-1}}{\partial \mathrm{c_{t-2}}}}_{t \ll \tau \;\rightarrow\; \text{short-term factors}} \cdot \underbrace{\ldots \cdot \frac{\partial c_{\tau+1}}{\partial \mathrm{c_\tau}}}_{t \gg \tau \;\rightarrow\; \text{long-term factors}} \leq \eta^{t-\tau} \frac{\partial \mathcal{L}_t}{\partial c_t}$$

- RNN gradients expanding product of $\frac{\partial c_t}{\partial \mathrm{c_{t-1}}}$
- With $\eta < 1$ long-term factors $\rightarrow 0$ exponentially fast

Pascanu, Mikolov, Bengio, On the difficulty of training recurrent neural networks, JMLR 2013

Some cases

- Let's assume we have 10 time steps and $\frac{\partial c_t}{\partial \mathrm{c}_{\mathrm{t-1}}} > 1$, e.g. $\frac{\partial c_t}{\partial \mathrm{c}_{\mathrm{t-1}}} = 1.5$
- What would happen to the total $\frac{\partial \mathcal{L}_t}{\partial W}$?

Some cases

- Let's assume we have 100 time steps and $\frac{\partial c_t}{\partial \mathrm{c}_{\mathrm{t}-1}} > 1$, e.g. $\frac{\partial c_t}{\partial \mathrm{c}_{\mathrm{t}-1}} = 1.5$
- What would happen to the total $\frac{\partial \mathcal{L}_t}{\partial W}$?

$$\frac{\partial \mathcal{L}}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \propto 1.5^{10} = 4.06 \cdot 10^{17}$$

Some cases

- Let's assume now that $\frac{\partial c_t}{\partial c_{t-1}} < 1$, e.g. $\frac{\partial c_t}{\partial c_{t-1}} = 0.5$
- What would happen to the total $\frac{\partial \mathcal{L}_t}{\partial W}$?

Some cases

- Let's assume now that $\frac{\partial c_t}{\partial c_{t-1}} < 1$, e.g. $\frac{\partial c_t}{\partial c_{t-1}} = 0.5$
- What would happen to the total $\frac{\partial \mathcal{L}_t}{\partial W}$?

$$\frac{\partial \mathcal{L}}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \propto 0.5^{10} = 9.7 \cdot 10^{-5}$$

- Do you think our optimizers like these kind of gradients?

Some cases

- Let's assume now that $\frac{\partial c_t}{\partial \mathrm{c}_{\mathrm{t}-1}} < 1$, e.g. $\frac{\partial c_t}{\partial \mathrm{c}_{\mathrm{t}-1}} = 0.5$
- What would happen to the total $\frac{\partial \mathcal{L}_t}{\partial W}$?

$$\frac{\partial \mathcal{L}}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \propto 0.5^{10} = 9.7 \cdot 10^{-5}$$

- Do you think our optimizers like these kind of gradients?
- Too large → unstable training, oscillations, divergence
- Too small → very slow training, has it converged?

Vanishing & Exploding Gradients

- In recurrent networks, and in very deep networks in general (an RNN is not very different from an MLP), gradients are much affected by depth

$$\frac{\partial \mathcal{L}}{\partial c_t} = \frac{\partial \mathcal{L}}{\partial \mathrm{c_T}} \cdot \frac{\partial c_T}{\partial \mathrm{c_{T-1}}} \cdot \frac{\partial c_{T-1}}{\partial \mathrm{c_{T-2}}} \cdot \ldots \cdot \frac{\partial c_{t+1}}{\partial \mathrm{c}_{c_t}} \text{ and } \frac{\partial c_{t+1}}{\partial \mathrm{c}_t} < 1 \ \Rightarrow \frac{\partial \mathcal{L}}{\partial W} \ll 1 \Rightarrow \text{Vanishing gradient}$$

$$\frac{\partial \mathcal{L}}{\partial c_t} = \frac{\partial \mathcal{L}}{\partial \mathrm{c_T}} \cdot \frac{\partial c_T}{\partial \mathrm{c_{T-1}}} \cdot \frac{\partial c_{T-1}}{\partial \mathrm{c_{T-2}}} \cdot \ldots \cdot \frac{\partial c_{t+1}}{\partial \mathrm{c}_{c_t}} \text{ and } \frac{\partial c_{t+1}}{\partial \mathrm{c}_t} > 1 \ \Rightarrow \frac{\partial \mathcal{L}}{\partial W} \gg 1 \Rightarrow \text{Exploding gradient}$$

Vanishing gradients & long memory

- Vanishing gradients are particularly a problem for long sequences
- Why?

Vanishing gradients & long memory

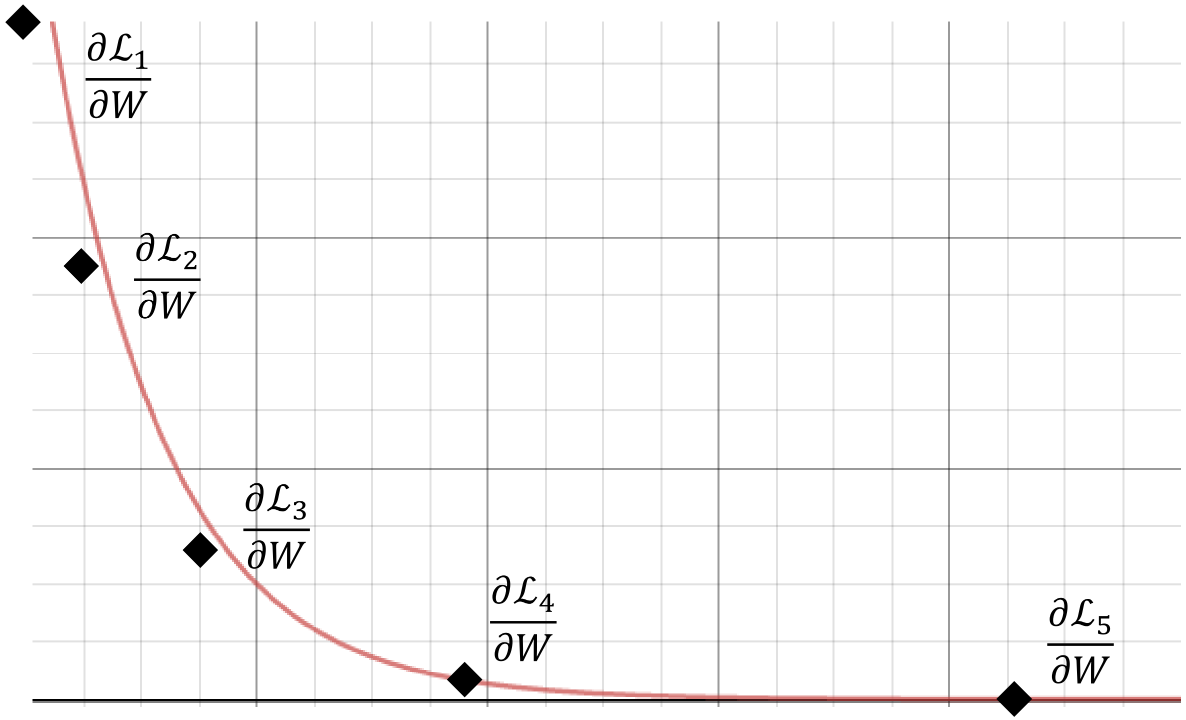
- Vanishing gradients are particularly a problem for long sequences
- Why?
- Exponential decay

$$\frac{\partial \mathcal{L}}{\partial c_t} = \prod_{t \geq k \geq \tau} \frac{\partial c_k}{\partial c_{k-1}} = \prod_{t \geq k \geq \tau} W \cdot \partial \tanh(c_{k-1})$$

- The further back we look (long-term dependencies), the smaller the weights automatically become
  - exponentially smaller weights

Why are vanishing gradients bad?

- The weight changes of earlier time steps become exponentially smaller
- Bad, even if we train the model exponentially longer
- The weights will quickly learn to "model" short-term transitions and ignore long-term transitions
- At best, even after longer training, they will try "fine-tune" the whatever bad "modelling" of long-term transitions
- But, as the short-term transitions are inherently more prevalent, they will dominate the learning and gradients



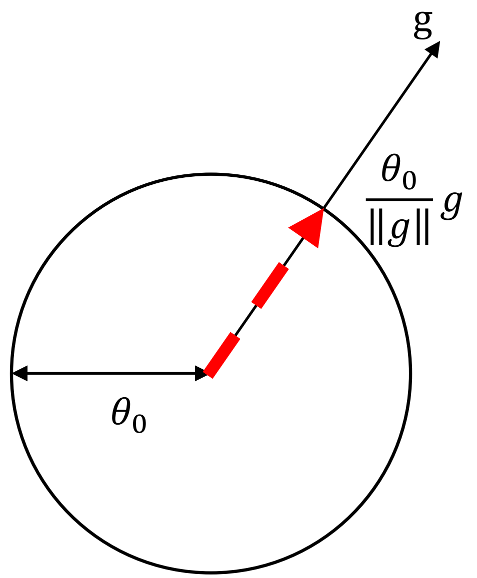
$$\frac{\partial \mathcal{L}}{\partial W} = \frac{\partial \mathcal{L}_1}{\partial W} + \frac{\partial \mathcal{L}_2}{\partial W} + \frac{\partial \mathcal{L}_3}{\partial W} + \frac{\partial \mathcal{L}_4}{\partial W} + \frac{\partial \mathcal{L}_5}{\partial W}$$

Quick fix for exploding gradients: Rescaling!

