Self-Attention For Generative Models

Ashish Vaswani and Anna Huang

Joint work with: Noam Shazeer, Niki Parmar, Lukasz Kaiser, Illia Polosukhin, Llion Jones, Justin Gilmer, David Bieber, Jonathan Frankle, Jakob Uszkoreit, and others.

Learning Representations of Variable Length Data

Basic building block of sequence-to-sequence learning

Neural machine translation, summarization, QA, …

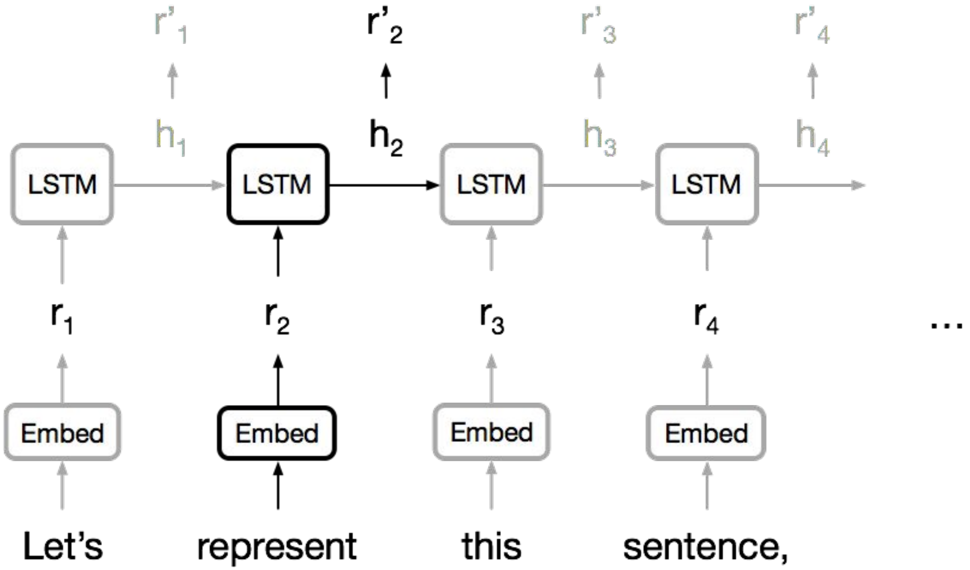
Recurrent Neural Networks

Model of choice for learning variable-length representations.

Natural fit for sentences and sequences of pixels.

LSTMs, GRUs and variants dominate recurrent models.

Recurrent Neural Networks



But…

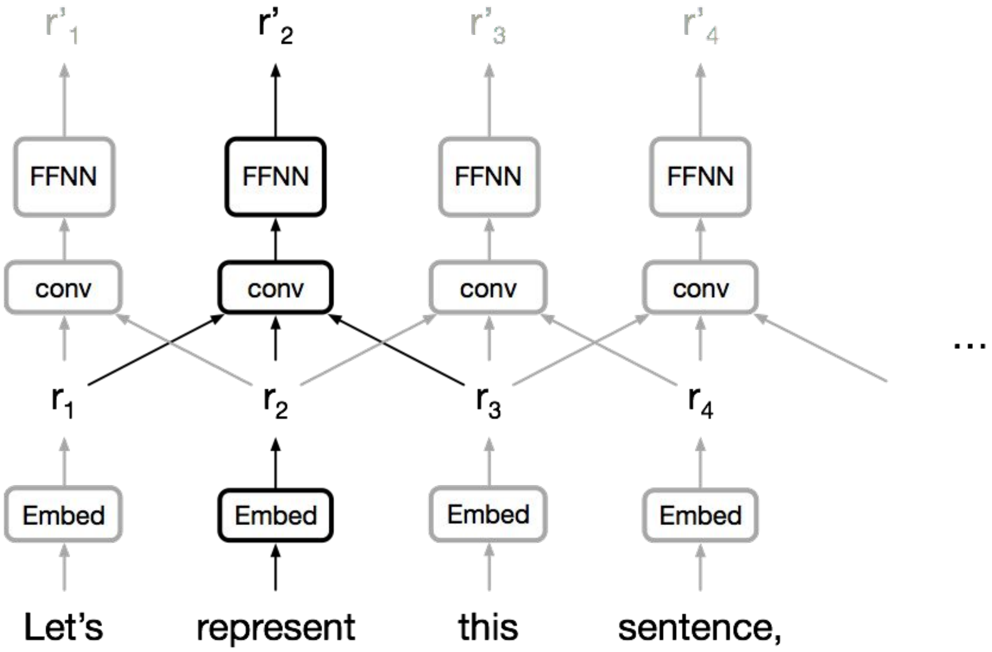
Sequential computation inhibits parallelization.

No explicit modeling of long and short range dependencies.

We want to model hierarchy.

RNNs (w/ sequence-aligned states) seem wasteful!

Convolutional Neural Networks?



Convolutional Neural Networks?

Trivial to parallelize (per layer).

Exploits local dependencies

‘Interaction distance’ between positions linear or logarithmic.

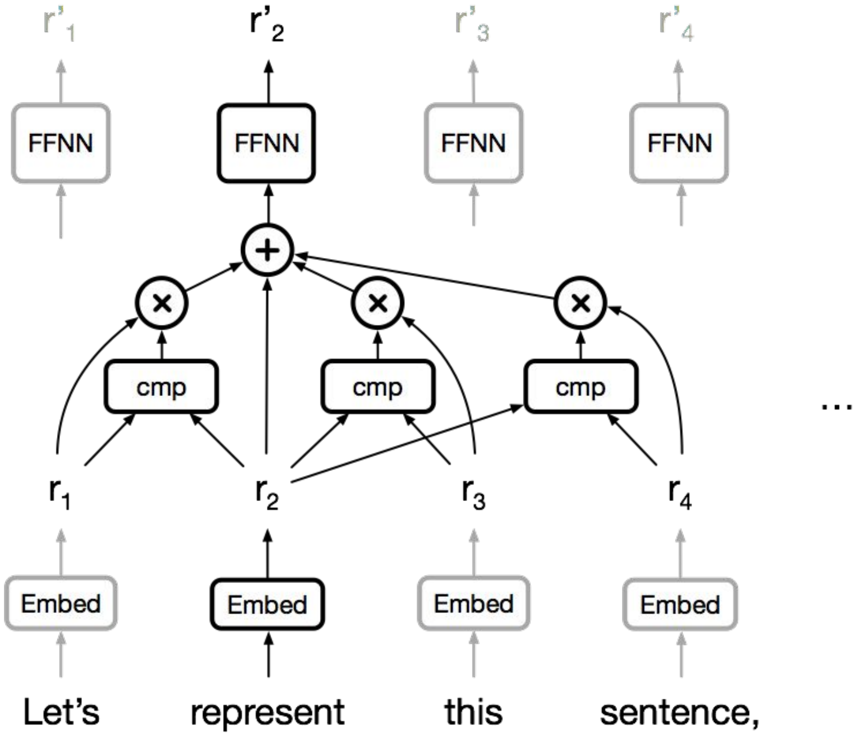
Long-distance dependencies require many layers.

Attention

Attention between encoder and decoder is crucial in NMT.

Why not use attention for representations?

Self-Attention



Text generation

Self-Attention

Constant ‘path length’ between any two positions.

Gating/multiplicative interactions.

Trivial to parallelize (per layer).

Can replace sequential computation entirely?

Previous work

Classification & regression with self-attention:

Parikh et al. (2016), Lin et al. (2016)

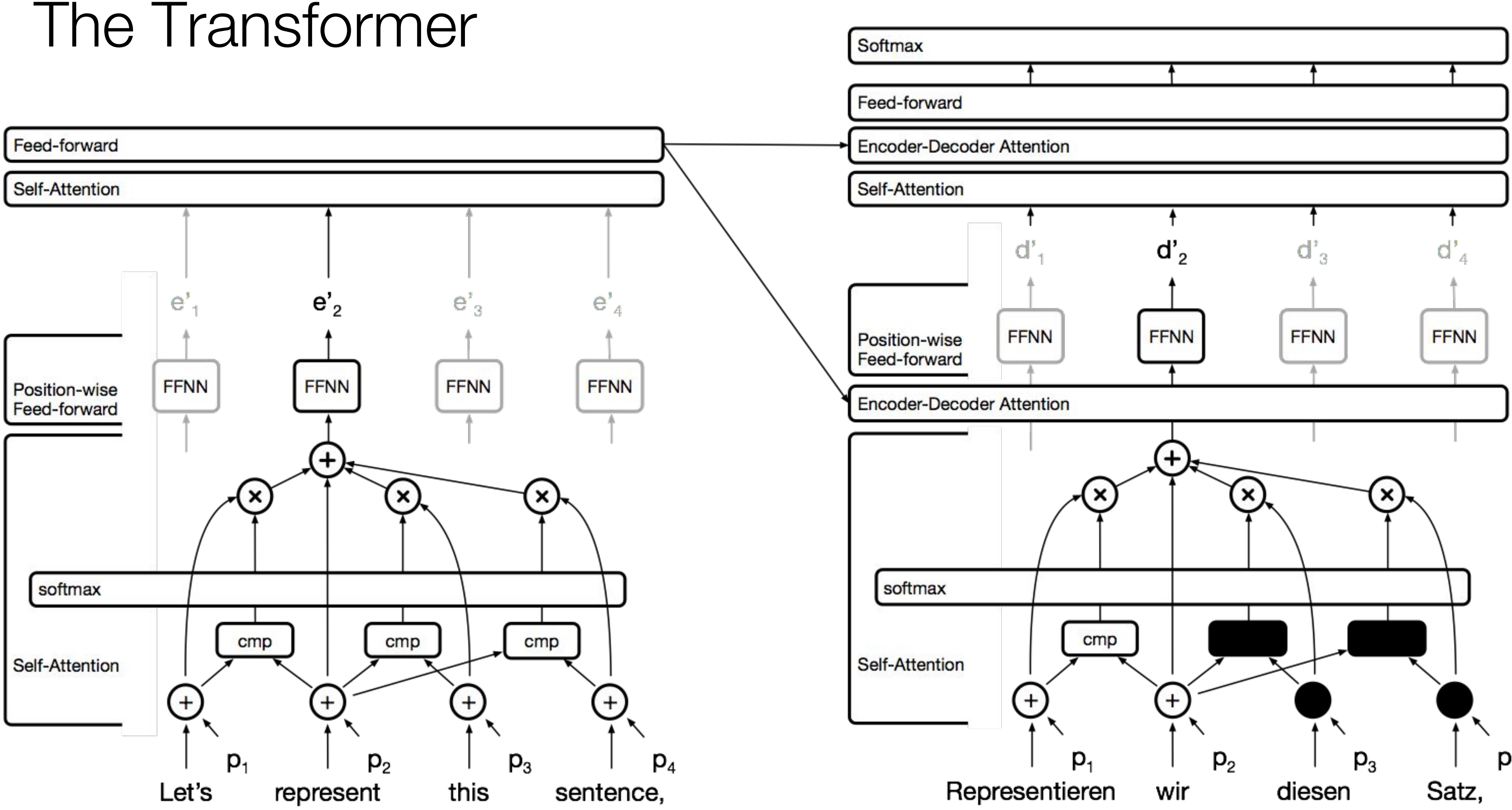
Self-attention with RNNs:

Long et al. (2016), Shao, Gows et al. (2017)

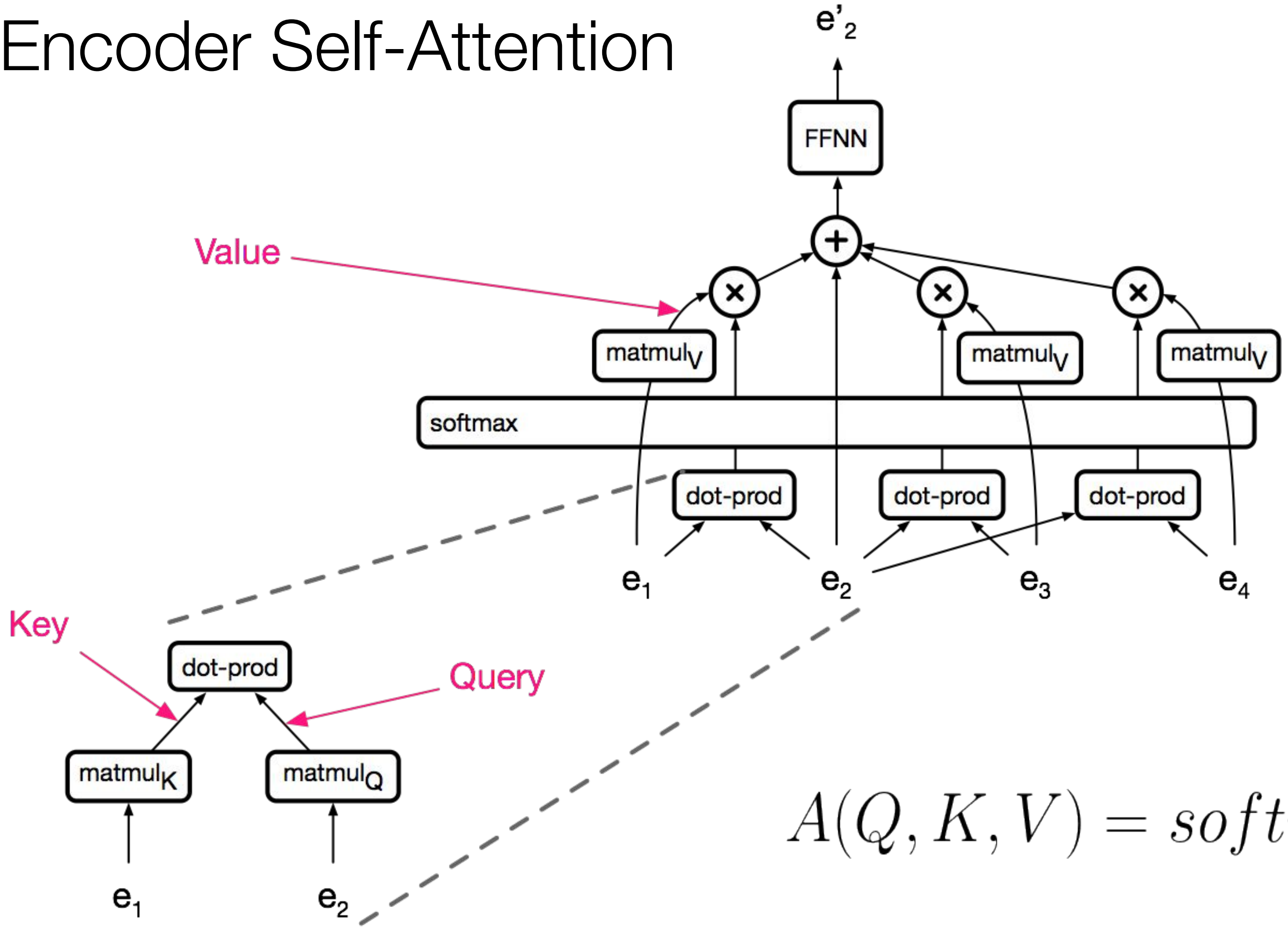
Recurrent attention:

Sukhbaatar et al. (2015)

The Transformer

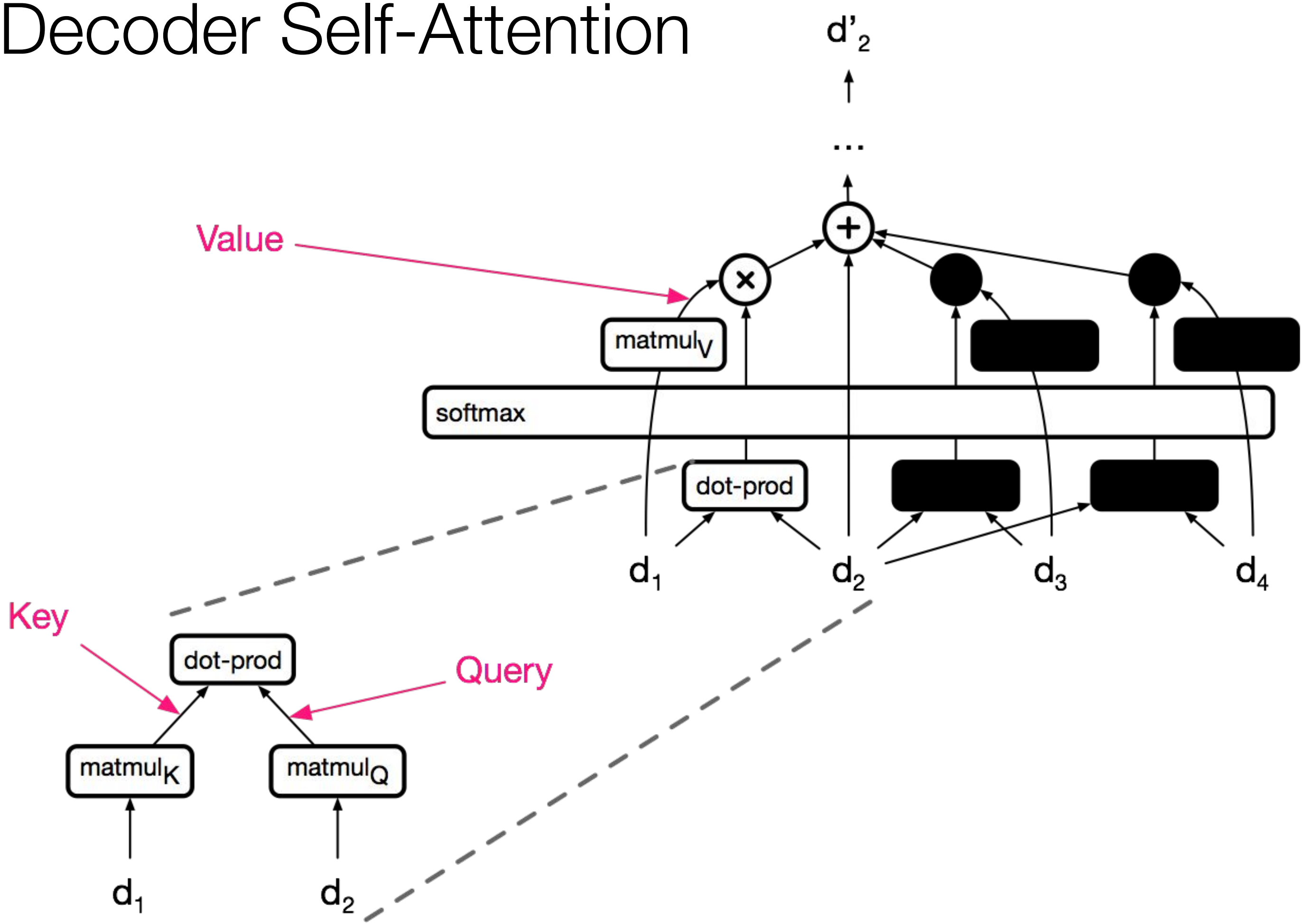


Encoder Self-Attention



$$A(Q,K,V) = softmax(\frac{QK^T}{\sqrt{d_k}})V$$

Decoder Self-Attention



Attention is Cheap!

