Increasing the Sequence Length in LLMs: Smoothness and Dynamics of Self-Attention

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University of Amsterdam, 27 May 2025

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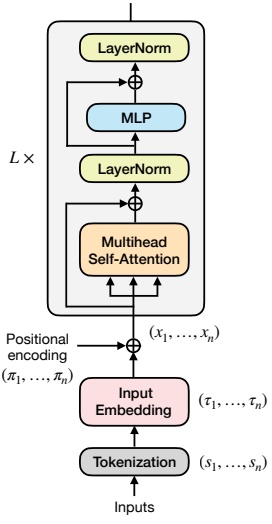
Apple Paris

A Unified Perspective on the Dynamics of Deep Transformers, Castin, Ablin, Carrillo, Peyré, *preprint 2025*

How Smooth Is Attention?, Castin, Ablin and Peyré, *in ICML 2024*

I - The dynamics of tokens processed by a Transformer

The Transformer architecture



- One input sentence $\rightarrow$ n tokens $X \coloneqq (x_1, \ldots, x_n) \in (\mathbb{R}^d)^n$

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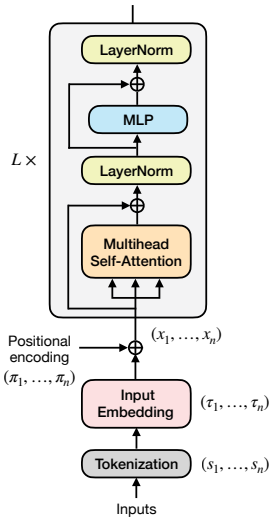

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- Self-attention with params Q, K, V:

$$f(x_1,\ldots,x_n) \coloneqq (\Gamma_X(x_1),\ldots,\Gamma_X(x_n)) \text{ where}$$

$$\Gamma_X(z) \coloneqq \sum_{j=1}^{n} p_j(z) V x_j \quad \text{with} \quad p_j(z) \coloneqq e^{\langle Qz, Kx_j\rangle} / \sum_{\ell=1}^{n} e^{\langle Qz, Kx_\ell\rangle}$$

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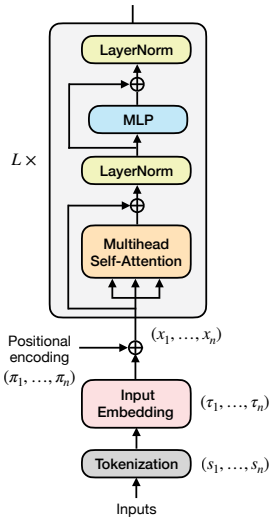

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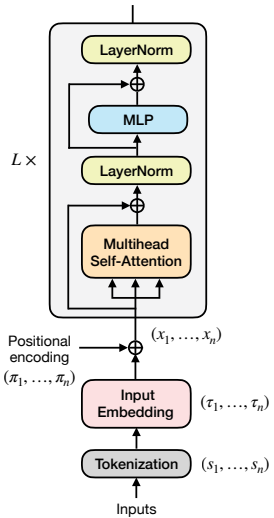

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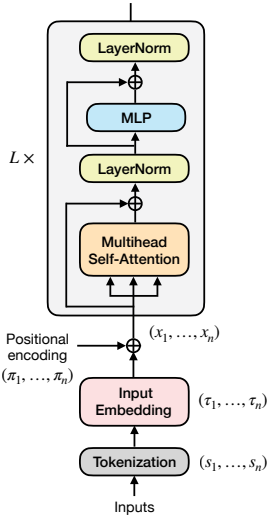
- Layer normalization $\mathrm{LN}\colon x \mapsto \beta \odot \frac{x}{|x|}\sqrt{d}$ (applied token-wise)
- Multilayer perceptron $g\colon \mathbb{R}^d \to \mathbb{R}^d, x \mapsto W\sigma(Ux + b)$ (applied token-wise)