- First, get the gradient $\mathrm{g} \leftarrow \frac{\partial \mathcal{L}}{\partial w}$
- Check if the norm is larger than a threshold θ_0
- If it is, rescale it to have same direction and threshold norm

$$\mathrm{g} \leftarrow \frac{\theta_0}{\|g\|} g$$

- Simple, but works!



Can we rescale gradients also for vanishing gradients?

- No!
- The nature of the problem is different
- Exploding gradients → you might have bouncing and unstable optimization
- Vanishing gradients → you simply do not have a gradient to begin with
  - Rescaling of what exactly?
- In any case, even with re-scaling we would still focus on the short-term gradients
  - Long-term dependencies would still be ignored

Biased gradients?

- Backpropagating all the way till infinity is unrealistic
  - We would backprop forever (or simply it would be computationally very expensive)
  - And in case, the gradients would be inaccurate because of intermediate updates
- What about truncating backprop to the last K steps

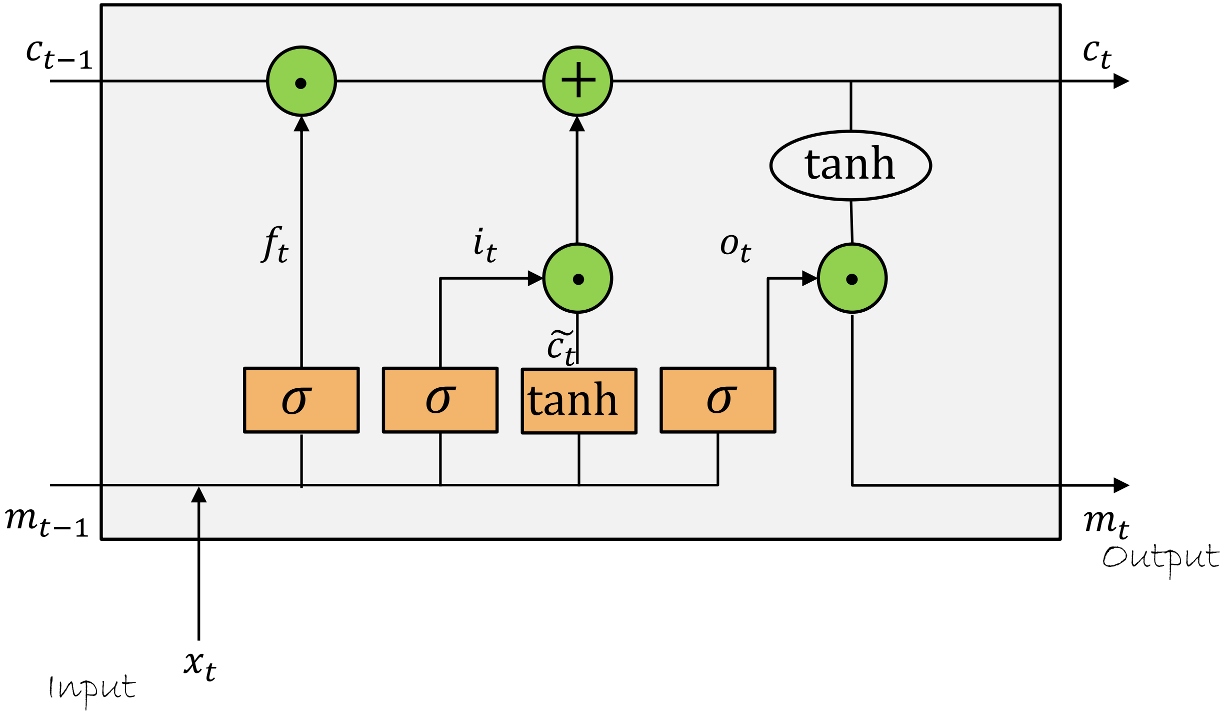
$$\tilde{g}_{t+1} \propto \frac{\partial \mathcal{L}}{\partial w}\Big|_{t=0}^{t=k}$$

- Unfortunately, this leads to biased gradients

$$g_{t+1} = \frac{\partial \mathcal{L}}{\partial w}\Big|_{t=0}^{t=\infty} \neq \tilde{g}_{t+1}$$

- Other algorithms exist but they are not as successful
  - We will visit them later

LSTM and variants



How to fix the vanishing gradients?

- Error signal over time must have not too large, not too small norm
- Let’s have a look at the loss function

$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{\tau=1}^{\mathrm{t}} \frac{\partial \mathcal{L}_r}{\partial y_t} \frac{\partial y_t}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \frac{\partial c_\tau}{\partial W}$$

$$\frac{\partial c_t}{\partial c_\tau} = \prod_{t \geq k \geq \tau} \frac{\partial c_k}{\partial c_{k-1}}$$

- How to make the product roughly the same no matter the length?

How to fix the vanishing gradients?

- Error signal over time must have not too large, not too small norm
- Let's have a look at the loss function

$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{\tau=1}^{\mathrm{t}} \frac{\partial \mathcal{L}_r}{\partial y_t} \frac{\partial y_t}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \frac{\partial c_\tau}{\partial W}$$

$$\frac{\partial c_t}{\partial c_\tau} = \prod_{t \geq k \geq \tau} \frac{\partial c_k}{\partial c_{k-1}}$$

- How to make the product roughly the same no matter the length?
- Use the identity function with gradient of 1

Main idea of LSTMs

- Over time the state change is $c_{t+1} = c_t + \Delta \mathrm{c}_{t+1}$
- This constant over-writing over long time steps leads to chaotic behavior

- Input weight conflict
  - Are all inputs important enough to write them down?

- Output conflict
  - Are all outputs important enough to be read?

- Forget conflict
  - Is all information important enough to be remembered over time?

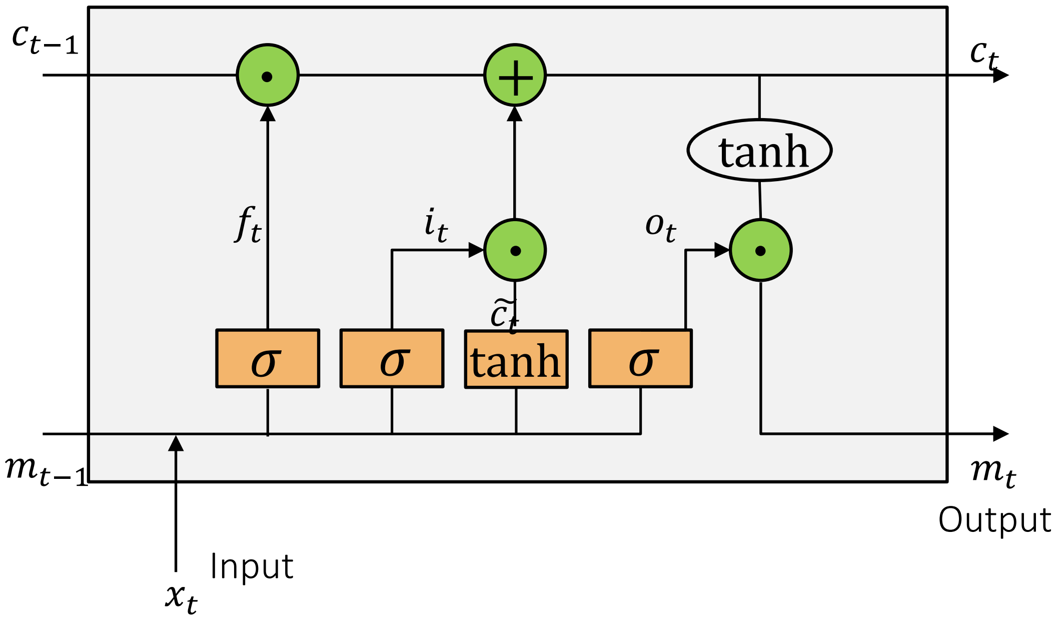
LSTMs

- RNNs

$$c_t = W \cdot \tanh(c_{t-1}) + U \cdot x_t + b$$

- LSTMs

$$i = \sigma\left(x_t U^{(i)} + m_{t-1} W^{(i)}\right)$$
$$f = \sigma\left(x_t U^{(f)} + m_{t-1} W^{(f)}\right)$$
$$o = \sigma\left(x_t U^{(o)} + m_{t-1} W^{(o)}\right)$$
$$\widetilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
$$c_t = c_{t-1} \odot f + \widetilde{c}_t \odot i$$
$$m_t = \tanh(c_t) \odot o$$



