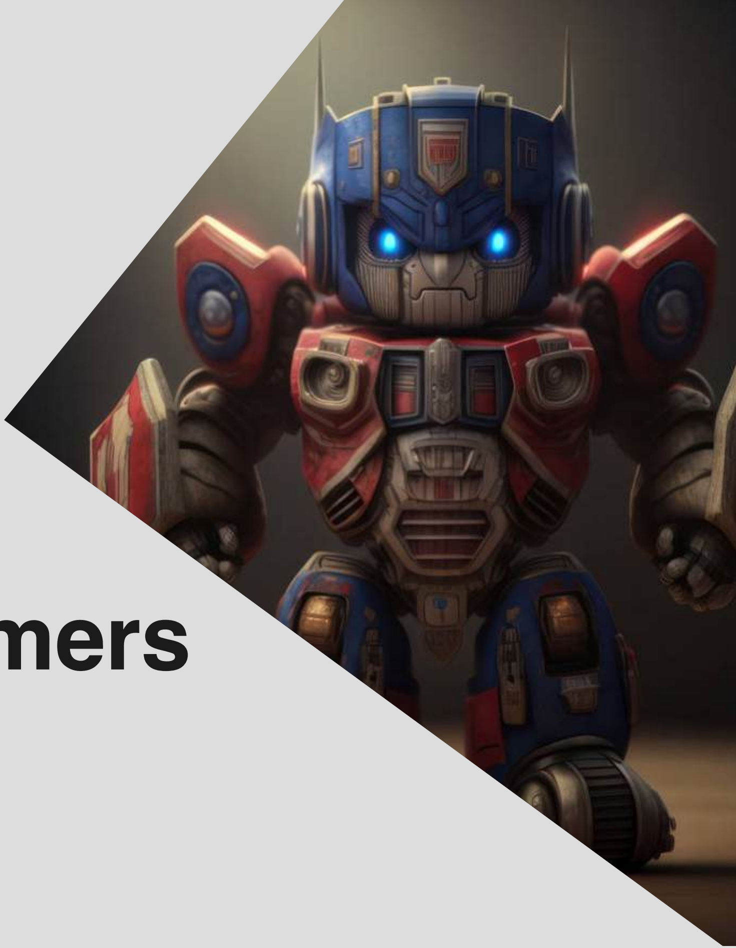
The Alan Turing Institute

# A perspective on the fundamentals of transformers

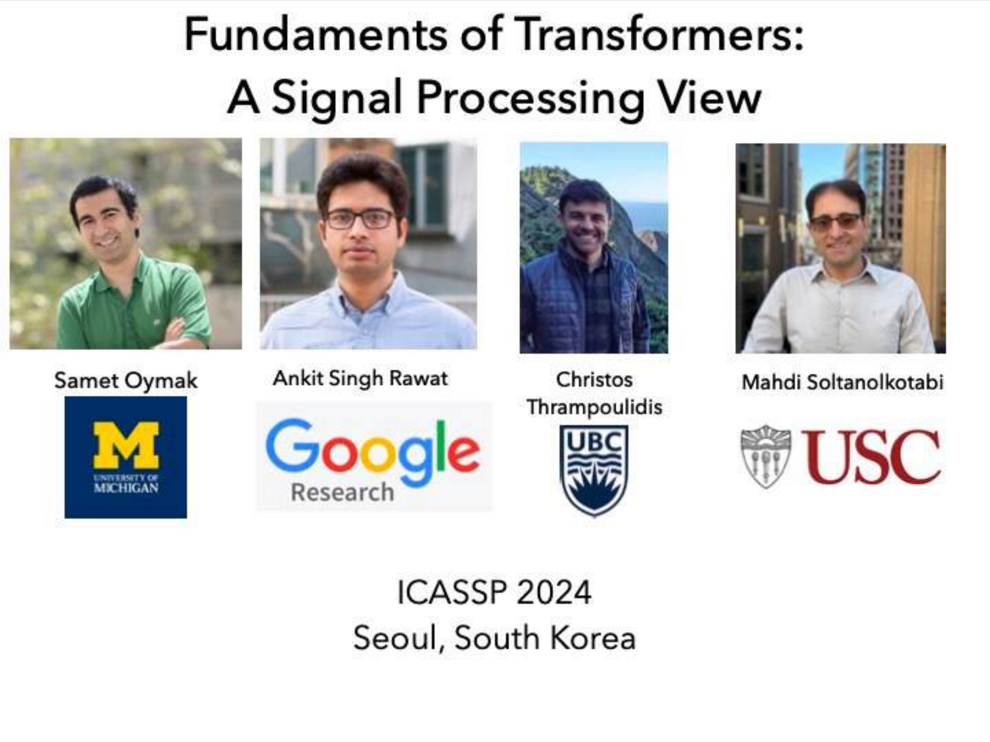


Edward Gunn, DARe

# Overview

- Transformers primer
- Optimisation
- Approximation
- Memorisation
- In-context learning

# Acknowledgements




[Link]

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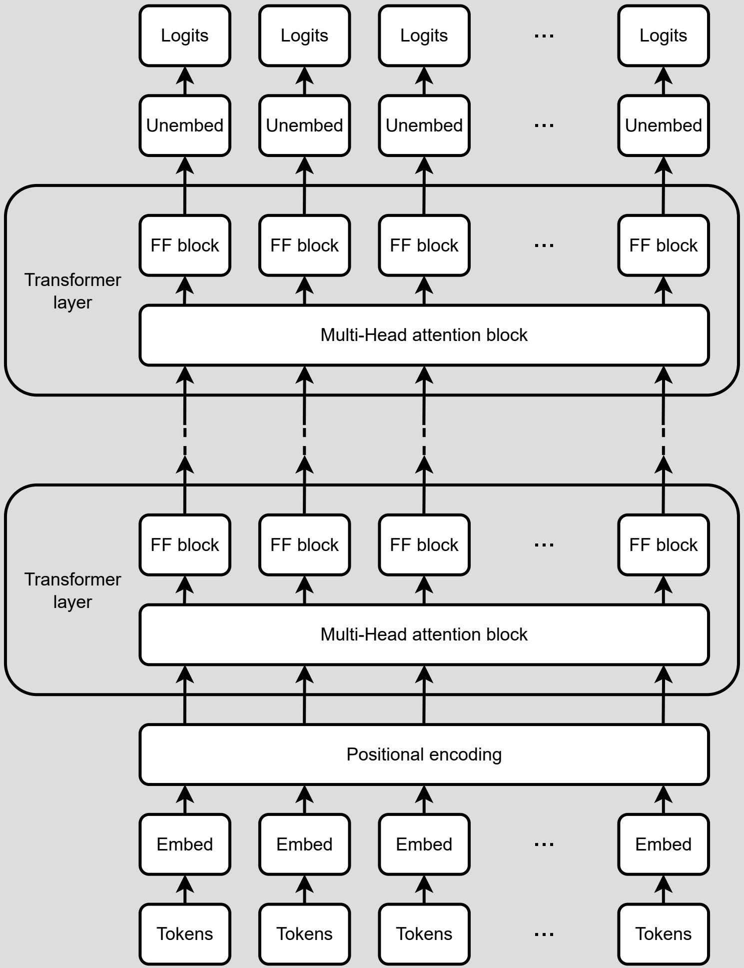
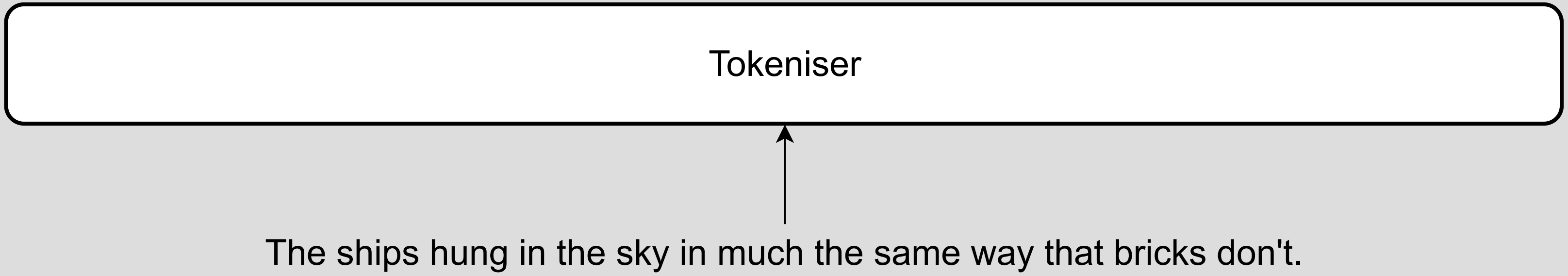
# Transformer




[Vaswani et al.'17]

# Tokenization



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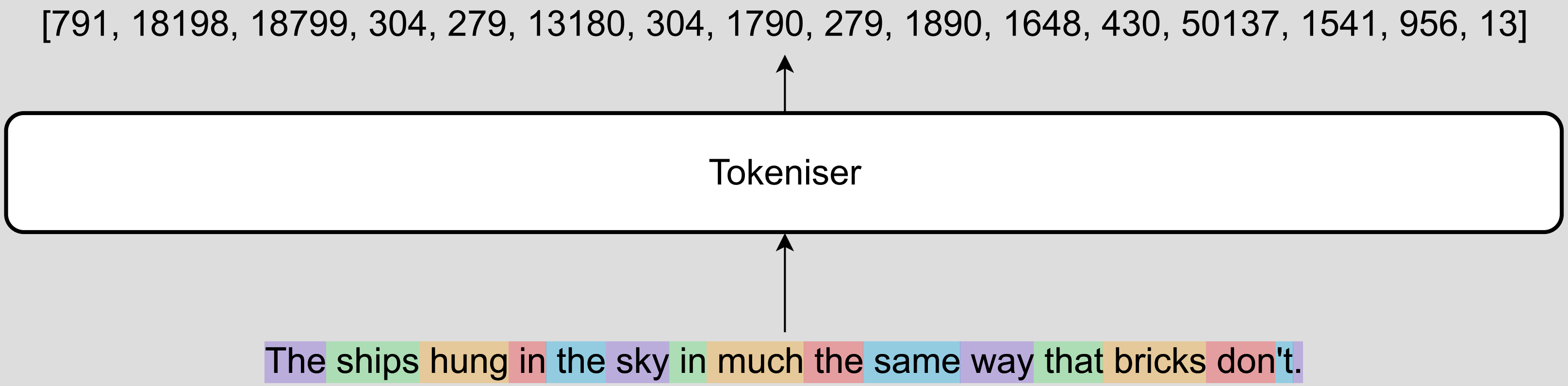

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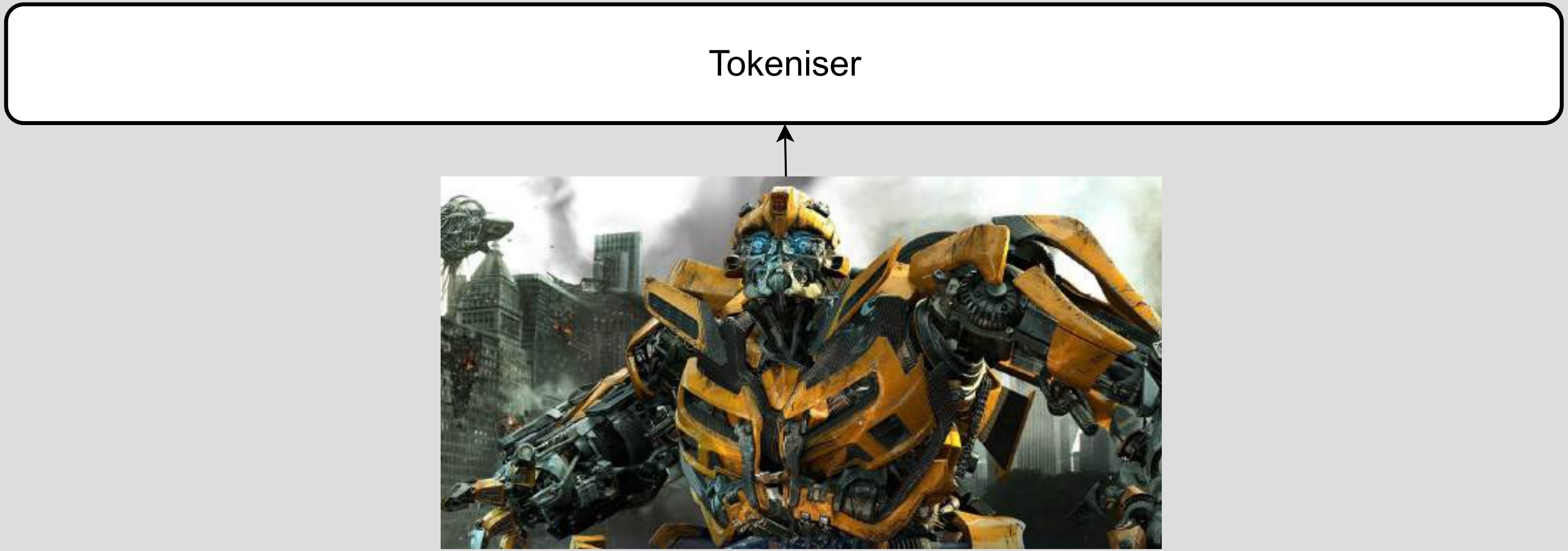

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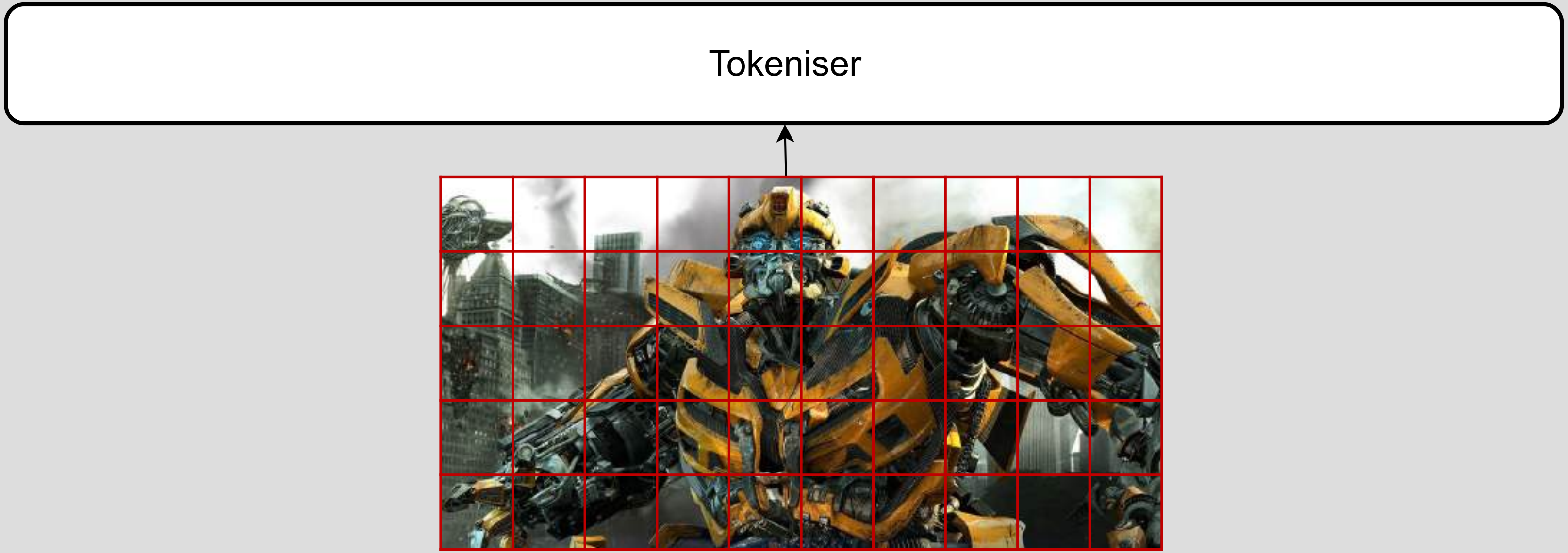

