A Theory on How LLMs Make Decisions

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LLMs can maximize rewards during inference

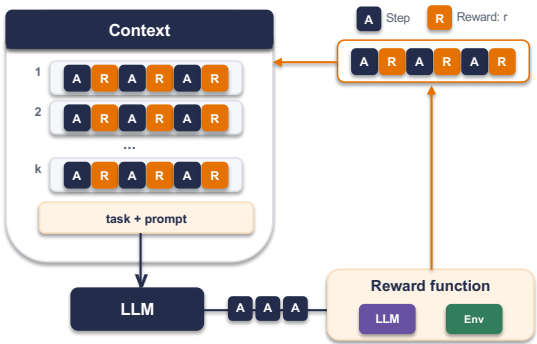
just like a reinforcement learning agent.

Game of 24

4	4	6	8

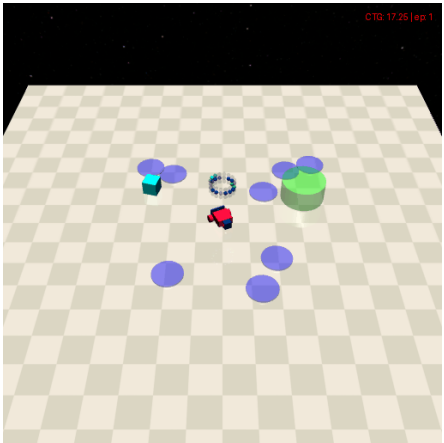
Prompt LLMs with Chain of Thought

Step 1	4 + 8 = 12	left: 4, 6, 12
Step 2	6 - 4 = 2	left: 2, 12
Step 3	2 * 12 = 24	left: 24
Answer	(6 - 4) * (4 + 8) = 24	



Transformers can maximize rewards and minimize costs simultaneously

also during inference.



- The **car** must reach the **green cylinder goal**.
- The **light blue cube** and **dark circle** are obstacles.
- The **car** receives only local observations.

Transformers can maximize rewards and minimize costs simultaneously

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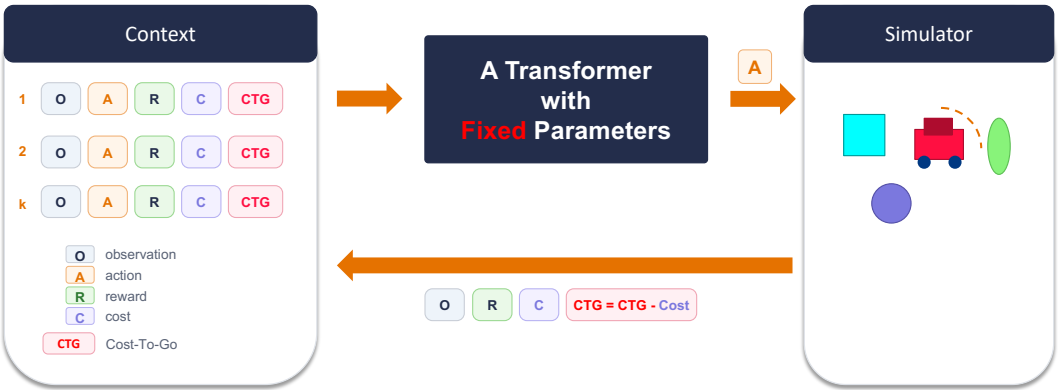

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Transformer’s forward pass implements some RL algorithm.

— An instance of the iterative inference hypothesis (Jastrzębski et al., 2017)

Layer-by-layer forward pass can be viewed as step-by-step update

of an iterative algorithm.

- Z_0: input tokens to a transformer
- $Z_{l+1} = Z_l + \text{Attention}_\theta(Z_l)$: the update rule for each layer
- $v_{l+1} = v_l + \text{TD-Error}(v_l)$: what an RL algorithm looks like

Transformers can implement temporal difference learning

in the forward pass.

What is TD?

- $A_t \sim \pi(\cdot|S_t), R_{t+1} = r(S_t, A_t), S_{t+1} \sim p(\cdot|S_t, A_t)$
- $v_\pi(s) = \mathbb{E}\left[\sum_{i=0}^{\infty} \gamma^i R_{t+i+1} \mid S_t = s\right]$
- $\phi : \mathcal{S} \to \mathbb{R}^d$: state feature map
- Goal of TD: find w such that $\phi(s)^\top w \approx v_\pi(s)$ for all s
- TD algorithm: $w_{t+1} = w_t + \alpha_t(R_{t+1} + \gamma w_t^\top \phi(S_{t+1}) - w_t^\top \phi(S_t))\phi(S_t)$

Transformers can implement temporal difference learning

in the forward pass.

