DeepSeek and GPT2 Architecture

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Contents

Math format

Let $X \in \{0,1\}^{T\times d}$ for input, where d is the dimension of tokens and T is the length of inputs.Then the **embedding layer** is defined as:

$$\mathrm{Enc}(X) = XE_1, \tag{1}$$

where $E \in \mathbb{R}^{d\times D}$.
The Enc module plus **positional encoding** reconstruct a new Enc module:

$$\mathrm{Enc}(X) = XE_1 + PE_2, \tag{2}$$

where $P \in \{0,1\}^{T\times T}$, $P_{i,i} = 1, P_{i\neq j} = 0$ and $E_2 \in \mathbb{R}^{T\times D}$
Remark: $\mathrm{Enc}(X) : \{0,1\}^{T\times d} \to \mathbb{R}^{T\times D}$.
Let $X \in \mathbb{R}^{T\times D}$ for the middle input, where D is the dimension of middle layer.
The **norm layer** is defined as:

$$\mathrm{Norm}(X) := \frac{X - \mathbb{E}X}{\mathrm{Var}(X)}, \tag{3}$$

where $\mathrm{E}(X), \mathrm{Var}(X) \in \mathbb{R}^{T\times D}$.
Norm: $\mathrm{ATT} : \mathbb{R}^{T\times D} \to \mathbb{R}^{T\times D}$.

Math format

Let H be the head number of multi-head attention, for the h-th head $W_{K,h} \in \mathbb{R}^{D\times D_K}$, $W_{Q,h} \in \mathbb{R}^{D\times D_K}$, $W_{V,h} \in \mathbb{R}^{D\times D_V}$ and $W_O \in \mathbb{R}^{HD_V\times D}$. Then the **multi-head attention** is defined as:

- Single head attention:

$$S_h = \mathrm{Softmax}(\frac{XW_{Q,h}(XW_{K,h})^T}{\sqrt{D_K}})XW_{V,h}, \tag{4}$$

- Masked single head attention:

$$S_h = \mathrm{Softmax}(\frac{XW_{Q,h}(XW_{K,h})^T + M}{\sqrt{D_K}})XW_{V,h}, \tag{5}$$

  where $M \in \{-\infty, 0\}^{T\times T}$, $M_{ij} = -\infty$ if $i < j$ else $M_{ij} = 0$.
  Remark: $\mathrm{S_h} : \mathbb{R}^{T\times D} \to \mathbb{R}^{T\times D_V}$.

- Concatenate & Residual

$$\mathrm{ATT}(X) := X + [S_1, \ldots, S_h, \ldots, S_H]W_O, \tag{6}$$

where $\mathrm{Softmax}(X)$ is row-wise.
Remark: $\mathrm{ATT} : \mathbb{R}^{T\times D} \to \mathbb{R}^{T\times D}$.

Math format

The **MLP** layer is defined as:

$$\mathrm{MLP}(X) := X + f_L(X) \circ \sigma \circ \cdots \sigma \circ f_1(X), \tag{7}$$

where $f_i(X) := XW_i + b_i,\ b_i \in \mathbb{R}^{D_i},\ W_1 \in \mathbb{R}^{D \times D_1},\ W_i \in \mathbb{R}^{D_{i-1} \times D_i}$ and $W_L \in \mathbb{R}^{D_{L-1} \times D}$.
Remark: $\mathrm{ATT} : \mathbb{R}^{T \times D} \to \mathbb{R}^{T \times D}$.
For each element x, the **active function** σ is defined as:

$$\begin{aligned} \mathrm{GeLU}(x) &:= xP(X \leq x) \\ &= x \int_{-\infty}^{x} \frac{\exp(\frac{-(t-\mu)^2}{2\sigma^2})}{\sqrt{2\pi}\sigma} dt \\ &\simeq 0.5x(1 + \tanh(\sqrt{\frac{2}{\pi}}(x + 0.044715x^3))). \end{aligned} \tag{8}$$