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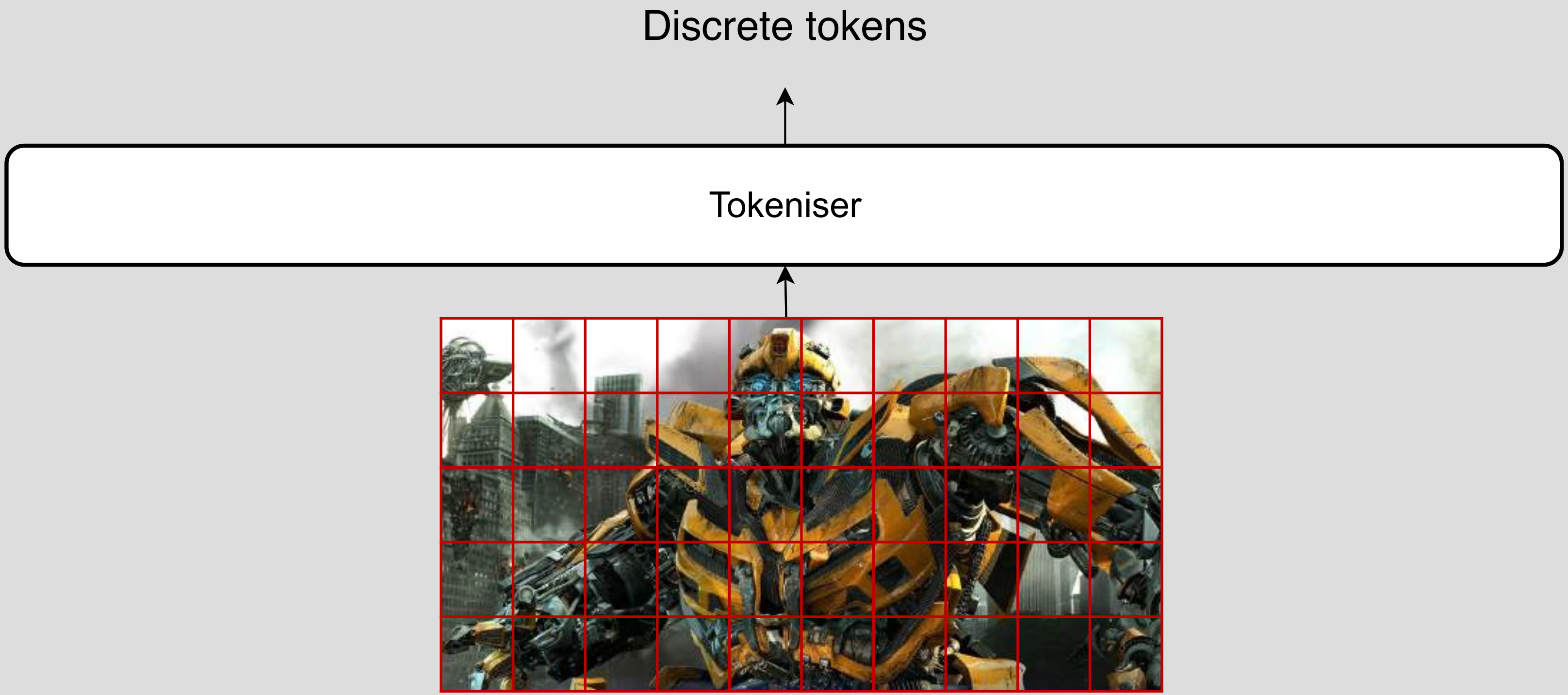
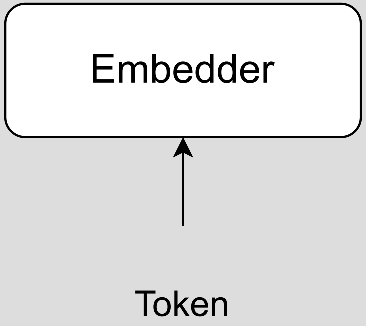


# Embeddings



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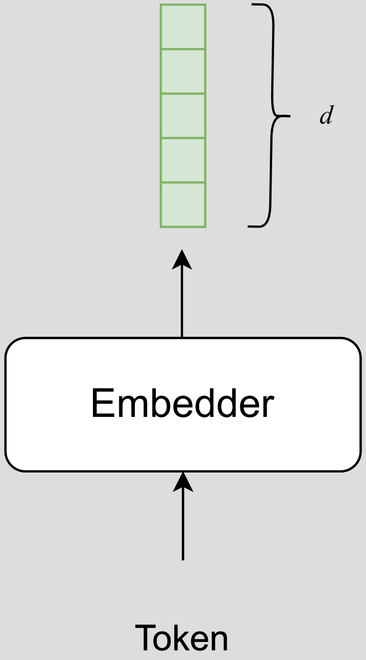

# Positional encodings

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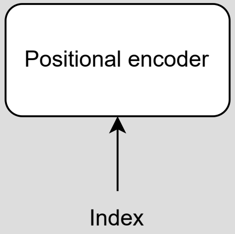

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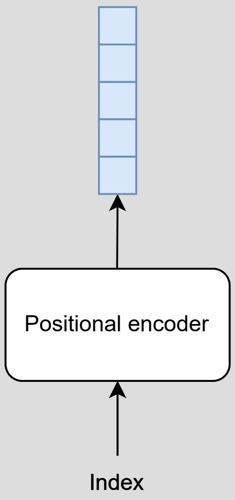

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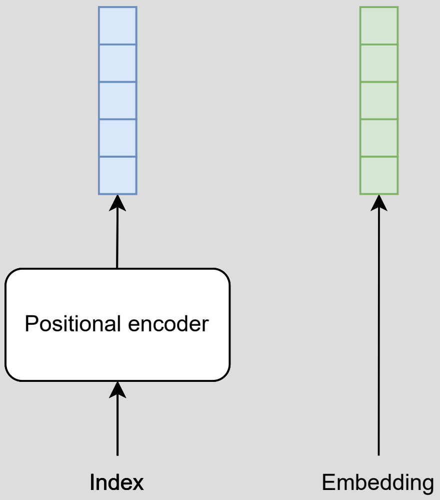

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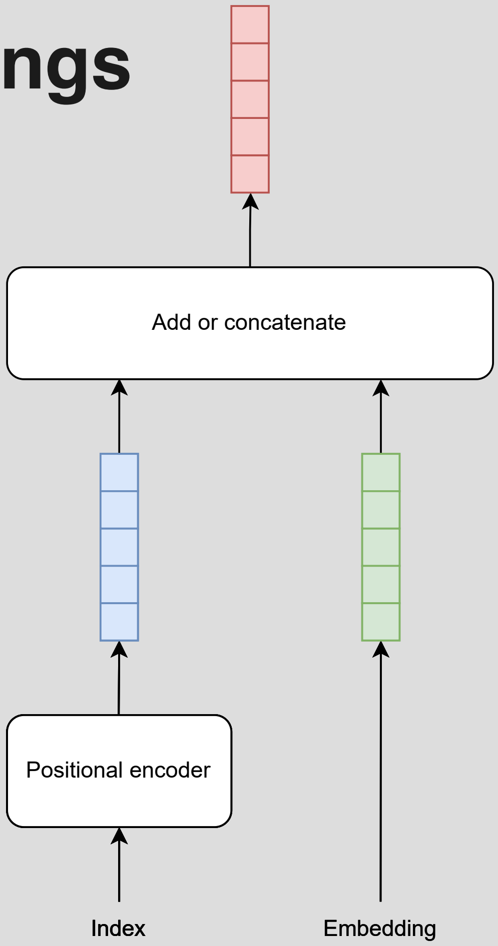
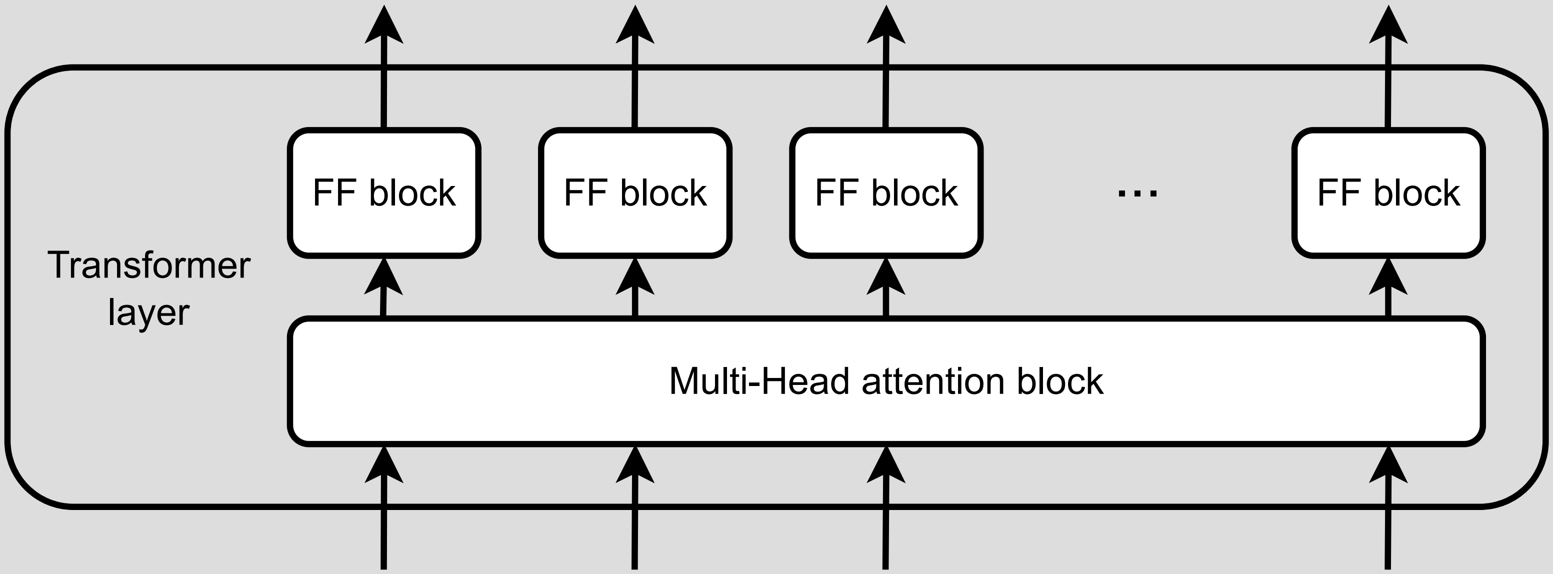


# Transformer layer




[Vaswani et al.'17]

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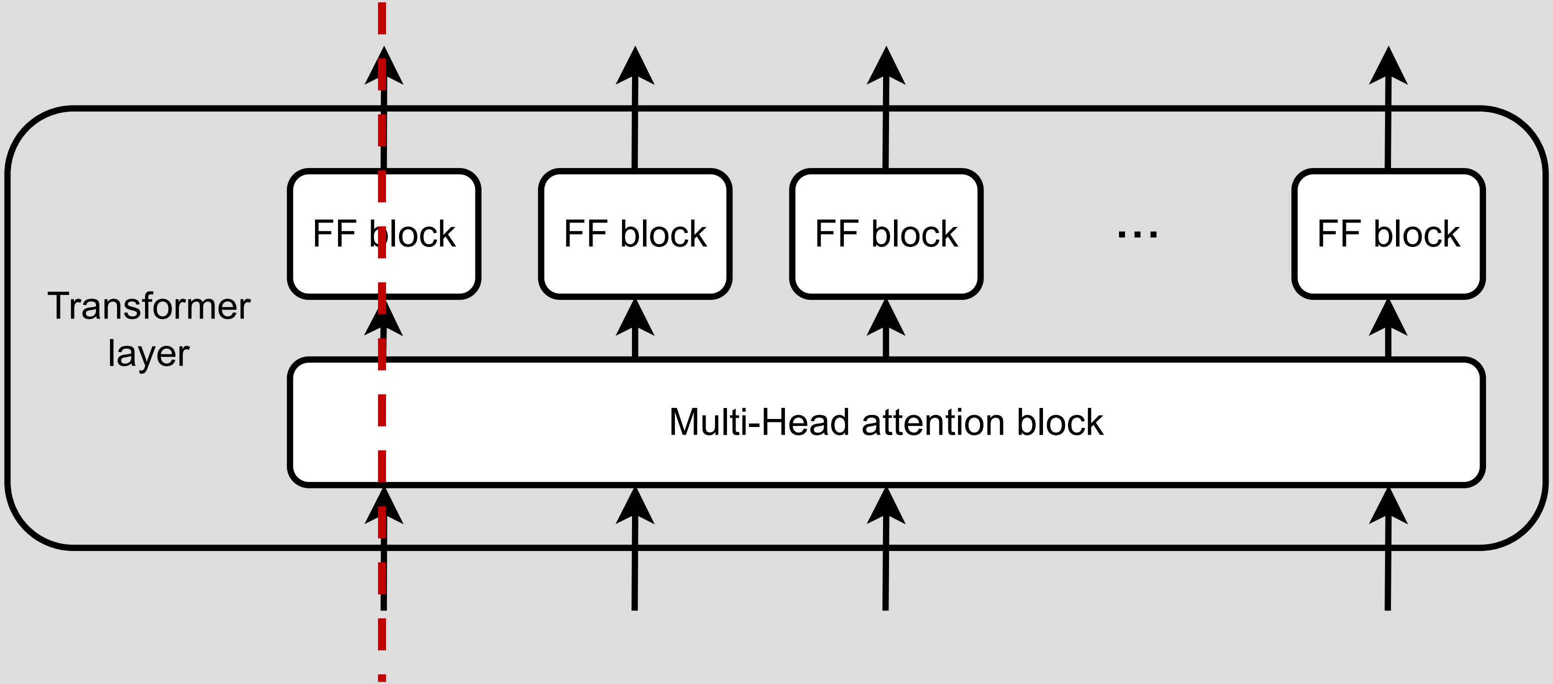


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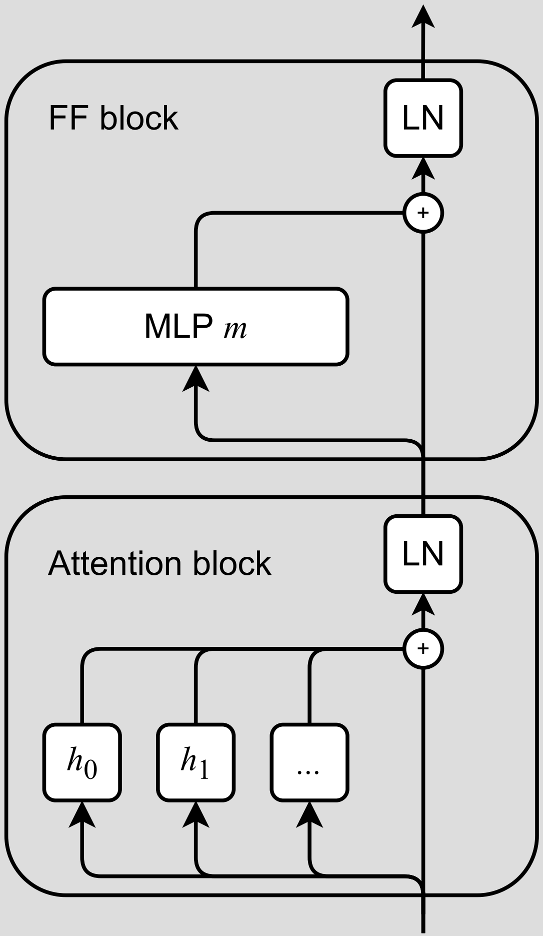


[Elhage et al.'21]

