CSE440: Natural Language Processing II

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Lecture 6: Neural Nets and RNN

Outline

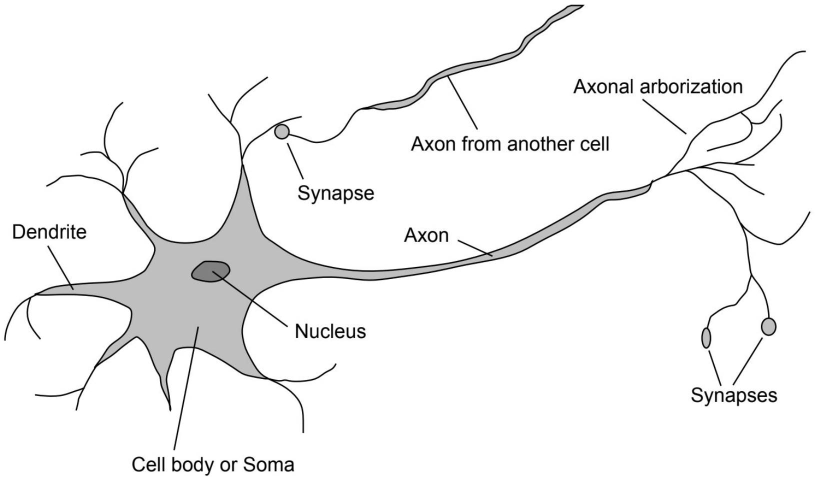
- Neural Networks (SLP 7 and lecture)
- Recurrent neural networks (SLP 9 and lecture)

Before starting learning sequence ….

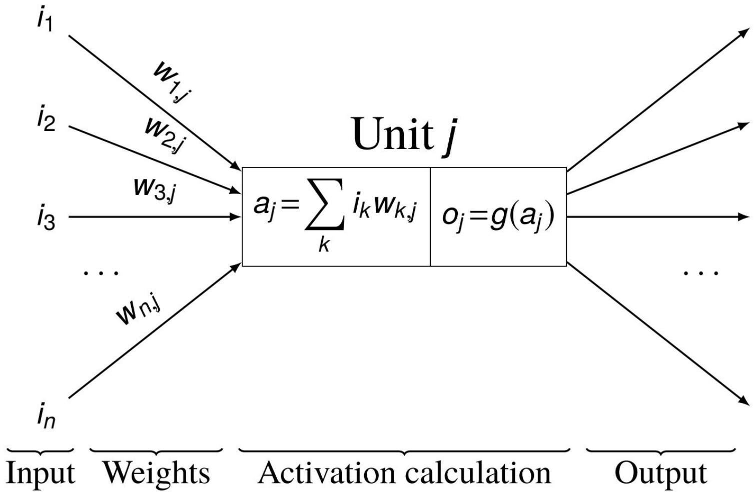
We need to remember some neural network basics.

