Geometry of Linear Neural Networks that are Equivariant / Invariant under Permutation Groups

Kathlén Kohn





joint work with

Anna-Laura Sattelberger

Vahid Shahverdi

Geometric questions:

- 1. How does the network architecture affect the geometry of the function space?
- 2. How does the geometry of the function space impact the training of the network?

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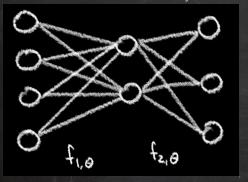
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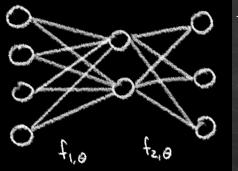
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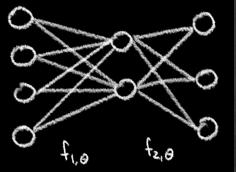
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This network parametrizes linear maps:

$$\mu: \mathbb{R}^{2\times 4} \times \mathbb{R}^{3\times 2} \longrightarrow \mathbb{R}^{3\times 4},$$
$$(W_1, W_2) \longmapsto W_2 W_1.$$

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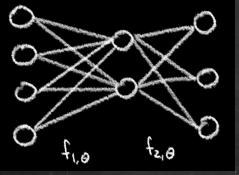
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In general:
$$\mu: \mathbb{R}^{k_1 \times k_0} \times \mathbb{R}^{k_2 \times k_1} \times \ldots \times \mathbb{R}^{k_L \times k_{L-1}} \longrightarrow \mathbb{R}^{k_L \times k_0},$$

$$(W_1, W_2, \ldots, W_L) \longmapsto W_L \cdots W_2 W_1.$$

Its function space $\mathcal{M}_r = \operatorname{im}(\mu) = \{W \in \mathbb{R}^{k_L \times k_0} \mid \operatorname{rank}(W) \leq r\}$, where $r := \min(k_0, \ldots, k_L)$, is an algebraic variety.

Running Example

Consider an autoencoder $\mu: \mathbb{R}^{2\times 9} \times \mathbb{R}^{9\times 2} \longrightarrow \mathbb{R}^{9\times 9}, \ (W_1, W_2) \longmapsto W_2 W_1$

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Its inputs and outputs are 3×3 images:

a ₁₁	a ₁₂	a ₁₃	
a ₂₁	a ₂₂	a ₂₃	$\in \mathbb{R}^9$
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Consider the clockwise rotation by 90°:

Which $W \in \mathcal{M}_2$ are equivariant under σ ? Which are invariant?



is represented by the permutation matrix

$$P_{\sigma} = egin{bmatrix} 0 & 0 & 0 & 1 \ 1 & 0 & 0 & 0 \ 0 & 1 & 0 & 0 \ 0 & 0 & 1 & 0 \ \end{pmatrix} egin{bmatrix} 0 & 0 & 0 & 1 \ 0 & 0 & 1 & 0 & 0 \ 0 & 0 & 1 & 0 & 0 \ \end{pmatrix} egin{bmatrix} 0 & 0 & 0 & 1 \ 0 & 0 & 1 & 0 & 0 \ \end{pmatrix} egin{bmatrix} 0 & 0 & 0 & 1 \ 0 & 0 & 1 & 0 \ \end{pmatrix} egin{bmatrix} 0 & 0 & 0 & 1 \ \end{pmatrix} egin{bmatrix} 0 & 0 & 0 & 1 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \ \end{bmatrix} egin{bmatrix} 0 & 0 & 0 & 0 \$$



$$\sigma: \mathbb{R}^9 \longrightarrow \mathbb{R}^9, egin{array}{c|ccccc} a_{11} & a_{12} & a_{13} \\ \hline a_{21} & a_{22} & a_{23} \\ \hline a_{31} & a_{32} & a_{33} \\ \hline \end{array} \longmapsto egin{array}{c|cccc} a_{31} & a_{21} & a_{11} \\ \hline a_{32} & a_{22} & a_{12} \\ \hline a_{33} & a_{23} & a_{13} \\ \hline \end{array}$$

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	0 1 0 0	0 1	0 0 0 1	0	1	(0		0
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		(1		1	0	0	0	0
		,	,		0	1	0	0	U
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 $W \in \mathbb{R}^{9 \times 9}$ is equivariant under σ \Leftrightarrow $W \cdot P_{\sigma} = P_{\sigma} \cdot W$.

