

RNNs and Transformers



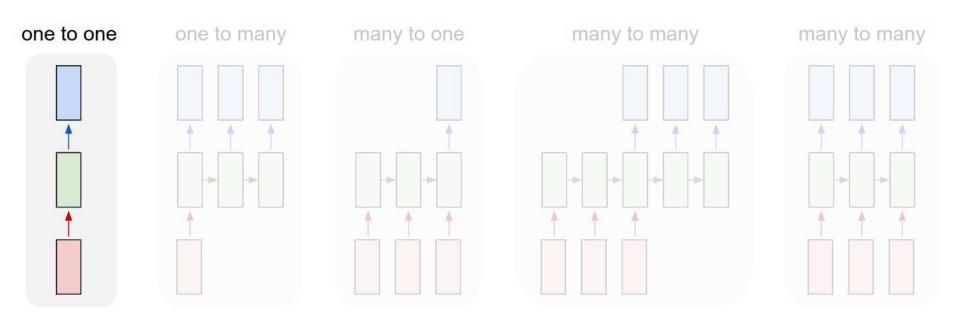
Recurrent Neural Networks

12DL: Prof. Da

Processing Sequences

Recurrent neural networks process sequence data

Input/output can be sequences



Classical neural networks for image classification

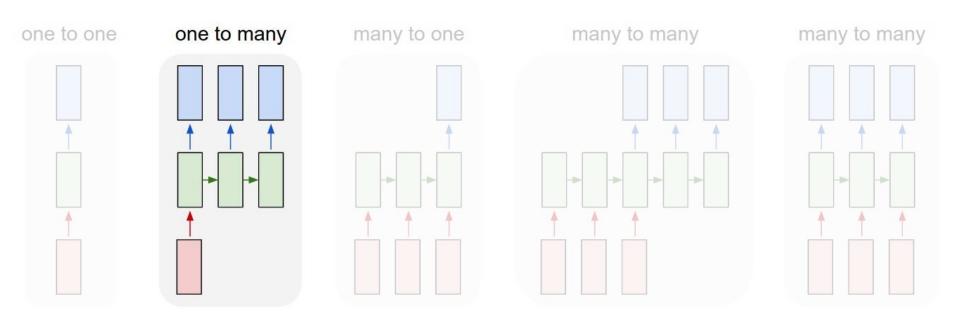
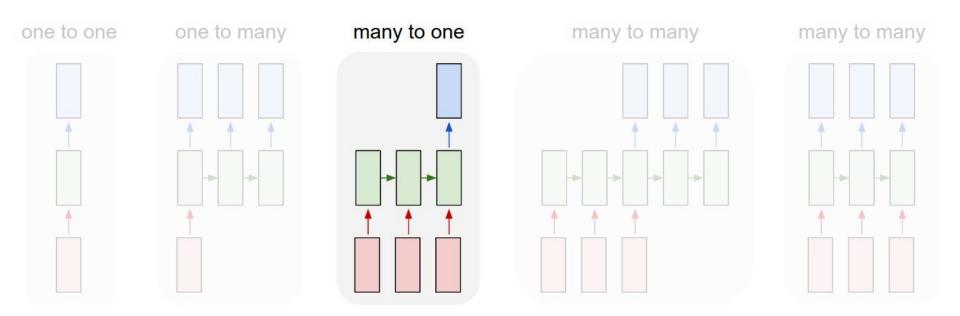
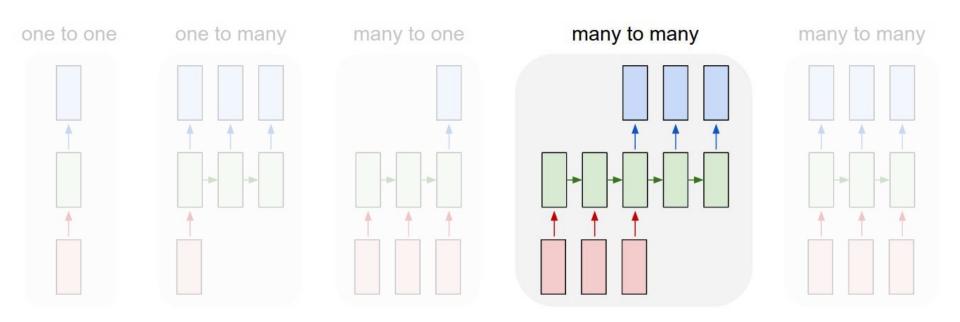


Image captioning

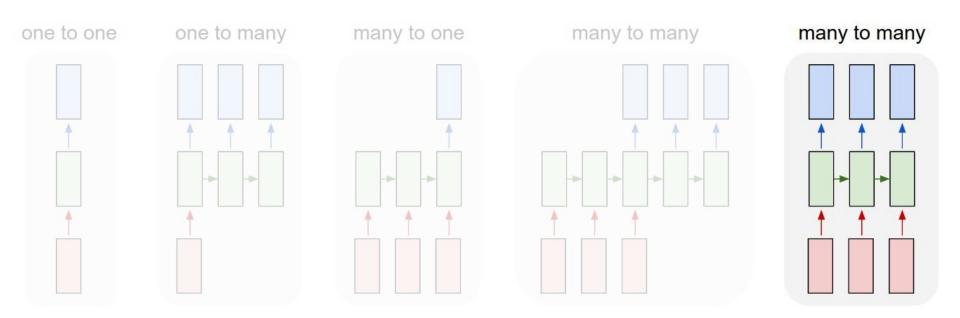


Language recognition



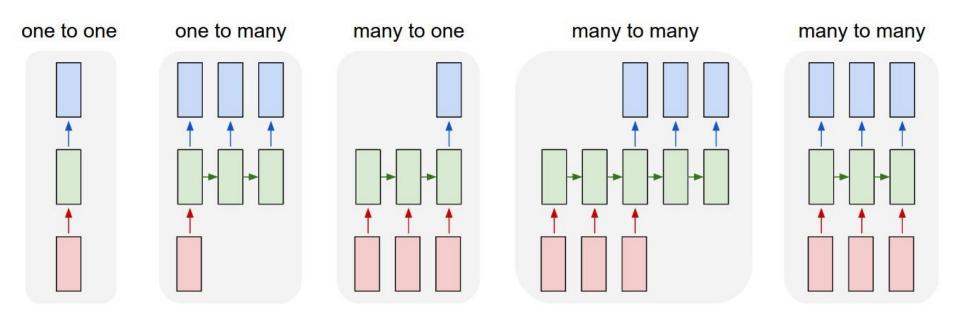
Machine translation

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



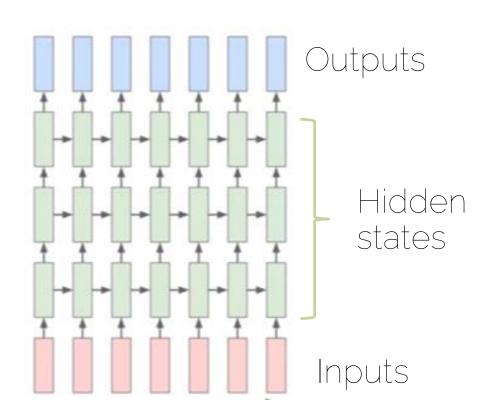
Event classification

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



Event classification

Multi-layer RNN

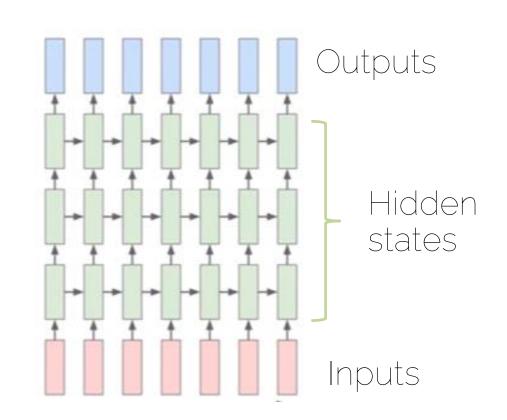


12DL: Prof. Dai

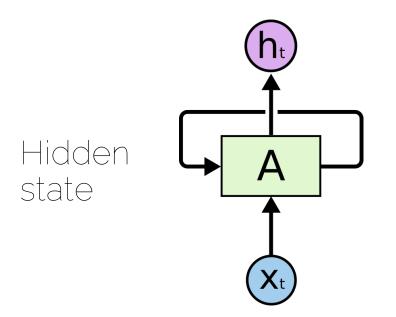
Multi-layer RNN

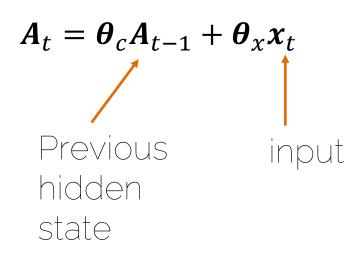
The hidden state will have its own internal dynamics

More expressive model!