Neural Networks

Neuron in a human brain

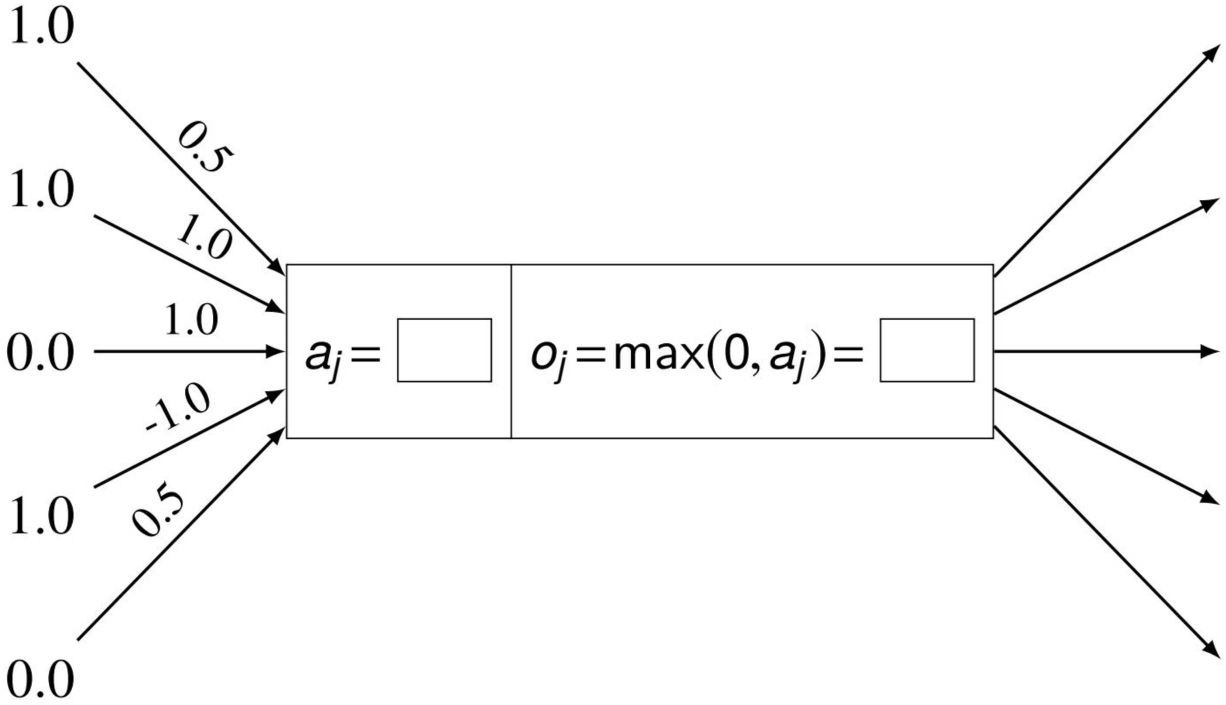


Neuron in an ML model



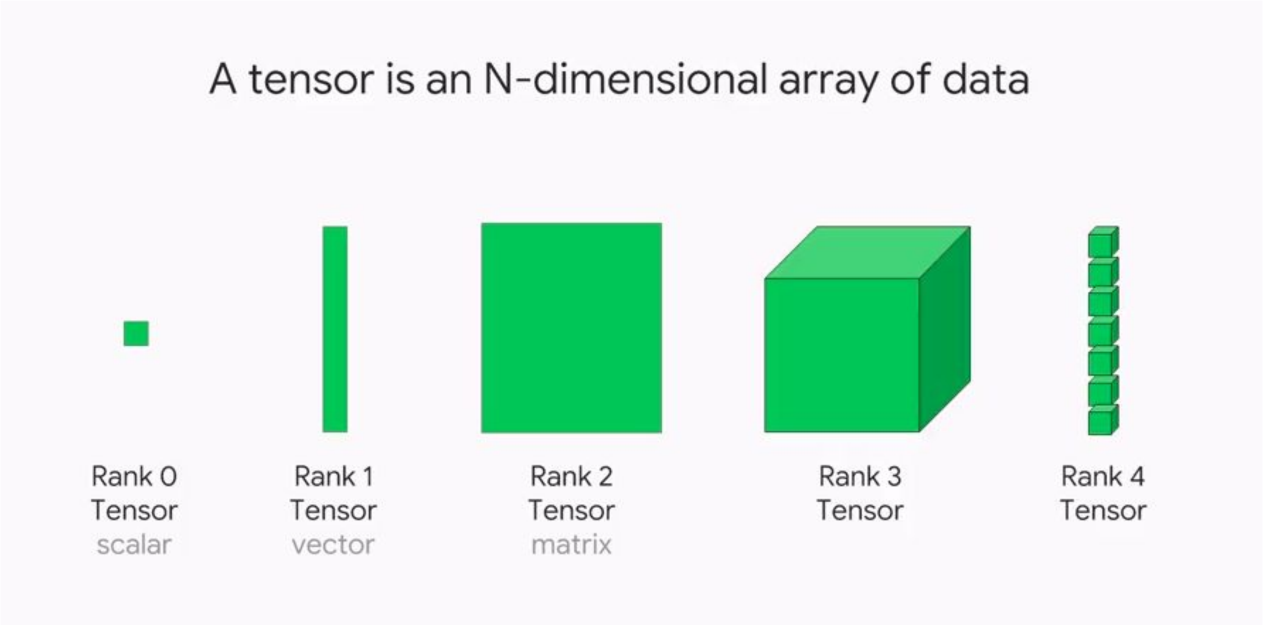
Class work

Calculate the output of this unit:



Unit calculations as tensor arithmetic

What is a tensor?



Unit calculations as tensor arithmetic

Summation for a single unit:

$$o_j = g\left(\sum_k i_k w_{k,j}\right)$$

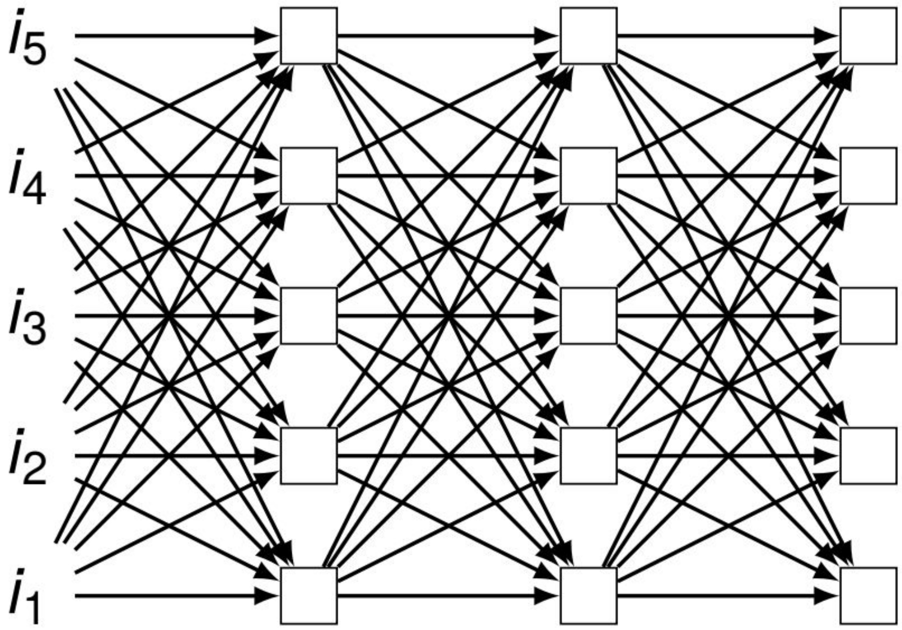
Vector arithmetic for a single unit:

$$o_j = g\left(\begin{bmatrix} i_1 & i_2 & \ldots & i_n \end{bmatrix} \begin{bmatrix} w_{1,j} \\ w_{2,j} \\ \ldots \\ w_{n,j} \end{bmatrix}\right) = g\left(\boldsymbol{i} \times \boldsymbol{w}_{*,j}\right)$$

Matrix arithmetic for multiple units:

$$\boldsymbol{o} = g\left(\boldsymbol{i} \times \boldsymbol{W}\right)$$

A feedforward network as composition



$$\boldsymbol{o} = g\left(g\left(g\left(\boldsymbol{i} \times \boldsymbol{W}^1\right) \times \boldsymbol{W}^2\right) \times \boldsymbol{W}^3\right)$$

Activation functions

- Why do we need activation functions?
- What types of activation functions do we have?

Learning the XOR

$$\boldsymbol{X} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \qquad \boldsymbol{y} = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$

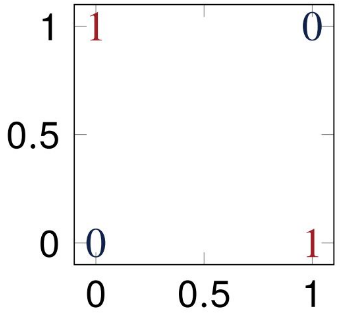
Can you solve it with linear regression?

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{W} + \boldsymbol{b}$$

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \boldsymbol{W} + \boldsymbol{b}$$

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} ? \\ ? \end{bmatrix} + ?$$

No such weights exist!



Solving XOR with NNs

$$f(\boldsymbol{X}; \boldsymbol{W}, \boldsymbol{c}, \boldsymbol{w}, b) = \max\left(0, \boldsymbol{X}\boldsymbol{W} + \boldsymbol{c}\right)\boldsymbol{w} + b$$

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} = \max\left(0, \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \boldsymbol{W} + \boldsymbol{c}\right)\boldsymbol{w} + b$$

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} = \max\left(0, \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix} + \begin{bmatrix} ? & ? \end{bmatrix}\right)\begin{bmatrix} ? \\ ? \end{bmatrix} + ?$$

Solving XOR with NNs

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} = \max\left(0, \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 & -1 \end{bmatrix}\right) \begin{bmatrix} 1 \\ -2 \end{bmatrix} + 0$$

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -2 \end{bmatrix} + 0$$

Common activation functions in hidden units

We have: affine transformation of input x, followed by nonlinear activation function

$$\boldsymbol{h} = g(\boldsymbol{W}^\top \boldsymbol{x} + \boldsymbol{b})$$

g could be just about anything! It can be linear, but a linear function is not preferred. Why?

Considerations:

- What specific behavior is needed?
- How will the gradients behave?

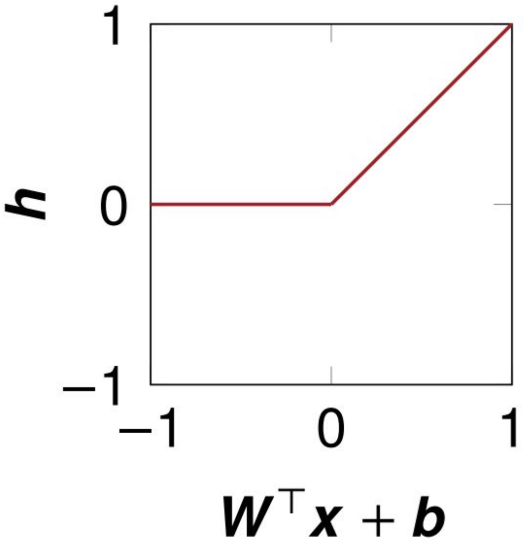
Why linear functions are not preferred?

