Token Selection in the Self-Attention Mechanism: Case Studies and Theoretical Understanding

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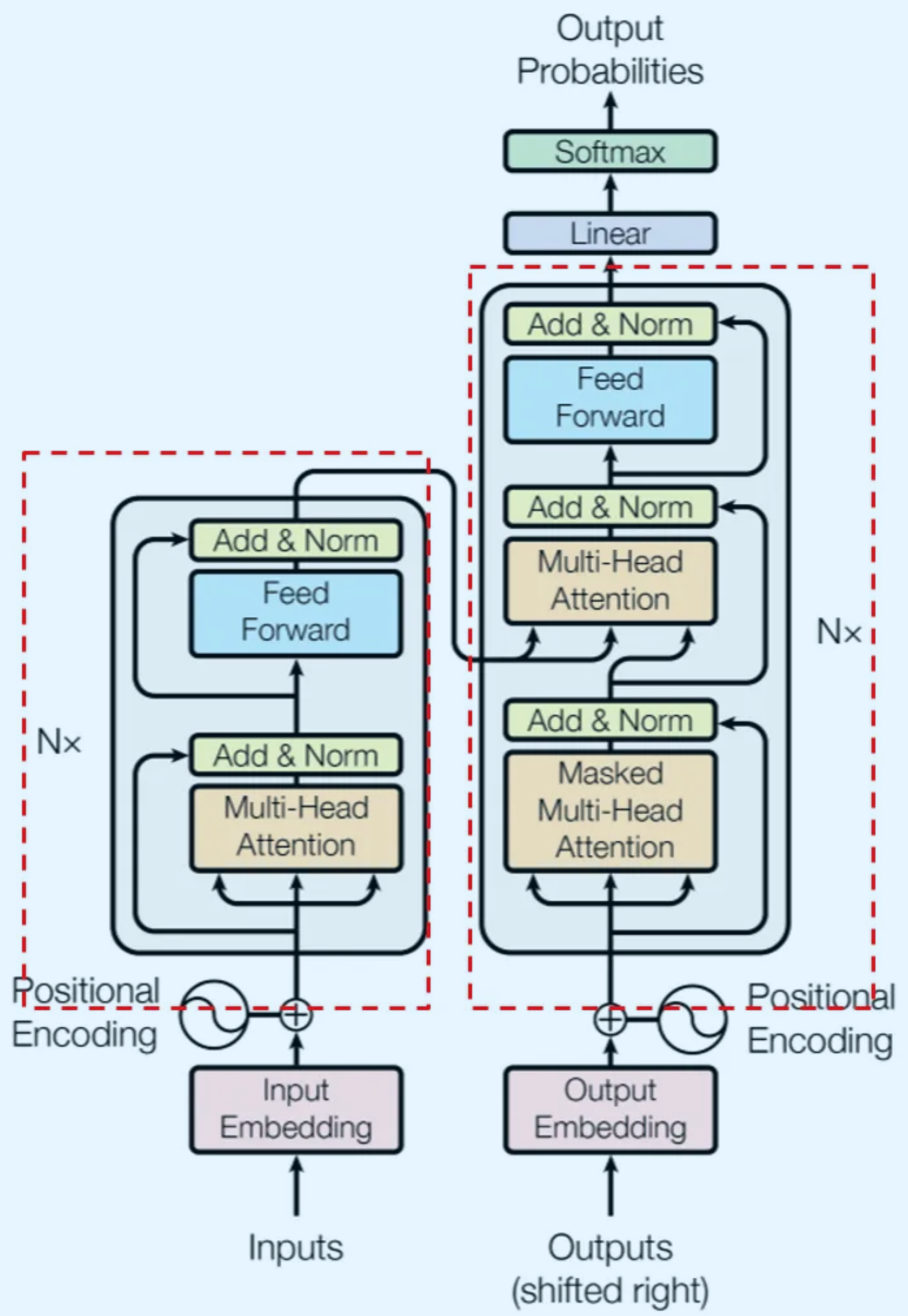
Joint work with: Zihao Li, Cheng Gao, Yihan He, Chenyang Zhang, Xuran Meng, Wei Shi, Han Liu, Jason Klusowski, Jianqing Fan, Mengdi Wang

Success of transformers

Theoretical understanding of transformers is limited



[Vaswani et al. 2017]

+

Large amount of natural language data

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Powerful language model

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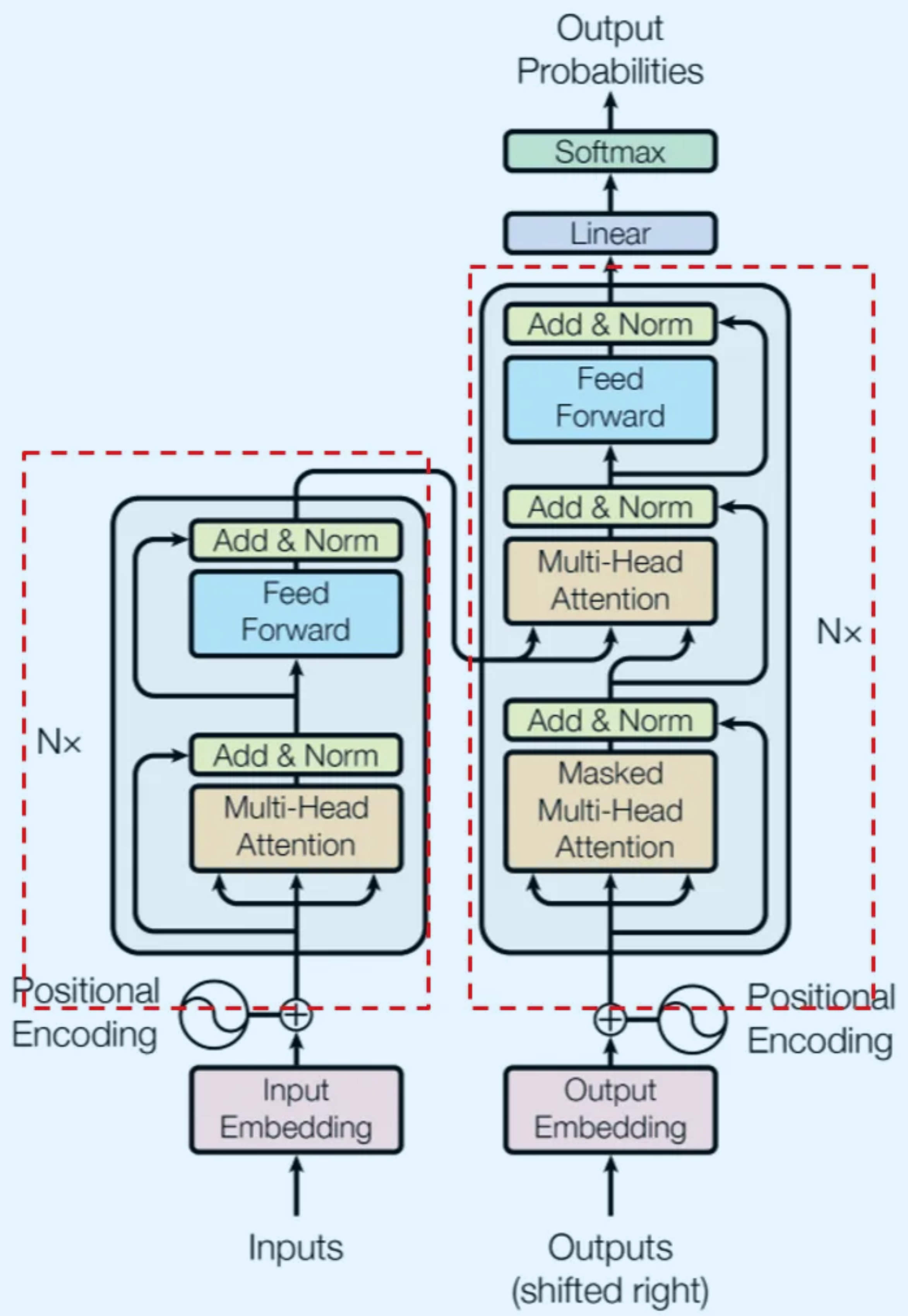

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Optimization/learning guarantees?

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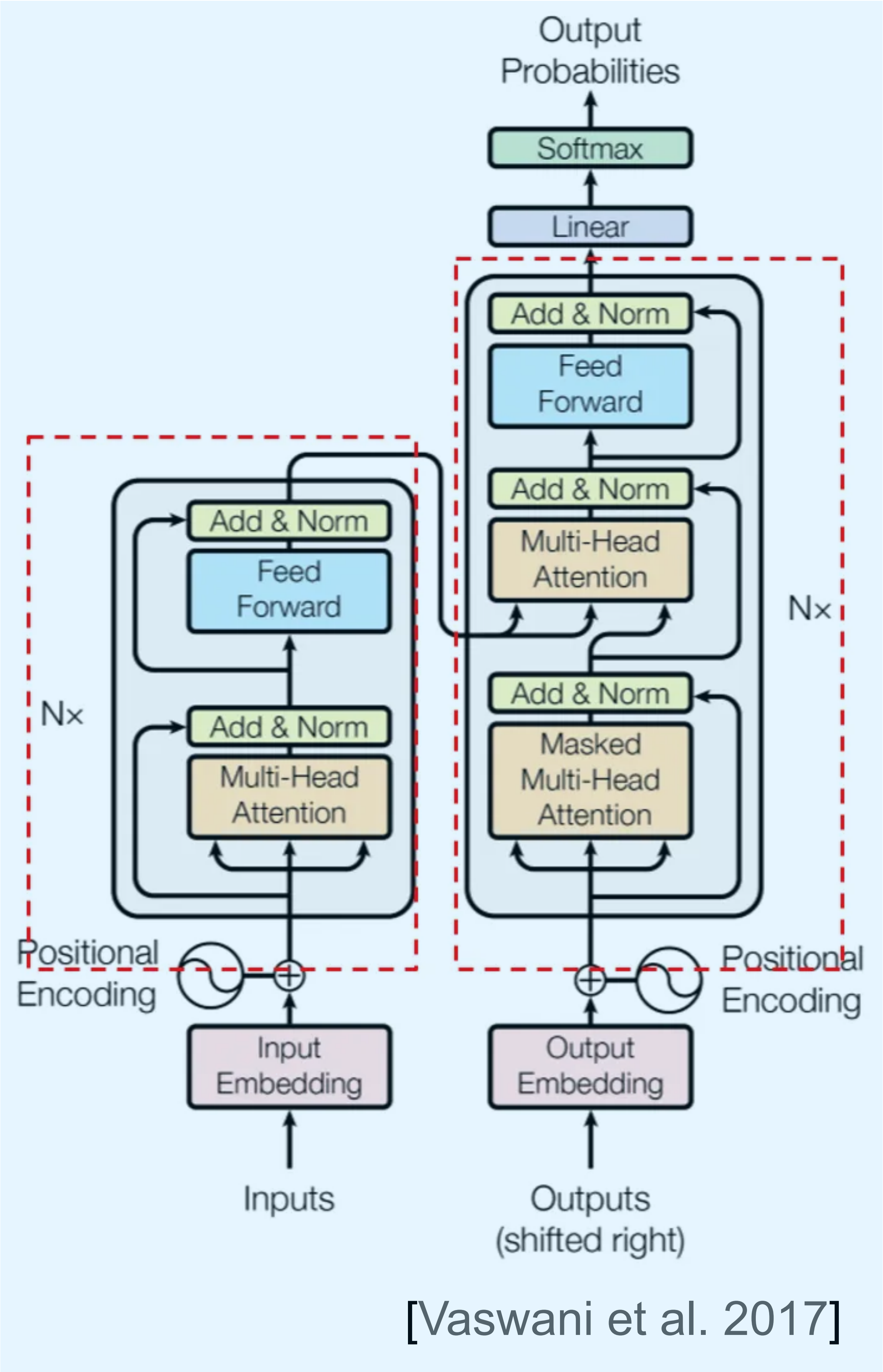

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Optimization/learning guarantees? **Interpretability?**

We consider...

Simple transformer $+$ **Data following classic statistical models** $= ?$

Nearest neighbor, group-sparse classification, random walk

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We will give **learning guarantees** & **interpretations of the trained model.**

Overview

Transformers as in-context one-nearest neighbor predictors

Zihao Li, Yuan Cao, Cheng Gao, Yihan He, Han Liu, Jason Klusowski, Jianqing Fan, and Mengdi Wang. "One-layer transformer provably learns one-nearest neighbor in context." NeurIPS 2024

Transformers as group-sparse linear predictors

Chenyang Zhang, Xuran Meng, and Yuan Cao. "Transformer learns optimal variable selection in group-sparse classification." ICLR 2025

Transformers as random walk predictors

Wei Shi and Yuan Cao. "Towards Understanding Transformers in Learning Random Walks." submitted.

Transformers Learn One-Nearest Neighbor In Context

In context learning

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Input matrix: $$\mathbf{H} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \dots & \mathbf{x}_N & \mathbf{x}_{\text{query}} \\ y_1 & y_2 & \dots & y_N & 0 \\ \mathbf{p}_1 & \mathbf{p}_2 & \dots & \mathbf{p}_N & \mathbf{p}_{\text{query}} \end{bmatrix}$$

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Output: $\boxed{[\text{self-attention}(\mathbf{H})]_{d+1,N+1}}$

The desired output should give the result of:

(i) performing linear regression on $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$ and obtain linear model $\hat{\mathbf{w}}$;

(ii) calculating the predicted value $\langle \hat{\mathbf{w}}, \mathbf{x}_{\text{query}} \rangle$.

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Can transformers be trained to perform one-nearest neighbor prediction?

In-context one-nearest neighbor prediction

Input matrix: $\mathbf{H} = [\mathbf{h}_1, \mathbf{h}_2, \ldots, \mathbf{h}_N, \mathbf{h}_{\text{query}}] = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \ldots & \mathbf{x}_N & \mathbf{x}_{\text{query}} \\ y_1 & y_2 & \ldots & y_N & 0 \\ 0 & 0 & \ldots & 0 & 1 \end{bmatrix} \in \mathbb{R}^{(d+2)\times(N+1)}$,

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$$y_{i*}, \quad i* = \arg\min_{j\in[N]} \|\mathbf{x}_{\text{query}} - \mathbf{x}_j\|_2.$$

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We suppose that the data are drawn from a distribution satisfying:

- $\mathbf{x}_i \in \mathbb{R}^d$: i.i.d. sampled from $U(\mathbb{S}^{d-1})$
- $y_i \in \{\pm 1\}$: $\mathbb{E}[y_i y_j \,|\, \mathbf{x}_{1:N}] = 0, \quad \mathbb{E}[y_i^2 \,|\, \mathbf{x}_{1:N}] = 1,$
- $\mathbb{P}(\mathbf{y}_{1:N} \,|\, \mathbf{x}_{1:N}) = \mathbb{P}(\mathbf{y}_{1:N} \,|\, -\mathbf{x}_{1:N})$

One-layer transformer model

Self-attention layer with the value matrix fixed as identity:

$$\text{self-attention}(\mathbf{H}) = \mathbf{H} \cdot \text{softmax}(\mathbf{H}^\top \mathbf{W} \mathbf{H}),$$

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We consider minimizing the population square loss with gradient descent:

Loss function: $$L(\mathbf{W}) = \frac{1}{2} \cdot \mathbb{E}_{\{\mathbf{x}_i,\mathbf{y}_i\}_{i\in[N]},\mathbf{x}_{\text{query}}}\left[\left(f_{\mathbf{W}}(\mathbf{H}) - \mathbf{y}_{i^*}\right)^2\right].$$

Gradient descent: $$\mathbf{W}^{(t+1)} - \mathbf{W}^{(t)} = \eta \cdot \nabla_{\mathbf{W}} L(\mathbf{W}^{(t)}), \quad \mathbf{W}^{(0)} = \begin{pmatrix} 0_{(d+1)\times(d+1)} & 0_{d+1} \\ 0_{d+1} & -\sigma \end{pmatrix}.$$

The constant $\sigma > 0$ serves as a mask to prevent the query from attending to itself.

One-layer transformer learns 1NN in context

Theorem. Suppose that

The mask σ in the initialization satisfies $\sigma = \Omega(\mathrm{poly}(d))$,

The length of context satisfies $N = \Omega\left(\sqrt{d}\log d\right)$,

Then $L(\mathbf{W}^{(t)})$ converges to zero.

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Target: $y_{i*}, \quad i* = \arg\min_{j \in [N]} \|\mathbf{x}_{\mathrm{query}} - \mathbf{x}_j\|_2$.

$$\boxed{L(\mathbf{W}) = 0 \quad \text{if and only if} \quad \mathrm{softmax}(\mathbf{H}^\top \mathbf{W} \mathbf{h}_{\mathrm{query}})) \equiv \mathbf{e}_{i*}}$$

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The transformer can be trained to perform appropriate token selection!

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"Nearest neighbor selector"

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Prediction performance under distribution shift

We also study the performance of the transformer trained by T gradient descent iterations on new test data with distribution shift.