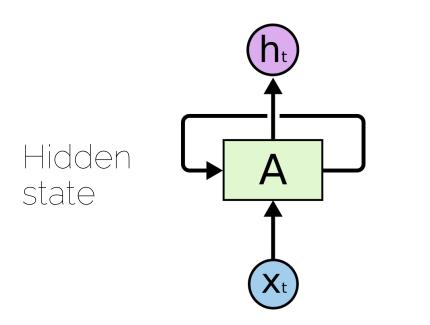


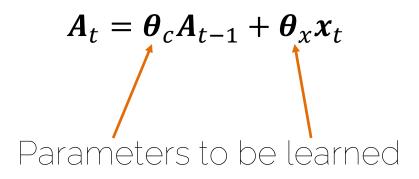
We want to have notion of "time" or "sequence"





We want to have notion of "time" or "sequence"

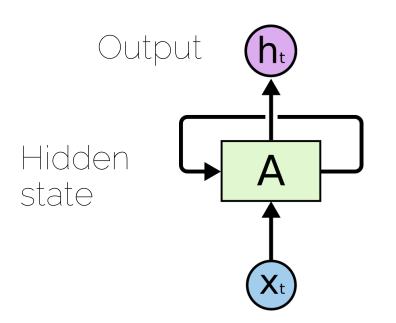




[Olah, https://colah.github.io '15] Understanding LSTMs

12DL: Prof. Dai

We want to have notion of "time" or "sequence"

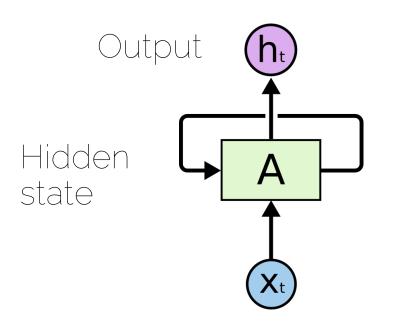


$$A_t = \boldsymbol{\theta}_c A_{t-1} + \boldsymbol{\theta}_{x} \boldsymbol{x}_t$$

$$h_t = \theta_h A_t$$

Note: non-linearities ignored for now

We want to have notion of "time" or "sequence"



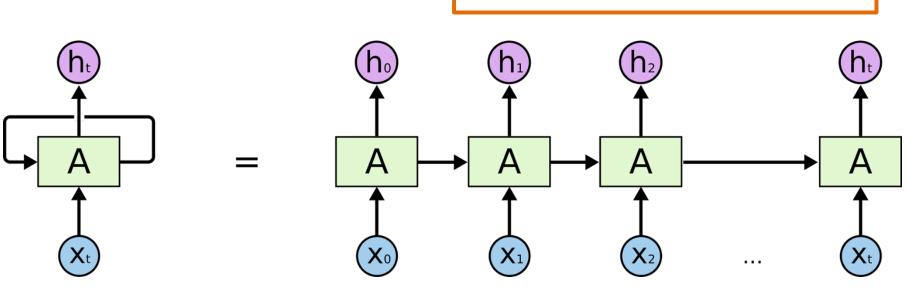
$$A_t = \theta_c A_{t-1} + \theta_x x_t$$

$$h_t = \theta_h A_t$$

Same parameters for each time step = generalization!

Unrolling RNNs

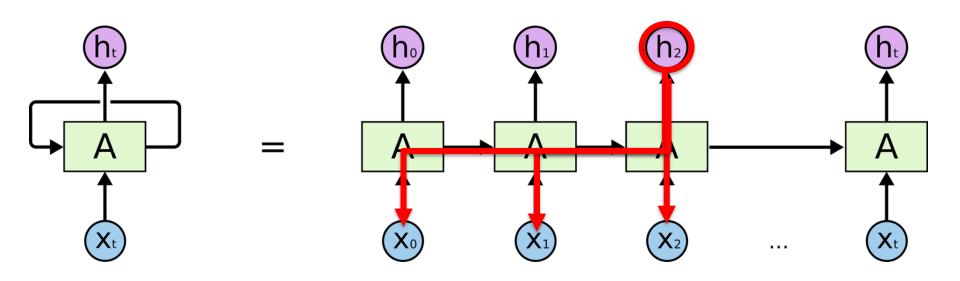
Same function for the hidden layers



[Olah, https://colah.github.io '15] Understanding LSTMs

12DL: Prof. Dai

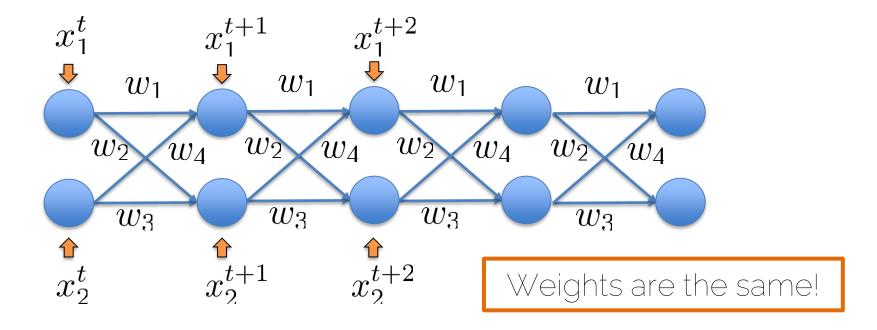
Unrolling RNNs



[Olah, https://colah.github.io '15] Understanding LSTMs

12DL: Prof. Dai

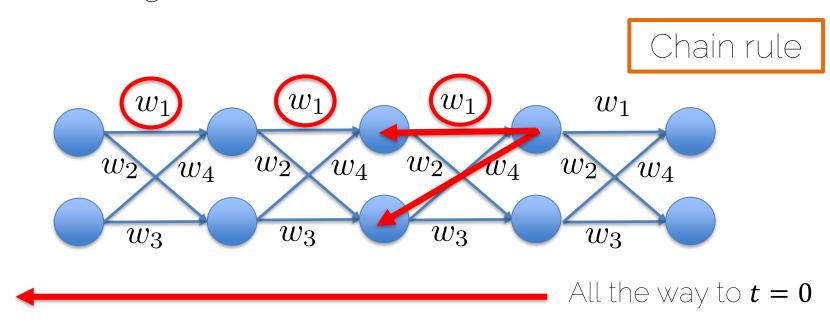
Unrolling RNNs as feedforward nets



18 Inches Prof. Dai

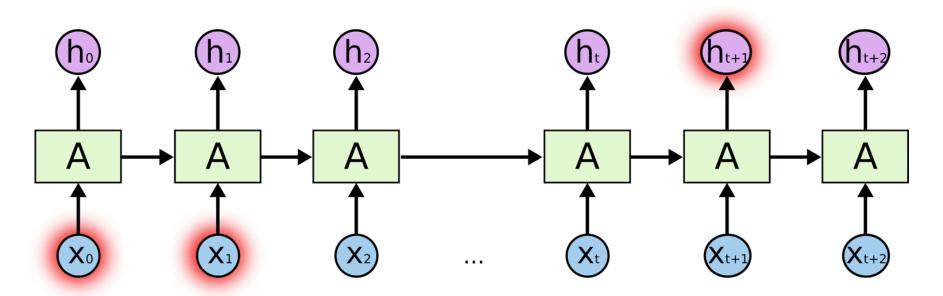
Backprop through an RNN

Unrolling RNNs as feedforward nets



Add the derivatives at different times for each weight

2DL: Prof. Dai



I moved to Germany ...

so I speak German fluently.