Because of the considerations.

- We need complex mappings between the inputs and the outputs
- All linear layers will translate the input linearly to output– that is, multiple linear transformation is basically one giant linear transformation
- Cannot use backpropagation as the derivative is constant

ReLU

$$\boldsymbol{h} = \max(0, \boldsymbol{W}^\top \boldsymbol{x} + \boldsymbol{b})$$



Behavior?

- Active only when input is positive

Gradients?

- 1 when positive
- 0 when negative

ReLU is non-differentiable

ReLU at $z = 0$:

- left derivative = 0
- right derivative = 1

So ReLU is not differentiable at $z = 0$!

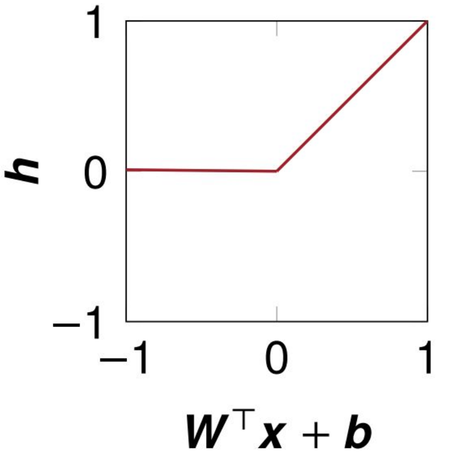
A few non-differentiable points are not a problem:

- Training rarely reaches a point with gradient 0 anyway
- Software simply returns either left or right derivative

Leaky ReLU

$$f(x) = max\ (0.1x, x)$$

$$\boldsymbol{h} = \max(0, \boldsymbol{W}^\top \boldsymbol{x} + \boldsymbol{b}) + 0.01 \min(0, \boldsymbol{W}^\top \boldsymbol{x} + \boldsymbol{b})$$



ReLU has a “dead neuron” problem!

Behavior?

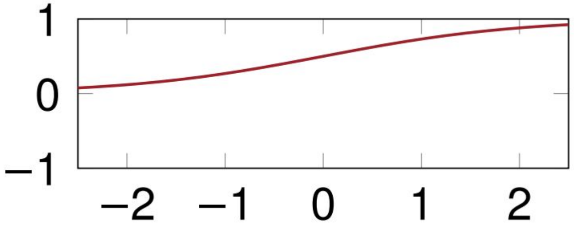
- Strong positive activation when positive
- Very weak negative activation when negative

Gradients?

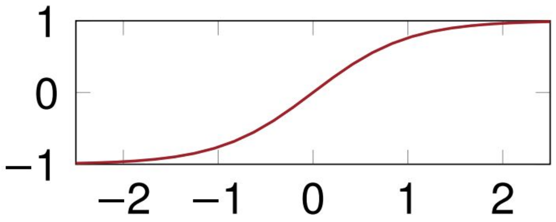
- 1 when positive
- 0.1 when negative

Sigmoid and tanh

Sigmoid: $f(x) = \frac{1}{1+e^{-x}}$



Tanh: $f(x) = \frac{(e^{x}-e^{-x})}{(e^{x}+e^{-x})}$



Behavior?

- Sigmoid: 0/1 switch
- Tanh: -1/+1 switch

Gradients?

- Saturate across most of their domain
- Tanh optimizes slightly better since it is similar to the identity function near 0

Hyperparameters

- Network parameters are the ones that are being learned throughout the training process (e.g. weights)
- There are parameters that we can control to facilitate this learning: they are called hyperparameters
- Activation function is one such hyperparameter
- We have others …

Optimizers

- Algorithms used to update the learnable parameters in order to reduce loss
- Common optimizers:
    - Gradient descent
    - Stochastic gradient descent
    - Mini-batch gradient descent
    - Momentum
    - Adagrad
    - RMSProp
    - AdaDelta
    - Adaptive moment estimation
- GD methods maintain a single learning rate (with/without decay for all parameters and are known as first order optimizers (works with the first order derivative)
- Adaptive methods like Adagrad provide learning rates for each parameter, thus improving the learnability, but are computationally expensive
- RMSProp not only provides LR for each parameter, it adapts based on the mean of recent magnitudes of the gradients for the weight → first order. AdaDelta is similar but works with squared gradients (second order)

Adaptive moment estimation

- Popularly known as Adam (not ADAM)
- Came out of OpenAI and University of Toronto
- Most likely the highest cited paper in recent history
- Why is it so popular?
    - Straightforward to implement
    - Little memory requirements
    - Well suited for problems that are large in terms of data and/or parameters
    - Needs little to no manual tuning

Adam

- Adam works with momentums of first and **second** order
- Instead of adapting the parameter learning rates based on the average first moment (the mean), m_t as in RMSProp, Adam also makes use of the average of the second moments of the gradients (the uncentered variance) v_t

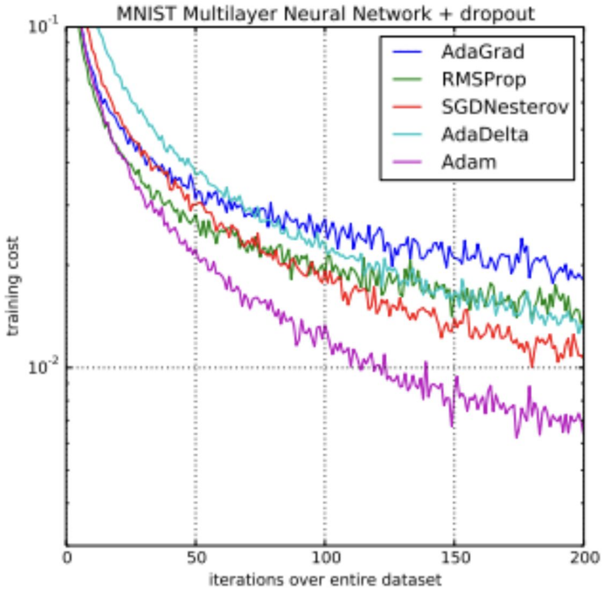
$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}.$$

$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}.$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t.$$

- The values for β1 is 0.9 , 0.999 for β2 and epsilon is an extremely small number to avoid zero division

Adam’s popularity



Sebastian Ruder: “... RMSprop, Adadelta, and Adam are very similar algorithms that do well in similar circumstances. ….. Adam might be the best overall choice.”
Andrej Karpathy: “In practice Adam is currently recommended as the default algorithm to use, and often works slightly better than RMSProp.”