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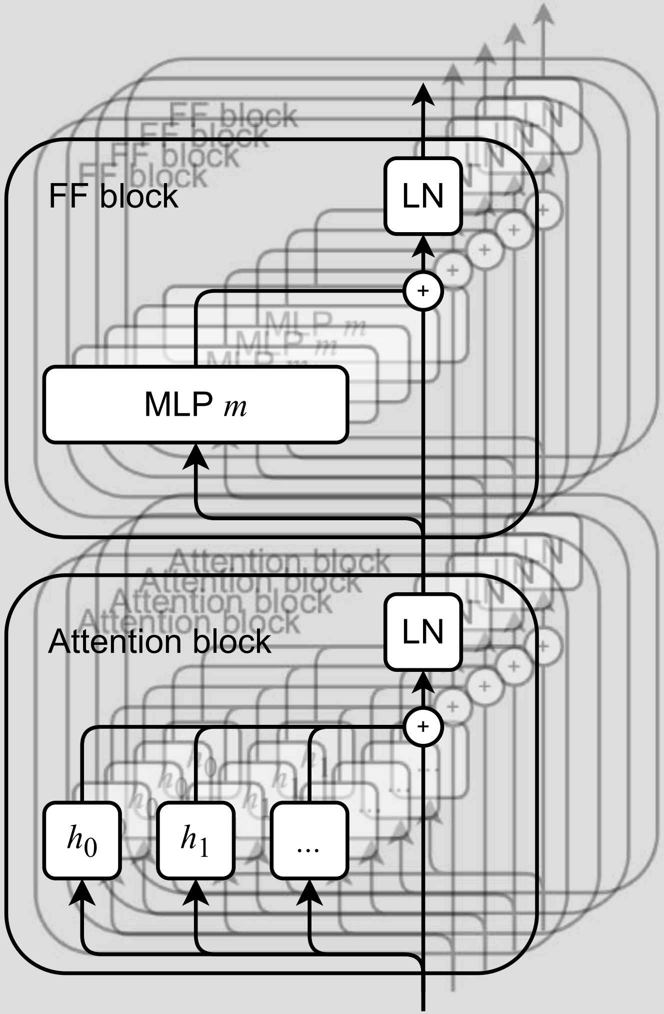


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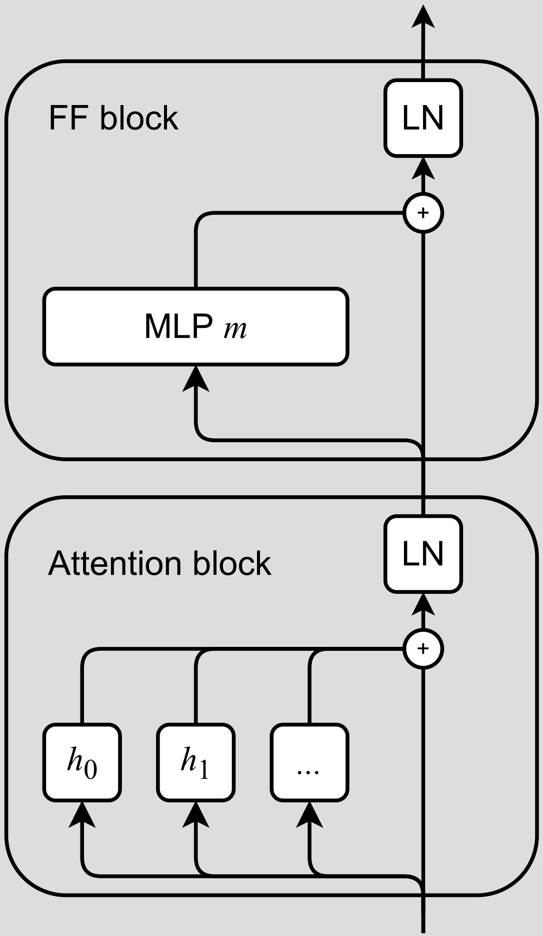


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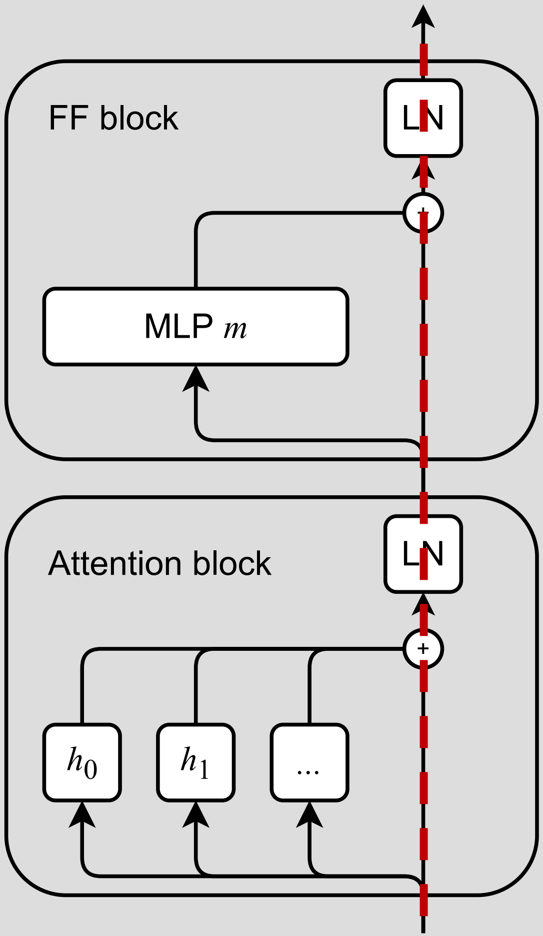


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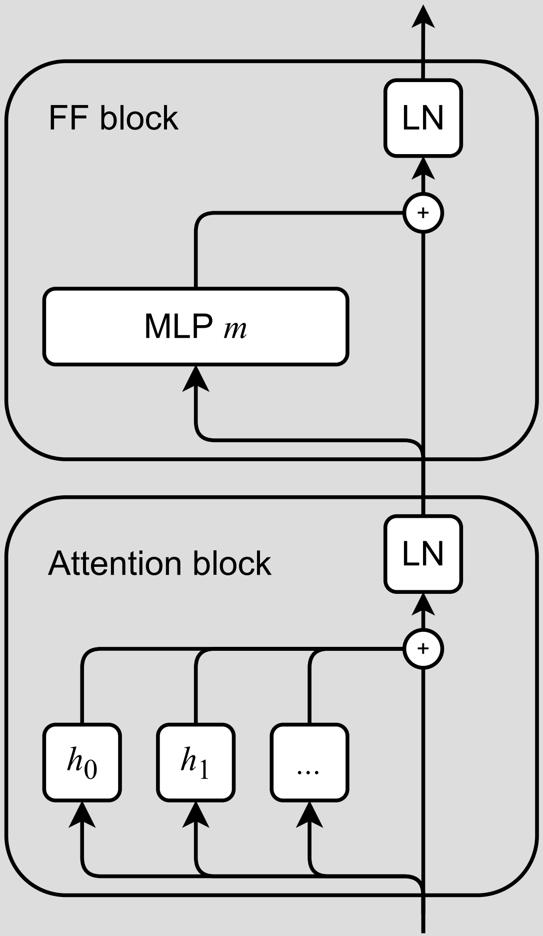


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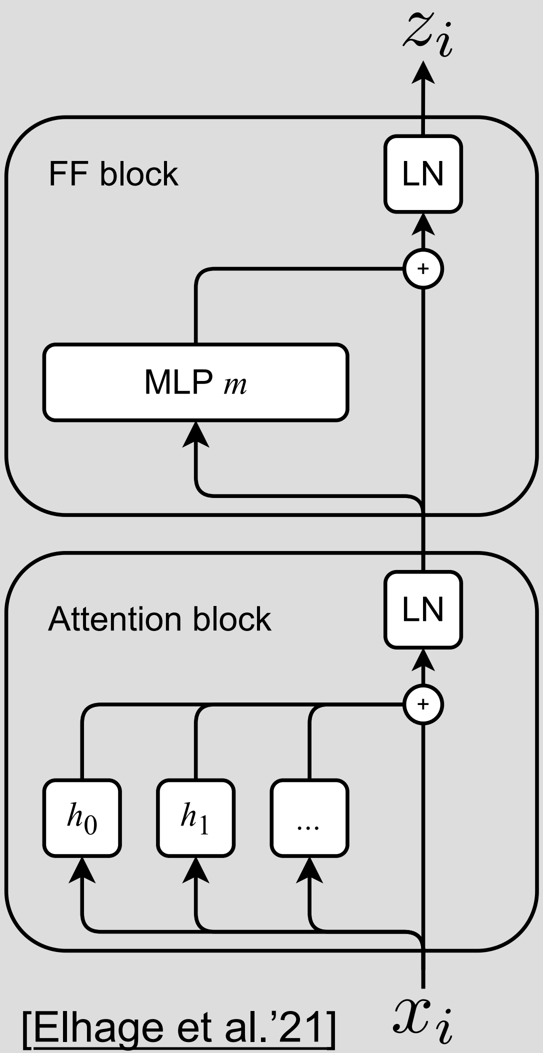
# Transformer layer

$$\hat{x}_i = \text{Attention}(X)$$
$$z_i = \text{FeedForward}(\hat{x}_i)$$

$$X = [x_1, x_2, \ldots, x_T]^\top$$



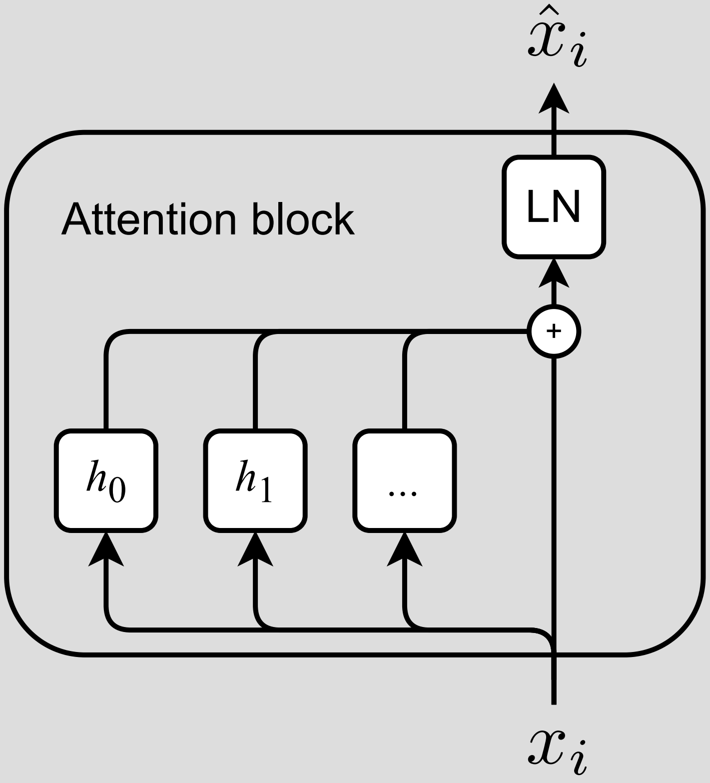

[Elhage et al.'21]

# Attention

$$\tilde{x}_i = x_i + \sum_{j=0}^{K} h_j(X)$$

$$\hat{x}_i = \mathrm{LN}(\tilde{x}_i)$$

$$X = [x_1, x_2, \ldots, x_T]^\top$$



# Attention heads $h$

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1. Compute the **value vector** for each token $x_i$

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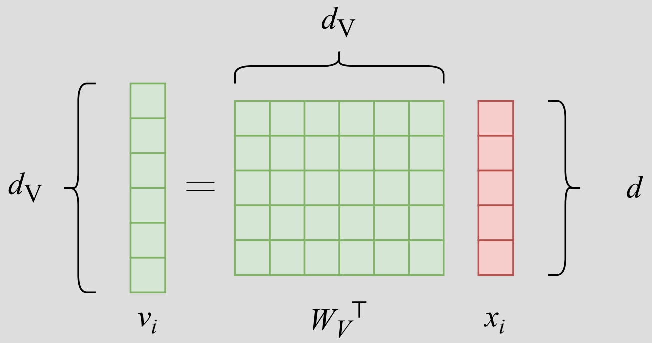

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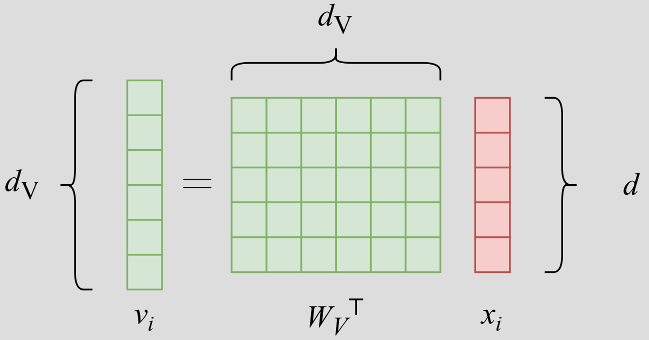


2. Compute the “result vector” by **linearly** combining value vectors according to the attention pattern

$$r_i = \sum_{j=1}^{T} A_{i,j} v_j$$

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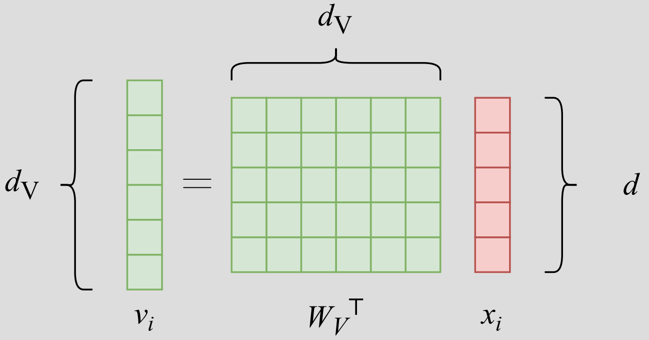


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3. Compute the output vector of the head for each token

$$h(X) = W_O r_i$$

$$X = [x_1, x_2, \ldots, x_T]^\top$$

# Attention patterns

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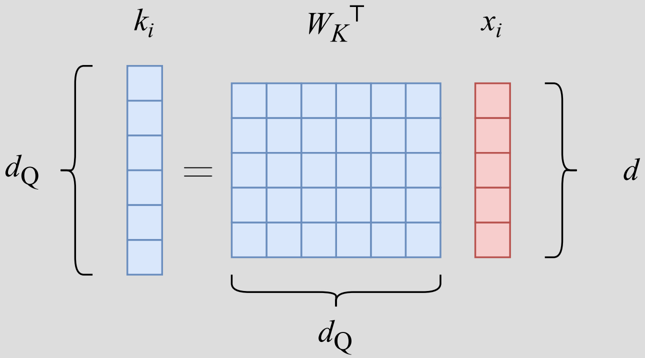

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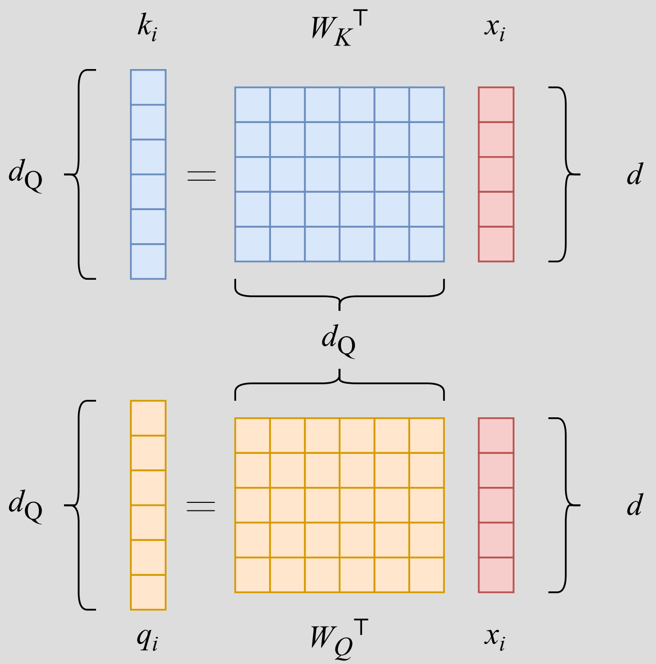