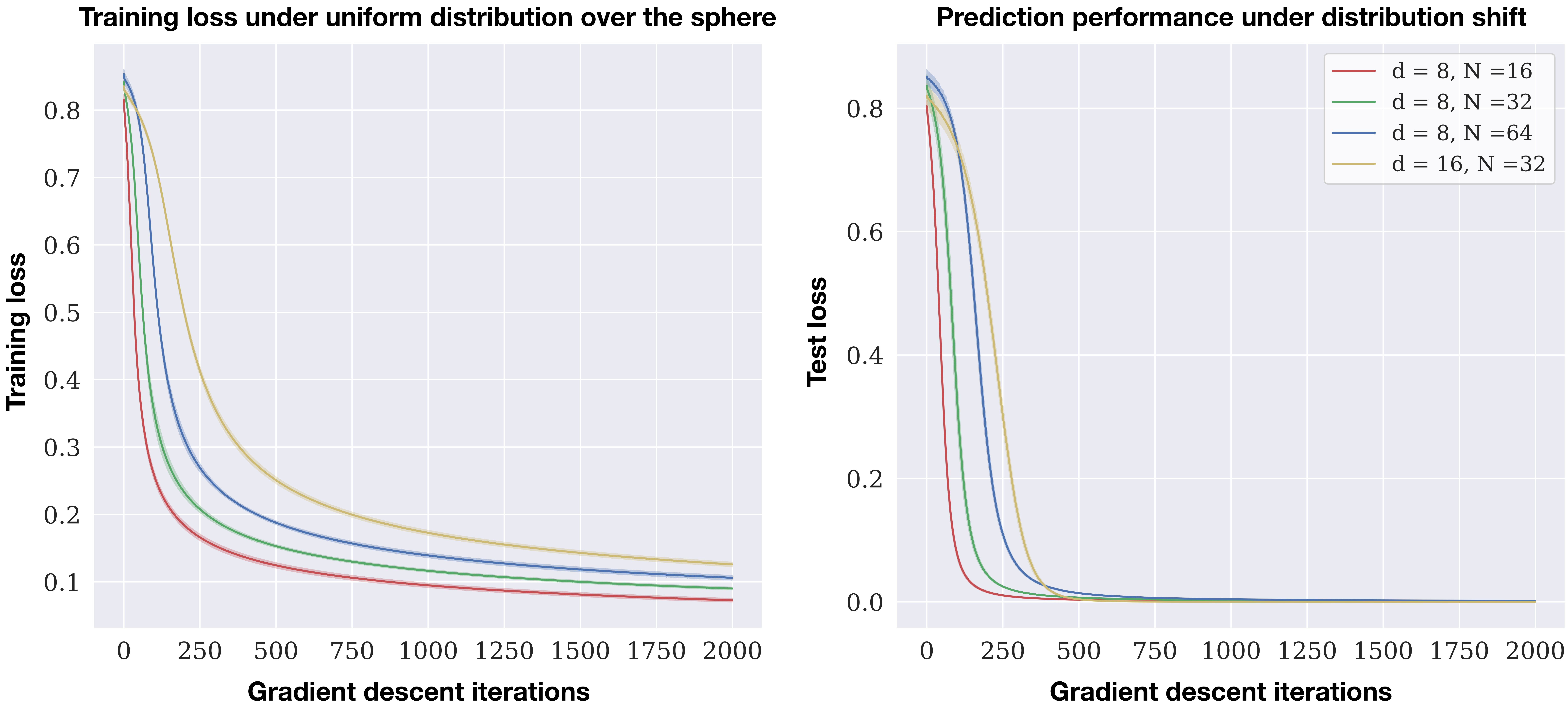
Theorem. For any data satisfying $|y_i| \leq R$, $\mathbf{x}_i \in \mathbb{S}^{d-1}$, and

$$\|\mathbf{x}_j - \mathbf{x}_{\text{query}}\|_2^2 \geq \|\mathbf{x}_{i*} - \mathbf{x}_{\text{query}}\|_2^2 + \delta \quad \text{for all } j \text{ with } y_j \neq y_{i*},$$

it holds that

$$\text{Test loss} \leq O\left(R^2 N^2 T^{-\text{poly}(N,d)\delta}\right).$$

Experiments



Training (left) and test loss (right) curves under gradient descent, with different dimensions and context sizes. The test contexts are generated with a boundary separation of $\delta = 0.1$.

Transformers Learn Optimal Variable Selection in Group-Sparse Classification

Group-sparse linear classification

Consider a classification task: $\overline{\mathbf{x}} \sim N(\mathbf{0}, \sigma_x^2 \cdot \mathbf{I}_p)$, $y = \operatorname{sign}(\langle \overline{\mathbf{x}}, \boldsymbol{\beta}^* \rangle)$.

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Suppose that index sets $G_1, \ldots, G_D$ give a predefined **partition** of $\{1, \ldots, p\}$.

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The learning problem is "group sparse" if $\boldsymbol{\beta}^*$ satisfies that

$$\mathrm{supp}(\boldsymbol{\beta}^*) := \{k \in [p] : [\boldsymbol{\beta}^*]_k \neq 0\} \subset G_{j^*},$$

where $j^* \in [D]$ is the index of label-relevant group.

Solving group-sparse classification with transformers

Let $p = dD$ with d denoting the dimension of each group. We can then reshape the feature vector $\bar{\mathbf{x}}$ into

$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_D],$$

where each column $\mathbf{x}_j = [\bar{\mathbf{x}}]_{G_j} \sim \mathcal{N}(\mathbf{0}, \sigma_x^2 \mathbf{I}_d)$.

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The desired output is then

$$y = \mathrm{sign}(\langle \mathbf{x}_{j^*}, \mathbf{v}^* \rangle),$$

where $\mathbf{v}^* = [\boldsymbol{\beta}^*]_{G_{j^*}} \in \mathbb{R}^d$.

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+ positional encodings

$\mathbf{p_j} \in \mathbb{R}^D$

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One-layer transformer

Consider a scalar-output one-layer transformer model:

$$f(\mathbf{H}, \mathbf{v}, \mathbf{W}) = \sum_{j=1}^{D} \mathbf{v}^\top \mathbf{H} \mathrm{softmax}(\mathbf{H}^\top \mathbf{W} \mathbf{h}_j)$$

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Population cross-entropy loss:

$$L(\mathbf{v}, \mathbf{W}) = \mathbb{E}_{(\mathbf{X}, y)} \left[\ell(y \cdot f(\mathbf{H}, \mathbf{v}, \mathbf{W})) \right],$$

where $\ell(a) = \log(1 + \exp(-a))$ is the cross-entropy loss.

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Gradient descent:

$$\mathbf{v}^{(t+1)} = \mathbf{v}^{(t)} - \eta \nabla_{\mathbf{v}} L(\mathbf{v}^{(t)}, \mathbf{W}^{(t)}); \;\; \mathbf{W}^{(t+1)} = \mathbf{W}^{(t)} - \eta \nabla_{\mathbf{W}} L(\mathbf{v}^{(t)}, \mathbf{W}^{(t)}),$$

with zero initialization: $\mathbf{v}^{(0)} = \mathbf{0}_{d+D}$, $\mathbf{W}^{(0)} = \mathbf{0}_{(d+D)\times(d+D)}$.

Transformers can solve group-sparse linear classification

Theorem. For any $\epsilon > 0$, suppose that $D = \omega(\log^2(1/\epsilon))$, $d \leq O(\mathrm{poly}(D))$, $\sigma_x, \eta = \Theta(1)$. Then there exists

$$T^* = \Theta\Big(D^3 \vee \frac{1}{D^3\epsilon^3}\Big),$$

such that the following conclusions hold:

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- Self-attention extracts the variables from the label-relevant group: w.h.p.,

$$\mathbf{S}_{j^*,j}^{(T^*)} \geq 1 - \exp(-\Theta(D)), \ \forall j \in [D]\,.$$

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- The value vector $\mathbf{v}$ successfully learns the ground truth classifier:

$$\mathbf{v}^{(T^*)} = [\mathbf{v}_1^{(T^*)\top}, \mathbf{0}_D^\top]^\top, \text{ and } \Big\|\mathrm{normalized}(\mathbf{v}_1^{(T^*)}) - \mathbf{v}^*\Big\|_2 \leq \epsilon D \exp(-\Theta(\sqrt{D}))\,.$$

Transformers can solve group-sparse linear classification

Theorem. For any $\epsilon > 0$, suppose that $D = \omega(\log^2(1/\epsilon))$, $d \leq O(\text{poly}(D))$, $\sigma_x, \eta = \Theta(1)$. Then there exists

$$T^* = \Theta\big(D^3 \vee \frac{1}{D^3 \epsilon^3}\big),$$

such that the following conclusions hold:

- Self-attention extracts the variables from the label-relevant group: w.h.p.,

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Optimal linear classification on selected variables

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- The loss is sufficiently minimized:

Optimal linear classification on selected variables

$$L(\mathbf{v}^{(T^*)}, \mathbf{W}^{(T^*)}) = \Theta(\epsilon \wedge D^{-2})\,.$$

Classification with variable selection

Recall the prediction model: $$f(\mathbf{H}, \mathbf{v}, \mathbf{W}) = \sum_{j=1}^{D} \mathbf{v}^\top \mathbf{H} \mathrm{softmax}(\mathbf{H}^\top \mathbf{W} \mathbf{h}_j)$$

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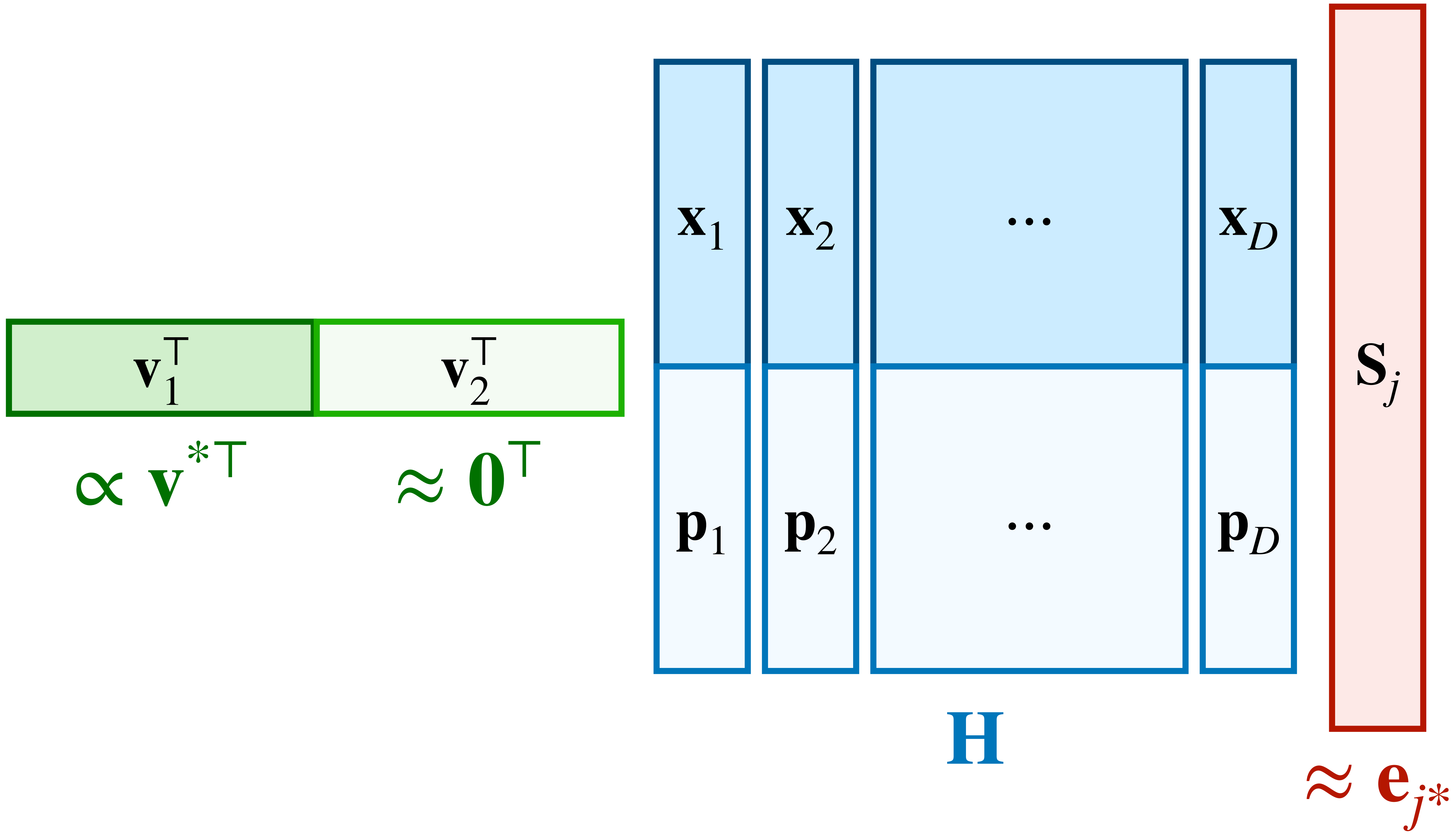

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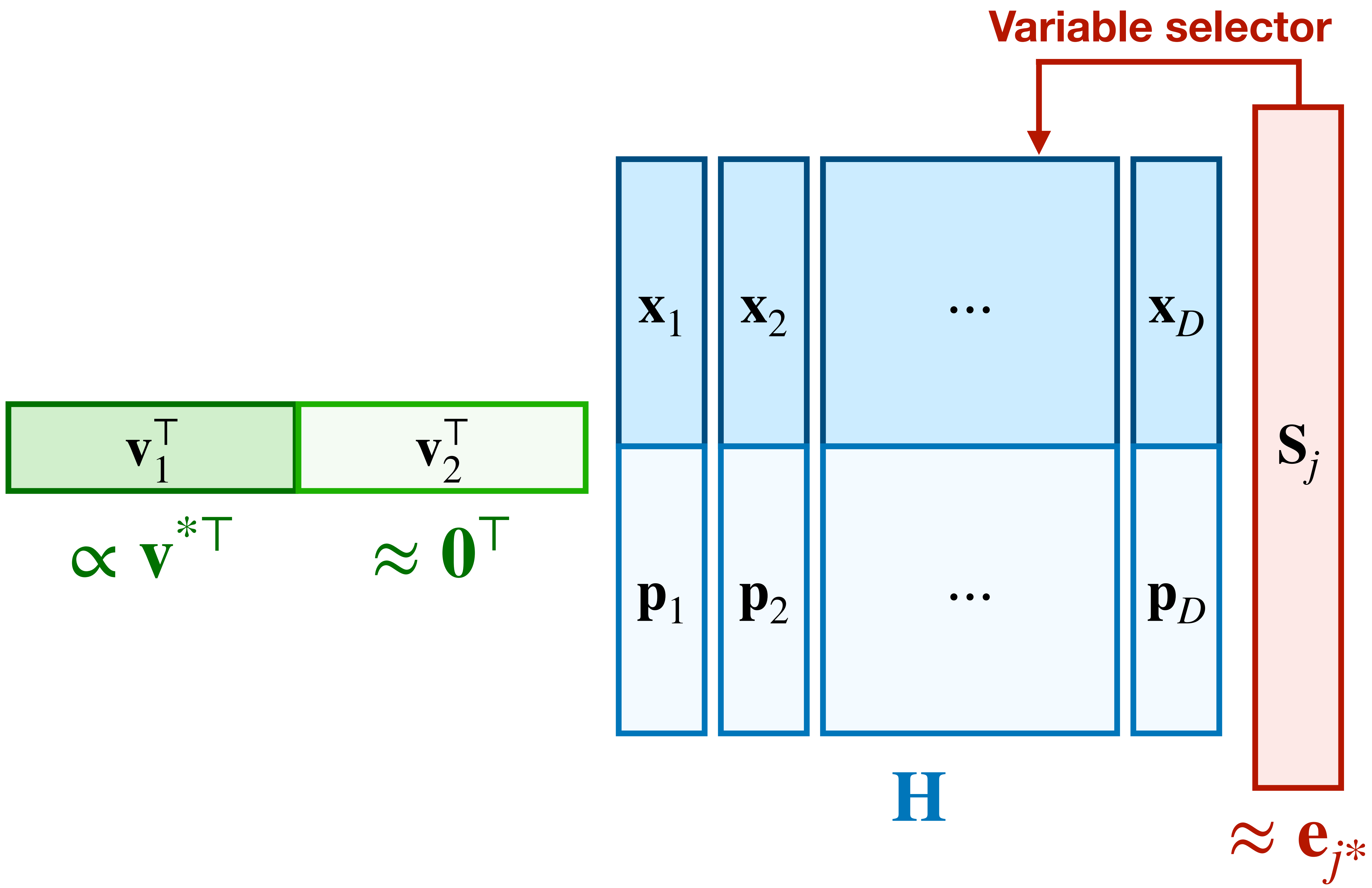

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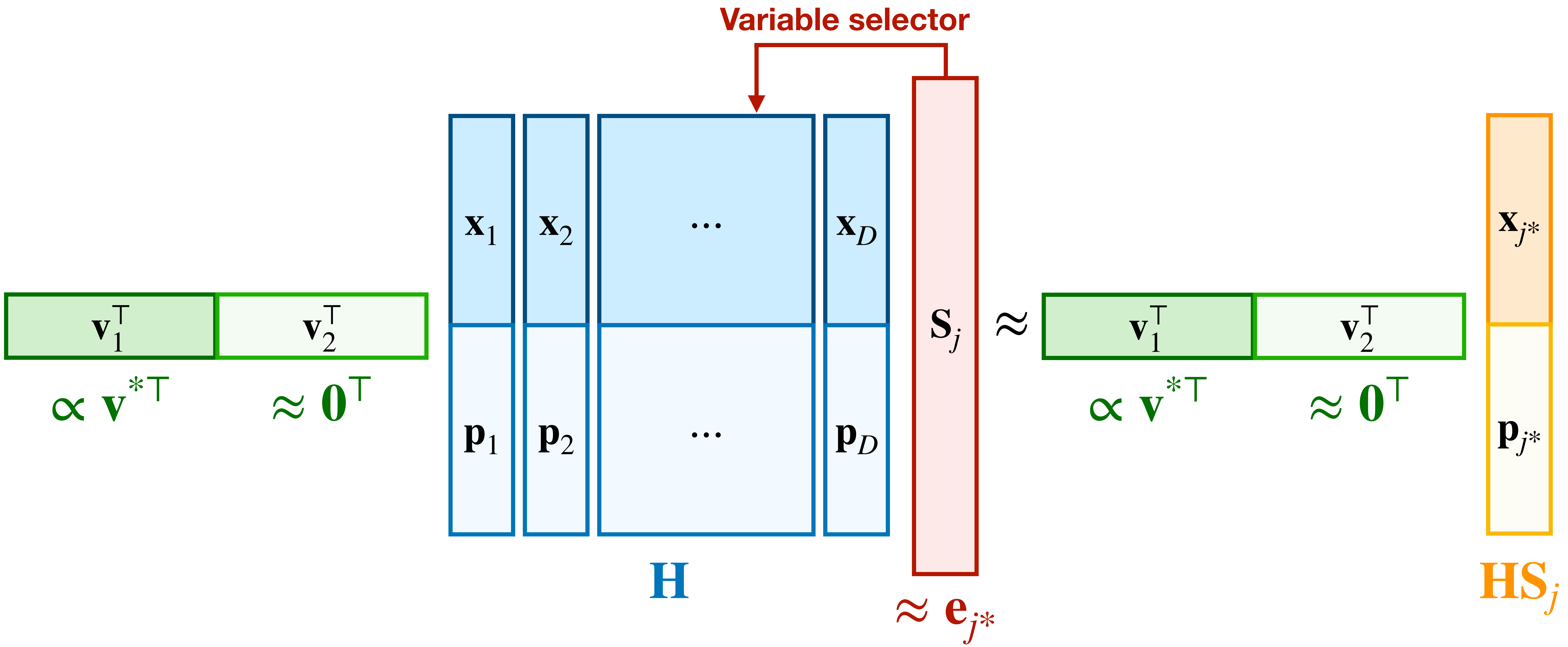

