Stat 9911
Principles of AI: LLMs
Large Language Model Architectures 04
Specific LLMs

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Plan

- We plan to discuss specific LLM families such as GPT, Llama, DeepSeek.

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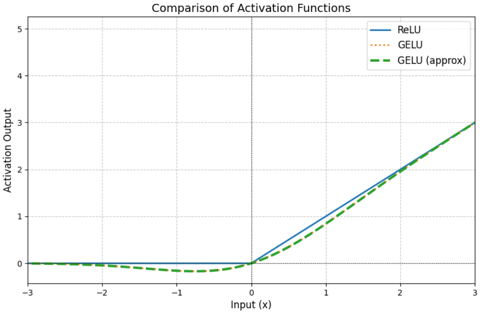
GPT Series

- GPT series (Radford et al., 2018, 2019; Brown et al., 2020; OpenAI, 2023)
- GPT-1: Gaussian Error Linear Unit (GELU) activation (Hendrycks and Gimpel, 2016): $x \mapsto x \cdot \Phi(x)$, where Φ is normal cdf, or approximate $x \mapsto 0.5x \left(1 + \tanh\left(\sqrt{\frac{2}{\pi}}\left(x + 0.044715x^3\right)\right)\right)$ (Choudhury, 2014).
- GPT-2: Modified initialization: "We scale the weights of residual layers at initialization by a factor of $1/N^{1/2}$ where N is the number of residual layers."



GPT-3 (Brown et al., 2020) Model Details

- "Alternating dense and locally banded sparse attention patterns (similar to the Sparse Transformer (Child et al., 2019))"
- GPT-3 with 175B parameters
  - Context window: $T = 2048$ tokens
  - Layers: 96
  - Embedding rep: $d = 12288$
  - Feedforward rep: $d' = 4d$
  - Number of attention heads: $H = 96$, Dimension per head: $d/H = 128$

GPT-3 "on a Napkin"

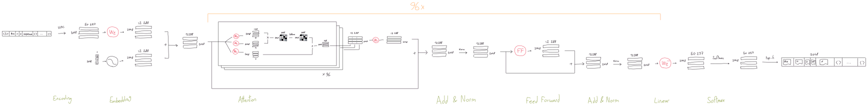


Figure: See source for a higher resolution.

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LLama Series

- LLama 1 (Touvron et al., 2023a):
  - RMSNorm pre-normalization (Zhang and Sennrich, 2019).
  - Activation: SwiGLU (Shazeer, 2020).
  - Rotary Position Embeddings (RoPE) (Su et al., 2024).
- LLama 2 (Touvron et al., 2023b):
  - Grouped-query attention (GQA) (Ainslie et al., 2023).
- LLama 3 (Dubey et al., 2024):
  - "Attention mask that prevents self-attention between different documents within the same sequence."
  - 405-B:
    - Context window: $T = 128K$ tokens
    - Layers: 126
    - Embedding rep: $d = 16,384$
    - Feedforward rep: $d' = 20,480$
    - Number of attention heads: $H = 128$. Key-value heads: 8

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DeepSeek-V2 (Liu et al., 2024)

- Multi-head Latent Attention
  - Map token emb e into an intermediate emb $e^{KV} = We$ of much lower dimension. Next, compute keys and values $k = W^K e^{KV}$, $v = W^V e^{KV}$ from this smaller dimensional rep.
  - Reduces size of the KV cache during inference, as only e^{KV} needs to be stored; leading to memory savings.
  - Weight decay can induce low-rank attention layers, see e.g., Kobayashi et al. (2024); so this architectural choice has some principled justification.
  - Same for the query, i.e., $e^Q = W^{Q'} e$, $q = W^Q e^Q$.
  - Compute MHA as usual.
  - Some linear maps become redundant, e.g., W^K and W^Q can be merged; also W^V and output projection W^O
- Decoupled Rotary Position Embedding (Bi et al., 2024)
  - Apply RoPE only to separate key-value projections