$\mathbb{S} = \mathrm{Softmax}$

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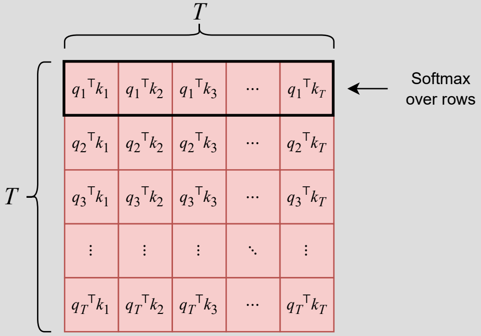
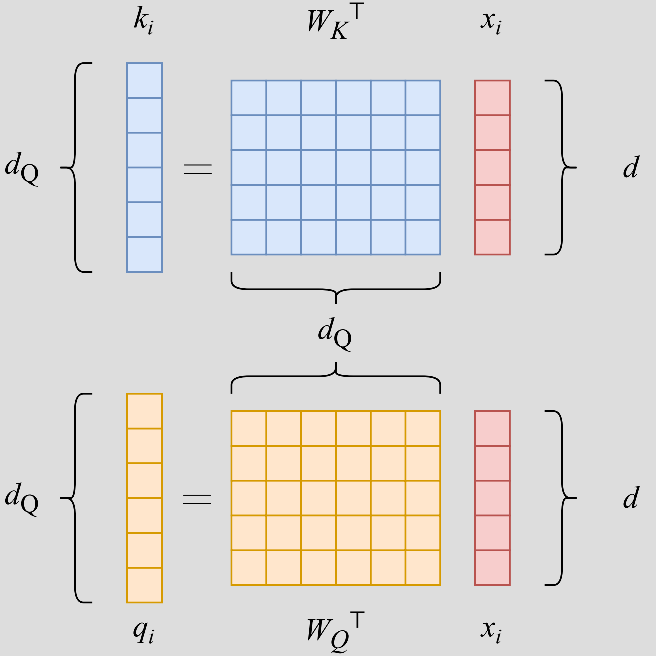
3. Take the **softmax**

$$A = \mathbb{S}(QK^\top)$$

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$$K = XW_K = [k_1, k_2, \ldots, k_T]^\top$$

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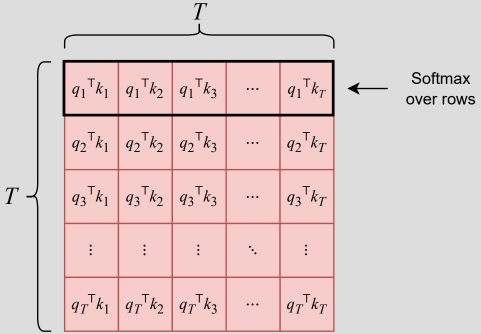
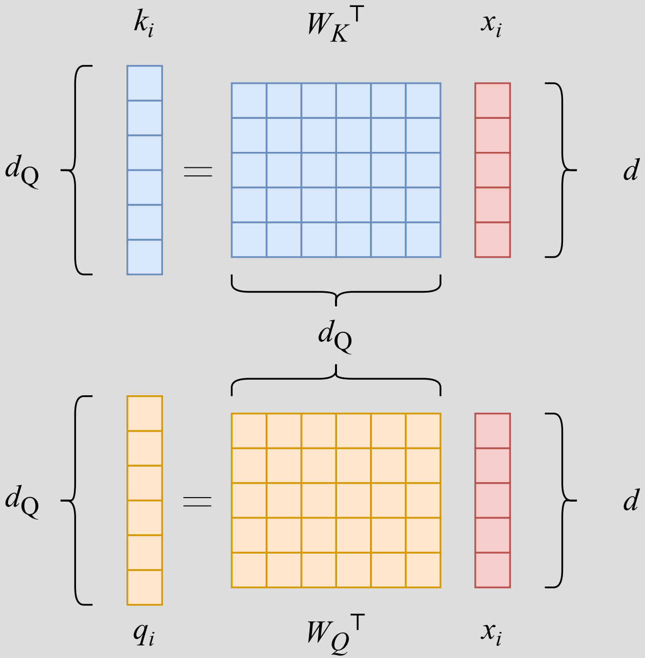



4. We can alternatively do it in one step

$$A = \mathbb{S}(XW_Q W_K^\top X^\top)$$

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$$T\left\{\overbrace{\begin{bmatrix} q_1{}^\top k_1 & q_1{}^\top k_2 & q_1{}^\top k_3 & \cdots & q_1{}^\top k_T \\ q_2{}^\top k_1 & q_2{}^\top k_2 & q_2{}^\top k_3 & \cdots & q_2{}^\top k_T \\ q_3{}^\top k_1 & q_3{}^\top k_2 & q_3{}^\top k_3 & \cdots & q_3{}^\top k_T \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ q_T{}^\top k_1 & q_T{}^\top k_2 & q_T{}^\top k_3 & \cdots & q_T{}^\top k_T \end{bmatrix}}^{T}\right.$$

← Softmax over rows

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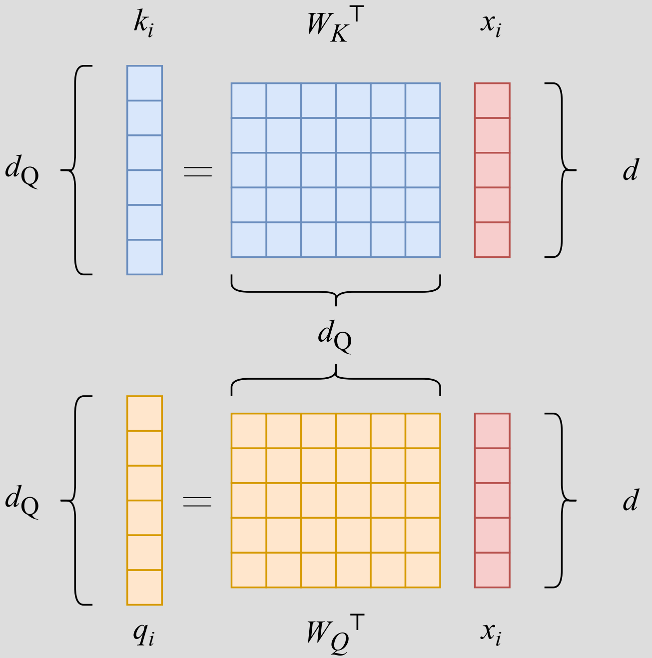


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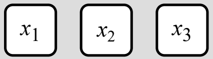

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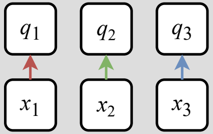

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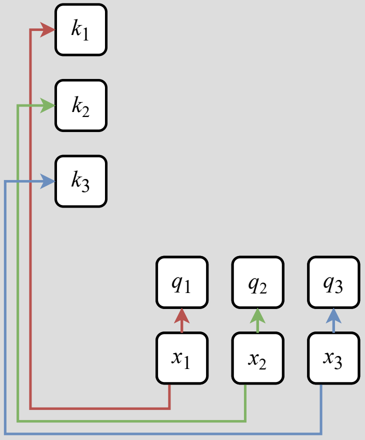

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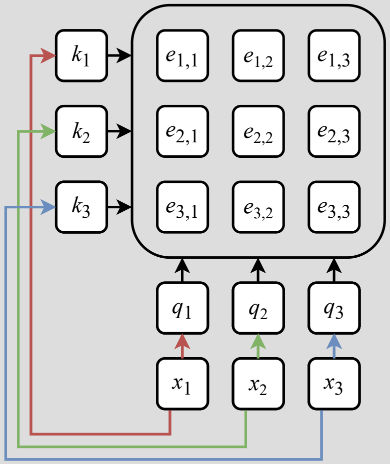

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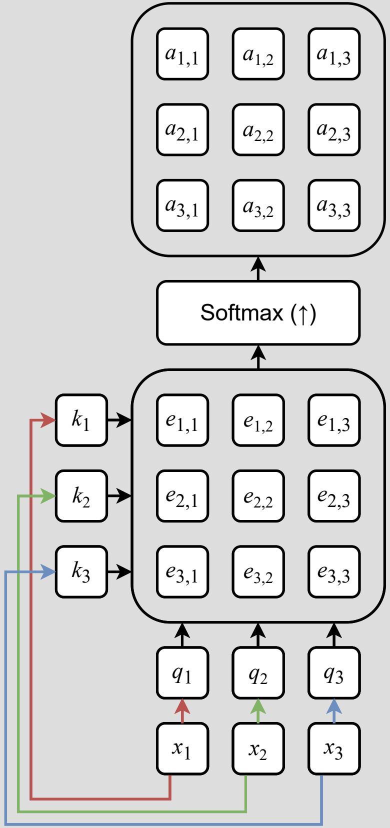
$$[a_{1,j}, \ldots, a_{T,j}] = \mathbb{S}([e_{1,j}, \ldots, e_{T,j}])$$

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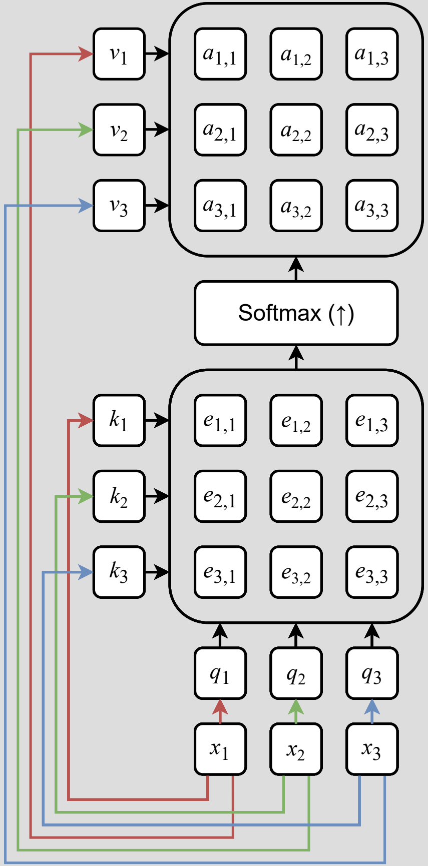


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$$\hat{x}_i = \sum_{j=1}^{T} a_{i,j} v_j$$

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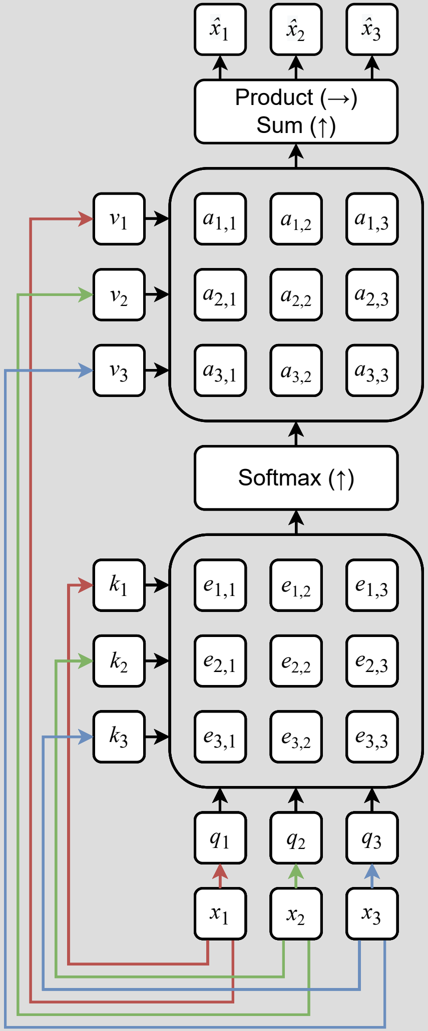

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- Putting it all together:

$$\hat{X} = \mathbb{S}(QK^\top)V$$

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$$\hat{X} = \mathbb{S}(QK^\top)V$$

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- In practice scale by dimension to avoid small gradients:

$$\hat{X} = \mathbb{S}(\frac{QK^\top}{\sqrt{d_k}})V$$

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# Overview

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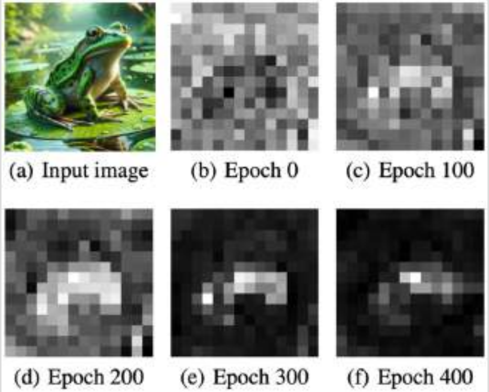
Optimiz prime

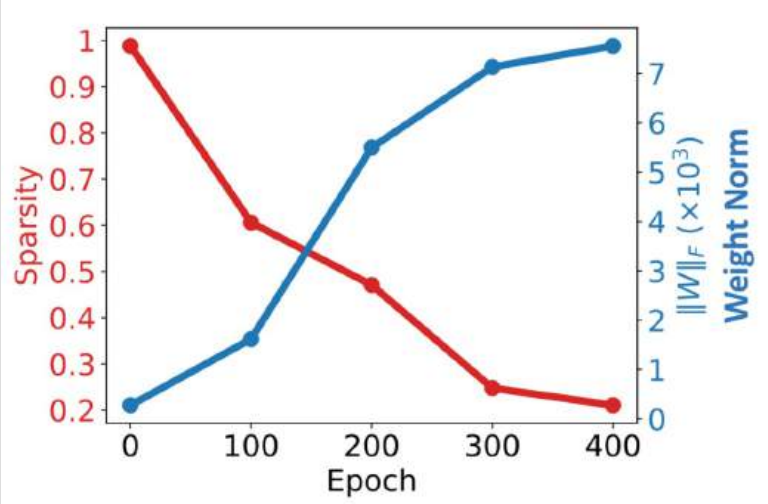
# Empirical motivations

1. Attention map is sparse

2. Attention map gets sparser as training evolves









3. Attention weights increase in norm

# Toy classification model

1. Classification: Map input sequence $X \in \mathbb{R}^{T \times d}$ to label $y \in \{-1, 1\}$

[Tarzanagh et al.'23b]

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    1. Read the token's last output: $x^{\mathrm{att}} = X^\top \mathbb{S}(XWz)$ (last token $z$)

[Tarzanagh et al.'23b]

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2. Prediction: $\hat{y}(X) = v^\top x^{\text{att}}$
3. Loss: $\ell$ strictly decreasing smooth loss (e.g. logistic)
4. Training objective:

$$\min_W \left\{ \mathcal{L}(W) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i \cdot v^\top x_i^{\text{att}}) \text{ where } x_i^{\text{att}} = X_i^\top \mathbb{S}(X_i W z_i) \right\}$$

[Tarzanagh et al.'23b]

# Gradient descent vs regularization paths

$$\mathcal{L}(W) = \frac{1}{n}\sum_{i=1}^{n} \ell\left(y_i \cdot v^\top X_i^\top \mathbb{S}(X_i W z_i)\right)$$

[Ji et al.'20]

# Gradient descent vs regularization paths

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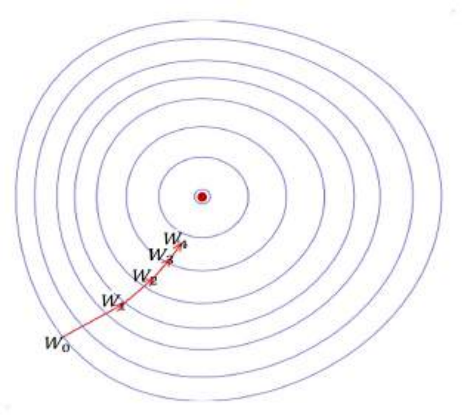


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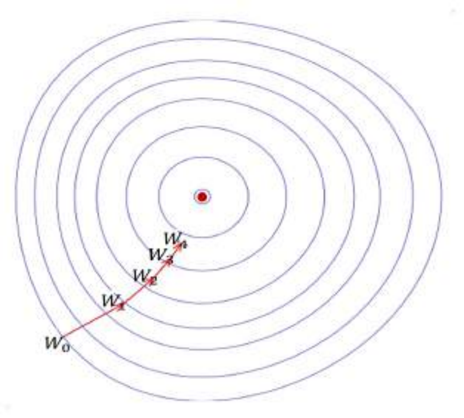


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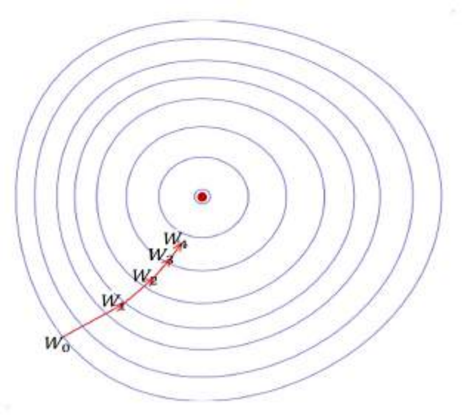

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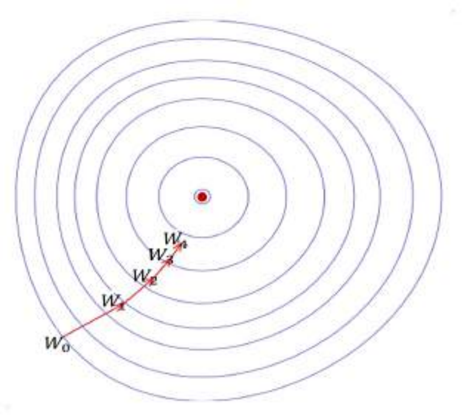


$$\lim_{k\to\infty} W_k = ???$$
$$\approx$$
$$\lim_{R\to\infty} W_R = ???$$

Regularization path proxy for GD

$$\text{Given } R > 0, \text{ find } d \times d \text{ matrix:}$$
$$\bar{W}_R = \arg \min_{\|W\|_F \le R}$$

[Ji et al.'20]

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- So **necessarily** $\|W\| \to \infty$

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$$x^{\text{att}} = \sum_{t=1}^{T} s_t \cdot x_t \text{ where } s_t = \mathbb{S}(XWz)_t$$

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The optimal softmax choice is to select token with the largest score!