[Olah, https://colah.github.io '15] Understanding LSTMs

I2DL: Prof. Dai

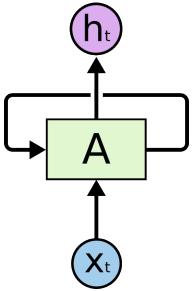
• Simple recurrence $A_t = \theta_c A_{t-1} + \theta_x x_t$

$$A_t = \boldsymbol{\theta}_c A_{t-1} + \boldsymbol{\theta}_{x} \boldsymbol{x}_t$$

• Let us forget the input $A_t = \theta_c^t A_0$

$$\mathbf{A}_t = \mathbf{\theta}_c^{\ t} \mathbf{A}_0$$

Same weights are multiplied over and over again



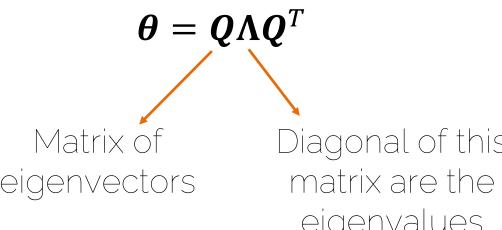
• Simple recurrence $A_t = \theta_c^{\ t} A_0$

What happens to small weights? Vanishing gradient

What happens to large weights? Exploding gradient

• Simple recurrence $A_t = \theta_c^t A_0$

• If $\boldsymbol{\theta}$ admits eigendecomposition

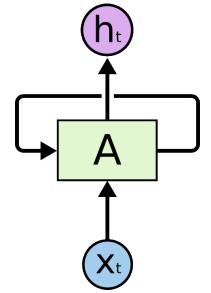


Diagonal of this eigenvectors eigenvalues

• Simple recurrence $A_t = \theta^t A_0$

• If θ admits eigendecomposition

$$\boldsymbol{\theta} = \boldsymbol{Q} \boldsymbol{\Lambda} \boldsymbol{Q}^T$$



• Orthogonal $\boldsymbol{\theta}$ allows us to simplify the recurrence

$$A_t = \mathbf{Q} \mathbf{\Lambda}^t \mathbf{Q}^T A_0$$

• Simple recurrence $A_t = Q \Lambda^t Q^T A_0$

What happens to eigenvalues with magnitude less than one?

Vanishing gradient

What happens to eigenvalues with magnitude larger than one?

Exploding gradient Gradient

Gradient clipping

12DL: Prof. Da

• Simple recurrence $A_t = \theta_c^t A_0$

$$t = \boldsymbol{\theta_c}^t \boldsymbol{A_0}$$

Let us just make a matrix with eigenvalues = 1

Allow the **cell** to maintain its "state"

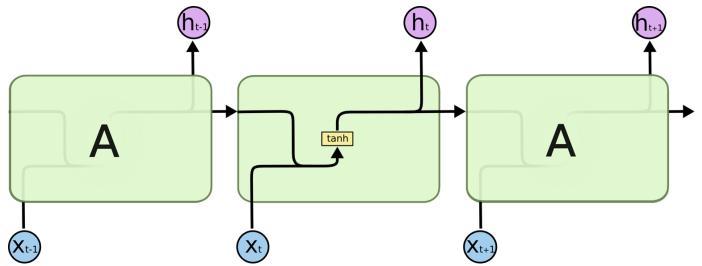
20 Li Prof. Dai

Vanishing Gradient

• 1. From the weights $A_t = \theta_c^{\ t} A_0$

$$A_t = \boldsymbol{\theta_c}^t A_0$$

• 2. From the activation functions (tanh)

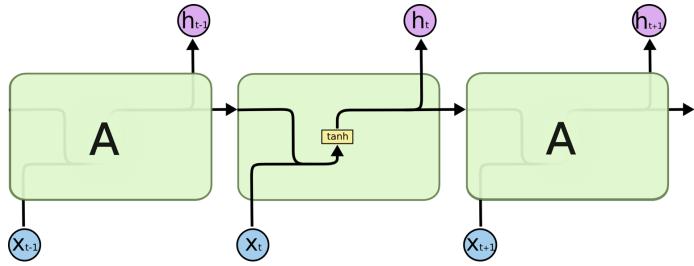


Vanishing Gradient

• 1. From the weights $A_t = \mathcal{D}^t A_0$

$$A_t = \mathbf{\beta}^t A_0$$

• 2. From the activation functions (tanh)



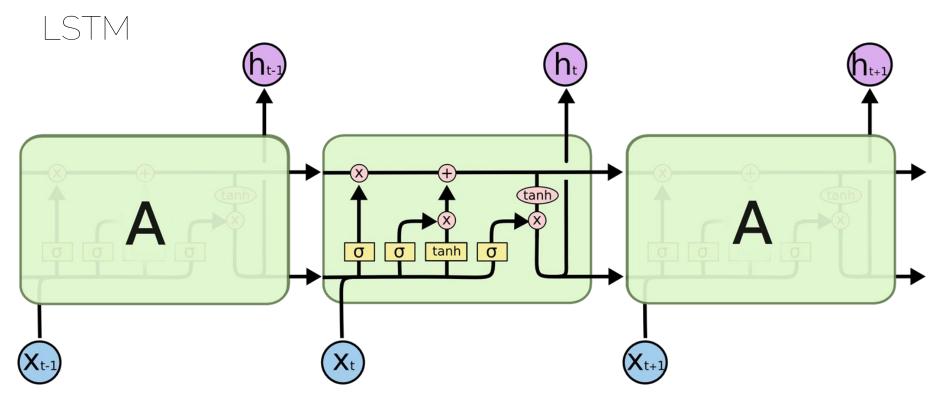


Long Short Term Memory

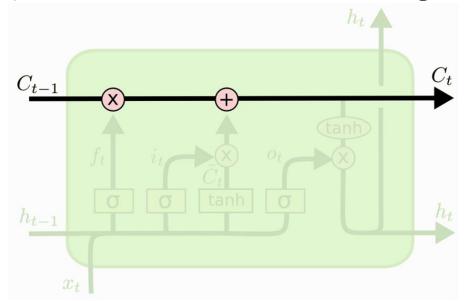
[Hochreiter et al., Neural Computation'97] Long Short-Term Memory

12DL: Prof. Dai

• Simple RNN has tanh as non-linearity tanh



- Key ingredients
- Cell = transports the information through the unit



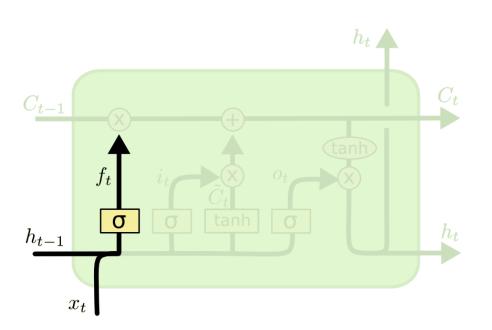
- Key ingredients
- Cell = transports the information through the unit
- Gate = remove or add information to the cell state



I2DL: Prof. Dai

LSTM: Step by Step

• Forget gate $f_t = sigm(\boldsymbol{\theta}_{xf} \boldsymbol{x}_t + \boldsymbol{\theta}_{hf} \boldsymbol{h}_{t-1} + \boldsymbol{b}_f)$

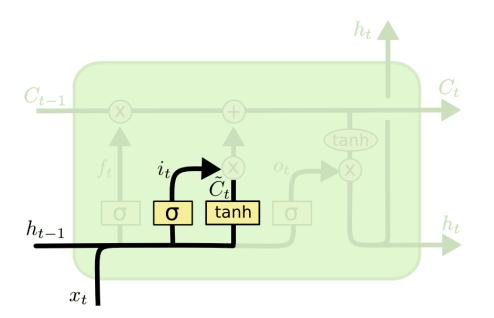


Decides when to erase the cell state

Sigmoid = output between **0** (forget) and **1** (keep)