Math format

The **block** in GPT is defined as:

$$\mathrm{Block}(X) := \mathrm{MLP} \circ \mathrm{Norm} \circ \mathrm{ATT} \circ \mathrm{Norm}(X) \tag{9}$$

The **embedding** is defined as:

$$X^e := \mathrm{Norm} \circ \mathrm{Block}_M \cdots \mathrm{Block}_1 \circ \mathrm{Enc}(X). \tag{10}$$

The **GPT** architecture is defined as:

$$\mathrm{GPT}(X) := \arg\max_{\mathrm{index}} X^l = X^e W_{\mathrm{head}}, \tag{11}$$

where $W_{\mathrm{head}} \in \mathbb{R}^{D \times d}$.
Remark: $\mathrm{ATT} : \{0, 1\}^{T \times d} \to \mathbb{R}^{T \times d}$.

GPT parameters

Table: Parameter setting.

Parameter	GPT-2(125M)	GPT-3/3.5(175B)	GPT-4(1800B)
d (vocab_size)	50304	*	*
T (block_size)	1024	2048	8000(p.t.)->32000(f.t.)
D (n_embd)	768	12288	*
D_V (n_embd)	768/12=64	12288/96 =128	*
D_K (n_embd)	768/12=64	12288/96 =128	*
H (n_head)	12	96	*
L (MLP layer)	2	2	*
W_1 (first layer)	$\mathbb{R}^{4D\times D}$	$\mathbb{R}^{4D\times D}$	*
W_2 (second layer)	$\mathbb{R}^{D\times 4D}$	$\mathbb{R}^{D\times 4D}$	*
M (n_layer)	12	96	120
N(data_number)	40G	570G	*

Loss functions

Then the loss function is:

$$-\sum_{i=1}^{T}\sum_{j=1}^{d} P_{ij} \log \mathrm{Softmax}(X^l)_{ij} \tag{12}$$

, where P_i is the probability of the next token. or

$$-\sum_{i=1}^{T} \log \mathrm{Softmax}(X^l)_{ij_{\mathrm{true}}} \tag{13}$$

, where j_{true} is the next token in the directory.

Contents

Math format

Let $X \in \{0,1\}^{T\times d}$ for input, where d is the dimension of tokens and T is the length of inputs.Then the **embedding layer** is defined as:

$$\mathrm{Enc}(X) = XE, \tag{14}$$

where $E \in \mathbb{R}^{d\times D}$.
Remark: $\mathrm{Enc}(X) : \{0,1\}^{T\times d} \to \mathbb{R}^{T\times D}$.
Let $X \in \mathbb{R}^{T\times D}$ be the hidden input and $X_{i\cdot}^T \in \mathbb{R}^D$, where D is the dimension of middle layer. Then **RMSNorm** layer is defined as:

$$\mathrm{RMSNorm}(X_{i\cdot}) := \frac{X_{i\cdot}}{\sqrt{\frac{1}{D}\|X_{i\cdot}\|_2^2}}, \forall i \in \{0,1,...,T\} \tag{15}$$

Remark: $\mathrm{RMSNorm}(X) : \mathbb{R}^{T\times D} \to \mathbb{R}^{T\times D}$.

Math format

Let $X \in \mathbb{R}^{T \times D}$ be the hidden input, then the Rotary Positional Embedding (**RoPE**) is defined as:

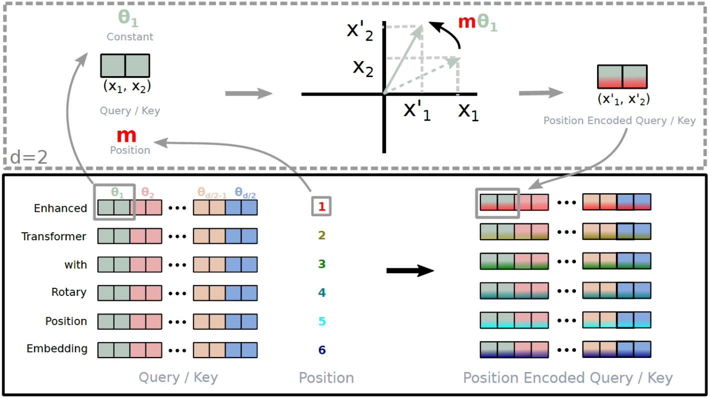
$$\mathrm{RoPE}(X; W_p, W_R) = XW_pW_R^T, \tag{16}$$