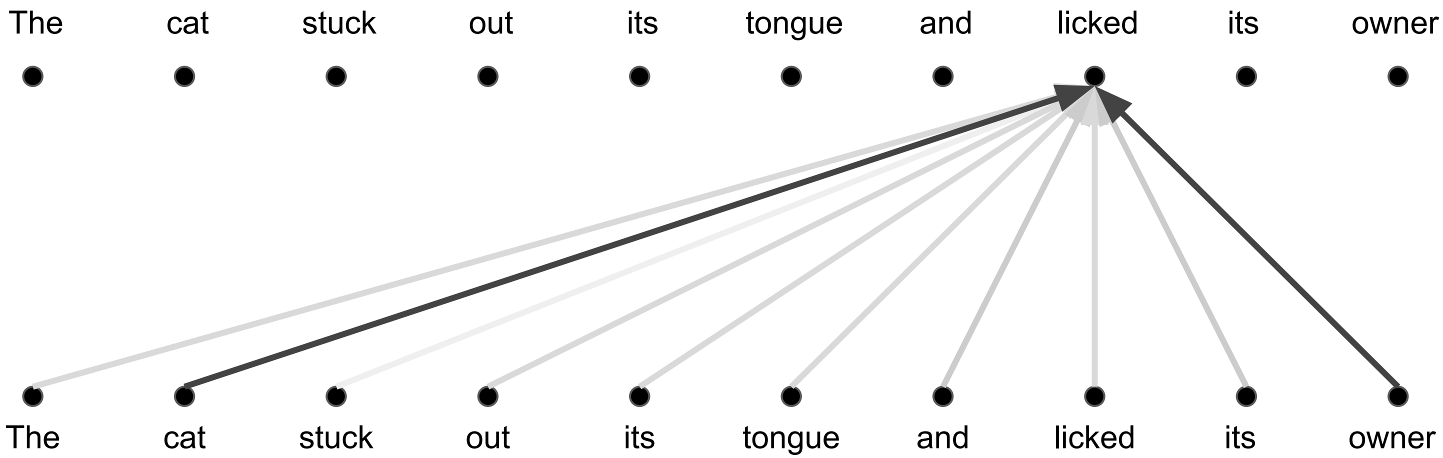
	FLOPs
Self-Attention	$O(\text{length}^2 \cdot \text{dim})$
RNN (LSTM)	$O(\text{length} \cdot \text{dim}^2)$
Convolution	$O(\text{length} \cdot \text{dim}^2 \cdot \text{kernel\_width})$

Attention is Cheap!

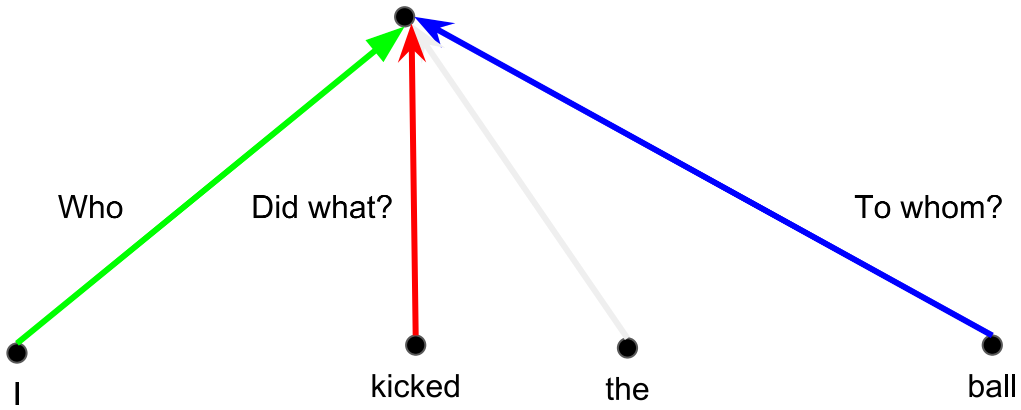
	FLOPs
Self-Attention	$O(\text{length}^2 \cdot \text{dim})$ $= 4{\cdot}10^9$
RNN (LSTM)	$O(\text{length} \cdot \text{dim}^2)$ $= 16{\cdot}10^9$
Convolution	$O(\text{length} \cdot \text{dim}^2 \cdot \text{kernel\_width})$ $= 6{\cdot}10^9$

