# X-formers

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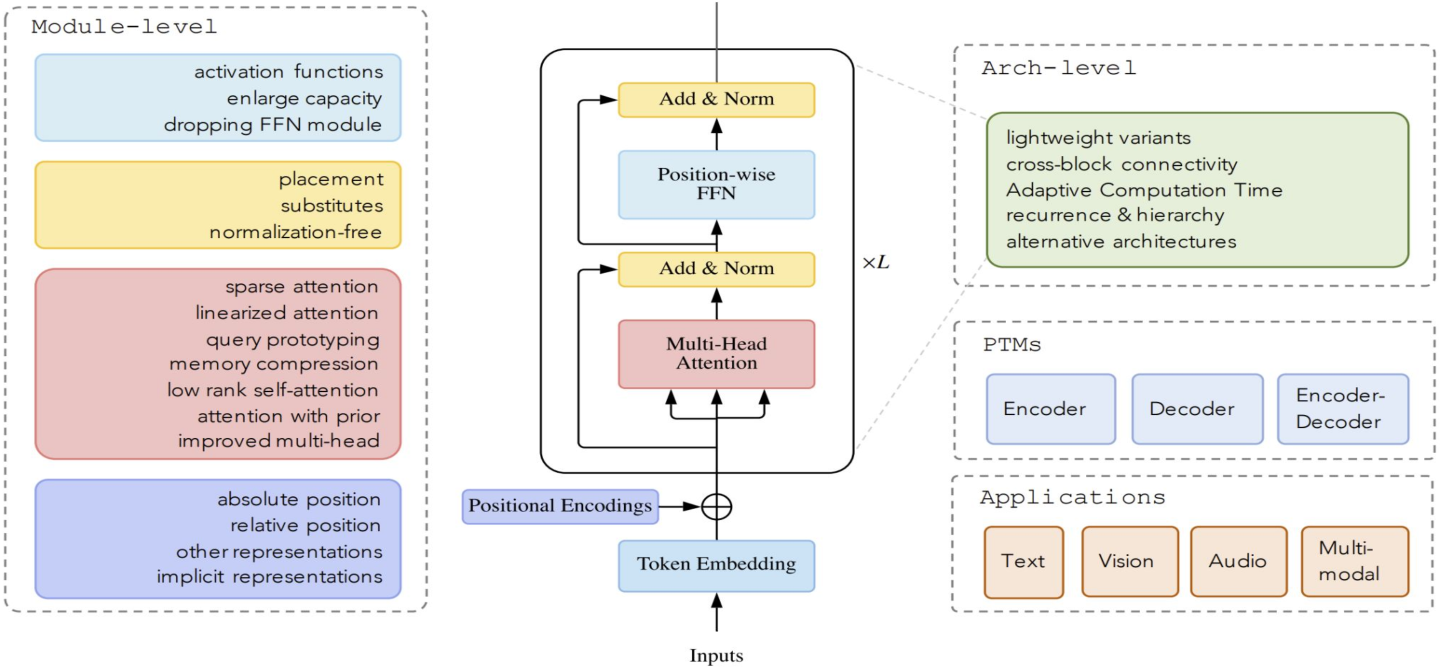
# Agenda

- Transformer Architecture and Variants overview
- Need for variants
- Vanilla Transformer components
- Data Movement vs Computation
- Transformer variants interesting to the compiler

# Transformer Variants Landscape



# Need for Transformer variants

- Vanilla transformers are inefficient at processing long sequences
    - Computation and memory complexity of self-attention is high
- Doesn’t use structural/inductive bias of input data
    - Variants: Introduce structural bias, regularization, pre-training on large-scale unlabeled data
- To handle specialized downstream tasks/applications

# Taxonomy for X-former variants

- Many variants address multiple needs
    - Example: Sparse Transformers - addresses computational requirements and adds structural prior
- Taxonomy should be based on the ways in which they improve vanilla x-former
    - Module level variants
    - Architecture modification
    - Pre-trained models (PTM)
    - Applications

# Vanilla Transformer

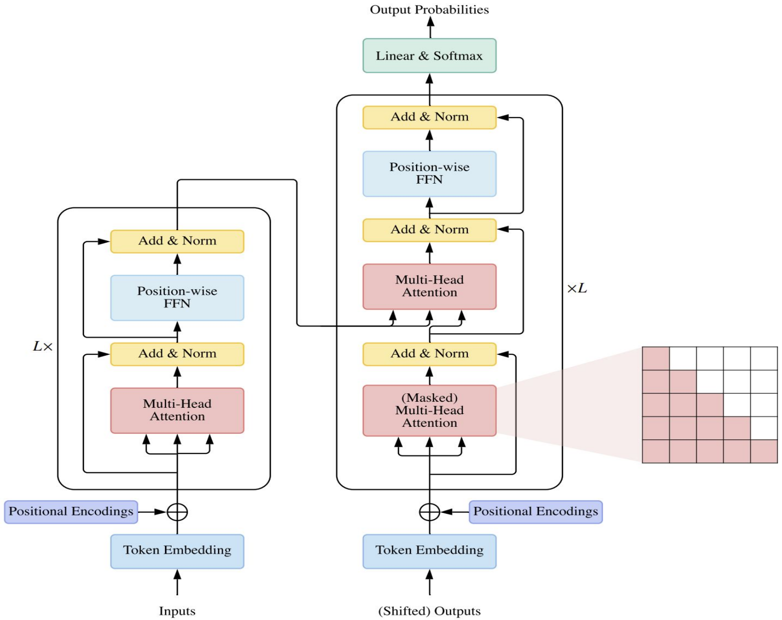


Fig. 1. Overview of vanilla Transformer architecture

# Attention Module

$$\mathrm{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \mathrm{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{D_k}}\right)\mathbf{V} = \mathbf{A}\mathbf{V},$$

$$\mathrm{MultiHeadAttn}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \mathrm{Concat}(\mathrm{head}_1, \cdots, \mathrm{head}_H)\mathbf{W}^O,$$

$$\text{where } \mathrm{head}_i = \mathrm{Attention}(\mathbf{Q}\mathbf{W}_i^Q, \mathbf{K}\mathbf{W}_i^K, \mathbf{V}\mathbf{W}_i^V).$$

# Self vs Masked vs Cross Attention

- Self: Q = K = V = X
- Masked: Restrict attention to certain parts of input. Ex: Decoder restricting attention to previous positions
- Cross-Attention:
  - Queries are projected from the previous layer.
  - Keys and values are projected from the encoder output

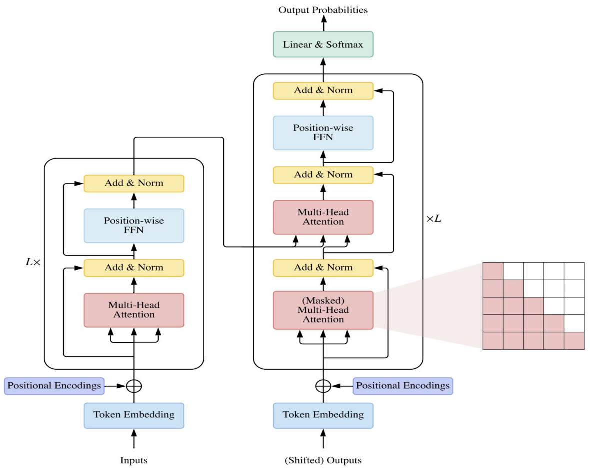


Fig. 1. Overview of vanilla Transformer architecture

# Position wise FFN

$$\mathrm{FFN}(\mathbf{H}') = \mathrm{ReLU}(\mathbf{H}'\mathbf{W}^1 + \mathbf{b}^1)\mathbf{W}^2 + \mathbf{b}^2,$$

- Provides rich representation to the attention outputs

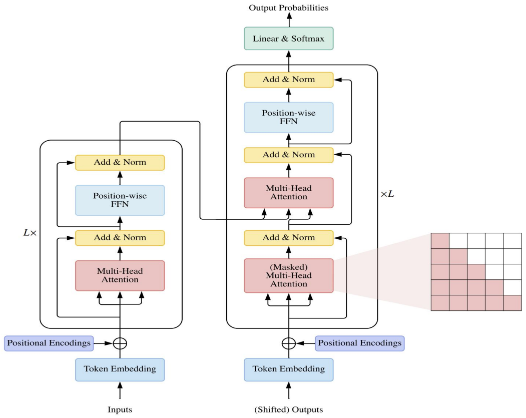


Fig. 1. Overview of vanilla Transformer architecture

# Residual connection + Layer Norm

$$\mathrm{H}' = \mathrm{LayerNorm}(\mathrm{SelfAttention}(\mathrm{X}) + \mathrm{X})$$

$$\mathrm{H} = \mathrm{LayerNorm}(\mathrm{FFN}(\mathrm{H}') + \mathrm{H}'),$$

- Residual connections
  - helps with vanishing gradient problem
  - retain information about the original input