LSTM: Step by Step

• Input gate $i_t = sigm(\theta_{xi}x_t + \theta_{hi}h_{t-1} + b_i)$

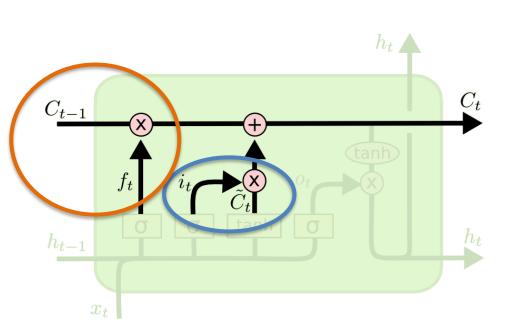


Decides which values will be updated

New cell state, output from a tanh (-1,1)

LSTM: Step by Step

• Element-wise operations





Previous states

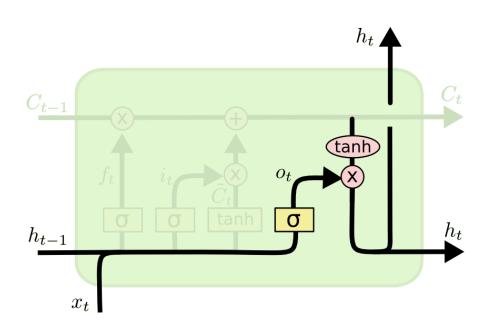
Current state

[Olah, https://colah.github.io '15] Understanding LSTMs

12DL: Prof. Dai

LSTM: Step by Step

• Output gate $h_t = o_t \odot \tanh(C_t)$



Decides which values will be outputted

Output from a tanh (-1,1)

[Olah, https://colah.github.io '15] Understanding LSTMs

LSTM: Step by Step

- Forget gate $f_t = sigm(\boldsymbol{\theta}_{xf} \boldsymbol{x}_t + \boldsymbol{\theta}_{hf} \boldsymbol{h}_{t-1} + \boldsymbol{b}_f)$
- Input gate $i_t = sigm(\theta_{xi}x_t + \theta_{hi}h_{t-1} + b_i)$
- Output gate $o_t = sigm(\theta_{xo}x_t + \theta_{ho}h_{t-1} + b_o)$
- Cell update $oldsymbol{g}_t = tanh(oldsymbol{ heta}_{xg}oldsymbol{x}_t + oldsymbol{ heta}_{hg}oldsymbol{h}_{t-1} + oldsymbol{b}_g)$
- Cell $C_t = f_t \odot C_{t-1} + i_t \odot g_t$
- Output $h_t = o_t \odot \tanh(C_t)$

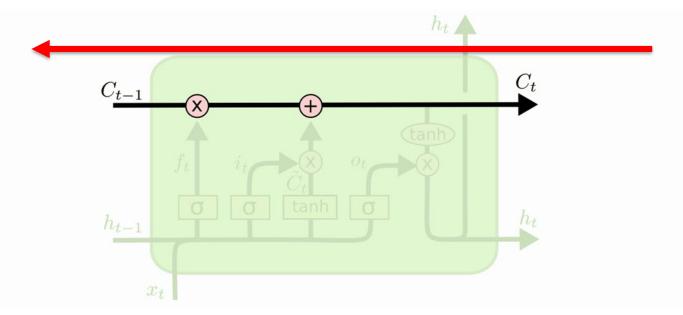
LSTM: Step by Step

- Forget gate $f_t = sigm(\boldsymbol{\theta}_{xf}\boldsymbol{x}_t + \boldsymbol{\theta}_{hf}\boldsymbol{h}_{t-1} + \boldsymbol{b}_f)$
- Input gate $i_t = sigm(\theta_{xi}x_t + \theta_{hi}h_{t-1} + b_i)$
- Output gate $o_t = sigm(\theta_{xo}x_t + \theta_{ho}h_{t-1} + b_o)$
- Cell update $g_t = tanh(\theta_{xg}x_1 + \theta_{hg}h_{t-1} + b_g)$
- Cell $oldsymbol{\mathcal{C}}_t = oldsymbol{f}_t \odot oldsymbol{\mathcal{C}}_{t-1} + oldsymbol{i}_t \odot oldsymbol{g}_t$
- Output $h_t = o_t \odot \tanh(C_t)$

Learned through backpropagation

LSTM

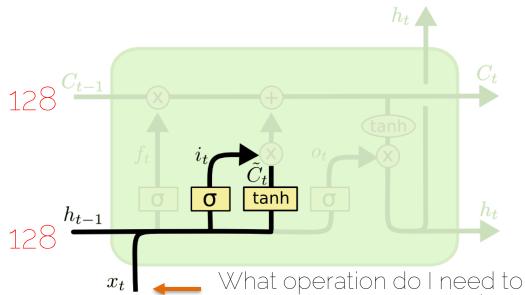
Highway for the gradient to flow



[Olah, https://colah.github.io '15] Understanding LSTMs

LSTM: Dimensions

• Cell update $\boldsymbol{g}_t = tanh(\boldsymbol{\theta}_{xg} \boldsymbol{x}_t + \boldsymbol{\theta}_{hg} \boldsymbol{h}_{t-1} + \boldsymbol{b}_g)$



When coding an LSTM, we have to define the size of the hidden state

Dimensions need to match

What operation do I need to do to my input to get a 128 vector representation?

[Olah, https://colah.github.io '15] Understanding LSTMs

LSTM in code

```
def lstm_step_forward(x, prev_h, prev_c, Wx, Wh, b):
 Forward pass for a single timestep of an LSTM.
 The input data has dimension D. the hidden state has dimension H. and we use
 a minibatch size of N.
 Inputs:
 - x: Input data, of shape (N, D)
 - prev h: Previous hidden state, of shape (N, H)
 - prev c: previous cell state, of shape (N. H)
 - Wx: Input-to-hidden weights, of shape (D, 4H)
 - Wh: Hidden-to-hidden weights, of shape (H, 4H)
 - b: Biases, of shape (4H,)
 Returns a tuple of:
 - next h: Next hidden state, of shape (N, H)
 - next c: Next cell state, of shape (N, H)
 - cache: Tuple of values needed for backward pass.
 next h, next c, cache = None, None, None
 N, H = prev h.shape
 a = np.dot(x, Wx) + np.dot(prev h, Wh) + b
 # 2
 ai = a[:, :H]
 af = a[:, H:2*H]
 ao = a[:, 2*H:3*H]
 aq = a[:. 3*H:]
 i = sigmoid(ai)
 f = sigmoid(af)
 o = sigmoid(ao)
 g = np.tanh(ag)
 next c = f * prev c + i * q
 # 5
 next h = o * np.tanh(next c)
 cache = i, f, o, g, a, ai, af, ao, ag, Wx, Wh, b, prev h, prev c, x, next c, next h
 return next h, next c, cache
```

```
def lstm step backward(dnext h. dnext c. cache):
  Backward pass for a single timestep of an LSTM.
 Inputs:
  - dnext h: Gradients of next hidden state, of shape (N, H)
  - dnext c: Gradients of next cell state, of shape (N, H)
  - cache: Values from the forward pass
 Returns a tuple of:
  - dx: Gradient of input data, of shape (N, D)
  - dprev h: Gradient of previous hidden state, of shape (N, H)
  - dprev c: Gradient of previous cell state, of shape (N, H)
  - dWx: Gradient of input-to-hidden weights, of shape (D, 4H)
  - dWh: Gradient of hidden-to-hidden weights, of shape (H. 4H)
  - db: Gradient of biases, of shape (4H,)
  dx. dh. dc. dWx. dWh. db = None, None, None, None, None, None
 i, f, o, q, a, ai, af, ao, aq, Wx, Wh, b, prev h, prev c, x, next c, next h = cache
  # backprop into step 5
  do = np.tanh(next c) * dnext h
  dnext c += o * (1 - np.tanh(next c) ** 2) * dnext h
  # backprop into 4
  df = prev c * dnext c
  dprev c = f * dnext c
  di = q * dnext c
  dq = i * dnext c
  # backprop into 3
  dai = sigmoid(ai) * (1 - sigmoid(ai)) * di
  daf = sigmoid(af) * (1 - sigmoid(af)) * df
  dao = sigmoid(ao) * (1 - sigmoid(ao)) * do
  dag = (1 - np.tanh(ag) ** 2) * dg
  # backprop into 2
  da = np.hstack((dai, daf, dao, dag))
  # backprop into 1
  db = np.sum(da, axis = 0)
  dprev h = np.dot(Wh, da.T).T
  dWh = np.dot(prev h.T, da)
  dx = np.dot(da, Wx.T)
  dWx = np.dot(x.T, da)
  return dx, dprev h, dprev c, dWx, dWh, db
```