LSTMs: A marking difference

- RNNs

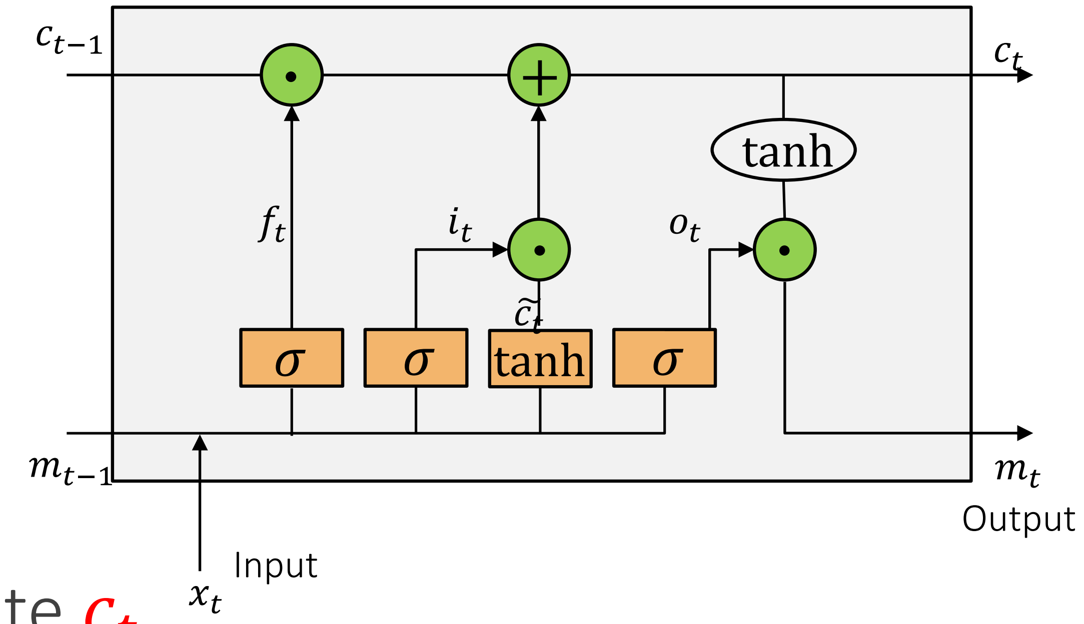
$$c_t = W \cdot \tanh(c_{t-1}) + U \cdot x_t + b$$

- LSTMs

$$i = \sigma\left(x_t U^{(i)} + m_{t-1} W^{(i)}\right)$$
$$f = \sigma\left(x_t U^{(f)} + m_{t-1} W^{(f)}\right)$$
$$o = \sigma\left(x_t U^{(o)} + m_{t-1} W^{(o)}\right)$$
$$\widetilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
$$c_t = c_{t-1} \odot f + \widetilde{c}_t \odot i$$
$$m_t = \tanh(c_t) \odot o$$

- The previous state c_{t-1} and the next state c_t are connected by addition

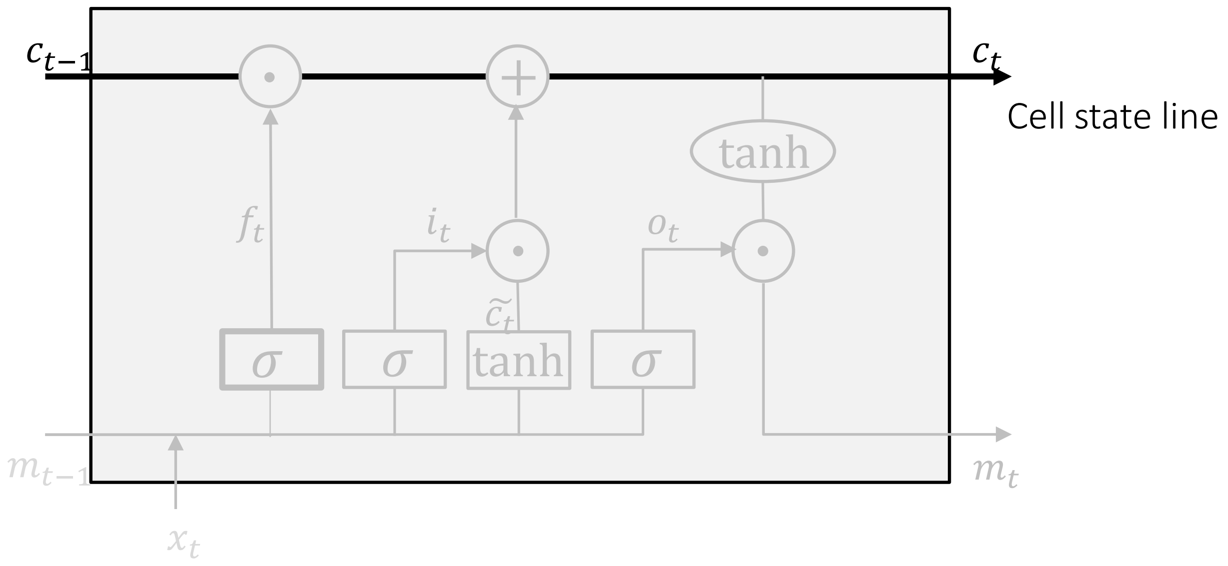
Additivity leads to strong gradients
Bounded by sigmoidal f



Nice tutorial: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

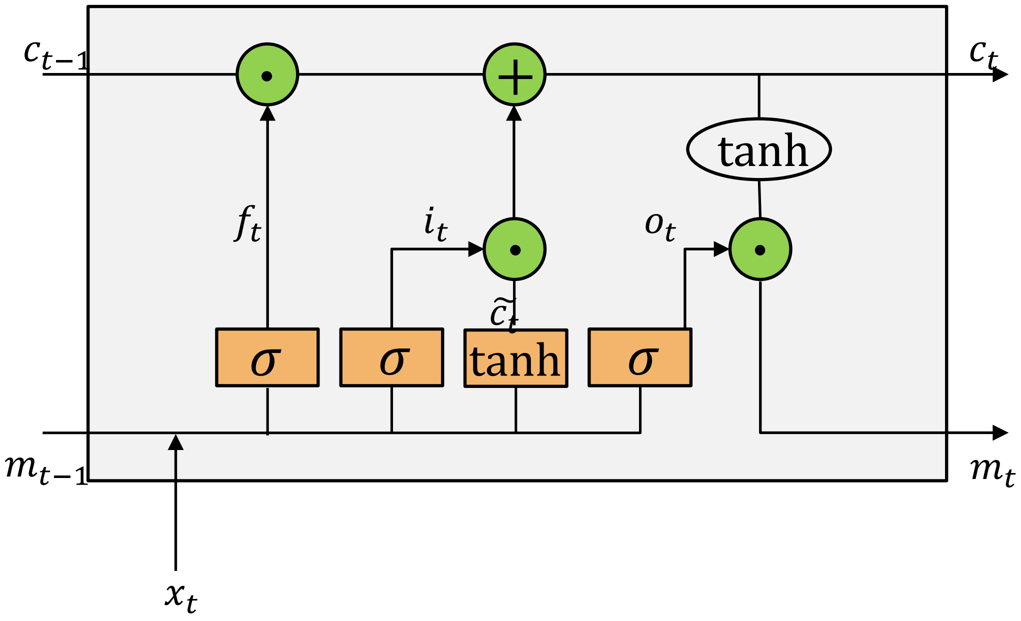
Cell state

$$i = \sigma\left(x_t U^{(i)} + m_{t-1} W^{(i)}\right)$$
$$f = \sigma\left(x_t U^{(f)} + m_{t-1} W^{(f)}\right)$$
$$o = \sigma\left(x_t U^{(o)} + m_{t-1} W^{(o)}\right)$$
$$\tilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
$$c_t = c_{t-1} \odot f + \tilde{c}_t \odot i$$
$$m_t = \tanh(c_t) \odot o$$