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But which one do GD and RP select?

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Weights go to ∞, but the direction converges to SVM solution!

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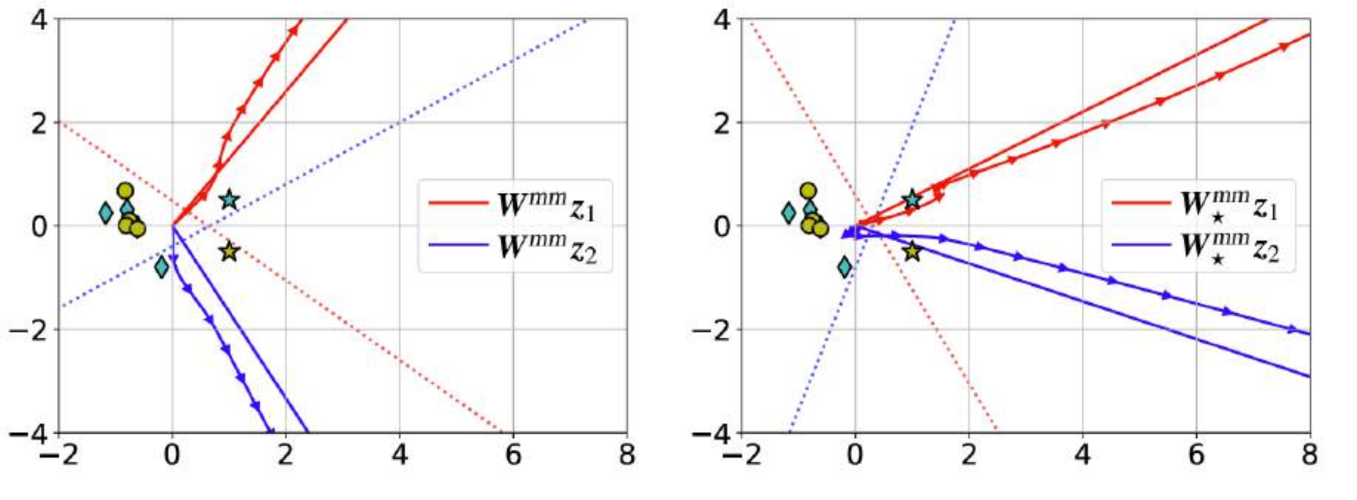


(a) $\boldsymbol{W}$-parameterization (b) $(\boldsymbol{K}, \boldsymbol{Q})$-parameterization

Arrows represent GD trajectory
Solid lines are SVM solution
Dotted lines represent separating hyperplanes

[Tarzanagh et al.’23b]

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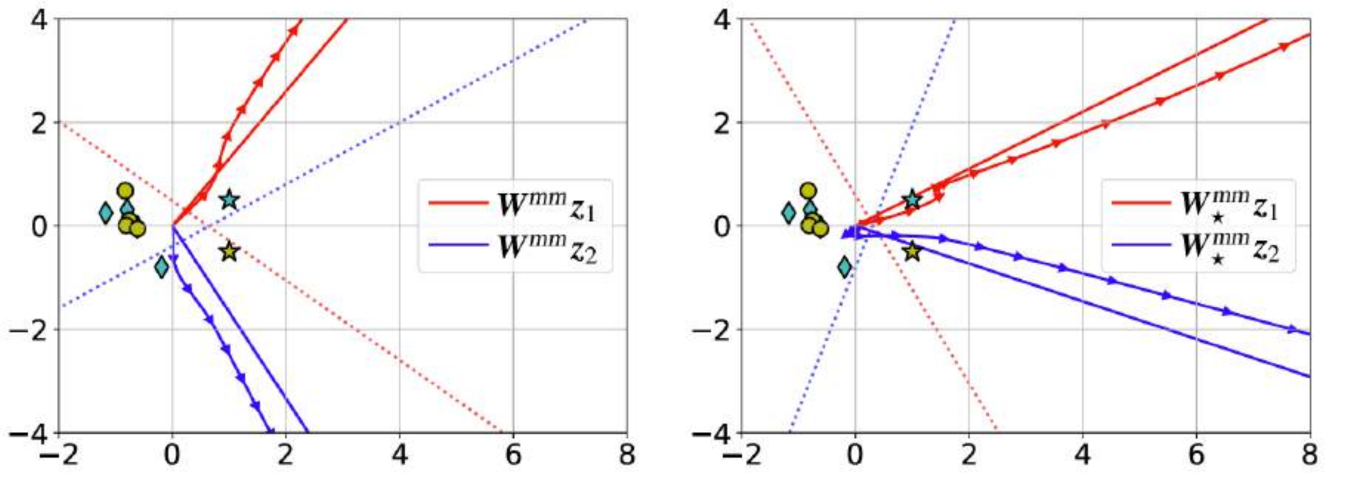


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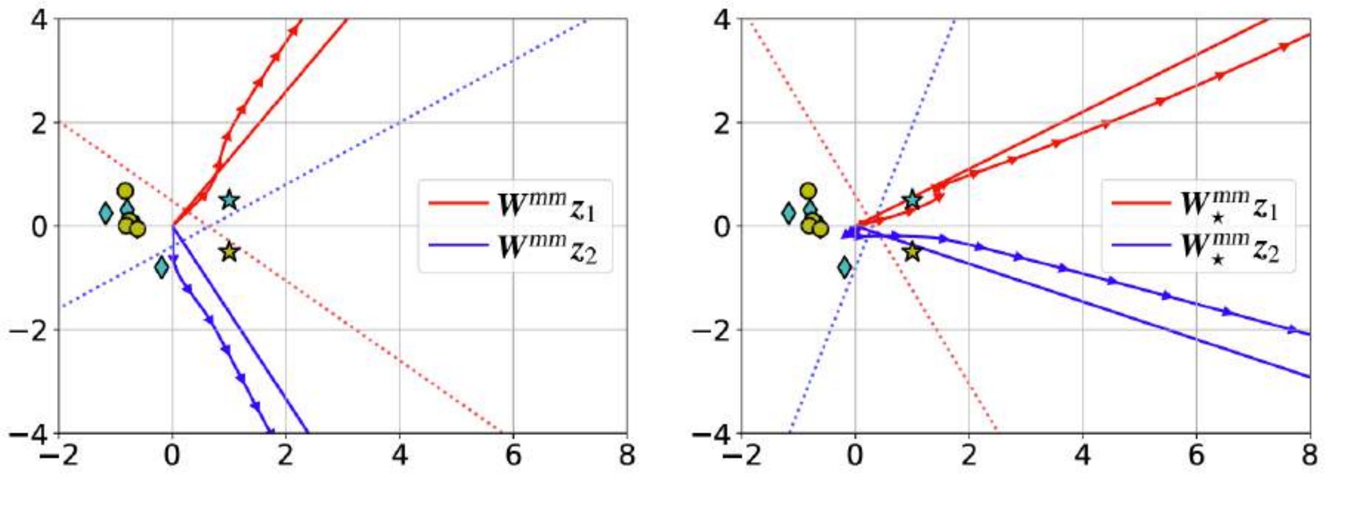


(a) $W$-parameterization (b) $(K, Q)$-parameterization

Weights diverge
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# Initialization dependence

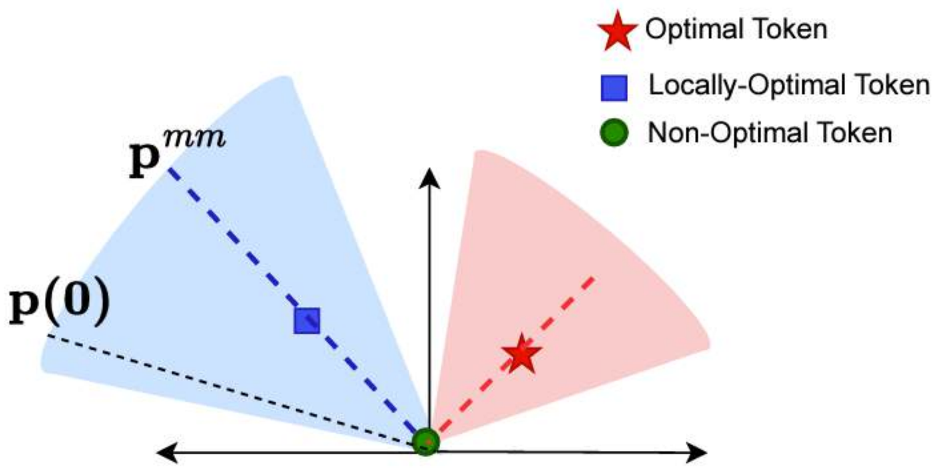


Figure 2: Gradient descent initialization $\boldsymbol{p}(0)$ inside the cone containing the locally-optimal solution $\boldsymbol{p}^{mm}$.

[Tarzanagh et al.'23a]

# Better models

What if the decoder is nonlinear? Or there is more than two classes?

[Tarzanagh et al.’23b]

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- $\mathcal{R}_i$ the set of optimal tokens per sequence $i$

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Conjecture: $W_k \approx W^{fin} + C_k W^{\mathrm{mm}}$ with $C_k \to \infty$

- $W^{\mathrm{mm}}$ : Directional component that diverges to infinity
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[Tarzanagh et al.'23b]

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# Faster optimizers

[Vasudeva et al.'24]

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Theorem (VDT24) (Informal) Assume nearly-orthogonal tokens and sub-optimal tokens. $x_{i,t}$ have equal scores $v^\top x_{i,t} = v^\top x_{i,t'}, \forall t, t' \neq \mathrm{opt}_i$. Then, NGD and Polyak-step both converge globally to Att-SVM with fast rate:

$$\left\langle \frac{W_k}{\|W_k\|}, \frac{W^{\mathrm{mm}}}{\|W^{\mathrm{mm}}\|} \right\rangle \geq 1 - C\frac{\log^2(k)}{k}$$

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# Overview

- Transformers primer
- Optimisation
- **Approximation**
- Memorisation
- In-context learning

Approximus prime?

# Goal of approximation

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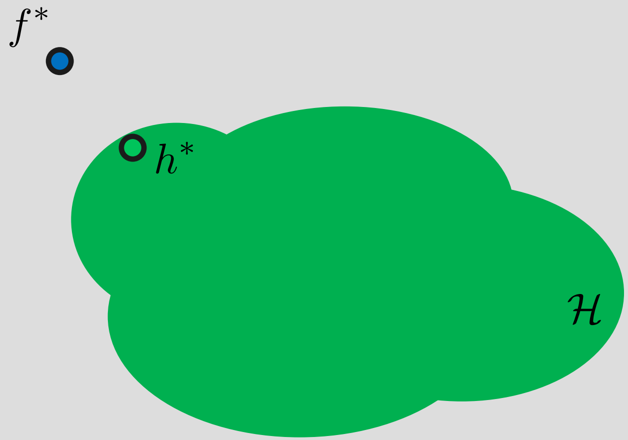

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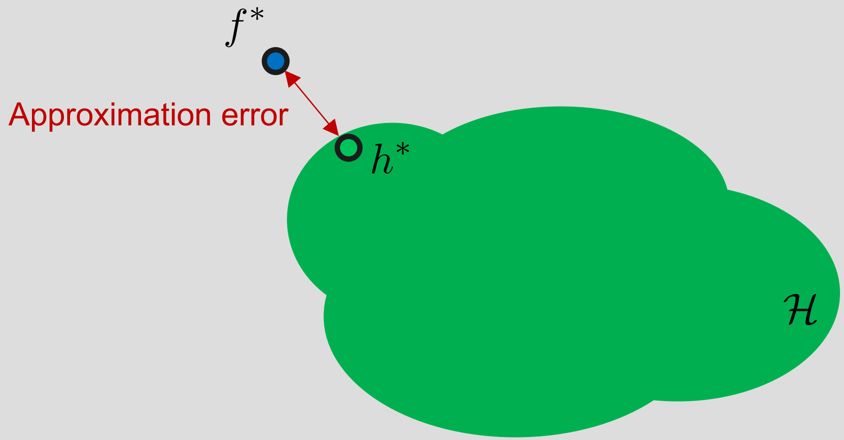

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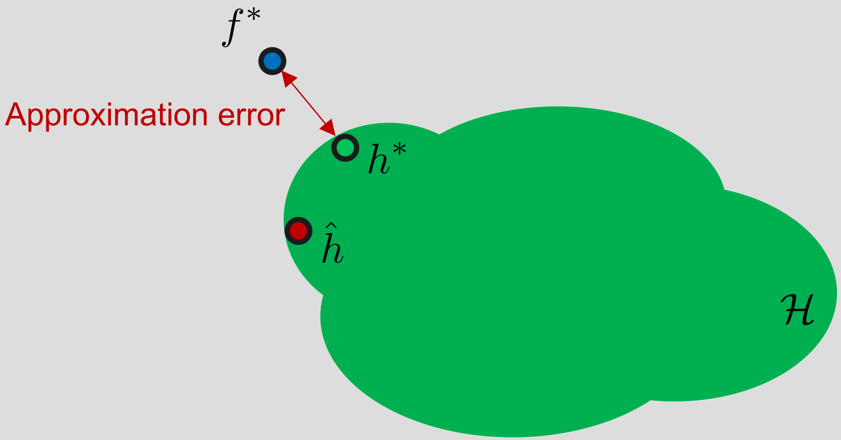

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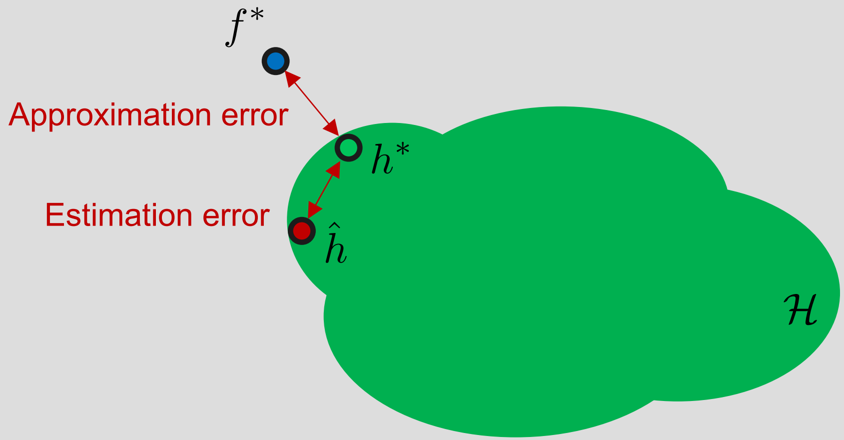