MLA + Decoupled RoPE

$$\mathbf{c}_t^Q = W^{DQ}\mathbf{h}_t, \tag{37}$$

$$[\mathbf{q}_{t,1}^C; \mathbf{q}_{t,2}^C; \ldots; \mathbf{q}_{t,n_h}^C] = \mathbf{q}_t^C = W^{UQ}\mathbf{c}_t^Q, \tag{38}$$

$$[\mathbf{q}_{t,1}^R; \mathbf{q}_{t,2}^R; \ldots; \mathbf{q}_{t,n_h}^R] = \mathbf{q}_t^R = \mathrm{RoPE}(W^{QR}\mathbf{c}_t^Q), \tag{39}$$

$$\mathbf{q}_{t,i} = [\mathbf{q}_{t,i}^C; \mathbf{q}_{t,i}^R], \tag{40}$$

$$\boxed{\mathbf{c}_t^{KV}} = W^{DKV}\mathbf{h}_t, \tag{41}$$

$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \ldots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK}\mathbf{c}_t^{KV}, \tag{42}$$

$$\boxed{\mathbf{k}_t^R} = \mathrm{RoPE}(W^{KR}\mathbf{h}_t), \tag{43}$$

$$\mathbf{k}_{t,i} = [\mathbf{k}_{t,i}^C; \mathbf{k}_t^R], \tag{44}$$

$$[\mathbf{v}_{t,1}^C; \mathbf{v}_{t,2}^C; \ldots; \mathbf{v}_{t,n_h}^C] = \mathbf{v}_t^C = W^{UV}\mathbf{c}_t^{KV}, \tag{45}$$

$$\mathbf{o}_{t,i} = \sum_{j=1}^{t} \mathrm{Softmax}_j\left(\frac{\mathbf{q}_{t,i}^T\mathbf{k}_{j,i}}{\sqrt{d_h + d_h^R}}\right)\mathbf{v}_{j,i}^C, \tag{46}$$

$$\mathbf{u}_t = W^O[\mathbf{o}_{t,1}; \mathbf{o}_{t,2}; \ldots; \mathbf{o}_{t,n_h}], \tag{47}$$

where the boxed vectors in blue need to be cached for generation. During inference, the naive formula needs to recover $\mathbf{k}_t^C$ and $\mathbf{v}_t^C$ from $\mathbf{c}_t^{KV}$ for attention. Fortunately, due to the associative law of matrix multiplication, we can absorb W^{UK} into W^{UQ}, and W^{UV} into W^O. Therefore, we do not need to compute keys and values out for each query. Through this optimization, we avoid the computational overhead for recomputing $\mathbf{k}_t^C$ and $\mathbf{v}_t^C$ during inference.

Figure: Our notation: $h \to e$, $c^Q \to e^Q$, $c^{KV} \to e^{KV}$, $o \to \hat{v}$, $u \to e'$

DeepSeek-V3 MoE

- Mixture of Experts (MoE): Shared and routed experts for efficiency (Dai et al., 2024). Compute the FFN output h' as

$$h' = u + \sum_{i=1}^{N_s} \phi_i^{(s)}(u) + \sum_{i=1}^{N_r} g_i \phi_i^{(r)}(u),$$

$$g_i = \begin{cases} s_i, & s_i \in \mathrm{Topk}\left(\{s_j \mid 1 \leqslant j \leqslant N_r\}, K_r\right), \\ 0, & \text{otherwise}, \end{cases}$$

$$s_i' = \mathrm{Sigmoid}\left({e'}_t^{\top} f_i\right), \quad s_i = s_i' / (\sum_{j=1}^{N_r} s_j)$$

where

- N_s and N_r denote the numbers of shared and routed experts, resp;
- $\phi_i^{(s)}(\cdot)$ and $\phi_i^{(r)}(\cdot)$ denote the i-th shared routed experts, resp;
- K_r denotes the number of activated routed experts;
- g_i is the gate value for the i-th expert; s_i is token-to-expert affinity;
- f_i is the mean over tokens of the activations of the i-th routed expert.