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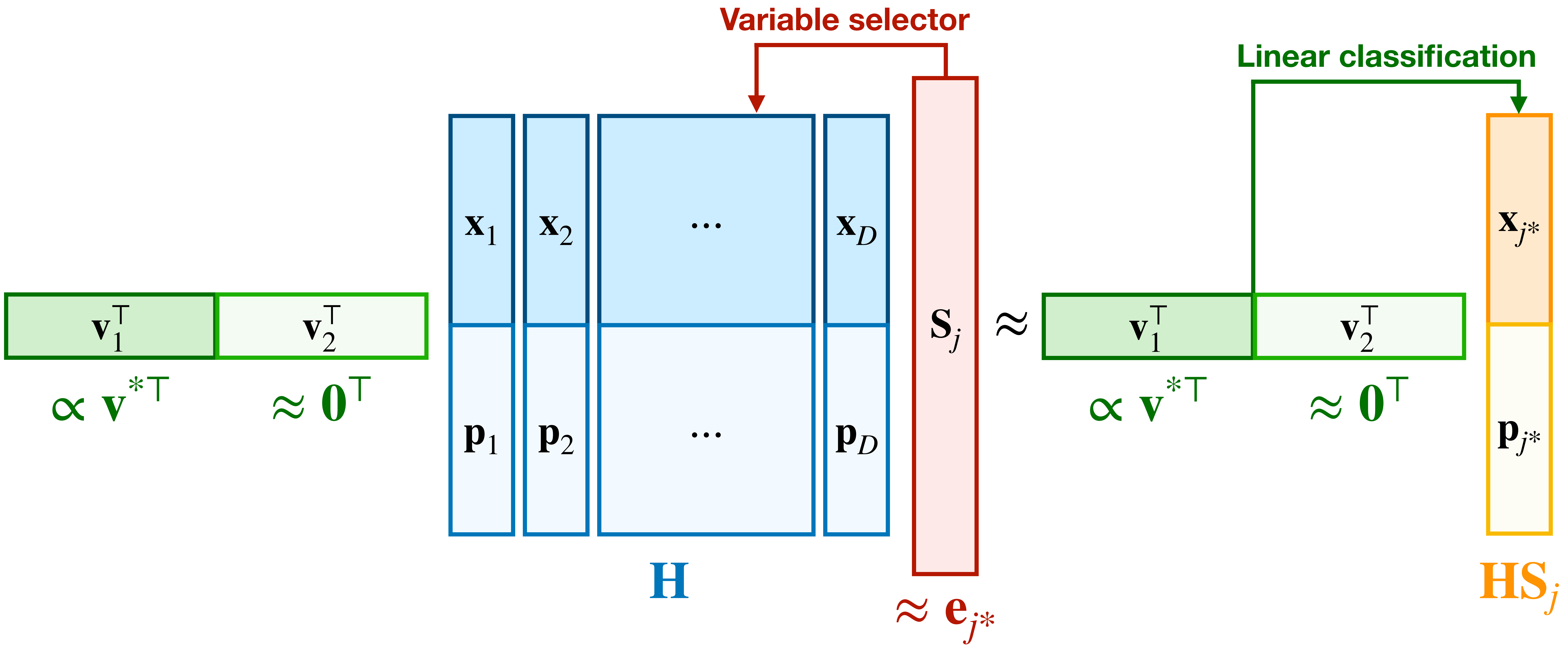

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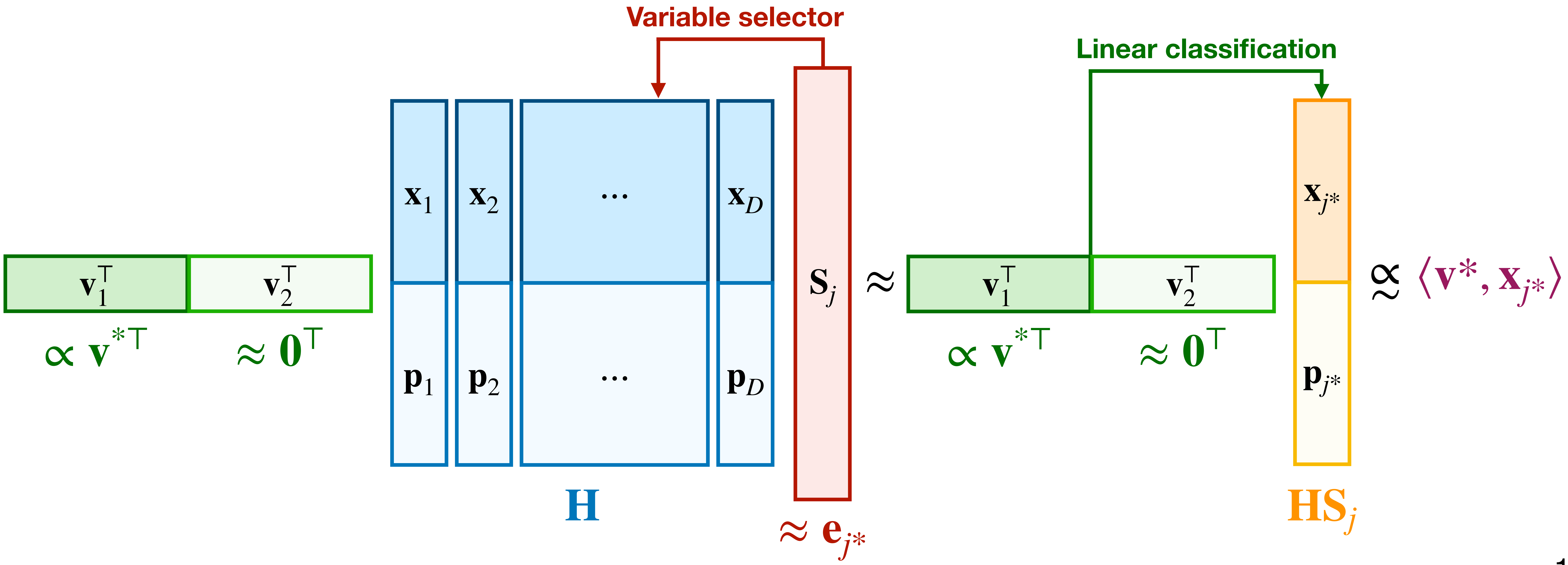
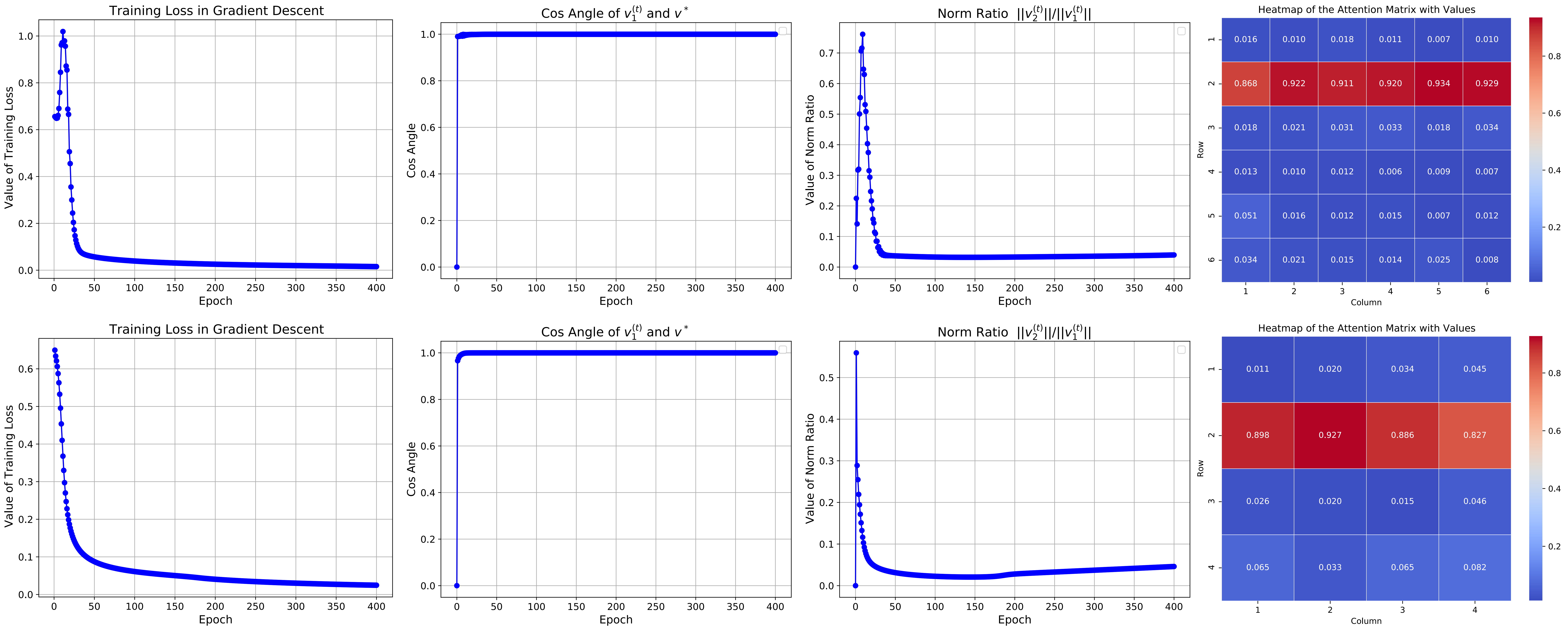


Experiments - pretraining

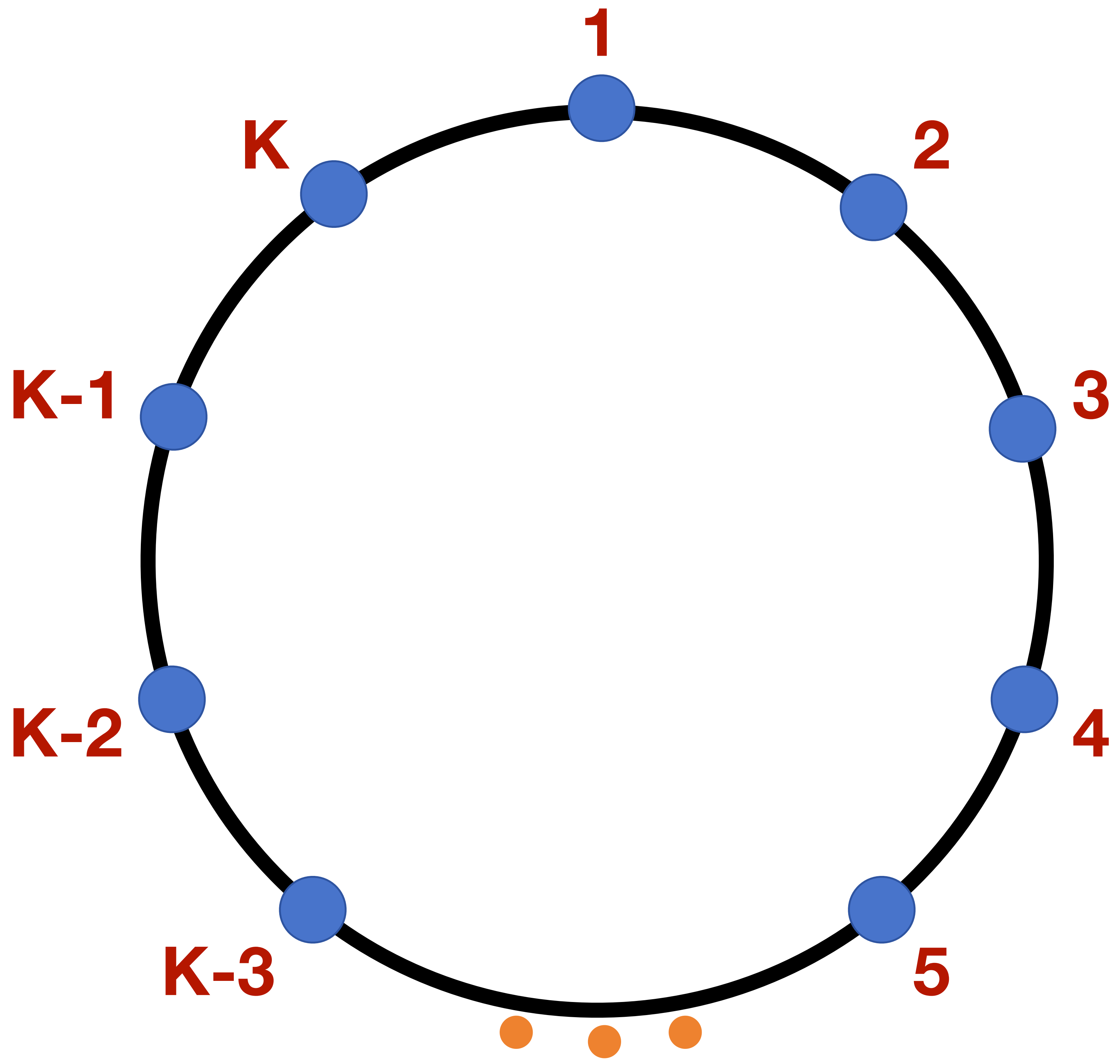


Training loss, cosine similarity, norm ratio, and attention score for $(n, d, D) = (500,4,6)$ and $(n, d, D) = (200,2,4)$ respectively when set $j^* = 2$.

Transformers Learn Random Walk Prediction by Attending to the Direct Parent State

A simple random walk prediction task

Consider a circle with K nodes.



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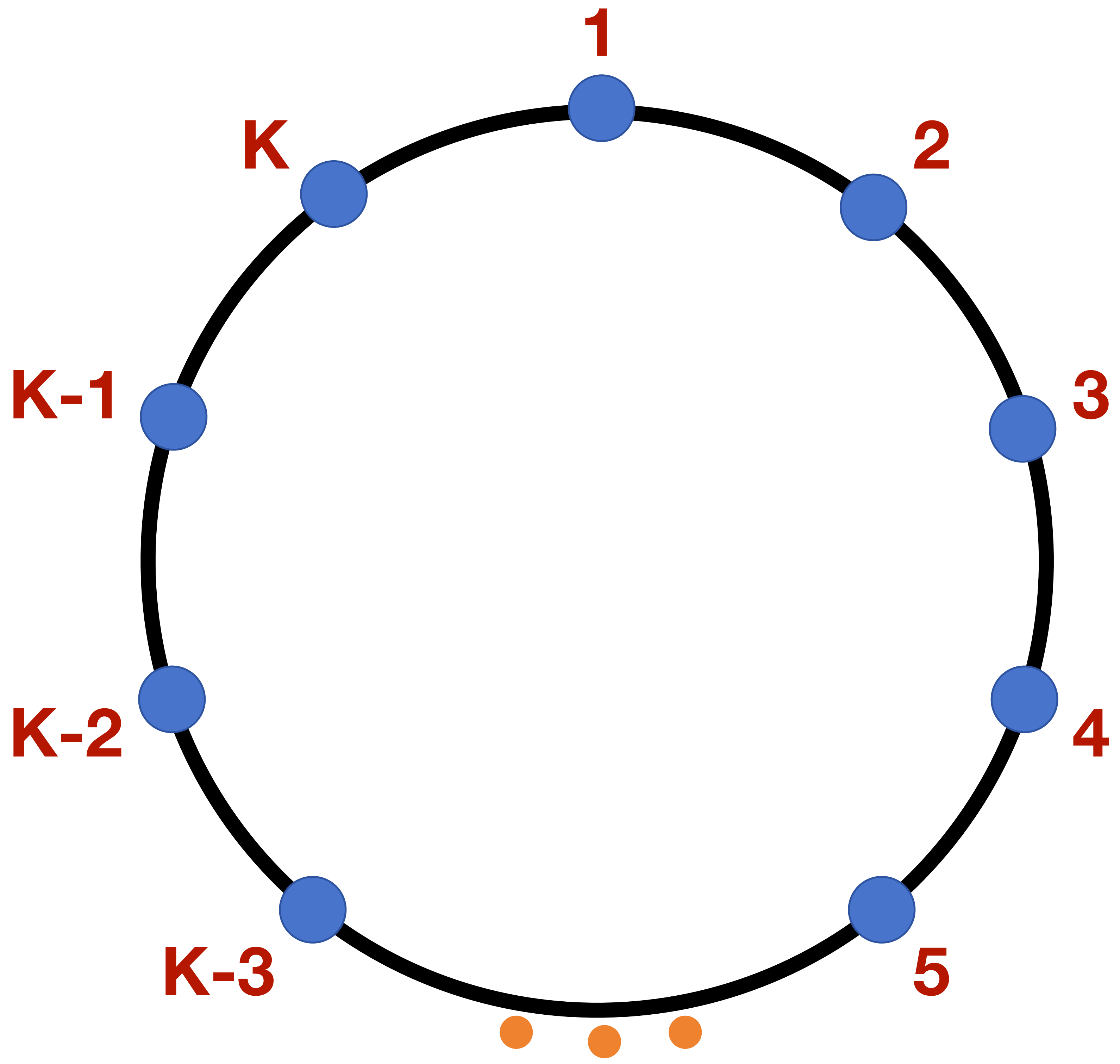
Consider a circle with K nodes.

A walk on the circle: the process where a ‘walker’ moves step-by-step among the nodes of the circle.