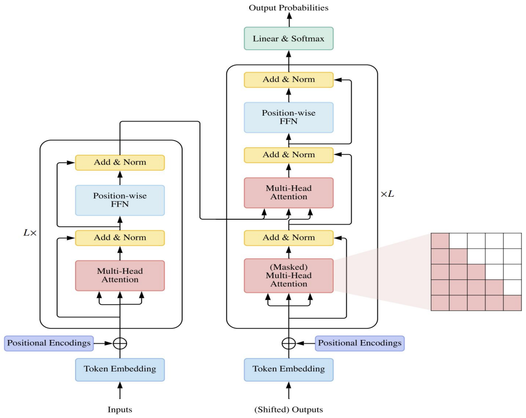


Fig. 1. Overview of vanilla Transformer architecture

# Vanilla Transformer - Class of Models

- Seq2Seq model - Example: NMT; Dalle
  - Encoder - usually multiple stacked on top of each other
  - Decoder - - usually multiple stacked on top of each other
- Encoder - Example: Sequence labeling, classification; BERT
  - Multi-head self-attention
  - Position-wise feed-forward network(FFN)
  - Residual connection
  - Layer Norm
- Decoder - Example: Sequence Generation; GPT
  - Multi-head self-attention (autoregressive in nature)
  - Cross attention with encoder state
  - FFN

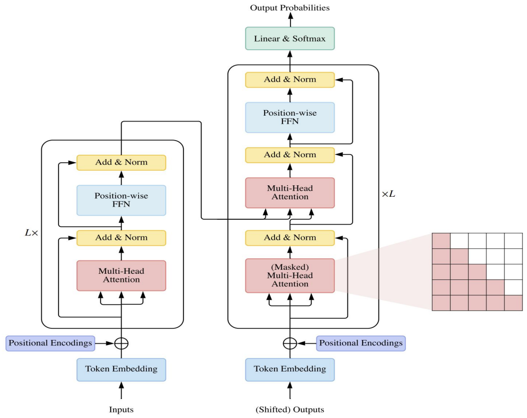
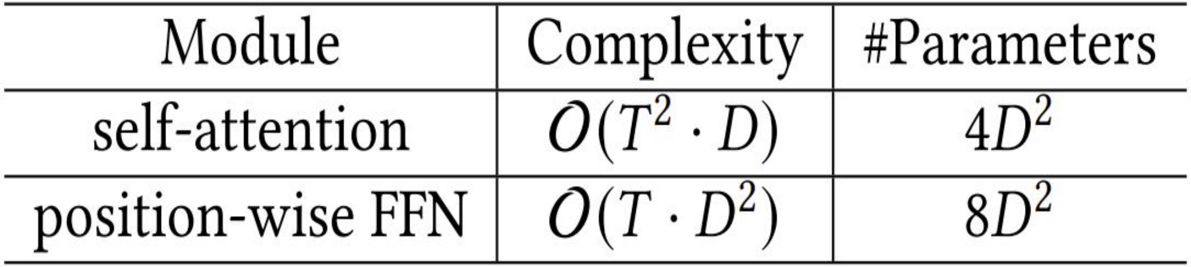


Fig. 1. Overview of vanilla Transformer architecture

# Model Analysis



| Module | Complexity | #Parameters |
|---|---|---|
| self-attention | $O(T^2 \cdot D)$ | $4D^2$ |
| position-wise FFN | $O(T \cdot D^2)$ | $8D^2$ |

- T - Sequence length; D - Hidden dimension
- Short-sequence: Bottleneck is FFN
- Long-sequence: Bottleneck Self-Attention; In computation and space
    - Pixel level image generation, long text document modeling are infeasible

# Computation Distribution

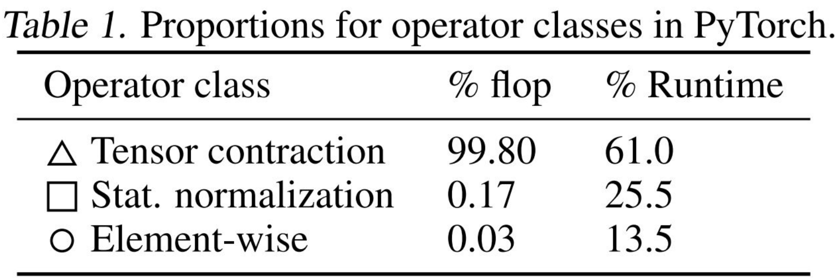


*Table 1.* Proportions for operator classes in PyTorch.

| Operator class | % flop | % Runtime |
|---|---|---|
| △ Tensor contraction | 99.80 | 61.0 |
| □ Stat. normalization | 0.17 | 25.5 |
| ○ Element-wise | 0.03 | 13.5 |

- Tensor contraction - Matmul
  - Data layout and tiling has significant impact
- Stat normalization - softmax, layer norms
  - Data layout and vectorization has significant impact
  - Reduction operators - Shared Iteration space promotes Fusion opportunities;
- Element-wise - dropout, residual connections, biases

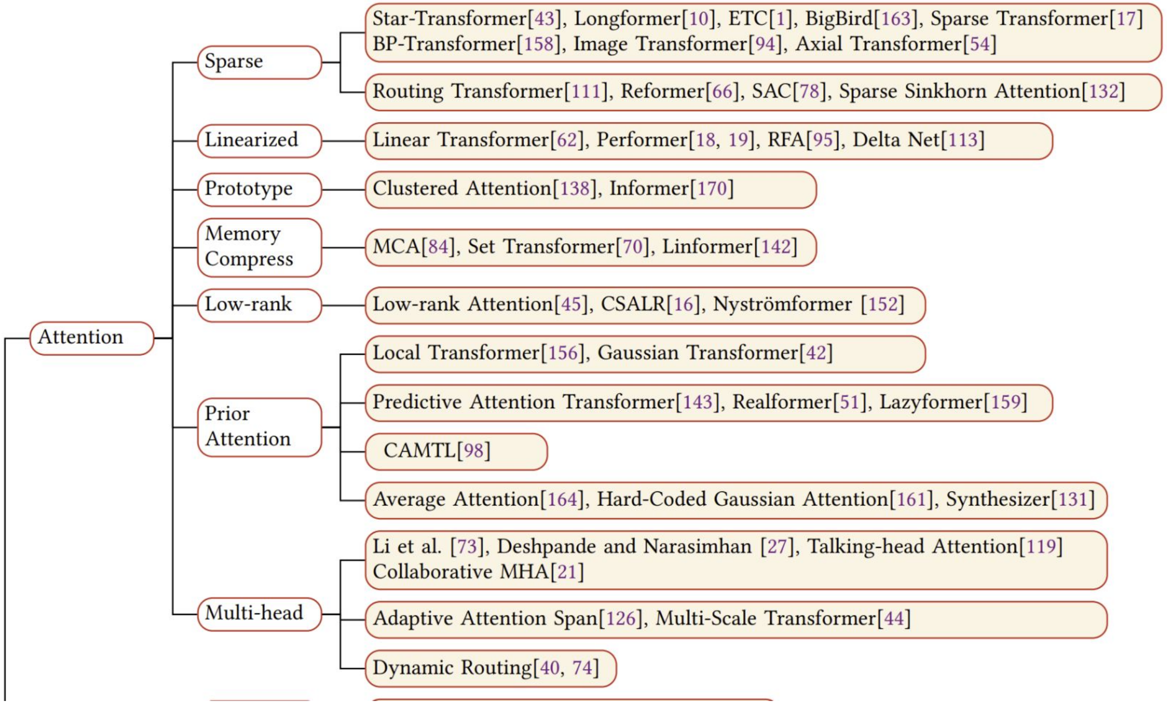
# Notes on Memory usage

- Computation cost is relatively small compared to the memory capacity and bandwidth costs
- Autoregressive nature of Decoders is a strain on latency
  - KV cache has to be maintained in memory for the duration of the decoding
  - KV cache changes for every sample in the batch
  - For smaller sequences, loading weights dominates performance
  - Data movement of KV cache dominates performance for longer sequences(T >= 2048) and batch size 512
  - On-chip memory tend to load the KV cache from off-chip memory for every token

# Self-Attention vs Conv vs FC vs Recurrent

- Conv vs SA: Convolutional network need to stack conv layers deep to get global receptive field. SA can get global receptive field with constant number of layers.
- FC vs SA: SA is flexible in handling variable-length inputs
- Recurrent vs SA: Constant sequential operations make SA more parallelizable and better at long-range modeling
- Inductive bias:
    - Conv layers impose translation invariance and locality with shared local kernel functions.
    - Recurrent layers impose temporal invariance and locality
    - TF make very little use of structural info and is prone to overfitting on small-scale data