The Transformer architecture



- One input sentence $\to$ n tokens $X := (x_1, \ldots, x_n) \in (\mathbb{R}^d)^n$
- Self-attention with params Q, K, V:

$$f(x_1, \ldots, x_n) := (\Gamma_X(x_1), \ldots, \Gamma_X(x_n)) \text{ where}$$

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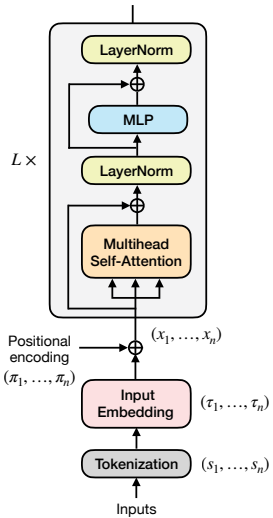
Without MLP and LN:

$$x_i(\ell + 1) = x_i(\ell) + \Gamma_{X_\ell}(x_i(\ell)) \qquad 1 \le i \le n$$

Studying the dynamics of tokens across layers



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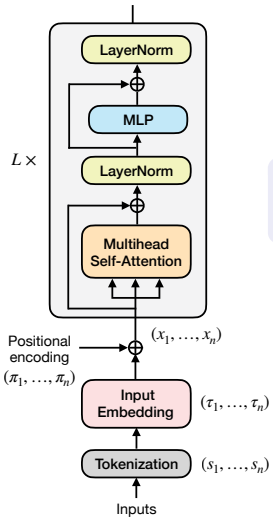

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What are the dynamics of tokens going through the Transformer? The geometry of learned representations?

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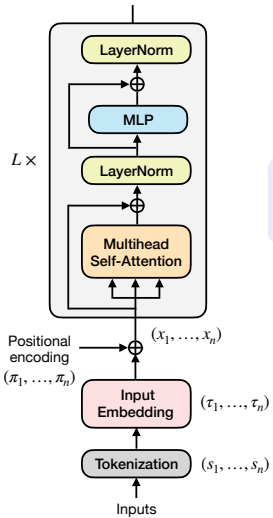

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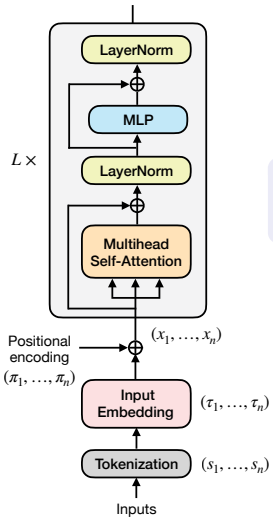

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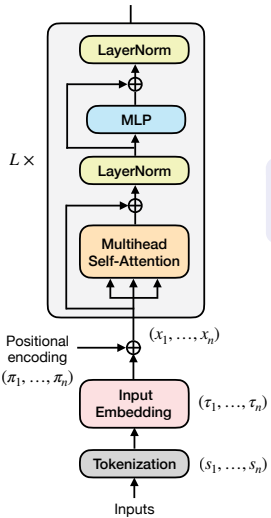

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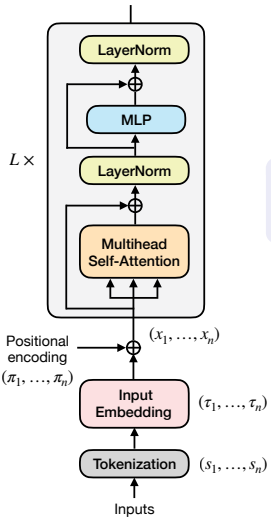

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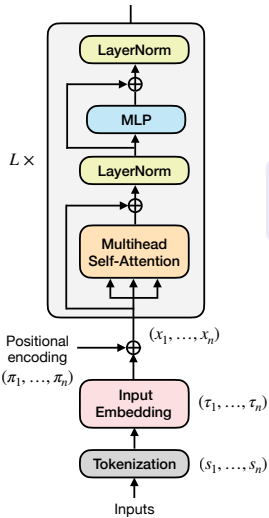