length=1000 dim=1000 kernel_width=3

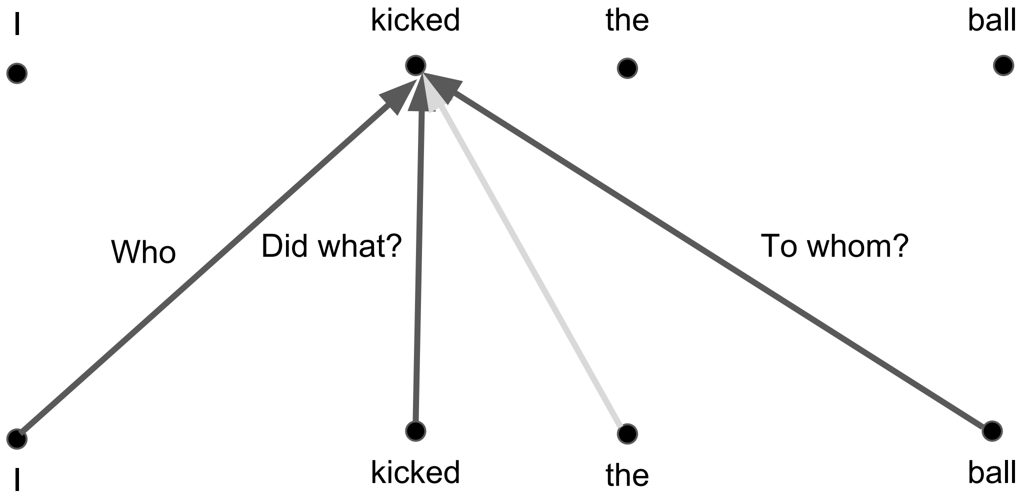
Attention: a weighted average



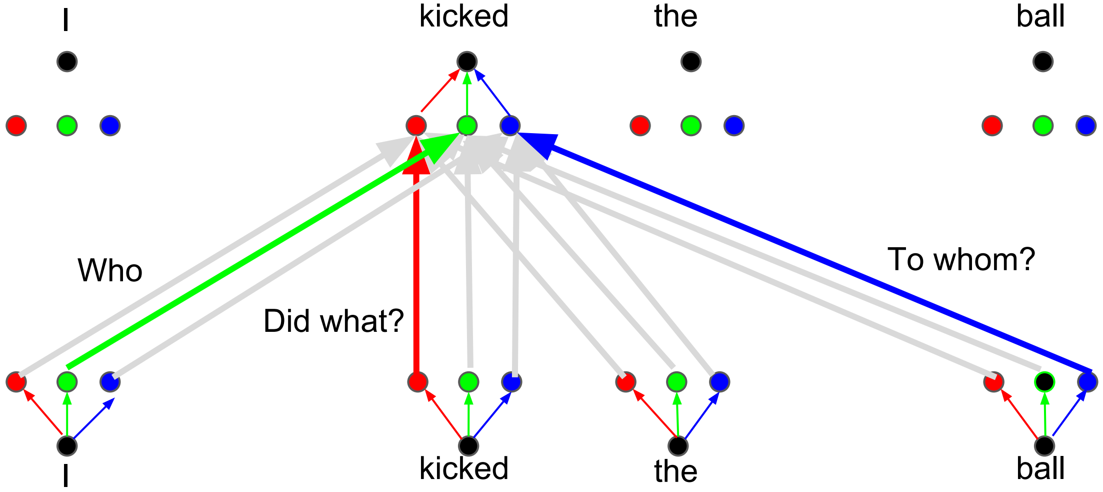
Convolutions



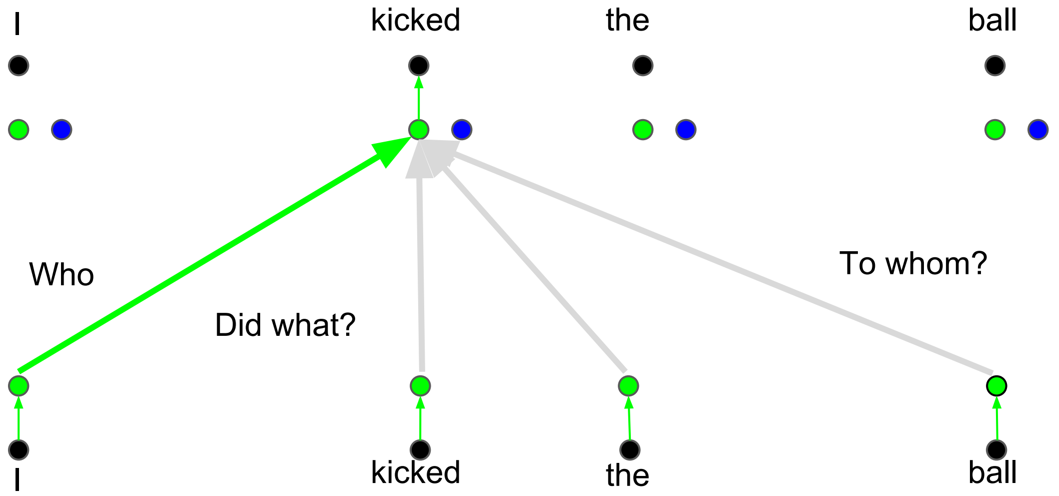
Self-Attention



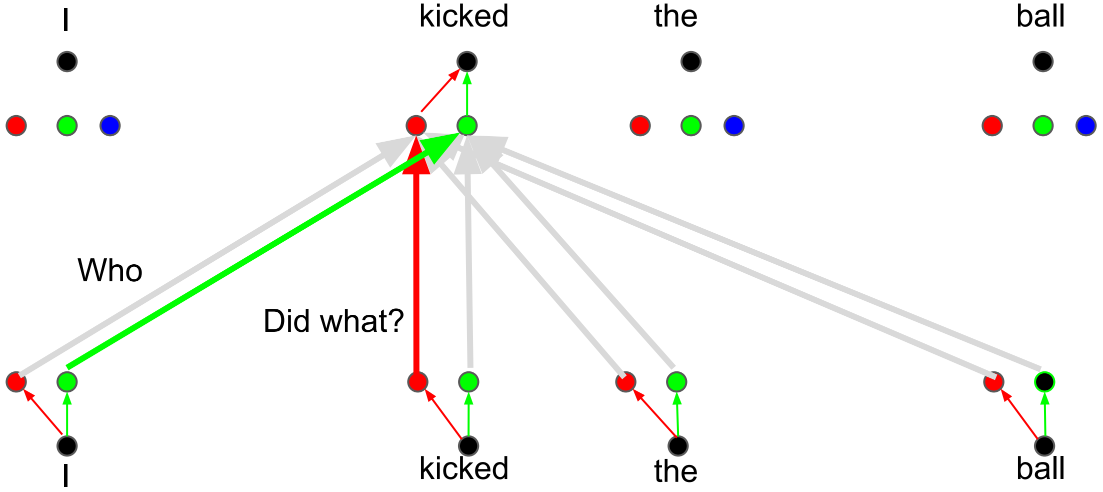
Parallel attention heads



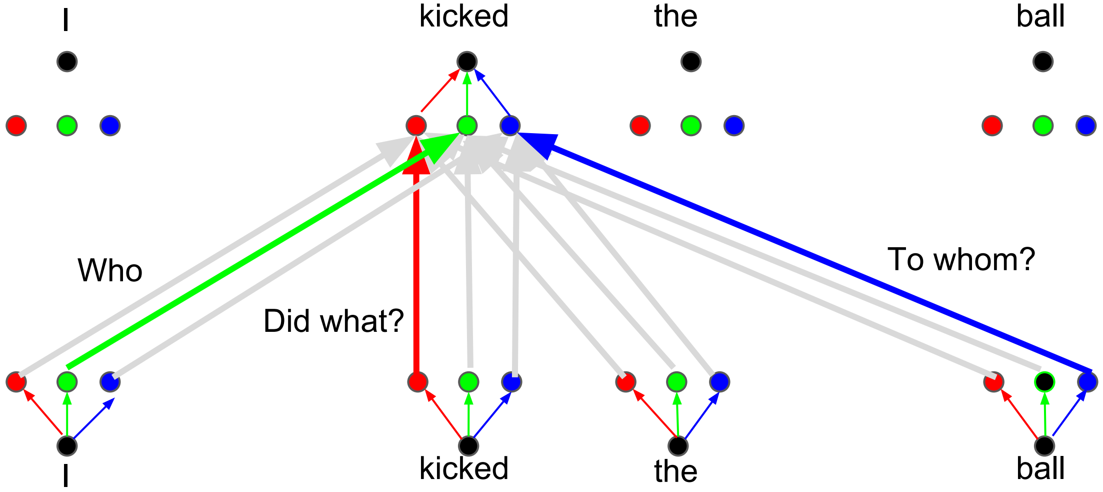
Attention head: Who



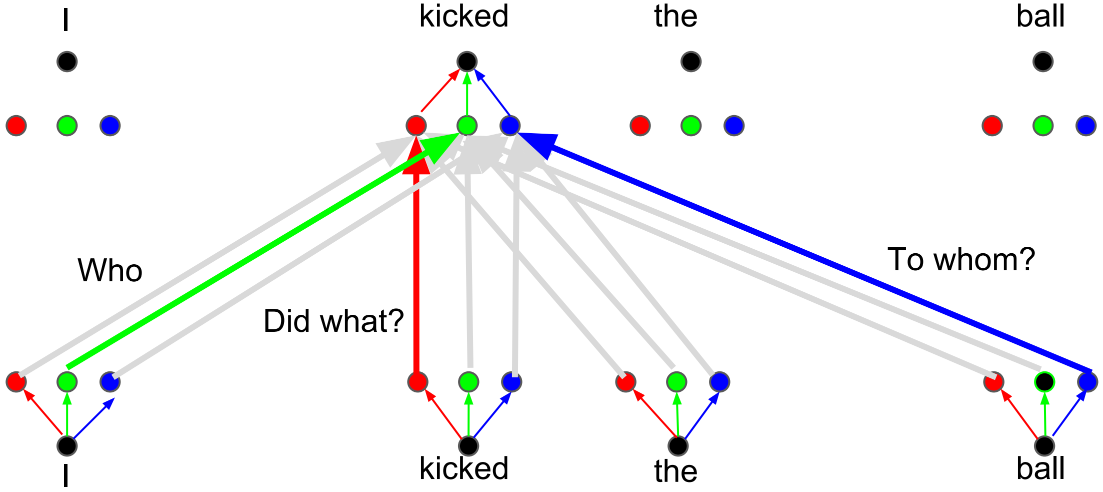
Parallel attention heads



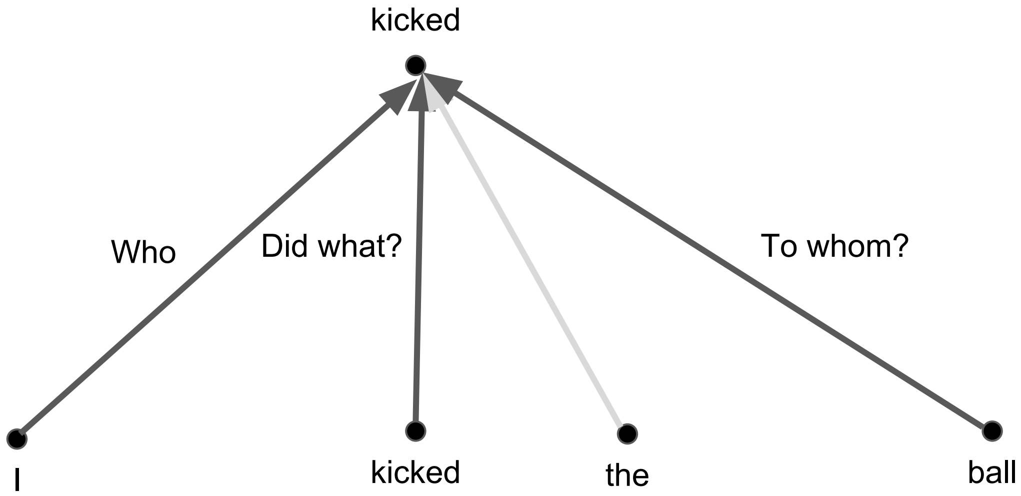
Parallel attention heads



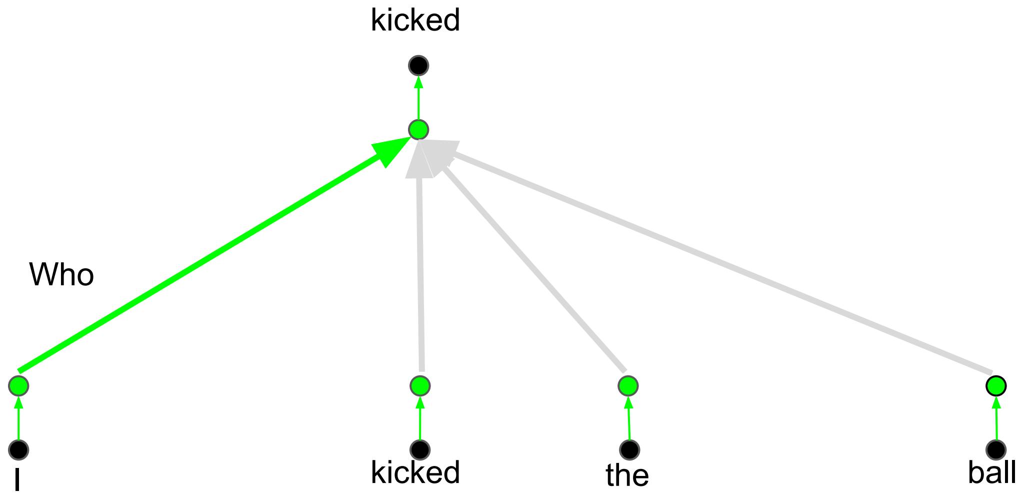
Parallel attention heads



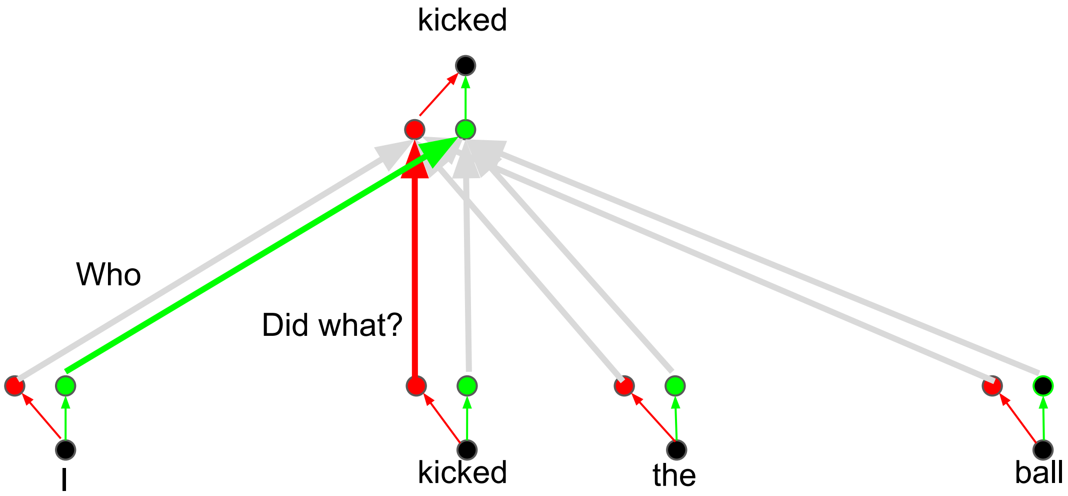
Self-Attention: Averaging



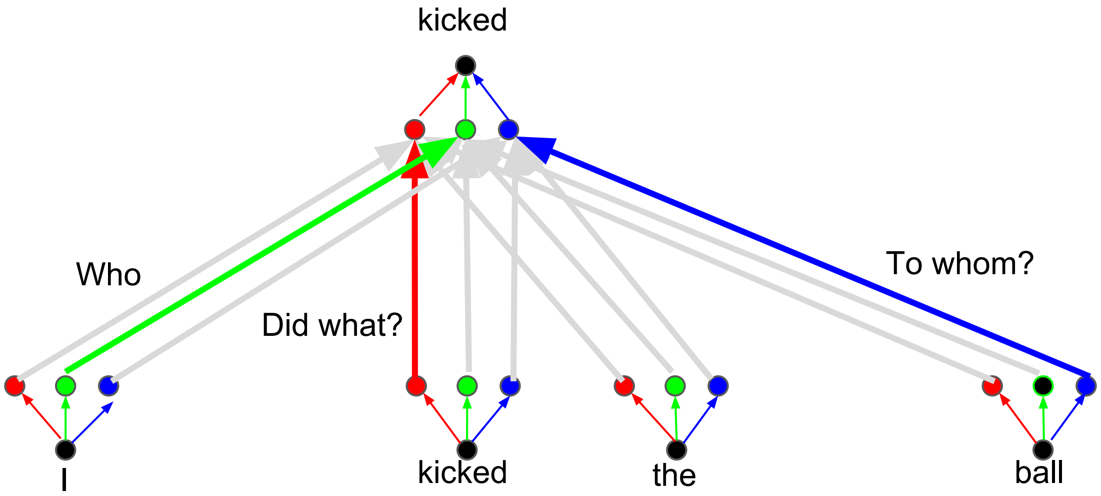
Attention head: Who



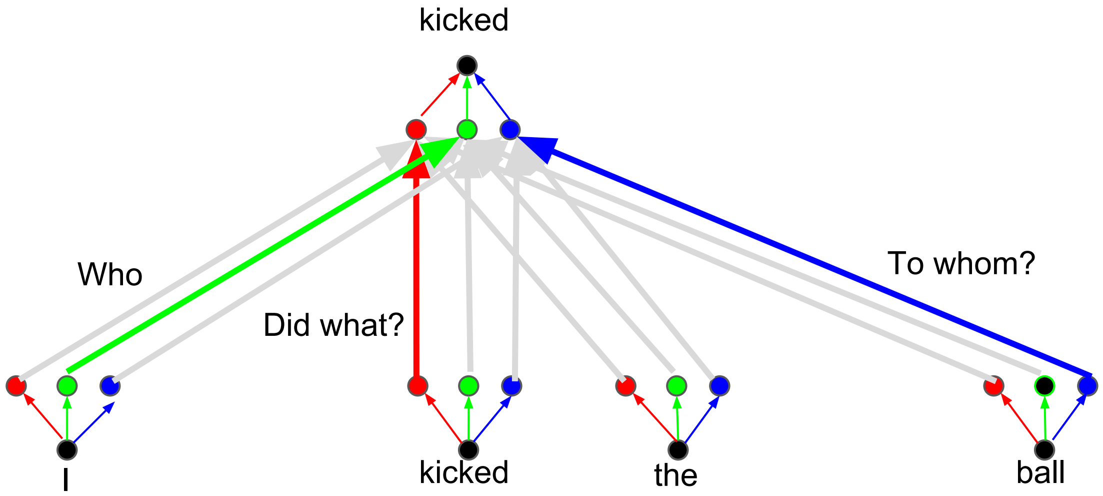
Attention head: Did What?



Attention head: To Whom?

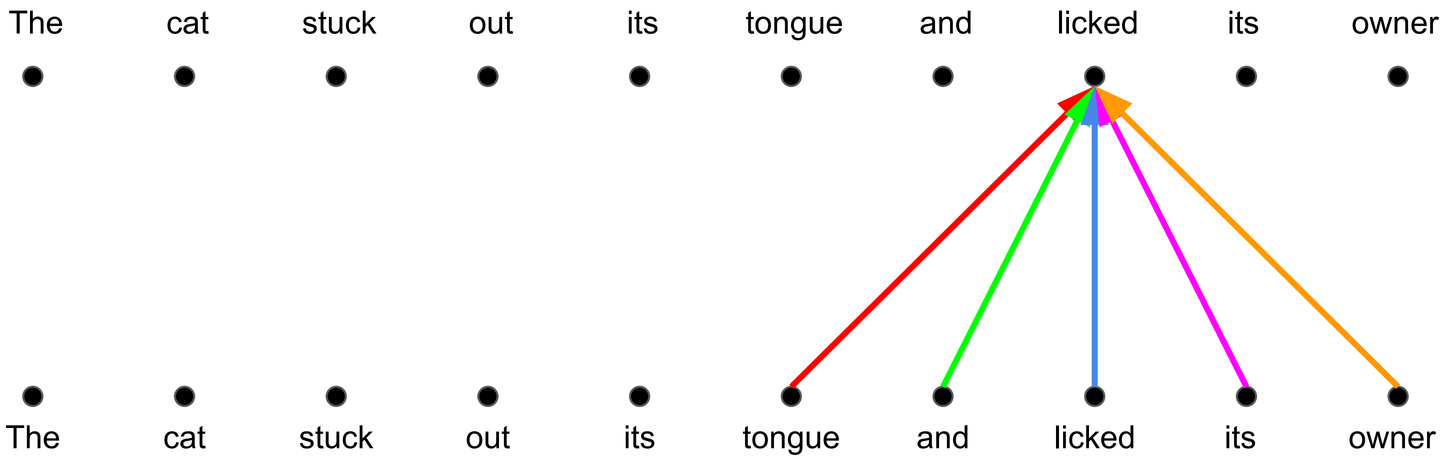


Multihead Attention

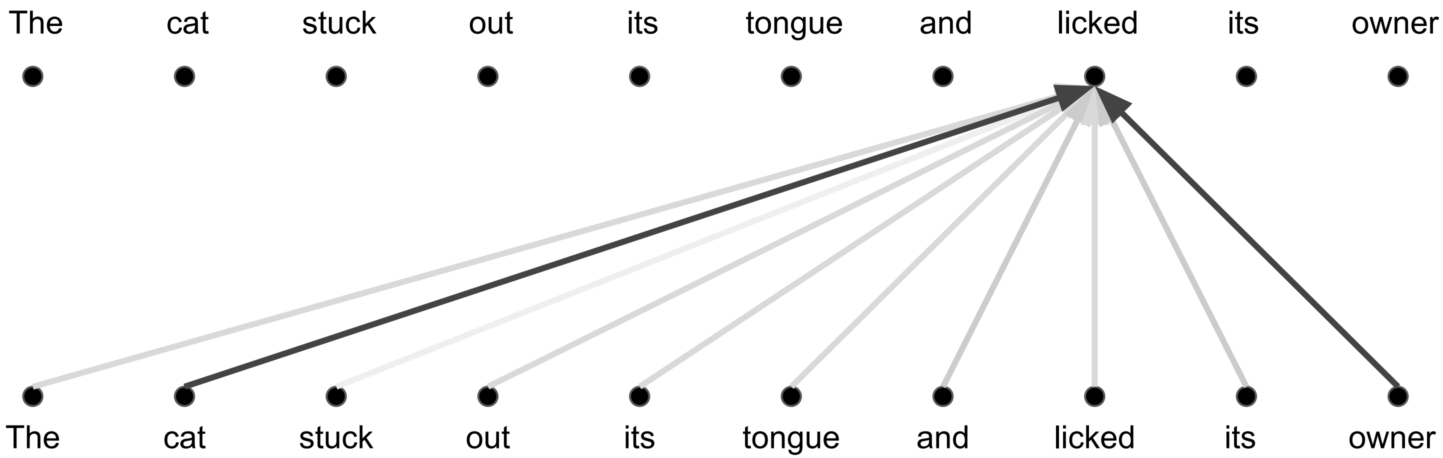


Convolution:

Different linear transformations by relative position.

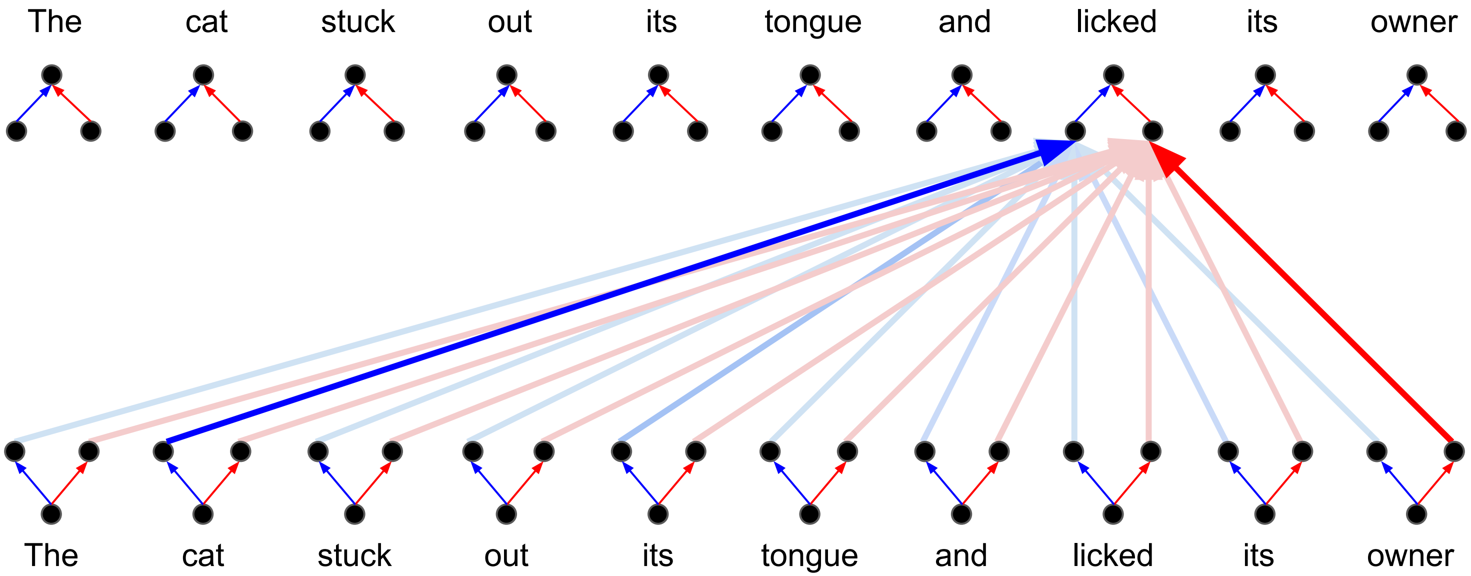


Attention: a weighted average



Multi-head Attention

Parallel attention layers with different linear transformations on input and output.



Results

Machine Translation: WMT-2014 BLEU

	EN-DE	EN-FR
GNMT (orig)	24.6	39.9
ConvSeq2Seq	25.2	40.5
Transformer*	**28.4**	**41.8**

*Transformer models trained >3x faster than the others.

Attention is All You Need (NeurIPS 2017) Vaswani*, Shazeer*, Parmar*, Uszkoreit*, Jones*, Kaiser*, Gomez*, Polosukhin*

Frameworks:

tensor2tensor

Sockeye

Importance of residuals

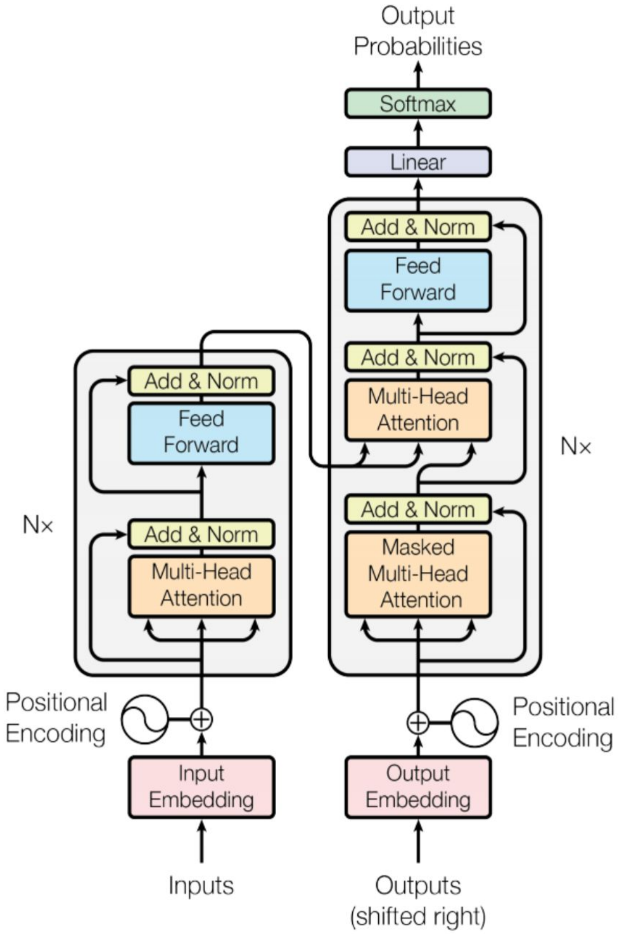
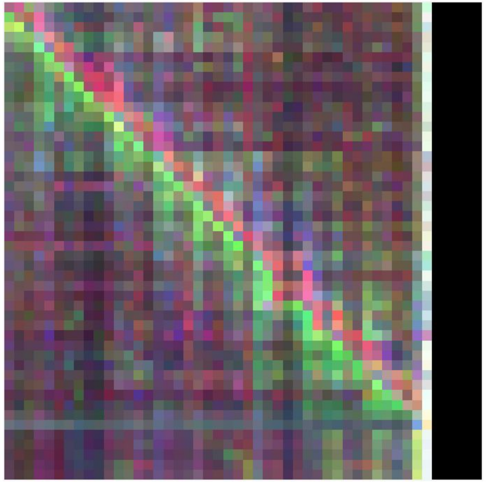


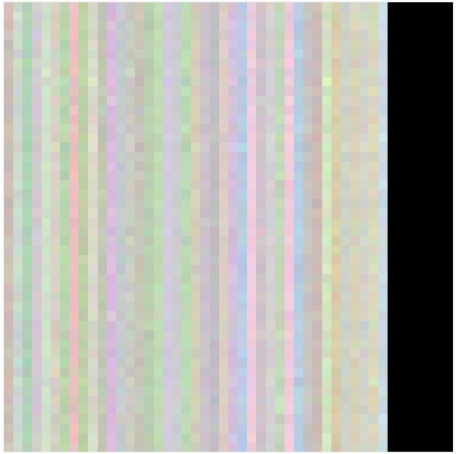
Figure 1: The Transformer - model architecture.

Importance of Residuals

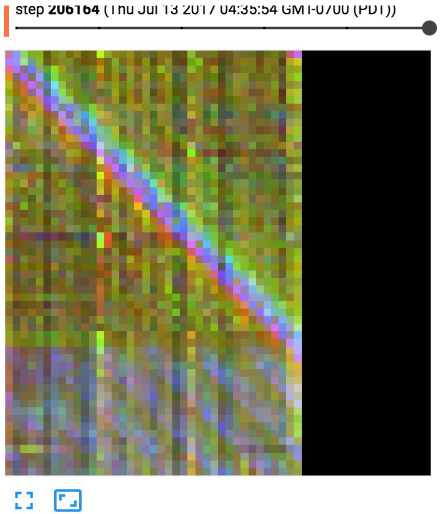
Residuals carry positional information to higher layers, among other information.



With residuals



Without residuals



step **206164** (Thu Jul 13 2017 04:35:54 GMT-0700 (PDT))

Without residuals,
with timing signals

Training Details

ADAM optimizer with a learning rate warmup (warmup + exponential decay)

Dropout during training at every layer just before adding residual

Layer-norm

Attention dropout (for some experiments)

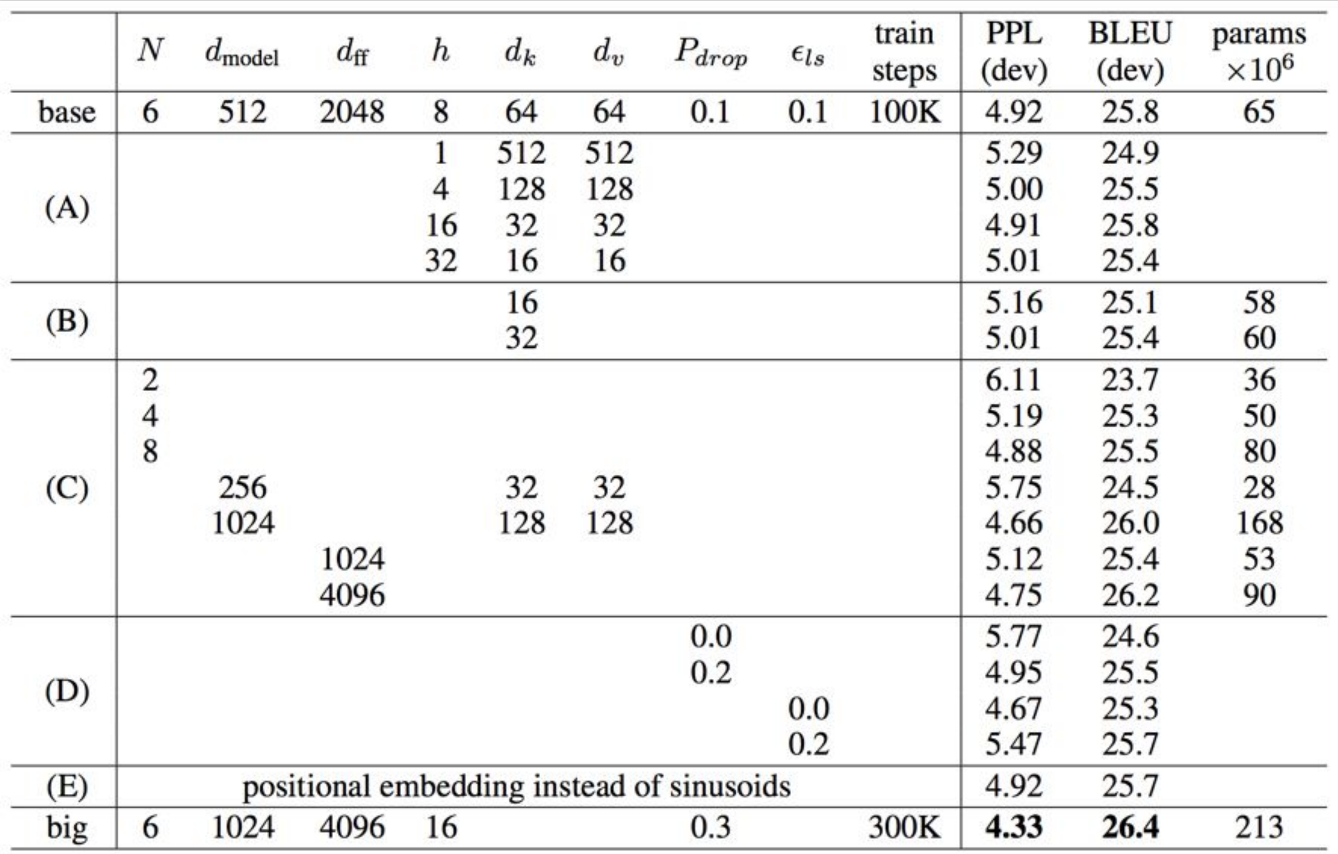
Checkpoint-averaging

Label smoothing

Auto-regressive decoding with beam search and length biasing
…

What Matters?

