Transformers, Large Language Models (LLMs), and Foundation Models

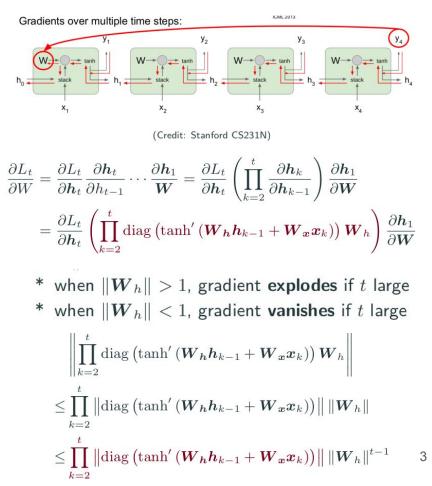
Ju Sun Computer Science & Engineering

Apr 08, 2025

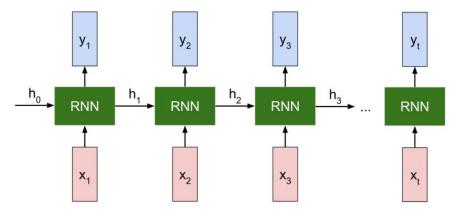


Quick recap

Vanishing/exploding gradient issue



RNN: model sequences

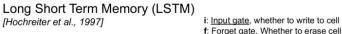


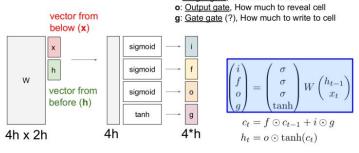
(Credit: Stanford CS231N)

$$egin{aligned} m{h}_t &= anh\left(m{W}_{m{h}}m{h}_{t-1} + m{W}_{m{x}}m{x}_t
ight) \ m{y}_t &= m{V}_ym{h}_t \end{aligned}$$

 ${old W}_h, {old W}_x$ and ${old V}_y$ are shared across the sequence

Gated RNNs





(Credit: Stanford CS231N)

u: **update gate**, control state update

r: **reset gate**, control how previous state affects new content

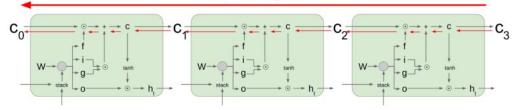
g: new content

Gated recurrent unit (GRU)

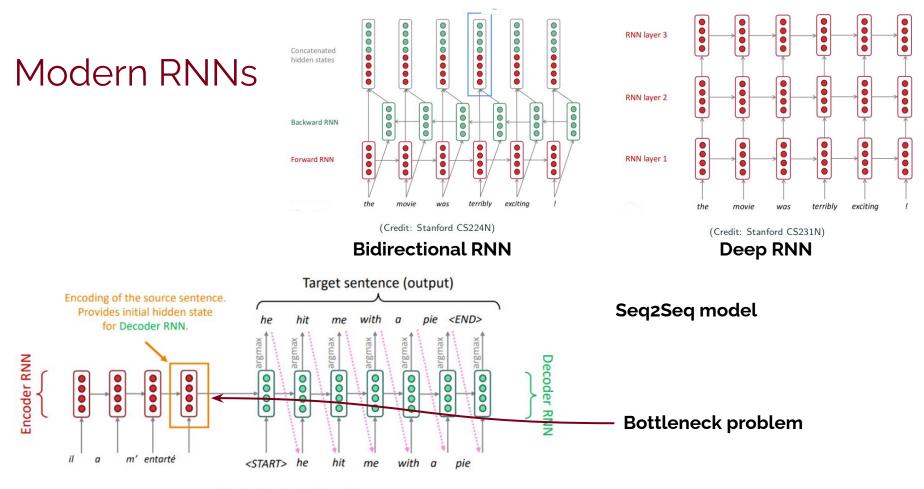
$$egin{aligned} egin{aligned} egin{aligne} egin{aligned} egin{aligned} egin{aligned} egin$$

f, i, o are merged

Uninterrupted gradient flow!

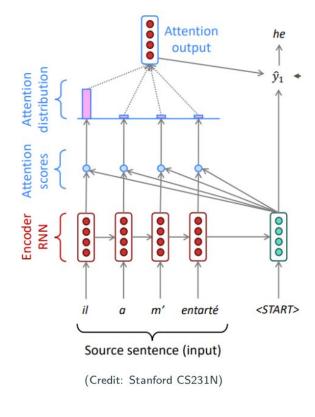


(Credit: Stanford CS231N)



⁽Credit: Stanford CS231N)

Attention mechanism



Input: source vectors $s_1, \ldots, s_N \in \mathbb{R}^h$, and target vector t

Output: weighted summation

$$\sum_{j=1}^N w_j oldsymbol{s}_j$$
 where $w_j = ext{similarity}(oldsymbol{s}_j,oldsymbol{t})$

Many possibilities:

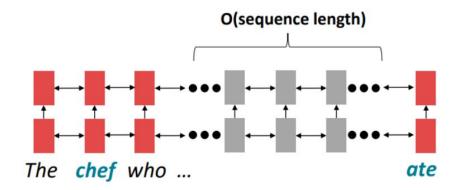
Attention scores

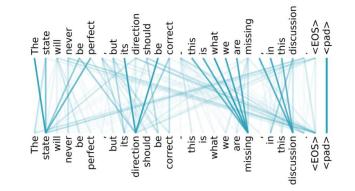
- dot-product attention: $\widehat{w_j} = \langle s_j, t \rangle$ (Is is better to normalize this or rescale it by the dimension factor?)
- multiplicative attention: $\widehat{w_j} = \langle s_j, oldsymbol{W} oldsymbol{t}
 angle$
- "additive attention": $\widehat{w_j} = \boldsymbol{v}^{\intercal} \sigma \left(\boldsymbol{W}_1 \boldsymbol{s}_j + \boldsymbol{W}_2 \boldsymbol{t} \right)$

The actual weights are attention scores passed through **softmax**

$$w_j = \frac{\exp\left(\widehat{w_j}\right)}{\sum_k \exp\left(\widehat{w_k}\right)}$$