LSTM nonlinearities

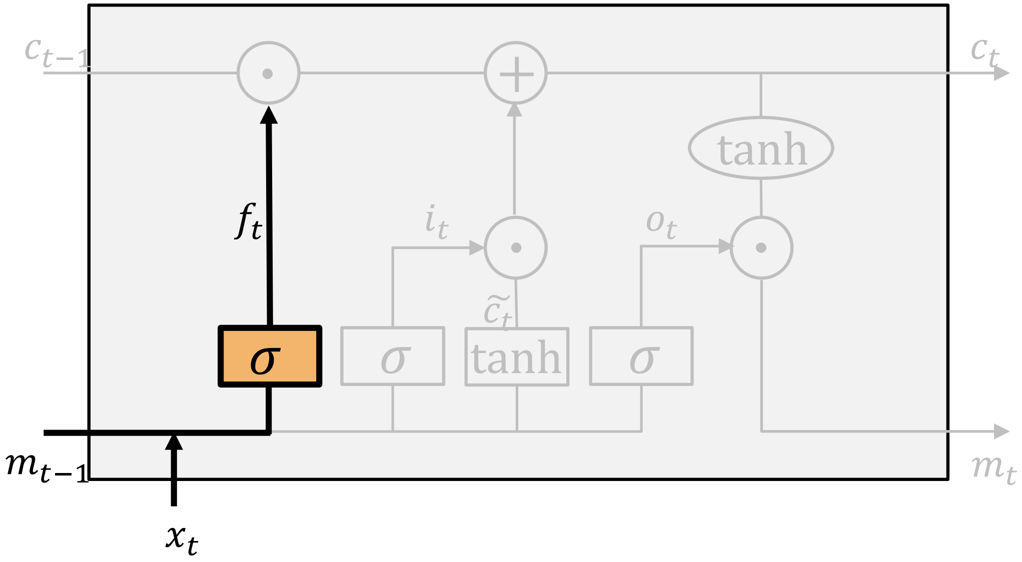
$$i = \sigma\left(x_t U^{(i)} + m_{t-1} W^{(i)}\right)$$
$$f = \sigma\left(x_t U^{(f)} + m_{t-1} W^{(f)}\right)$$
$$o = \sigma\left(x_t U^{(o)} + m_{t-1} W^{(o)}\right)$$
$$\widetilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
$$c_t = c_{t-1} \odot f + \widetilde{c}_t \odot i$$
$$m_t = \tanh(c_t) \odot o$$



- $\sigma \in (0, 1)$: control gate – something like a switch
- $\tanh \in (-1, 1)$: recurrent nonlinearity

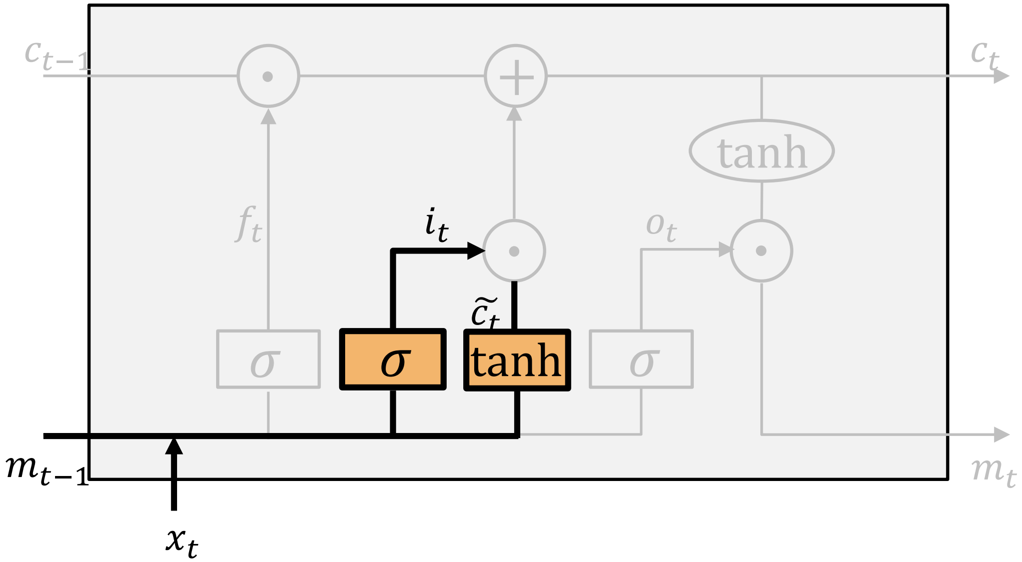
LSTM Step by Step #1

$$i = \sigma\left(x_t U^{(i)} + m_{t-1} W^{(i)}\right)$$
$$f = \sigma\left(x_t U^{(f)} + m_{t-1} W^{(f)}\right)$$
$$o = \sigma\left(x_t U^{(o)} + m_{t-1} W^{(o)}\right)$$
$$\widetilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
$$c_t = c_{t-1} \odot f + \widetilde{c}_t \odot i$$
$$m_t = \tanh(c_t) \odot o$$



LSTM Step by Step #2

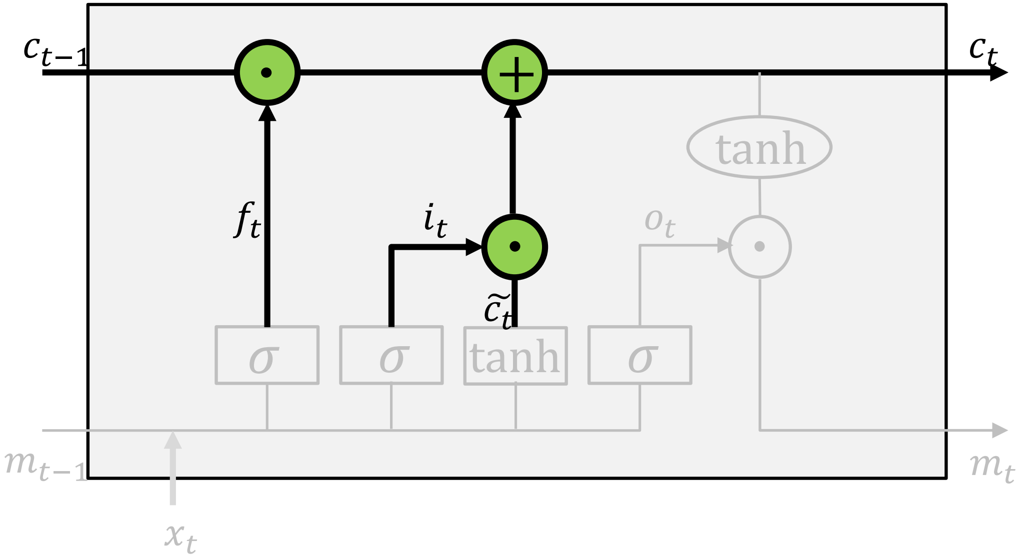
$$i = \sigma\left(x_t U^{(i)} + m_{t-1} W^{(i)}\right)$$
$$f = \sigma\left(x_t U^{(f)} + m_{t-1} W^{(f)}\right)$$
$$o = \sigma\left(x_t U^{(o)} + m_{t-1} W^{(o)}\right)$$
$$\widetilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
$$c_t = c_{t-1} \odot f + \widetilde{c}_t \odot i$$
$$m_t = \tanh(c_t) \odot o$$



- Decide what new information is relevant from the new input and should be added to the new memory
  - Modulate the input i_t
  - Generate candidate memories $\widetilde{c}_t$

LSTM Step by Step #3

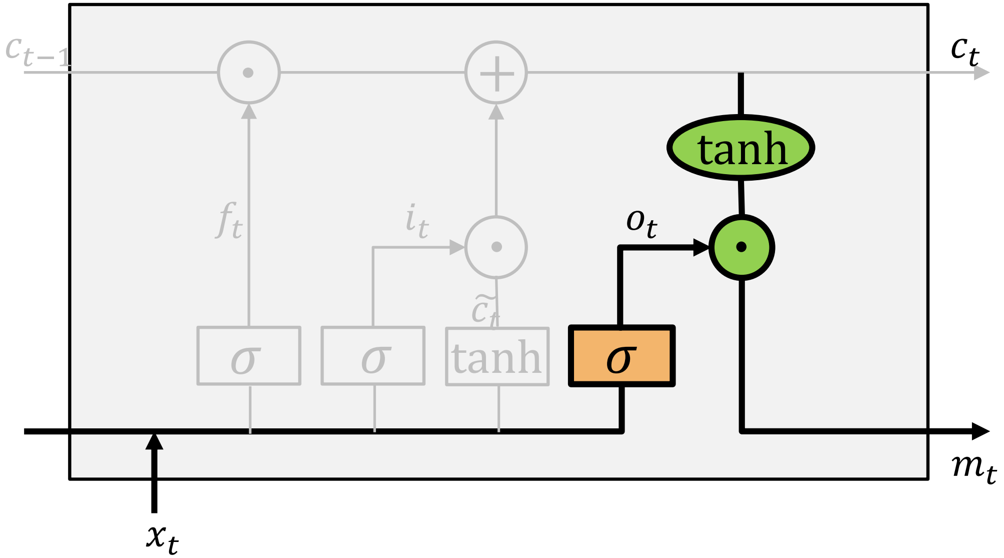
$$i = \sigma\left(x_t U^{(i)} + m_{t-1} W^{(i)}\right)$$
$$f = \sigma\left(x_t U^{(f)} + m_{t-1} W^{(f)}\right)$$
$$o = \sigma\left(x_t U^{(o)} + m_{t-1} W^{(o)}\right)$$
$$\tilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
$$c_t = c_{t-1} \odot f + \tilde{c}_t \odot i$$
$$m_t = \tanh(c_t) \odot o$$