# Attention level variants



- Attention
  - Sparse
    - Star-Transformer[43], Longformer[10], ETC[1], BigBird[163], Sparse Transformer[17] BP-Transformer[158], Image Transformer[94], Axial Transformer[54]
    - Routing Transformer[111], Reformer[66], SAC[78], Sparse Sinkhorn Attention[132]
  - Linearized
    - Linear Transformer[62], Performer[18, 19], RFA[95], Delta Net[113]
  - Prototype
    - Clustered Attention[138], Informer[170]
  - Memory Compress
    - MCA[84], Set Transformer[70], Linformer[142]
  - Low-rank
    - Low-rank Attention[45], CSALR[16], Nyströmformer [152]
  - Prior Attention
    - Local Transformer[156], Gaussian Transformer[42]
    - Predictive Attention Transformer[143], Realformer[51], Lazyformer[159]
    - CAMTL[98]
    - Average Attention[164], Hard-Coded Gaussian Attention[161], Synthesizer[131]
  - Multi-head
    - Li et al. [73], Deshpande and Narasimhan [27], Talking-head Attention[119] Collaborative MHA[21]
    - Adaptive Attention Span[126], Multi-Scale Transformer[44]
    - Dynamic Routing[40, 74]

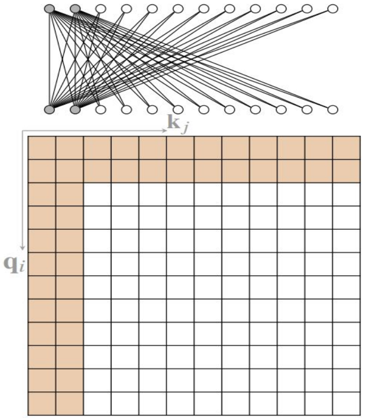
# Sparse Attention

- Learned Attention matrix is often sparse across most data points
- Incorporate this information to reduce the number of query-key pairs computed

$$\hat{\mathbf{A}}_{ij} = \begin{cases} \mathbf{q}_i \mathbf{k}_j^\top & \text{if token } i \text{ attends to token } j, \\ -\infty & \text{if token } i \text{ does not attend to token } j, \end{cases}$$

# Sparse Attention - Global Attention

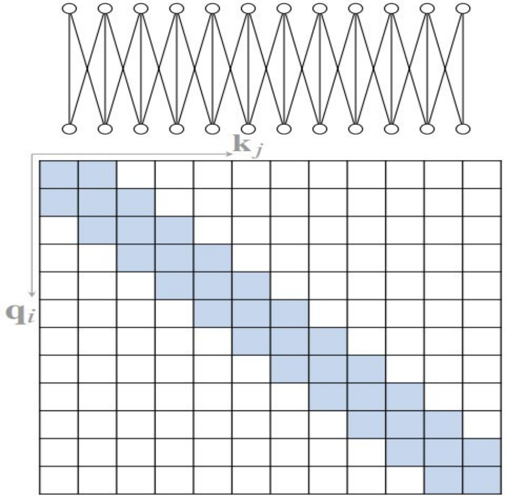
- Sparse Attention: Loses ability to model long deps
- Global nodes: Retain the ability to model long range deps
- Serve as the hub for information propagation between nodes
- Global nodes attend to all nodes in the sequence



(a) global

# Sparse Attention - Band Attention

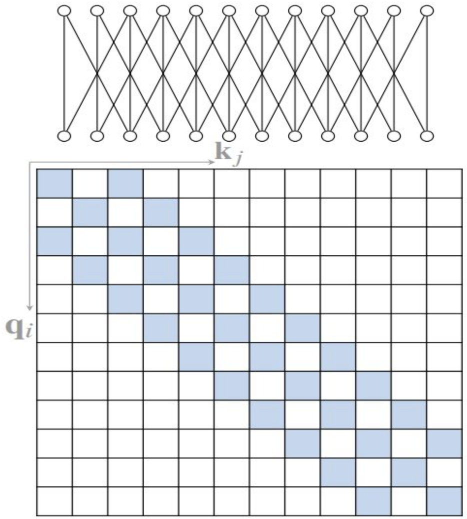
- Sliding window attention
- Aka local attention
- Restrict each query to attend to it its neighbor nodes



(b) band

# Dilated Attention

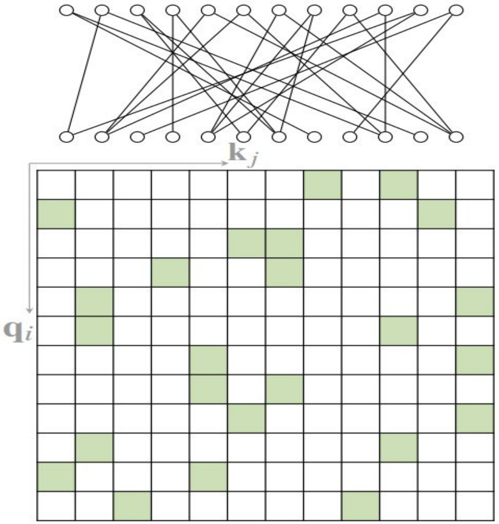
- Idea is similar to dilation in CNN
- Increased receptive field without increasing computation
- Aka strided attention



(c) dilated

# Random Attention

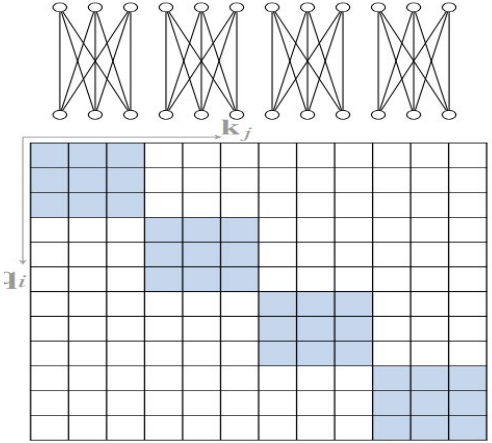
- Randomly sampled nodes for each query
- Random graphs can have similar spectral properties with complete graphs that leads to fast mixing time for random walking on graphs



(d) random

# Block Local Attention

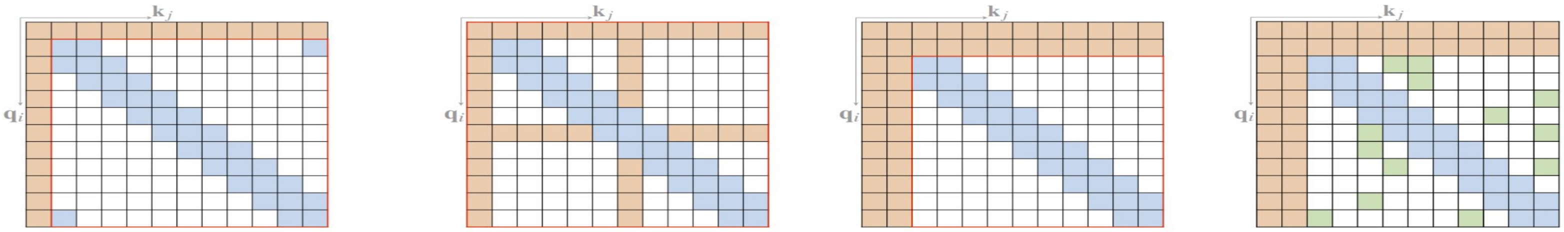
- Segments input sequence into several non-overlapping query blocks
- Queries in a query block attend to only the keys in the corresponding block



(e) block local

# Compound Sparse Attention

- Combination of multiple attention patterns
- Star-Transformer: Band Attention + Global Attention
- Longformer: Band Attention + Internal global-node attention + dilated window attention in upper layers
- Extended Transformer Construction(ETC): Band + External-node global attention
- BigBird: Band + Global + Random Attention to approximate full attention



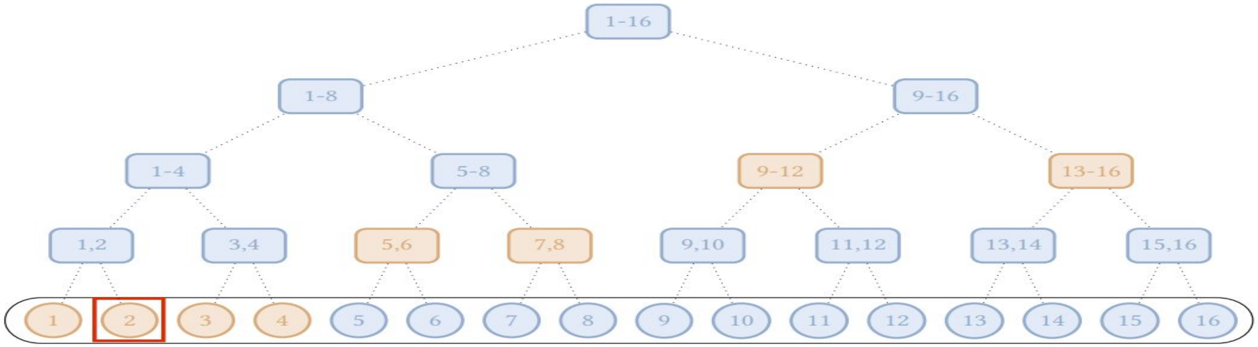
(a) Star-Transformer (b) Longformer (c) ETC (d) BigBird