Self-attention





RNN

- Long interaction distance
- Resistant to parallelization

Self-attention

- O(1) interaction distance
- Highly parallelizable

Each token gets a selective summary of information from all others

Self-attention

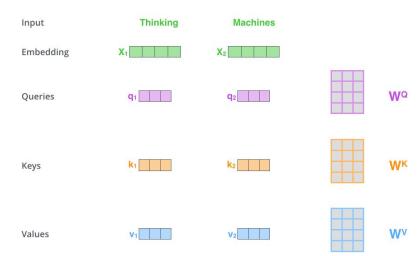


Image credit: https://jalammar.github.io/illustrated-transformer/

- Each word now encoded as (query, key, value) triple
- For an input x_i , we have:

 $\boldsymbol{q}_i = (\boldsymbol{W}^Q)^{\mathsf{T}} \boldsymbol{x}_i, \quad \boldsymbol{k}_i = (\boldsymbol{W}^K)^{\mathsf{T}} \boldsymbol{x}_i, \quad \boldsymbol{v}_i = (\boldsymbol{W}^V)^{\mathsf{T}} \boldsymbol{x}_i$

- Calculate attention scores between query and all keys: $e_{ij} = \langle m{q}_i, m{k}_j
 angle$
- softmax normalization $w_{ij} = \exp(e_{ij}) / \sum_k \exp(e_{ik})$
- output the weighted sum of values $\sum_j w_{ij} v_j$

In matrix notation

- Compute queries, keys, and values

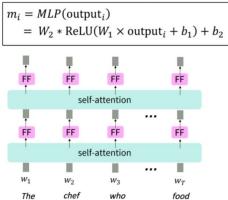
$$Q = XW^Q, \quad K = XW^K, \quad V = XW^V$$

- Calculate attention scores between query and all keys: $oldsymbol{E}=oldsymbol{Q}oldsymbol{K}^{\intercal}$
- softmax normalization $oldsymbol{A} = \operatorname{softmax}(oldsymbol{E})$
- output the weighted sum of values AV

output = softmax $(QK^{\mathsf{T}})V$

Question: why we need both query and key?

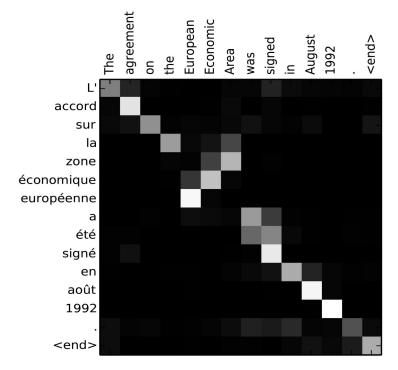
Equation for Feed Forward Layer



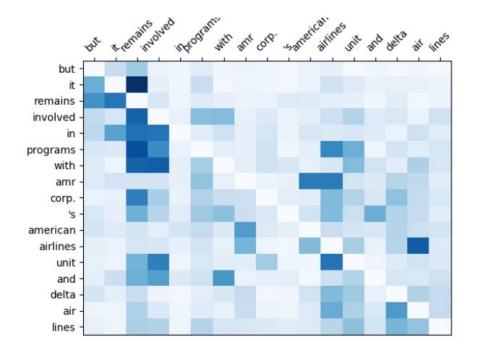
Adding in nonlinearity!

First step toward Transformers!

Attention matrices—visualizing correlations



General attention



Self-attention

Transformers

Transformers

Attention Is All You Need

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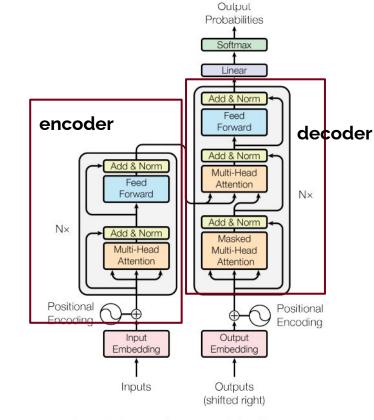


Figure 1: The Transformer - model architecture.

NIPS 2017; <u>https://arxiv.org/abs/1706.03762</u>

Transformers reign in NLP!

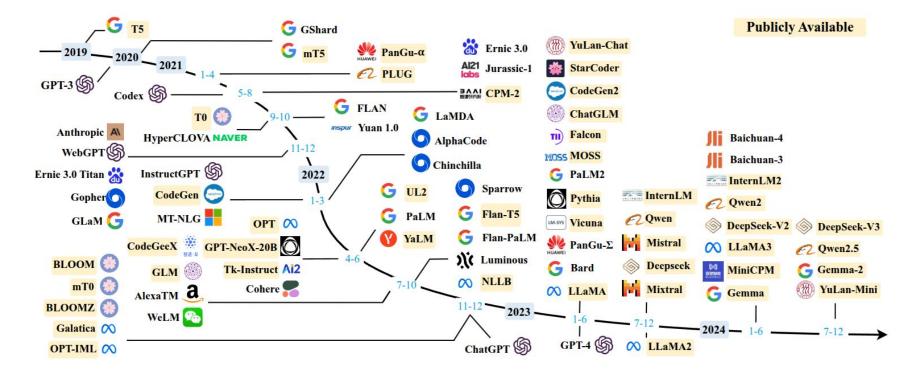
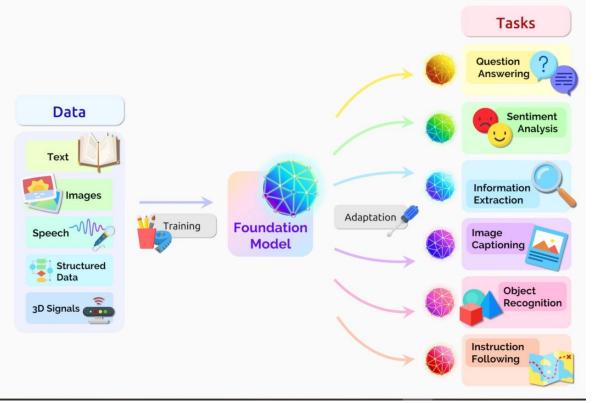


Image credit: A Survey of Large Language Models https://arxiv.org/abs/2303.18223

Transformers for everything!