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- influence of sequence length
- compare attention variants

Clustering for the time-continuous interacting particle system

$$x_i(\ell+1) = x_i(\ell) + \Gamma_{X_\ell}(x_i(\ell)) \quad \longleftrightarrow \quad \dot{x}_i(t) = \Gamma_{X(t)}(x_i(t)) \quad \text{[Sander et al., 2021]}$$

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Clustering result [Geshkovski et al., 2024]

- Assume $A \succ 0$ constant and $V = I_d$
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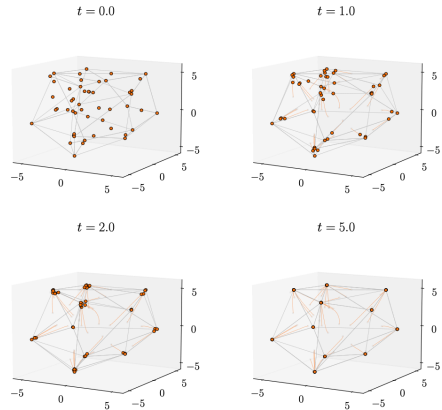
- typically $\sharp\text{vertices}(K) \ll n$



Mean-field attention and the Transformer PDE

Self-attention $f(X) = (\Gamma_X(x_1), \dots, \Gamma_X(x_n))$ where

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- Well-defined for μ compactly supported, Gaussian...
- Covers discrete case: view X as $\frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$

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$$\dot{x}_i(t) = \Gamma_{X(t)}(x_i(t)) \quad \longrightarrow \quad \partial_t \mu + \mathrm{div}(\mu \Gamma_\mu) = 0 \tag{1}$$

I - 1) Studying the Transformer PDE with compactly supported initial data

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The Transformer PDE in the compactly supported case

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Well-posedness [Geshkovski et al., 2024, Castin et al., 2025]

- Assume $A(t), V(t)$ continuous
- Assume $\operatorname{supp} \mu_0 \subset B(0, R_0)$

Then (1) has a unique global weak solution μ, such that

$$\operatorname{supp} \mu(t) \subset B(0, e^{\int_0^t \|V(s)\|_2 \mathrm{d}s} R_0).$$

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If $\operatorname{supp} \nu_0 \subset B(0, R_0)$ then

$$W_p(\mu(t), \nu(t)) \leq C(t, R_0) W_p(\mu_0, \nu_0) \quad \forall p \geq 1$$

with $C(t, R_0) \propto e^{tR(t)^2}$

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Central estimates for proof

1. $\sup_{x\in\mathbb{R}^d} |\Gamma_\mu(x)| \leq \|V\|_2 R$,
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- Modular framework $\rightarrow$ extends to attention variants!

Extending to attention variants

Attention map: $\Gamma_\mu(z) = \int k(z,y) V y \mathrm{d}\mu(y)$

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- ✓ Masked attention
- ✓ Multihead attention: $\Gamma_\mu = \sum_{h=1}^H \Gamma_\mu^{(h)}$

Extending to attention variants

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- ✗ Linear attention: $k(z,y) = \langle Az, y\rangle$
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I - 2) Beyond compactly supported data:
the Gaussian case [Castin et al., 2025]

$$\partial_t \mu + \mathrm{div}(\mu \Gamma_\mu) = 0$$

The Transformer PDE in the Gaussian case

Lemma: attention map on Gaussians

If $\mu = \mathcal{N}(\alpha, \Sigma)$ then

$$\Gamma_\mu(x) = V(\alpha + \Sigma A x)$$

Similar for L2 and Sinkhorn attention!