# Compound Sparse Attention

- Sparse Transformer: Different sparse patterns for different types of data
- Data with periodic structure(Images):
  - Composition of band attention and strided attention
- Data without periodic structure(text):
  - Block local attention + global attention

# Extended Sparse Attention

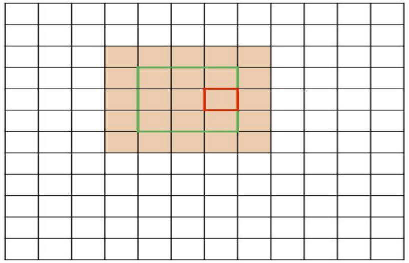
- For text: BP transformer
  - Binary tree with tokens as leaf nodes and internal nodes as span nodes containing many tokens



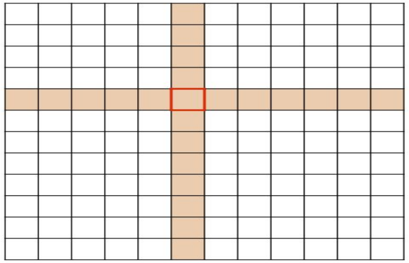
(a) BPT

# Extended Sparse Attention

- Image Transformer:
  - flattens image pixels in raster-scan order and applies block local sparse attention
  - 2D block local attention with query and memory blocks arranged in 2D
- Axial Transformer:
  - Applies independent attention modules over each axis of the image
  - Mixes information along one axis while keeping information from the other axis independent



(b) block local (2D)



(c) axial (2D)

# Content-based Sparse Attention

- Sparse graph is created based on the input content
- Idea: Select those keys that are likely to have large similarity scores with the given query
- Routing Transformer:
  - K-means clustering to cluster both queries and keys to the same set of centroid vectors
  - Each query attends only to the keys that belong to the same cluster
- Reformer
  - Locality sensitive hashing to select key-value pairs for each query
  - Each query attends only to the keys within the same hashing bucket
  - LSH function to hash queries and keys into several buckets with similar items fall in the same bucket with high probability

# Content-based Sparse Attention

- Sparse Adaptive Connection(SAC)
  - Input sequence as a graph and learns to construct attention edges to improve task specific performances
  - Uses adaptive sparse connection using LSTM edge predictor to construct edges between tokens
  - Uses reinforcement learning to predict edges
- Sparse Sinkhorn Attention
  - Splits queries and keys into several blocks and assigns a key block to each query block
  - The assignment of key block to query block is done via sorting network which uses Sinkhorn normalization
  - Permutation  matrix representing the assignment

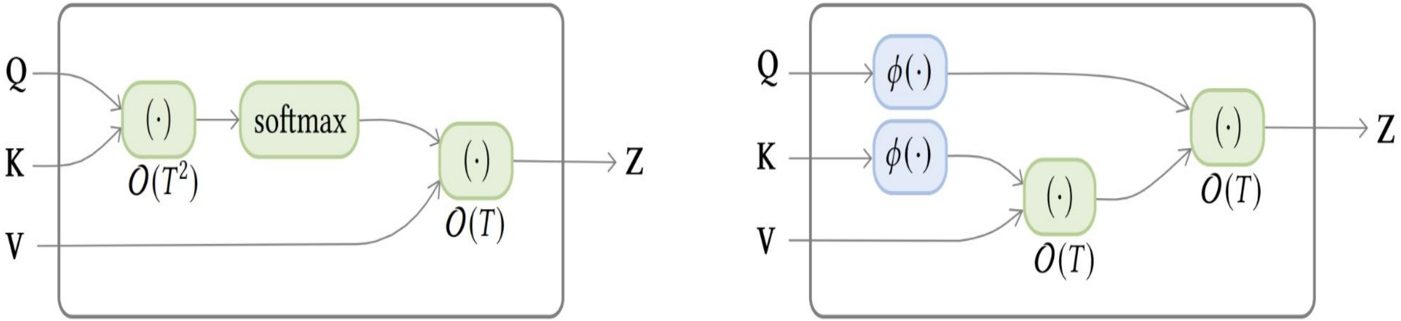
# Linearized Attention

- Attention computation is quadratic in sequence length T.
- O(T^2 D)
- How to get linear computation complexity?

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{D_k}}\right)\mathbf{V} = \mathbf{A}\mathbf{V},$$

- N, M - sequence lengths of queries and keys/values
- Dk; Dv - dimensions of queries/keys and values
- Q - N x Dk ; K - M x Dk; V - M x Dv;
- Q.K^T - N x M; (Q.K^T)V = N x Dv => O(T^2.D) => O(T^2) when T >> D
- Q(K^T.V) - O(T.D^2) => O(T) when T >> D

# Linearized Attention



(a) standard self-attention

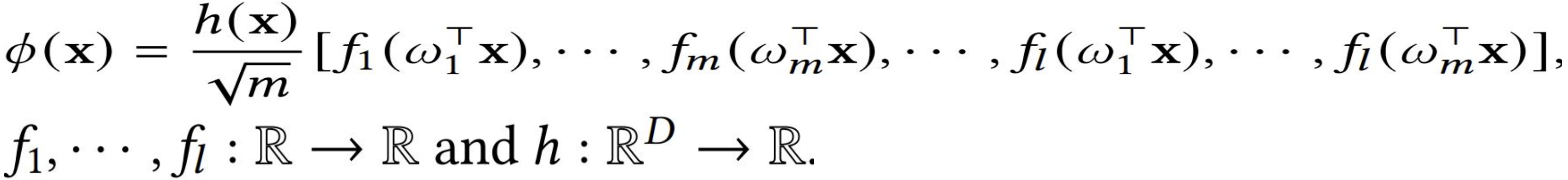
(b) linearized self-attention

# Linearized Attention

- Unnormalized attention - A_hat = exp(Q.K^T)
- Replace this unnormalized attention with a torch.matmul(phi(Q), phi(K)^T)
- Phi - feature map applied in row-wise manner
- Standard Self-Attention $Z = D^{-1}\hat{A}V, \text{ where } D = \text{diag}(\hat{A}1_T^T);$
- Because A_hat = exp(Q.K^T) = phi(Q).phi(K)^T
- phi(Q).(phi(K)^T . V)

# Linearized Attention

- Feature map used in Linear Transformer: phi(x) = elu(x) + 1
- The feature map doesn’t approximate dot product attention
- Empirically performs on par with standard transformer
- Performer
  - Uses random feature maps that approximate the scoring function of Transformer



$$\phi(\mathbf{x}) = \frac{h(\mathbf{x})}{\sqrt{m}} [f_1(\omega_1^\top \mathbf{x}), \cdots, f_m(\omega_m^\top \mathbf{x}), \cdots, f_l(\omega_1^\top \mathbf{x}), \cdots, f_l(\omega_m^\top \mathbf{x})],$$

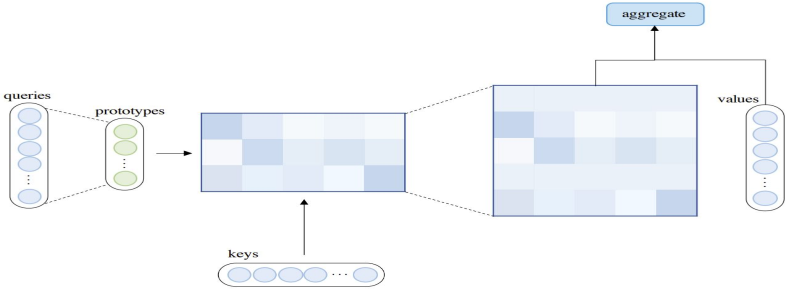
$$f_1, \cdots, f_l : \mathbb{R} \to \mathbb{R} \text{ and } h : \mathbb{R}^D \to \mathbb{R}.$$

# Performer variants

- They vary in the number of functions the feature maps take and h(x)
- Some variants
  - L = 2; f1 = sin; f2 = cos; h(x) = exp( l2norm(x))/2
  - L=1; f1 = exp; h(x) = exp(-l2norm(x))/2
  - L=1; f1 = RELU; h(x)=1 (Protein sequence modeling and NMT find this effective)

# Query Prototyping and Memory Compression

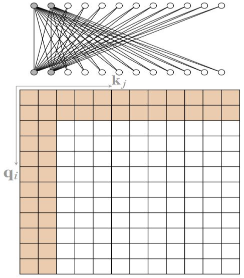
- Idea: Reduce the number of queries or key-value pairs
- Prototype queries:
  - Several prototype queries serve as the main source to compute attention matrix
  - Clustered Attention: groups queries into clusters and compute attention distribution for cluster centroids. All queries in the cluster share the attention distribution of the centroid
  - Informer selects prototype queries using sparsity measurement
    - KL divergence between query's attention distribution and discrete uniform distribution.
    - Select Top-u queries as prototype