Resul



	N	d_{model}	d_{ff}	h	d_k	d_v	P_{drop}	ϵ_{ls}	train steps	PPL (dev)	BLEU (dev)	params $\times 10^6$
base	6	512	2048	8	64	64	0.1	0.1	100K	4.92	25.8	65
(A)				1	512	512				5.29	24.9	
				4	128	128				5.00	25.5	
				16	32	32				4.91	25.8	
				32	16	16				5.01	25.4	
(B)					16					5.16	25.1	58
					32					5.01	25.4	60
(C)	2									6.11	23.7	36
	4									5.19	25.3	50
	8									4.88	25.5	80
		256			32	32				5.75	24.5	28
		1024			128	128				4.66	26.0	168
			1024							5.12	25.4	53
			4096							4.75	26.2	90
(D)							0.0			5.77	24.6	
							0.2			4.95	25.5	
								0.0		4.67	25.3	
								0.2		5.47	25.7	
(E)	positional embedding instead of sinusoids									4.92	25.7	
big	6	1024	4096	16			0.3		300K	**4.33**	**26.4**	213

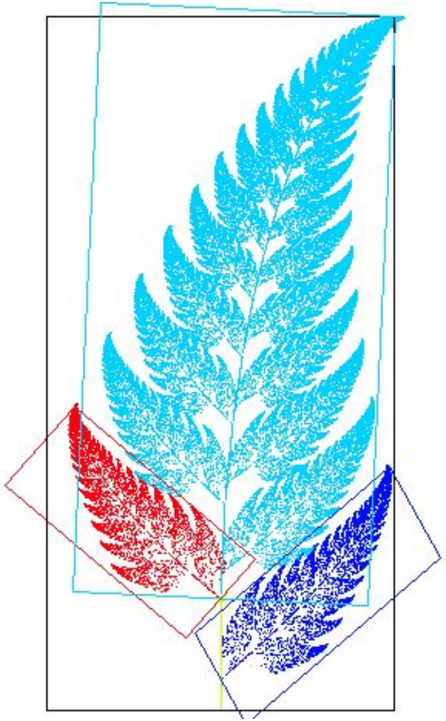
Generating Wikipedia by Summarizing Long Sequences

msaleh@ et al. submission to ICLR’18

	ROUGE
seq2seq-attention	12.7
Transformer-ED (L=500)	34.2
Transformer-DMCA (L=11000)	**36.2**

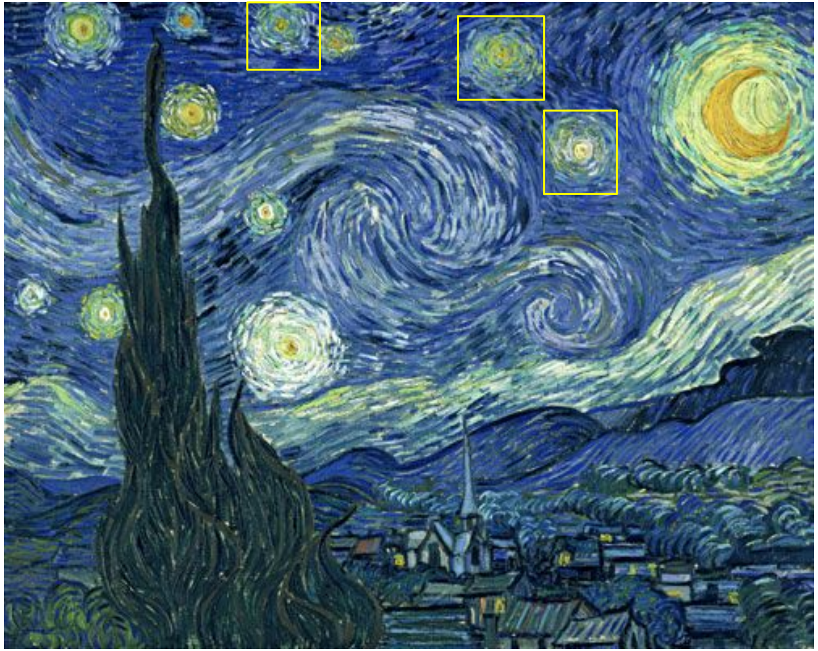
Self-Similarity, Image and Music Generation

Self-similarity in images



https://en.wikipedia.org/wiki/Self-similarity

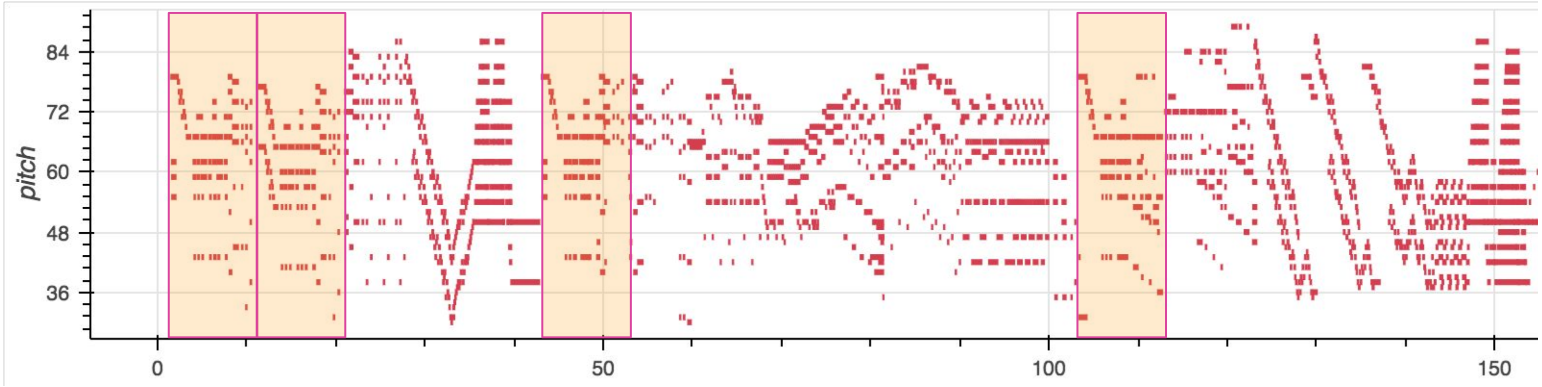
Self-Similarity in Images



Starry Night (Van Gogh, June 1889)

Self-similarity in music

Motifs repeat, immediately and also at a distance



Probabilistic Image Generation

Model the joint distribution of pixels

Turning it into a sequence modeling problem

Assigning probabilities allows measuring generalization

Probabilistic Image Generation

RNNs and CNNs are state-of-the-art (PixelRNN, PixelCNN)

CNNs incorporating gating now match RNNs in quality

CNNs are much faster due to parallelization

A Oord et al. (2016), Salimans et al. (2017), Kalchbrenner et al. (2016)

Probabilistic Image Generation

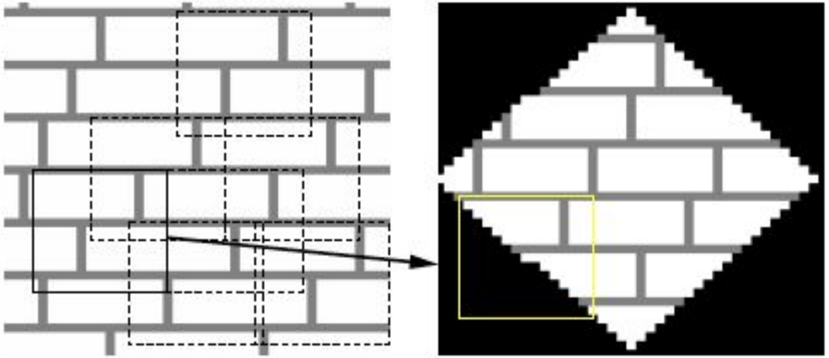
Long-range dependencies matter for images (e.g. symmetry)

Likely increasingly important with increasing image size

Modeling long-range dependencies with CNNs requires either

- **Many layers** likely making training harder
- **Large kernels** at large parameter/computational cost

Texture Synthesis with Self-Similarity



Texture Synthesis by Non-parametric Sampling (Efros and Leung, 1999)

Non-local Means

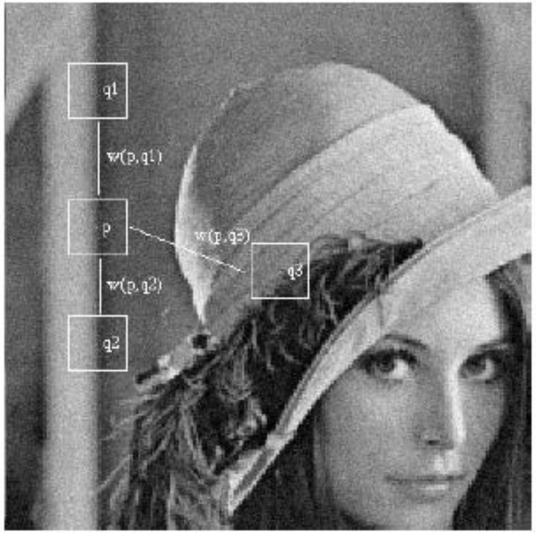


Figure 1. Scheme of NL-means strategy. Similar pixel neighborhoods give a large weight, w(p,q1) and w(p,q2), while much different neighborhoods give a small weight w(p,q3).

BCM 2005

Non-local Means

A Non-local Algorithm for Image Denoising (Buades, Coll, and Morel. CVPR 2005)

Non-local Neural Networks (Wang et al., 2018)

Previous work

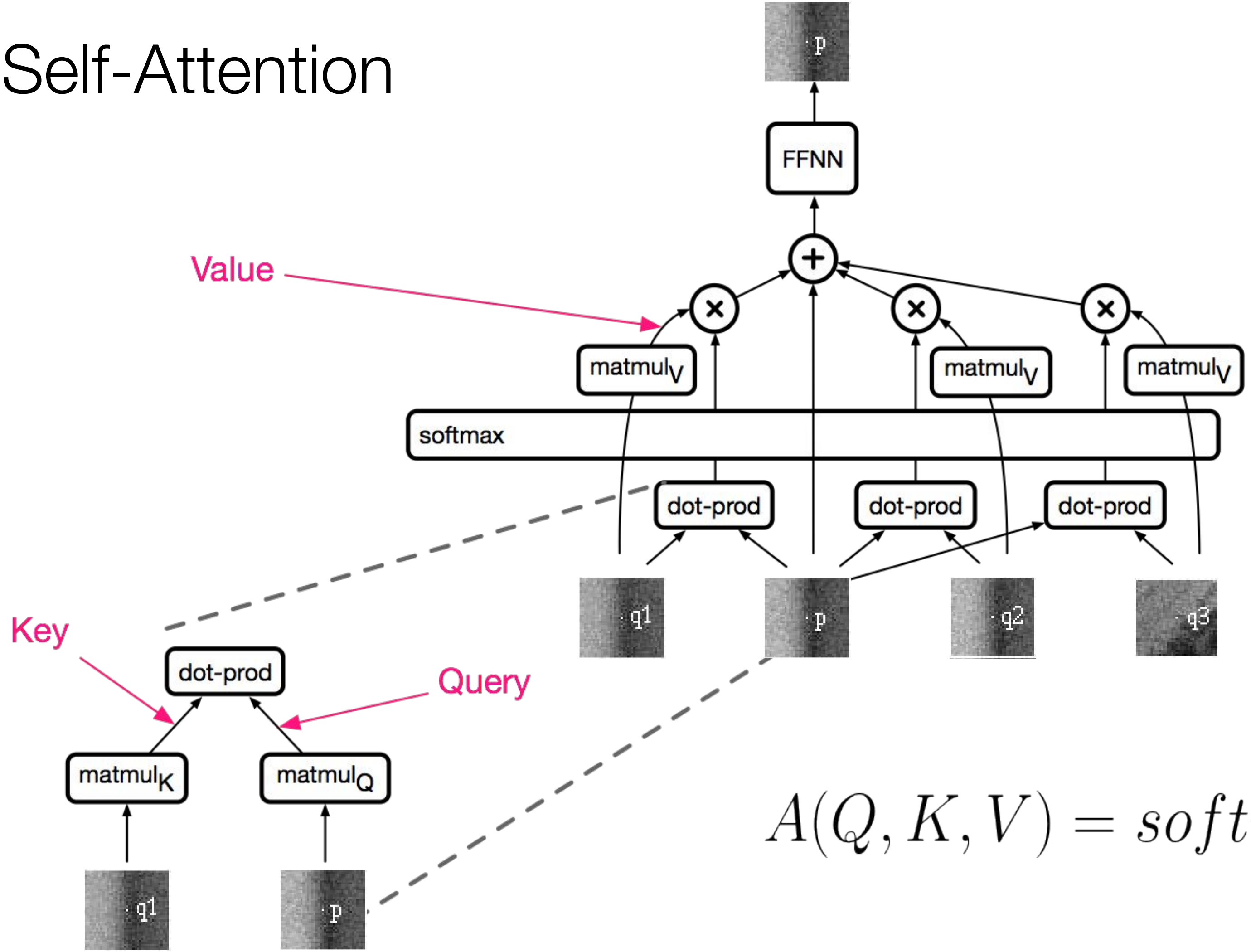
Self-attention:

Parikh et al. (2016), Lin et al. (2016), Vaswani et al. (2017)

Autoregressive Image Generation:

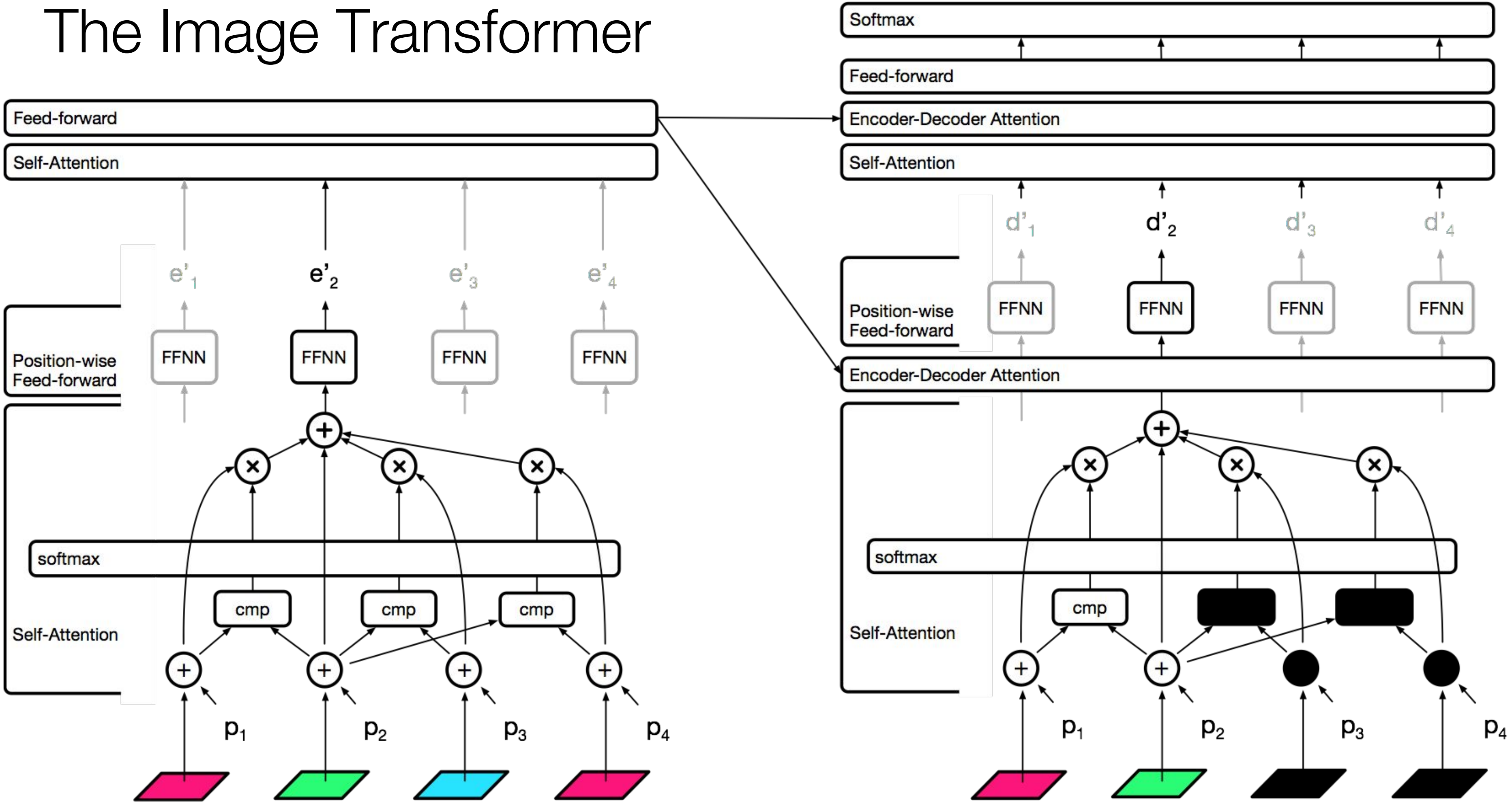
A Oord et al. (2016), Salimans et al. (2017)