Attention

Attention is all you need

Attention Is All You Need

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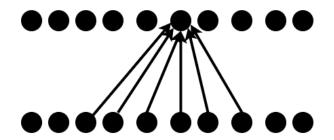
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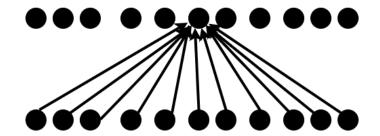
Illia Polosukhin* † illia.polosukhin@gmail.com

Attention vs convolution

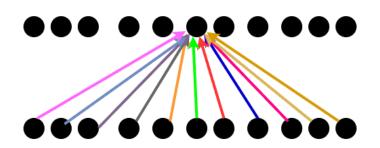
Convolution



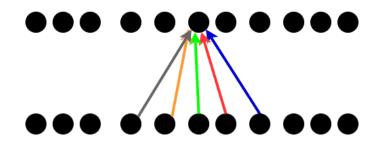
Fully Connected layer



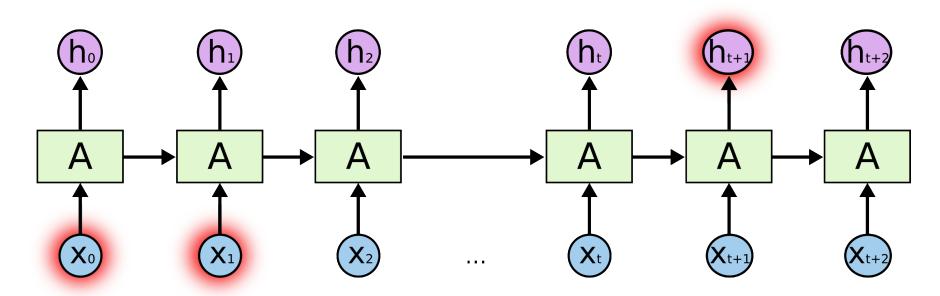
Global attention



Local attention



Long-Term Dependencies

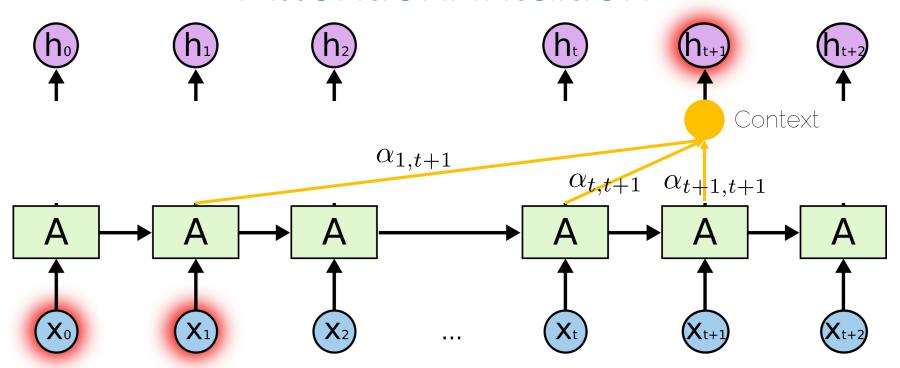


I moved to Germany ...

so I speak German fluently.

Source: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

Attention: Intuition



I moved to Germany ...

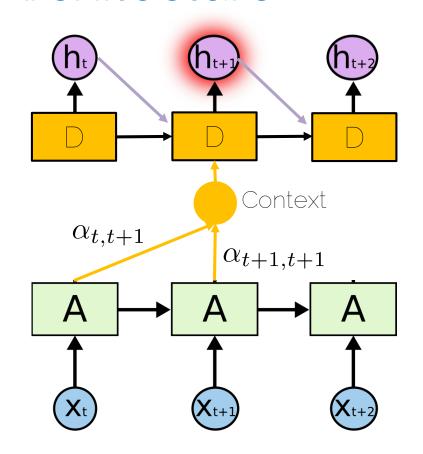
so I speak German fluently

laDL: Prof. Dail

Attention: Architecture

 A decoder processes the information

- Decoders take as input:
 - Previous decoder hidden state
 - Previous output
 - Attention





Transformers

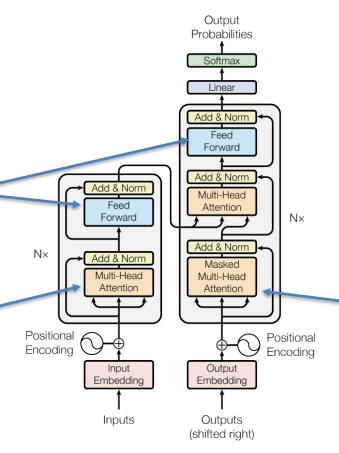
Deep Learning Revolution

	Deep Learning	Deep Learning 2.0
Main idea	Convolution	Attention
Field invented	Computer vision	NLP
Started	NeurIPS 2012	NeurIPS 2017
Paper	AlexNet	Transformers
Conquered vision	Around 2014-2015	Around 2020-2021
Replaced (Augmented)	Traditional ML/CV	CNNs, RNNs

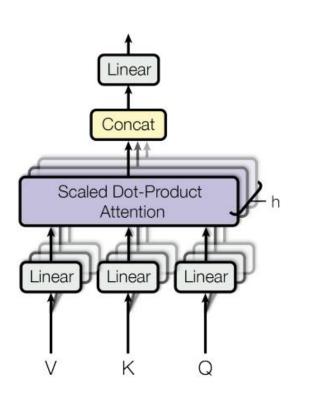
Transformers

Fully connected layer

Multi-Head Attention on the "encoder"



Masked Multi-Head Attention on the "decoder"



Intuition: Take the query Q, find the most similar key K, and then find the value V that corresponds to the key.

In other words, learn V, K, Q where:

- V here is a bunch of interesting things.
- K here is how we can index some things.
- Q I would like to know this interesting thing.

Loosely connected to Neural Turing Machines (Graves et al.).

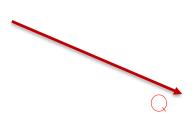
Index the values via a differentiable operator.

Multiply queries with keys

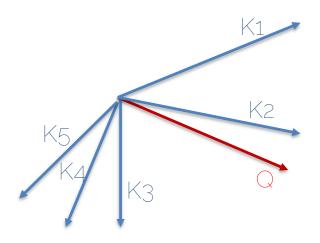
Get the values

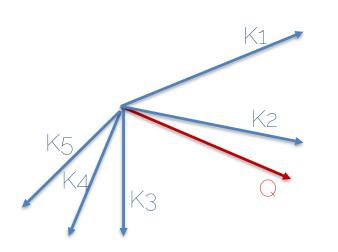
Attention
$$(Q, K, V) = \operatorname{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

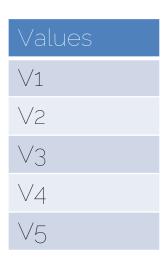
To train them well, divide by $\sqrt{d_k}$, "probably" because for large values of the key's dimension, the dot product grows large in magnitude, pushing the softmax function into regions where it has extremely small gradients.