(a) Query prototyping

# Memory Compressed Attention

- Idea: Reduce the number of key-value pairs before applying attention
- MCA:
  - Uses strided convolution on Keys and Values with local attention
  - Can capture global context
  - Reduces number of keys and values by a factor of kernel size k
- Set Transformer
  - External trainable global nodes(From Global Attention)
    - Summarizes information from inputs
    - Summarized representations serve as a compressed memory that the inputs attend to
    - Shown to perform with linear computational complexity in sequence length



(a) global

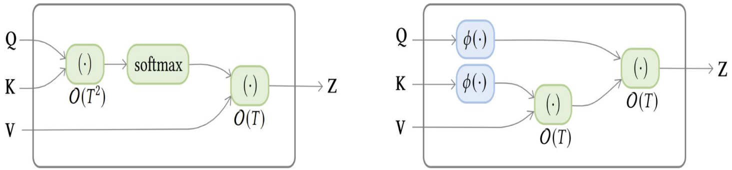
# Other Compressed variants

- Linformer
  - Linear projections to project keys and values from length n to smaller length k
  - Assumes a fixed input sequence length
  - Cannot be used autoregressively
- Poolingformer
  - Two-level attention
    - Sliding window
    - Compressed memory attention
  - Compression achieved by max pooling, pooling with dynamic convolution

# Low rank Self-Attention

$$\text{Attention}(\mathbf{Q},\mathbf{K},\mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^{\top}}{\sqrt{D_k}}\right)\mathbf{V} = \mathbf{A}\mathbf{V},$$

- Idea: Self-Attention matrix is often low-rank
- Low-rank parameterization:
  - Model the low-rank property as inductive bias by limiting the dimension of query/keys Dk
  - Self-attention matrix - decomposed into low-rank attention module with small Dk to capture long-range non-local interactions and a band attention module to capture local dependencies
- Low-rank Approximation:
  - Performer variants were inspired from kernel approximation with feature maps
  - Decompose attention matrix A into (C.G.C) where feature maps are used to approximate G



(a) standard self-attention

(b) linearized self-attention

# Nyström based Attention approximation

- Another form of low rank approximation
- Idea:
    - Select m landmark nodes from T inputs with down-sampling(strided average pooling)

$$\tilde{\mathbf{A}} = \mathrm{softmax}\left(\mathbf{Q}\tilde{\mathbf{K}}^{\top}\right)\left(\mathrm{softmax}\left(\tilde{\mathbf{Q}}\tilde{\mathbf{K}}^{\top}\right)\right)^{-1}\mathrm{softmax}\left(\tilde{\mathbf{Q}}\mathbf{K}^{\top}\right)$$

- Inverse doesn’t always exist
- Identity matrix could be added to make sure that the inverse always exists
- Nyström-former used Moore-Penrose pseudoinverse in place of inverse

# Attention with Prior

- Attention matrix = softmax(QK^T)
  - Generated using input sequences
- Prior: Attention distribution stemming from source other than input, referred as prior
  - Common priors are information about location of the input token
- Fusion of two attention distribution matrices can be done by computing a weighted sum of the scores corresponding to the prior and generated attention before applying softmax
  - Softmax( Prior + Q.K^T)

# Priors that model locality

- Text data usually exhibits preference for locality
- This can be modelled as a prior attention
- Multiply the generated attention distribution with some Gaussian density
  - Gaussian density Gij indicates higher probability that the i-th input attend to j-th input
  - Pi predicts a central position for each query Qi using a FFN

$$G_{ij} = -\frac{(j - p_i)^2}{2\sigma^2},$$

- Gaussian Transfomer
  - $G_{ij} = -|w(i - j)^2 + b|$,

# Priors from lower modules

- Observation: Attention distributions are similar in adjacent layers
- Idea: Use attention distribution from previous layer as a prior

$$\hat{\mathbf{A}}^{(l)} = w_1 \cdot \mathbf{A}^{(l)} + w_2 \cdot g(\mathbf{A}^{(l-1)}),$$

- Predictive Attention Transformer
  - Apply a 2D convolution to previous attention scores
  - Final attention = convex combination of generated attention score and convoluted scores
- Realformer
  - Directly adds previous attention scores resembling a residual skip connection
- Lazyformer
  - Shares attention maps between a number of adjacent layers
  - Attention maps computed once but reused several times as prior

# Multi-task adapters

- Adapters: Task-dependent modules attached in specific locations of a pre-trained network for cross-task efficient parameter sharing
- Idea: Use trainable attention priors that depends on task encoding

$$M(\mathbf{z}_i) = \bigoplus_{j=1}^{m} A'_j(\mathbf{z}_i), \qquad A'_j(\mathbf{z}_i) = A_j \gamma_i(\mathbf{z}_i) + \beta_i(\mathbf{z}_i)$$

- Zi depends on task specific encoding
- Gamma and Beta are Feature wise linear modulation functions
- This trainable prior is added to attention scores of upper layers in pre-trained transformers

# Attention with only prior

- Idea: No generated attention. Only prior attention distribution
- Average Attention network:
  - Discrete uniform distribution as the only source of attention distribution
  - A FFN gating layer on top of the average attention module
  - Used in decoder side
  - Decoder like RNN and avoids O(T^2) complexity
- Gaussian distribution as prior
  - Achieves comparable performance to baseline machine translation
- Synthesizer
  - Replace generated attention with learnable, randomly initialized attention scores
  - Replace attention score with a FFN that is conditioned on the querying input

# Multi-head Attention variants

- Multi-heads: Allows to attend to information from different representation subspaces at different positions
- Do the attention heads capture distinct features?
- Attention heads don’t interact with each other
- Variants
  - Encourage distinction learned features between attention heads
  - Add mechanisms to guide attention head behaviors
  - Regularization terms to loss function to encourage diversity among attention heads
- Observation: Multiple attention heads pay attention to CLS and SEP tokens
  - Auxillary loss: Frobenius norm between attention distribution maps and predefined attention patterns

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^{\top}}{\sqrt{D_k}}\right)\mathbf{V} = \mathbf{A}\mathbf{V},$$

$$\text{MultiHeadAttn}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{Concat}(\text{head}_1, \cdots, \text{head}_H)\mathbf{W}^O,$$

$$\text{where } \text{head}_i = \text{Attention}(\mathbf{Q}\mathbf{W}_i^Q, \mathbf{K}\mathbf{W}_i^K, \mathbf{V}\mathbf{W}_i^V).$$

# Multi-head Attention variants

$$\mathrm{MultiHeadAttn}(Q, K, V) = \mathrm{Concat}(\mathrm{head}_1, \cdots, \mathrm{head}_H)\mathbf{W}^O,$$

$$\text{where } \mathrm{head}_i = \mathrm{Attention}(Q\mathbf{W}_i^Q, K\mathbf{W}_i^K, V\mathbf{W}_i^V).$$

- Talking-head Attention
  - Linearly projects the generated attention scores from h_k to h heads
  - Applies softmax
  - Projects output to h_v heads for value aggregation
    - This moves information between attention heads in a learnable fashion
- Collaborative Multi-head Attention
  - Shared query and key projection
  - In the normal attention shown below, Wq and Wk are different for each head

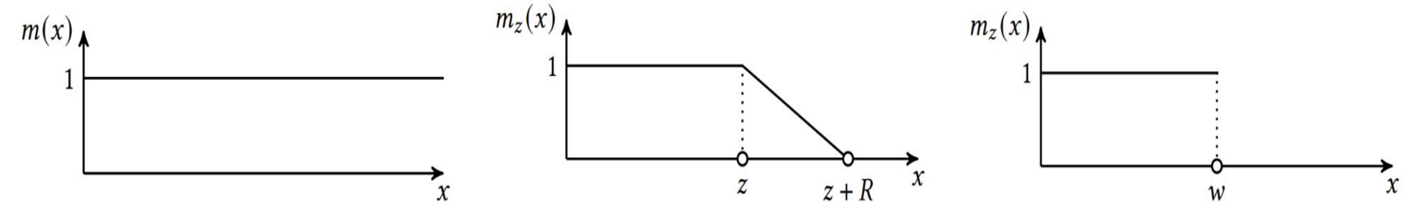
$$\mathrm{head}_i = \mathrm{Attention}(\mathbf{Q}\mathbf{W}^Q \mathrm{diag}(\mathbf{m}_i), \mathbf{K}\mathbf{W}^K, \mathbf{V}\mathbf{W}_i^V),$$

# Multi-head with Restricted spans

- Full attention span: A query can attend to all key-value pairs
- Observation: Some heads focus on local context and some heads attend to broader contexts
- Restricting attention spans on some heads can save memory footprint and computational time while allowing to extend to long sequences
- Learnable attention span
    - Restricted attention span are implemented via attention masks
    - Learnable scalar z represents a distance/span value
    - Character-level language modeling show adaptive-span models outperform baseline models

# Multi-head with Restricted span

- Multi-scale Transformer
  - Fixed attention span with different heads in different layers using a different max span
  - Scales are designed from an intuitive linguistic perspective and empirical observation
  - Higher layers have more scale/span length
  - Lower layers are confined to smaller scale



(a) mask function for vanilla attention (b) mask function for adaptive span (c) mask function for fixed span