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 $W \in \mathbb{R}^{9 \times 9}$ is invariant under σ \Leftrightarrow

$$\Leftrightarrow W \cdot P_{\sigma} = W.$$



 $W \in \mathbb{R}^{9 imes 9}$ is equivariant under σ iff

$$W = \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \beta_1 & \beta_2 & \beta_3 & \beta_4 & \varepsilon_3 \\ \alpha_4 & \alpha_1 & \alpha_2 & \alpha_3 & \beta_4 & \beta_1 & \beta_2 & \beta_3 & \varepsilon_3 \\ \alpha_3 & \alpha_4 & \alpha_1 & \alpha_2 & \beta_3 & \beta_4 & \beta_1 & \beta_2 & \varepsilon_3 \\ \alpha_2 & \alpha_3 & \alpha_4 & \alpha_1 & \beta_2 & \beta_3 & \beta_4 & \beta_1 & \varepsilon_3 \\ \hline \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \delta_1 & \delta_2 & \delta_3 & \delta_4 & \varepsilon_4 \\ \gamma_4 & \gamma_1 & \gamma_2 & \gamma_3 & \delta_4 & \delta_1 & \delta_2 & \delta_3 & \varepsilon_4 \\ \gamma_3 & \gamma_4 & \gamma_1 & \gamma_2 & \delta_3 & \delta_4 & \delta_1 & \delta_2 & \varepsilon_4 \\ \hline \gamma_2 & \gamma_3 & \gamma_4 & \gamma_1 & \delta_2 & \delta_3 & \delta_4 & \delta_1 & \varepsilon_4 \\ \hline \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_5 \end{bmatrix}$$

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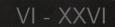
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- ◆ 10 irreducible components over ℂ
- ullet 4 irreducible components over ${\mathbb R}$



takeaway message

There is no neural network whose function space is $\mathcal{E}^{\sigma} \cap \mathcal{M}_2$!

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Any neural network can parametrize at most one of the real irreducible components of $\mathcal{E}^{\sigma}\cap\mathcal{M}_{2}.$



 $W \in \mathbb{R}^{9 \times 9}$ is invariant under σ iff

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The linear space \mathcal{I}^{σ} of σ -invariant $W \in \mathbb{R}^{9 \times 9}$ intersected with the function space $\mathcal{M}_2 = \{W \in \mathbb{R}^{9 \times 9} \mid \operatorname{rank}(W) \leq 2\}$ is an irreducible algebraic variety $\cong \{A \in \mathbb{R}^{9 \times 3} \mid \operatorname{rank}(A) \leq 2\}.$

Consider $\mathcal{M}_r = \{W \in \mathbb{R}^{m \times n} \mid \text{rank}(W) \leq r\}$ and $\sigma \in \mathcal{S}_n$.

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The set of G-invariant $W \in \mathbb{R}^{m \times n}$ is \mathcal{I}^{σ} for some $\sigma \in \mathcal{S}_n$.

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Invariance

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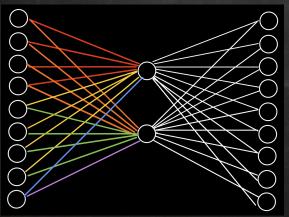
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Lemma: $\{(A, B) \in \mathbb{R}^{m \times k} \times \mathbb{R}^{k \times n} \mid \operatorname{rank}(AB) = k, AB \in \mathcal{I}^{\sigma}\} = \{A \in \mathbb{R}^{m \times k} \mid \operatorname{rank}(A) = k\} \times \{B \in \mathbb{R}^{k \times n} \mid \text{columns indexed by } \pi_i \text{ are equal}\}$ $\Rightarrow \sigma \text{ induces weight sharing on the encoder!}$



$$\sigma: \mathbb{R}^9 \longrightarrow \mathbb{R}^9, egin{array}{c|cccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ \hline \end{array} \longmapsto egin{array}{c|cccc} a_{31} & a_{21} & a_{11} \\ a_{32} & a_{22} & a_{12} \\ a_{33} & a_{23} & a_{13} \\ \hline \end{array}$$



has function space $\mathcal{I}^{\sigma} \cap \mathcal{M}_2$

Consider
$$\mathcal{M}_r = \{W \in \mathbb{R}^{n \times n} \mid \text{rank}(W) \leq r\}$$
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Idea: Let $T \in GL_n$.