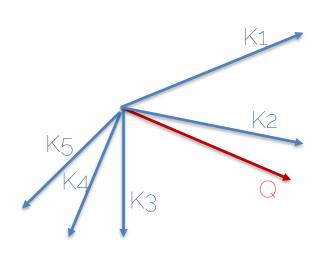


Adapted from Y. Kilcher





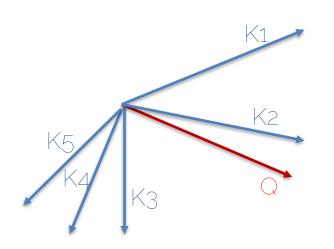




Values
V1
V2
V3
V4
V5

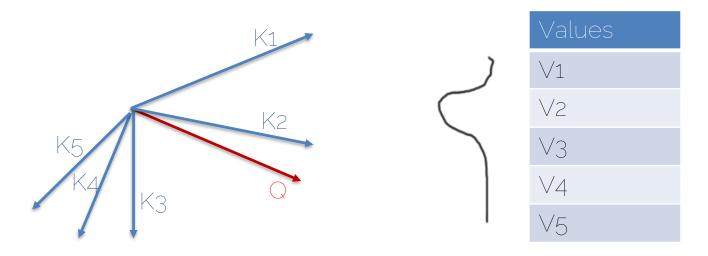
 QK^T

Essentially, dot product between (<Q,K1>), (<Q,K2>), (<Q,K3>), (<Q,K4>), (<Q,K5>).



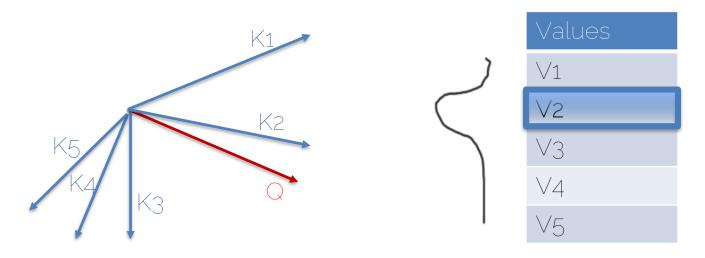
Values
V1
V2
V 3
V4
V5

$$\operatorname{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)$$



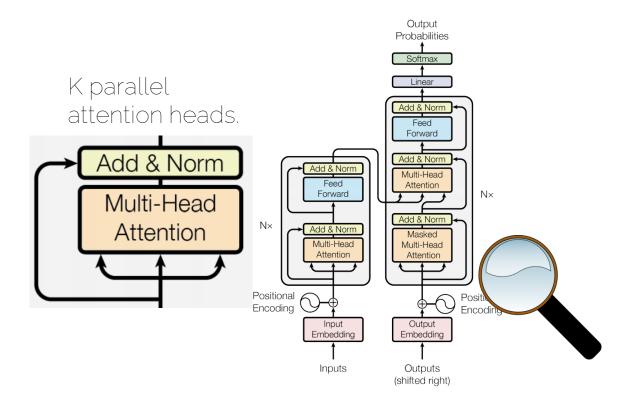
$$\operatorname{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)$$

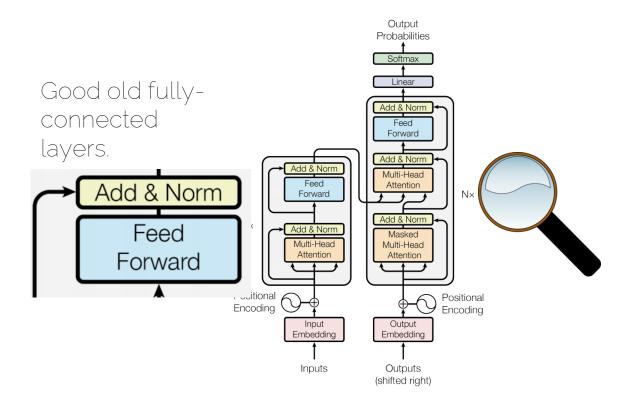
softmax $\left(\frac{QK^T}{\sqrt{d_k}}\right)$ Is simply inducing a distribution over the values. The larger a value is, the higher is its softmax value. Can be interpreted as a differentiable soft indexing.

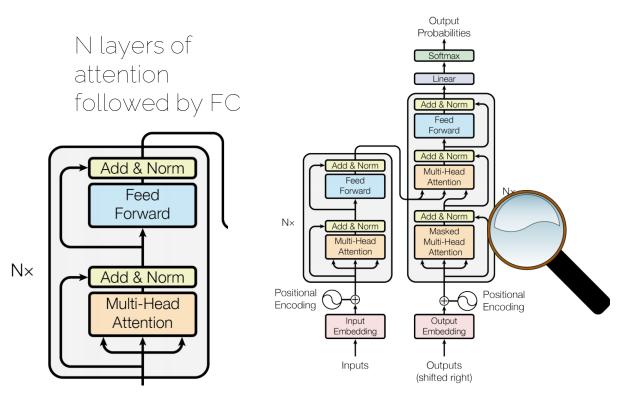


$$\operatorname{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)$$

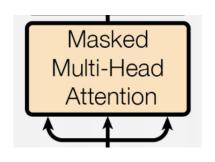
Selecting the value V where the network needs to attend...

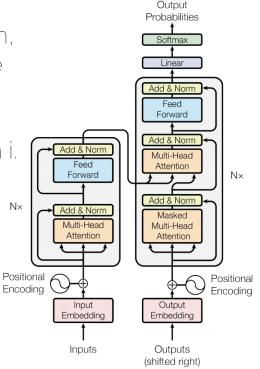




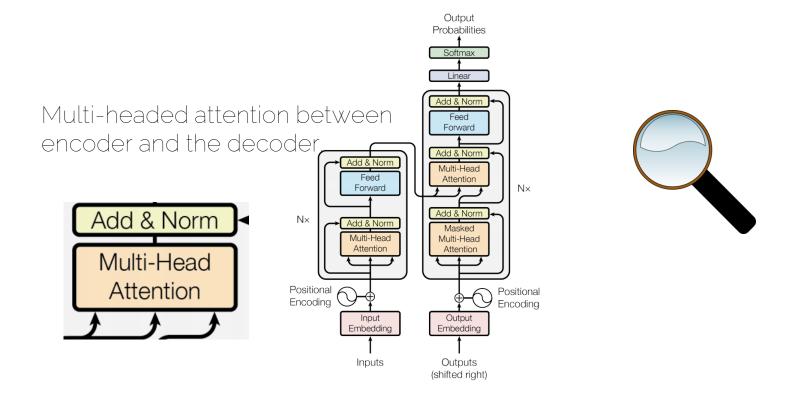


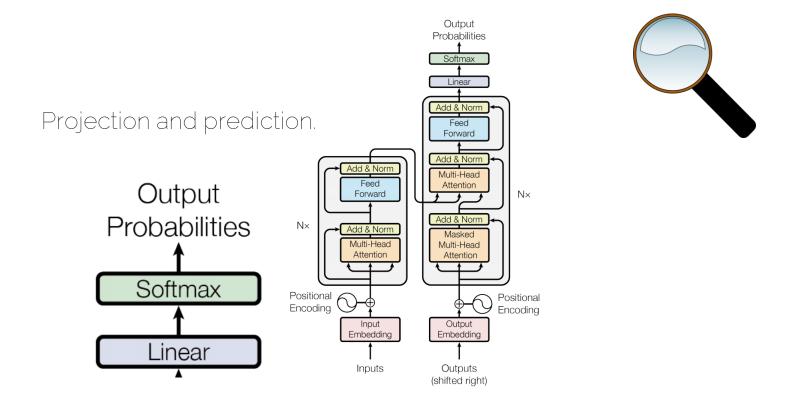
Same as multi-head attention, but masked. Ensures that the predictions for position i can depend only on the known outputs at positions less than i.





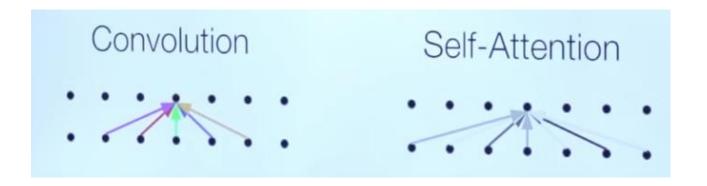




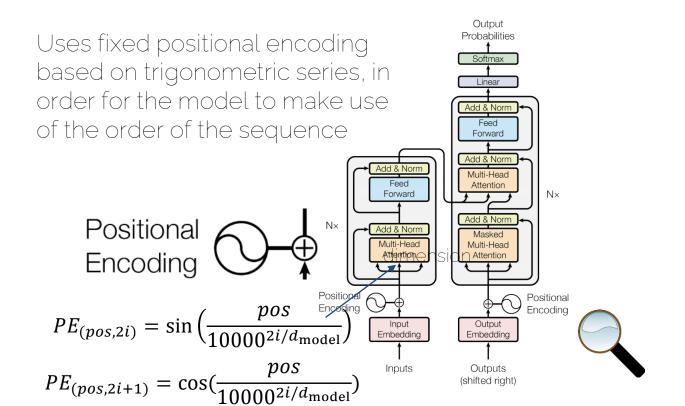


What is missing from self-attention?