# Multi-head with Refined Aggregation

- Multi-head attention usually concatenates attention head outputs and projects them to final output representation

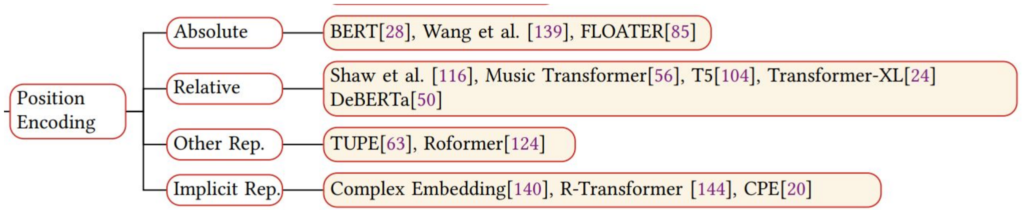
$$\mathrm{MultiHeadAttn}(Q, K, V) = \sum_{i=1}^{H} \mathrm{Attention}(Q\mathbf{W}_i^Q, K\mathbf{W}_i^K, V\mathbf{W}_i^V\mathbf{W}_i^O).$$

- Idea: This aggregation doesn’t fully exploit the expressiveness of multi-head attention
- Alternate aggregation:
  - Dynamic routing
  - EM routing
- Computational overhead is alleviated by applying complex aggregation to lower layers

# Multi-head variants

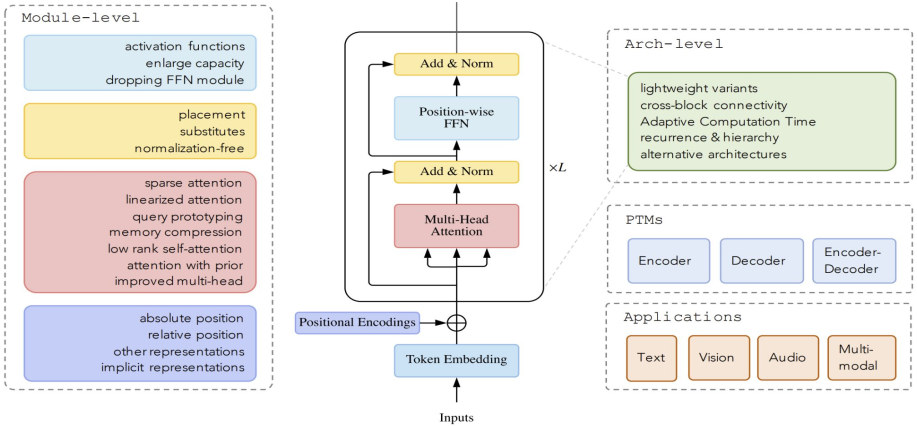
- Multi-query attention
  - Key-value pairs are shared among attention heads
  - Faster decode operations with minimal quality loss
- Usual Head size: Key dimension / Number of heads
  - Variant: Attention head size to be same as input sequence length

# Position level variants



Position Encoding

- Absolute: BERT[28], Wang et al. [139], FLOATER[85]
- Relative: Shaw et al. [116], Music Transformer[56], T5[104], Transformer-XL[24] DeBERTa[50]
- Other Rep.: TUPE[63], Roformer[124]
- Implicit Rep.: Complex Embedding[140], R-Transformer [144], CPE[20]



# Module-level variant - Position

- Self-Attention and position-wise FFN are permutation equivariant
    - Same set of inputs regardless of permutation will product same set of outputs with permutation matching the input permutation
- Position information has to be added as a separate step.
- Variants:
    - Absolute position representations
        - Position encoding for index t of size Dm is generated
        - Position encoding is added to token embeddings and fed to transformer

$$\mathrm{PE}(t)_i = \begin{cases} \sin(\omega_i t) & \text{if } i \text{ is even,} \\ \cos(\omega_i t) & \text{if } i \text{ is odd,} \end{cases}$$

# Position Encoding variants

- Learned position embeddings for each position
  - Number of embeddings is limited to a maximum sequence length
  - Loses inductive bias
- Sinusoidal position representation with each frequency learned from data
  - More robust compared to hand-crafted position representation
- FLOATER
  - Positional representation as continuous dynamical system and adopts Neural ODE to enable end-to-end training
  - Inductive and flexible with a fully learnable approach
- Add positional encodings to each layer input and not just the first layer since positional information gets lost after first few layers

# Relative Position Representation

- Represent positional relationships between tokens as opposed to position of tokens
- Pairwise positional relationships between input elements could be more beneficial than position of elements
- Music Transformer uses relative position representation
- Transformer-XL use a sinusoidal encoding to represent positional relationship but fuses contents and position information
- DeBERTa utilizes position embeddings similar to Transformer-XL

# Other Representations

- TUPE - Transformers with Untied Position Encoding
  - absolute position-to-position term
  - Relative content-to-content term
  - Bias term representing relative positional relationships
- Roformer
  - Rotary Position Embedding to represent the position of a token by multiplying the affine transformed embedding of the input by a rotatory matrix
  - Combines absolute and relative information

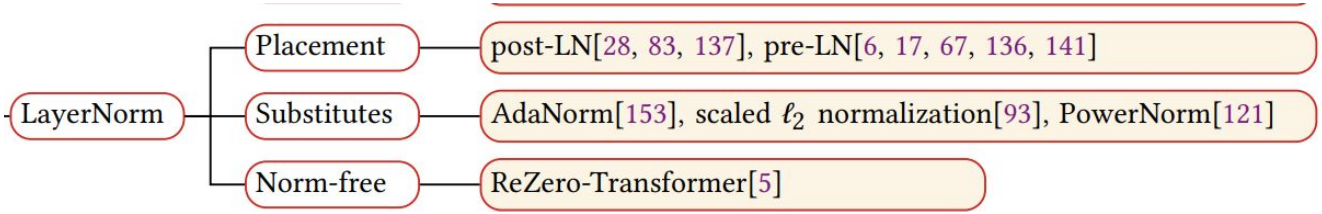
# Implicit encoding of position

- Encode positional information in word embeddings
- Embedding function generalized to continuous function over positions
- R-Transformer
  - Model locality of sequential data with a local RNN
  - Inputs fed to local RNN and then to MHSA
- Conditional Positional Encoding:
  - Generate conditional position encodings with a 2-D convolution with zero-padding at each layer input
  - Convolution implicitly encodes position information

# Position Representation on Decoder

- Decoders use cross attention and masks (to limit attention to previous inputs)
- Masked self-attention is not permutation equivariant
- A model that only uses the decoder is capable of sensing position information without explicit position representation
- Removing explicit position information on decoders improve performance

# Layer Norm



LayerNorm

Placement

post-LN[28, 83, 137], pre-LN[6, 17, 67, 136, 141]

Substitutes

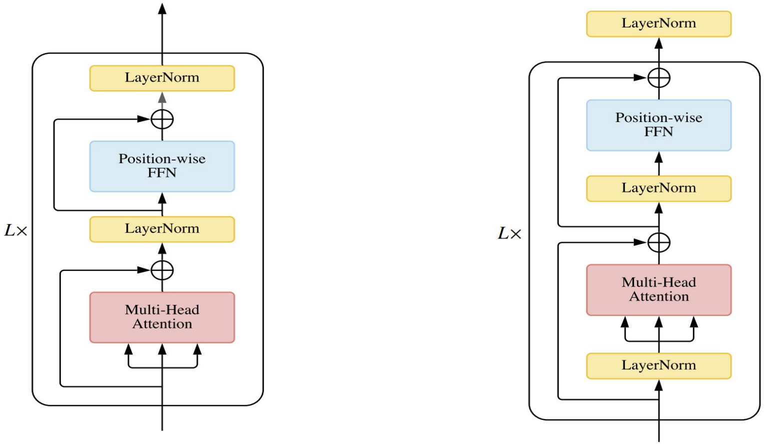
AdaNorm[153], scaled $\ell_2$ normalization[93], PowerNorm[121]

Norm-free

ReZero-Transformer[5]

# Layer Norm

- Layer Norm + Residual connection stabilize training of deep networks
- Where to apply Layer Norm?
  - Vanilla Transformer used Post-LN
  - Later transformers used Pre-LN



(a) post-LN

(b) pre-LN

# Layer Norm based variants

- Empirical results show post-LN without learning rate warm-up lead to unstable training
  - Because of large gradients near output layer at initialization
  - Pre-LN doesn’t suffer from this problem
- Post-LN outperforms pre-LN variants after convergence
- post-LN variants don’t suffer from gradient imbalance
  - Amplification effect is the cause
    - Heavier dependency on residual branch leads to larger output shift in post-LN transformers
    - Remedy: Initialize parameters based on activation variations of sample data