- Transformers have been modified to deal with almost all kinds of structured and unstructured data
- Enable multimodal data integration and interaction

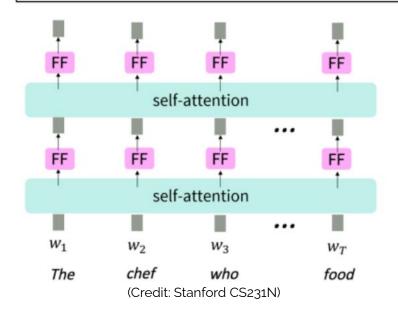
Image credit: https://blogs.nvidia.com/blog/2022/03/25/what-is-a-transformer-model/

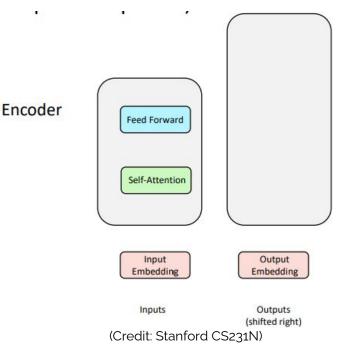
Starting from self-attention

Equation for Feed Forward Layer

 $m_i = MLP(\text{output}_i)$

 $= W_2 * \text{ReLU}(W_1 \times \text{output}_i + b_1) + b_2$



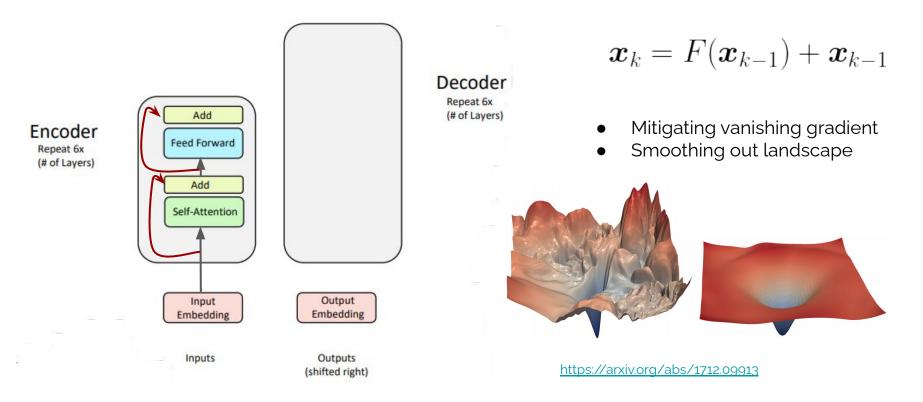


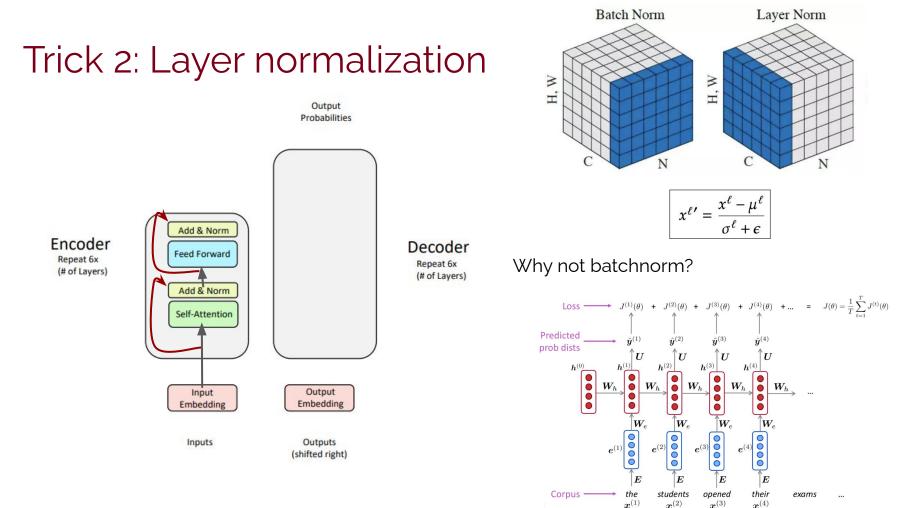
Three tricks to build in depth:

- Residual connection
- Layer normalization
- Scaled inner product attention

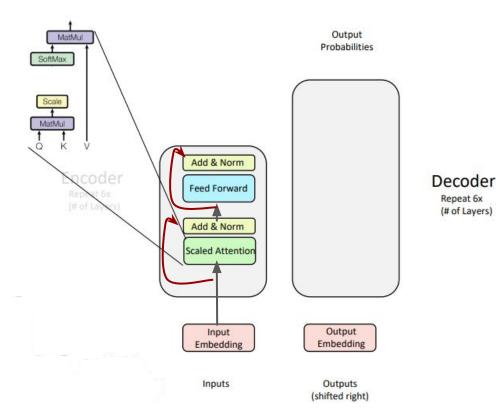
Decoder

Trick 1: Residual connection





Trick 3: Scaled inner product attention



 $output = softmax(QK^{\mathsf{T}})V$

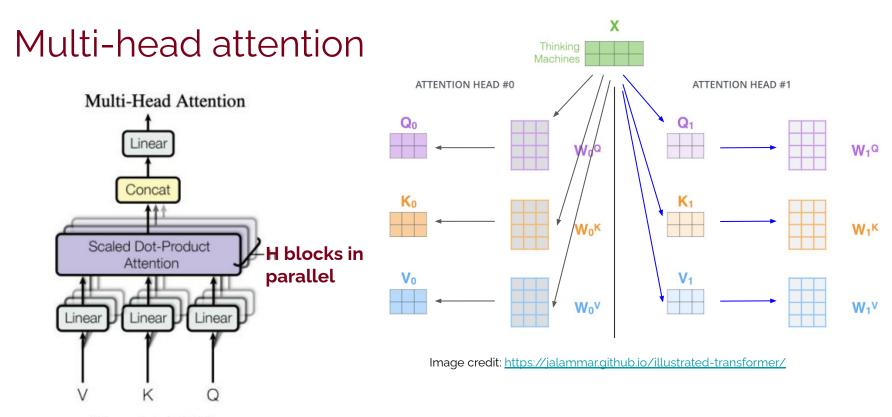
• Suppose that entries of Q and K behaves like IID zero-mean, unit variance