- Convolution: a different linear transformation for each relative position. Allows you to distinguish what information came from where.
- Self-attention: a weighted average.

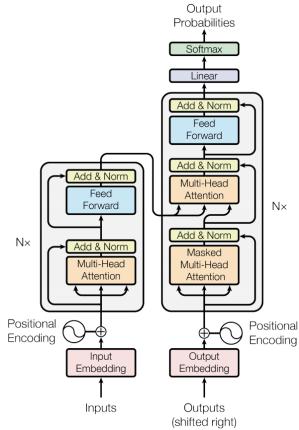


laDL: Prof. Dail





Transformers – a final look



Self-attention: complexity

Layer Type	Complexity per Layer	Sequential	Maximum Path Length
		Operations	
Self-Attention	$O(n^2 \cdot d)$	O(1)	O(1)
Recurrent	$O(n \cdot d^2)$	O(n)	O(n)
Convolutional	$O(k \cdot n \cdot d^2)$	O(1)	$O(log_k(n))$
Self-Attention (restricted)	$O(r \cdot n \cdot d)$	O(1)	O(n/r)

where n is the sequence length, d is the representation dimension, k is the convolutional kernel size, and r is the size of the neighborhood.

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where n is the sequence length, d is the representation dimension, k is the convolutional kernel size, and r is the size of the neighborhood.

Considering that most sentences have a smaller dimension than the representation dimension (in the paper, it is 512), self-attention is very efficient.

Transformers – training tricks

ADAM optimizer with proportional learning rate:

$$lrate = d_{\text{model}}^{-0.5} \cdot \min(step_num^{-0.5}, step_num \cdot warmup_steps^{-1.5})$$

- Residual dropout
- Label smoothing
- Checkpoint averaging

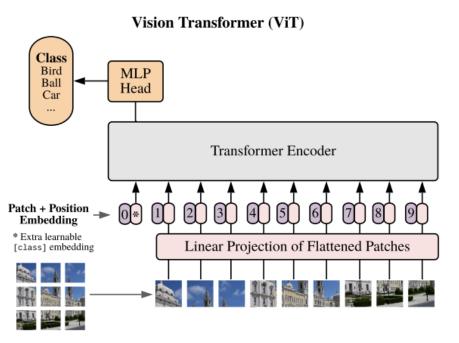
Transformers - results

Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on the English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [15]	23.75			
Deep-Att + PosUnk [32]		39.2		$1.0\cdot 10^{20}$
GNMT + RL [31]	24.6	39.92	$2.3\cdot 10^{19}$	$1.4\cdot 10^{20}$
ConvS2S [8]	25.16	40.46	$9.6\cdot 10^{18}$	$1.5\cdot 10^{20}$
MoE [26]	26.03	40.56	$2.0\cdot 10^{19}$	$1.2\cdot 10^{20}$
Deep-Att + PosUnk Ensemble [32]		40.4		$8.0\cdot 10^{20}$
GNMT + RL Ensemble [31]	26.30	41.16	$1.8\cdot 10^{20}$	$1.1\cdot 10^{21}$
ConvS2S Ensemble [8]	26.36	41.29	$7.7\cdot 10^{19}$	$1.2\cdot 10^{21}$
Transformer (base model)	27.3	38.1	$3.3\cdot 10^{18}$	
Transformer (big)	28.4	41.0	$2.3\cdot 10^{19}$	

Transformers for Images

Vision Transformers (ViTs)



*Dosovitskiy et al. "An image is worth 16x16 words: Transformers for image recognition at scale", ICLR 2020.

Transformers - summary

- Significantly improved SOTA in machine translation
- Launched a new deep-learning revolution in MLP
- Building block of NLP models like BERT (Google) or GPT/ChatGPT (OpenAI)
- BERT has been heavily used in Google Search

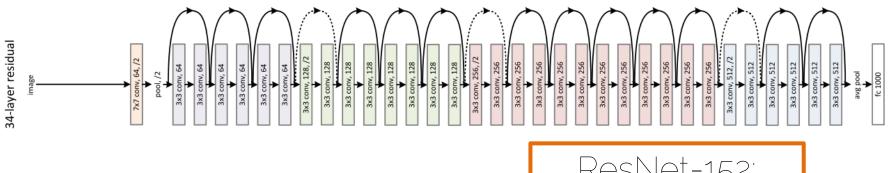
 And eventually made its way to computer vision (and other related fields)*

*Dosovitskiy et al. "An image is worth 16x16 words: Transformers for image recognition at scale", ICLR 2020.



Transfer Learning

ResNet



ResNet-152: 60M parameters

[He et al. CVPR'16] ResNet

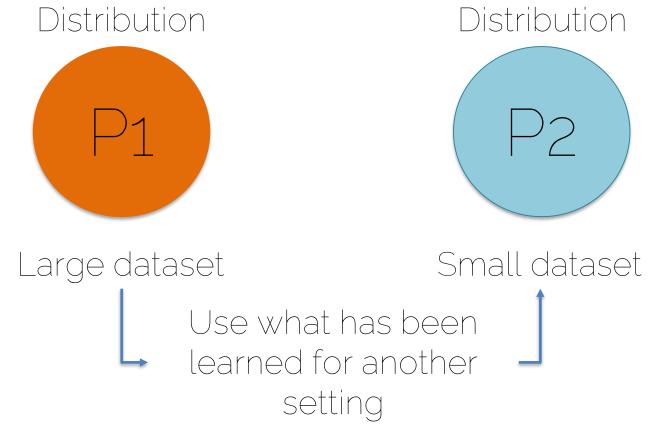
Transfer Learning

 Training your own model can be difficult with limited data and other resources

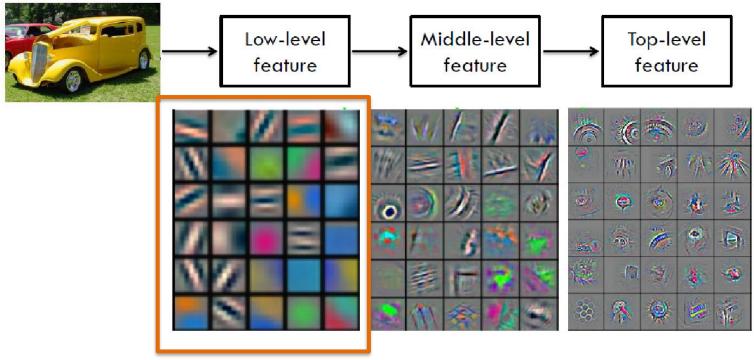
e.g.,

- It is a laborious task to manually annotate your own training dataset
- Why not reuse already pre-trained models?