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Assume A, V continuous and $\mu_0 = \mathcal{N}(\alpha_0, \Sigma_0)$. Then (1) has a unique maximal solution on $[0, t_{\max})$, Gaussian for all t. Denoting $\mu(t) = \mathcal{N}(\alpha(t), \Sigma(t))$:

$$\begin{cases} \dot{\alpha} = V(I_d + \Sigma A)\alpha \\ \dot{\Sigma} = V\Sigma A\Sigma + \Sigma A^\top \Sigma V^\top \end{cases}$$

Clustering emerges in the Gaussian case

Proposition: closed-form analysis

Consider

$$\dot{\Sigma} = V\Sigma A\Sigma + \Sigma A^\top \Sigma V^\top.$$

Assume

- A, V constant
- V commutes with $VA + A^\top V^\top$ and Σ_0

Then

$$\Sigma(t) = (\Sigma_0^{-1} - t(VA + A^\top V^\top))^{-1}$$

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- If $VA + A^\top V^\top \preceq 0$ the solution is global and converges to Σ^* such that

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- Otherwise $\lambda_1(\Sigma(t)) \to +\infty$ in finite time

Clustering emerges in the Gaussian case

Proposition: limiting covariances have low-rank

Let Σ such that

$$V\Sigma A\Sigma + \Sigma A^\top \Sigma V^\top = 0$$

Assume

- A constant and symmetric
- $V = I_d$

Then

$$\operatorname{rk}\Sigma \leq \dim\ker A + \min(\sharp\text{pos. eigvals of } A, \sharp\text{neg. eigvals of } A)$$

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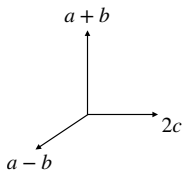
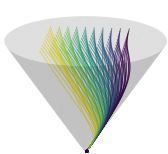
- Numerically: holds for V random

Clustering emerges in the Gaussian case

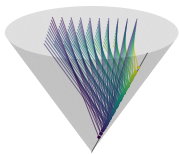
Plot the covariance evolution for $d = 2$:



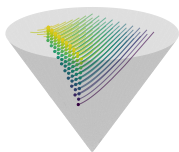
(a) Conv. to zero



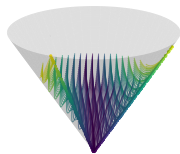
(b) Conv. to a line



(c) Conv. to a plane



(d) Conv. to two lines



$$\begin{pmatrix} a & c \\ c & b \end{pmatrix} \in \mathcal{S}_2^+ \mapsto (x, y, z) \coloneqq (a - b, 2c, a + b)$$

Comparing attention variants

- Softmax, L2, Sinkhorn attention $\rightarrow$ similar behavior when converge
- L2 does not blow-up in finite time $\rightarrow$ more regular

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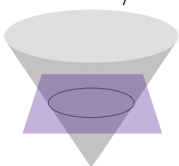
$\Sigma \mapsto \Sigma/\mathrm{Tr}\Sigma$



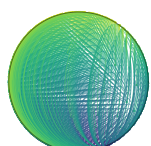
(a) Blow-up

SM att.

(b) Blow-up

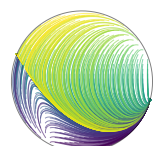
MH att.

(c) Div.



L2 att.

(d) Conv./blow-up



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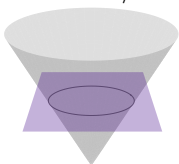

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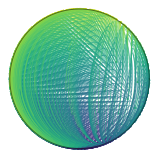

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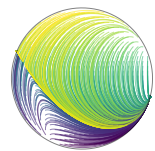

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Open question: beyond Gaussians?

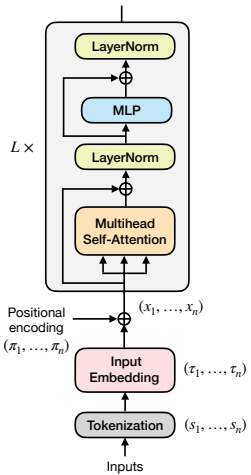
Conclusion of part I

- Mean-field attention and the Transformer PDE generalize dynamics to infinitely many tokens
- Attention variants should have a normalized kernel to induce well-posed dynamics
- The Gaussian case reduces to a system of matrix equations $\rightarrow$ theoretical and numerical analysis, variety of behaviors, clustering
- LayerNorm changes a lot the dynamics

- What about next-token prediction? (Masked attention dynamics)
- From discrete to continuous time, what changes?