•
$$\mathbb{E}\langle \boldsymbol{q}^i, \boldsymbol{k}^j
angle = 0$$
 but
 $\operatorname{Var}\langle \boldsymbol{q}^i, \boldsymbol{k}^j
angle = d_k$

This can blow up exp computation in the softmax normalization for large $d_k!$

Solution: normalize by standard deviation

output = softmax $(\boldsymbol{Q}\boldsymbol{K}^{\intercal}/\sqrt{d_k})\boldsymbol{V}$



[Vaswani et al. 2017]

Multiple, independent self-attention blocks in parallel

Intuition: allow the flexibility of capturing different kinds of "relevance"/correlations

Multi-head attention

1) Concatenate all the attention heads



Concatenate



3) The result would be the Z matrix that captures information from all the attention heads. We can send this forward to the FFNN

=

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Output

Image credit: https://jalammar.github.io/illustrated-transformer/

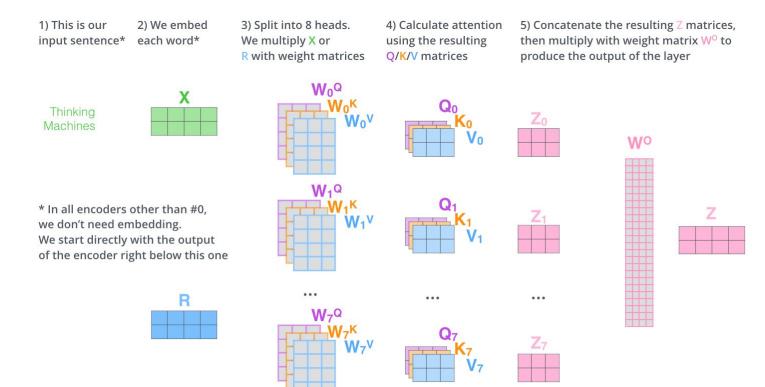


2) Multiply with a weight matrix W^o that was trained jointly with the model

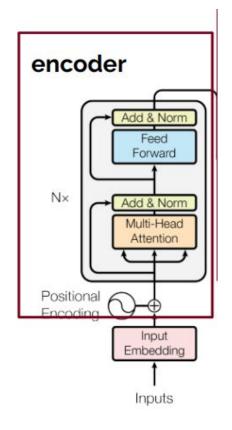
Х

Multiply

Multi-head attention



Positional encoding



Does the input order matter or not?

$$Q = XW^Q$$
, $K = XW^K$, $V = XW^V$
output = softmax $(QK^{\intercal}/\sqrt{d_k})V$

Positional encoding to break the order invariance

• Idea: a positional vector to (hopefully) encode the position information

E.g.,
$$\boldsymbol{X}_p = \boldsymbol{X} + \boldsymbol{P}, \text{ or } \boldsymbol{X}_p = [\boldsymbol{X}, \boldsymbol{P}]$$

• P can be pre-defined, or made learnable

Sinusoidal positional encoding

L: sequence length d: embedding dimension

$$ext{PE}(i,\delta) = egin{cases} \sin(rac{i}{10000^{2\delta'/d}}) & ext{if } \delta = 2\delta' \ \cos(rac{i}{10000^{2\delta'/d}}) & ext{if } \delta = 2\delta' + 1 \end{cases}$$

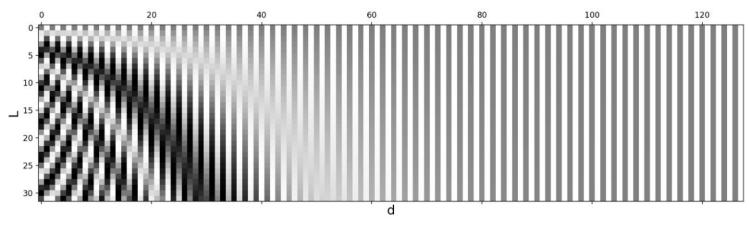
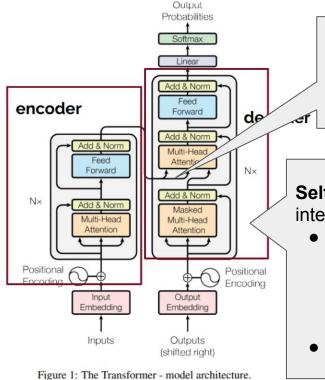


Image credit: <u>https://lilianweng.github.io/posts/2020-04-07-the-transformer-family/</u>

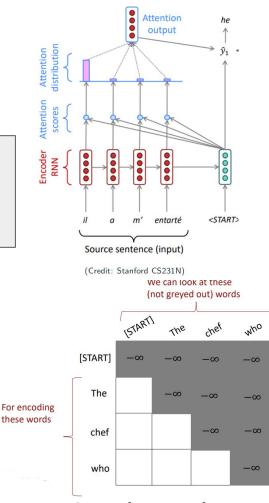
Decoder



Cross-attention (to model the interaction between the encoder key-values and the current decoder query)

Self-attention (to model the interaction within itself)

- Respect the sequential nature (e.g., language modeling, assuming access to the future is cheating!)
- Masked out future tokens



