Transformers and Associative Memories

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$$f(x) = W_L \sigma(W_{L-1} \cdots \sigma(W_1 x) \cdots)$$

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Q: Why does it work?

Breaking the curse of dimensionality I: feature learning

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- Image/text/genomics/etc. data are **high-dimensional**: $x \in \mathbb{R}^d$, d large
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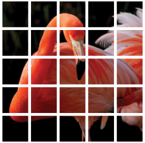
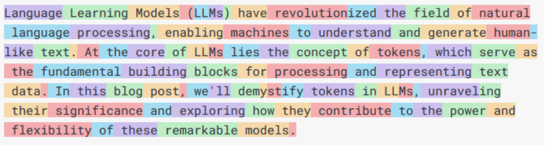
- **Goal**: $O(n^{-1/r})$ instead of $O(n^{-1/d})$ rates (Bach, 2017)
- Gradient descent on **first layer** of shallow neural network can achieve this
  - Well-studied for Gaussian data, harmonic analysis over Hermite basis
  - (e.g., Ben Arous et al., 2021; Ba et al., 2022; B. et al., 2022; Damian et al., 2022; B. et al., 2023a)

Breaking the curse of dimensionality II: locality + architecture

- **Local structure**: split input into small local patches / "tokens": $x = (x_1, \ldots, x_T)$





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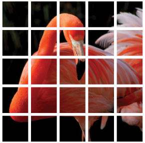

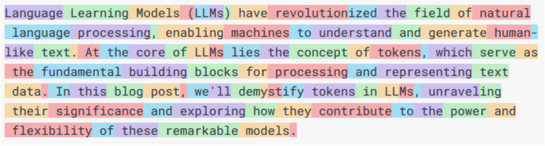

- Target may involve **interactions** between tokens, e.g. (Wahba, 1990)

$$\mathbb{E}[y|x] = \sum_i f_i^*(x_i) + \sum_{i,j} f_{ij}^*(x_i, x_j)$$

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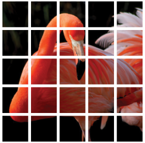

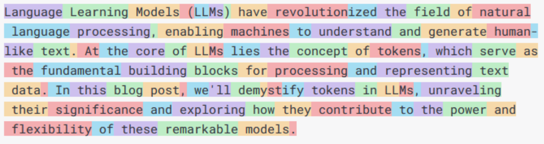

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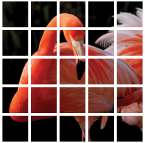

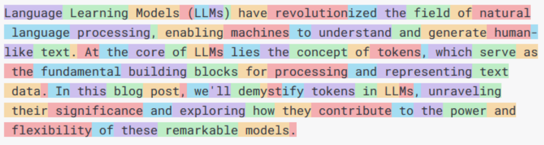

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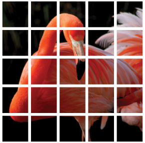

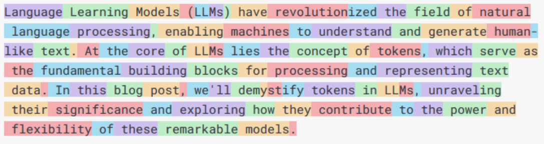

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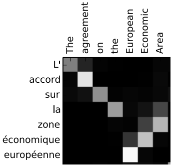
- **Convolution**: local interactions at different scales
- **Attention**: non-local interactions



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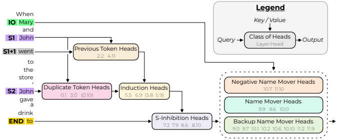
What about intermediate layers?

- (discrete) communication/computation in feature space (??)
- $\Longrightarrow$ **associative** mappings (input-output, or across tokens)



(Wang et al., 2022)

Matrices as associative memories

- Consider sets of **nearly orthonormal embeddings** $\{u_i\}_{i \in \mathcal{I}}$ and $\{v_j\}_{j \in \mathcal{J}}$:

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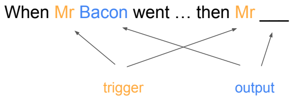
Q: how do these play a role in Transformers?