Self-Attention

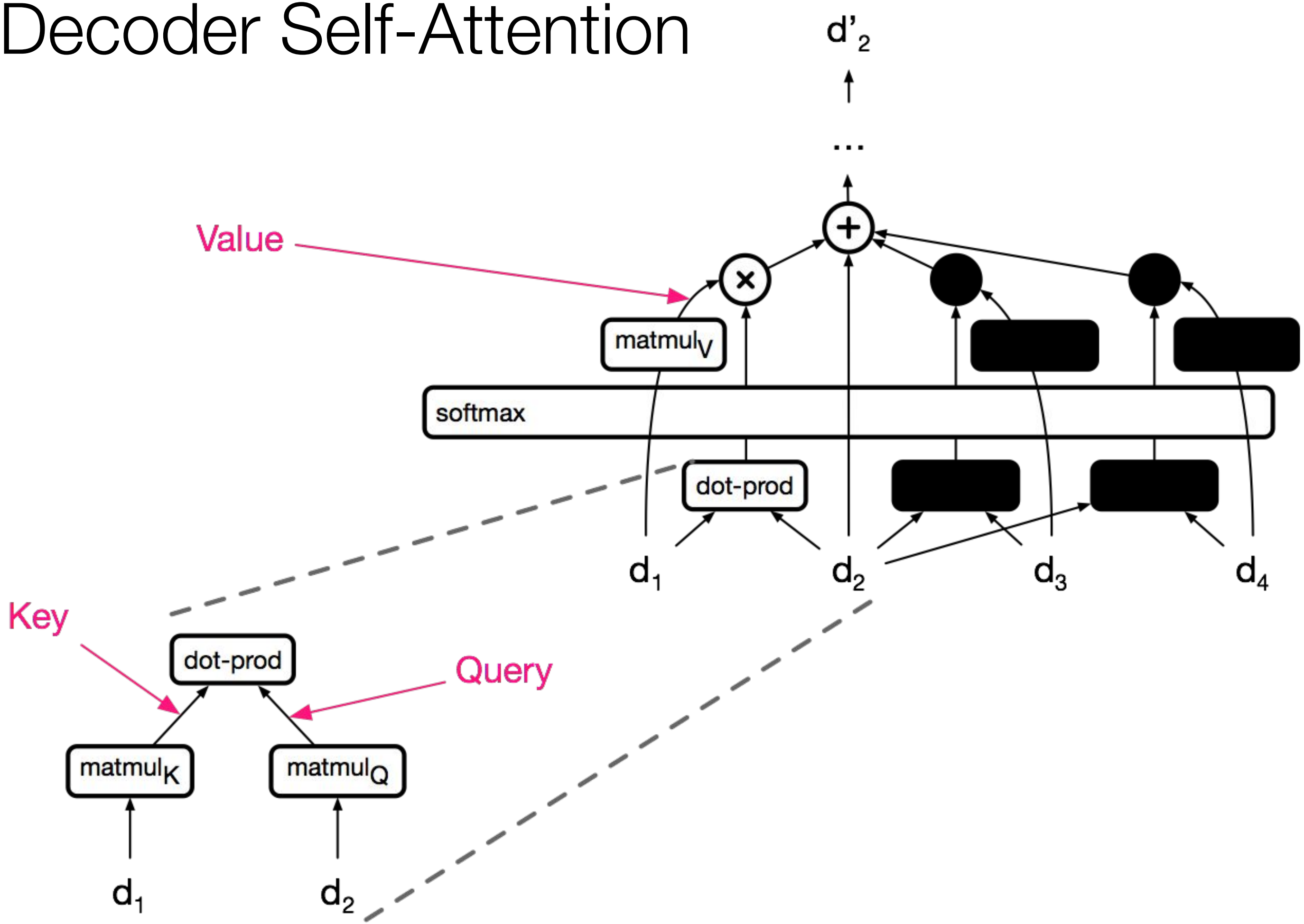


$$A(Q,K,V) = softmax(\frac{QK^T}{\sqrt{d_k}})V$$

The Image Transformer



Decoder Self-Attention



Attention is Cheap!

	FLOPs
Self-Attention	$O(\text{length}^2 \cdot \text{dim})$
RNN (LSTM)	$O(\text{length} \cdot \text{dim}^2)$
Convolution	$O(\text{length} \cdot \text{dim}^2 \cdot \text{kernel\_width})$

Attention is Cheap if length << dim!

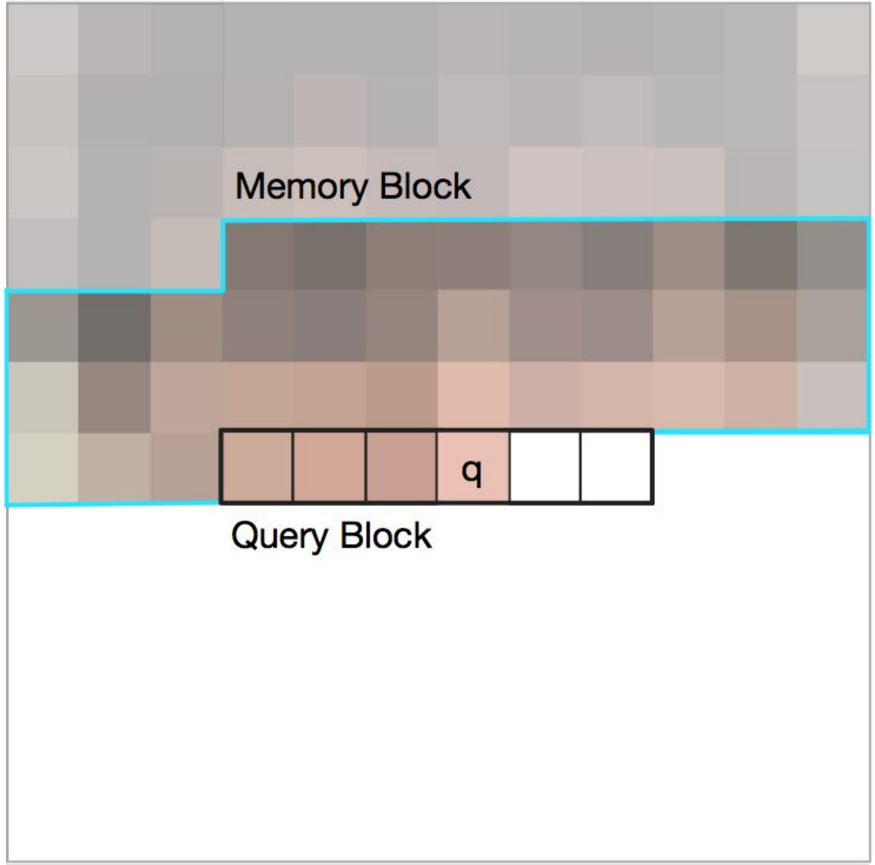
	FLOPs
Self-Attention	$O(\text{length}^2 \cdot \text{dim})$ (length=3072 for images)
RNN (LSTM)	$O(\text{length} \cdot \text{dim}^2)$
Convolution	$O(\text{length} \cdot \text{dim}^2 \cdot \text{kernel\_width})$

Combining Locality with Self-Attention

Restrict the attention windows to be local neighborhoods

Good assumption for images because of spatial locality

Local 1D Attention



Local 2D Attention

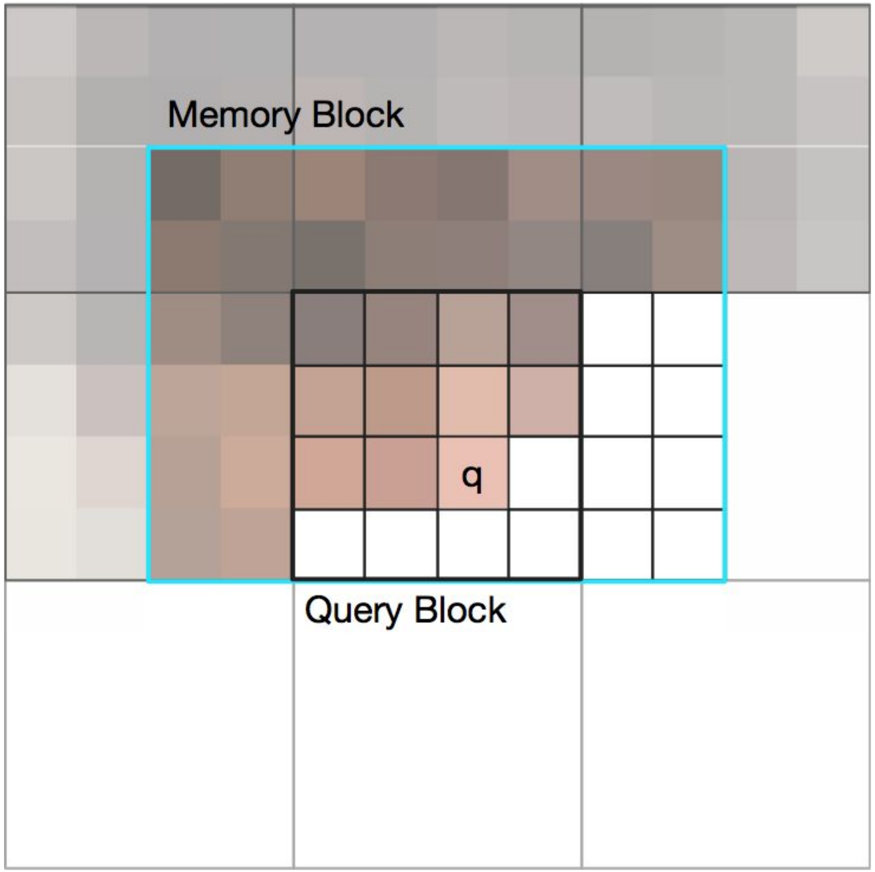
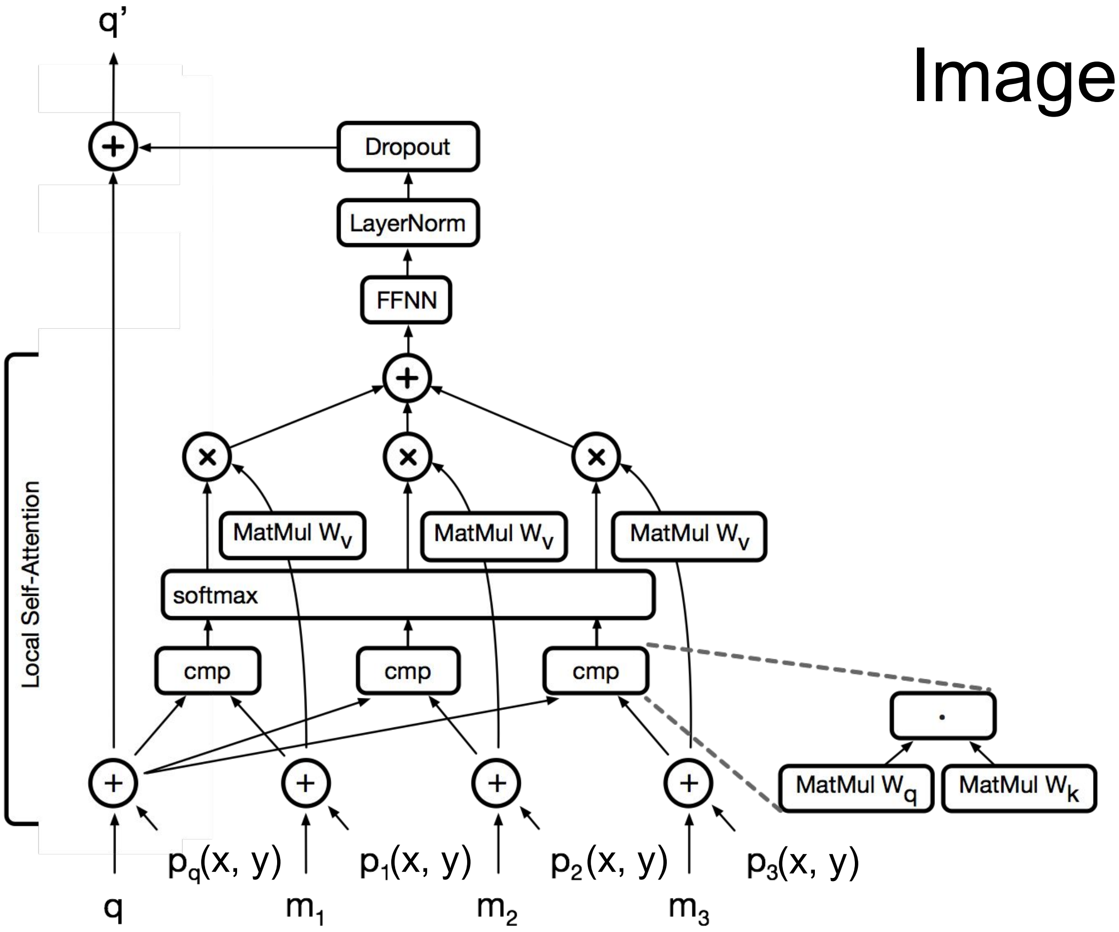


Image Transformer Layer



Tasks

Super-resolution

Unconditional and Conditional Image generation

Results

Image Transformer

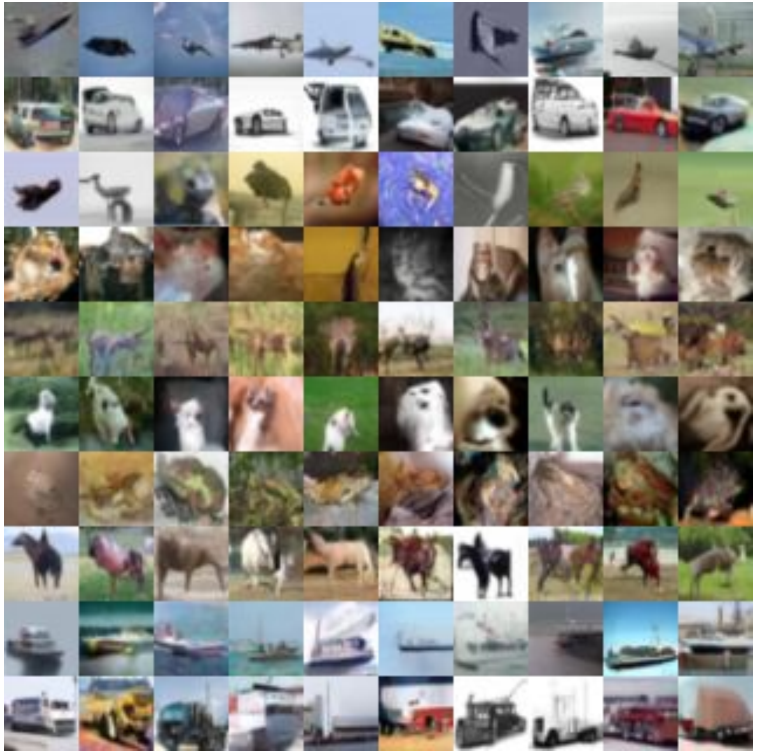
Parmar*, Vaswani*, Uszkoreit, Kaiser, Shazeer, Ku, and Tran. ICML 2018

Unconditional Image Generation

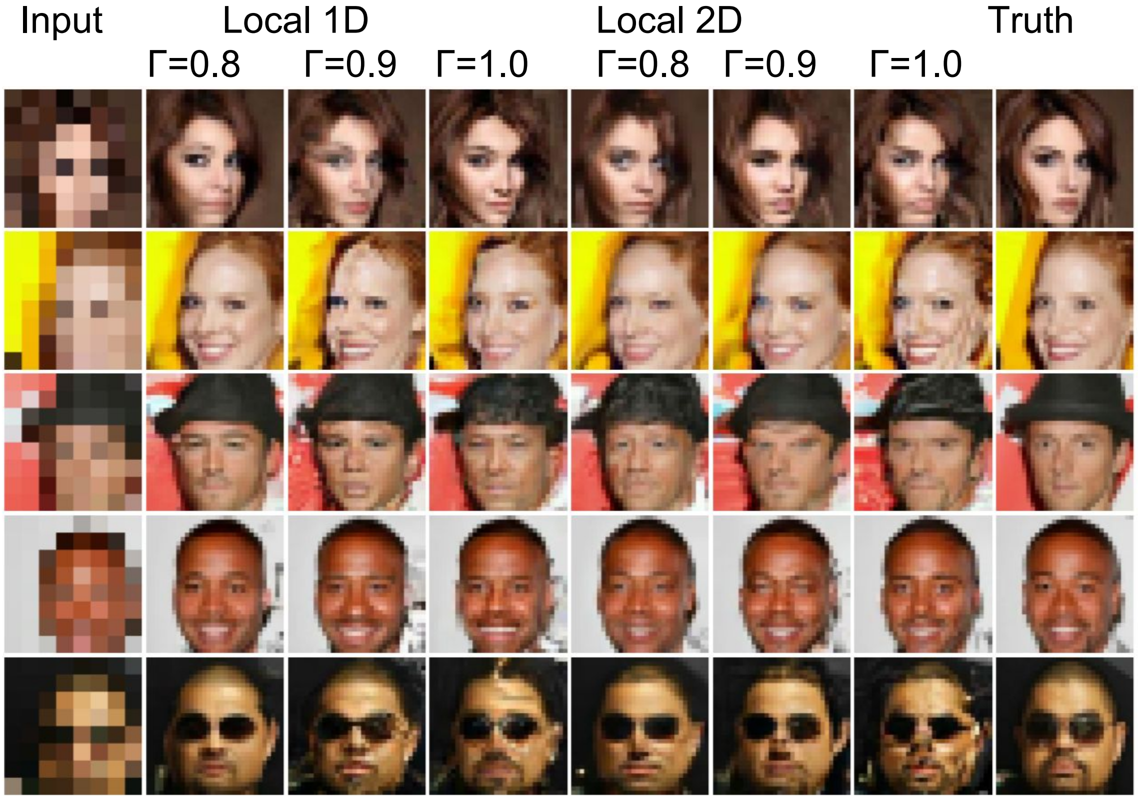
	Cifar-10 (Test)	Imagenet (Validation)
PixelRNN	3.00	3.86
Gated PixelCNN	3.03	3.83
PixelCNN++	2.92 (dmol)	-
PixelSNAIL	**2.85**	3.8
Image Transformer, 1D local	2.9 (xent)	**3.77**
Image Transformer, 1D local	2.9 (dmol)	3.78

Cross entropy of various models on CIFAR-10 and Imagenet datasets.