Regularization

- A set of strategies used in Machine Learning to reduce the generalization error
- Why?
- Bias-variance tradeoff
- Bias: error from wrong assumptions in the learning algorithm
    - High bias can cause an algorithm to miss the relevant relations between features and target outputs → Observations don't matter
    - Underfitting
- Variance: error from sensitivity to small fluctuations in the training set
    - High variance may result in modeling the random noise in the training data → focusing too much on observations
    - Overfitting

Regularization

- A good model needs to balance bias and variance
- Regularization helps us do that

Regularization techniques

- Introduce regularization term to the loss function
  - Introduces a small amount of bias to counter variance → reduce overfitting
  - Loss function: negative log likelihood or binary cross entropy
  - Most common terms:
    - L2 regularizer: Ridge regression → adds the “squared magnitude” of the coefficient as the penalty term to the loss function
    - L1 regularizer: Lasso regression → adds the “absolute value of magnitude” of the coefficient as a penalty term to the loss function
    - Uses λ that controls the sensitivity of`the model to the input → less sensitive, less likely to overfit
    - L2 focuses on larger weights, so higher λ means L2 penalizes higher value weights more than lower ones → no feature essentially goes away
    - L1 has equal focus, so, higher λ → low weight features go away → feature selection

Regularization techniques

- Dropout: Drops out (ignore) a layer’s output with a probability *p*
    - Choice of p depends on the architecture
- Early stopping: Stops when performance gets saturated
    - Stops model from being overfit
    - Returns the best current model
- Data augmentation
    - Introduce new training data with variation
    - Injects noise

Other common hyperparameters

- Learning rate: how quickly a network updates its parameters
  - Low learning rate slows down the learning process but converges smoothly
  - Larger learning rate speeds up the learning but may not converge
  - Decaying learning rate is preferred
- Epochs: How many times the entire training dataset has passed through the model
- Batch size: (Mini) batch size refers to a subset of the training data. Weights are updated after each mini batch training
  - Small mini batch → too many updates
  - Large mini batch → too few updates, too many epochs to converge

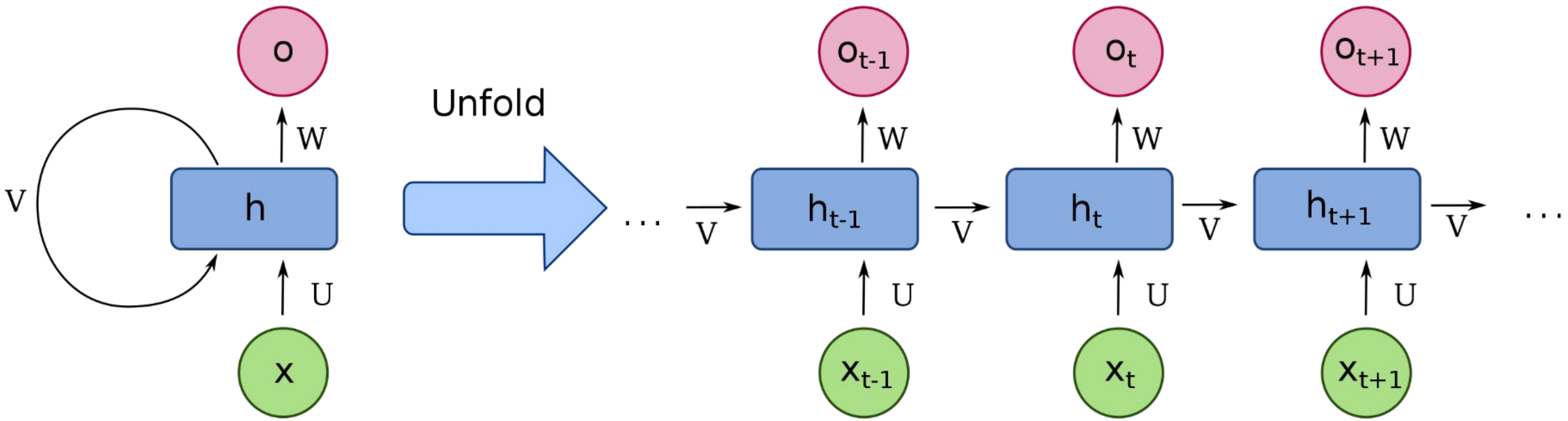
Recurrent Neural Networks (RNN)

- Simple recurrent networks
- Bidirectional and gated recurrent networks
- Recurrent architectures
- Seq2Seq models
- Attention

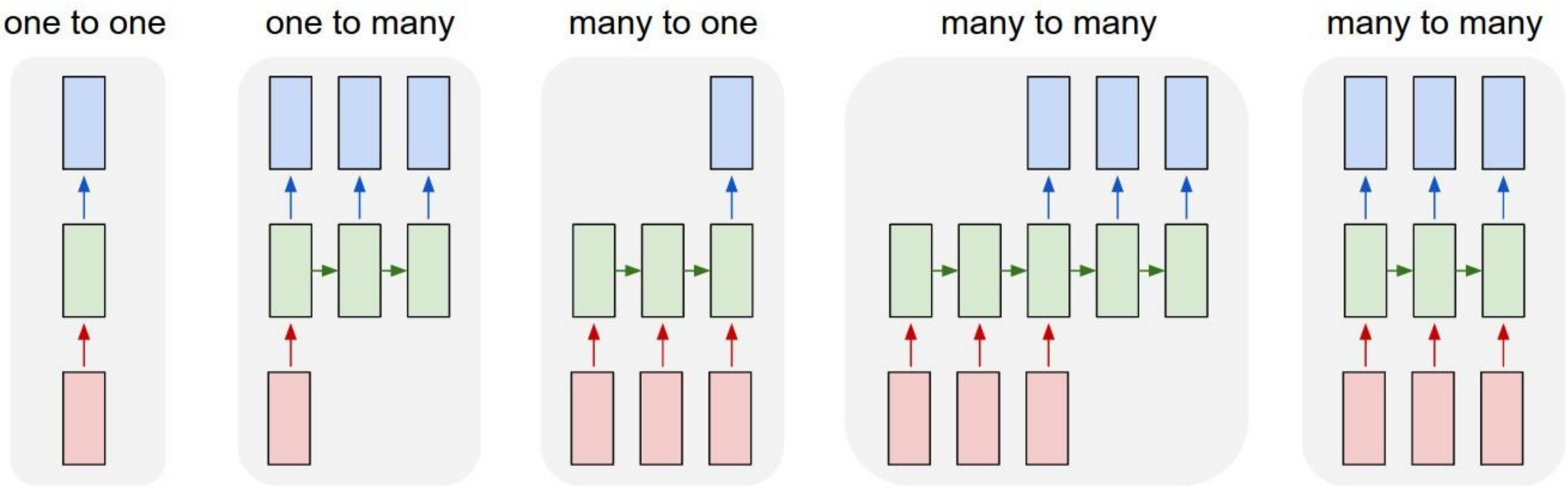
Short history of RNN

- 1986: RNNs are Introduced by David Rumelhart
- 1995: LSTMs are introduced by Sepp Hochreiter and Jürgen Schmidhuber based on Hochreiter's 1991 research on vanishing gradient problem
- 2001: Gers and Schmidhuber trained LSTMs to learn language models (unlearnable by HMMs)
- 2009: Graves et al. won ICDAR handwriting recognition competition using LSTMs
- 2013: Hinton and his team destroyed previous record for speech recognition using LSTM
- 2014: GRU is introduced by Cho et al.
- 2015: Widespread use in both academia and industry due to Google's adaptation of LSTM in their Google Voice speech recognition system