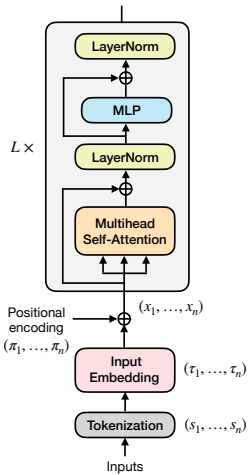
II - The Lipschitz constant of self-attention [Castin et al., 2024]

Studying the robustness of Transformers



How much can the output of a Transformer change when slightly perturbing the input?

Studying the robustness of Transformers



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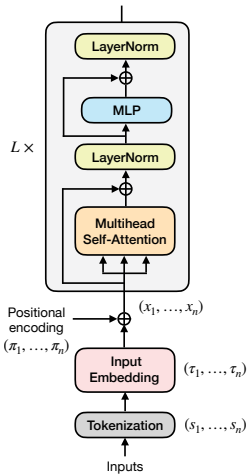

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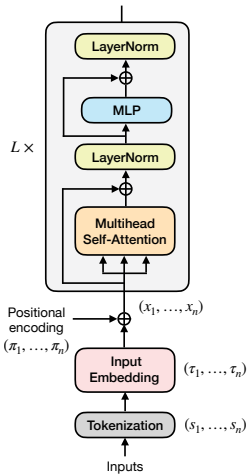

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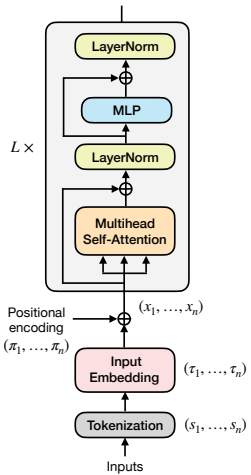

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Does the robustness of an input depend on the sequence length?

Measuring regularity with the local Lipschitz constant

$f\colon (\mathbb{R}^d)^n \to (\mathbb{R}^d)^n$ self-attention

Local Lipschitz constant

Norm on $(\mathbb{R}^d)^n$: $\|X\|^2 := \sum_{i=1}^n |x_i|^2$

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$$\operatorname{Lip}_X(f) \coloneqq \|D_X f\|_2 = \sup_{\|\varepsilon\|=1} \|D_X f(\varepsilon)\|$$

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Gives global guarantees:

$$\sup_{X \neq Y \in B_R^n} \frac{\|f(X) - f(Y)\|}{\|X - Y\|} = \sup_{X \in B_R^n} \mathrm{Lip}_X(f)$$

Theoretical dependency on the sequence length n

Theorem 1 [Castin et al., 2024]

$$\mathrm{Lip}(f_{|B_R^n}) \leq \sqrt{3}\,\|V\|_2 \left(\|A\|_2^2\, R^4(4n+1) + n\right)^{1/2} \approx R^2\sqrt{n}$$

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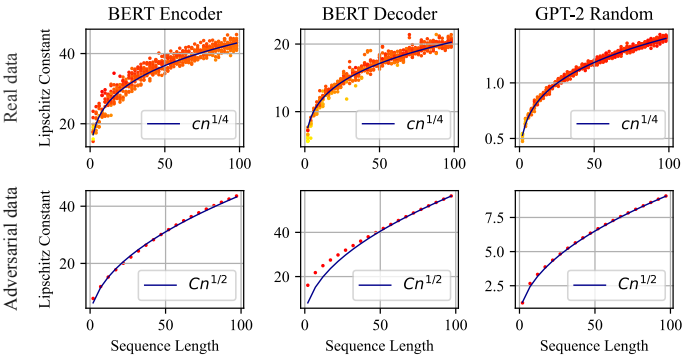
- R fixed by layer normalization
- n not too large: $\mathrm{Lip}(f_{|B_R^n})$ grows like $C\sqrt{n}$
- mean-field bound: $\mathrm{Lip}(f_{|B_R^n}) \leq c(A, V)R^2 e^{1\|A\|_2 R^2}$