Cifar10 Samples



CelebA Super Resolution



Input

Local 1D

Γ=0.8 Γ=0.9 Γ=1.0

Local 2D

Γ=0.8 Γ=0.9 Γ=1.0

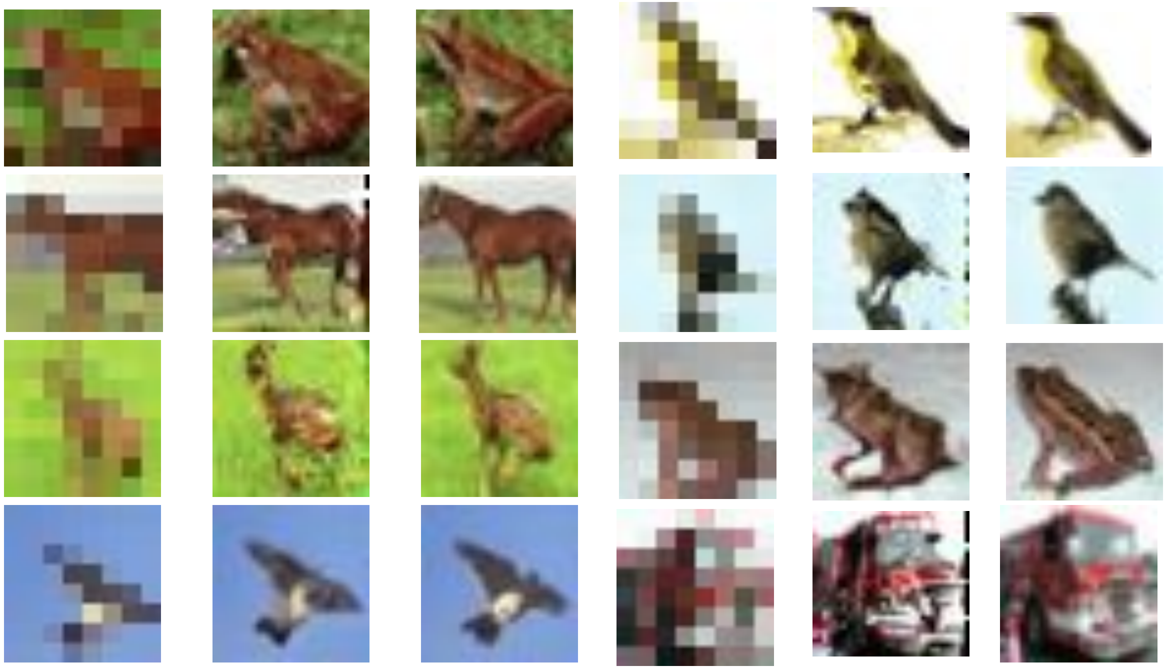
Truth

CelebA Super Resolution

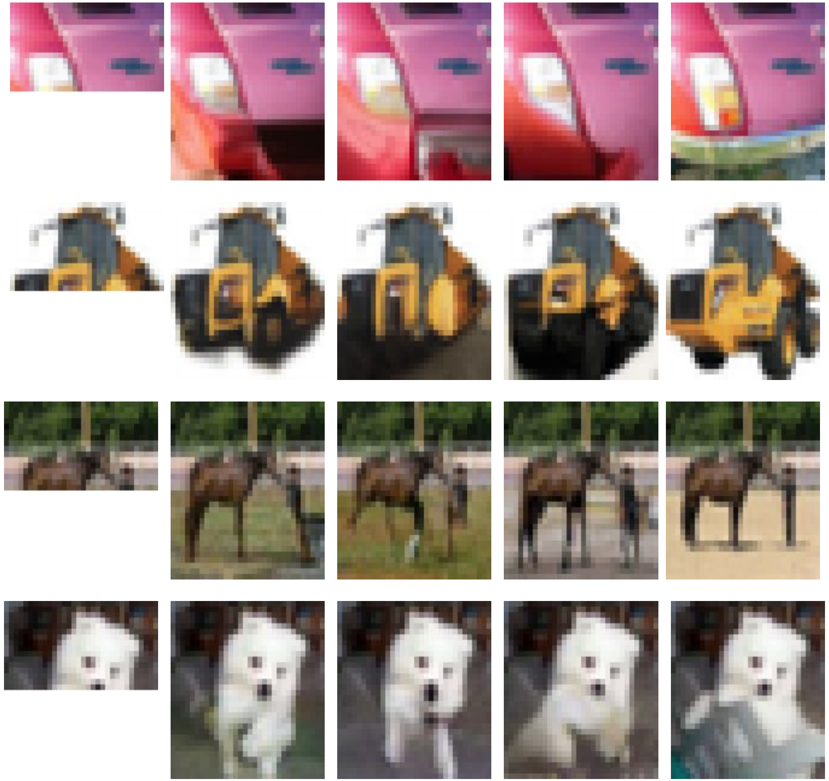
	% Fooled			
	Γ = n/a	Γ = 1.0	Γ = 0.9	Γ = 0.8
ResNet	4.0	-	-	-
srez GAN (Garcia, 2016)	8.5	-	-	-
Pixel Recursive (Dahl et al., 2017)	-	11.0	10.4	10.25
Image Transformer, 1D local		**35.94** ± 3.0	33.5 ± 3.5	29.6 ± 4.0
Image Transformer, 2D local		**36.11** ±2.5	34 ± 3.5	30.64 ± 4.0

Human Eval performance for the Image Transformer on CelebA. The fraction of humans fooled is significantly better than the previous state of art.

Cifar10 SuperResolution



Conditional Image Completion



Music generation using relative self-attention

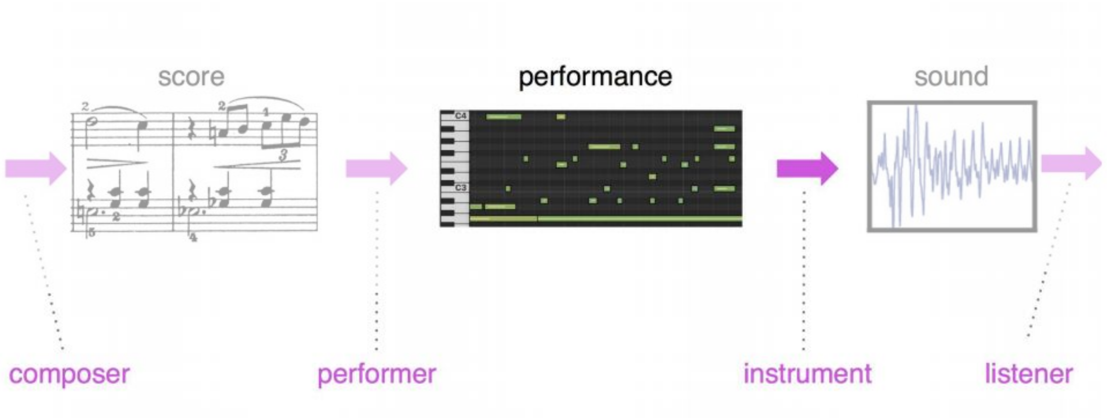
Music Transformer (ICLR 2019) by Cheng-Zhi Anna Huang, Ashish Vaswani, Jakob Uszkoreit, Noam Shazeer, Ian Simon, Curtis Hawthorne, Andrew M. Dai, Matthew D. Hoffman, Monica Dinculescu and Douglas Eck.

Blog post: https://magenta.tensorflow.org/music-transformer

Raw representations in music and language

Language text → speech

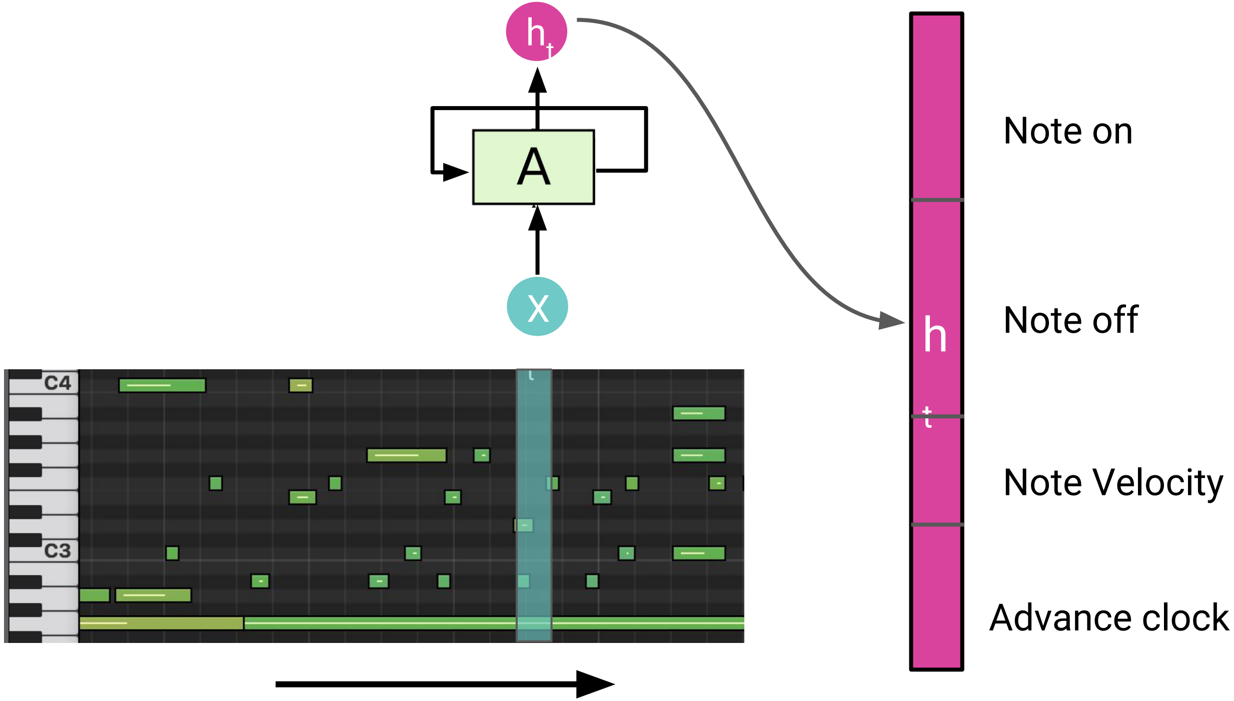
Music



(Image from Simon & Oore, 2016)

Music Language model:

Prior work Performance RNN (Simon & Oore, 2016)



Note on

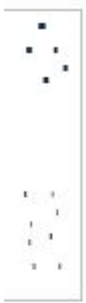
Note off

Note Velocity

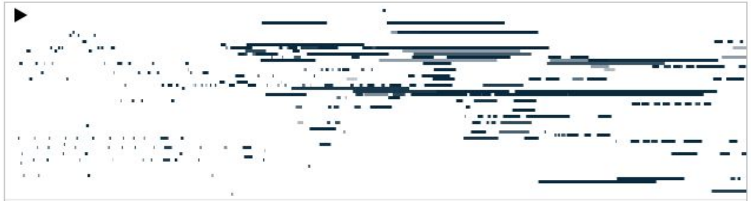
Advance clock

Continuations to given initial motif

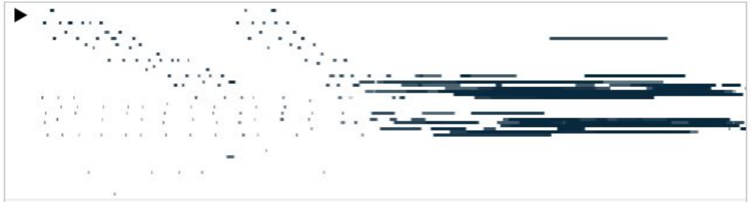
Given motif



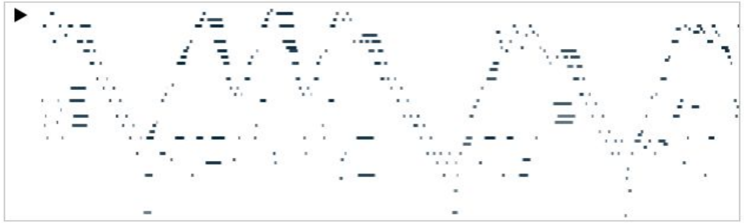
RNN-LSTM



Transformer



Music Transformer



Continuations to given initial motif

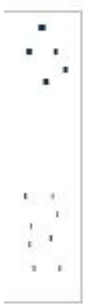
Given
motif

Continuations to given initial motif

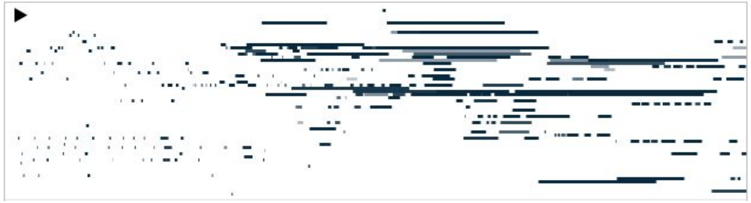
Given
motif

Continuations to given initial motif

Given motif



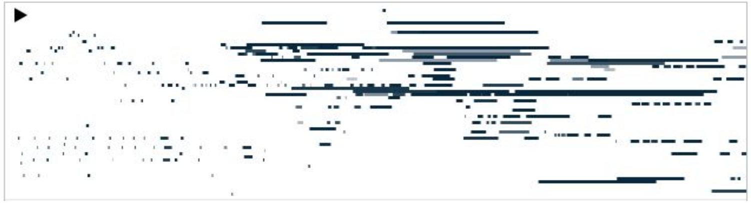
RNN-LSTM



Continuations to given initial motif

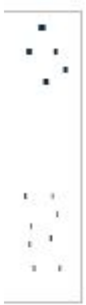
Given motif

RNN-LSTM 🔊

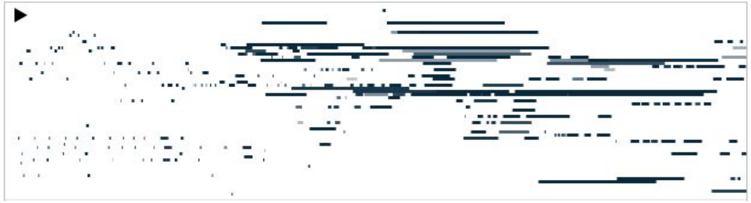


Continuations to given initial motif

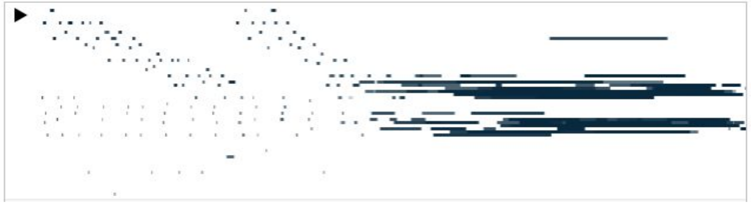
Given motif



RNN-LSTM

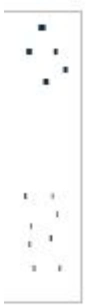


Transformer



Continuations to given initial motif

Given motif



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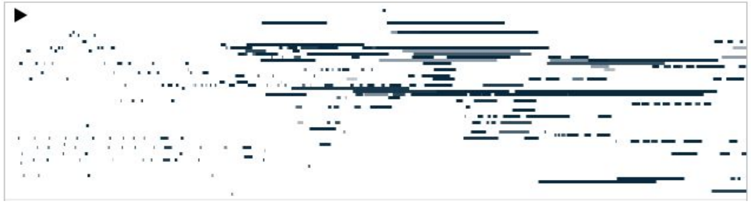
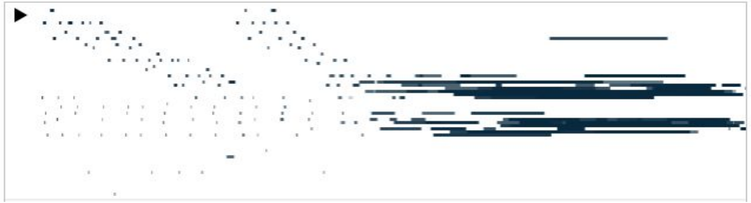
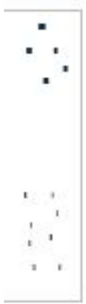