- Compute and update the current cell state c_t
  - Depends on the previous cell state
  - What we decide to forget
  - What inputs we allow
  - The candidate memories

LSTM Step by Step #4

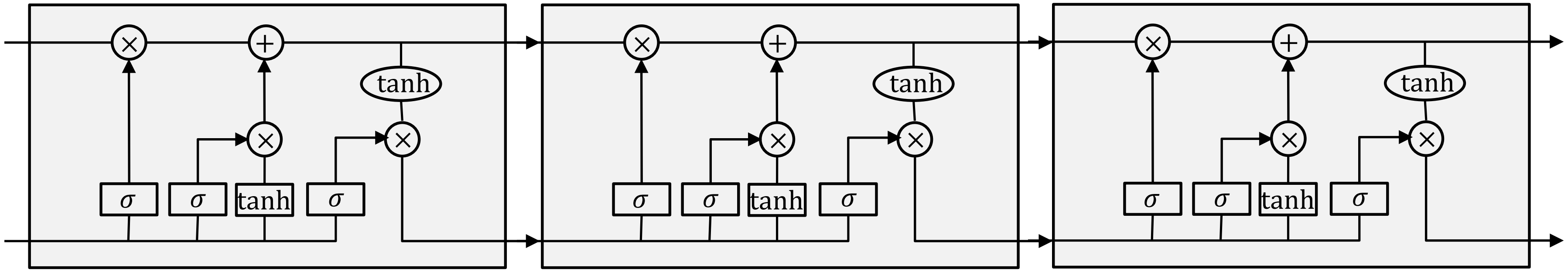
$$i = \sigma\left(x_t U^{(i)} + m_{t-1} W^{(i)}\right)$$
$$f = \sigma\left(x_t U^{(f)} + m_{t-1} W^{(f)}\right)$$
$$o = \sigma\left(x_t U^{(o)} + m_{t-1} W^{(o)}\right)$$
$$\widetilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
$$c_t = c_{t-1} \odot f + \widetilde{c}_t \odot i$$
$$m_t = \tanh(c_t) \odot o$$



- Modulate the output
  - Does the new cell state relevant? → Sigmoid 1
  - If not → Sigmoid 0
- Generate the new memory

Unrolling the LSTMs

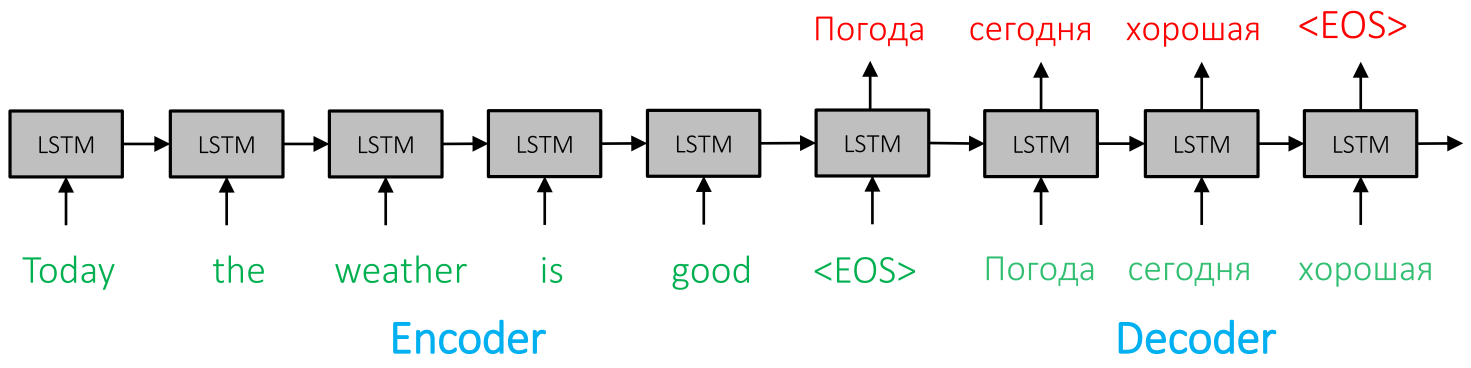
- Just the same like for RNNs
- The engine is a bit different (more complicated)
  - Because of their gates LSTMs capture long and short term dependencies



LSTM variants

- LSTM with peephole connections
- Gates have access also to the previous cell states $c\_(t-1)$ (not only memories)
- Bi-directional recurrent networks
- Gated Recurrent Units (GRU)
- Phased LSTMs
- Skip LSTMs
- And many more …

Encoder-Decoder Architectures



Machine translation

- The phrase in the source language is one sequence
  - “Today the weather is good”
- It is captured by an Encoder LSTM
- The phrase in the target language is also a sequence
  - “Погода сегодня хорошая”
- It is captured by a Decoder LSTM

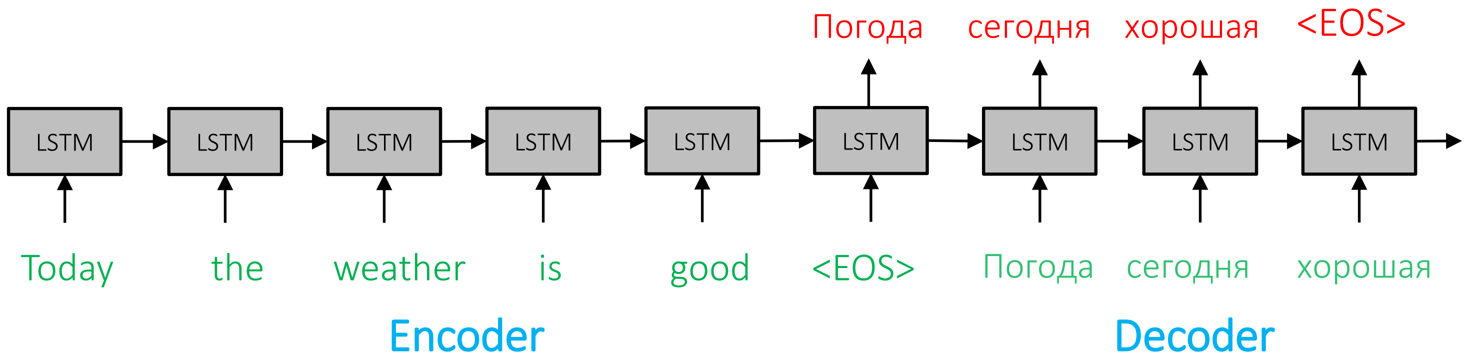


Image captioning

- Similar to image translation
- The only difference is that the Encoder LSTM is an image ConvNet
  - VGG, ResNet, …
- Keep decoder the same