where

$$W_R = \begin{pmatrix} \cos m\theta_1 & -\sin m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ \sin m\theta_1 & \cos m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cos m\theta_2 & -\sin m\theta_2 & \cdots & 0 & 0 \\ 0 & 0 & \sin m\theta_2 & \cos m\theta_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cos m\theta_{D^R}/2 & -\sin m\theta_{D^R}/2 \\ 0 & 0 & 0 & 0 & \cdots & \sin m\theta_{D^R}/2 & \cos m\theta_{D^R}/2 \end{pmatrix}$$

, $\theta_i = 10000^{-2(i-1)/d}, i \in [1, 2, \ldots, D^R/2]$ and $W_p \in \mathbb{R}^{D \times D^R}$.
Remark:$\mathrm{RoPE}(X) : T \times D \to T \times D^R$.

RoPE


θ_1
Constant
(x_1, x_2)
Query / Key
m
Position
d=2
x'_2
x_2
x'_1
x_1
$m\theta_1$
(x'_1, x'_2)
Position Encoded Query / Key
θ_1 θ_2 $\theta_{d/2-1}$ $\theta_{d/2}$
Enhanced
Transformer
with
Rotary
Position
Embedding
1
2
3
4
5
6
Query / Key
Position
Position Encoded Query / Key

Math format

Let $X \in \mathbb{R}^{T \times D}$ be the hidden input, then the **LoRA** layer is defined as:

$$\mathrm{LoRA}(X; W_{down}, W_{up}) := XW_{down}W_{up}, \tag{17}$$

where $W_{down} \in \mathbb{R}^{D \times d_{down}}$, $W_{up} \in \mathbb{R}^{d_{down} \times d_h n_h}$, $d_{down} = d_c$ for keys and values, $d_{down} = d'_c$ for queries, d_h is the hidden dimension before attention layer and h_n is the number of heads in multi-head attention layer.
Remark:$\mathrm{LoRA}(X; W_{down}, W_{up}) : T \times D \to T \times d_h h_n$.
Let $L \in T \times d_h h_n$, Define an extract operator as follows:

$$L_{\cdot\cdot h} = L_{i, j \times h_n + h}, \forall i \in \{1, \cdots, T\}, j \in \{1, \cdots, d_h\} \tag{18}$$

where $h \in \{1, \cdots, h_n\}$.
Remark: $L_{\cdot\cdot h} : T \times d_h h_n \to T \times d_h$

Math format

Let $X \in \mathbb{R}^{T \times D}$ be the hidden input, $W_O \in \mathbb{R}^{d_h n_h \times D}$, $\mathrm{Softmax}(X)$ is a row-wise operator, then the multi-head attention (**MLA**) is defined as follows:

- LoRA layer:

$$\begin{cases} L_Q = LoRA(X; W^{DQ}, W^{UQ}), \\ L_K = LoRA(X; W^{DKV}, W^{UK}), \\ V = LoRA(X; W^{DKV}, W^{UV}). \end{cases} \tag{19}$$

- RoPE layer:

$$R_Q = \mathrm{RoPE}(X; W_{DQ}, W_{QR}), R_K = \mathrm{RoPE}(X; W_{DKV}, W_{KR}) \tag{20}$$

- Cat the output of LoRA and ROPE for one head:

$$Q_h = [L_{Q \cdot \cdot h}, R_{Q \cdot \cdot h}], K_h = [L_{k \cdot \cdot h}, R_{K \cdot \cdot h}], \tag{21}$$

where $Q_h, R_K \in \mathbb{R}^{T \times (d_h + D^R)}$.