Transformer

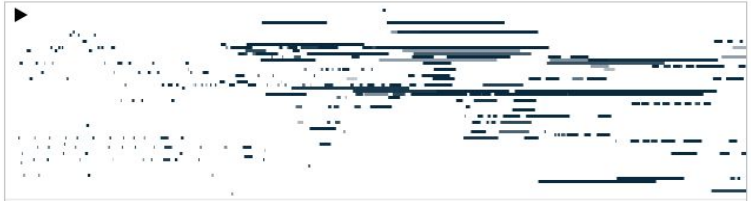


Continuations to given initial motif

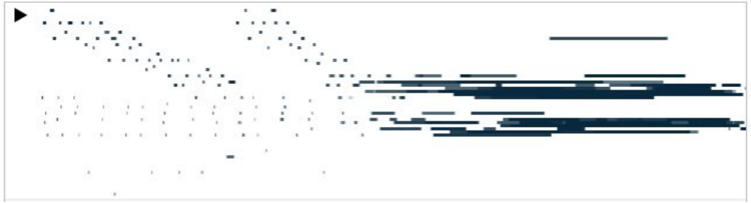
Given motif



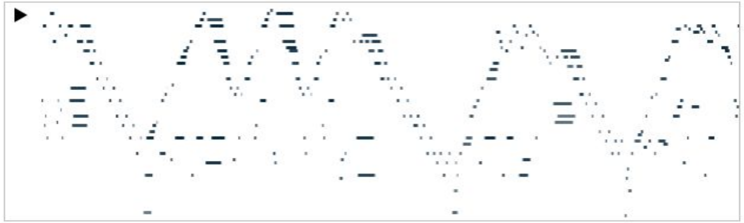
RNN-LSTM



Transformer

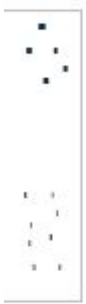


Music Transformer

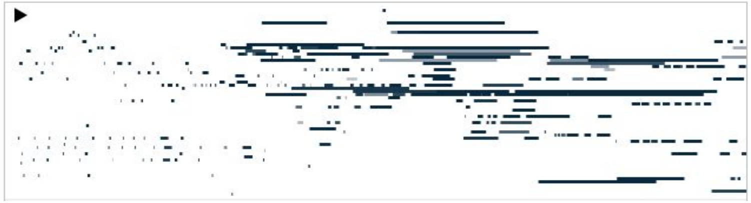


Continuations to given initial motif

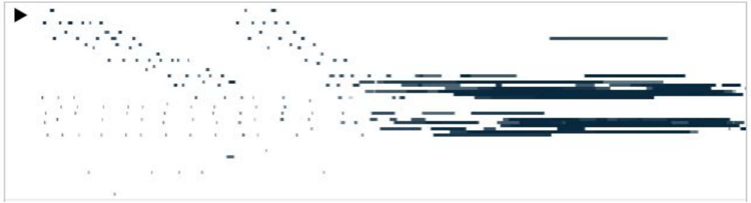
Given motif



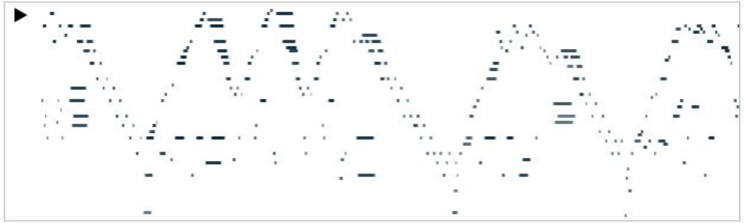
RNN-LSTM



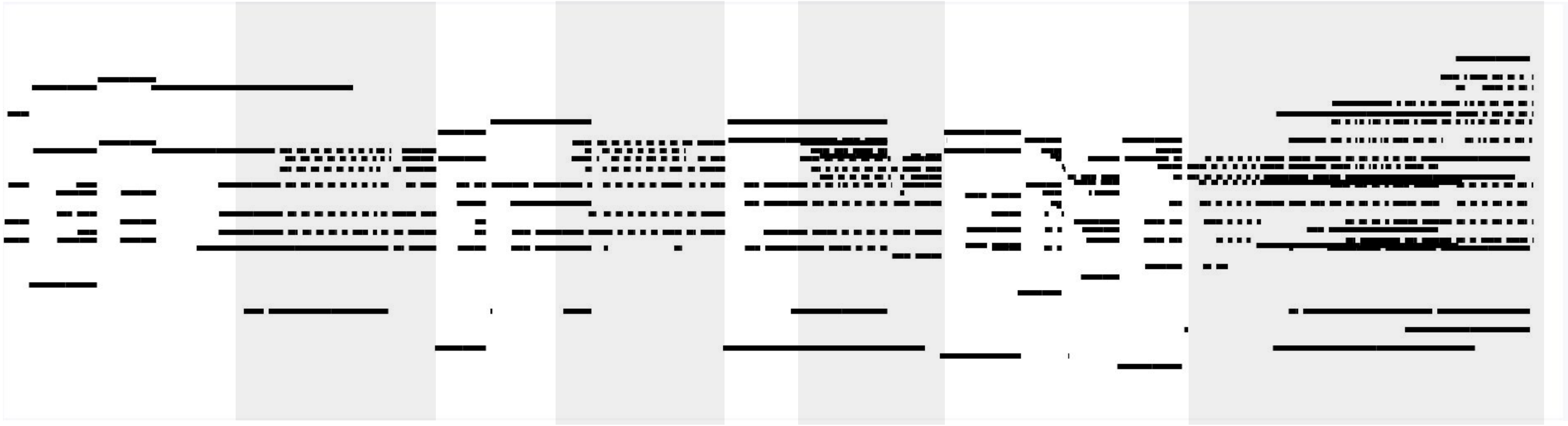
Transformer



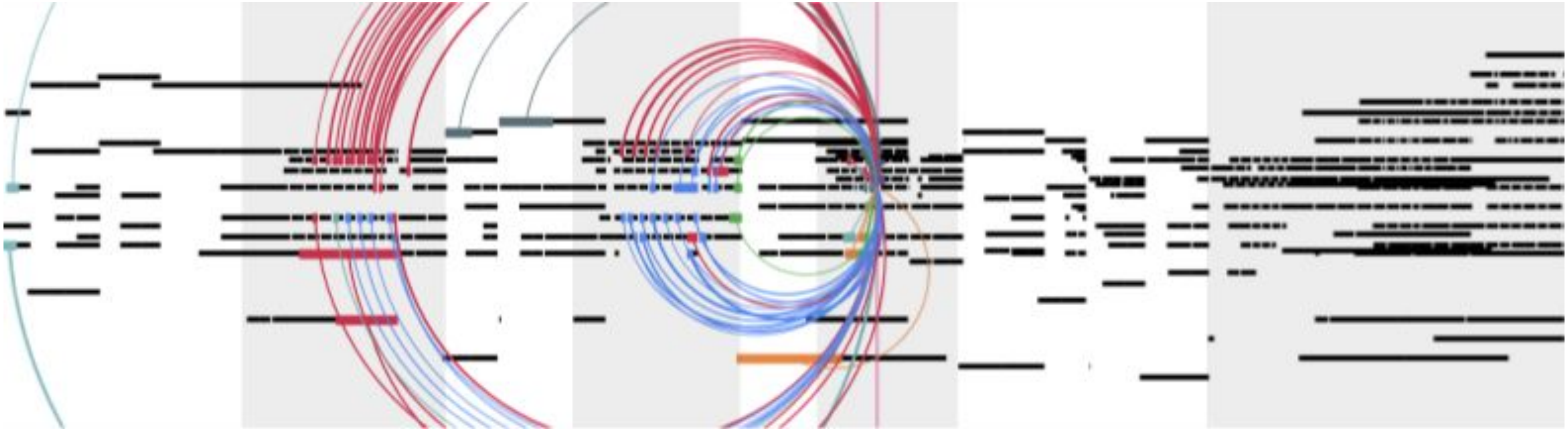
Music Transformer



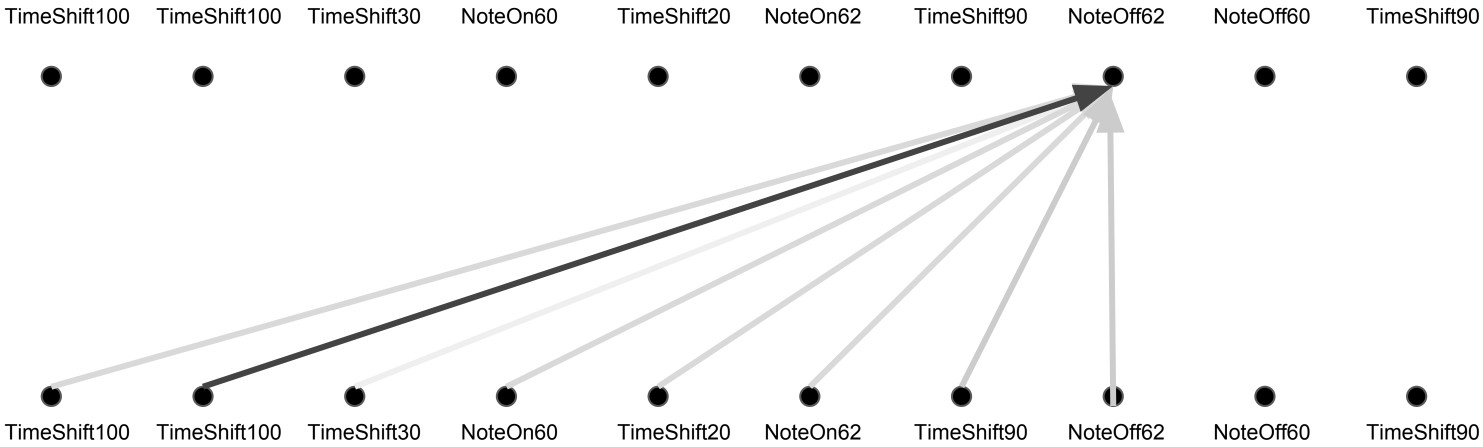
Self-Similarity in Music



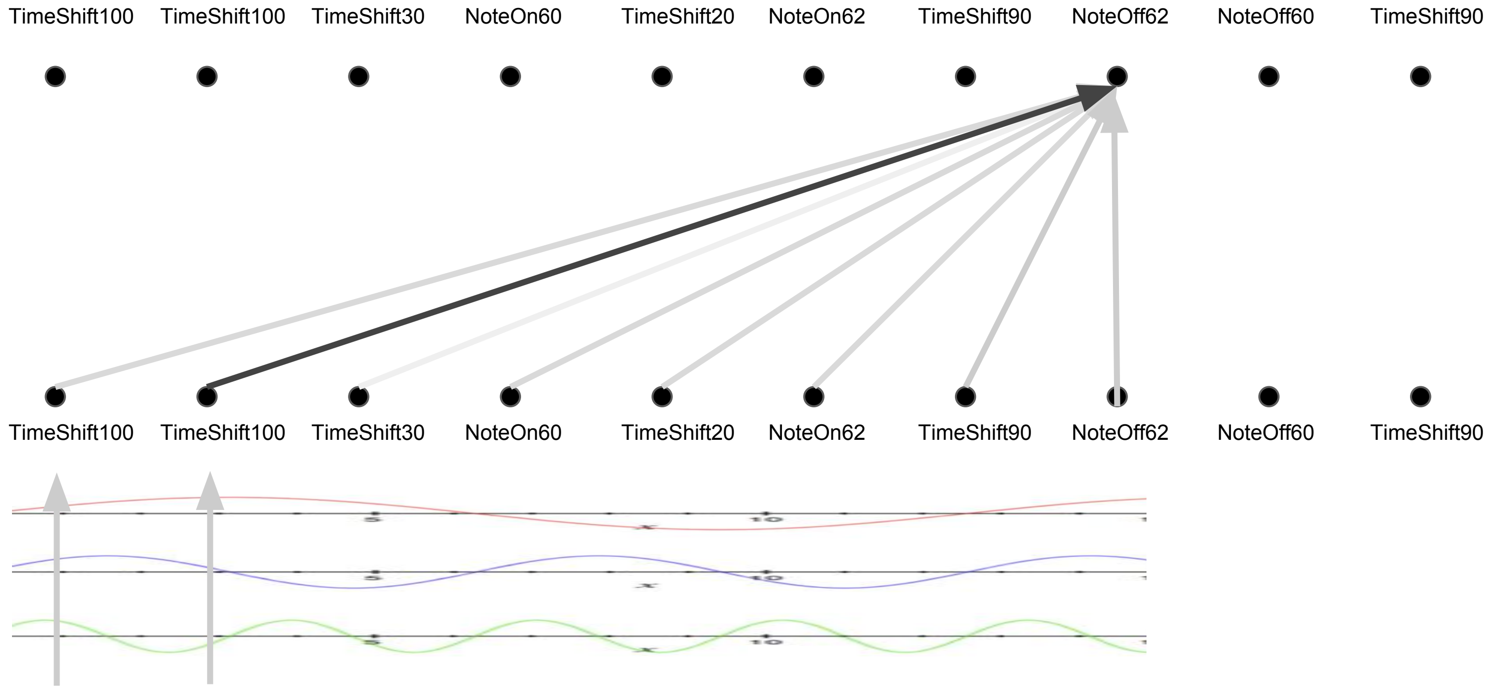
Sample from Music Transformer



Attention: a weighted average



Attention: a weighted average

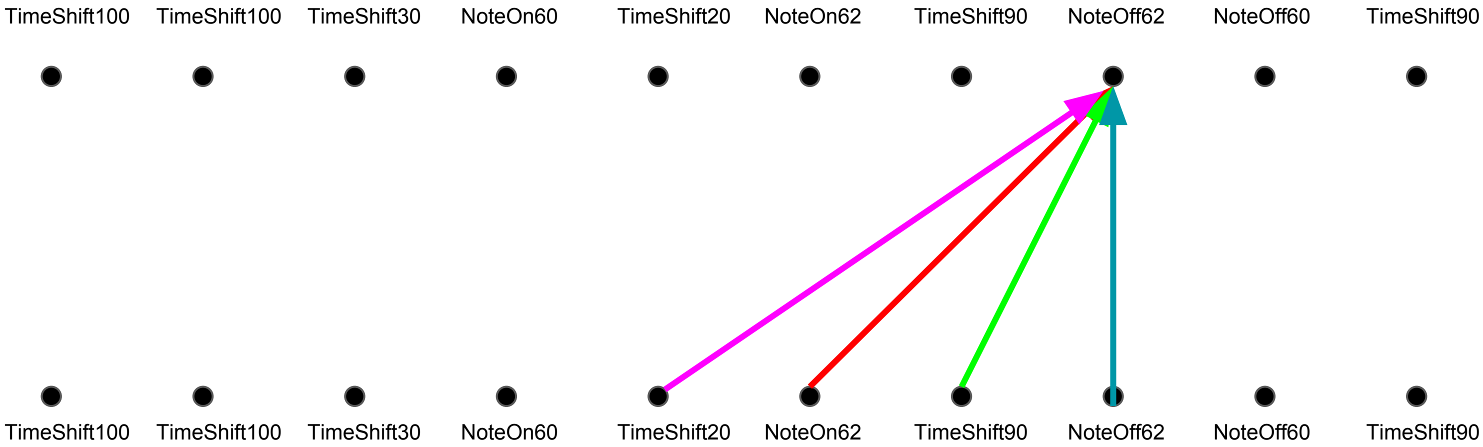


TimeShift100 TimeShift100 TimeShift30 NoteOn60 TimeShift20 NoteOn62 TimeShift90 NoteOff62 NoteOff60 TimeShift90

TimeShift100 TimeShift100 TimeShift30 NoteOn60 TimeShift20 NoteOn62 TimeShift90 NoteOff62 NoteOff60 TimeShift90

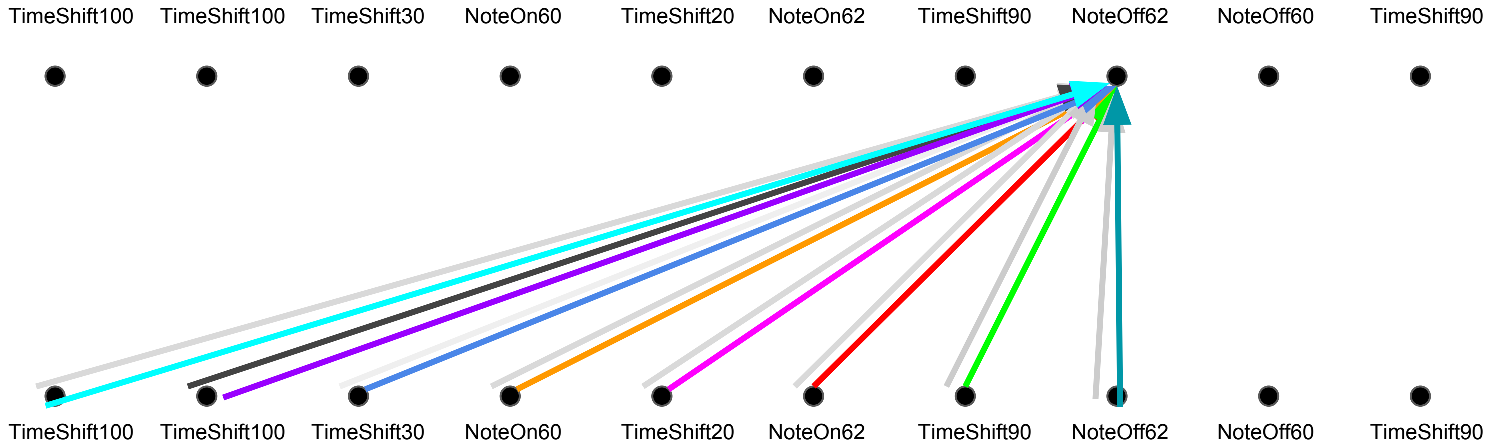
Convolution:

Different linear transformations by relative position.



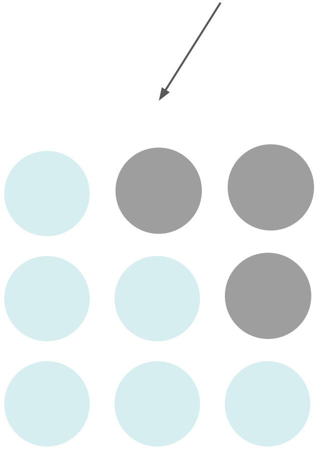
Relative attention (Shaw et al, 2018)

Multihead attention + convolution?



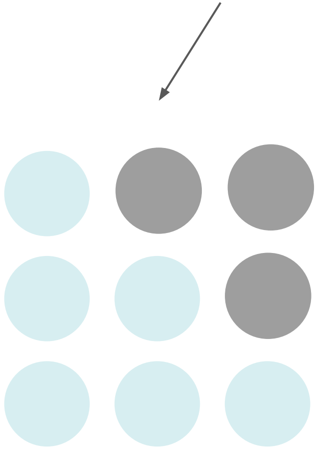
Closer look at attention

$$softmax(QK^\top)$$

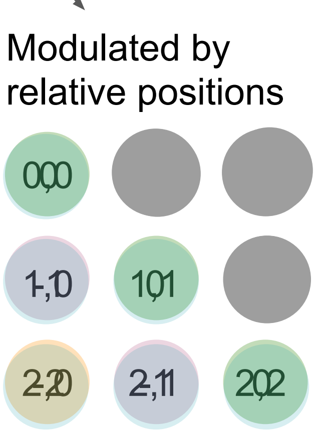


Closer look at relative attention

$$softmax(QK^\top + Qf(E_{rel}))$$



Modulated by relative positions



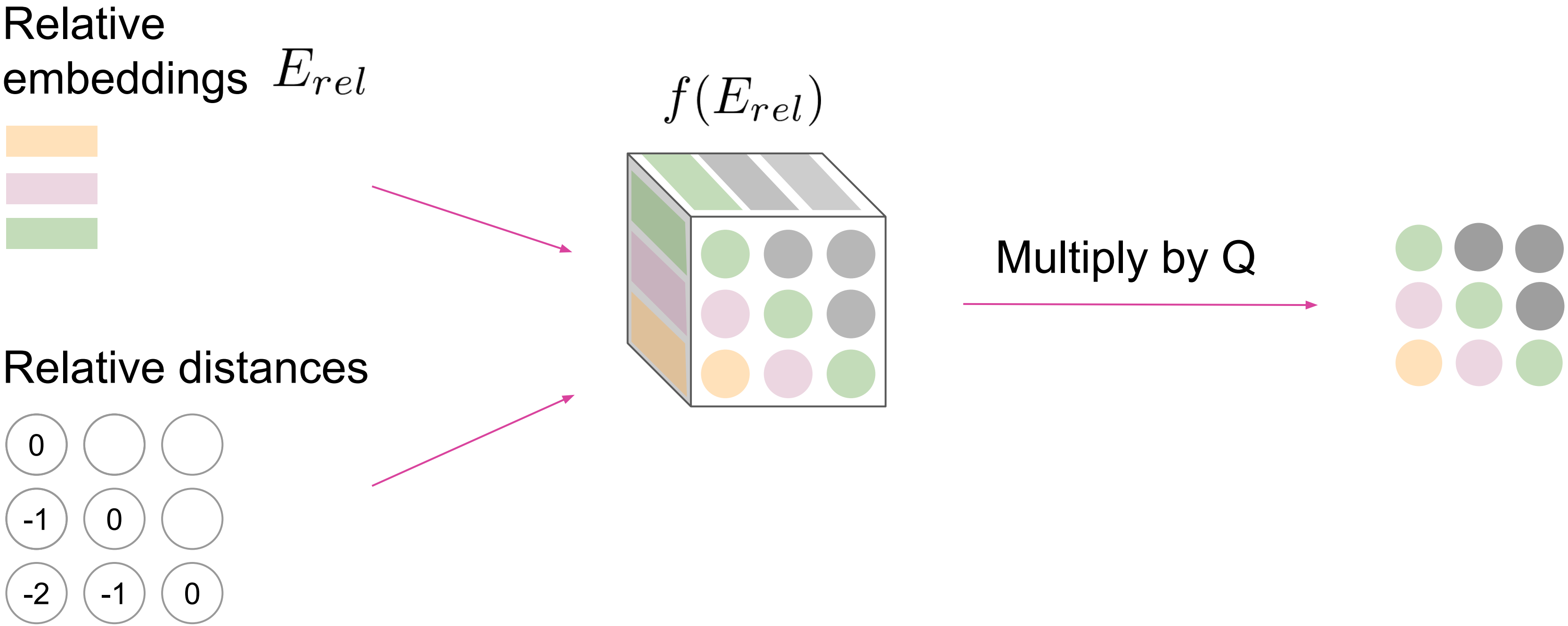
Machine Translation (Shaw et al, 2018)

Model	Position Representation	BLEU En-De	BLEU En-Fr
Transformer Big	Absolute	27.9	41.3
Transformer Big	Relative	**29.2**	**41.5**

Previous work O(L²D): **8.5 GB** per layer (Shaw et al, 2018)