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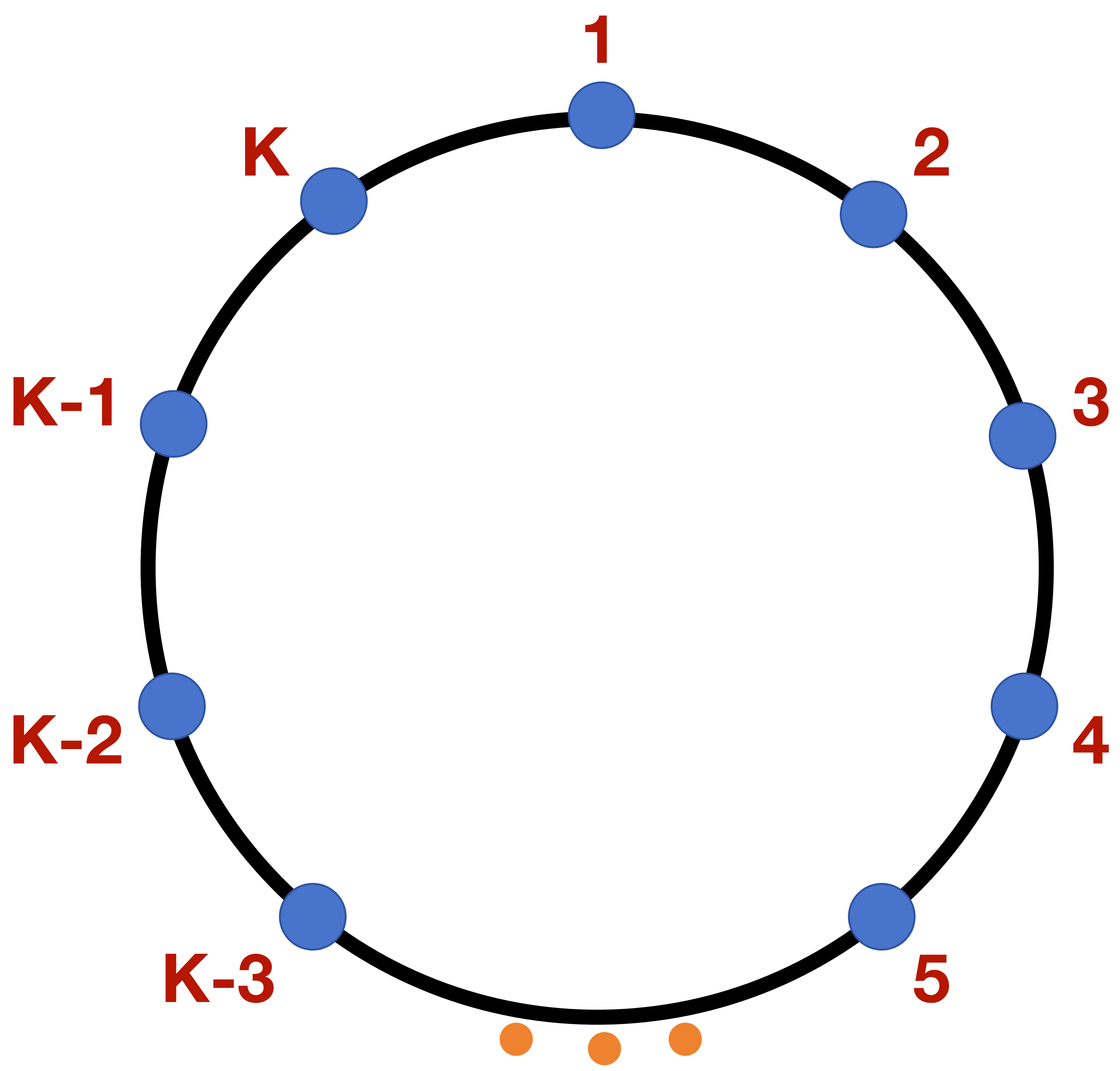

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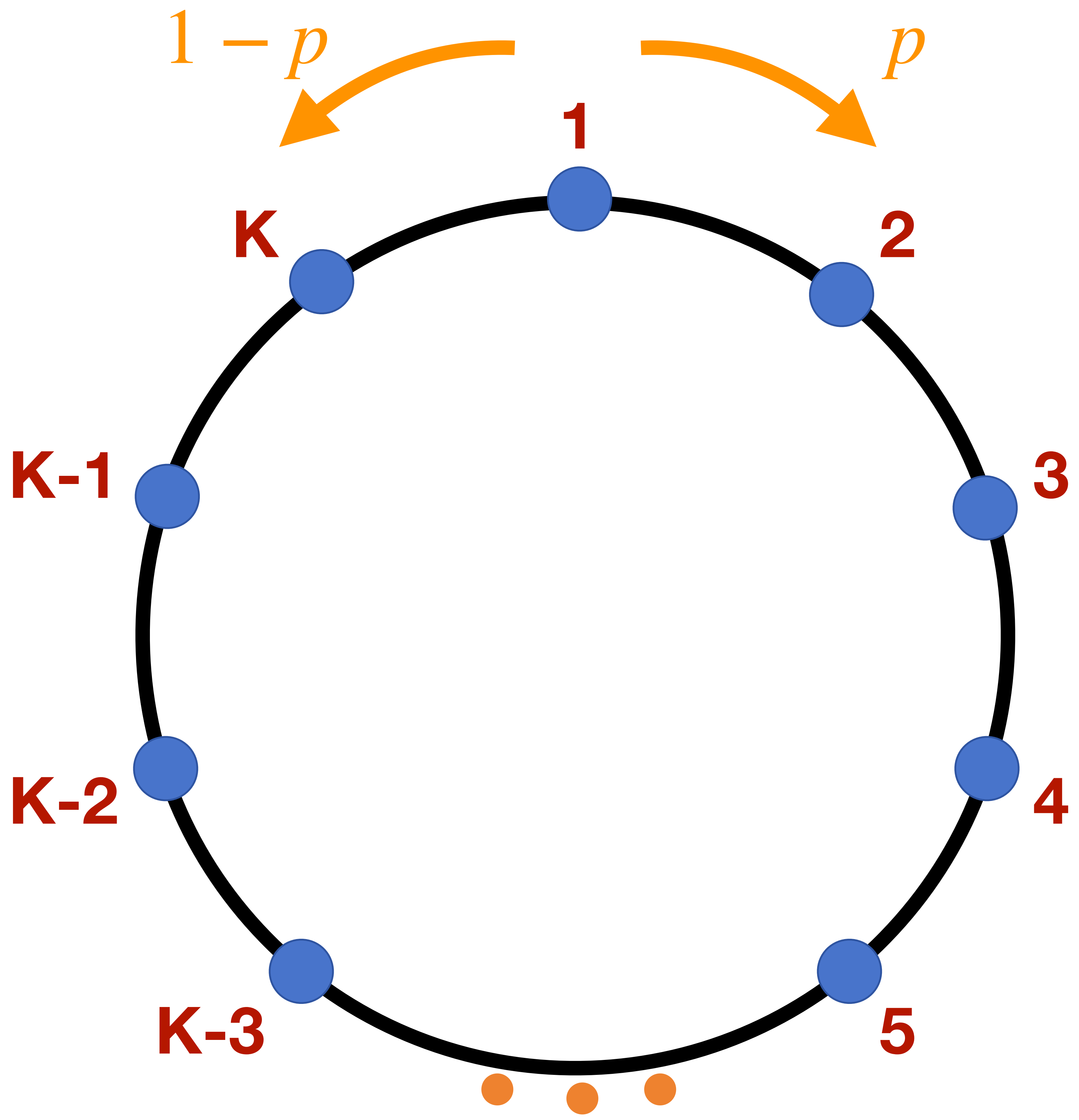
Suppose that $s_1 \in [K]$ is uniformly chosen. At each step, the walker goes **clockwise w.p. p** or **counter-clockwise w.p. $1 - p$**.



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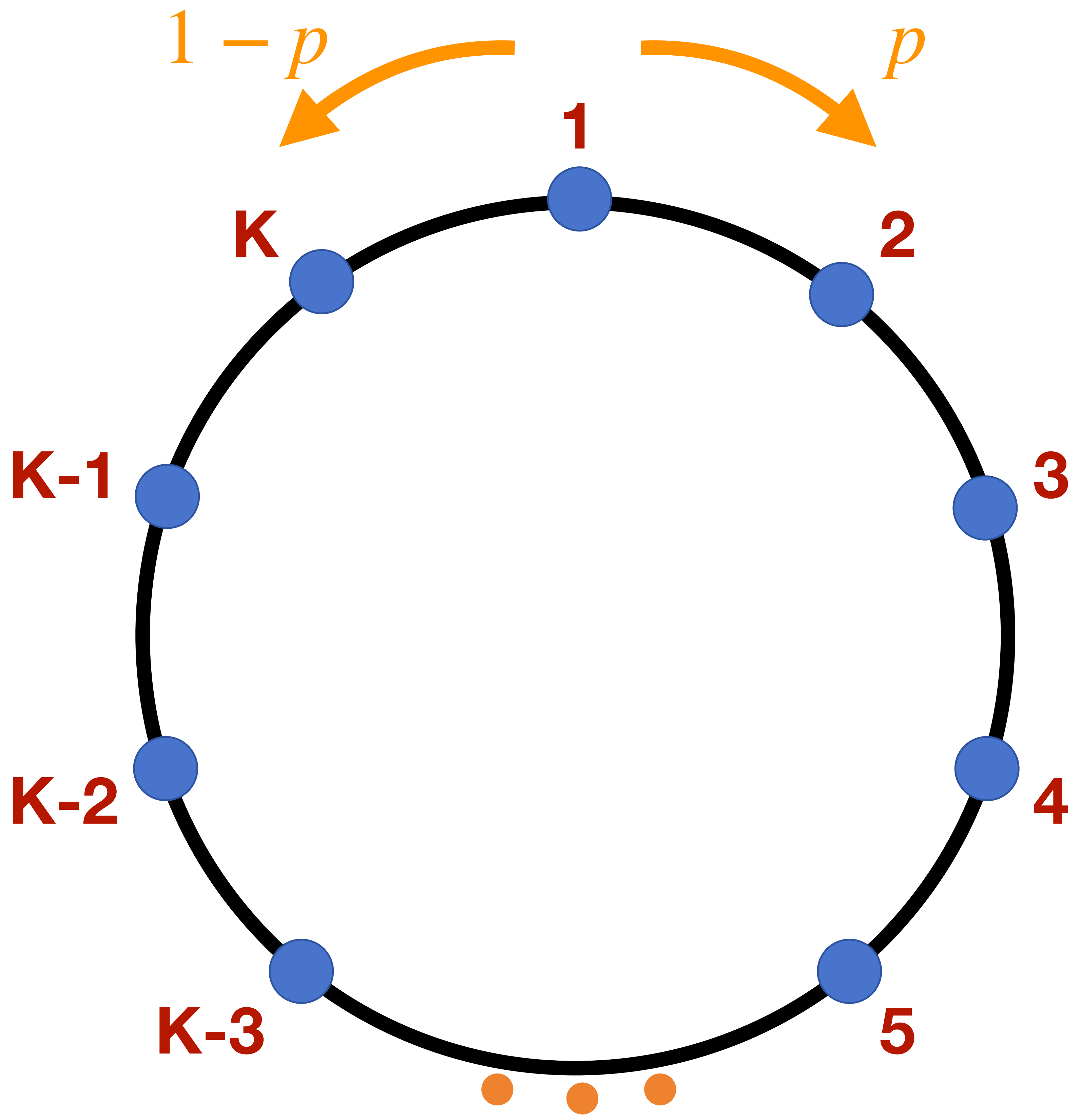
Goal: predict the location of the next step s_N based on the historical locations $s_1, \ldots, s_{N-1}$.

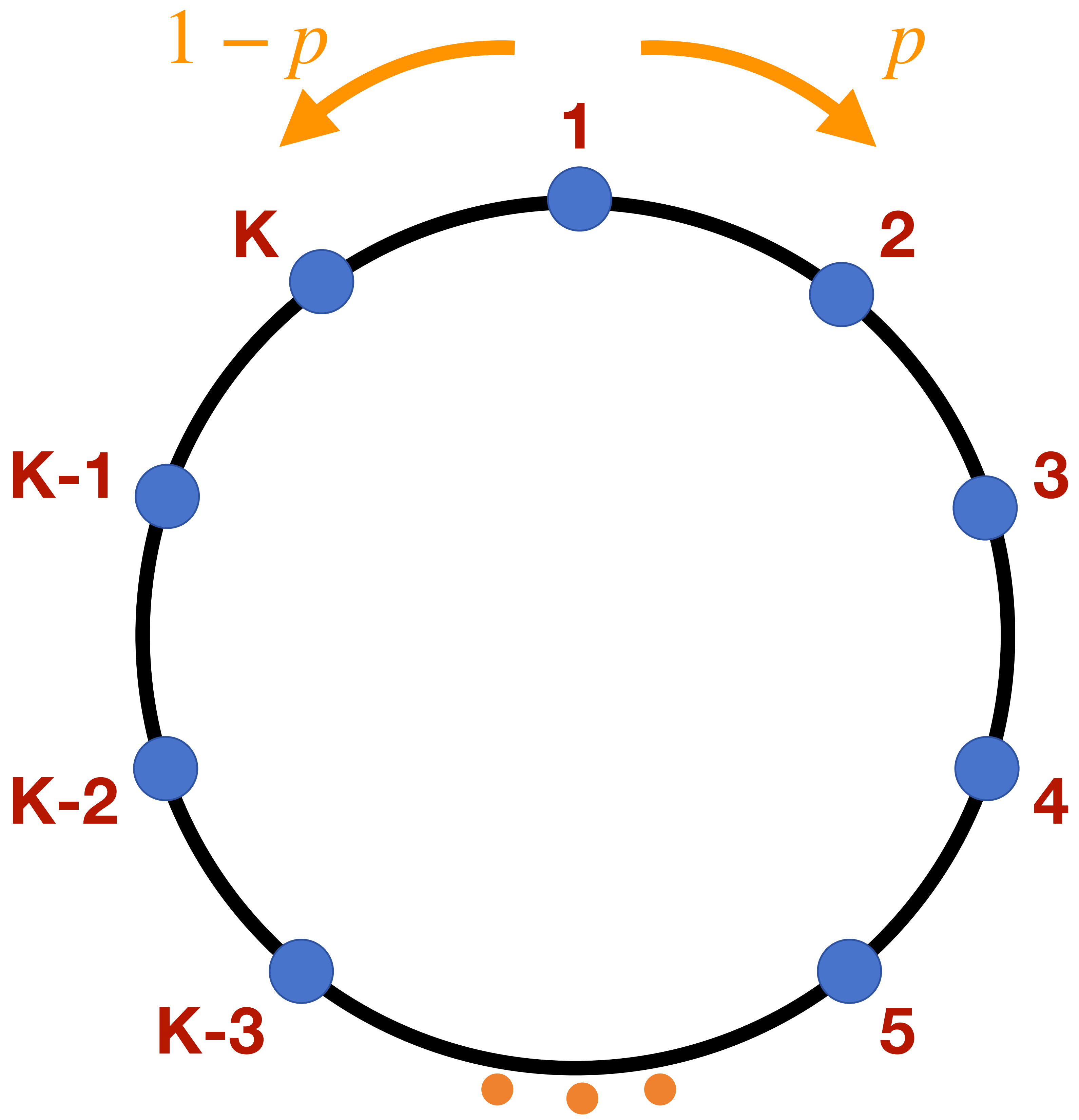


A simple random walk prediction task

Goal: predict the location of the next step s_N based on the historical locations $s_1, \ldots, s_{N-1}$.

For $i \in [N-1]$, denote by $\mathbf{x}_i \in \mathbb{R}^K$ the one-hot encoding of $s_i \in [K]$. Then

$$\mathbb{P}(\mathbf{x}_i \,|\, \mathbf{x}_1, \ldots, \mathbf{x}_{i-1}) = \mathbb{P}(\mathbf{x}_i \,|\, \mathbf{x}_{i-1}) = \mathbf{\Pi}^{*\top} \mathbf{x}_{i-1},$$



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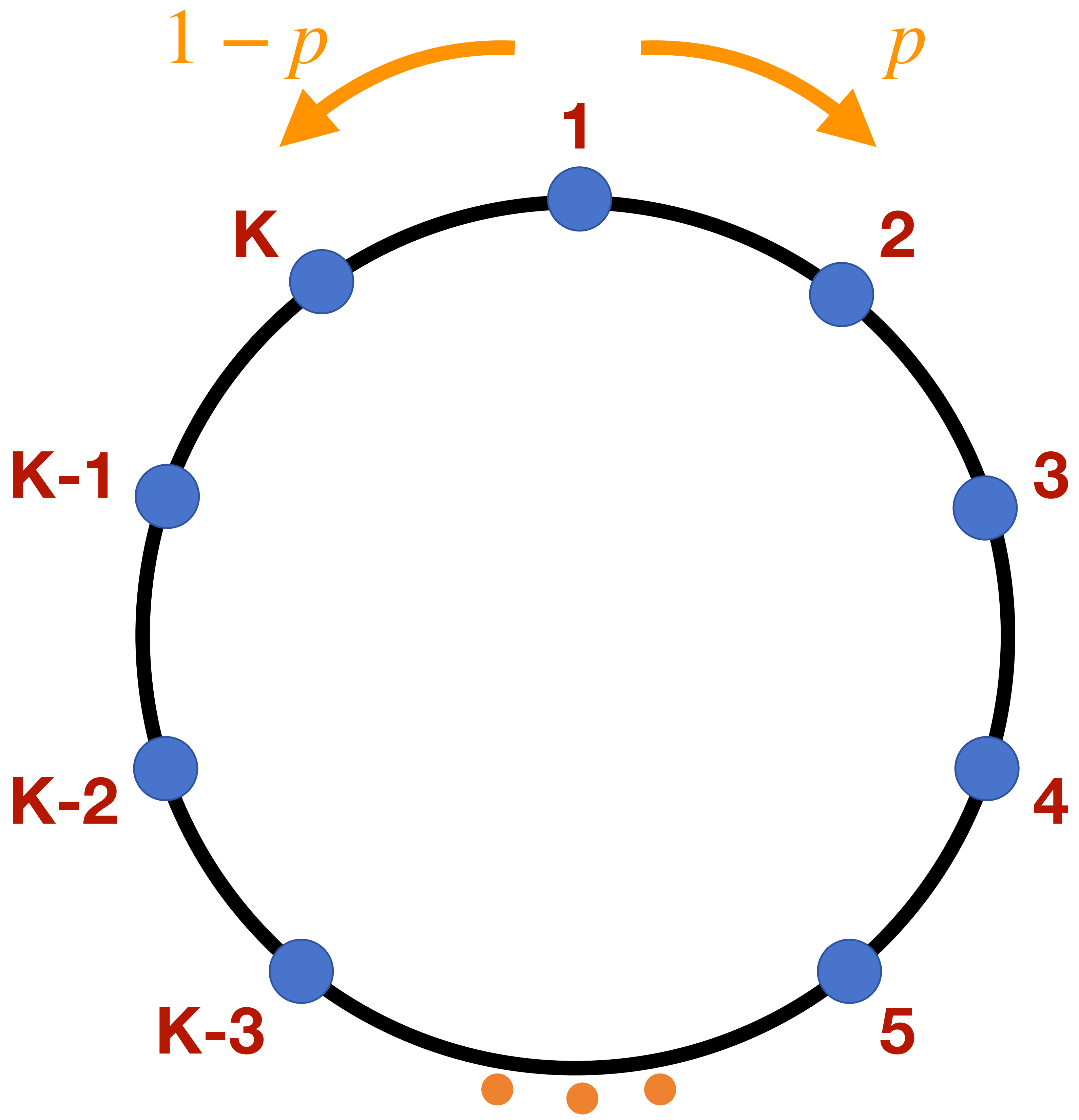