Math format

- Single head attention:

$$S_h = \mathrm{Softmax}(\frac{Q_h K_h^T + M}{\sqrt{D^R + d_h}}) V_{\cdot\cdot h}, \tag{22}$$

where $M \in \{-\infty, 0\}^{T \times T}$, $M_{ij} = -\infty$ if $i < j$ else $M_{ij} = 0$.
Remark: $\mathrm{S_h} \in \mathbb{R}^{T \times T}$.

- Concatenate & Residual

$$\mathrm{MLA}(X) := [S_1, \dots, S_h, \dots, S_{h_n}] W_O, \tag{23}$$

Remark: $\mathrm{MLA} : \mathbb{R}^{T \times D} \to \mathbb{R}^{T \times D}$.

Math format

The **MLP** layer is defined as:

$$\mathrm{MLP}(X) := f_3 \circ (\sigma(f_2(X)) \odot f_1(X)), \tag{24}$$

where $f_i(X) := XW_i + b_i$, $b_i \in \mathbb{R}^{D_i}$, $W_1 \in \mathbb{R}^{D \times D_1}$, $W_i \in \mathbb{R}^{D_{i-1} \times D_i}$ and $W_L \in \mathbb{R}^{D_{L-1} \times D}$.

Remark: $\mathrm{MLP} : \mathbb{R}^{T \times D} \to \mathbb{R}^{T \times D}$.

For each element x, the **active function** σ is defined as:

$$\mathrm{SiLU}(x) := \frac{x}{1 + e^{-x}}. \tag{25}$$

Math format

Let $X \in \mathbb{R}^{T\times D}$ be the hidden input, the **Gate** is defined as follows:

- Obtain the weights of N_r experts for every tokens:

$$G = \mathrm{Sigmoid}(XW_{experts}), \tag{26}$$

  where $W_{experts} \in \mathbb{R}^{D\times N_r}$ and Sigmoid is a row-wise operator.

- Select top K_r experts for every tokens:

$$g'_{i,t} = \begin{cases} G_{i,t}, & G_{i,t} \in \mathrm{Topk}(\{G_{i,k} \mid 1 \le k \le N_r\}, K_r) \\ 0, & \text{otherwise}, \end{cases} \tag{27}$$

- Normalization:

$$\mathrm{Gate}(X)_{it} := \frac{g'_{i,t}}{\sum_{t=1}^{N_r} g'_{j,t}} \tag{28}$$

Remark: $\mathrm{Gate}(X) : \mathbb{R}^{T\times D} \to \mathbb{R}^{T\times N_r}$. In the code only need $T \times K_r$ because the remains are zero.

Math format

Let $X \in \mathbb{R}^{T\times D}$ be the hidden input. There are N_r routed experts (**MLP**^{r}) and N_s shared experts (**MLP**^{s}), then the **MOE** layer is defined as:

$$\mathrm{MoE}(X) = \sum_{i=1}^{N_s} \mathrm{MLP}_i^s(X) + \sum_{j=1}^{N_r} \mathrm{Gate}(X)_{\cdot j}\, \mathrm{MLP}_j^r(X), \tag{29}$$

Remark:$\mathrm{MoE}(X) : \mathbb{R}^{T\times D} \to \mathbb{R}^{T\times D}$.

Math format

The **Block** in DeepSeek is defined as follows:

- The attention layer

$$\mathrm{ResMLA}(X) := X + \mathrm{MLA} \circ \mathrm{RMSNorm}(X) \tag{30}$$

- If the block number less than the number of dense layers (n_dense_layers).

$$\mathrm{ResMLP}(X) := X + \mathrm{MLP} \circ \mathrm{RMSNorm}(X), \tag{31}$$

- For the other blocks

$$\mathrm{ResMoE}(X) := X + \mathrm{MoE} \circ \mathrm{RMSNorm}(X), \tag{32}$$

- The i-th block is defined as:

$$\mathrm{Block_i}(X) = \begin{cases} \mathrm{ResMLP} \circ \mathrm{ResMLA}(X), i < \mathrm{n\_dense\_layers}, \\ \mathrm{ResMoE} \circ \mathrm{ResMLA}(X), \textit{others} \end{cases} \tag{33}$$