With certain attention parameters θ_* and Z_0

$$Z_{l+1} = Z_l + \text{LinAttention}_{\theta_*}(Z_l)$$

With $w_0 = 0$

$$w_{l+1} = \text{BatchTD}(w_l)$$

$$Z_l[-1, -1] = w_l^\top \phi(s) \quad \forall l$$

Linear attention replaces softmax with identity

- $\text{Attention}_\theta(Z) = \text{softmax}\big((ZW_Q)(ZW_K)^\top\big)ZW_V$
- $\text{LinAttention}_\theta(Z) = ZW_Q(ZW_K)^\top ZW_V$

BatchTD applies TD in a fixed dataset

- A dataset $\mathcal{D} = \{(s_i, r_i, s_{i+1})\}_{i=1}^{N}$ of transitions sampled from (π, p)
- $w_{l+1} = w_l + \frac{\alpha_l}{N} \sum_{i=1}^{N} (r_i + \gamma w_l^\top \phi(s_{i+1}) - w_l^\top \phi(s_i)) \phi(s_i)$

Transformers can implement temporal difference learning

in the forward pass.

Task: given $\mathcal{D}$ and a state s, estimate $v_\pi(s)$

With certain attention parameters θ_*

$$Z_0 = \begin{bmatrix} \phi(s_1) & \dots & \phi(s_N) & \phi(s) \\ \gamma\phi(s_2) & \dots & \gamma\phi(s_{N+1}) & 0 \\ r_1 & \dots & r_N & 0 \end{bmatrix}$$

$$Z_{l+1} = Z_l + \text{LinAttention}_{\theta_*}(Z_l)$$

With $w_0 = 0$

$$w_{l+1} = \text{BatchTD}(w_l)$$

$$Z_l[-1, -1] = w_l^\top \phi(s) \quad \forall l$$

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Multi-task pretraining discovers θ_*, i.e., discovers the TD algorithm, in a few minutes.

— It took humans more than 20 years to invent TD.

Pretraining is to use DQN to train a transformer in multiple Atari games

... an analogy to our pretraining process.

- Sample a task (π, p, r)
- Sample a trajectory $S_0, A_0, R_1, S_1, \ldots$
- DQN-style update

$$\theta_{t+1} = \theta_t + \alpha_t(R_{t+1} + \gamma \mathrm{TF}_{\theta_t}(S_{t+1}) - \mathrm{TF}_{\theta_t}(S_t))\nabla_\theta \mathrm{TF}_{\theta_t}(S_t)$$

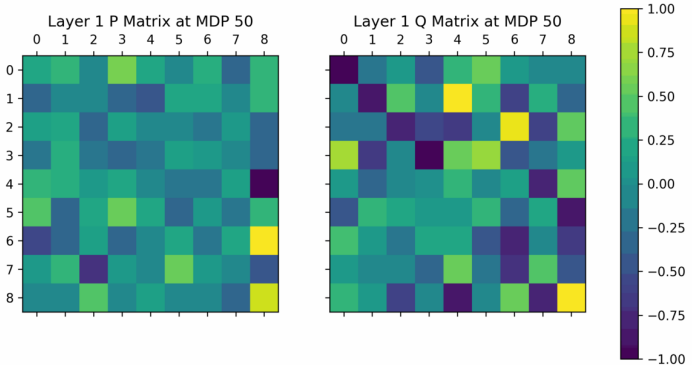
$$Z_0 \doteq \begin{bmatrix} \phi(S_0) & \ldots & \phi(S_{t-1}) & \phi(S_t) \\ \gamma\phi(S_1) & \ldots & \gamma\phi(S_t) & 0 \\ R_1 & \ldots & R_t & 0 \end{bmatrix} \xrightarrow{\theta} Z_1 \xrightarrow{\theta} \ldots \xrightarrow{\theta} \mathrm{TF}_\theta(S_t) \doteq Z_L[-1, -1]$$

Wang, J., Blaser, E., Daneshmand, H., and Zhang, S. (2025a). Transformers can learn temporal difference methods for in-context reinforcement learning. In *Proceedings of the International Conference on Learning Representations*

Transformer parameters converge to θ_* during pretraining

with random initialization

$$\text{LinAttention}_\theta(Z) = ZW_Q(ZW_K)^\top ZW_V = Z\left(W_Q W_K^\top\right)Z^\top ZW_V, \quad \theta = \left\{W_Q W_K^\top, W_V\right\}$$



Pretraining tasks can be very different from evaluation tasks

enabling maximal out-of-distribution generalization.