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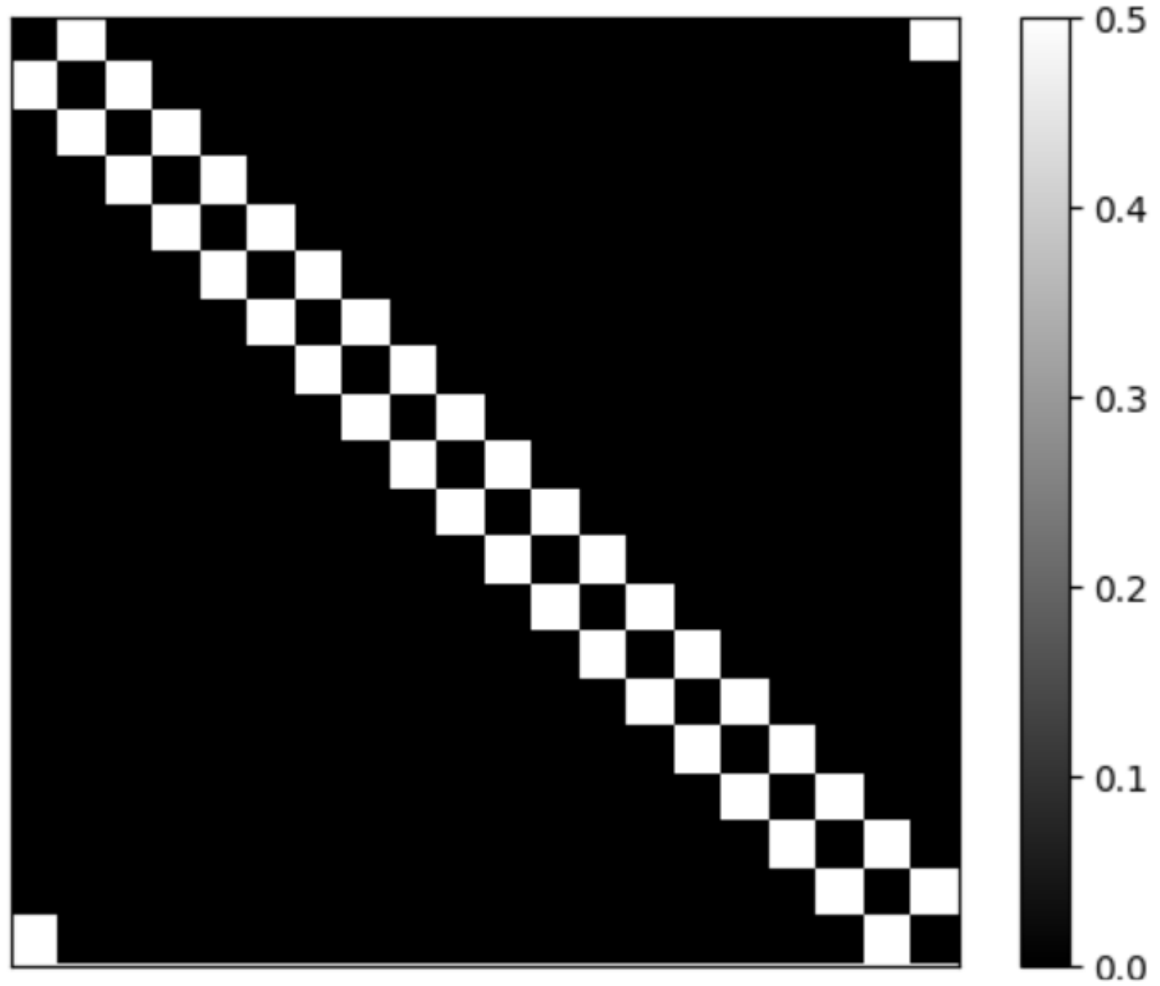
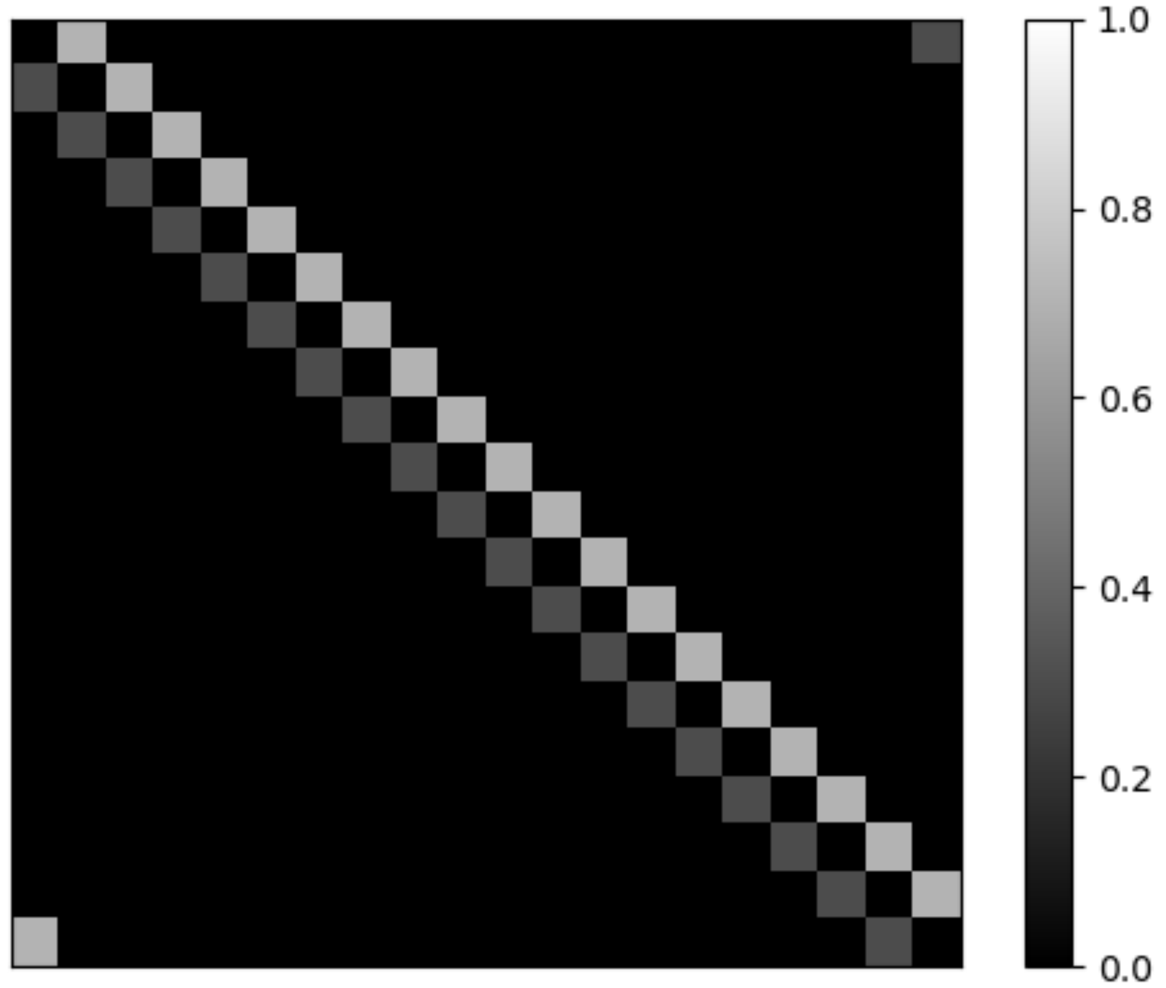
Markov property

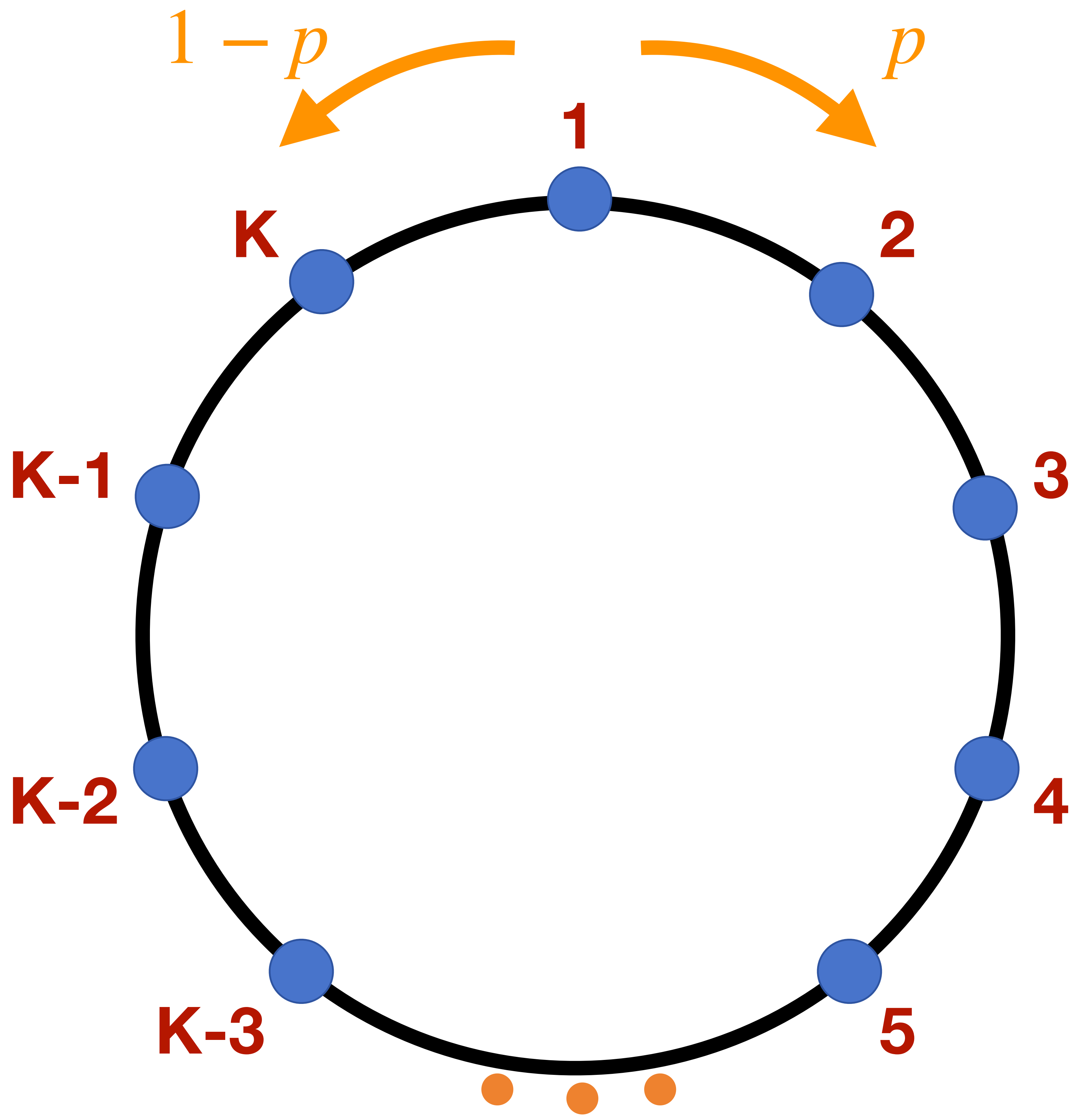
where $\mathbf{\Pi}^*$ is the ground-truth transition matrix:

$p = 0.5$





$p = 0.7$



Random walk prediction with transformers

Input matrix: $\mathbf{H} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \dots & \mathbf{x}_{N-1} & \mathbf{0} \\ \mathbf{p}_1 & \mathbf{p}_2 & \dots & \mathbf{p}_{N-1} & \mathbf{p}_N \end{bmatrix} \in \mathbb{R}^{(K+M)\times N}$

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Mutually orthogonal positional encodings

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Label: $y = s_N \sim \boldsymbol{\Pi}^{*\top}\mathbf{x}_{i-1}$

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Population log loss: $L(\mathbf{V}, \mathbf{W}) = \mathbb{E}_{(\mathbf{X},y)} \log[\mathbf{e}_y^\top \mathbf{f}(\mathbf{H}, \mathbf{V}, \mathbf{W}) + \epsilon]$

Gradient descent:

$$\mathbf{V}^{(t+1)} = \mathbf{V}^{(t)} - \eta \nabla_{\mathbf{V}} L(\mathbf{V}^{(t)}, \mathbf{W}^{(t)});\ \ \mathbf{W}^{(t+1)} = \mathbf{W}^{(t)} - \eta \nabla_{\mathbf{W}} L(\mathbf{V}^{(t)}, \mathbf{W}^{(t)}),$$

with zero initialization: $\mathbf{v}^{(0)} = \mathbf{0}_{K\times K}$, $\mathbf{W}^{(0)} = \mathbf{0}_{(K+M)\times(K+M)}$.

Transformers learn random walk prediction

Theorem. Suppose that $0 < p < 1$, and $\eta, \epsilon = \Theta(1)$. Under certain conditions, there exists $T_0 = \Theta(1)$, such that for any polynomial iteration number $T \geq T_0$, the following results hold:

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Theorem. Suppose that $0 < p < 1$, and $\eta, \epsilon = \Theta(1)$. Under certain conditions, there exists $T_0 = \Theta(1)$, such that for any polynomial iteration number $T \geq T_0$, the following results hold:

- Softmax attention selects the "direct parent" token:

$$\left[\mathrm{softmax}(\mathbf{H}^\top \mathbf{W}^{(T)} \mathbf{h}_N)\right]_{N-1} \geq 1 - \exp(-\Omega(N)), \quad \left[\mathrm{softmax}(\mathbf{H}^\top \mathbf{W}^{(T)} \mathbf{h}_N)\right]_j \leq \exp(-\Omega(N)) \,.$$

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$$\left\| \frac{\mathbf{V}^{(T)}}{\|\mathbf{V}^{(T)}\|_F} - \frac{\mathbf{\Pi}^{*\top}}{\|\mathbf{\Pi}^{*\top}\|_F} \right\|_F = O\left(\frac{1}{\sqrt{T}}\right).$$

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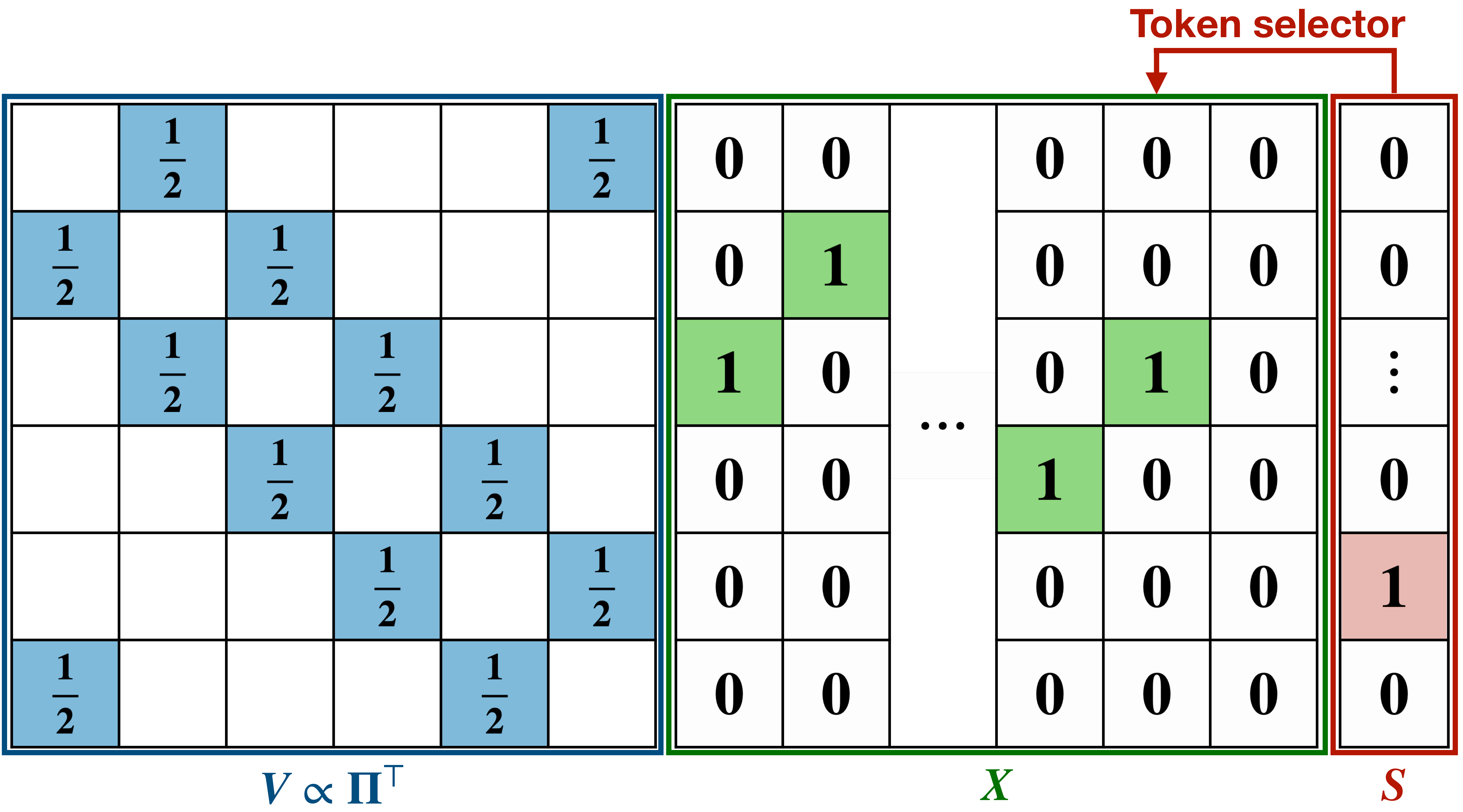
Optimal probability transition on the parent token

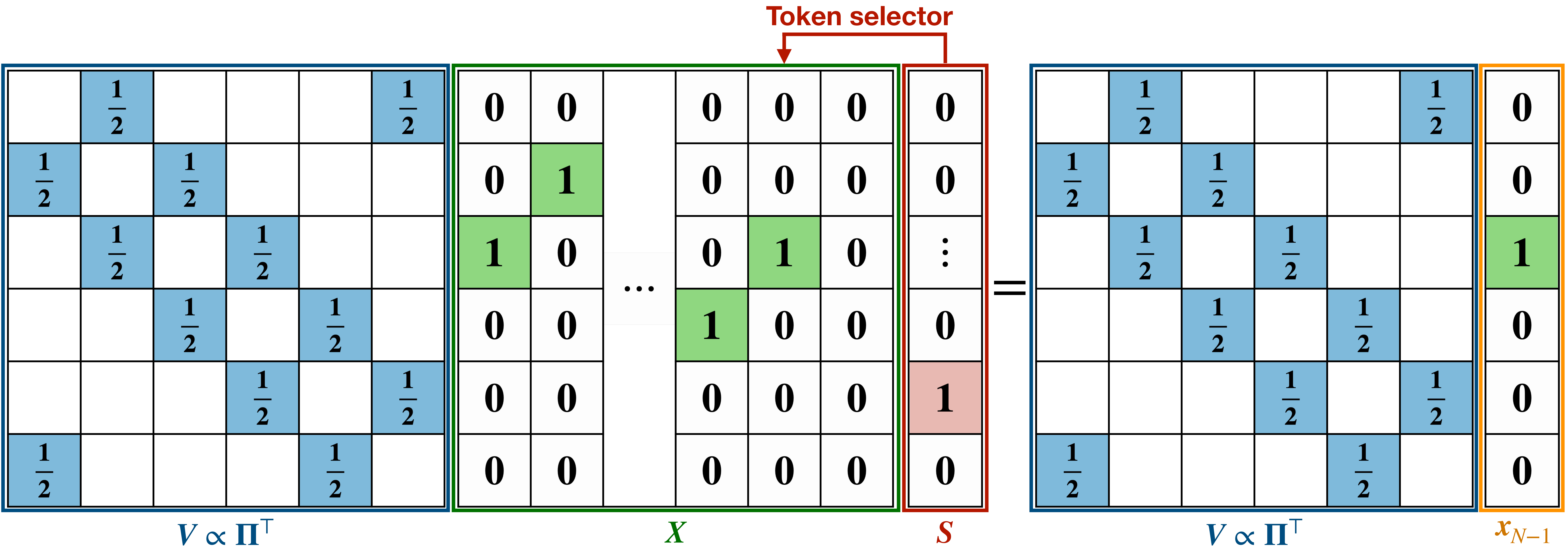
Transformers learn random walk prediction

$$
\underbrace{\begin{bmatrix} & \frac{1}{2} & & & & \frac{1}{2} \\ \frac{1}{2} & & \frac{1}{2} & & & \\ & \frac{1}{2} & & \frac{1}{2} & & \\ & & \frac{1}{2} & & \frac{1}{2} & \\ & & & \frac{1}{2} & & \frac{1}{2} \\ \frac{1}{2} & & & & \frac{1}{2} & \end{bmatrix}}_{\boldsymbol{V} \propto \boldsymbol{\Pi}^\top}
\underbrace{\begin{bmatrix} 0 & 0 & & 0 & 0 & 0 \\ 0 & 1 & & 0 & 0 & 0 \\ 1 & 0 & & 0 & 1 & 0 \\ 0 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 0 & & 0 & 0 & 0 \\ 0 & 0 & & 0 & 0 & 0 \end{bmatrix}}_{\boldsymbol{X}}
\underbrace{\begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \end{bmatrix}}_{\boldsymbol{S}}
$$