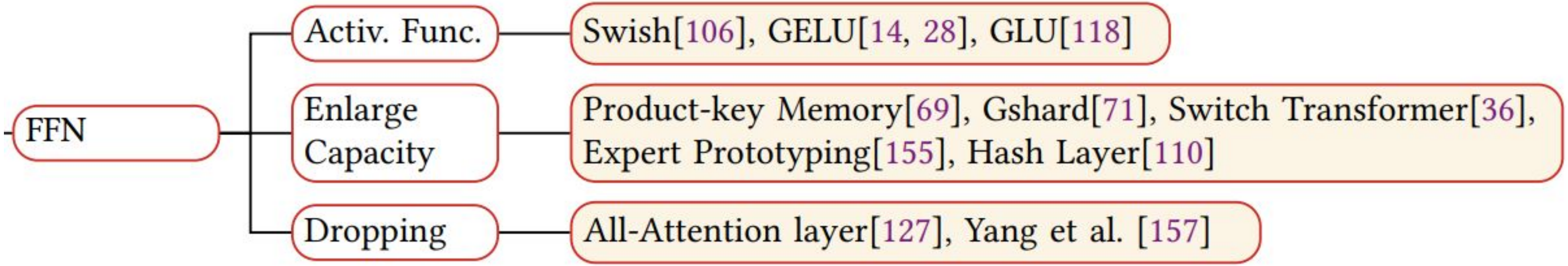
# Layer Norm substitutes

- Layer Norm has learnable parameters which aren’t very useful and increase risk of overfitting
- AdaNorm - a normalization technique without learnable parameters
- Scaled L2 normalization
- PowerNorm
    - Modifies BatchNorm
        - Relaxes zero-mean normalization
        - Uses quadratic mean of the signal instead of variance
        - Uses running statistics of quadratic mean instead of using per-batch statistics

# Normalization-free Transformers

- ReZero
    - Replaces LN module with a learnable residual connection
    - $H' = H + \text{alpha} * F(H)$
    - alpha is a learnable parameter with zero-initialization
    - Better dynamic isometry for input signals and leads to faster convergence

# FFN Variants

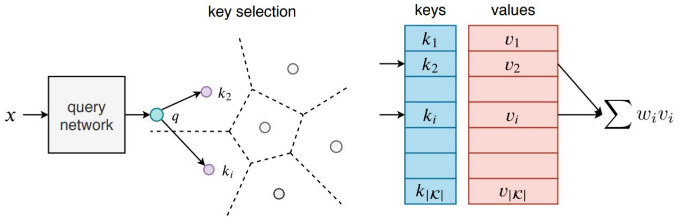

FFN
Activ. Func.
Swish[106], GELU[14, 28], GLU[118]
Enlarge Capacity
Product-key Memory[69], Gshard[71], Switch Transformer[36], Expert Prototyping[155], Hash Layer[110]
Dropping
All-Attention layer[127], Yang et al. [157]

# Position-wise FFN

- Simply stacking self-attention modules causes a rank-collapse
  - Token-uniformity inductive bias
- FFN mitigates this issue
- Variants:
  - Replace ReLU with Swish function f(x) = x * sigmoid(beta * x)
  - GPT replaces ReLU with GELU
  - Mini-dalle replaces ReLU with GLU

# Replacing FFN

- Idea: Replace FFN with similar structures with more parameters thereby improving model capacity
- Product-Key memory layers
  - A query network
  - A key selection module containing two sets of sub-keys
  - Value lookup table
  - Project input to a latency space using query network
  - Compare generated query to keys that are cartesian product of two sub-keys
  - Get K-nearest neighbors; Aggregate them to produce final output
  - Experiments on large-scale language modeling improved performance with negligible overhead



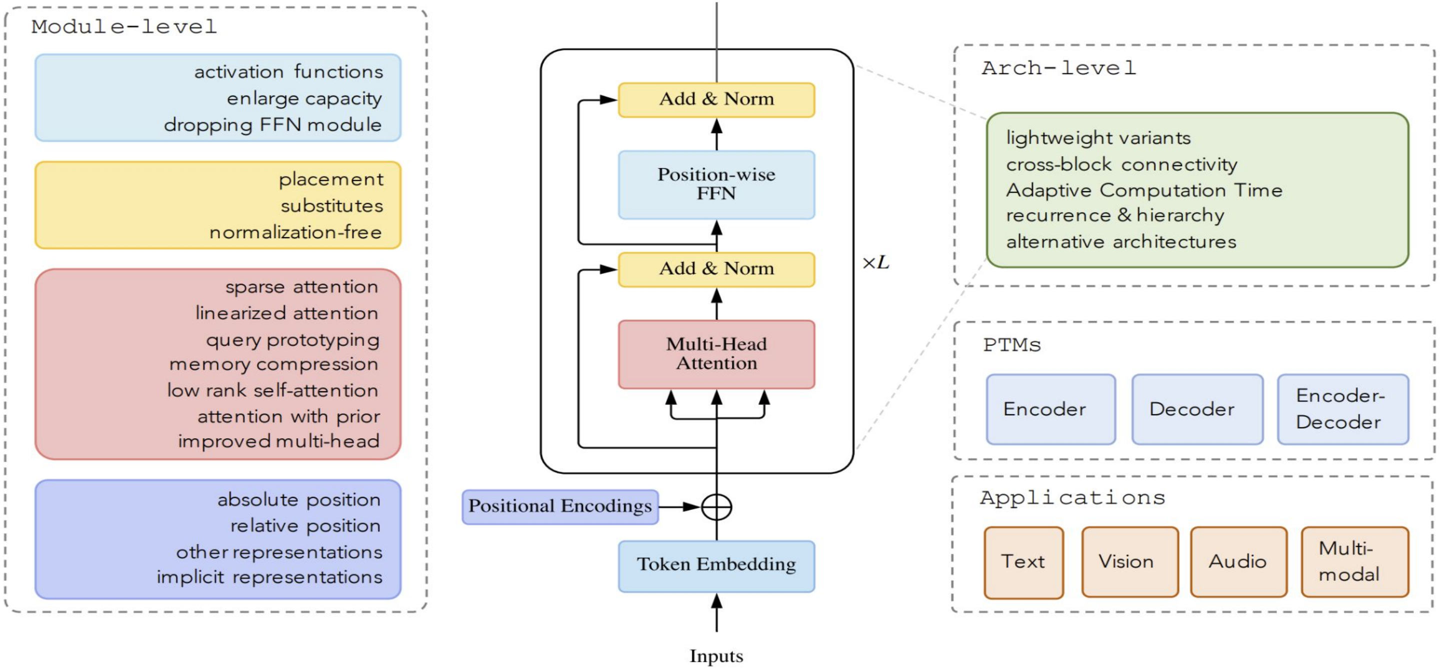
# Replacing FFN

- Mixture-of-Experts(MoE)
  - Sparsely-gated MoE instead of FFN
    - Experts are several FFNs
    - Outputs: weighted sum of FFN outputs using gate values computed by routing function
    - Routing function is learnable. Assigns tokens to experts
    - Only the experts with top-k gate values are activated in forward pass
- Switch Transformer
  - Routes using only a single expert with the largest gate value
  - Auxillary loss function to load balance between experts
- Top-k routing with expert prototyping
  - Top-k prototype groups and top-1 routing within group
- Instead of learnable routing function, hash function can be used
  - Tokens are hashed to fixed number of buckets(experts)

# Dropping FFN

- Observation: Replacing ReLU activation in FFN with softmax and dropping bias term turns FFN into an attention module where position-wise inputs attend to a global key-value memory
- Idea: Drop FFN by adding a set of learnable global key-value pairs
- In the decoder of a transformer, FFNs contribute very little with their large number of parameters.
    - Empirical results show improvement in inference and training with little loss of performance

# Architecture Level variants



# Architecture-level variants

- Lite-Transformer
  - Replaces attention module with a two-branch structure
    - Attention to capture long-range contexts
    - Depth-wise convolution and linear layers to capture local dependencies
- Funnel Transformer
  - Length of the hidden sequence is gradually reduced using pooling along the sequence dimension and recovered using up-sampling
  - Reduces FLOPs and memory
- DeLighT Transformer
  - Replaces transformer block with three sub-modules
    - Expand-and-reduce - to learn wider representations with low computation requirements
    - Single-head self-attention to learn pairwise interaction
    - Reduce-and-expand FFN
  - Leads to a deeper network with fewer parameters and FLOPs

# Cross-Block connectivity

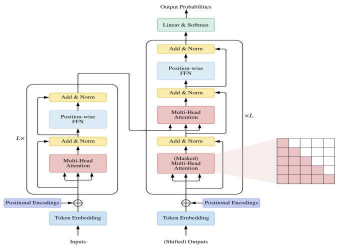


Fig. 1. Overview of vanilla Transformer architecture

- In a deep encoder-decoder transformer
  - Cross-attention module in the decoder only utilize the final outputs of the encoder
  - The error/feedback signal has to traverse along the depth of the encoder
  - Transformers are more susceptible to optimization issues like vanishing gradients
- Transparent Attention:
  - Weighted sum of encoder representations at all encoder layers
  - Use that as input in the cross attention module
  - This shortens the path for the error signal to the encoders and eases the optimization of deeper Transformers
- Feedback Transformer
  - Vanilla Transformer: Decoders were attending history representations of lower layers
  - Feedback mechanism where each position in the decoder can attend to history representation from all layers