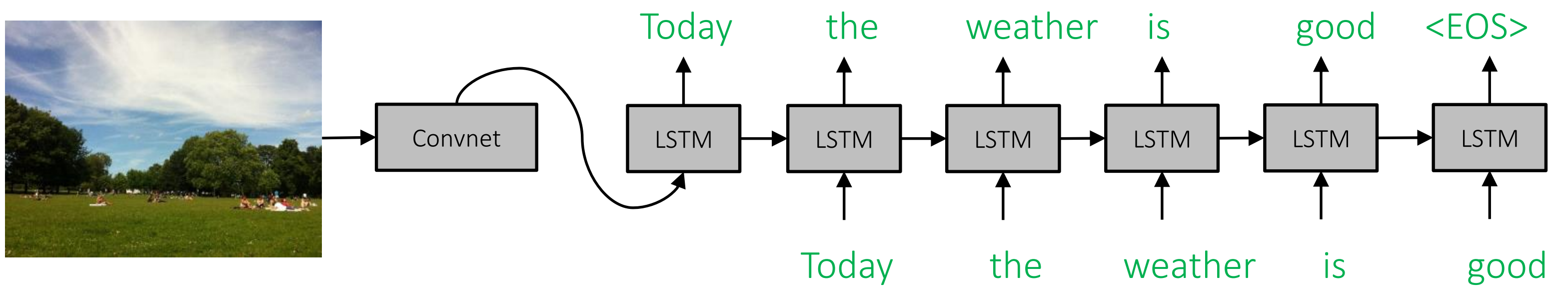
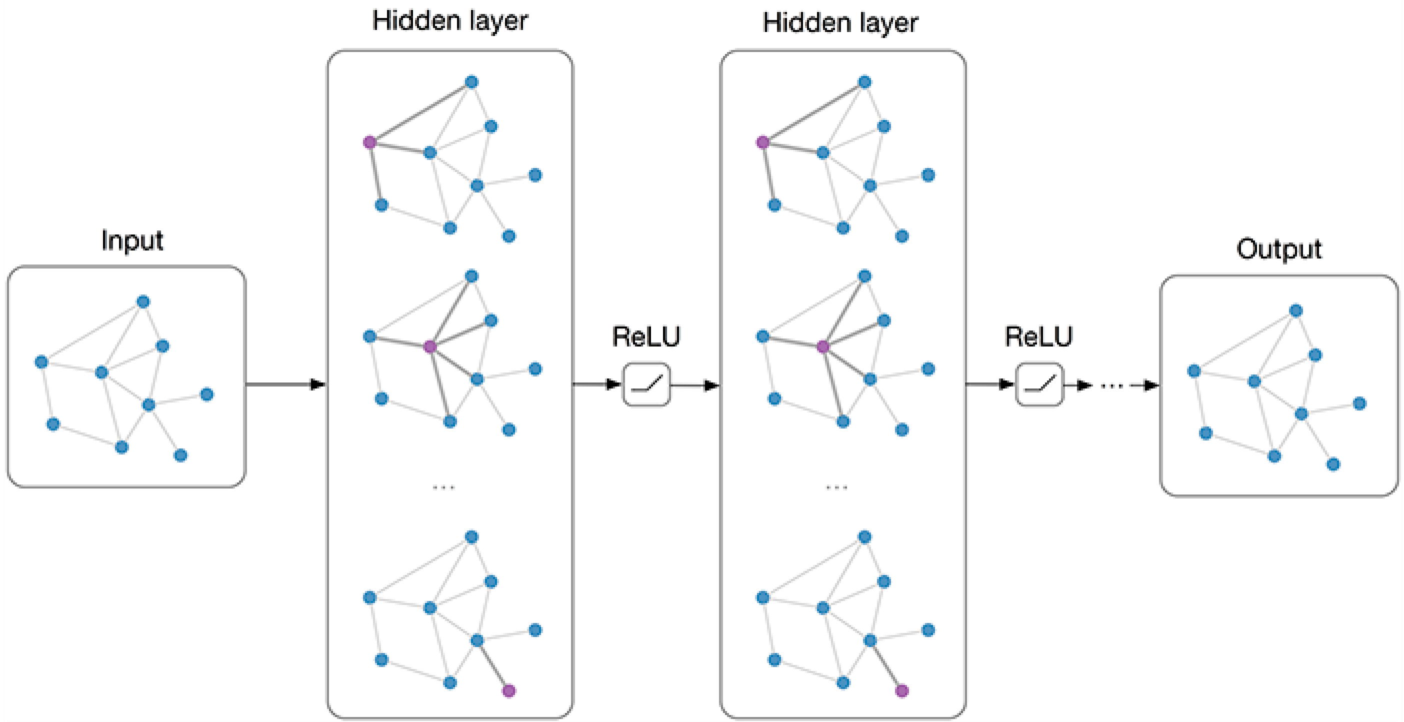


Image captioning demo

[Click to go to the video in Youtube]

NeuralTalk and Walk, recognition, text description of the image while walking

Graph Neural Networks

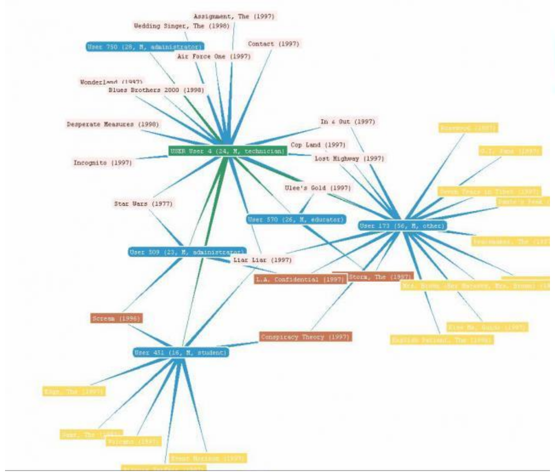


Why Graphs?

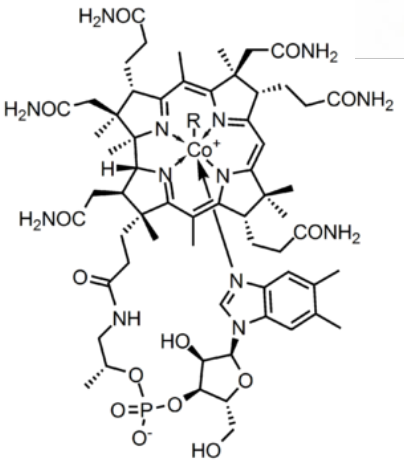
- Many domains & data have graph structure
- Examples?

Why Graphs?

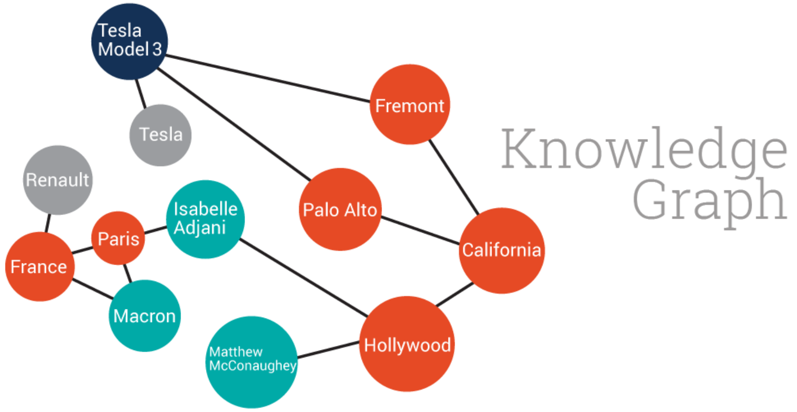
- Many domains & data have graph structure



- Social networks
- Knowledge graphs
- Recommender systems
- Chemical compounds
- And more



R = 5'-deoxyadenosyl, Me, OH, CN



Predictions tasks on graphs?

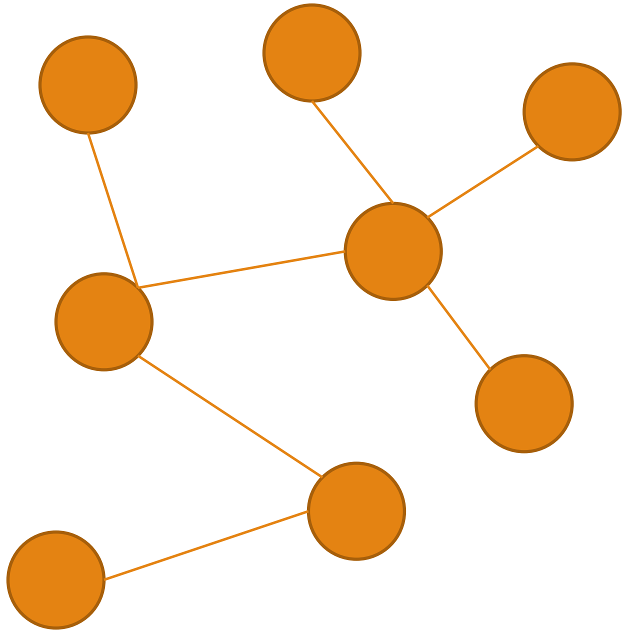
Predictions tasks on graphs?

- Node classification
- Filling out missing edges
- Filling out missing nodes
- Novel graph generation

DeepWalk

Algorithm

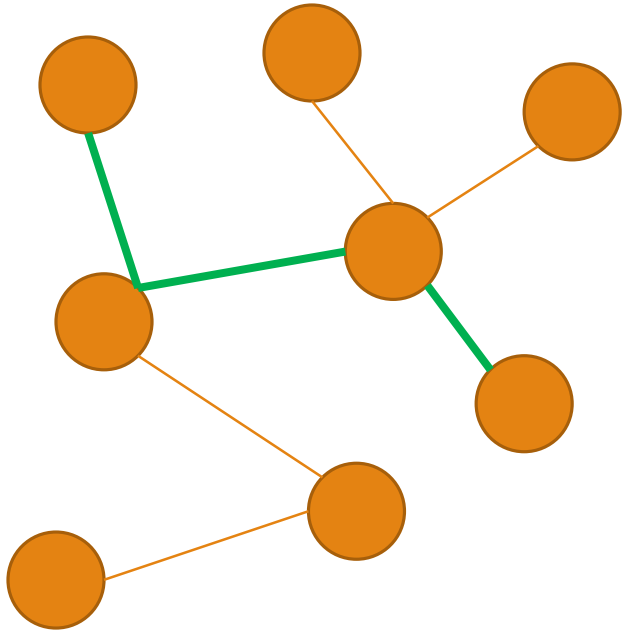
1. Perform random walks on the graph to generate node sequences