Transformers learn random walk prediction



Transformers learn random walk prediction



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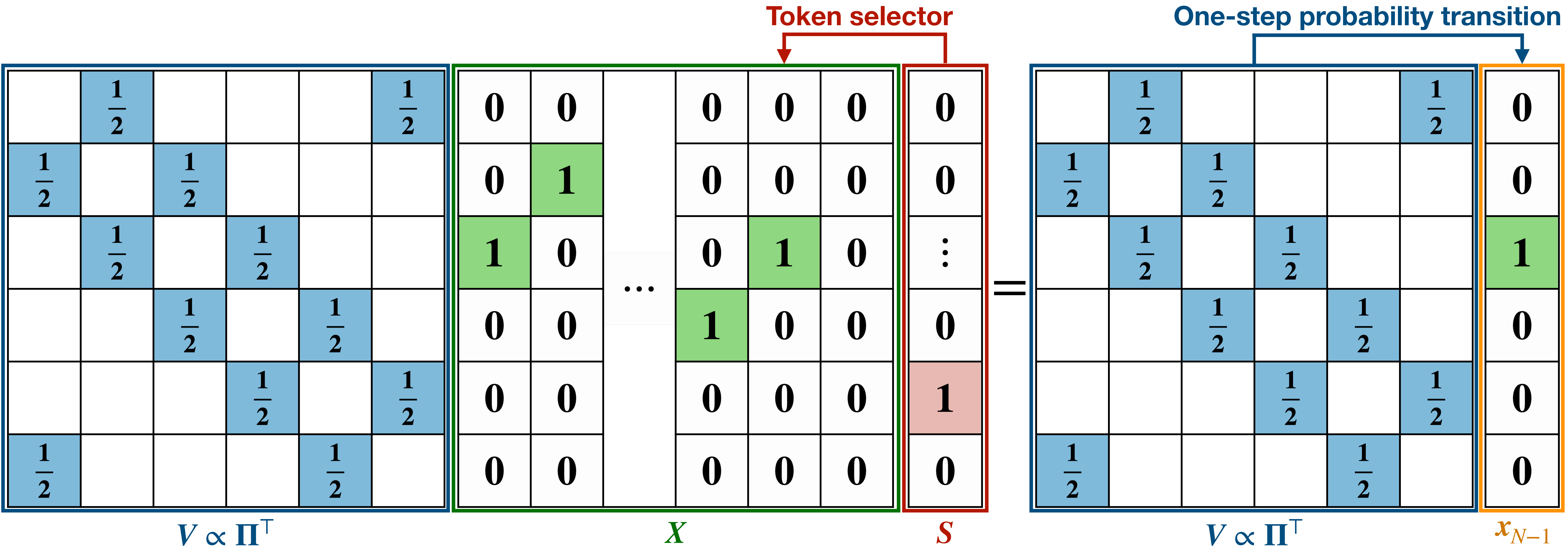

Transformers learn random walk prediction

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Corollary. Suppose that $0 < p < 1$, and $\eta, \epsilon = \Theta(1)$. Under certain conditions, there exists $T_0 = \Theta(1)$, such that for any polynomial iteration number $T \geq T_0$, the following results hold:

Transformers learn random walk prediction

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- The transformer converges to the optimal predictor:

$$\left\| \frac{\mathbf{f}(\mathbf{H}, \mathbf{V}^{(T)}, \mathbf{W}^{(T)})}{\|\mathbf{f}(\mathbf{H}, \mathbf{V}^{(T)}, \mathbf{W}^{(T)})\|_2} - \mathbf{\Pi}^{*\top}\mathbf{x}_{N-1} \right\|_2 = O\left(\frac{1}{\sqrt{T}}\right).$$

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- The trained transformer achieves optimal prediction accuracy:

$$\mathbb{P}_{(\mathbf{X},y)}\left[\mathrm{Pred}[\mathbf{f}(\mathbf{X}, \mathbf{V}^{(T)}, \mathbf{W}^{(T)})] = y\right] = \max\{p, 1-p\}.$$

Here we define: $\mathrm{Pred}(\mathbf{f}) = \min\left\{ j \in [K] : [\mathbf{f}]_j = \max_{i \in [K]}\{[\mathbf{f}]_i\} \right\}.$

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Failure in learning “deterministic walks” with $p = 0 \text{ or } 1$

Theorem. Suppose that $p = 0 \text{ or } 1$, K is a constant integer, and $N = rK + 1$ with $r \geq 1$. Then for any loss function $\ell(\,\cdot\,)$, any learning rate $\eta > 0$, and any $T \geq 0$, it holds that

$$\mathbb{P}_{(\mathbf{X},y)}\big[\mathrm{Pred}[\mathbf{f}(\mathbf{X}, \mathbf{V}^{(T)}, \mathbf{W}^{(T)})] = y\big] = \frac{1}{K}.$$

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Random guess

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Random guess

Moreover, with probability 1, for all $T \geq 0$, it holds that

$$\mathbf{V}^{(T)} \propto \mathbf{1}_{K \times K}, \quad \left[\mathrm{softmax}(\mathbf{H}^\top \mathbf{W}^{(T)} \mathbf{h}_N)\right]_1 = \cdots = \left[\mathrm{softmax}(\mathbf{H}^\top \mathbf{W}^{(T)} \mathbf{h}_N)\right]_{N-1}.$$

Failure in learning "deterministic walks" with $p = 0 \text{ or } 1$

Theorem. Suppose that $p = 0 \text{ or } 1$, K is a constant integer, and $N = rK + 1$ with $r \geq 1$. Then for any loss function $\ell(\cdot)$, any learning rate $\eta > 0$, and any $T \geq 0$, it holds that

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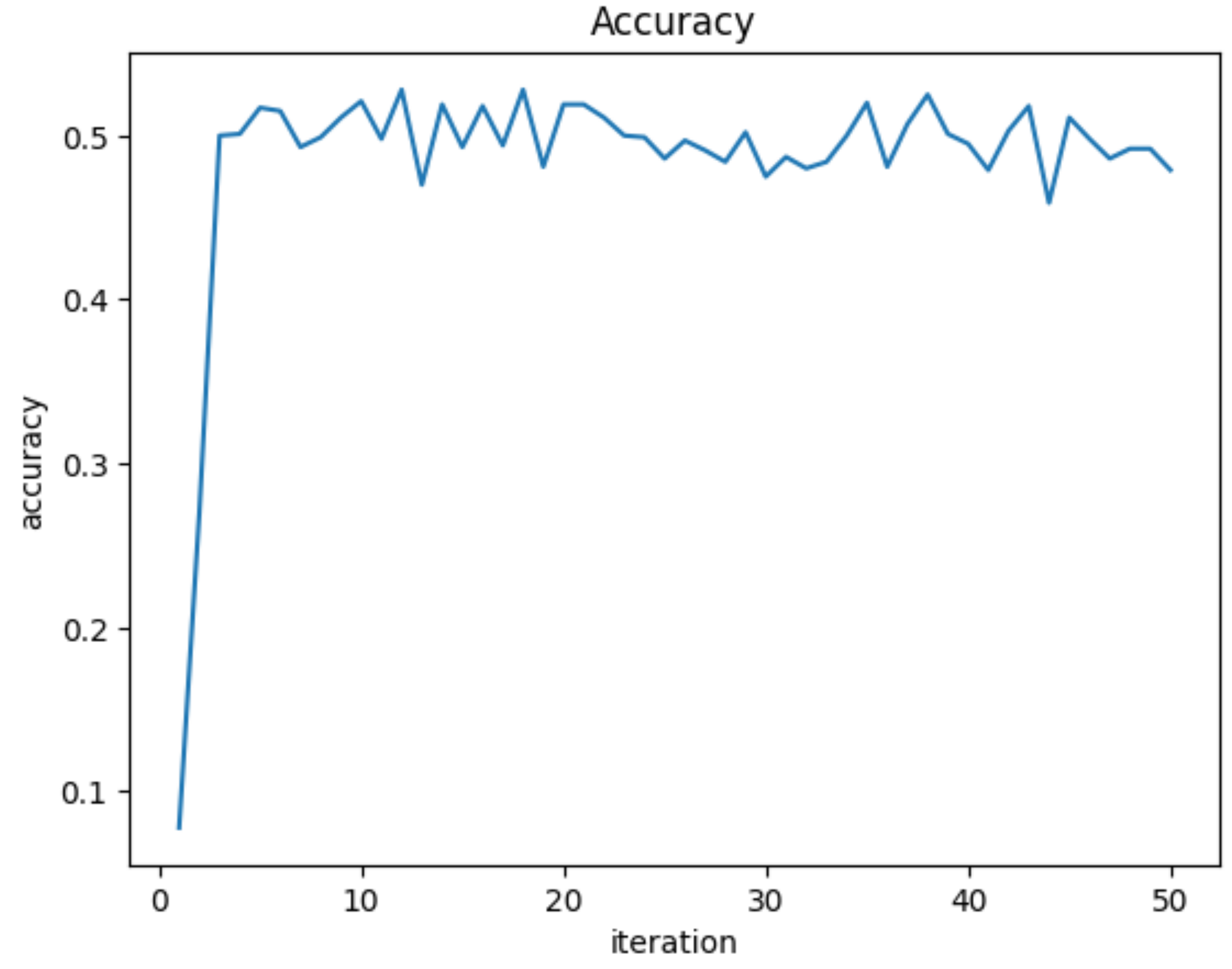
Random initialization overcomes the issue to a certain extent.

Experiments

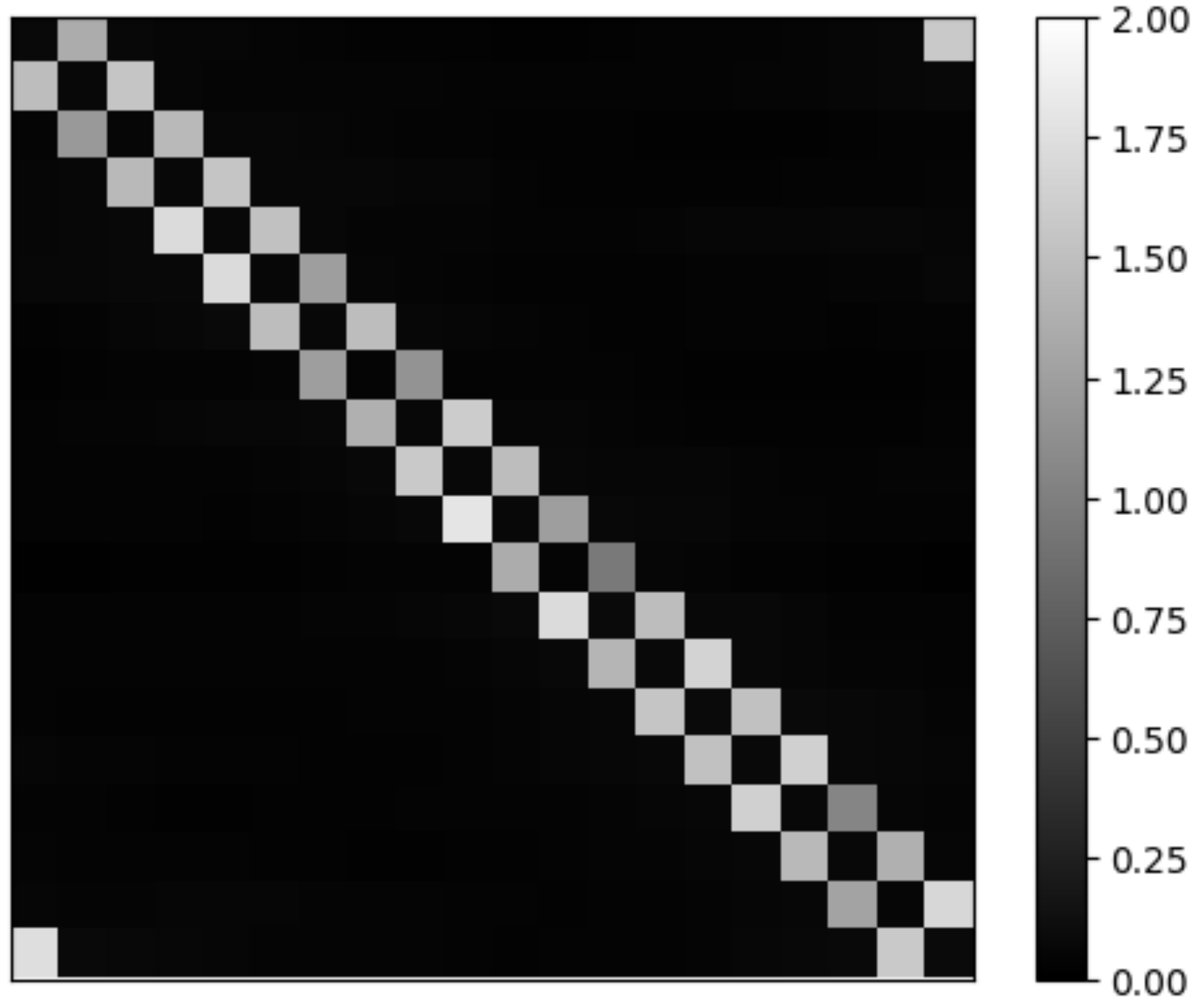
$p = 1/2$:

$K = 20,\ N = 101$

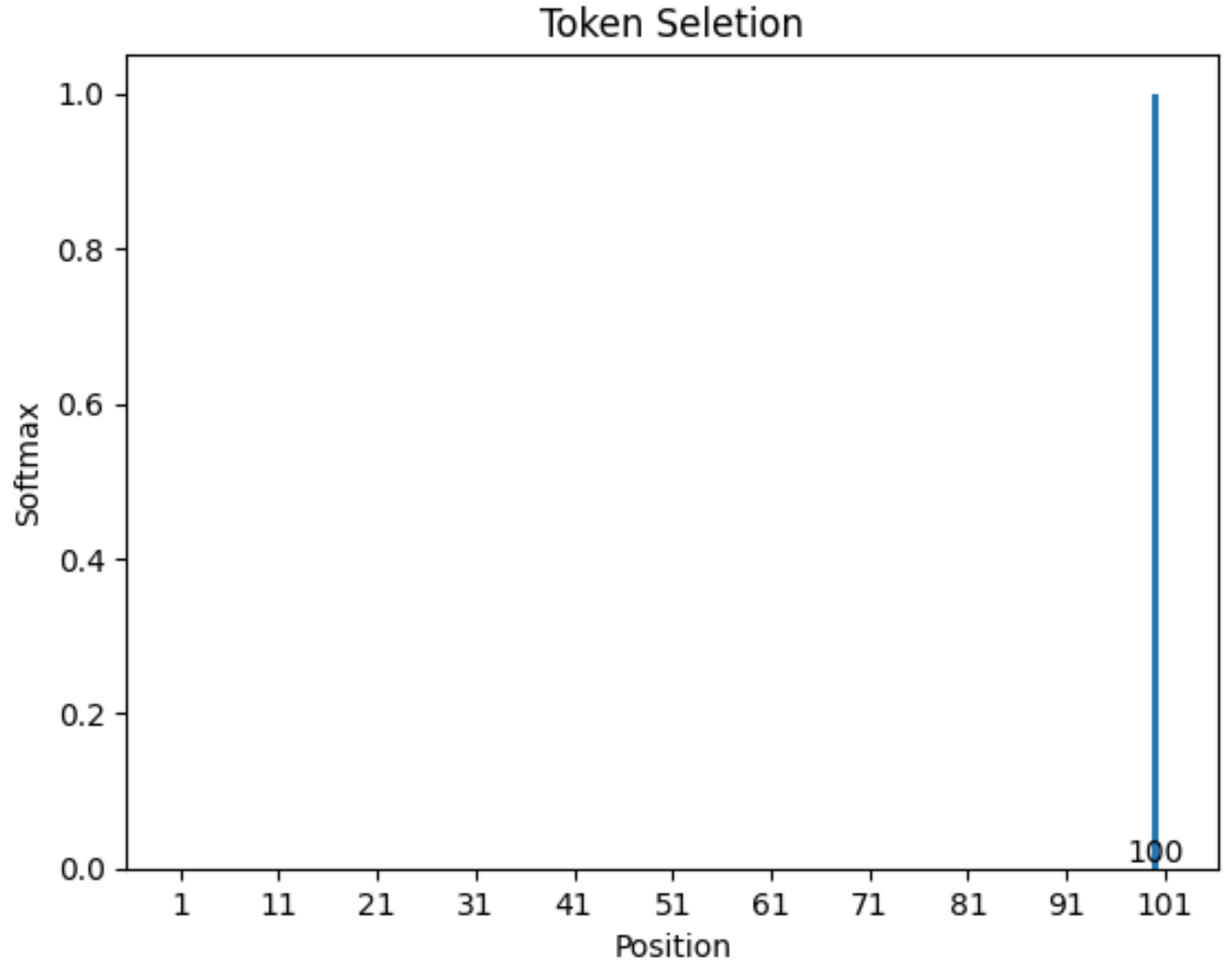
Accuracy



$\mathbf{V}^{(T)}$



Softmax attention



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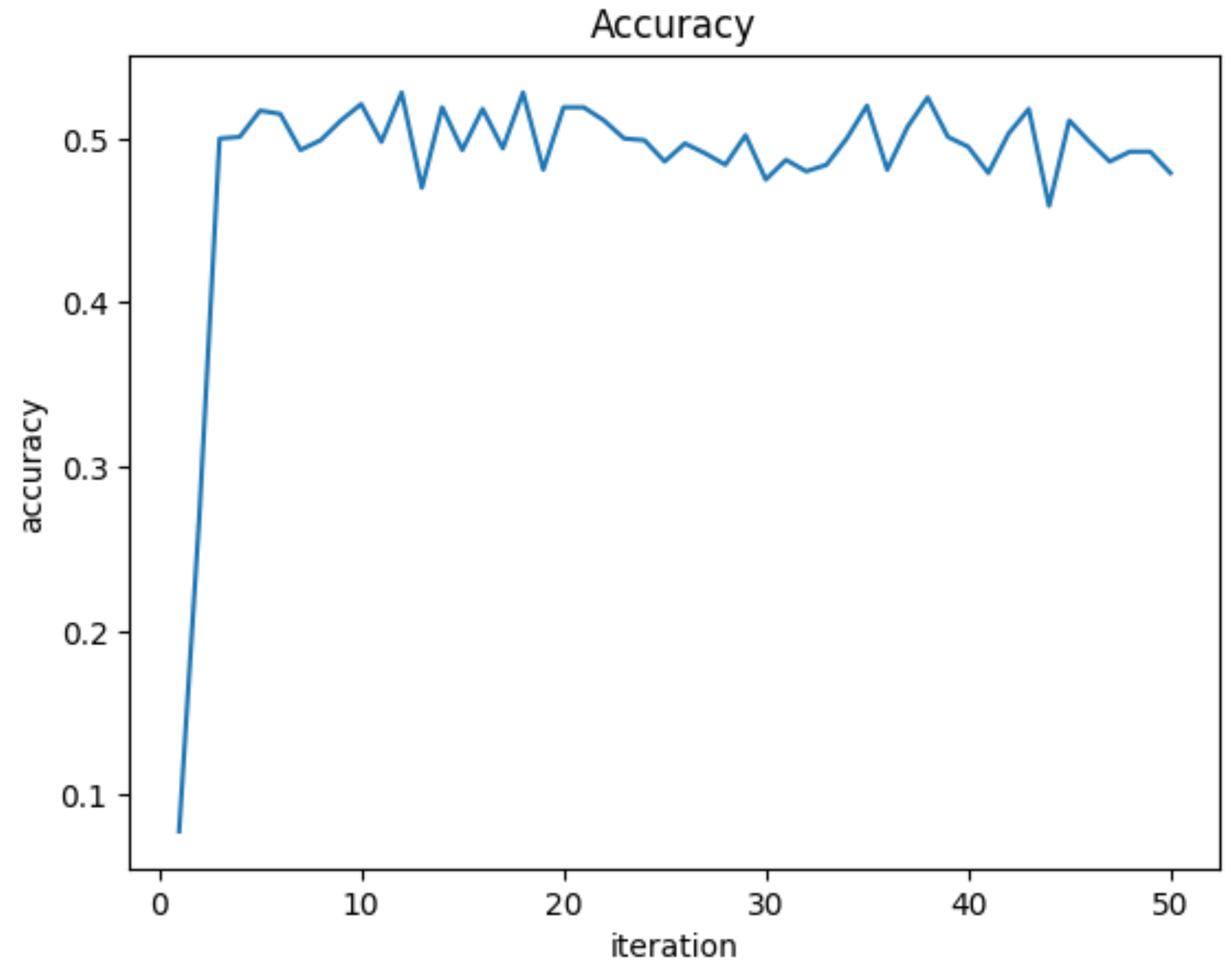