# Adaptive Computation Time

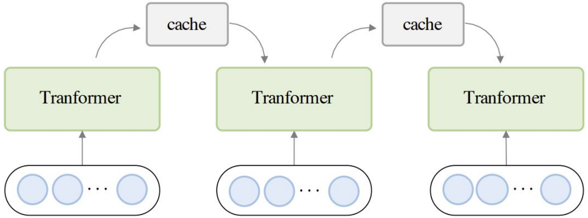
- Idea: Computation time conditioned on the inputs
- More computation for harder data and less computation for easy data
  - Efficiency for easy examples
  - Feature refinement for hard examples
- Universal Transformer
  - Recurrence-over-depth mechanism that iteratively refines representations for all symbols using a module that is shared over depth
  - Per-position dynamic halting mechanism that calculates a halting probability for each symbol at every time step
  - If halting prob > threshold, representation for subsequent time steps is unchanged
  - Recurrence is stopped when all symbols halt or max number of steps is reached

# Adaptive Computation Time

- Conditional Computation Transformer
  - Adds a gating module to each self-attention and FFN to decide whether to skip the current layer
  - Auxillary loss that encourages the model to adjust the gating modules to match the practical computation cost to the available computation budget
- Adapt the number of layers to each input in order to achieve good speed-accuracy trade-off
  - Choosing to exit early
  - Add an internal classifier at each layer and jointly train all classifiers
  - Classifier output says yes or no to the exit question
  - Criteria:
    - Entropy of output probability distribution of current layer
    - Number of times predictions remain unchanged to decide to whether to exit
    - Window-based uncertainty criterion to achieve token-level partial exiting in sequence labeling tasks
    - Voting-based exit strategy that considers each layer predictions of all past internal classifiers to infer the correct label and to decide whether to exit

# Divide and Conquer

- Decompose input sequence into finer segments
- Transformers are reused for different input segments
- Recurrent Transformers
  - A cache memory is maintained to incorporate history information
  - Cache is an additional input to the network
  - Network writes hidden state to cache
  - Example: Transformer-XL
- Compressive Transformer
  - Extends the cache with two levels of memory
    - Activations from previous segment
    - Compressed activations from older segments
- Memformer
  - Introduces cross attention to encoder
    - Allows encoder to attend to the memory
    - Memory slot attention on top of the encoder output to write the memory for next segment



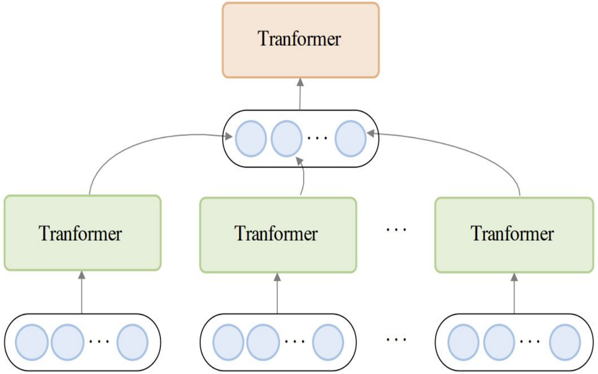
(a) Recurrent Transformer

# Recurrent Transformer

- Extended context:
  - Transformer-XL: L x Nmem; Nmem is the length of cached memory sequence
  - Compressive Transformer: L x (Nmem + c Ncm); c is compression rate; Ncm is length of compressed memory
- Notes to avoid expensive BPTT:
  - Local loss functions where original memories are constructed from compressed memories
  - Memformer uses: Memory Replay Back-Propagation algorithm which replays the memory at each timestep to accomplish back propagation over long unrolls
- Alternate ways to add recurrence to transformers
  - ERNIE-Doc
  - Compressed single vector representation of divided segments

# Hierarchical Transformer

- Decompose inputs hierarchically into elements of finer granularity
- Low-level features are first fed to a Transformer encoder
  - Outputs are aggregated to form a high level feature -> High-level transformer
- Allows modeling of long inputs with limited resources
- Potential to generate richer representations that are beneficial to tasks



(b) Hierarchical Transformer

# Hierarchical Transformers

- Document translation
  - Previous sentences from both source and target are used in translating a new sentence
  - Attention is used to summarize low-level information
- HIBERT
  - Encodes a document of text by first learning sentence representations
  - Then uses sentence representations to encode document-level representations
- Hi-Transformer
  - Sentence Transformer
  - Document Transformer
  - Learns hierarchically document context aware sentence representations
  - Document context-aware sentence representations are fed to another sentence transformer to improve sentence context modeling

# Hierarchical TF for richer representation

- Task specific rich representations
- TENER
  - Low-level TF encoder to encoder character features which is concatenated to word embeddings as input to high-level TF encoder
- Vision Transformer
  - Divide input image into several patches that serve as basic input elements to TF
  - Loses pixel information within patches
  - TNT: Fixes this issue by using inner TF block that transforms pixel representations and an outer TF block that takes fused vectors of patch representations and pixel representations as input

# Alternate Architectures

- Macaron Transformer
    - Replaces each transformer block with FFN-attention-FFN variant
- Sandwich Transformer
    - Reorganizes attention modules and FFN modules such that attention modules are mainly located in lower layers and FFN modules in upper layers
    - Improves perplexity on multiple language models without increasing parameters
- Mask Attention Network
    - Prepends a dynamic mask attention module to self-attention module in each TF block
    - Mask is conditioned on token representations
    - Effectively models model locality in text data
- Evolved Transformer
    - Uses Evolution based architecture search to come up with a TF architecture
    - Shows consistent improved performance on language tasks
- DARTSformer
    - Uses Differentiable architecture search for searching architecture and outperforms ET

# Pre-trained Transformer Variants

- Transformers are suitable for learning universal representations
- Transformers are used for producing pre-trained that can be later fine-tuned for downstream tasks
- Pre-training is usually combined with self-supervised tasks
- Encoder only
  - BERT with Masked Language Modeling and Next Sentence Prediction as self-supervision
  - RoBERTa: Removed NSP from BERT
- Decoder only
  - GPT, GPT-2, GPT-3
  - Impressive few shot performance
- Encoder-Decoder
  - BART - model is able to perform both natural language understanding and generation

# Hugging Face Transformers

ALBERT - Factorized embedding parameterization and cross-layer parameter sharing

BART - Standard Transformer with bidirectional encoder

BARThez - Seq2Seq model in French; Standard Transformer

BARTPho - BART in Vietnamese; Standard Transformer

BeIT - BERT for Image Transformers; Standard Transformer

BERT - Standard Transformer

# HF

BigBird Pegasus/RoBERT-a - Sparse attention;

BlenderBot - Standard Transformer

BLOOM - Like GPT-3; Standard Transformer

Bort - Neural Architecture Search based; Compressed BERT

ByT5 - Token free; Robust to noise; Standard Transformer

CamemBert - French language model

Canine - Deep Transformer stack; Performer/BigBird -as drop in replacement

Codegen, CLIP, CLIPSeg - Standard Transformer

Conditional DETR - Cross Attention

Conv BERT - Mixed Attention; Some Self-Attention heads are replaced with conv

ConvNexT - Pure ConvNet inspired from Transformers. Outperforms Swin-T

CTRL - Standard Transformer with sinusoidal position embedding

Data2vec - Standard Transformer

DeBERTa - Disentangled attention; Word - two vectors; Disentangled attn matrix

Decision Transformer - Reinforcement Learning

# HF

Deformable DETR - DETR that attends to a small set of key sampling points

DeIT - Teacher-student strategy specific to transformers. Token-based distillation

DETR - Detection Transformer

DistilBERT - BERT with Knowledge distillation

DIT - Document Image Transformer; Uses ViT as backbone

Donut - Doc Understanding; Swin-T

Dense Prediction Transformer - ViT as backbone

FNET - Replaces Self-Attention with linear transformations of input - Fourier Transform

HF

Funnel Transformer - Compresses sequence of hidden state to save FLOPs

LeViT - Activation maps with different resolutions + Attention bias(for position)

Longformer - Sparse Attention

LongT5 - ETC like local/global attention - Extended Transformer Construction

Maskformer - Per-pixel classification - predicts a set of binary masks to each class

Metaformer - Poolformer with pooling layer generalized as “token mixer”

HF

Pyramid Vision Transformer - Stacks multiple ViT

Roformer - Replace dot product with locality sensitive hashing

Segformer - Hierarchically placed Transformer encoder - Segmentation

Switchformers - Variant on FFN

Table Transformer - DETR on table data

Transjectory Transformer - RL based Transformer

ViLT - Convolution free processing of visual inputs similar to text

HF

- Visual Attention Network - Large Kernel Attention replaces Self Attention
- YOSO - Linear Attention with LSH and Bernoulli Sampling

# References

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- Efficiently Scaling Transformers - https://arxiv.org/pdf/2211.05102.pdf