Experiments: typical case and worst case



Local Lipschitz constant of real vs. adversarial data

- Growth in $Cn^{1/4}$ for real data

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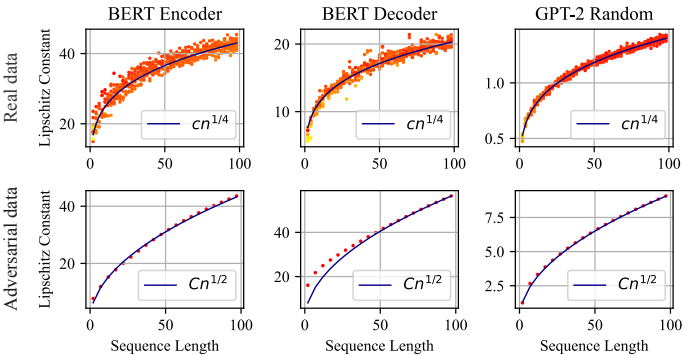

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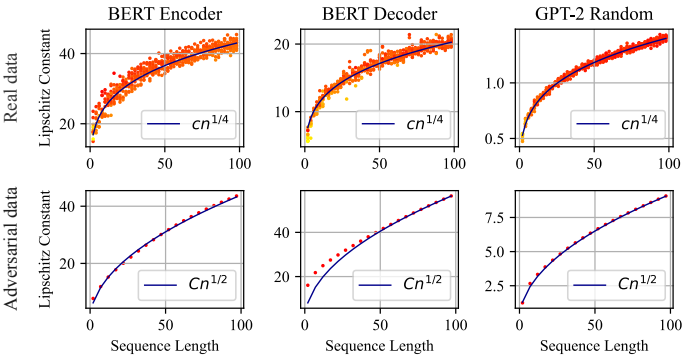

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Obstacle to Lipschitz attention (GPT-4o context window: 128k)

Thank you!

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III - Masked self-attention

Masked self-attention processes tokens sequentially

Masked self-attention $f^m \colon (\mathbb{R}^d)^n \to (\mathbb{R}^d)^n$ such that

$$f^m(X)_i := f(x_1, \ldots, x_i)_i$$

with params $A, V \in \mathbb{R}^{d \times d}$

Mean-field regime? $\to$ not permutation equivariant!

Generalizing masked self-attention to measures

Mean-field self-attention $F : \mu \in \mathcal{P}_c(\mathbb{R}^d) \mapsto (\Gamma_\mu)_\sharp \mu$ where

$$\Gamma_\mu : x \in \mathbb{R}^d \mapsto \int_{\mathbb{R}^d} k(x,y) V y \mathrm{d}\mu(y) \quad \text{with} \quad k(x,y) \coloneqq e^{\langle Ax, y \rangle} / \int e^{\langle Ax, z \rangle} \mathrm{d}\mu(z)$$

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Mean-field masked self-attention [Castin et al., 2024]

Replace $\mu \in \mathcal{P}_c(\mathbb{R}^d)$ by $\bar{\mu} \in \mathcal{P}_c([0,1] \times \mathbb{R}^d)$:

$$F^m\colon \bar{\mu} \mapsto (\Gamma_{\bar{\mu}})_\sharp \bar{\mu} \quad \text{where} \quad \Gamma_{\bar{\mu}}(s,x) \coloneqq \left(s, \int_{[0,1]\times\mathbb{R}^d} V y k_s(x,y) \mathrm{d}\bar{\mu}(\tau, y) \right)$$

with

$$k_s(x,y) \coloneqq e^{\langle Ax, y\rangle} 1_{\tau \le s} / \int_{[0,1]\times\mathbb{R}^d} e^{\langle Ax, y\rangle} 1_{\tau \le s} \mathrm{d}\bar{\mu}(\tau, y)$$