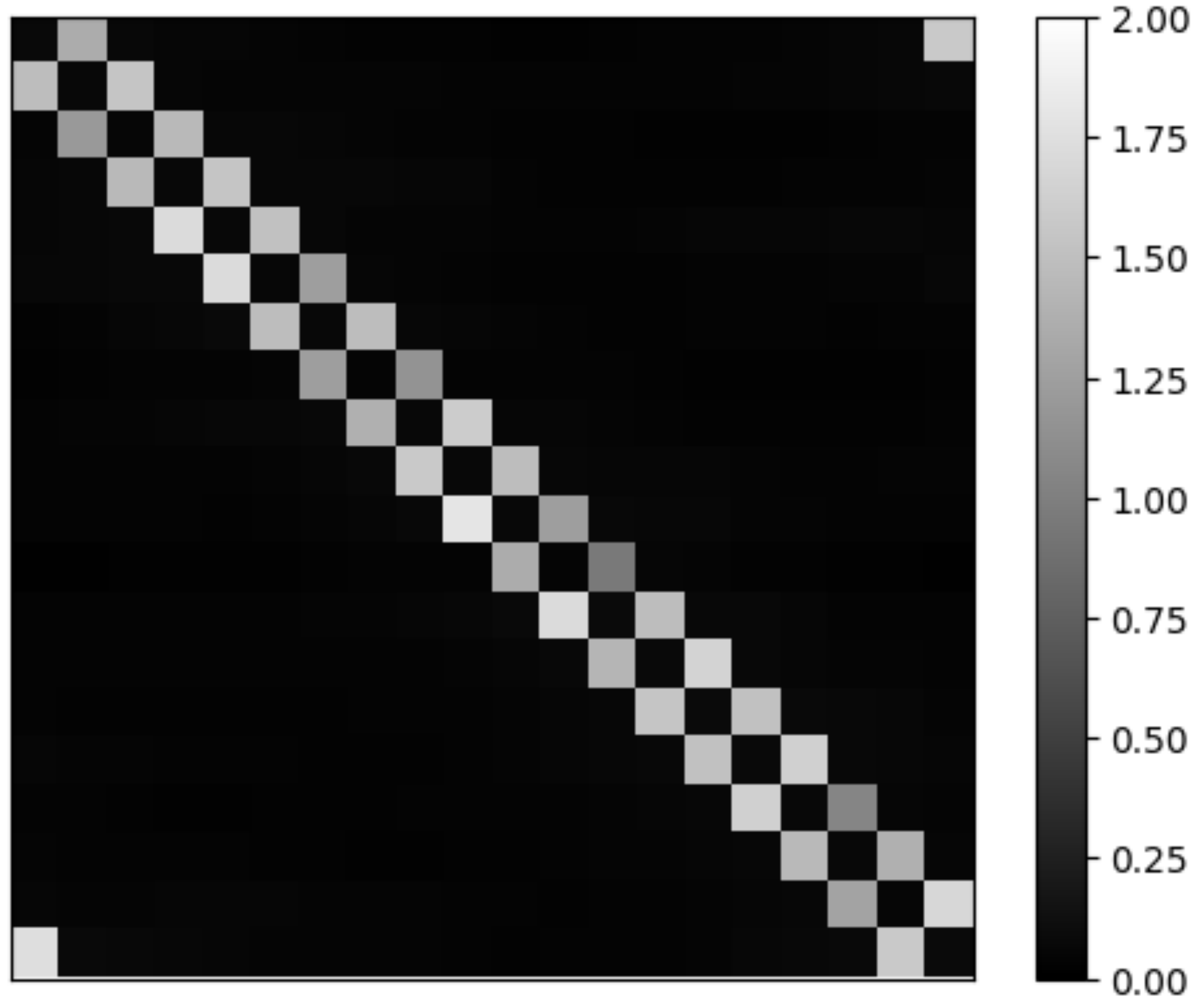

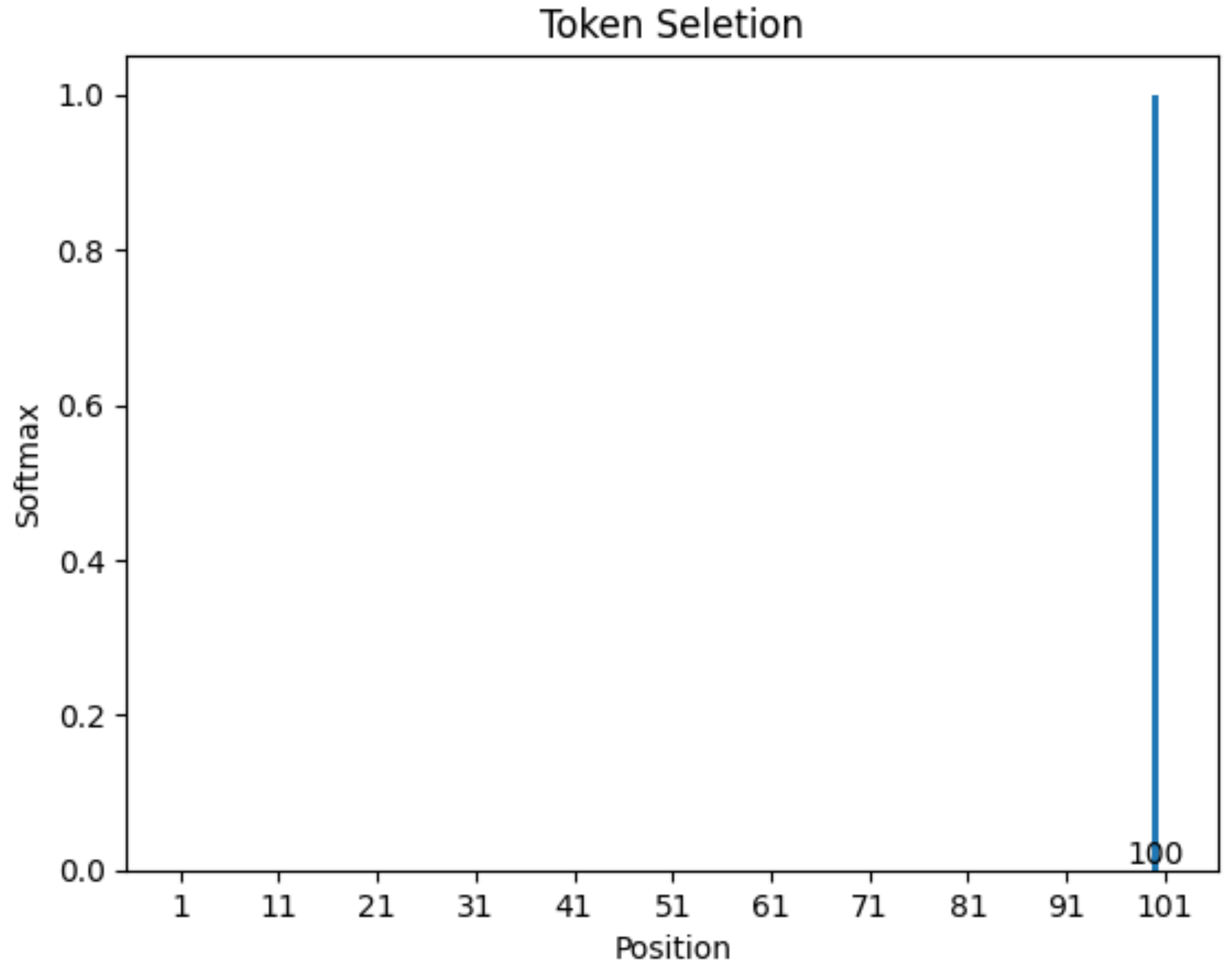

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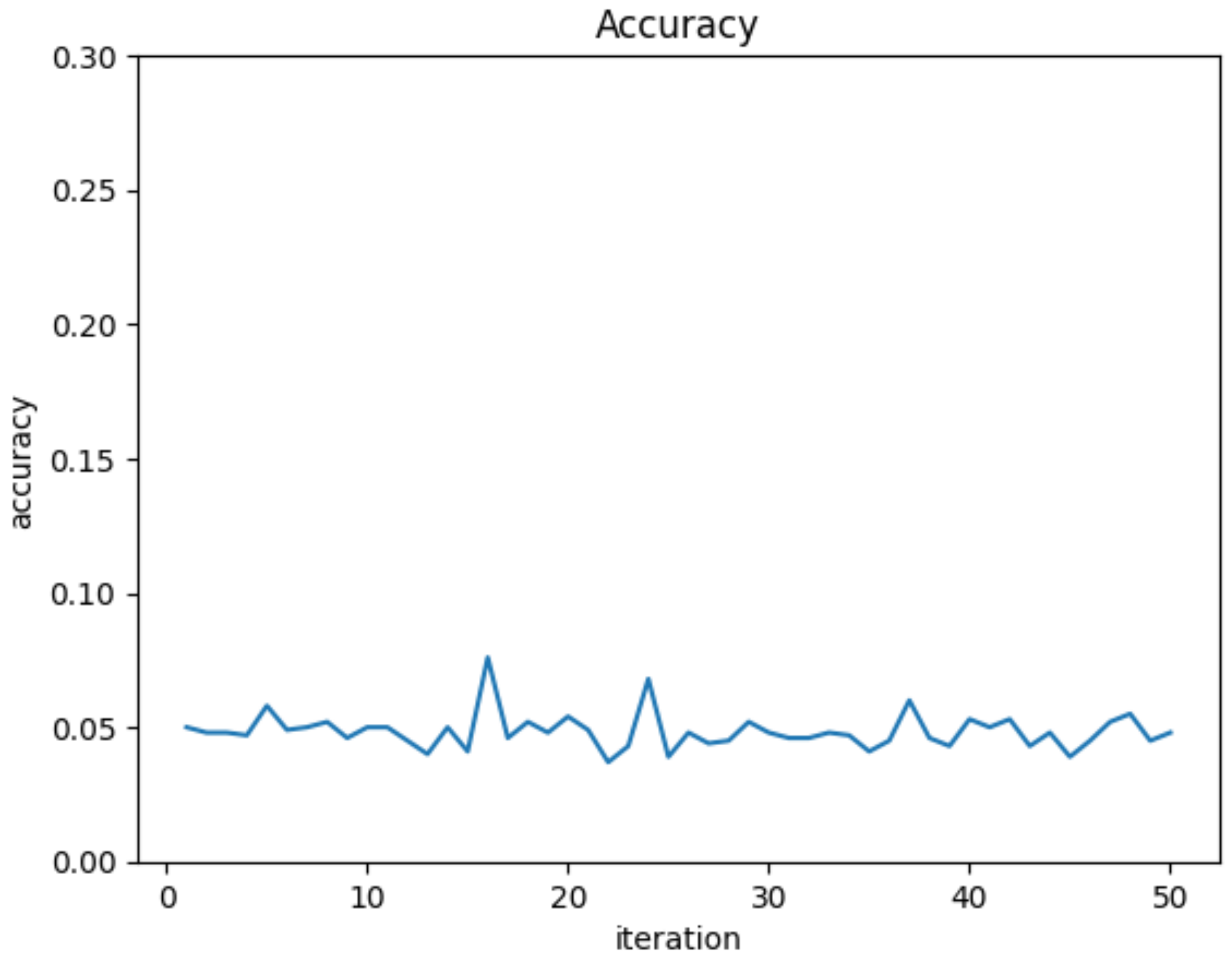

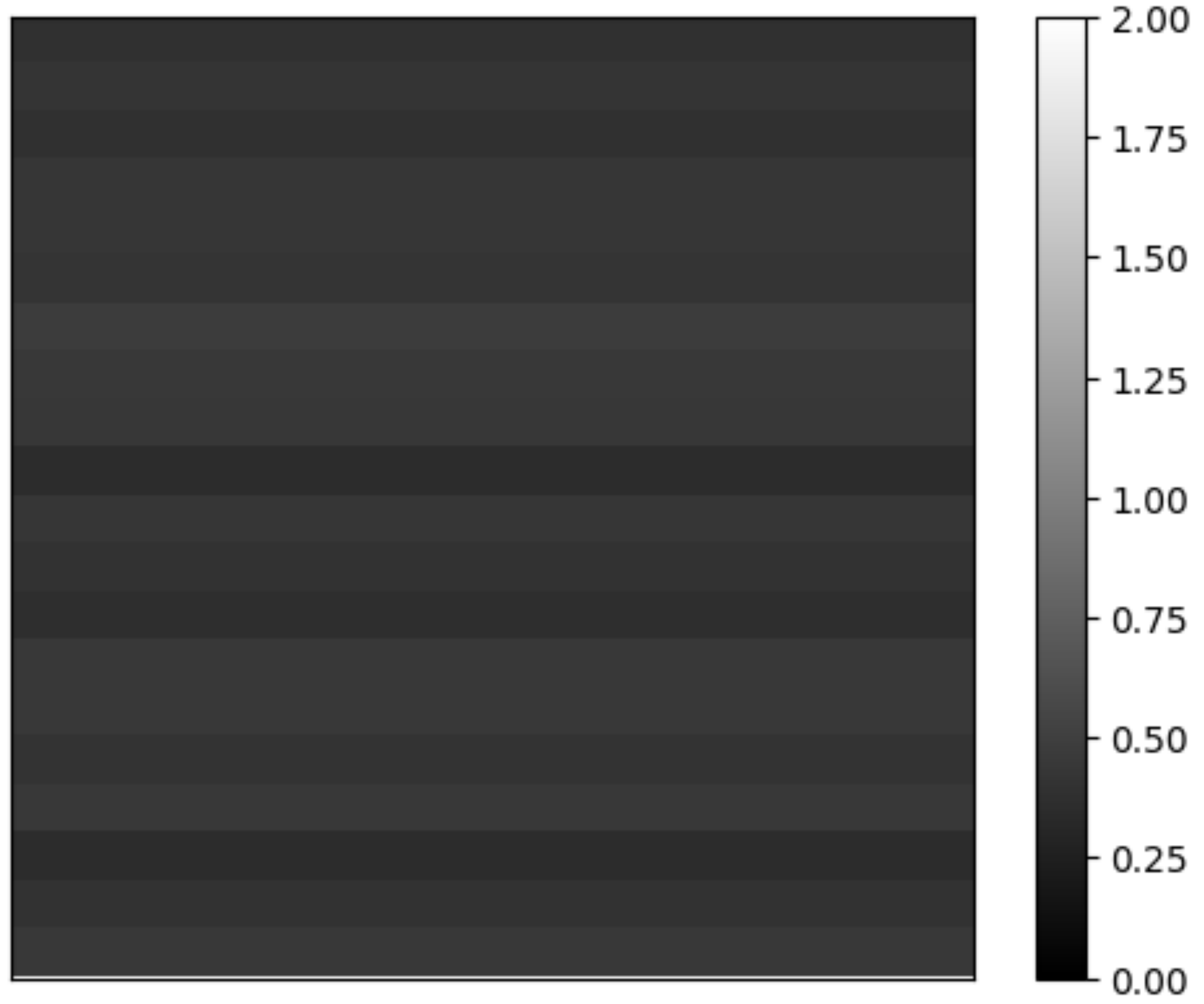

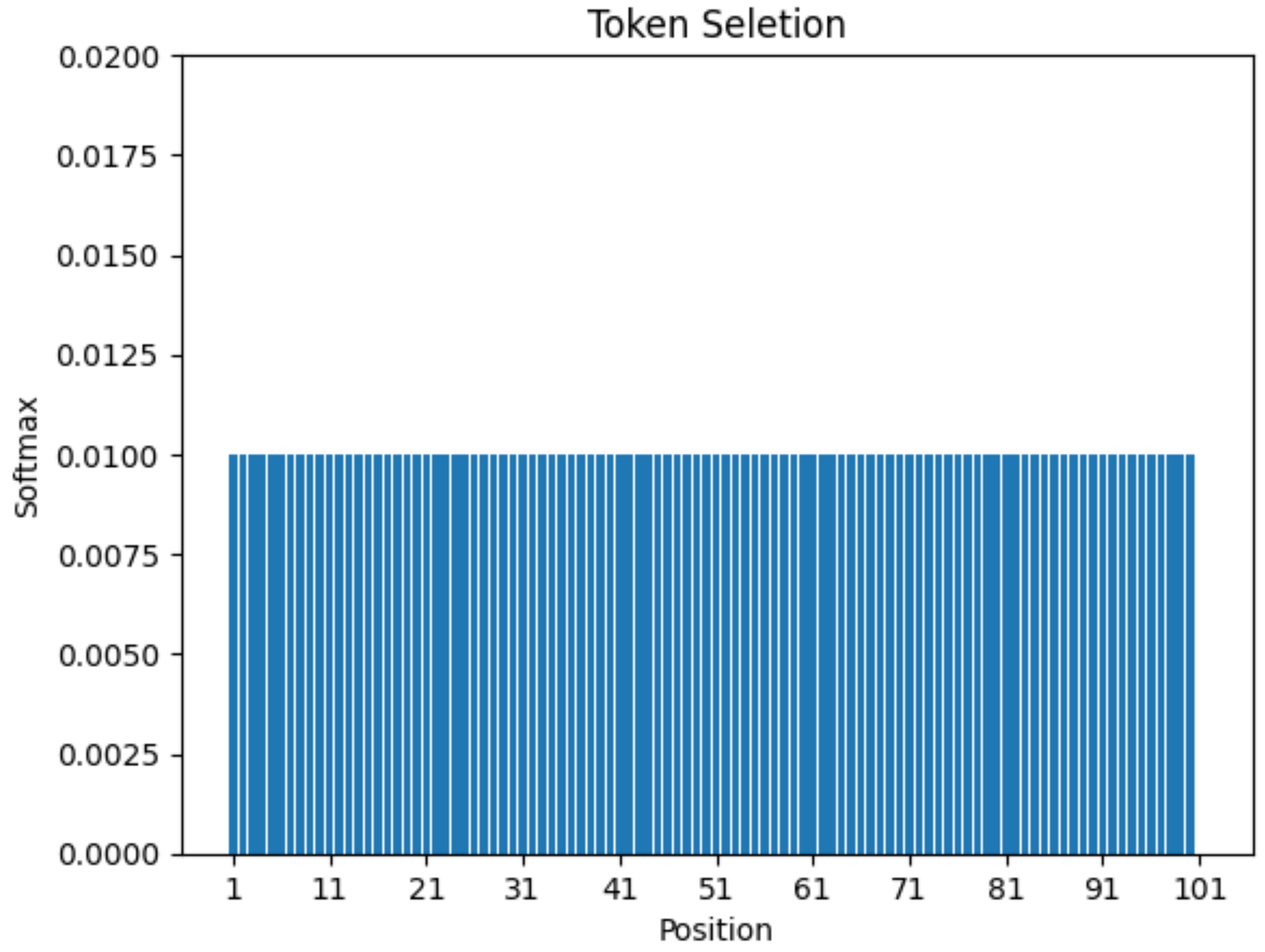

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Thank you!