DeepWalk

Algorithm

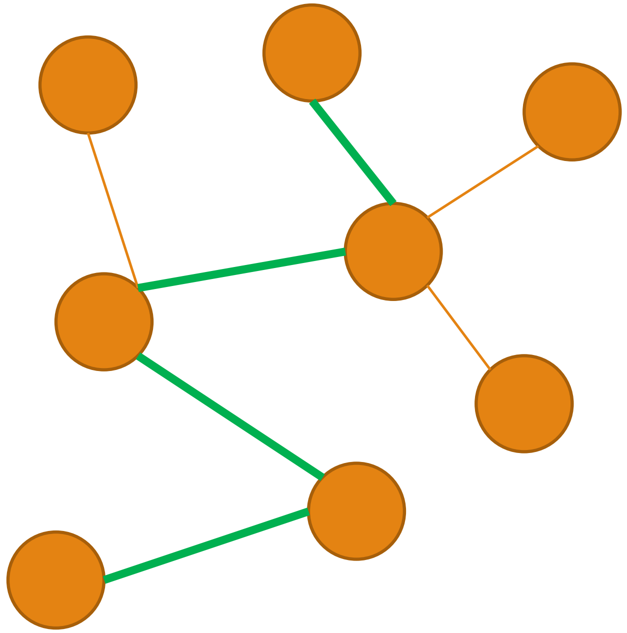
1. Perform random walks on the graph to generate node sequences
2. Run skip-gram to learn the node embedding



DeepWalk

Algorithm

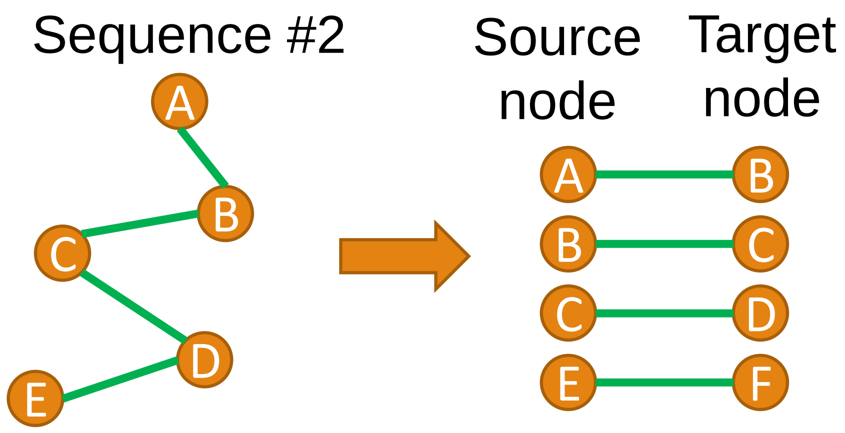
1. Perform random walks on the graph to generate node sequences



DeepWalk

Algorithm

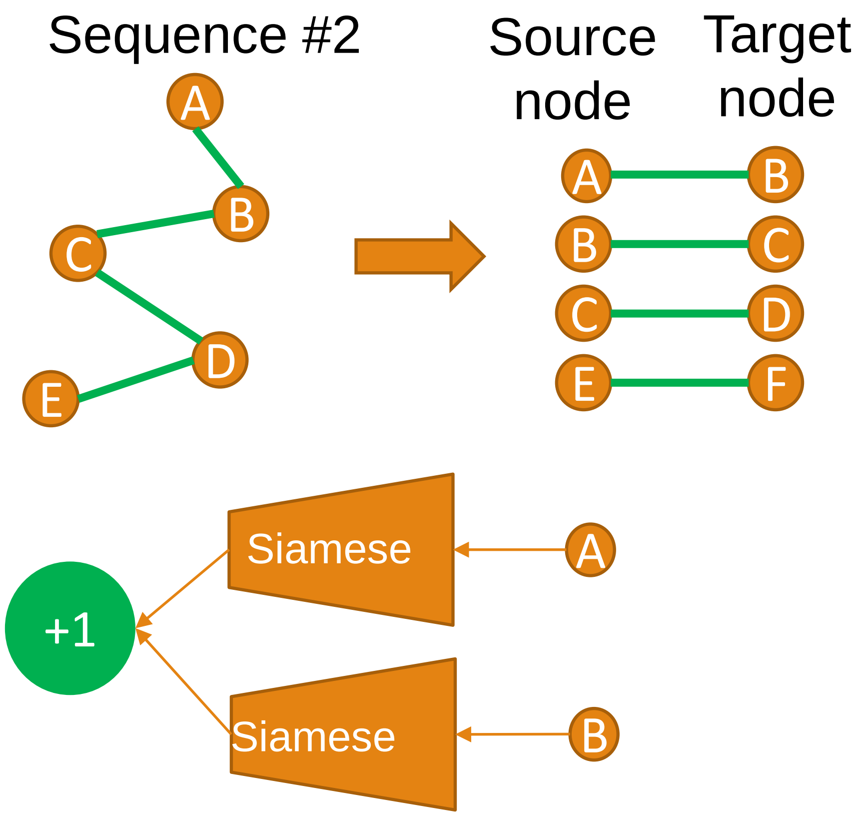
1. Perform random walks on the graph to generate node sequences
2. Run skip-gram to learn node embeddings



DeepWalk

Algorithm

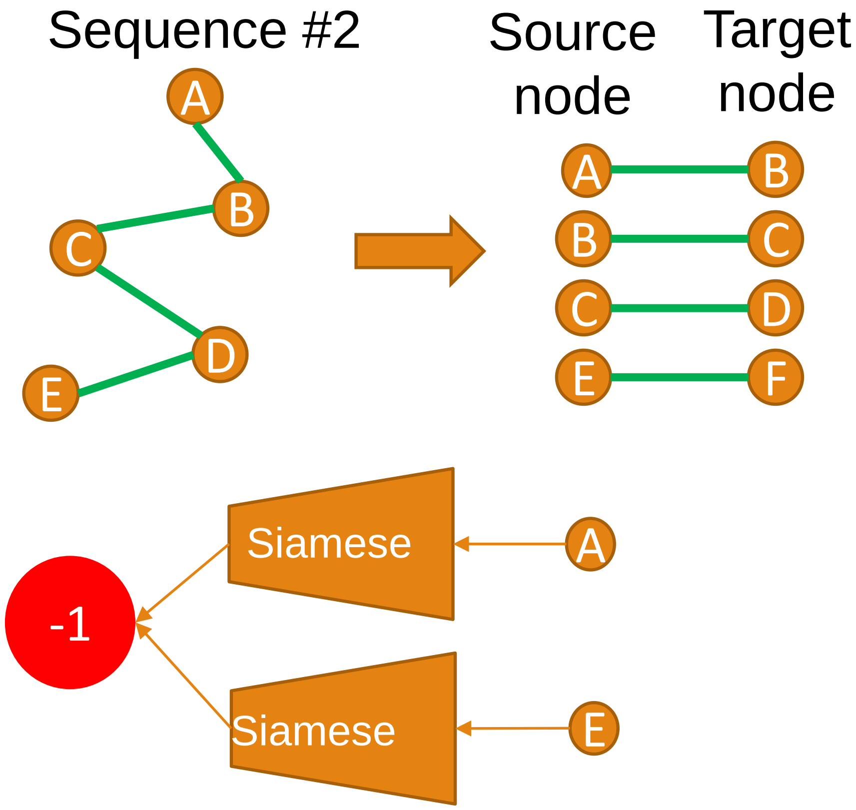
1. Perform random walks on the graph to generate node sequences
2. Run skip-gram to learn node embeddings



DeepWalk

Algorithm

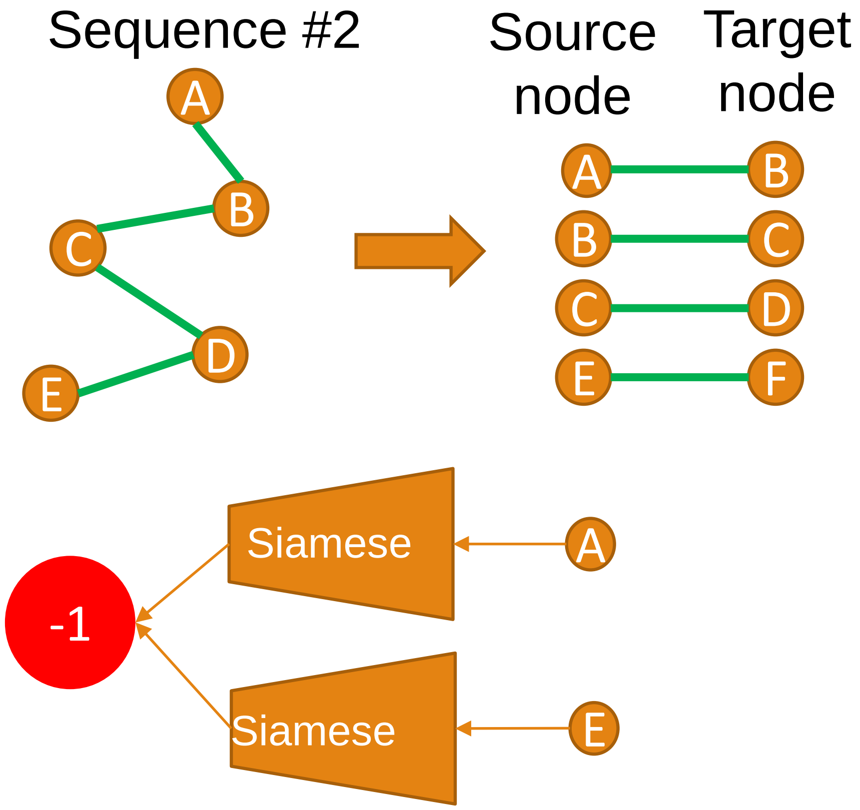
1. Perform random walks on the graph to generate node sequences
2. Run skip-gram to learn node embeddings