Per layer, L=2048, D=512

$$softmax(QK^\top + Qf(E_{rel}))$$



Relative embeddings E_{rel}

Relative distances

0		
-1	0	
-2	-1	0

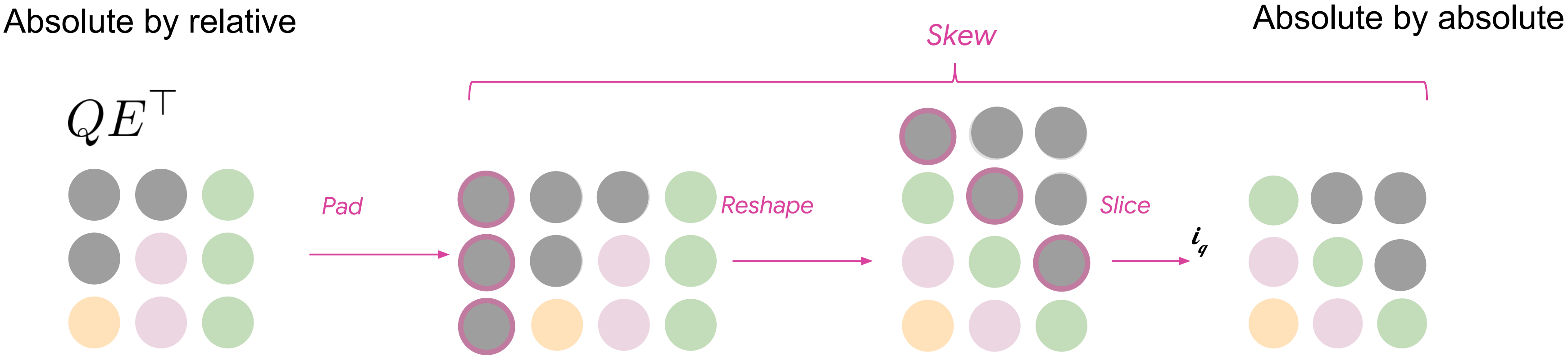
$f(E_{rel})$

Multiply by Q

Our formulation O(LD): **4.2 MB** per layer

$$softmax(QK^\top + skew(QE_{rel}^\top))$$

Per layer, L=2048, D=512

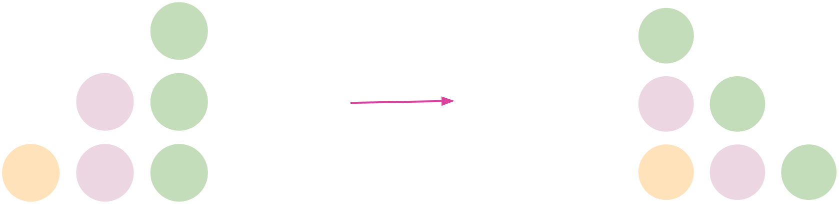


Goal of skewing procedure

Indexed by

absolute by relative

absolute by absolute



Skewing to reduce relative memory from $O(L^2D)$ to $O(LD)$

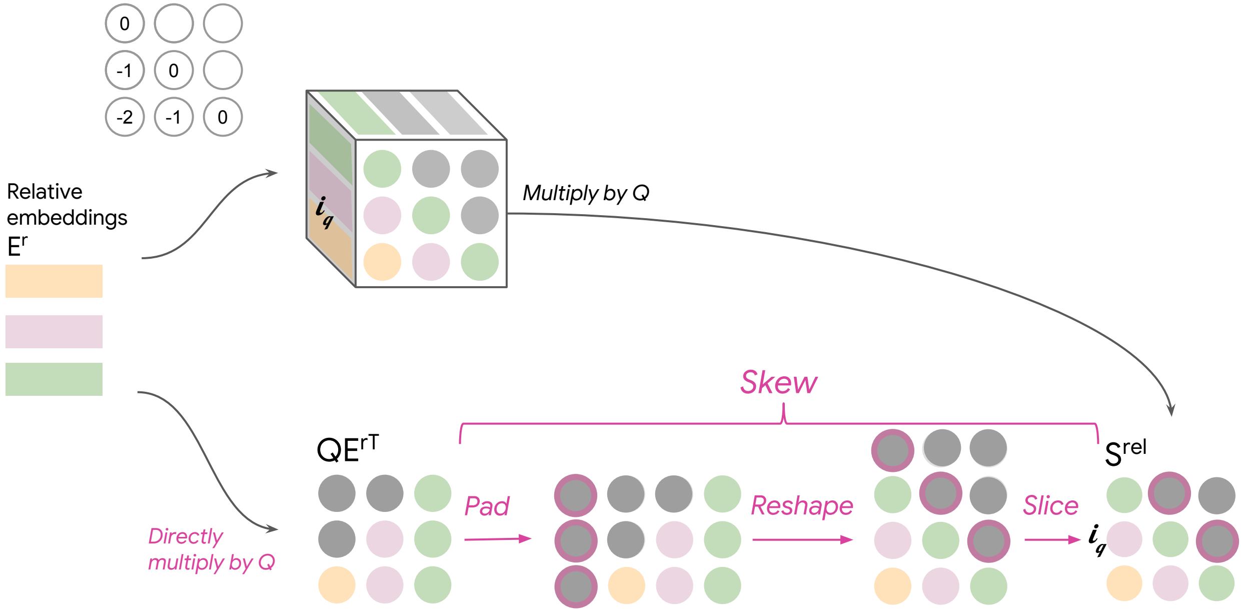
Per layer, L=2048, D=512

Previous work

$O(L^2D)$: **8.5 GB**

Our work

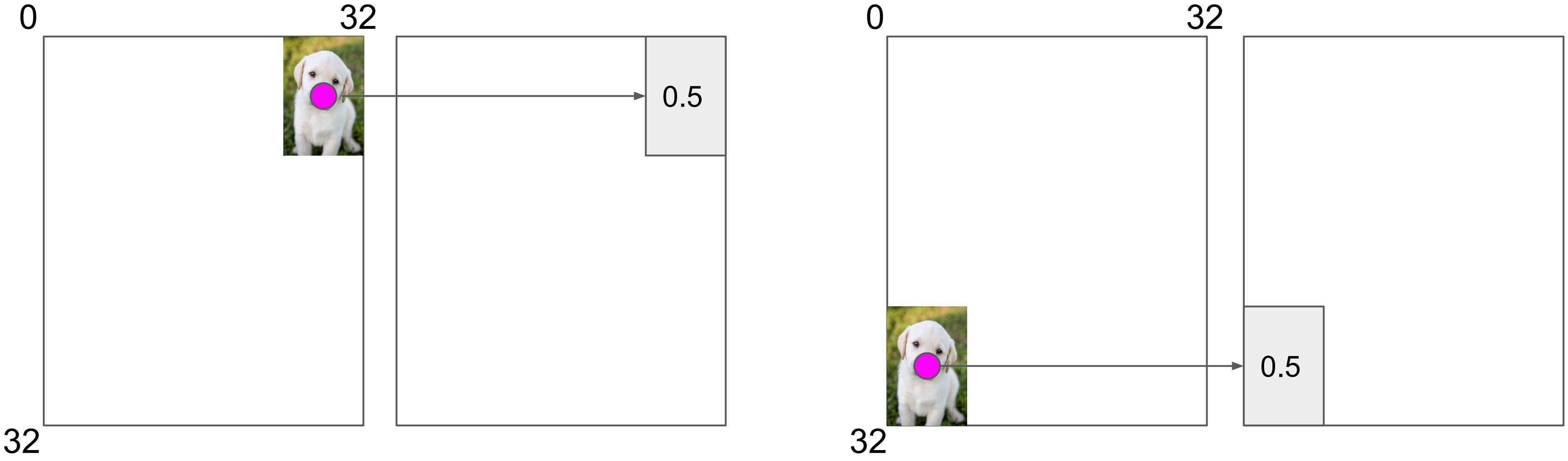
$O(LD)$: **4.2 MB**



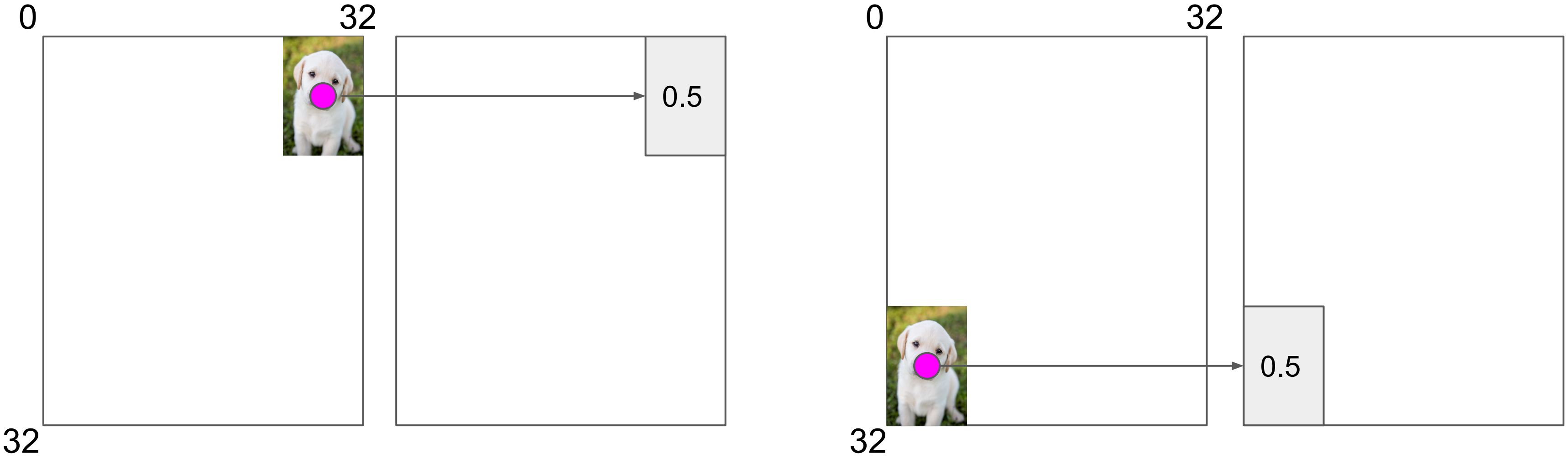
A Jazz sample from Music Transformer

A Jazz sample from Music Transformer

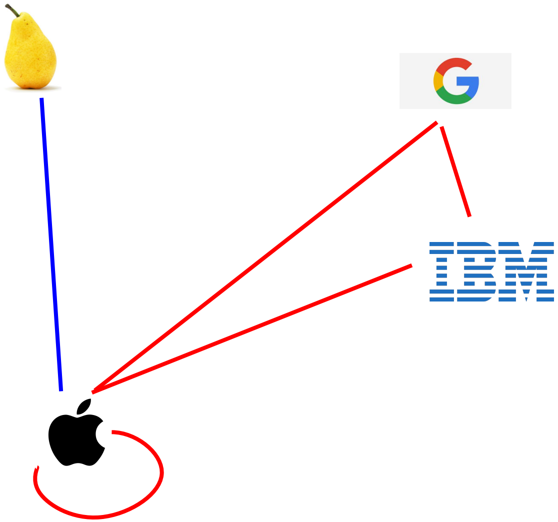
Convolutions and Translational Equivariance



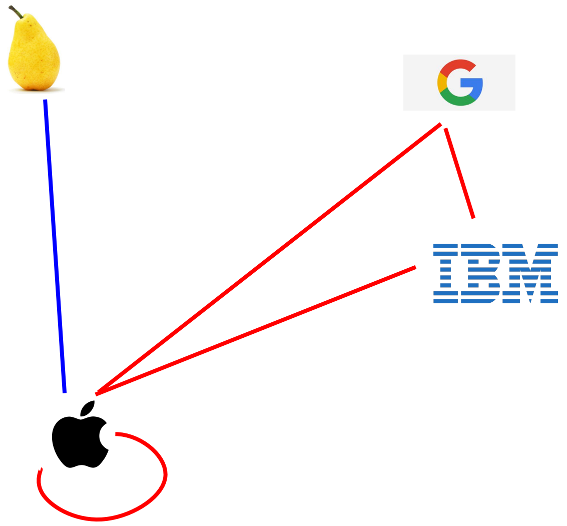
Relative positions Translational Equivariance

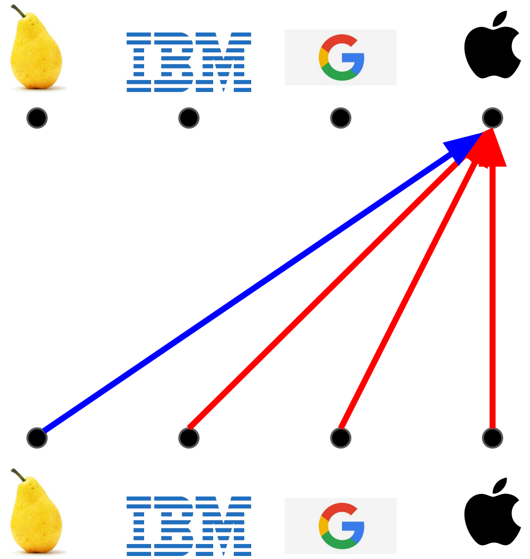


Relative Attention And Graphs



Relative Attention And Graphs

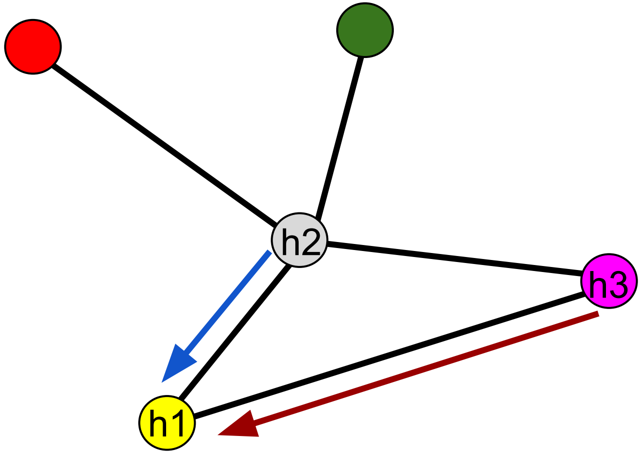




Relational inductive biases, deep learning, and graph networks. (Battaglia et al., 2018)

Self-Attention With Relative Position Representations (Shaw et al., 2018)

Message Passing Neural Networks



$$m_v^{t+1} = \sum_{w \in N(v)} M_t(h_v^t, h_w^t, e_{vw})$$

$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1})$$

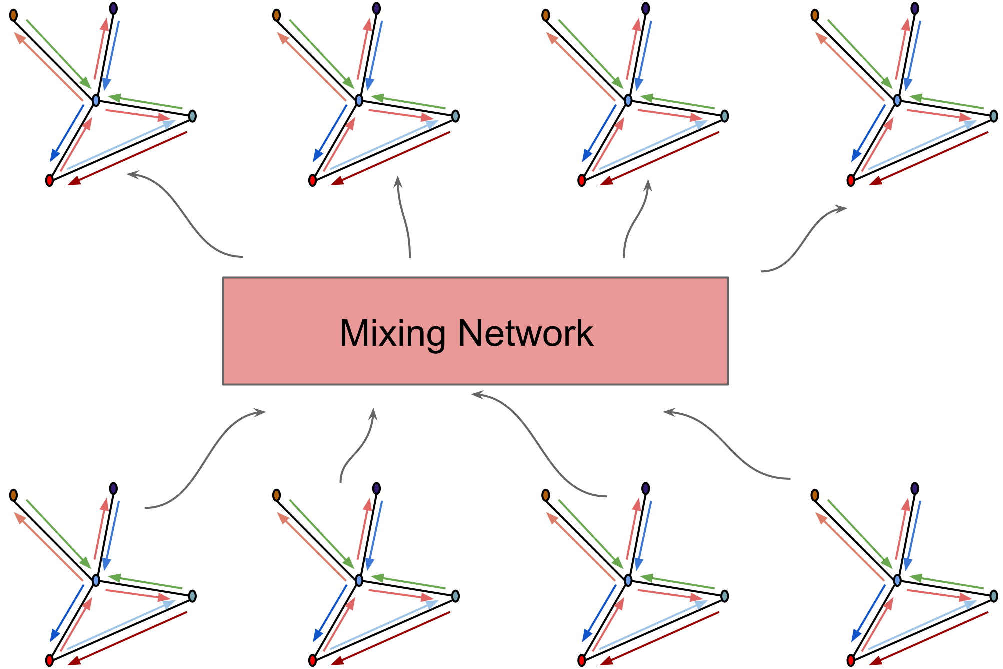
$$\hat{y} = R(\{h_v^T | v \in G\})$$

Neural Message Passing For Quantum Chemistry. Gilmer et al. ICML 2017

Google

Slide credit: Justin Gilmer

Multiple Towers



- Run k smaller copies of the MPNN in parallel.
- Mix node states after each message pass.
- Offers a factor of k speedup for the same node dimension d (> 2x speedup when d=200).
- Also helped improve performance when used with matrix multiply message function.

Slide credit: Justin Gilmer

Graph Library

Code

With Justin Gilmer, Jonathan Frankle, and David Bieber

Self-Attention

Constant ‘path length’ between any two positions.

Unbounded memory.

Trivial to parallelize (per layer).

Models Self-Similarity.

Relative attention provides expressive timing, equivariance, and extends naturally to graphs.

Active Research Area

Non autoregressive transformer (Gu and Bradbury et al., 2018)

Deterministic Non-Autoregressive Neural Sequence Modeling by Iterative Refinement
(Lee, Manismov, and Cho, 2018)

Fast Decoding in Sequence Models Using Discrete Latent Variables (ICML 2018)
Kaiser, Roy, Vaswani, Pamar, Bengio, Uszkoreit, Shazeer

Towards a Better Understanding of Vector Quantized Autoencoders
Roy, Vaswani, Parmar, Neelakantan, 2018

Blockwise Parallel Decoding For Deep Autogressive Models (NeurIPS 2019)
Stern, Shazeer, Uszkoreit,

Transfer learning

Improving Language Understanding by Generative Pre-Training (Radford, Narsimhan, Salimans, and Sutskever)

BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding (Devlin, Chang, Lee, and Toutanova)

Optimization and Large Models

Adafactor: Adaptive Learning Rates with Sublinear Memory Cost (ICML 2018). Shazeer, Stern.

Memory-Efficient Adaptive Optimization for Large-Scale Learning (2019). Anil, Gupta, Koren, Singer.

Mesh-TensorFlow: Deep Learning for Supercomputers (NeurIPS 2019). Shazeer, Cheng, Parmar, Tran, Vaswani, Koanantakool, Hawkins, Lee, Hong, Young, Sepassi, Hechtman) Code (5 billion parameters)

Self-attention in Other Work.

Generating Wikipedia by Summarizing Long sequences. (ICLR 2018). Liu, Saleh, Pot, Goodrich, Sepassi, Shazeer, Kaiser.

Universal Transformers (ICLR 2019). Deghiani*, Gouws*, Vinyals, Uszkoreit, Kaiser.

Transformer-XL: Attentive Language Models Beyond a Fixed-Length Context (2019). Dai, Yang, Yang, Carbonell, Le, Salakhutdinov.

A Time-Restricted Self-Attention Layer for ASR (ICASSP 2018). Povey, Hadian, Gharemani, Li, Khudanpur.

Character-Level Language Modeling with Deeper Self-Attention (2018). Roufou*, Choe*, Guo*, Constant*, Jones*

Ongoing and Future Work

Ongoing

Self-supervision and classification for images and video

Understanding Transfer

Future

Multitask learning

Long-range attention