The **embedding** is defined as:

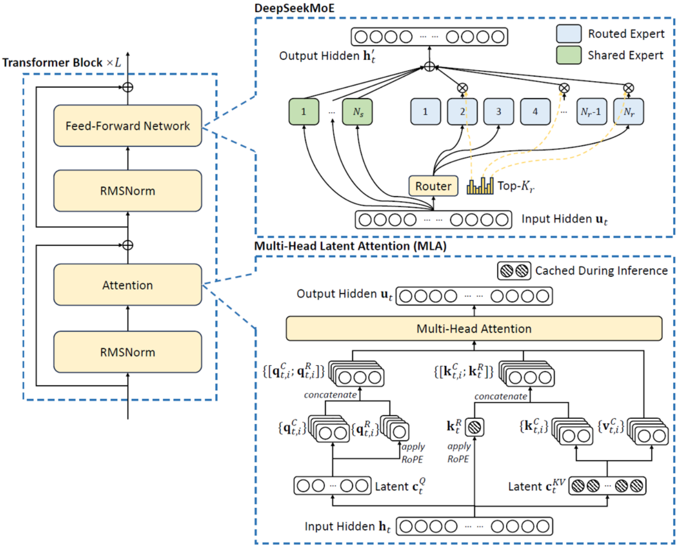
$$X^e := \mathrm{RMSNorm} \circ \mathrm{Block}_M \cdots \mathrm{Block}_1 \circ \mathrm{Enc}(X), \tag{34}$$

where $X^e \in \mathbb{R}^{T \times D}$. The output of **DeepSeek** is defined as:

$$\mathrm{DeepSeek} := \operatorname*{arg\,max}_{\mathrm{index}} X^l = X^e W_{\mathrm{head}}, \tag{35}$$

where $W_{\mathrm{head}} \in \mathbb{R}^{D \times d}$.

MLA and MOE


DeepSeekMoE
Transformer Block ×L
Feed-Forward Network
RMSNorm
Attention
RMSNorm
Output Hidden $\mathbf{h}_t'$
Routed Expert
Shared Expert
1
N_s
1
2
3
4
N_r-1
N_r
Router
Top-K_r
Input Hidden $\mathbf{u}_t$
Multi-Head Latent Attention (MLA)
Cached During Inference
Output Hidden $\mathbf{u}_t$
Multi-Head Attention
$\{[\mathbf{q}_{t,i}^C; \mathbf{q}_{t,i}^R]\}$
$\{[\mathbf{k}_{t,i}^C; \mathbf{k}_t^R]\}$
concatenate
concatenate
$\{\mathbf{q}_{t,i}^C\}$
$\{\mathbf{q}_{t,i}^R\}$
$\mathbf{k}_t^R$
$\{\mathbf{k}_{t,i}^C\}$
$\{\mathbf{v}_{t,i}^C\}$
apply RoPE
apply RoPE
Latent $\mathbf{c}_t^Q$
Latent $\mathbf{c}_t^{KV}$
Input Hidden $\mathbf{h}_t$

DeepSeek parameters

Parameter	168B	236B	671B
vocab_size (d)	102400	102400	129280
dim (D)	2048	5120	7168
inter_dim (MLP)	10944	12288	18432
moe_inter_dim (MoE)	1408	1536	2048
n_layers (M)	27	60	61
n_dense_layers	1	1	3
n_heads (n_h)	16	128	128
n_routed_experts (N_r)	64	160	256
n_shared_experts (N_s)	2	2	1
n_activated_experts (K_r)	6	6	8
q_lora_rank (LoRA)	0	1536	1536
kv_lora_rank (LoRA)	512	512	512
v_head_dim (h_n)	128	128	128