Structure of an RNN

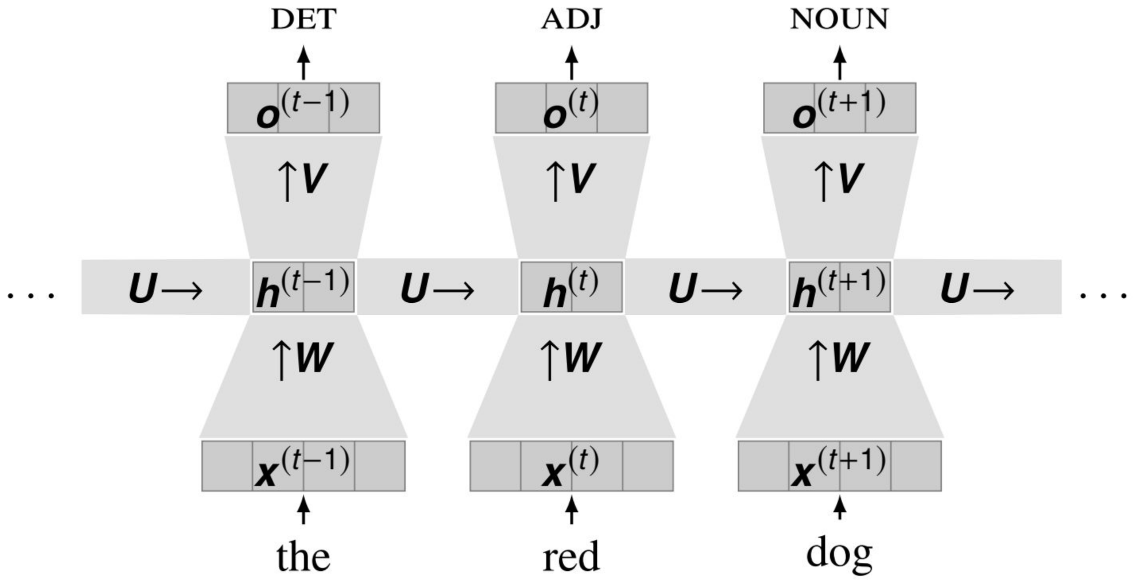


Types of RNNs



https://karpathy.github.io/2015/05/21/rnn-effectiveness/

A completely unrolled Simple RNN



$$\boldsymbol{o}^{(t)} = \text{softmax}(\boldsymbol{V}\boldsymbol{h}^{(t)})$$

$$\boldsymbol{h}^{(t)} = \tanh(\boldsymbol{U}\boldsymbol{h}^{(t-1)} + \boldsymbol{W}\boldsymbol{x}^{(t)})$$

Simple RNN

Intuitions:

- Each step combines the current input with the history
- Each prediction is made based on this combination

Observations:

- The input and hidden state change at each time step
- The parameters W, U, V are the same at each step

Equations:

$$\boldsymbol{h}^{(t)} = \tanh(\boldsymbol{U}\boldsymbol{h}^{(t-1)} + \boldsymbol{W}\boldsymbol{x}^{(t)})$$

$$\boldsymbol{o}^{(t)} = \mathrm{softmax}(\boldsymbol{V}\boldsymbol{h}^{(t)})$$

Classwork

Consider an RNN that predicts as:

$$\boldsymbol{o}^{(t)} = \mathrm{softmax}(\boldsymbol{V}\boldsymbol{h}^{(t)})$$

$$\boldsymbol{h}^{(t)} = \boldsymbol{U}\boldsymbol{h}^{(t-1)} + \boldsymbol{W}\boldsymbol{x}^{(t)}$$

whose parameters have been set to:

$$\boldsymbol{U} = \begin{bmatrix} 2 & 0 \\ 1 & 2 \end{bmatrix} \quad \boldsymbol{W} = \begin{bmatrix} 2 & 0 & -1 \\ 1 & -1 & 1 \end{bmatrix} \quad \boldsymbol{V} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 3 \end{bmatrix}$$

If you are given the following input:

$$h^{(0)} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad x^{(1)} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad x^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Which label will be predicted for each word if in the final softmax, index 0=ADJ, index 1=DET, and index 2=NOUN?

Drawbacks of simple RNN

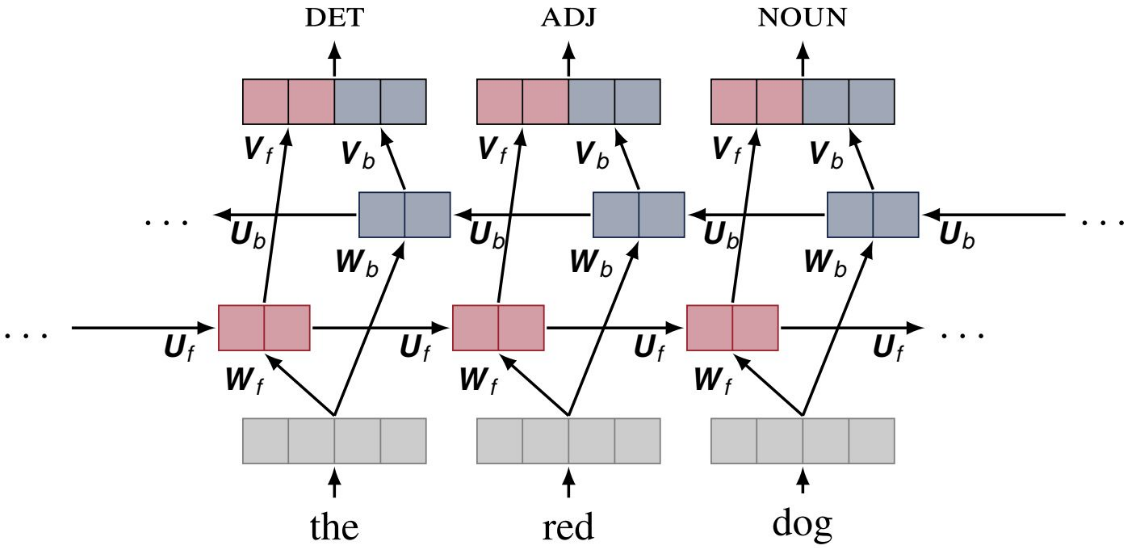
- They can only see the past, not the future
- They must forget the same amount of history at each time step
    - Theoretically, they don't have to
    - Maintaining long term memory is difficult