The θ_* minimizes the norm of the expected updates (NEU)

under some (arguably restrictive) assumptions

$$\theta_{t+1} = \theta_t + \alpha_t(R_{t+1} + \gamma \mathrm{TF}_{\theta_t}(S_{t+1}) - \mathrm{TF}_{\theta_t}(S_t))\nabla_\theta \mathrm{TF}_{\theta_t}(S_t)$$

Assume

- Enumeration of states in the context
- Expected next state features

$$\begin{bmatrix} \phi(S_0) & \dots & \phi(S_{t-1}) & \phi(S_t) \\ \gamma\phi(S_1) & \dots & \gamma\phi(S_t) & 0 \\ R_1 & \dots & R_t & 0 \end{bmatrix} \rightarrow \begin{bmatrix} \phi(s_1) & \dots & \phi(s_{|\mathcal{S}|}) & \phi(S_t) \\ \gamma \sum_{s'} p_\pi(s'|s_1)\phi(s_1) & \dots & \gamma \sum_{s'} p(s'|s_{|\mathcal{S}|})\phi(s_{|\mathcal{S}|}) & 0 \\ r_\pi(s_1) & \dots & r_\pi(s_{|\mathcal{S}|}) & 0 \end{bmatrix}$$

Then

$$\lim_{l \to \infty} \|\mathbb{E}[(R_{t+1} + \gamma \mathrm{TF}_{\theta_*}(S_{t+1}) - \mathrm{TF}_{\theta_*}(S_t))\nabla_\theta \mathrm{TF}_{\theta_t}(S_t)]\| = 0$$

A single-layer Transformer can also implement TD

if we use Chain-of-Thought prompting.

- CoT is to allow intermediate data
- Without CoT:

$$Z_L \leftarrow \mathrm{TF}_\theta(Z_0)$$

- With CoT:

$$\begin{aligned}
&Z_L \leftarrow \mathrm{TF}_\theta(Z_0) \xleftarrow{L=1} w_1 \\
&Z_0 \leftarrow [Z_0, Z_L] \\
&Z_L \leftarrow \mathrm{TF}_\theta(Z_0) \xleftarrow{L=1} w_2 \\
&Z_0 \leftarrow [Z_0, Z_L] \\
&\quad \ldots \\
&Z_L \leftarrow \mathrm{TF}_\theta(Z_0) \xleftarrow{L=1} w_k
\end{aligned}$$

Transformers with softmax attention implement a kernel TD

Given $(S_t, A_t, R_{t+1}, S_{t+1})$

- TD:

$$v(S_t) \leftarrow v(S_t) + \alpha(R_{t+1} + \gamma v(S_{t+1}) - v(S_t))$$

- Kernel TD:

$$\forall s, v(s) \leftarrow v(s) + \alpha(R_{t+1} + \gamma v(S_{t+1}) - v(S_t))\kappa(s, S_t)$$

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LLMs (Transformers) make good decisions because they are computational machines

— not just statistical models that fit data.

Thanks & Questions

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Jastrzębski, S., Arpit, D., Ballas, N., Verma, V., Che, T., and Bengio, Y. (2017). Residual connections encourage iterative inference. *arXiv Preprint*.

Moeini, A., Kwon, M., Bozkurt, A. K., Motai, Y., Chandra, R., Feng, L., and Zhang, S. (2026). Safe in-context reinforcement learning. In *Proceedings of the International Conference on Machine Learning*.

Song, K., Moeini, A., Wang, P., Gong, L., Chandra, R., Zhang, S., and Qi, Y. (2026). Reward is enough: LLMs are in-context reinforcement learners. In *Proceedings of the International Conference on Learning Representations*.

Wang, J., Blaser, E., Daneshmand, H., and Zhang, S. (2025a). Transformers can learn temporal difference methods for in-context reinforcement learning. In *Proceedings of the International Conference on Learning Representations*.

Wang, J., Chandra, R., and Zhang, S. (2025b). Towards provable emergence of in-context reinforcement learning. In *Advances in Neural Information Processing Systems*.

Xie, Z., Liu, X., Chandra, R., and Zhang, S. (2026a). Convergence and emergence of in-context reinforcement learning with chain of thought. *arXiv Preprint*.

Xie, Z., Liu, X., Chen, C., Liu, S., Chandra, R., and Zhang, S. (2026b). Beyond linear attention: Softmax transformers implement in-context reinforcement learning. *arXiv Preprint*.