Strong performance in machine translation

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)		
WIOUEI	EN-DE	EN-FR	EN-DE	EN-FR	
ByteNet [18]	23.75				
Deep-Att + PosUnk [39]		39.2		$1.0\cdot10^{20}$	
GNMT + RL [38]	24.6	39.92	$2.3\cdot 10^{19}$	$1.4\cdot10^{20}$	
ConvS2S [9]	25.16	40.46	$9.6\cdot10^{18}$	$1.5\cdot 10^{20}$	
MoE [32]	26.03	40.56	$2.0\cdot10^{19}$	$1.2\cdot 10^{20}$	
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$	
GNMT + RL Ensemble [38]	26.30	41.16	$1.8\cdot 10^{20}$	$1.1\cdot 10^{21}$	
ConvS2S Ensemble [9]	26.36	41.29	$7.7\cdot 10^{19}$	$1.2\cdot10^{21}$	
Transformer (base model)	27.3	38.1	3.3 •	10^{18}	
Transformer (big)	28.4	41.8	$2.3\cdot 10^{19}$		

Computation

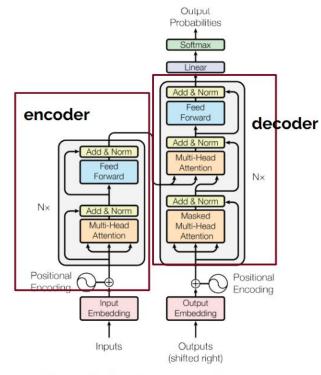


Figure 1: The Transformer - model architecture.

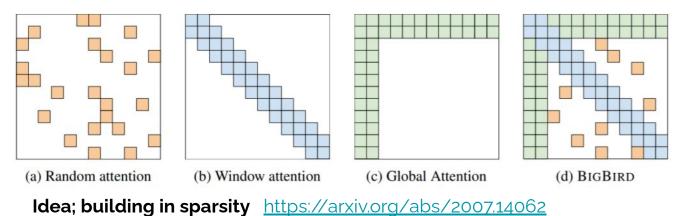
What's the total computation?

$$oldsymbol{Q} = oldsymbol{X}oldsymbol{W}^Q, \quad oldsymbol{K} = oldsymbol{X}oldsymbol{W}^K, \quad oldsymbol{V} = oldsymbol{X}oldsymbol{W}^V$$

output = softmax $(oldsymbol{Q}oldsymbol{K}^\intercal/\sqrt{d_k})oldsymbol{V}$
 $O(T^2d)$

Quadratic computation vs. linear computation in RNNs (**T** is the length of each input sequence, **d** is the embedding dimension)





Do Transformer Modifications Transfer Across Implementations and Applications?

Sharan Narang*	Hyung Won Chung	Yi Tay	William Fedus
Thibault Fevry †	${\bf Michael}~{\bf Matena}^{\dagger}$	Karishma Malkan †	Noah Fiedel
Noam Shazeer	$\mathbf{Zhenzhong}\ \mathbf{Lan}^{\dagger}$	Yanqi Zhou	Wei Li
Nan Ding	Jake Marcus	Adam Roberts	${\bf Colin} \ {\bf Raffel}^{\dagger}$

But not much consistent improvement so far https://arxiv.org/abs/2102.11972

Large language models (LLMs)

Transformers reign in NLP!

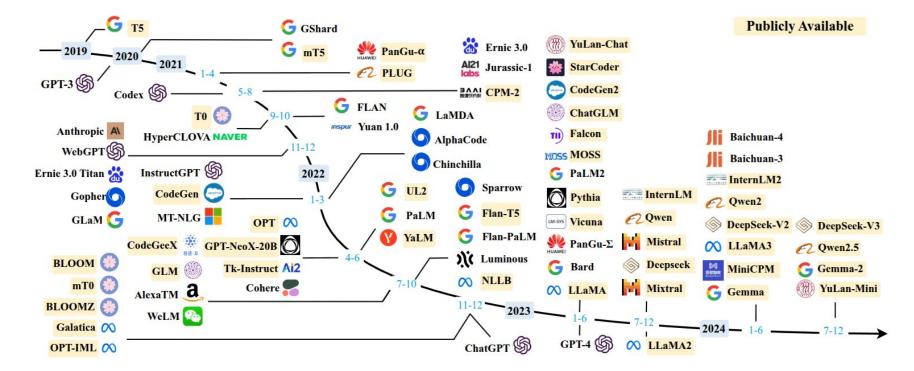


Image credit: A Survey of Large Language Models https://arxiv.org/abs/2303.18223

LLMs: large models trained on large datasets

	Model	Release Time	Size (B)
6	T5 73	Oct-2019	11
	mT5 74	Oct-2020	13
	PanGu- α 75	Apr-2021	13*
	CPM-2 76	Jun-2021	198
	T0 28	Oct-2021	11
	CodeGen 77	Mar-2022	16
	GPT-NeoX-20B 78	Apr-2022	20
	Tk-Instruct 79	Apr-2022	11
	UL2 80	May-2022	20
	OPT 81	May-2022	175
	NLLB 82	Jul-2022	54.5
	CodeGeeX 83	Sep-2022	13
	GLM 84	Oct-2022	130
	Flan-T5 64	Oct-2022	11
Publicly	BLOOM 69	Nov-2022	176
Available	mT0 85	Nov-2022	13
	Galactica 35	Nov-2022	120
	BLOOMZ 85	Nov-2022	176
	OPT-IML 86	Dec-2022	175
	LLaMA 57	Feb-2023	65
	Pythia <mark>87</mark>	Apr-2023	12
	CodeGen2 88	May-2023	16
	StarCoder 89	May-2023	15.5
	LLaMA2 90	Jul-2023	70