Transfer Learning



Transfer Learning for Images



[Zeiler al., ECCV'14] Visualizing and Understanding Convolutional Networks

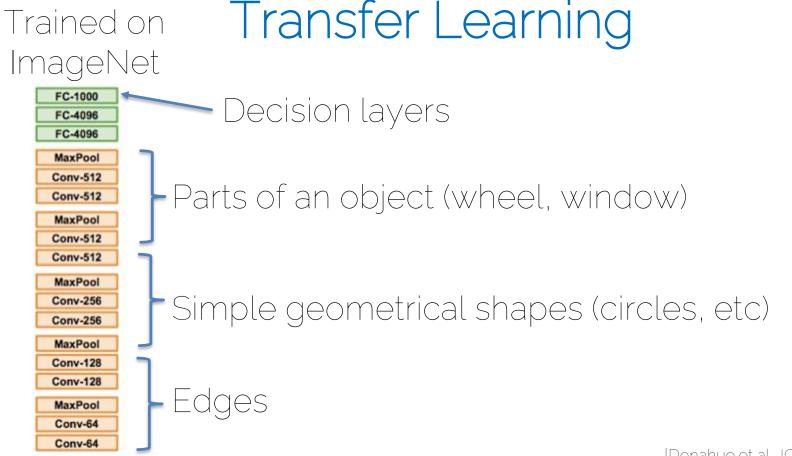
ImageNet

Trained on Transfer Learning

FC-1000 FC-4096 FC-4096 MaxPool Conv-512 Conv-512 MaxPool Conv-512 Conv-512 MaxPool Conv-256 Conv-256 MaxPool Conv-128 Conv-128 MaxPool Conv-64 Conv-64 Image

Feature extraction

> [Donahue et al., ICML'14] DeCAF, [Razavian et al., CVPRW'14] CNN Features off-the-shelf



[Donahue et al., ICML'14] DeCAF, [Razavian et al., CVPRW'14] CNN Features off-the-shelf

2DL: Prof. Dai

Image

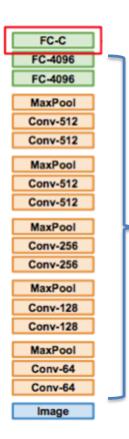
Trained on ImageNet

Transfer Learning



Image

TRAIN



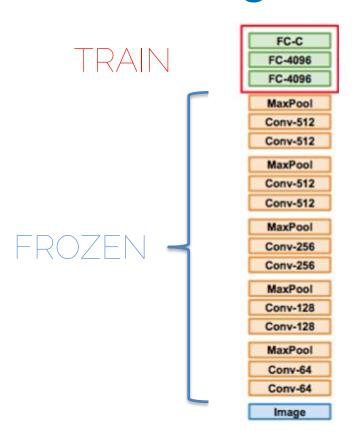
New dataset with C classes

FROZEN

[Donahue et al., ICML'14] DeCAF, [Razavian et al., CVPRW'14] CNN Features off-the-shelf

Transfer Learning

If the dataset is big enough train more layers with a low learning rate



When Transfer Learning Makes Sense

 When task T1 and T2 have the same input (e.g. an RGB image)

When you have more data for task T1 than for task T2

• When the low-level features for T1 could be useful to learn T2



Representation Learning

Learning Good Features

- Good features are essential for successful machine learning
- (Supervised) deep learning depends on training data used: input/target labels
- Change in inputs (noise, irregularities, etc.) can result in drastically different results

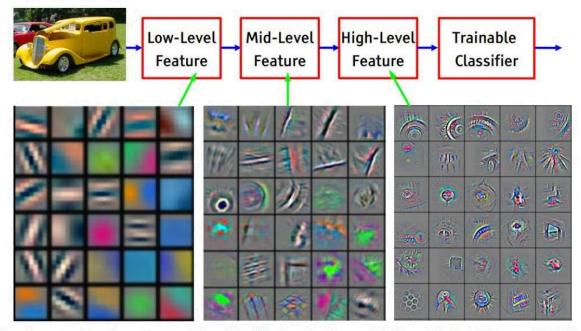
Representation Learning

Allows for discovery of representations required for various tasks

• Deep representation learning: model maps input \boldsymbol{X} to output \boldsymbol{Y}

Deep Representation Learning

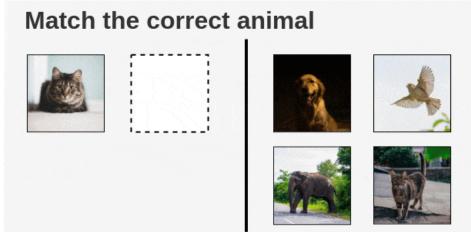
 Intuitively, deep networks learn multiple levels of abstraction



How to Learn Good Features?

Determine desired feature invariances

Teach machines to distinguish between similar and dissimilar things



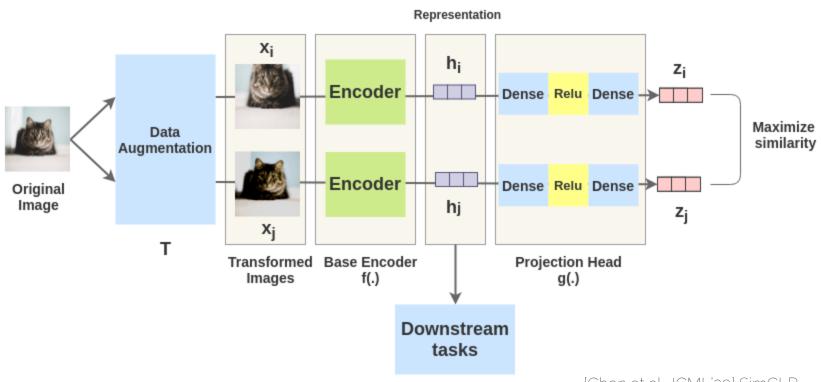
https://amitness.com/2020/03/illustrated-simclr/

Self-Supervised Representation Learning

- Why not just supervised learning?
 - Relies heavily on labeled data
 - Learns task-specific features

 Want general useful internal features that are transferable to many tasks

How to Learn Good Features?

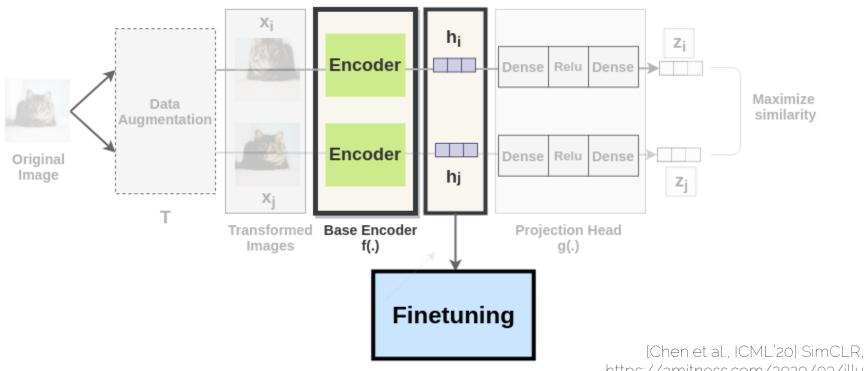


[Chen et al., ICML'20] SimCLR, https://amitness.com/2020/03/illustrated-simclr/

Apply to Downstream Tasks

Usage on downstream tasks

Representation



classification, detection, ...

[Chen et al., ICML'20] SimCLR, https://amitness.com/2020/03/illu strated-simclr/

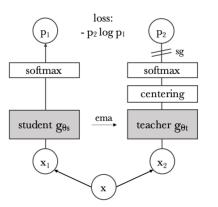
DINO

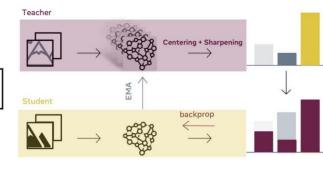
Self-supervised learning

 Trains a vision transformer (ViT) to produce meaningful representations using self-distillation w/

minibatch

no labels



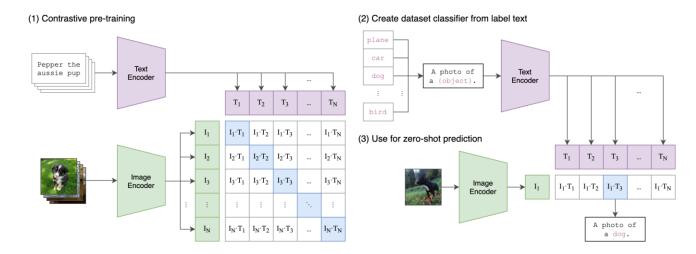


 $heta_{ ext{teacher}} \leftarrow au \cdot heta_{ ext{teacher}} + (1 - au) \cdot heta_{ ext{student}}$

[Caron et al., ICCV'21] Emerging Properties in Self-Supervised Vision Transformers

CLIP: Contrastive Language-Image Pre-training

 Connects images and text by training on massive dataset of (image, caption) pairs scraped from the internet



Transfer & Representation Learning

Transfer learning can be done via representation learning

• Effectiveness of representation learning often demonstrated by transfer learning performance (but also other factors, e.g., smoothness of the manifold)



See you next time!