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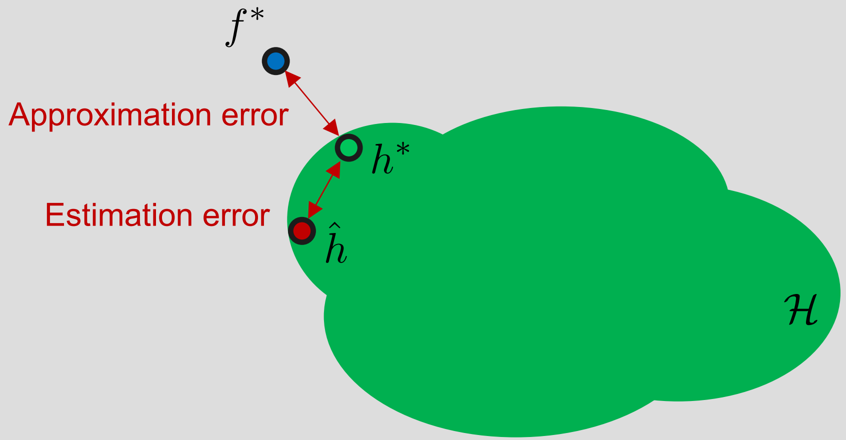

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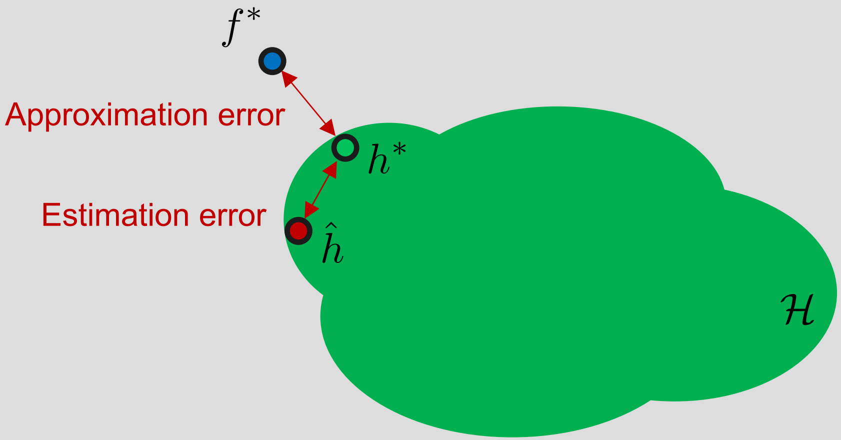

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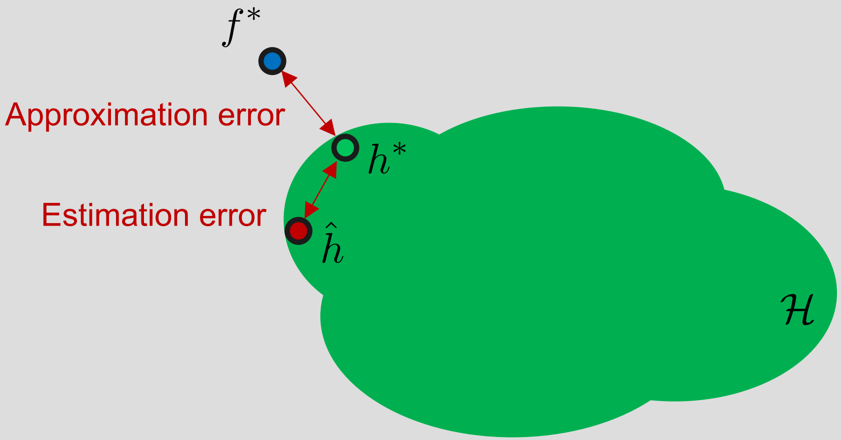

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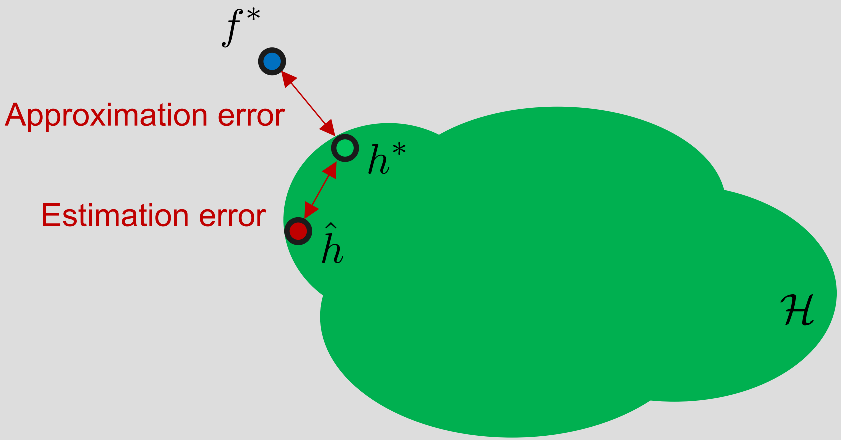
Universal approximation

Given $\epsilon > 0$ and any $f^* \in \mathcal{C}$, there exists $h \in \mathcal{H}$ such that the approximation error $D(h, f^*) \leq \epsilon$



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**Theorem 2 [Yun et al.'19]:** Transformer networks with constant width and large enough depth can universally approximate $\mathcal{C}$. In particular, for any given $\epsilon > 0$ and $f^* \in \mathcal{C}$, there exists an $h \in \mathcal{H}$ satisfying

$$D_p(h, f^*) := \left( \int \|h(X) - f^*(X)\|_p^p \, dX \right)^{1/p} \leq \epsilon$$

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**Theorem [Kajitsuka & Sato'23]:** For any given $\epsilon > 0$ and $f^* \in \mathcal{C}$, there exists an $h \in \mathcal{H}$ With **one layer** and **single-head attention** such that the following holds:

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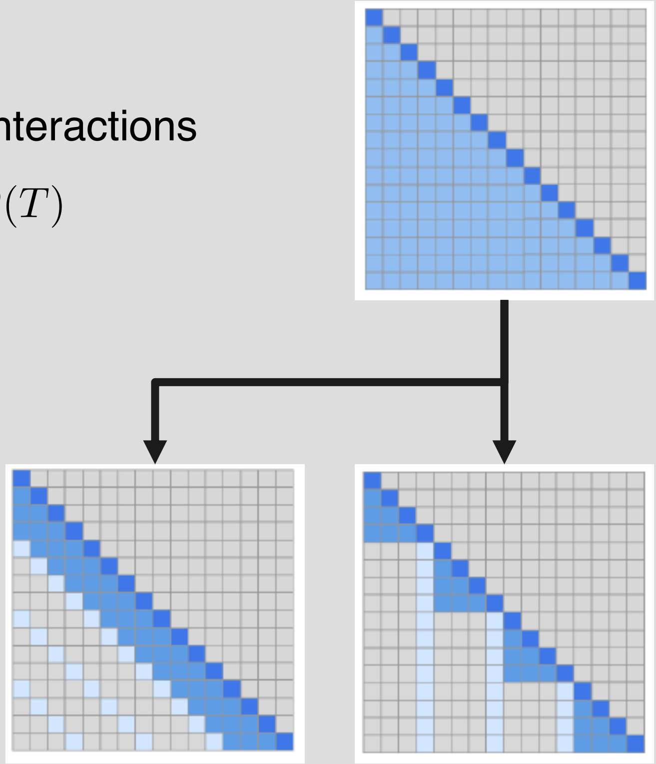

Strided

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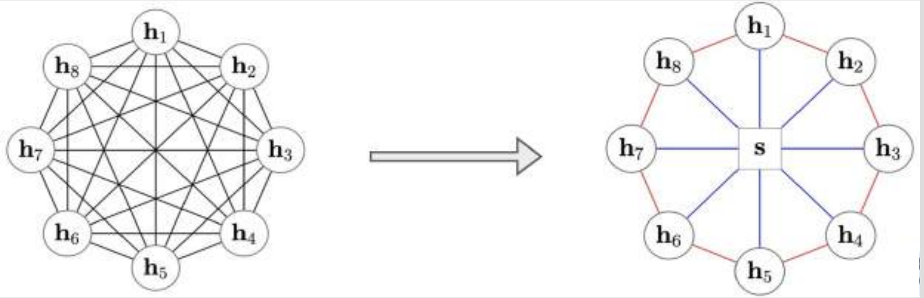


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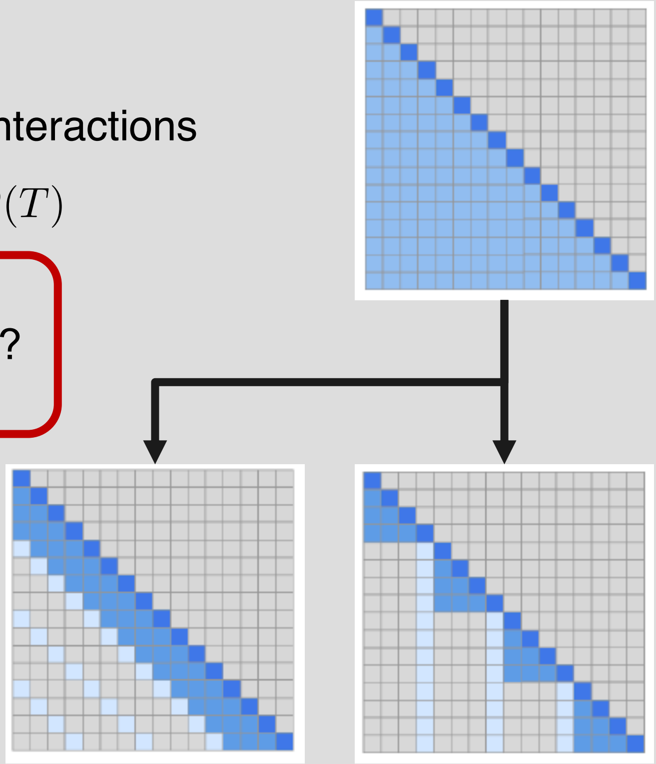
Can sparse transformers be universal approximators?
- If so, what are the requirements on the sparsity pattern?
- How sparse can attention be?

Transformer



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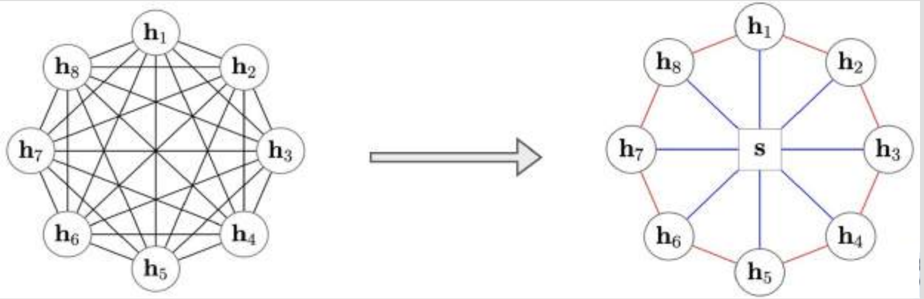


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**Corollary.** There are sparse Transformers with $\mathcal{O}(T)$ connections per attention layer that are universal approximators ([Guo et al.'19, Beltagy et al.'20, Zaheer et al.'20])

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  - E.g., memory-augmented NLP models
- **Hopfield networks:** A model for memorization via neural networks
  - Can shed light on memorization mechanism in many existing architectures, e.g., Transformers
  - Can provide a framework to design/analyze iterative model architectures

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[Blog]
[Hopfield ’82]

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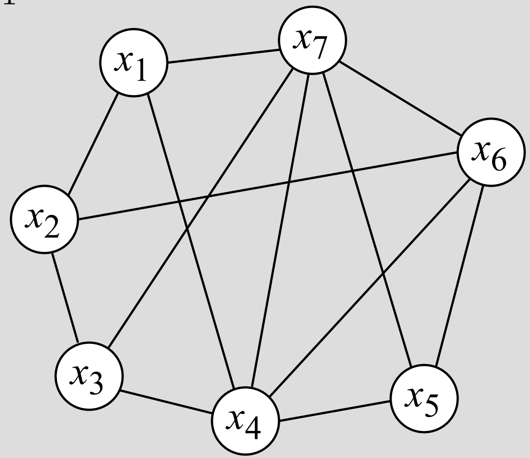

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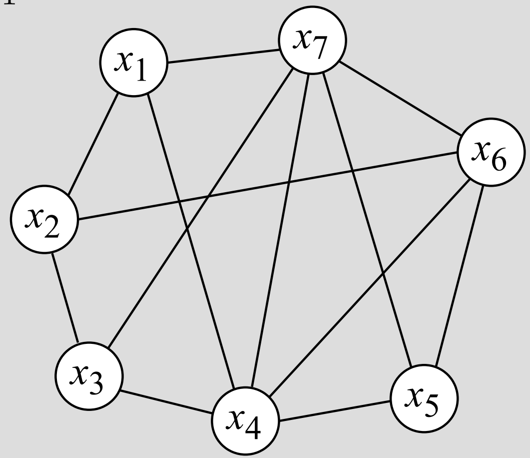

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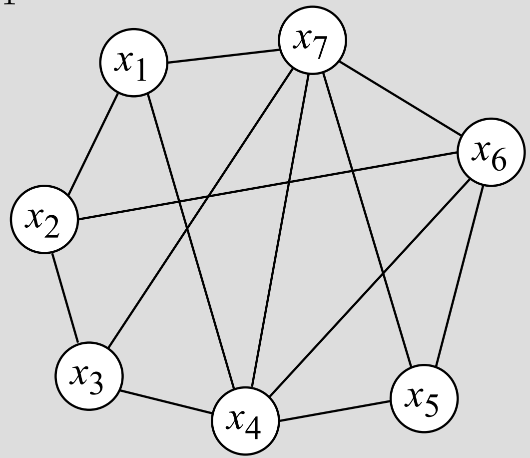

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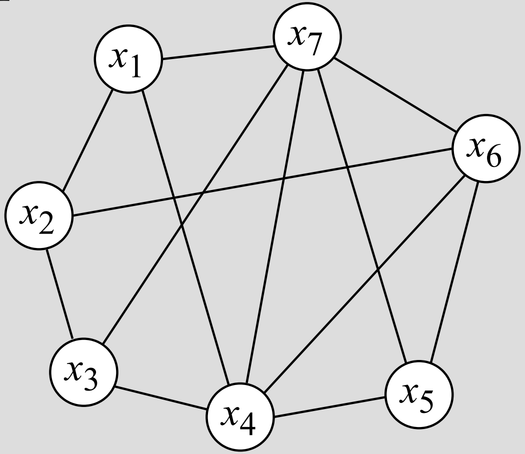

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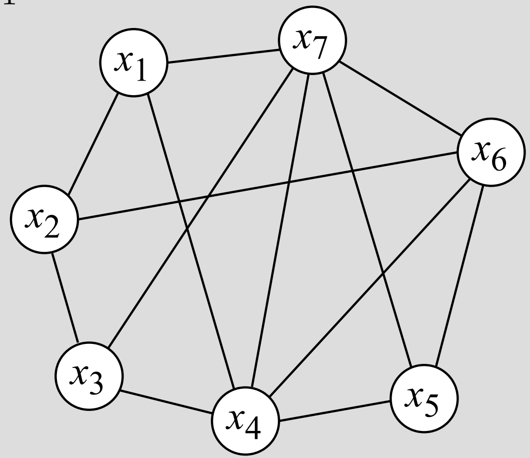