GPT-3 55	May-2020	175
GShard 91	Jun-2020	600
Codex 92	Jul-2021	12
ERNIE 3.0 93	Jul-2021	10
Jurassic-1 94	Aug-2021	178
HyperCLOVA 95	Sep-2021	82
FLÂN 62	Sep-2021	137
Yuan 1.0 96	Oct-2021	245
Anthropic 97	Dec-2021	52
WebGPT 72	Dec-2021	175
Gopher 59	Dec-2021	280
ERNIE 3.0 Titan 98	Dec-2021	260
GLaM 99	Dec-2021	1200
LaMDA 63	Jan-2022	137
MT-NLG 100	Jan-2022	530
AlphaCode 101	Feb-2022	41
InstructGPT 61	Mar-2022	175
Chinchilla 34	Mar-2022	70
PaLM 56	Apr-2022	540
AlexaTM 102	Aug-2022	20
Sparrow 103	Sep-2022	70
WeLM 104	Sep-2022	10
U-PaLM 105	Oct-2022	540
Flan-PaLM 64	Oct-2022	540
Flan-U-PaLM 64	Oct-2022	540
GPT-4 46	Mar-2023	-
	Mar-2023	1085
PaLM2 107	Mav-2023	16
	GShard 91 Codex 92 ERNIE 3.0 93 Jurassic-1 94 HyperCLOVA 95 FLAN 62 Yuan 1.0 96 Anthropic 97 WebGPT 72 Gopher 59 ERNIE 3.0 Titan 98 GLaM 99 LaMDA 63 MT-NLG 100 AlphaCode 101 InstructGPT 61 Chinchilla 34 PaLM 56 AlexaTM 102 Sparrow 103 WeLM 104 U-PaLM 105 Flan-PaLM 64 Flan-U-PaLM 64 GPT-4 46 PanGu-Σ 106	GShard 91 Jun-2020 Codex 92 Jul-2021 ERNIE 3.0 93 Jul-2021 Jurassic-1 94 Aug-2021 HyperCLOVA 95 Sep-2021 FLAN 62 Sep-2021 Yuan 1.0 96 Oct-2021 Anthropic 97 Dec-2021 WebGPT 72 Dec-2021 Gopher 59 Dec-2021 Gamber 59 Dec-2021 LaMDA 63 Jan-2022 MT-NLG 100 Jan-2022 AlphaCode 101 Feb-2022 InstructGPT 61 Mar-2022 PaLM 56 Apr-2022 VeLM 102 Aug-2022 WeLM

LLMs: large models trained on large datasets

TABLE 2: Statistics of commonly-used data sources.

Corpora	Size	Source	Latest Update Time
BookCorpus 138	5GB	Books	Dec-2015
Gutenberg 139	_	Books	Dec-2021
C4 73	800GB	CommonCrawl	Apr-2019
CC-Stories-R 140	31GB	CommonCrawl	Sep-2019
CC-NEWS 27	78GB	CommonCrawl	Feb-2019
REALNEWs 141	120GB	CommonCrawl	Apr-2019
OpenWebText 142	38GB	Reddit links	Mar-2023
Pushift.io 143	2TB	Reddit links	Mar-2023
Wikipedia 144	21GB	Wikipedia	Mar-2023
BigQuery 145	_	Codes	Mar-2023
the Pile 146	800GB	Other	Dec-2020
ROOTS 147	1.6TB	Other	Jun-2022

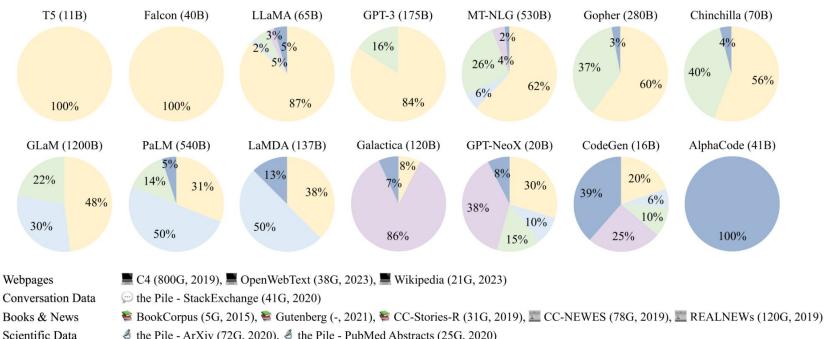
Two crucial technical steps toward LLMs

• Pretraining

• Finetuning (Adaptation)

Recall transfer learning?

Pretraining: data collection



- 🛓 the Pile ArXiv (72G, 2020), 🛓 the Pile PubMed Abstracts (25G, 2020)
 - BigQuery (-, 2023), the Pile GitHub (61G, 2020)

Code

Image credit: A Survey of Large Language Models https://arxiv.org/abs/2303.18223

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Pretraining: data collection

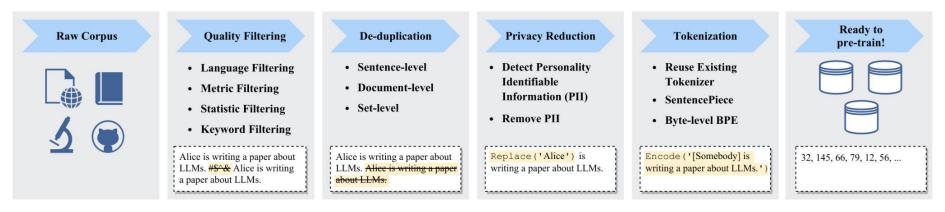
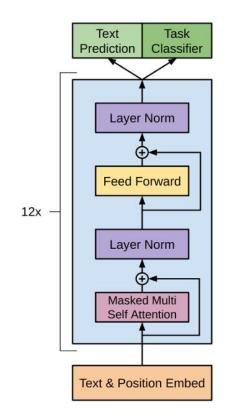
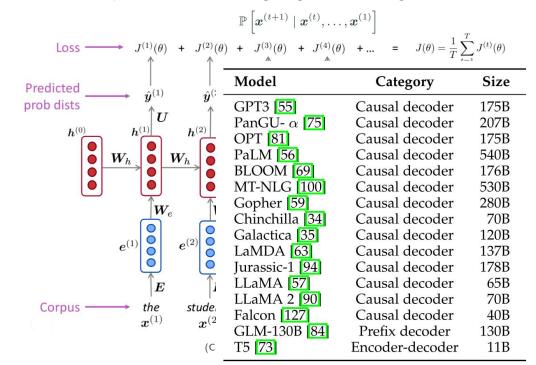


Fig. 6: An illustration of a typical data preprocessing pipeline for pre-training large language models.