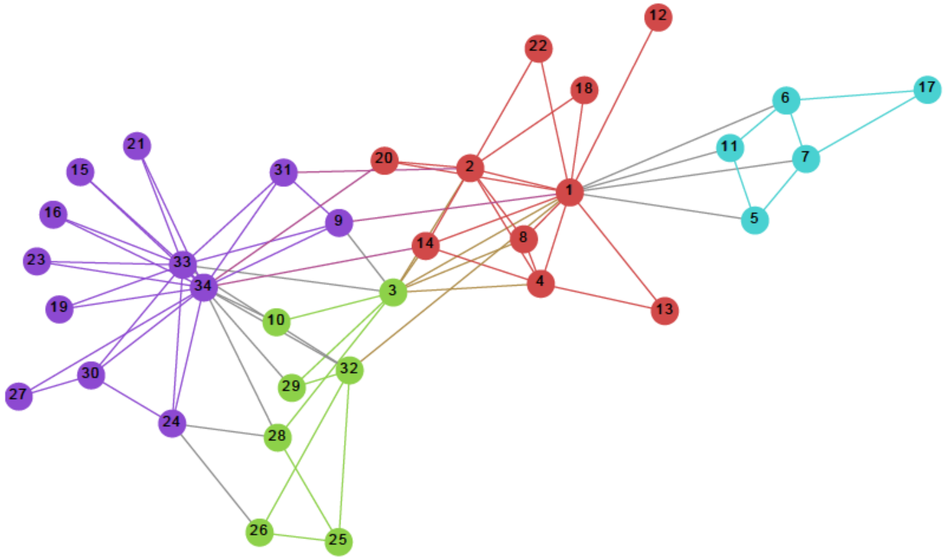
DeepWalk

Algorithm

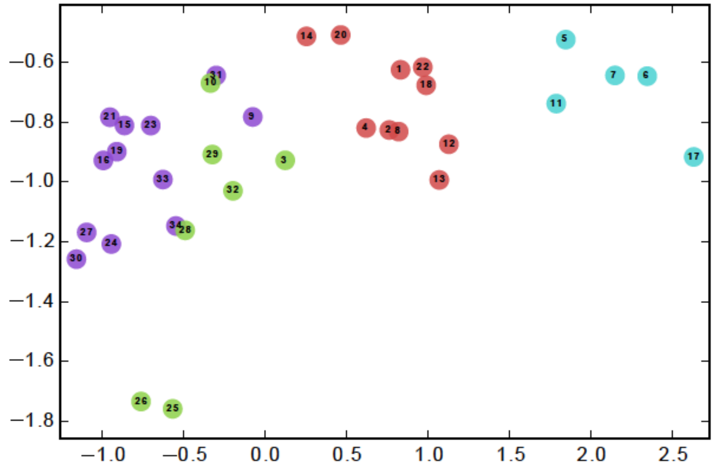
1. Perform random walks on the graph to generate node sequences
2. Run skip-gram to learn node embeddings



DeepWalk: Results



(a) Input: Karate Graph



(b) Output: Representation

DeepWalk: A problem

- The method is transductive
- Whenever a new node is added to the graph, the model must be retrained
- This is not useful for dynamic graphs

GraphSage

Algorithm 1: GraphSAGE embedding generation (i.e., forward propagation) algorithm

Input : Graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$; input features $\{\mathbf{x}_v, \forall v \in \mathcal{V}\}$; depth K; weight matrices $\mathbf{W}^k, \forall k \in \{1, ..., K\}$; non-linearity σ; differentiable aggregator functions $\text{AGGREGATE}_k, \forall k \in \{1, ..., K\}$; neighborhood function $\mathcal{N} : v \rightarrow 2^{\mathcal{V}}$

Output : Vector representations $\mathbf{z}_v$ for all $v \in \mathcal{V}$

$\mathbf{h}_v^0 \leftarrow \mathbf{x}_v, \forall v \in \mathcal{V}$;
for $k = 1 ... K$ **do**
    for $v \in \mathcal{V}$ **do**
        $\mathbf{h}_{\mathcal{N}(v)}^k \leftarrow \text{AGGREGATE}_k(\{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\})$;
        $\mathbf{h}_v^k \leftarrow \sigma\left(\mathbf{W}^k \cdot \text{CONCAT}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}(v)}^k)\right)$
    end
    $\mathbf{h}_v^k \leftarrow \mathbf{h}_v^k / \|\mathbf{h}_v^k\|_2, \forall v \in \mathcal{V}$
end
$\mathbf{z}_v \leftarrow \mathbf{h}_v^K, \forall v \in \mathcal{V}$

GraphSage: How to aggregate?

- Mean aggregation $\mathbf{h}_v^k \leftarrow \sigma(\mathbf{W} \cdot \text{MEAN}(\{\mathbf{h}_v^{k-1}\} \cup \{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\})$

- LSTM aggregation

- Pooling aggregation $\text{AGGREGATE}_k^{\text{pool}} = \max(\{\sigma\left(\mathbf{W}_{\text{pool}}\mathbf{h}_{u_i}^k + \mathbf{b}\right), \forall u_i \in \mathcal{N}(v)\})$

- Loss $J_{\mathcal{G}}(\mathbf{z}_u) = -\log\left(\sigma(\mathbf{z}_u^\top \mathbf{z}_v)\right) - Q \cdot \mathbb{E}_{v_n \sim P_n(v)} \log\left(\sigma(-\mathbf{z}_u^\top \mathbf{z}_{v_n})\right)$

Graph Convolutional Networks

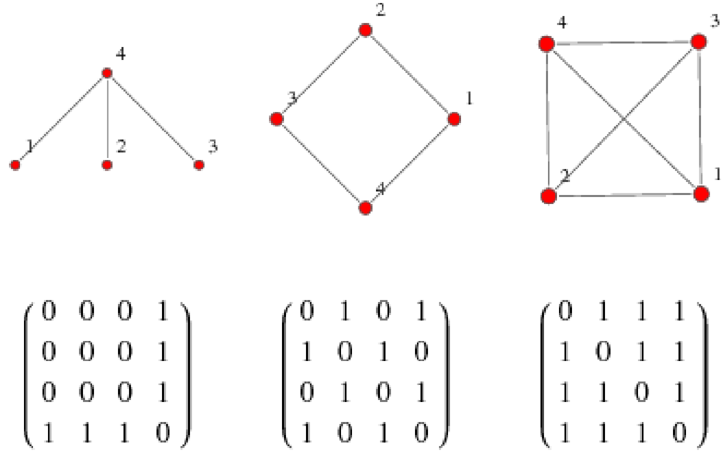
- Assuming a graph $G = (\mathcal{V}, \mathcal{E})$

- A node has a description x_i, all stored in a $N \times D$ matrix $X = [\dots, x_i, \dots]$

- The graph structure is encoded by the adjacency matrix A

- A neural network on this graph then is

$$H^{(l+1)} = h(H^{(l)}, A)$$



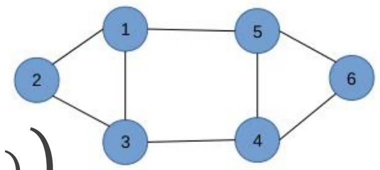
Graph Convolutional Networks: A simple example

- $h(H^{(l)}, A) = \sigma(AH^{(l)}W^{(l)})$
- Two problems
  - Given a node, the adjacency matrix A considers neighboring nodes but not the node itself → Aggregation does not use the node itself
  - A node might have different numbers of neighbors and change the scale of the multiplication
- Add the identity matrix to A
- Left multiply by $D^{-1}A$: D is the degree matrix
- Combining all, we have the following module

$$h(H^{(l)}, A) = \sigma\left(D^{-\frac{1}{2}}\hat{A}D^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$
$$\hat{A} = A + I$$

Degree matrix

$$D_{ij} = \begin{cases} d(i) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$



$$D = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

Summary

- Sequential data
- Recurrent Neural Networks
- Backpropagation through time
- Exploding and vanishing gradients
- LSTMs and variants
- Encoder-Decoder Architectures
- Graph Neural Networks