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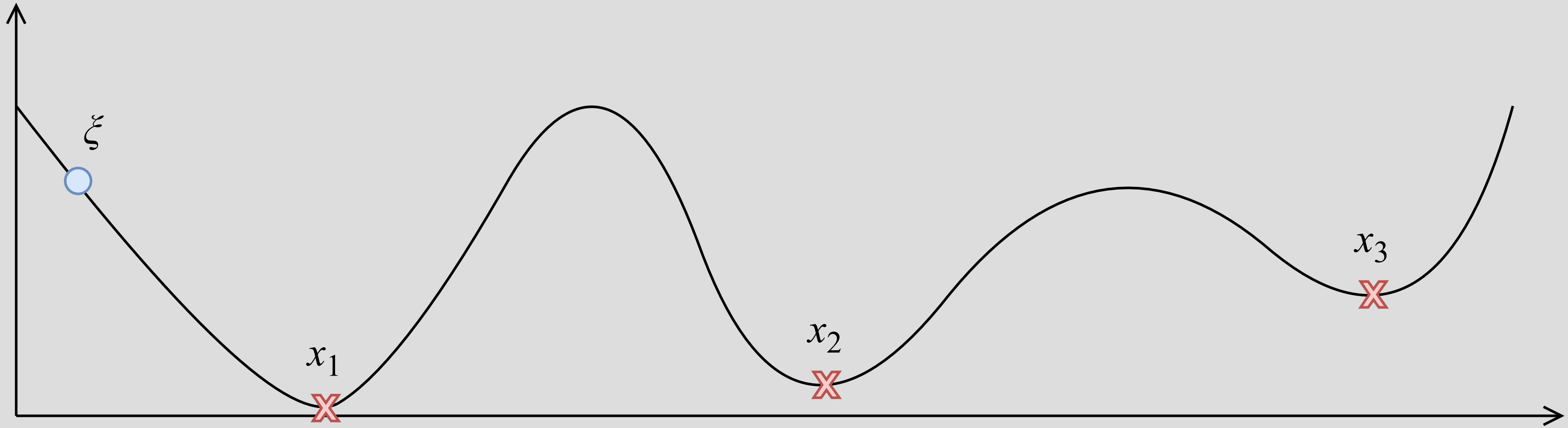

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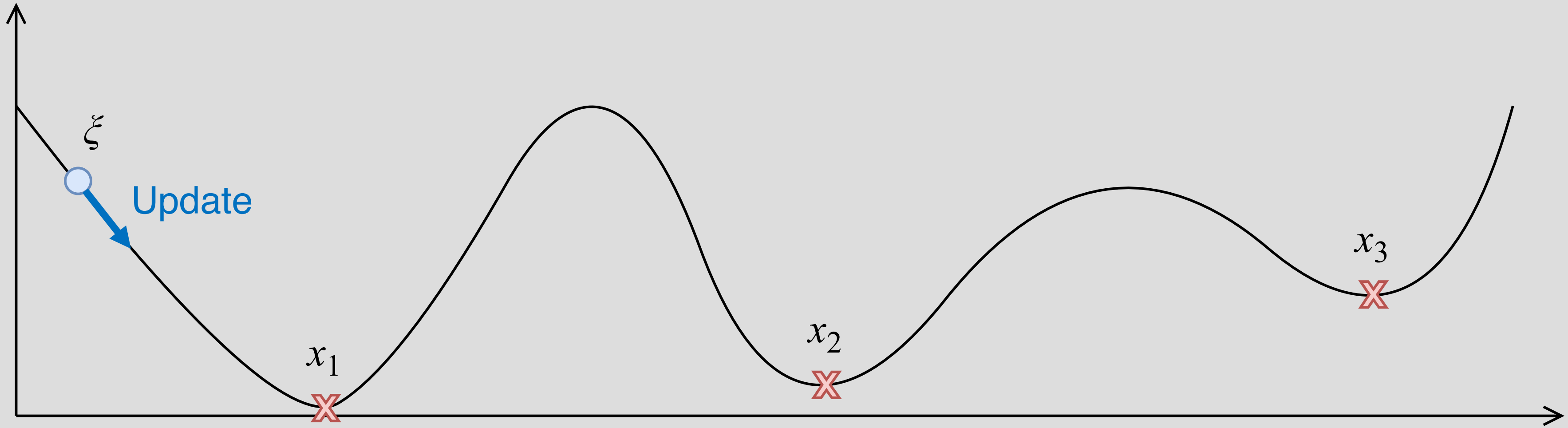

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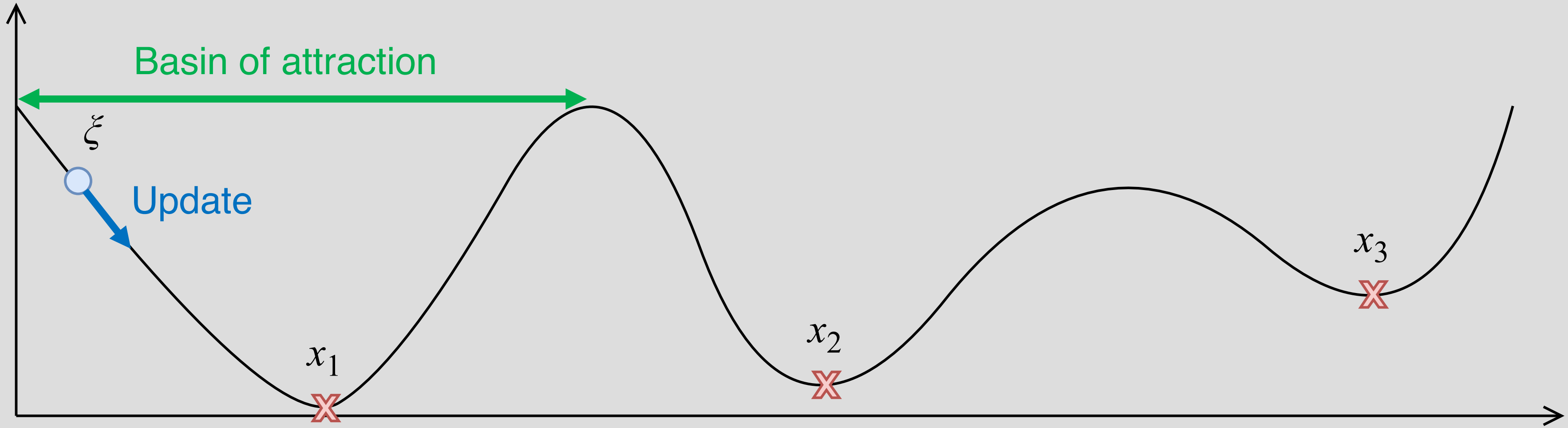

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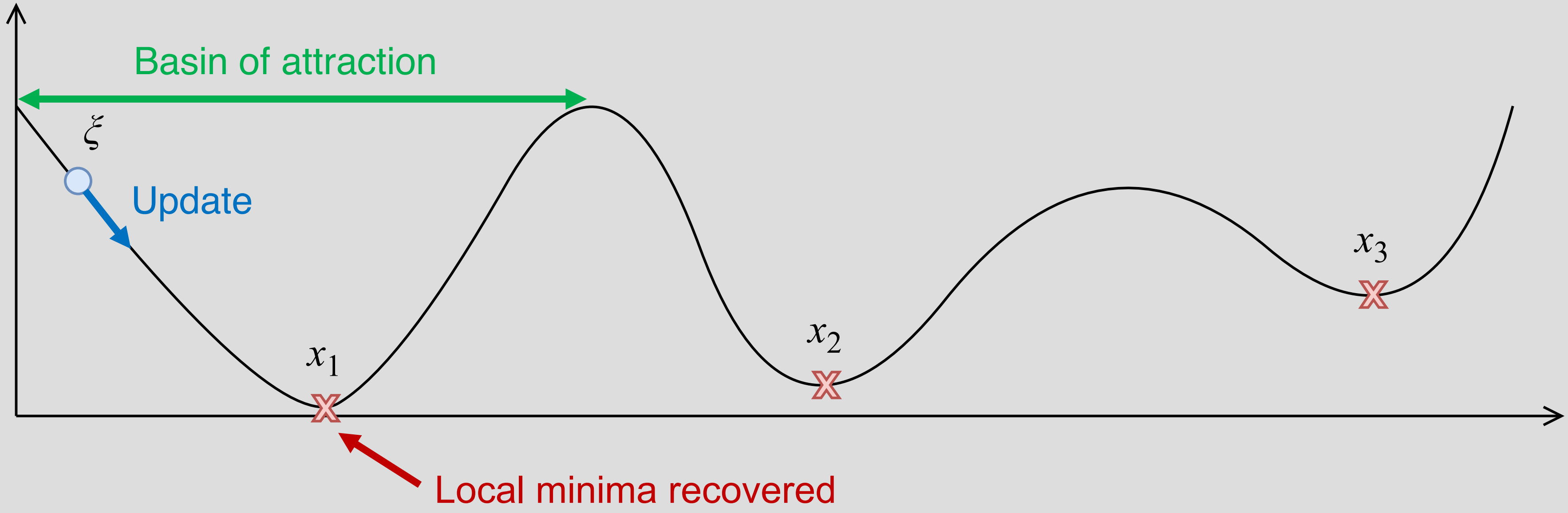

# Example

[Blog]

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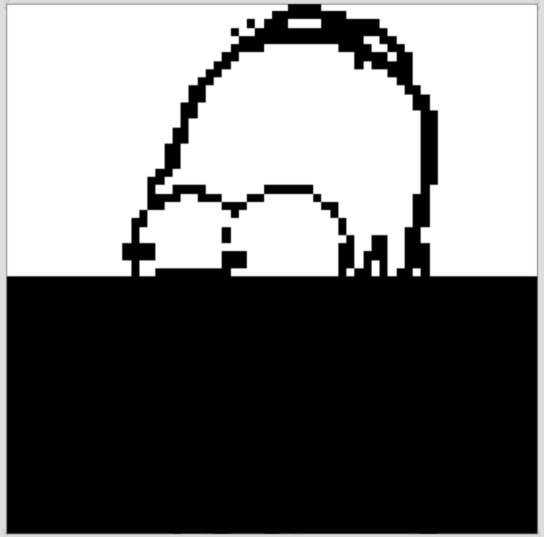

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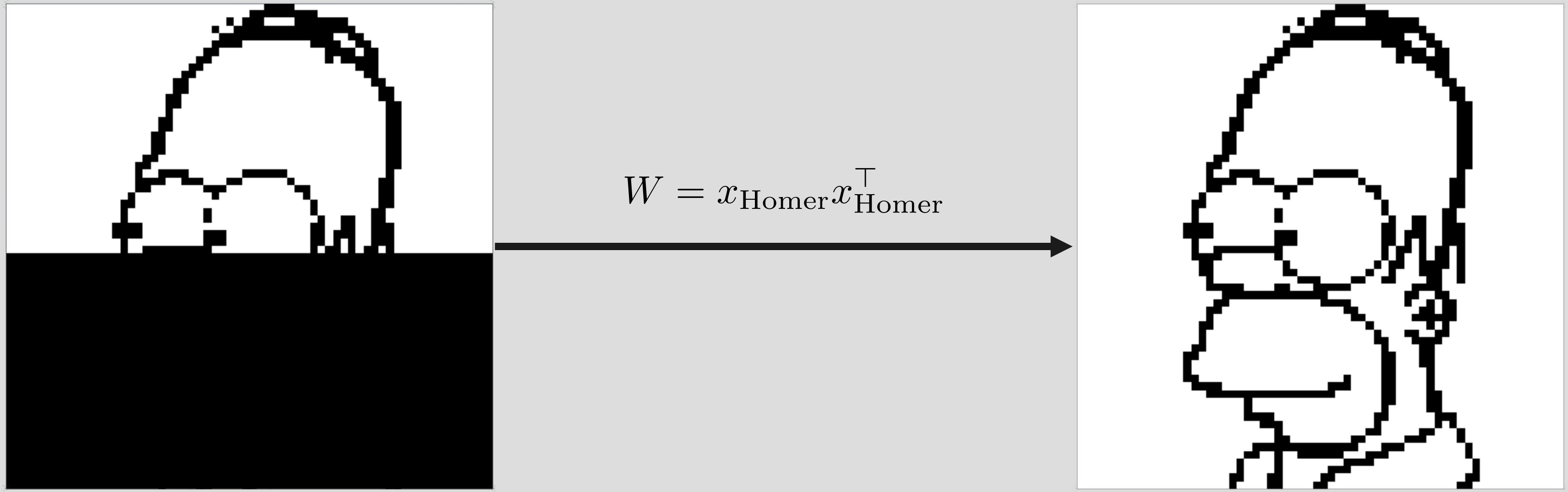

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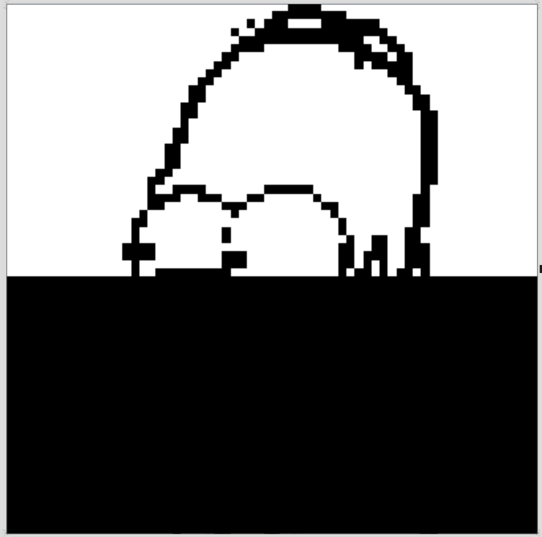

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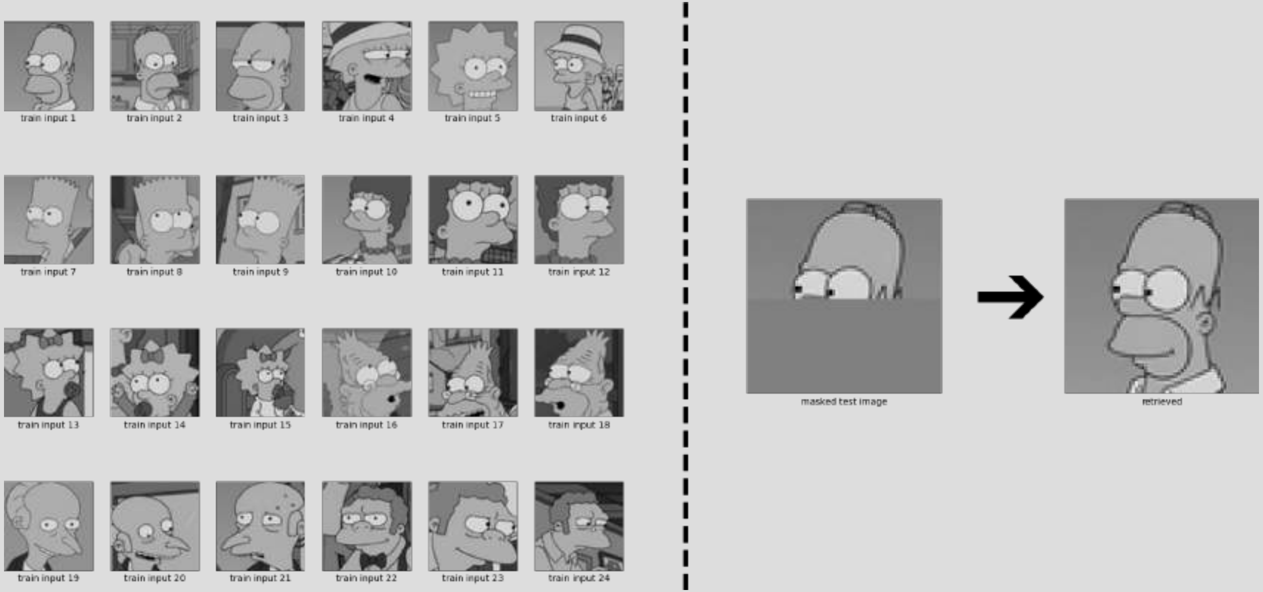


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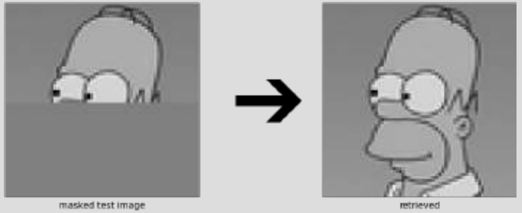