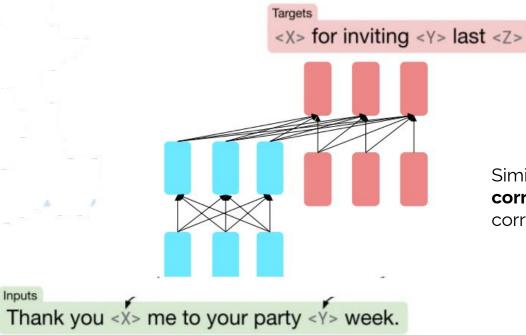
Pretraining: architecture & task



Most popular: (transformer-based) **decoder-only** architectures pretrained on **language modeling**, i.e. model



Pretraining: architecture & task — alternative



Similar to pretraining encoder, **corruption removal**! (called span corruption)

Pretraining: architecture details

Configuration	Method	Equation	
Normalization position	Post Norm 22 Pre Norm 26 Sandwich Norm 201	$ \begin{vmatrix} Norm(\mathbf{x}+Sublayer(\mathbf{x})) \\ \mathbf{x}+Sublayer(Norm(\mathbf{x})) \\ \mathbf{x}+Norm(Sublayer(Norm(\mathbf{x}))) \end{vmatrix} $	
Normalization method	LayerNorm 202 RMSNorm 203 DeepNorm 204	$\begin{vmatrix} \frac{\mathbf{x}-\mu}{\sqrt{\sigma}} \cdot \gamma + \beta, & \mu = \frac{1}{d} \sum_{i=1}^{d} x_i, & \sigma = \sqrt{\frac{1}{d} \sum_{i=1}^{d} (x_i - \mu)} \\ \frac{\mathbf{x}}{\text{RMS}(\mathbf{x})} \cdot \gamma, & \text{RMS}(\mathbf{x}) = \sqrt{\frac{1}{d} \sum_{i=1}^{d} x_i^2} \\ \text{LayerNorm}(\alpha \cdot \mathbf{x} + \text{Sublayer}(\mathbf{x})) \end{vmatrix}$	
Activation function	ReLU 205 GeLU 206 Swish 207 SwiGLU 208 GeGLU 208	$\begin{vmatrix} \operatorname{ReLU}(\mathbf{x}) = \max(\mathbf{x}, 0) \\ \operatorname{GeLU}(\mathbf{x}) = 0.5\mathbf{x} \otimes [1 + \operatorname{erf}(\mathbf{x}/\sqrt{2})], & \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \\ \operatorname{Swish}(\mathbf{x}) = \mathbf{x} \otimes \operatorname{sigmoid}(\mathbf{x}) \\ \operatorname{SwiGLU}(\mathbf{x}_1, \mathbf{x}_2) = \operatorname{Swish}(\mathbf{x}_1) \otimes \mathbf{x}_2 \\ \operatorname{GeGLU}(\mathbf{x}_1, \mathbf{x}_2) = \operatorname{GeLU}(\mathbf{x}_1) \otimes \mathbf{x}_2 \end{vmatrix}$	
Position embedding	Absolute 22 Relative 73 RoPE 209 Alibi 210	$\begin{vmatrix} \mathbf{x}_{i} = \mathbf{x}_{i} + \mathbf{p}_{i} \\ A_{ij} = \mathbf{W}_{q} \mathbf{x}_{i} \mathbf{x}_{j}^{T} \mathbf{W}_{k}^{T} + r_{i-j} \\ A_{ij} = \mathbf{W}_{q} \mathbf{x}_{i} \mathbf{R}_{\theta, i-j} \mathbf{x}_{j}^{T} \mathbf{W}_{k}^{T} \\ A_{ij} = \mathbf{W}_{q} \mathbf{x}_{i} \mathbf{R}_{\theta, i-j} \mathbf{x}_{j}^{T} \mathbf{W}_{k}^{T} A_{ij} = \mathbf{W}_{q} \mathbf{x}_{i} \mathbf{x}_{j}^{T} \mathbf{W}_{k}^{T} - m(i-j) \end{vmatrix}$	

Image credit: A Survey of Large Language Models https://arxiv.org/abs/2303.18223

Pretraining: optimization details

Model	Batch Size (#tokens)	Learning Rate	Warmup	Decay Method	Optimizer	Precision Type	Weight Decay	Grad Clip	Dropout
GPT3 (175B)	32K→3.2M	6×10^{-5}	yes	cosine decay to 10%	Adam	FP16	0.1	1.0	-
PanGu- α (200B)	-	2×10^{-5}	-	-	Adam	-	0.1	-	-
OPT (175B)	2M	1.2×10^{-4}	yes	manual decay	AdamW	FP16	0.1	-	0.1
PaLM (540B)	$1M \rightarrow 4M$	1×10^{-2}	no	inverse square root	Adafactor	BF16	lr^2	1.0	0.1
BLOOM (176B)	4M	6×10^{-5}	yes	cosine decay to 10%	Adam	BF16	0.1	1.0	0.0
MT-NLG (530B)	64 K→3.75M	5×10^{-5}	yes	cosine decay to 10%	Adam	BF16	0.1	1.0	-
Gopher (280B)	3M→6M	4×10^{-5}	yes	cosine decay to 10%	Adam	BF16	_	1.0	-
Chinchilla (70B)	$1.5M \rightarrow 3M$	1×10^{-4}	yes	cosine decay to 10%	AdamW	BF16	-	-	-
Galactica (120B)	2M	7×10^{-6}	yes	linear decay to 10%	AdamW	-	0.1	1.0	0.1
LaMDA (137B)	256K	-	-	-	-	BF16	-	-	-
Jurassic-1 (178B)	32 K→3.2M	6×10^{-5}	yes	-	-	-	-	-	-
LLaMA (65B)	4M	$1.5 imes 10^{-4}$	yes	cosine decay to 10%	AdamW	-	0.1	1.0	-
LLaMA 2 (70B)	4M	1.5×10^{-4}	yes	cosine decay to 10%	AdamW	-	0.1	1.0	-
Falcon (40B)	2M	$1.85 imes 10^{-4}$	yes	cosine decay to 10%	AdamW	BF16	0.1	-	-
GLM (130B)	$0.4M \rightarrow 8.25M$	8×10^{-5}	yes	cosine decay to 10%	AdamW	FP16	0.1	1.0	0.1
T5 (11B)	64K	1×10^{-2}	no	inverse square root	AdaFactor	-	-	-	0.1
ERNIE 3.0 Titan (260B)	-	1×10^{-4}	-	-	Adam	FP16	0.1	1.0	-
PanGu- Σ (1.085T)	0.5M	2×10^{-5}	yes	-	Adam	FP16	-	-	-

TABLE 5: Detailed optimization settings of several existing LLMs.