Bidirectional RNNs

Intuition:

- Run one forward RNN
- Run one backward RNN
- Combine their outputs

Bidirectional RNNs



$$o^{(t)} = \text{softmax}(V_f h_f^{(t)} + V_b h_b^{(t)})$$

$$h_b^{(t)} = \tanh(U_b h^{(t+1)} + W_b x^{(t)})$$

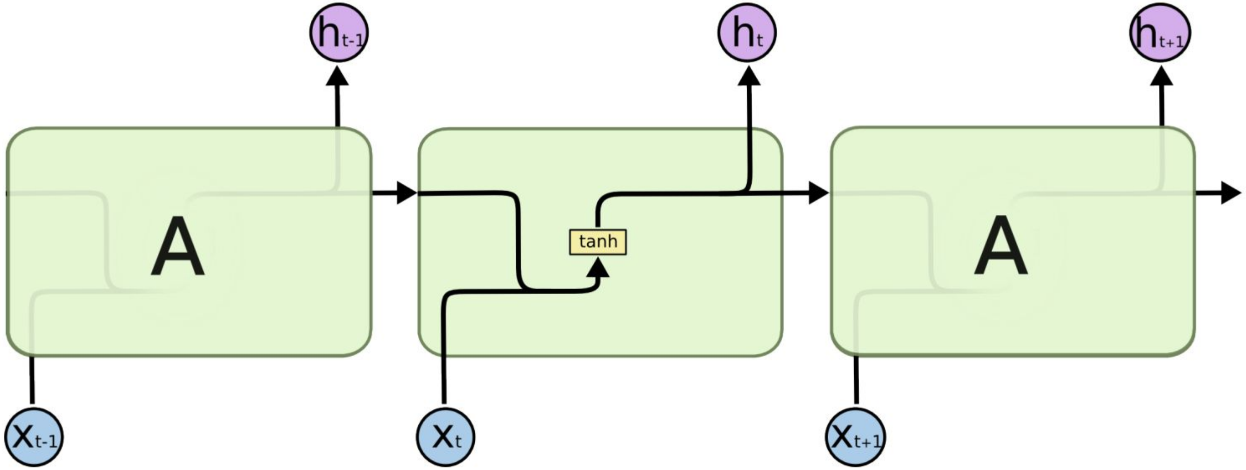
$$h_f^{(t)} = \tanh(U_f h^{(t-1)} + W_f x^{(t)})$$

Gated RNNs

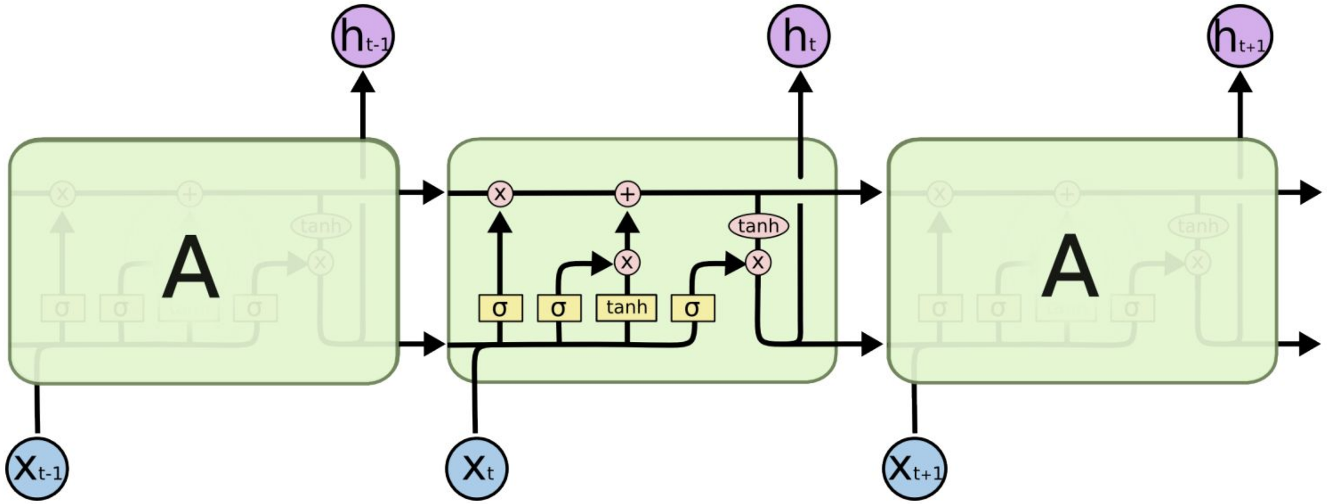
Intuition:

- Simple RNNs forget the same amount at each time step
- Look at the previous hidden state and the current input
- Decide how much to forget based on those
- Two gated RNNs
    - Long Short-Term Memory (LSTM)
    - Gated Recurrent Units (GRU)