Outline

1. Application to Transformers (B., Cabannes, Bouchacourt, Jegou, and Bottou, 2023b)
2. Scaling laws for associative memories (Cabannes, Dohmatob, and B., 2024a)
3. Learning with gradient steps (B. et al., 2023b; Cabannes et al., 2024a,b)

The bigram data model for in-context reasoning

Goal: capture both in-context and global knowledge (*e.g.*, nouns vs syntax)



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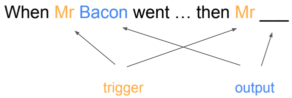

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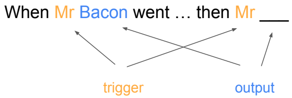

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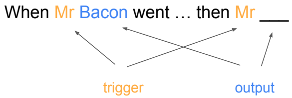

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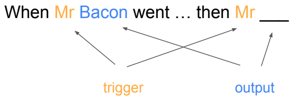

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π_b: **global bigrams** model (estimated from Karpathy's character-level Shakespeare)

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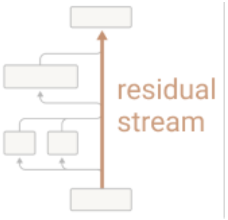

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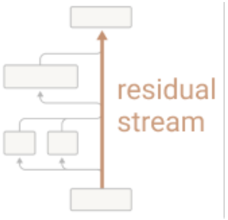
- **Loss** for next-token prediction (ℓ: cross-entropy)

$$\sum_{t=1}^{T-1} \ell(z_{t+1}, \xi_t)$$



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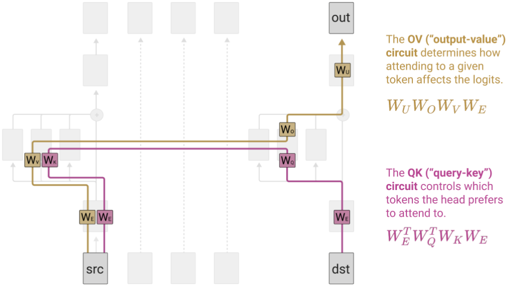

Causal self-attention layer (single head):

$$x'_t = \sum_{s=1}^{t} \beta_s W_O^T W_V x_s, \qquad \text{with } \beta_s = \frac{\exp(x_s{}^\top W_K^\top W_Q x_t)}{\sum_{s=1}^t \exp(x_s{}^\top W_K^\top W_Q x_t)}$$

- $W_K, W_Q \in \mathbb{R}^{d_h \times d}$: **key/query** matrices, $W_O, W_V \in \mathbb{R}^{d_h \times d}$: **output/value** matrices
- β_s: attention weights, $\sum_{s=1}^t \beta_s = 1$

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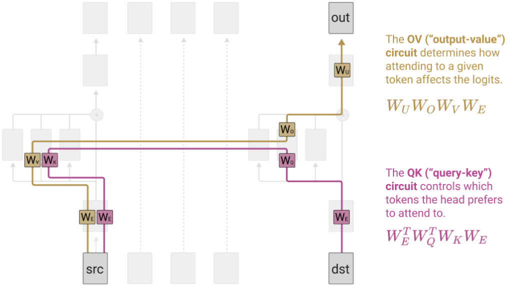

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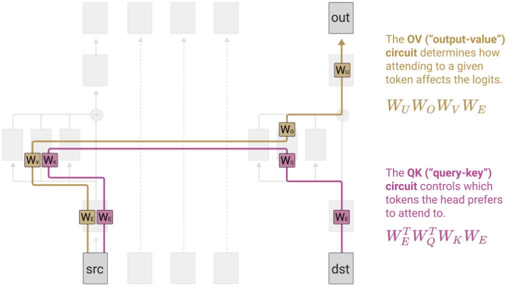

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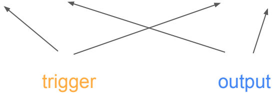
- β_s: attention weights, $\sum_{s=1}^{t} \beta_s = 1$
- Each x'_t is then added to the corresponding residual stream

$$x_t := x_t + x'_t$$

Transformers on the bigram task

When Mr Bacon went … then Mr ___



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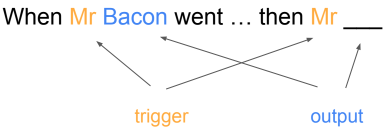

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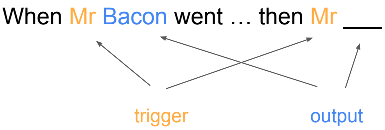