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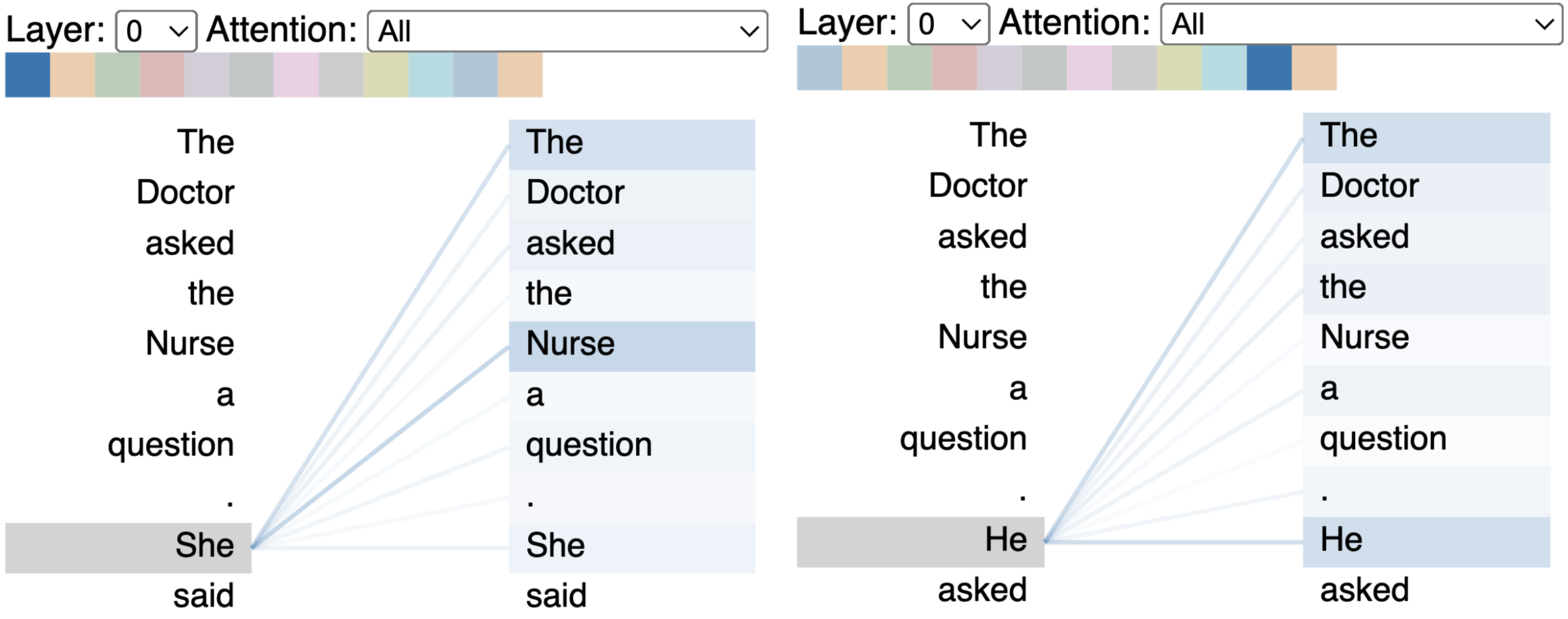

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Proof sketch of in-context nearest neighbor predictor

Consider the parameter matrix $\mathbf{W}$ as a block matrix:

$$\mathbf{W} = \begin{bmatrix} \mathbf{W}_{11} & \mathbf{W}_{12} & \mathbf{W}_{13} \\ \mathbf{W}_{21} & \mathbf{W}_{22} & \mathbf{W}_{23} \\ \mathbf{W}_{31} & \mathbf{W}_{32} & \mathbf{W}_{33} \end{bmatrix}.$$

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A key observation is that

$$\nabla_{\mathbf{W}_{11}} L(\mathbf{W}^{(t)}) = \mathbb{E}\left[\sum_{i=1}^{N} g_i^{(t)}(\mathbf{x}_i^\top \mathbf{x}_{N+1}) \cdot \mathbf{x}_i \mathbf{x}_{N+1}^\top + g_*^{(t)}(\mathbf{x}_{i*}^\top \mathbf{x}_{N+1}) \cdot \mathbf{x}_{i*} \mathbf{x}_{N+1}^\top\right],$$

where $g_i^k(x) : \mathbb{R} \to \mathbb{R}, i \in [N]$ are functions that map scalars to scalars.

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Moreover, $\nabla_{\mathbf{W}_{ij}} L(\mathbf{W}^k) = 0$ for all i, j except for $\mathbf{W}_{11}$ and $\mathbf{W}_{33}$!

Proof sketch of in-context nearest neighbor predictor

Proposition.

Along the optimization path of gradient descent, the weights has the form

$$\mathbf{W}^{(t)} = \mathrm{diag}\{\underbrace{\xi_1^{(t)}, \ldots, \xi_1^{(t)}}_{d \text{ times}}, 0, -\xi_2^{(t)}\}, \text{ with } \xi_1^k, \xi_2^k > 0.$$

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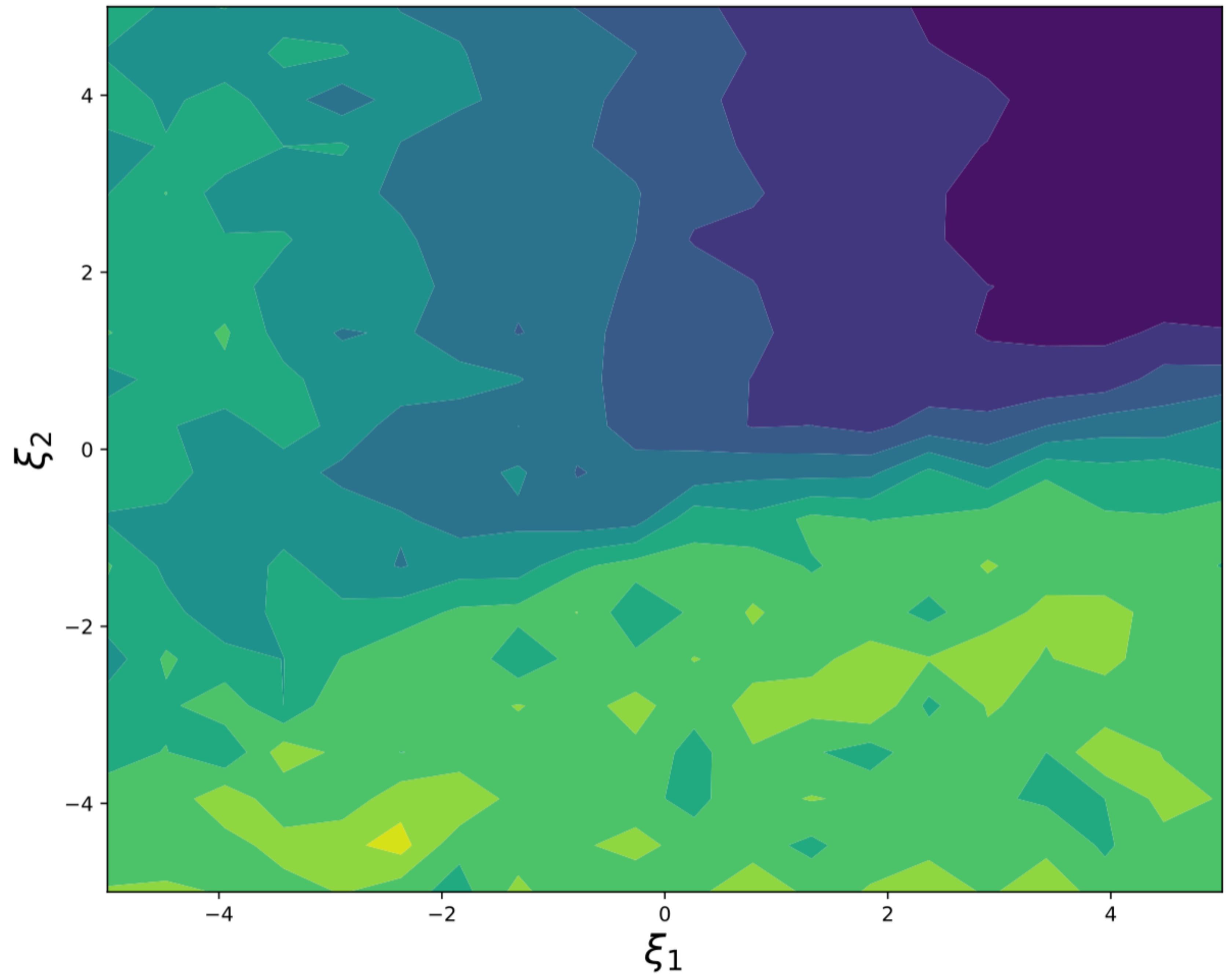

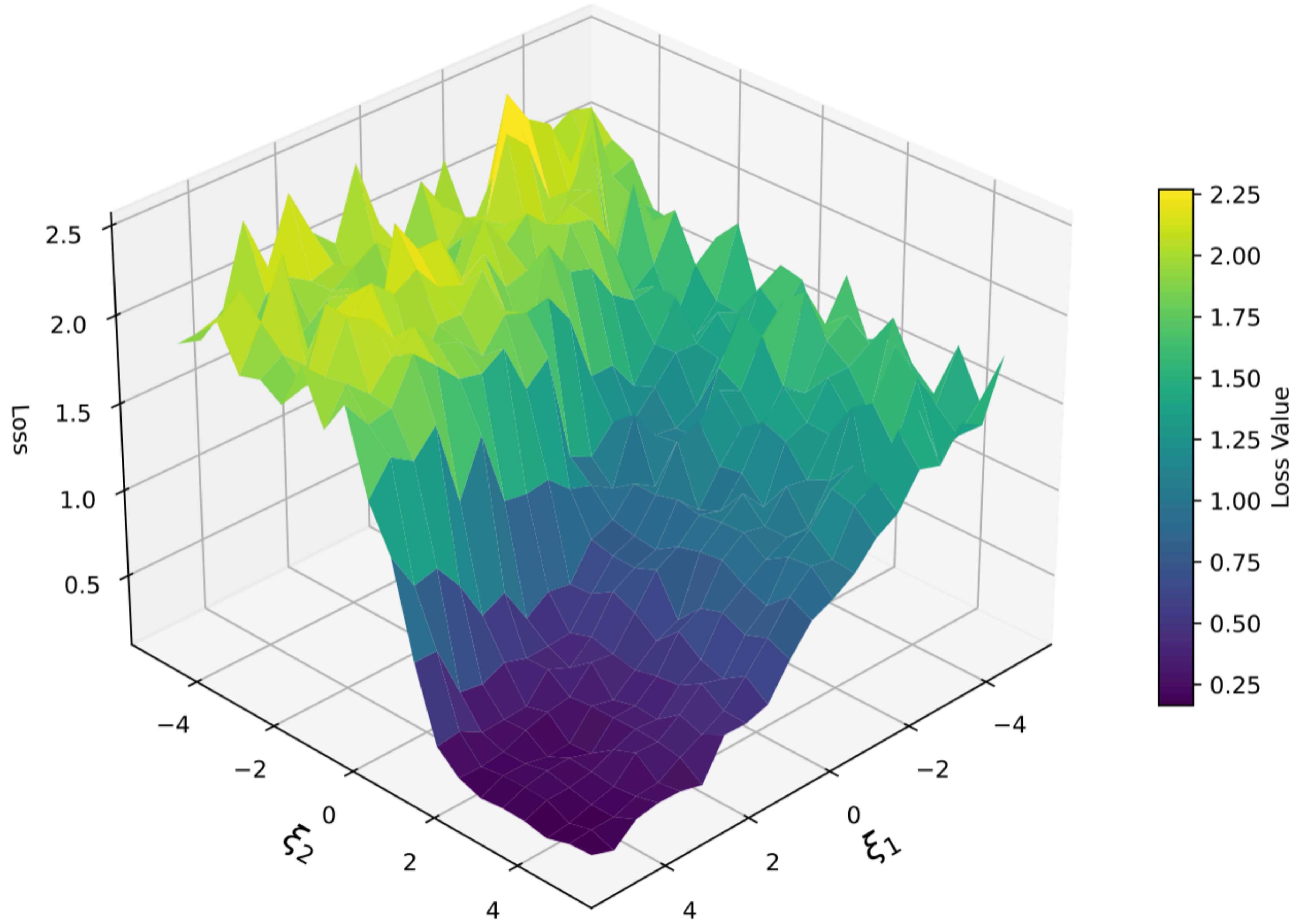

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$$\mathrm{softmax}(\mathbf{H}^\top \mathbf{W}^{(t)} \mathbf{H}) = \mathrm{softmax}\left(\begin{bmatrix} \xi_1^{(t)} \cdot \langle \mathbf{x}_1, \mathbf{x}_{\text{query}} \rangle \\ \xi_1^{(t)} \cdot \langle \mathbf{x}_2, \mathbf{x}_{\text{query}} \rangle \\ \vdots \\ \xi_1^{(t)} \cdot \langle \mathbf{x}_N, \mathbf{x}_{\text{query}} \rangle \\ -\xi_2^{(t)} \end{bmatrix} \right)$$

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As $\xi_1^{(t)} \gg \xi_2^{(t)} \to +\infty$.

Downstream task for group-sparse classification

Consider a downstream task, where the data $\{(\tilde{\mathbf{X}}^{(i)}, \tilde{y}^{(i)})\}_{i=1}^{n}$ follow an arbitrary distribution satisfying (i) $\tilde{\mathbf{X}}$ is sub-Gaussian, and (ii) $\tilde{y} \cdot \langle \tilde{\mathbf{v}}^*, \tilde{\mathbf{x}}_{j^*} \rangle \geq \gamma$ almost surely.

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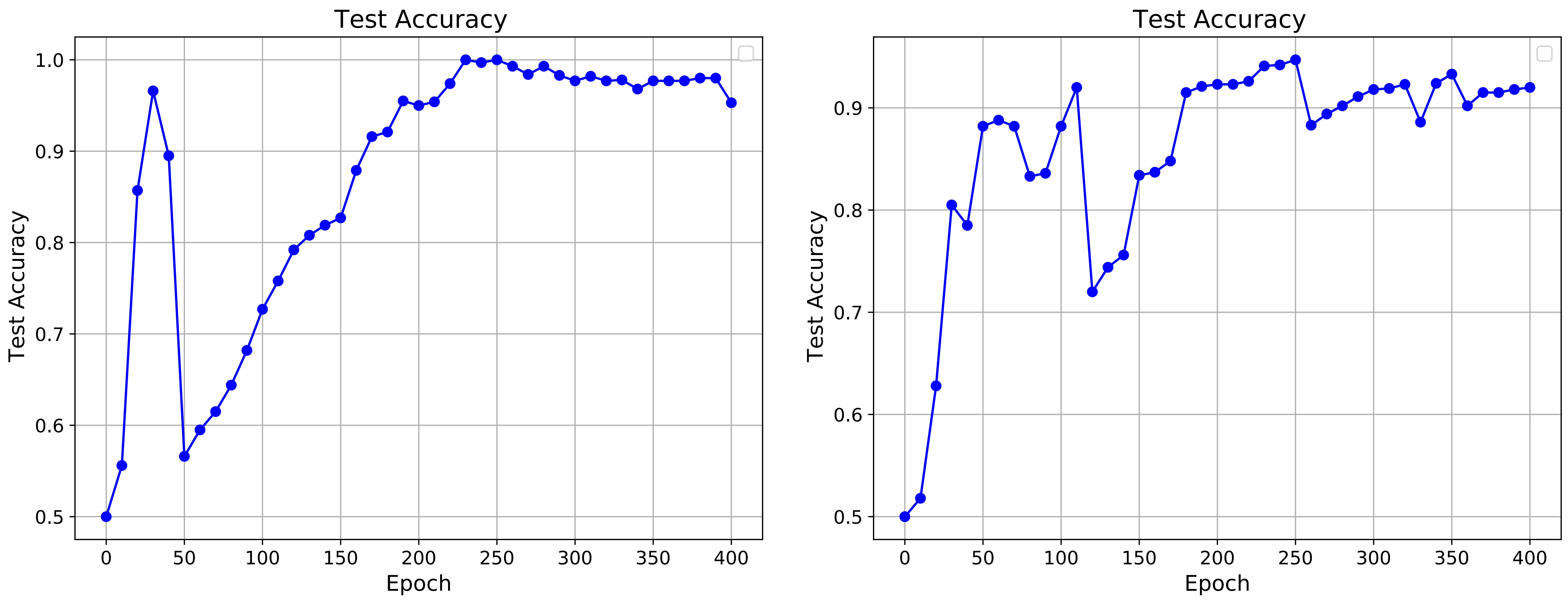
Sample complexity lower bound of linear logistic regression on $\mathrm{vec}(\tilde{\mathbf{X}})$ is $\tilde{\Omega}(dD/\epsilon)$.

Experiments - downstream task



Test accuracy in the downstream task when utilizing the pre-trained $\mathbf{W}^{(T^*)}$.