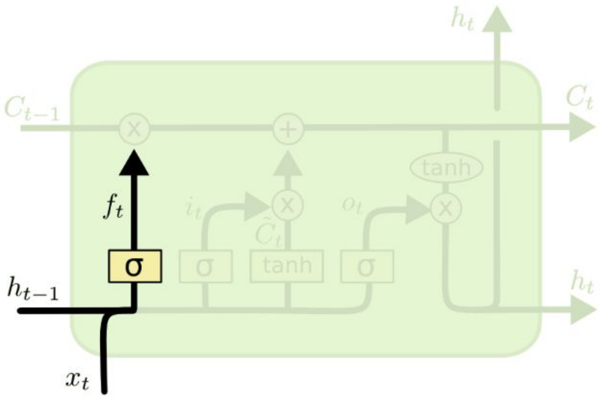
Simple RNN



LSTM

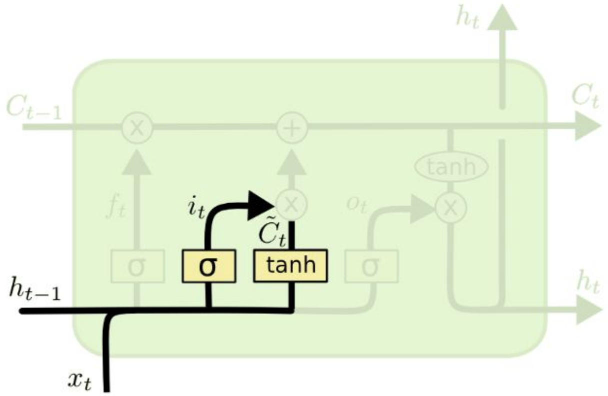


Forget gate



$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \;+\; b_f\right)$$

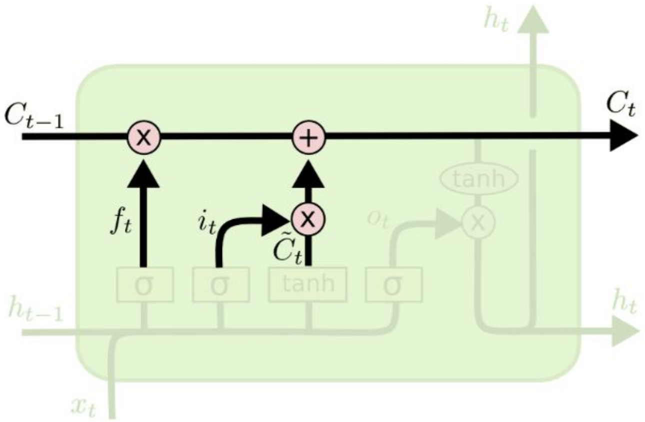
Input gate



$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \ + \ b_i\right)$$

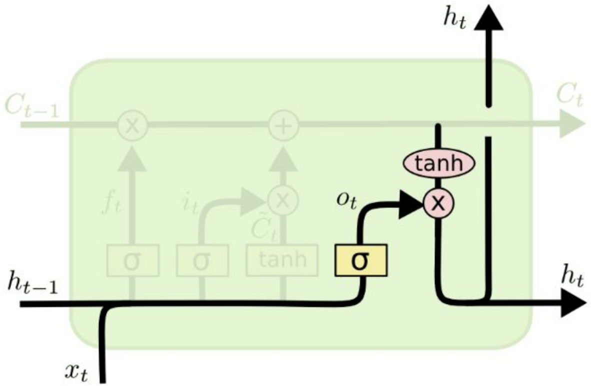
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \ + \ b_C)$$

Cell update



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

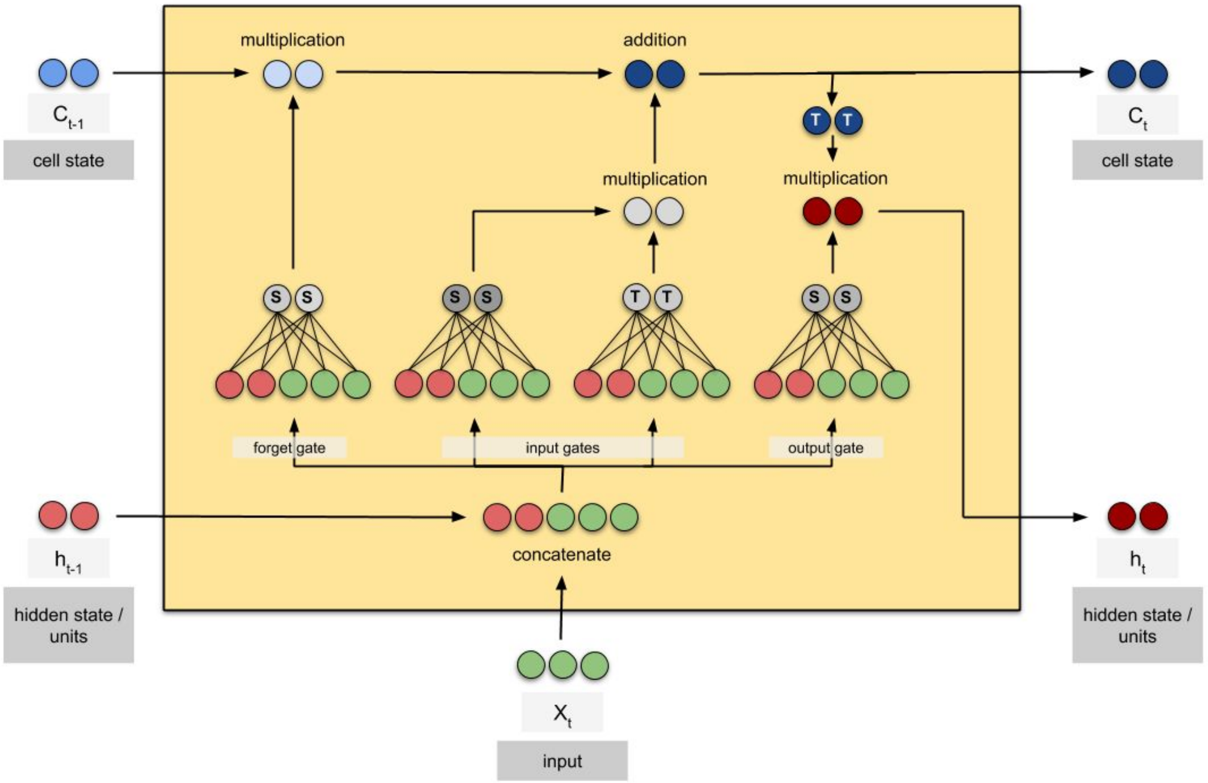
Output gate



$$o_t = \sigma\left(W_o\ [h_{t-1}, x_t]\ +\ b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

One LSTM cell



LSTM

Step 1: calculate forget, input, and output gates

$$\boldsymbol{f}^{(t)} = \sigma(\boldsymbol{b}_f + \boldsymbol{W}_f\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_f\boldsymbol{x}^{(t)})$$

$$\boldsymbol{i}^{(t)} = \sigma(\boldsymbol{b}_i + \boldsymbol{W}_i\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_i\boldsymbol{x}^{(t)})$$

$$\boldsymbol{o}^{(t)} = \sigma(\boldsymbol{b}_o + \boldsymbol{W}_o\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_o\boldsymbol{x}^{(t)})$$