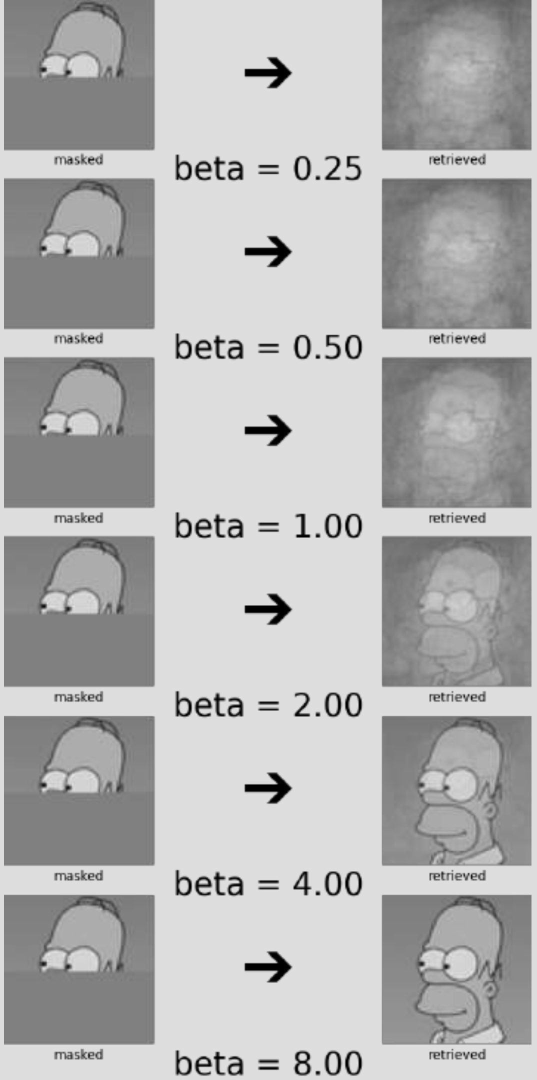


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4. The **attention mechanism** carries out the **update rule** for a continuous Hopfield network

# Overview

- Transformers primer
- Optimisation
- Approximation
- Memorisation
- **In-context learning**

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**Example 1:**

Lemon -> Yellow
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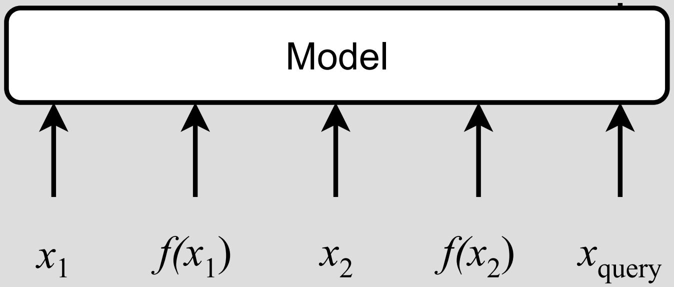


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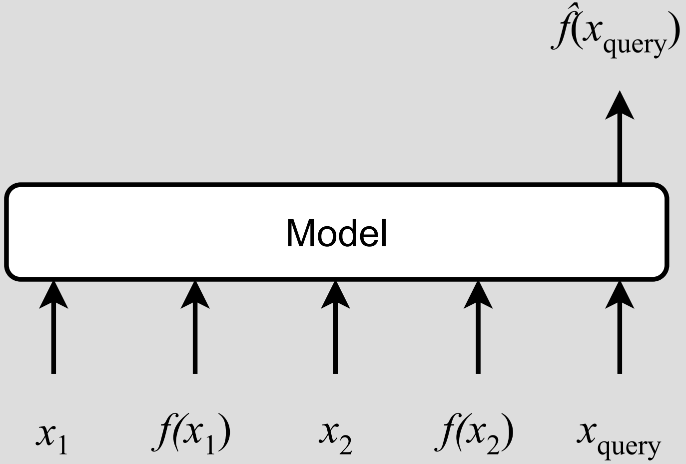


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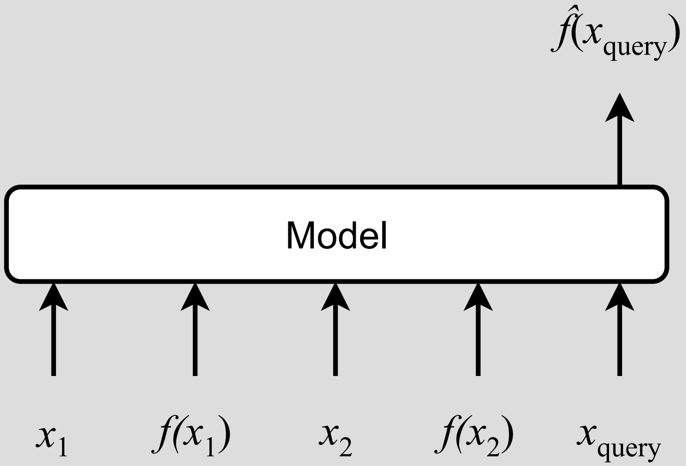


A model $M$ can ICL a function class $\mathcal{F}$ up to $\epsilon$ with respect to $(D_{\mathcal{X}}, D_{\mathcal{F}})$ for a loss function $\ell$ if:

$$\mathbb{E}_{(x,f)\sim(D_{\mathcal{X}},D_{\mathcal{F}})}\left[\ell(M(P), f(x_{query}))\right] \leq \epsilon$$

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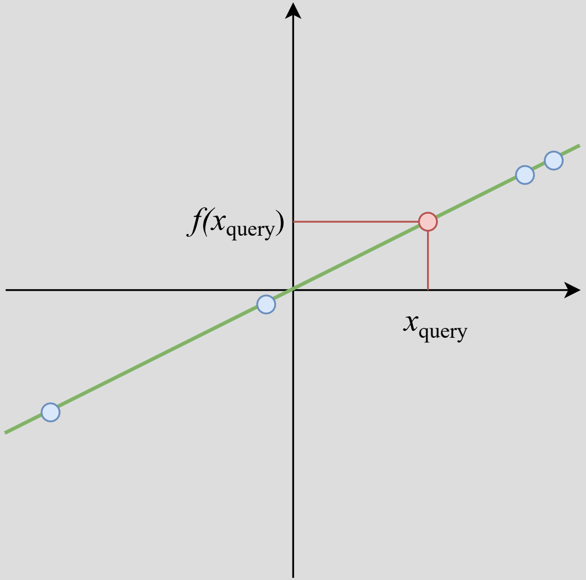
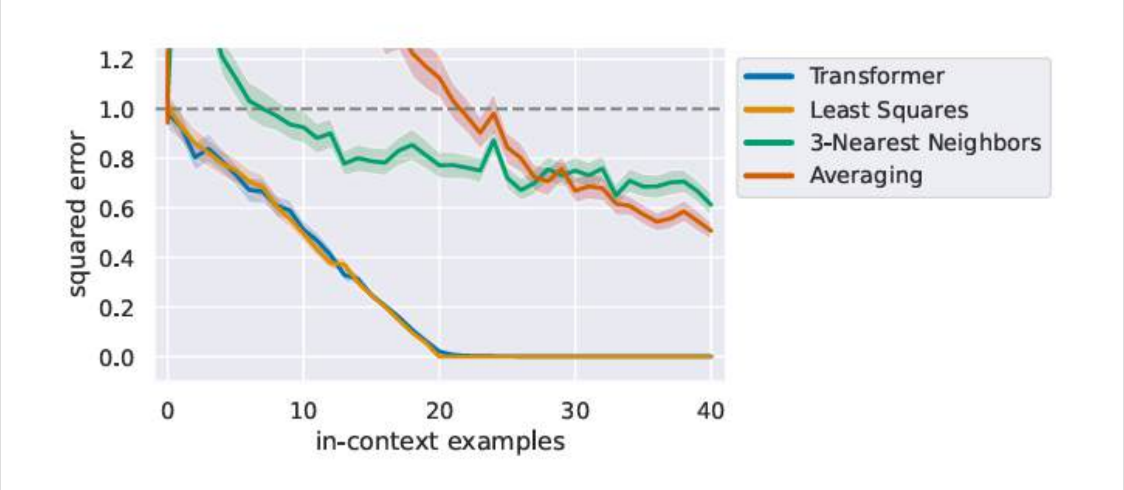
- **Hypothesis #2**: ICL is learning
  - It can identify novel functions from within a function class (e.g., puzzle-solving tasks)

# Linear regression

$$\mathcal{F} = \{f : f(x) = w^\top x\} \quad w \sim \mathcal{N}(0, I)$$

$$\mathcal{X} = \mathbb{R}^d \quad x \sim \mathcal{N}(0, I)$$

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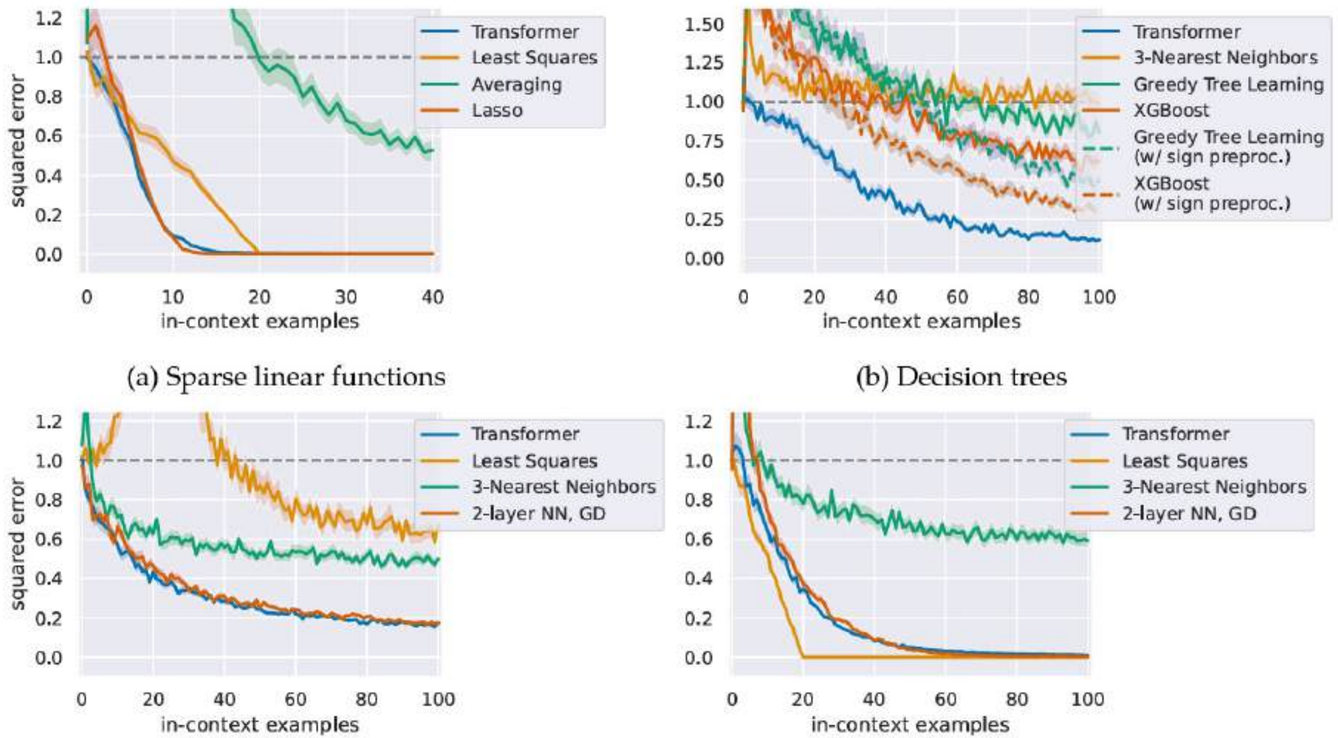
# Non-linear regression




(a) Sparse linear functions

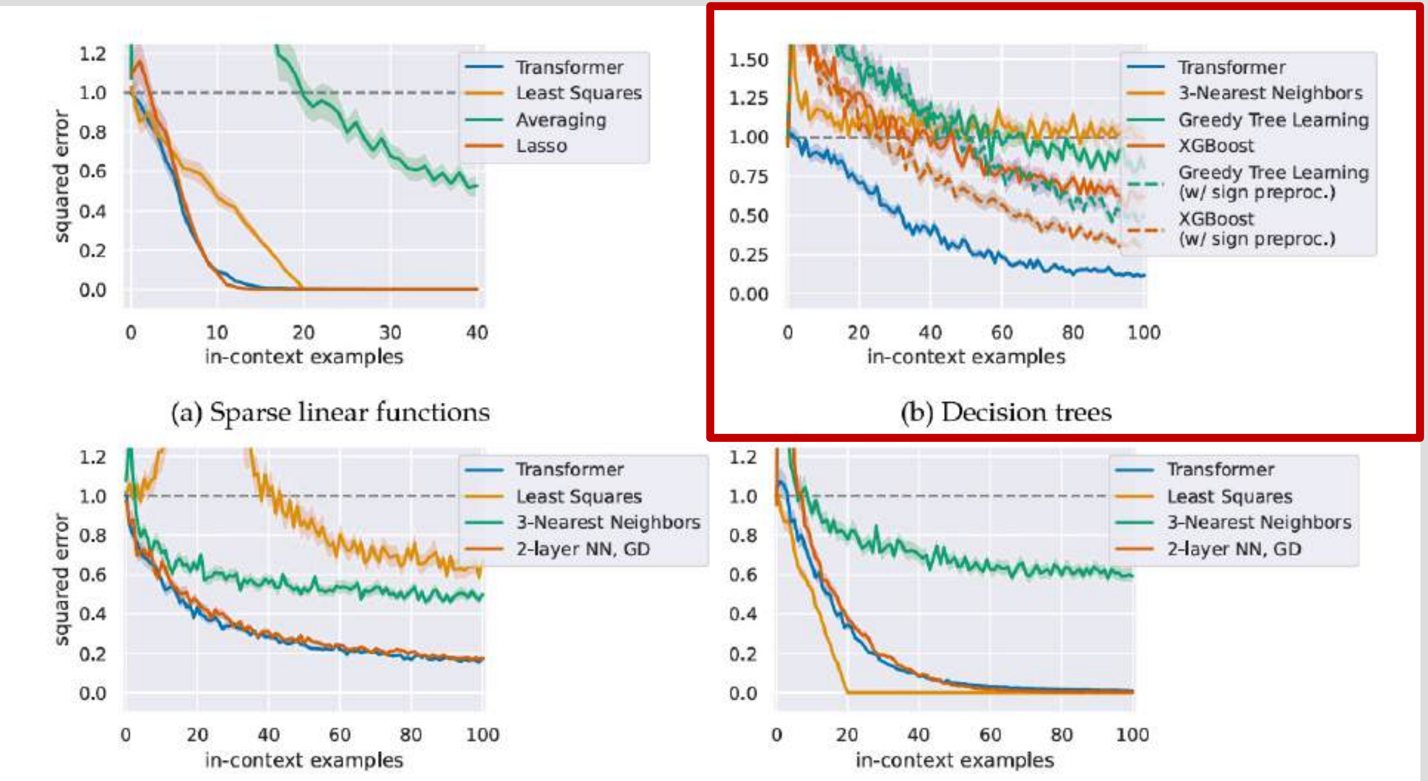
(b) Decision trees

(c) 2-layer NN

(d) 2-layer NN, eval on linear functions

[Oswald et al.'22]

# Non-linear regression




(a) Sparse linear functions

(b) Decision trees

(c) 2-layer NN

(d) 2-layer NN, eval on linear functions

# Gradient descent

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**Claim [Oswald et al.'22]:** We can construct a 1-head linear attention layer such that a Transformer step on every token $e_j$ is $e_j \leftarrow (x_j, y_j) + (0, -\Delta W x_j) = (x_j, y_j) + PVK^\top q_j$ where $e_j = (x_j, y_j - \Delta y_j)$

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2. They can learn more sample efficient algorithms than are known
3. 1-head Linear attention transformers **can and do** learn to do a single step of gradient descent

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# Questions?