Supervised adaptation—instruction tuning

TABLE 6: A detailed list of available collections for instruction tuning.

Categories	Collections	Time	#Examples
	Nat. Inst. 264	Apr-2021	193K
	FLAN 62	Sep-2021	4.4M
	P3 265	Oct-2021	12.1M
Task	Super Nat. Inst. 79	Apr-2022	5M
	MVPCorpus 266	Jun-2022	41M
	xP3 85	Nov-2022	81M
	OIC ²²	Mar-2023	43M
	HH-RLHF 267	Apr-2022	160K
	HC3 268	Jan-2023	87K
Chat	ShareGPT ²³	Mar-2023	90K
	Dolly ²⁴	Apr-2023	15K
	OpenAssistant 269	Apr-2023	161K
	Self-Instruct 129	Dec-2022	82K
	Alpaca 123	Mar-2023	52K
Synthetic	Guanaco ²⁵	Mar-2023	535K
	Baize 270	Apr-2023	158K
	BELLE 271	Apr-2023	1.5M

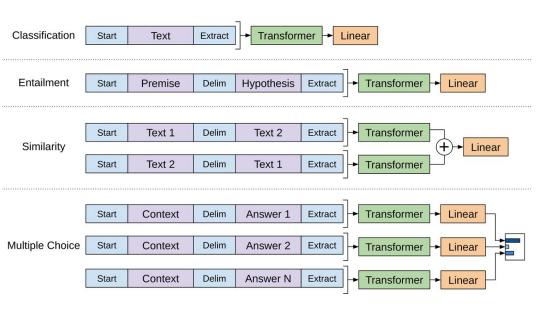


Image credit: Improving Language Understanding by Generative Pre-Training, https://gwern.net/doc/www/s3-us-west-2.amazonaws.com/d73fdc5ffa8627bce4.pdf

Image credit: A Survey of Large Language Models <u>https://arxiv.org/abs/2303.18223</u>

Constructing the instruction sets

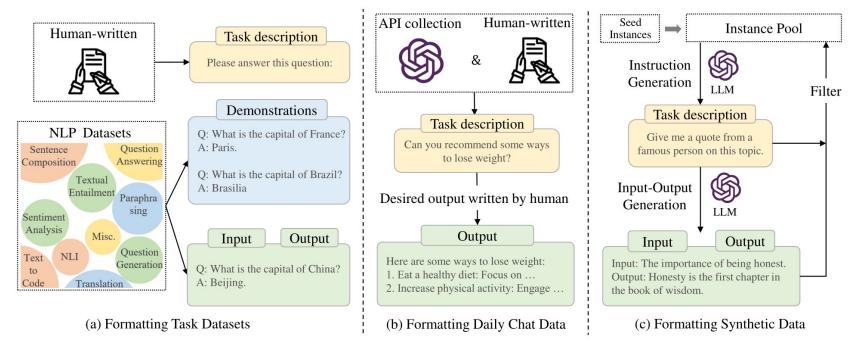
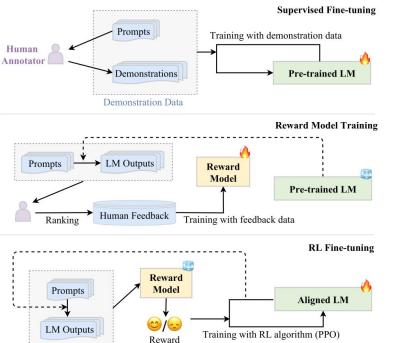


Fig. 9: An illustration of instance formatting and three different methods for constructing the instruction-formatted instances.

Supervised adaptation—alignment tuning



Make sure the output is aligned with human values and not harmful

Reinforcement learning with human feedback (RLHF)

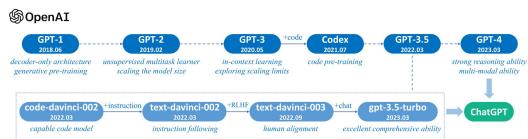


Fig. 3: A brief illustration for the technical evolution of GPT-series models. We plot this figure mainly based on the papers, blog articles and official APIs from OpenAI. Here, *solid lines* denote that there exists an explicit evidence (*e.g.*, the official statement that a new model is developed based on a base model) on the evolution path between two models, while *dashed lines* denote a relatively weaker evolution relation.

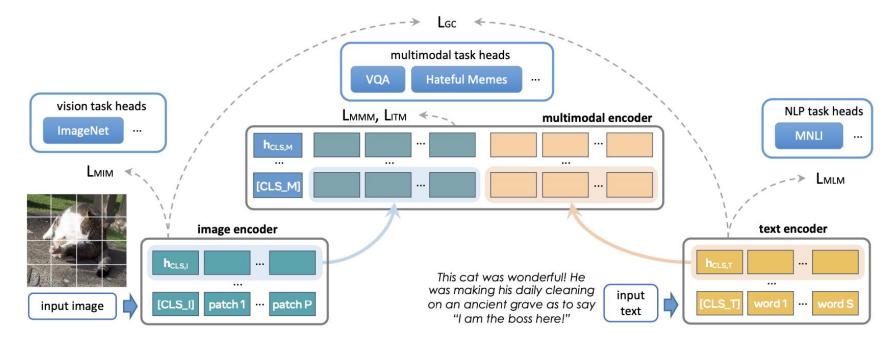
Image credit: A Survey of Large Language Models https://arxiv.org/abs/2303.18223

Transformers for other domains

Vision Transformers

Transformers | Davide Coccomini | 2021

Multimodal foundation models



https://pytorch.org/blog/scaling-multimodal-foundation-models-in-torchmultimodal-with-pytorch-distributed/