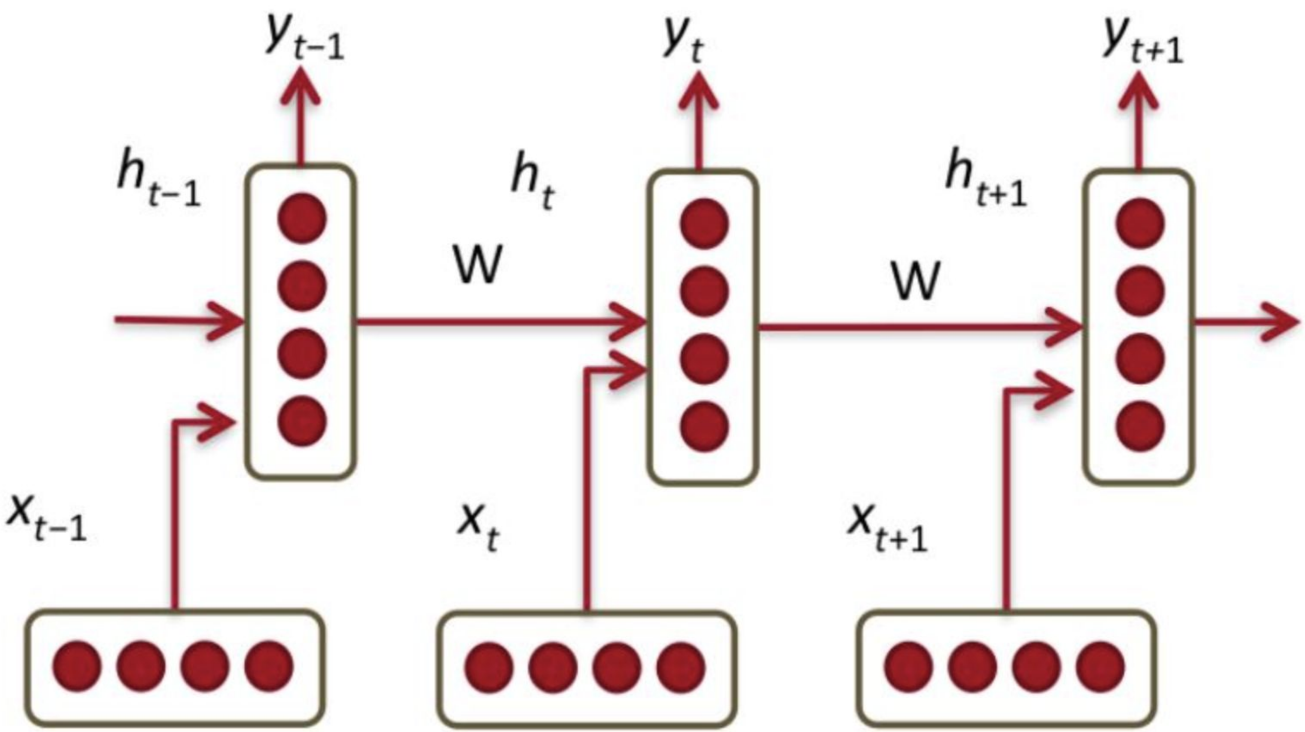
Step 2: update "cell": forget some old, add some new

$$\boldsymbol{c}^{(t)} = \boldsymbol{f}^{(t)} \odot \boldsymbol{c}^{(t-1)} + \boldsymbol{i}^{(t)} \odot \tanh(\boldsymbol{b}_c + \boldsymbol{W}_c\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_c\boldsymbol{x}^{(t)})$$

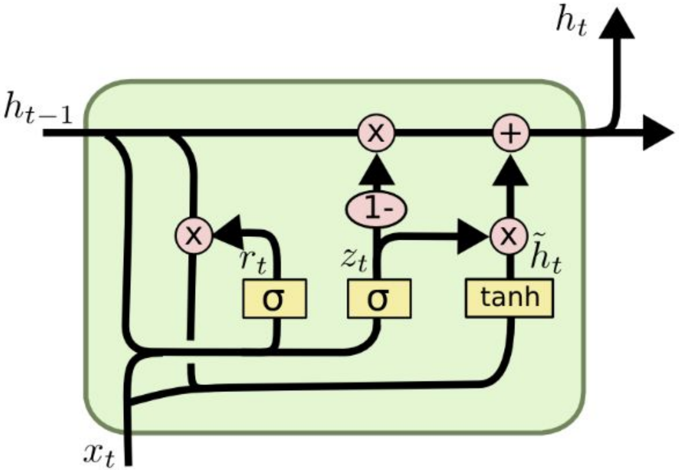
Step 3: update hidden state: output some of the cell

$$\boldsymbol{h}^{(t)} = \boldsymbol{o}^{(t)} \odot \tanh(\boldsymbol{c}^{(t)})$$

LSTM Network



GRU



$$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$$

$$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$$

$$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$$

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

GRU

Step 1: calculate update and reset gates

$$\boldsymbol{u}^{(t)} = \sigma(\boldsymbol{b}_u + \boldsymbol{W}_u\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_u\boldsymbol{x}^{(t)})$$

$$\boldsymbol{r}^{(t)} = \sigma(\boldsymbol{b}_r + \boldsymbol{W}_r\boldsymbol{h}^{(t-1)} + \boldsymbol{U}_r\boldsymbol{x}^{(t)})$$

Step 2: update hidden: forget some old, add some new

$$\begin{aligned}\boldsymbol{h}^{(t)} = {} & (1 - \boldsymbol{u}^{(t)}) \odot \boldsymbol{h}^{(t-1)} \\ & + \boldsymbol{u}^{(t)} \odot \tanh(\boldsymbol{b}_h + \boldsymbol{W}_h(\boldsymbol{r}^{(t)} \odot \boldsymbol{h}^{(t-1)}) + \boldsymbol{U}_h\boldsymbol{x}^{(t)})\end{aligned}$$

GRUs generally perform as well or better than LSTMs, with fewer parameters

Gated RNNs

Properties:

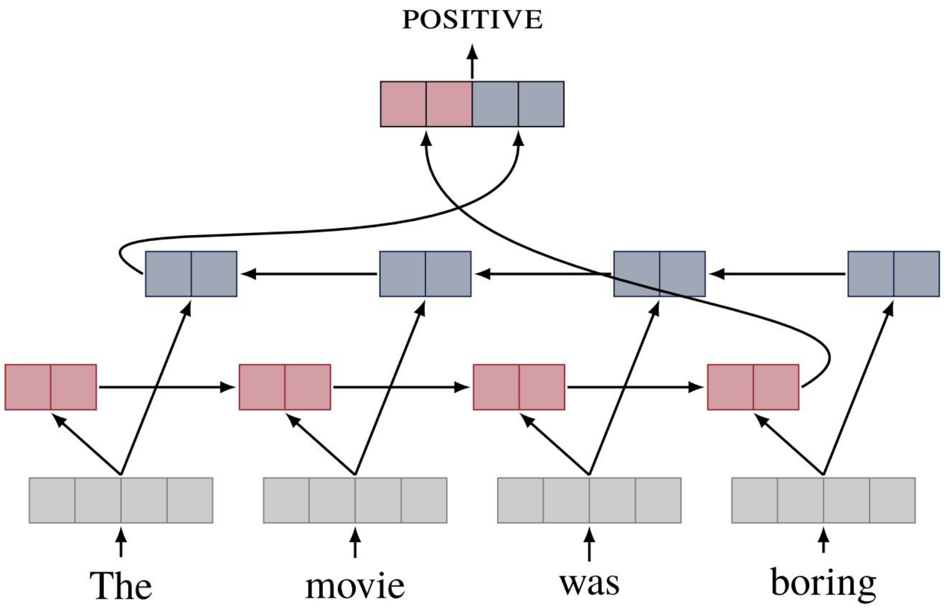
- Can forget different amounts at each time step
- Much better at using long distance information

A bidirectional GRU is a good starting point for many sequence tagging tasks

Recurrent architectures for related tasks

RNNs for text classification

- Last hidden state of the RNN represents the entire sentence.



Recurrent architectures for related tasks

What other tasks can RNNs handle?

Next to come

- Seq2seq models
  - Encoders and decoders
- Attention
- Autoregressive models
- Transformers
- A whole lotta variations
  - Transformer-encoders vs. transformer-decoders