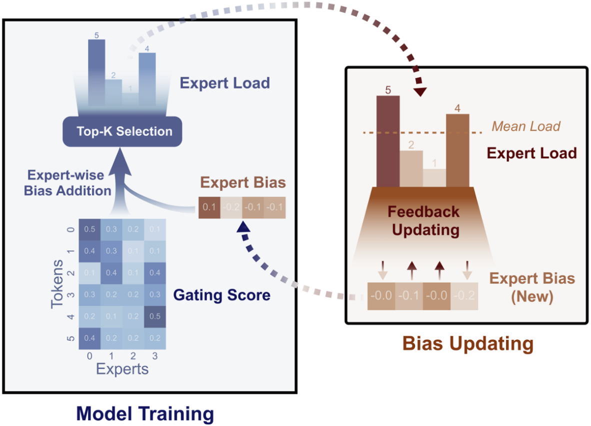
Main Loss Function

The main loss function is:

$$L_{main} = -\sum_{i=1}^{T} \log \mathrm{Softmax}(X^{l})_{ij_{\mathrm{true}}} \tag{36}$$

, where j_{true} is the next token in the directory.

Auxiliary-Loss-Free Load Balancing



An unbalanced expert load will lead to routing collapse and diminish computational efficiency in scenarios with expert parallelism.

Auxiliary-Loss-Free Load Balancing

Algorithm 1: Adjusting the per-expert bias b_i during training

Input: MoE model θ, training batch iterator B, bias update rate u.
1. Initialize $b_i = 0$ for each expert;
for *a batch* $\{(\mathbf{x}_k, \mathbf{y}_k)\}_k$ *in* B **do**
    2. Train MoE model θ on the batch data $\{(\mathbf{x}_k, \mathbf{y}_k)\}_k$, with gating scores calculated according to Eq. (3);
    3. Count the number of assigned tokens c_i for each expert, and the average number $\overline{c_i}$;
    4. Calculate the load violation error $e_i = \overline{c_i} - c_i$;
    4. Update $\mathbf{b}_i$ by $b_i = b_i + u * \text{sign}(e_i)$;
end
Output: trained model θ, corresponding bias $\mathbf{b}_i$

$$g'_{i,t} = \begin{cases} s_{i,t}, & s_{i,t} + b_i \in \operatorname{Topk}(\{s_{j,t} + b_j | 1 \leqslant j \leqslant N_r\}, K_r), \\ 0, & \text{otherwise.} \end{cases}$$

Complementary Sequence-Wise Auxiliary Loss

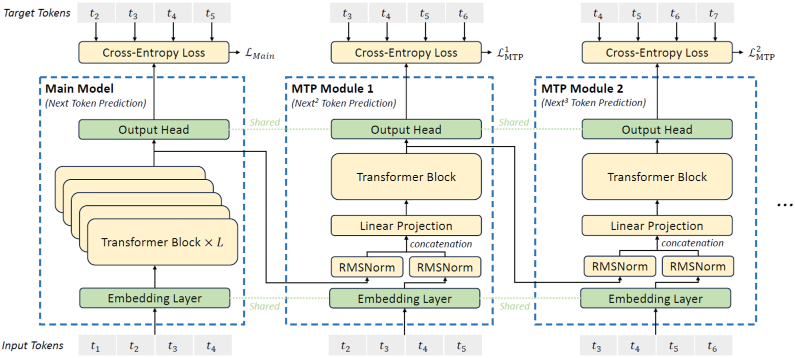
$$\mathcal{L}_{\text{Bal}} = \alpha \sum_{i=1}^{N_r} f_i P_i,$$

$$f_i = \frac{N_r}{K_r T} \sum_{t=1}^{T} \mathbb{1} \left(s_{i,t} \in \operatorname{Topk}(\{s_{j,t} | 1 \leqslant j \leqslant N_r\}, K_r) \right),$$

$$s'_{i,t} = \frac{s_{i,t}}{\sum_{j=1}^{N_r} s_{j,t}},$$

$$P_i = \frac{1}{T} \sum_{t=1}^{T} s'_{i,t},$$

Multi-Token Prediction



$$\mathcal{L}_{\mathrm{MTP}}^{k} = \mathrm{CrossEntropy}(P_{2+k:T+1}^{k}, t_{2+k:T+1}) = -\frac{1}{T}\sum_{i=2+k}^{T+1} \log P_i^k[t_i],$$

THANKS!