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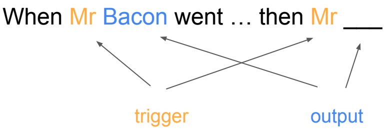

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See also (Sanford, Hsu, and Telgarsky, 2023, 2024) for representational lower bounds

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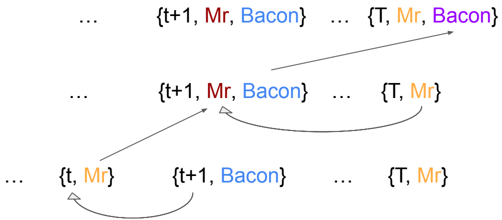

- 1st layer: **previous-token head**
  - attends to previous token and copies it to residual stream

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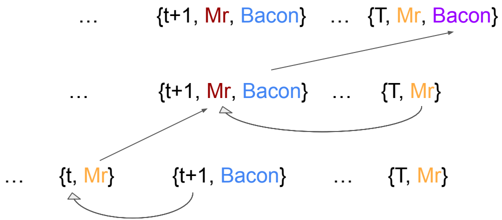

- 1st layer: **previous-token head**
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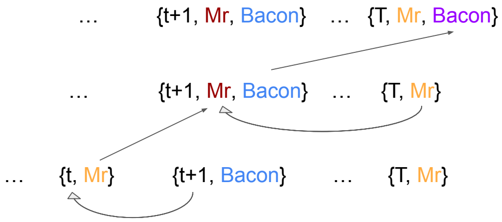

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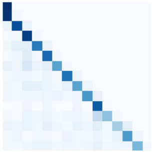
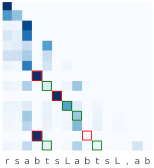
- Matches observed attention scores:





Random embeddings in high dimension

- We consider **random** embeddings u_i with i.i.d. $N(0, 1/d)$ entries and d large

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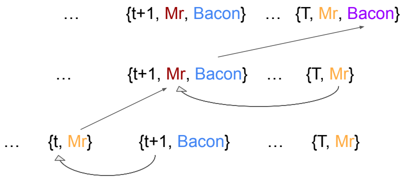
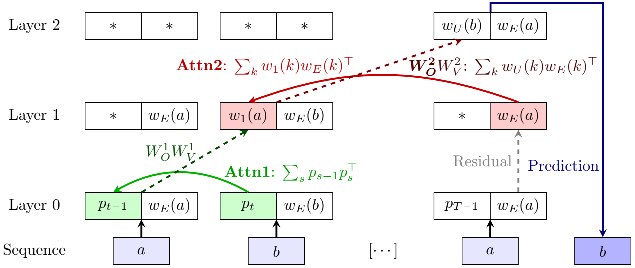
- Value/Output matrices help with token remapping: Mr $\mapsto$ Mr, Bacon $\mapsto$ Bacon



Induction head with associative memories



$$W_{KQ}^1 = \sum_{t=2}^{T} p_t p_{t-1}^\top, \quad W_{KQ}^2 = \sum_{k \in Q} w_E(k) w_1(k)^\top, \quad W_{OV}^2 = \sum_{k=1}^{N} w_U(k) w_E(k)^\top,$$

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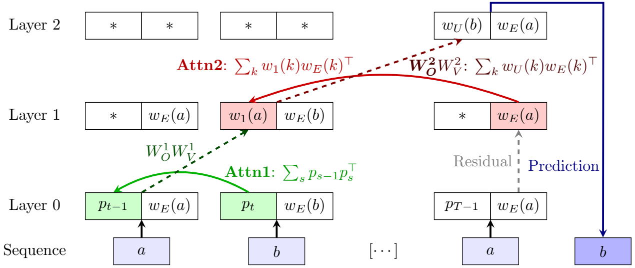

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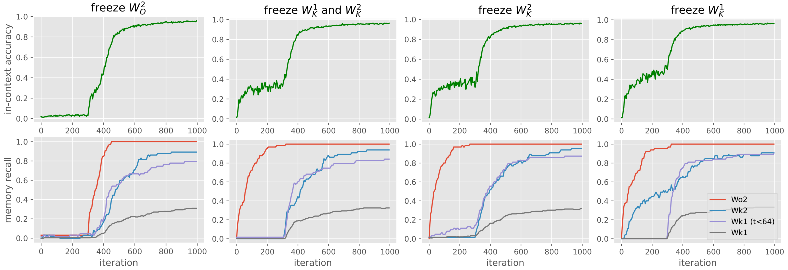
Q: Does this match practice?