DeepSeek-V3

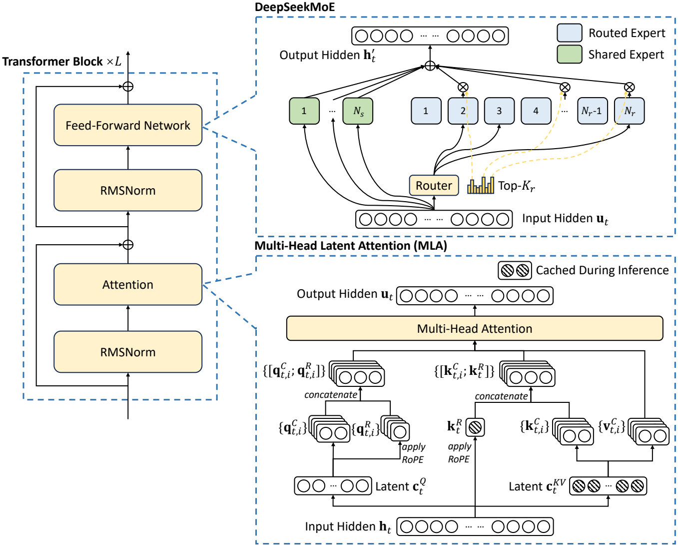

Figure: Our notation: $h \to e$, $c^Q \to e^Q$, $c^{KV} \to e^{KV}$, $o \to \hat{v}$, $u \to e'$

DeepSeek-V3 MoE

- Auxiliary-Loss-Free Load Balancing (Wang et al., 2024).
  - Add a constant c_i to the affinities when determining which experts to choose as in $s_i + c_i \in \operatorname{Topk}\left(\{s_j + c_j \mid 1 \leqslant j \leqslant N_r\}, K_r\right)$. These values are constant across tokens.
  - Update them heuristically during training to balance loads.

Loss-based balancing in MoE

- Loss-based balancing (Lepikhin et al., 2020; Fedus et al., 2022), with a small weight: For a sequence of length T, define auxiliary loss $\mathcal{L}_{\text{Balance}} = \alpha \sum_{i=1}^{N} f_i P_i$, where

$$f_i = \frac{N}{KT} \sum_{t=1}^{T} I(\text{Token } t \text{ selects Expert } i), \quad P_i = \frac{1}{T} \sum_{t=1}^{T} s_{i,t}.$$

  Here:
  - N is the total number of experts.
  - K is the number of experts selected for each token.
  - $s_{i,t}$ is the routing score of Expert i for Token t.
  - f_i represents the fraction of tokens routed to Expert i.
  - P_i denotes the average gating scores of Expert i.
  - α is a hyper-parameter controlling the strength of the auxiliary loss.

  This loss promotes balance, if f_i is correlated with P_i across tokens;
  - larger average scores (across tokens) for an expert correspond to larger selection frequencies (across tokens) of that specific expert.

DeepSeek-V3

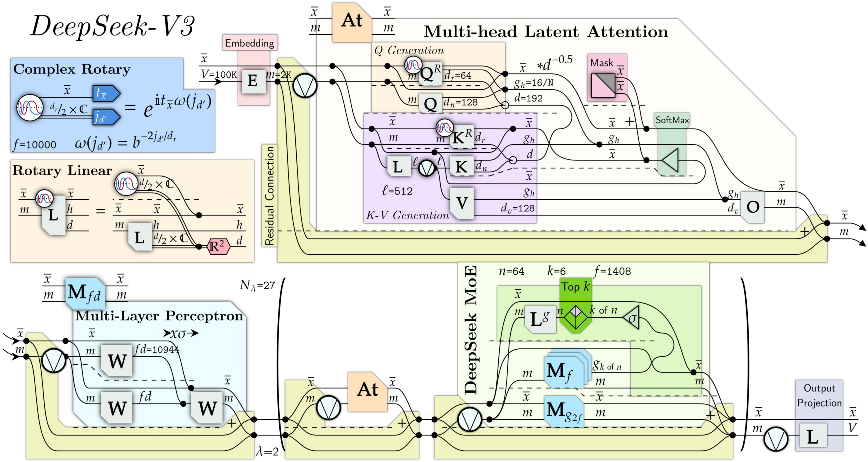

Figure: Via X (suspended account)

DeepSeek-V3

- Long context extension: YaRN (Peng et al., 2023).

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