Empirically probing the dynamics

Train only W_K^1, W_K^2, W_O^2, loss on deterministic output tokens only



- "Memory recall **probes**": for target memory $W_* = \sum_{(i,j)\in\mathcal{M}} v_j u_i^\top$, compute

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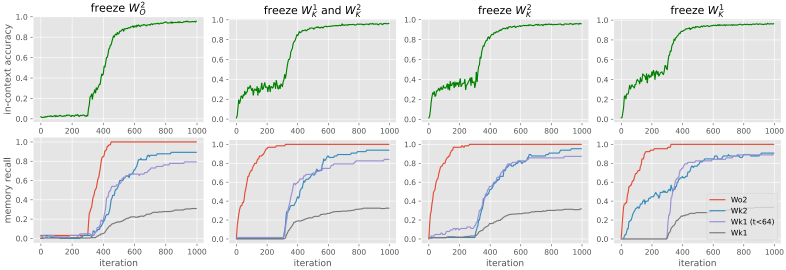

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- Natural learning "**order**": W_{OV}^2 first, W_{KQ}^2 next, W_{KQ}^1 last
- Joint learning is faster (motivates our theory below)

Outline

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Q: What about finite capacity?

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- Recover all associations when $\mathrm{Var}[\gamma_{z,y}] \lesssim 1$. Examples:
  - $f^*(z) = z$: can store up to $N \approx d^2$ associations
  - $f^*(z) = z \mod 2$: can store up to $N \approx d$ associations

Scaling laws with finite capacity

- **Random embeddings** $u_z, v_y \in \mathbb{R}^d$ with i.i.d. $\mathcal{N}(0, 1/d)$ entries
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Outline

Gradients as associative memories

- **Simple model** to learn associative memories:

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Example: one gradient step

- **Data model**: $z \sim \mathrm{Unif}([N]), \quad y = f_*(z) \in [N]$
- After **one gradient step** from $W_0 = 0$, step-size η:

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Note: related to (Ba et al., 2022; Damian et al., 2022; Yang and Hu, 2021)

Gradient associative memories with noisy inputs

- In practice, inputs are often a collection of tokens / sum of embeddings

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Example: filter out exogenous noise with one gradient step

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Gradient steps for the bigram task

Setting: transformer on the bigram task

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Key ideas

- Attention is uniform at initialization $\implies$ inputs are sums of embeddings
- W_O^2: correct output appears w.p. 1, while other tokens are noisy and cond. indep. of z_T
- $W_K^{1/2}$: correct associations lead to more focused attention

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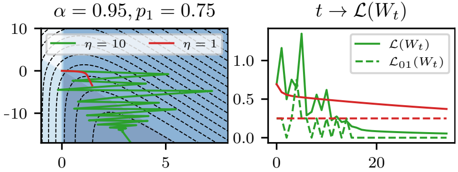
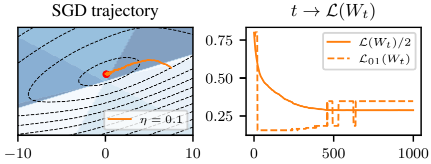
Benefits of large step-sizes + oscillations: (Cabannes, Simsek, and B., 2024b)

- Orthogonal embeddings $\implies$ logarithmic growth of margins for any step-size
- Correlated embeddings + imbalance $\implies$ oscillatory regimes
- Large step-sizes help reach perfect accuracy faster despite oscillations (empirically)
- Over-optimization can hurt in under-parameterized settings (empirically)





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- Beyond text data: images and scientific data
- Applications: interpretability, model editing, factual recall, efficient fine-tuning

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- Applications: interpretability, model editing, factual recall, efficient fine-tuning

Thank you!

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Learning associations

Motivation:

- DL theory often focuses on learning/approximation of **continuous** target functions
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- Typically $\hat{f}(z) = \arg\max_y f_y(z)$ with $f_y : [N] \to \mathbb{R}$ for each $y \in [M]$

Matrices as associative memories

- Consider sets of **nearly orthonormal embeddings** $\{u_i\}_{i\in\mathcal{I}}$ and $\{v_j\}_{j\in\mathcal{J}}$:

$$\|u_i\| \approx 1 \quad \text{and} \quad {u_i}^\top u_j \approx 0$$
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note: closely related to Hopfield (1982); Kohonen (1972); Willshaw et al. (1969)

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- Simple **differentiable model** to learn such associative memories:

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$$\nabla L(W) = \sum_{k=1}^{M} \mathbb{E}_z[(\hat{p}_W(y = k|z) - p(y = k|z)) v_k {u_z}^\top],$$

with $\hat{p}_W(y = k|z) = \exp(\xi_W(z)_k) / \sum_j \exp(\xi_W(z)_j)$.

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Note: related to (Ba et al., 2022; Damian et al., 2022; Yang and Hu, 2021)

Gradient associative memories with noisy inputs

- In practice, inputs are often a collection of tokens / sum of embeddings

$$\mathbf{z} = \{z_1, \ldots, z_s\} \subset [N], \quad x = \sum_{j=1}^{s} u_{z_s} \in \mathbb{R}^d$$

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Link with feature learning

Maximal updates:

- First gradient update from standard initialization ($[W_0]_{ij} \sim \mathcal{N}(0, 1/d)$) take the form

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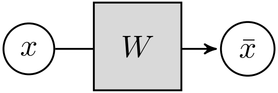
Large gradient steps on shallow networks:

- Useful for feature learning in **single-index** and **multi-index** models

$$y = f^*(x) + \text{noise}, \quad f^*(x) = g^*(Wx), \quad W \in \mathbb{R}^{r \times d}$$

- Sufficient to break the curse of dimensionality when $r \ll d$
- (Ba et al., 2022; Damian et al., 2022; Dandi et al., 2023; Nichani et al., 2023)

Associative memories inside deep models



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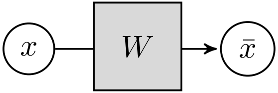

- Consider W that connects two nodes $x, \bar{x}$ in a feedforward computational graph
- The loss gradient takes the form

$$\nabla_W L = \mathbb{E}[\nabla_{\bar{x}} \ell \cdot x^\top]$$

  where $\nabla_{\bar{x}} \ell$ is the **backward** vector (loss gradient w.r.t. $\bar{x}$)
- Often, this expectation may lead to associative memories as before
- A similar form can arise in attention matrices (see later!)

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- **Finite samples?** how well can we learn with finite data?
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$\Longrightarrow$ **study through scaling laws** (a.k.a. generalization bounds/statistical rates)

Setup with heavy-tailed data

Setting

- $z_i \sim p(z)$, $y_i = f^*(z_i)$, n samples: $S_n = \{z_1, \dots, z_n\}$, 0/1 loss:

$$L(\hat{f}_n) = \mathbb{P}(y \neq \hat{f}_n(z))$$

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- **Q: What about finite capacity?**

Scaling laws with finite capacity

- Random embeddings $u_z, v_y \in \mathbb{R}^d$ with $\mathcal{N}(0, 1/d)$ entries
- Estimator: $\hat{f}_{n,d}(x) = \arg\max_y v_y^\top W_{n,d} u_z$, with

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Theorem (Cabannes, Dohmatob, B., 2023, informal)

1. *For* $q(z) = \sum_i \mathbb{1}\{z = z_i\}$*:* $L(\hat{f}_{n,d}) \lesssim n^{-\frac{\alpha-1}{\alpha}} + d^{-\frac{\alpha-1}{2\alpha}}$

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- $n^{-\frac{\alpha-1}{\alpha}}$ is the same as (Hutter, 2021)
- $q = 1$ is best if we have enough capacity
- Can store at most d memories (approximation error: $d^{-\alpha+1}$)

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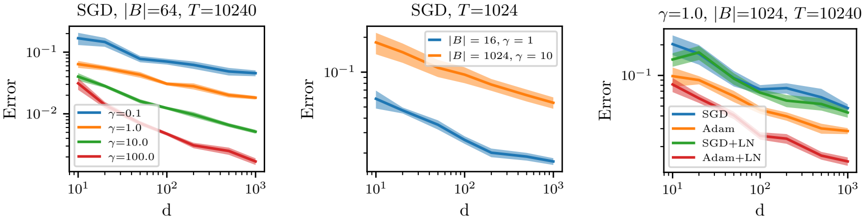

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Main idea: there are $\exp(d)$ near-orthogonal directions on the sphere

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But: higher computational cost, more sensitive to noise, harder to learn