W is P_{σ} -equivariant iff $T^{-1}WT$ is $T^{-1}P_{\sigma}T$ -equivariant.

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W is P_{σ} -equivariant iff $T^{-1}WT$ is $T^{-1}P_{\sigma}T$ -equivariant.

This base change also preserves rank!

		a ₁₂					a ₁₁
$\sigma: \mathbb{R}^9 \longrightarrow \mathbb{R}^9, \mid$	a ₂₁	a ₂₂	a ₂₃	\longmapsto	a ₃₂	a ₂₂	a ₁₂
	a ₃₁	a ₃₂	a ₃₃		a ₃₃	a ₂₃	a ₁₃

$$P = P_{\sigma}$$



α_1	α_2	α_3	α_{4}	β_1	β_2	β_3	β_4	ε_3
α_{4}	α_1	α_2	α_3	β_4	β_1	β_2	β_3	ε_3
α_3	α_{4}	α_1	α_2	β_3	β_4	β_1	β_2	ε_3
α_2	α_3	α_{4}	α_1	β_2	β_3	β_4	β_1	ε_3
γ_1	γ_2	γ_3	γ_4	δ_1	δ_2	δ_3	δ_4	ε_{4}
γ_4	γ_1	γ_2	γ_3	1,000		δ_2		ε_{4}
γ_3	γ_4	γ_1	γ_2	δ_3	δ_4	δ_1	δ_2	ε_{4}
γ_2	γ_3	γ_4	γ_1	δ_2	δ_3	δ_4	δ_1	ε_{4}
ε_1	ε_1	ε_1	ε_1	ε_2	ε_2	ε_2	ε_2	ε_5 _
$\begin{array}{c} \gamma_1 \\ \gamma_4 \\ \gamma_3 \\ \gamma_2 \end{array}$	$\begin{array}{c} \gamma_2 \\ \gamma_1 \\ \gamma_4 \\ \gamma_3 \end{array}$	γ_3 γ_2 γ_1 γ_4	γ ₄ γ ₃ γ ₂ γ ₁	$\begin{array}{c c} \delta_1 \\ \delta_4 \\ \delta_3 \\ \delta_2 \end{array}$	δ_2 δ_1 δ_4 δ_3	δ_3 δ_2 δ_1 δ_4	$ \delta_4 $ $ \delta_3 $ $ \delta_2 $ $ \delta_1 $	ε ₄ ε ₄ ε ₄ ε ₄

$$\sigma: \mathbb{R}^9 \longrightarrow \mathbb{R}^9, egin{array}{c|cccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ \hline \end{array} \longmapsto egin{array}{c|cccc} a_{31} & a_{21} & a_{11} \\ a_{32} & a_{22} & a_{12} \\ a_{33} & a_{23} & a_{13} \\ \hline \end{array}$$

 $P = \text{diagonalization of } P_{\sigma}$

0 0 0	i	$\begin{array}{c} 0 \\ 0 \\ -1 \\ 0 \end{array}$	0 0 0 -i			0		0
		3 4		1	0	0	0	1/8
		0		0	i	0	0	0
		U		0	0	-1	0	0
				0	0	0	-i	
		0				0		1

a ₁₁	0	0	0	a ₁₂	0	0	0	a ₁₃ -
0	c ₁₁	0	0	0	c ₁₂	0	0	0
0	0	b_{11}	0	0	0	b_{12}	0	0
0	0	0	d_{11}	0	0	0	d_{12}	0
a ₂₁	0	0	0	a ₂₂	0	0	0	a ₂₃
0	c ₂₁	0	0	0	C ₂₂	0	- 0	0
0	0	b ₂₁	0	0	0	b ₂₂	0	0
0	0	0	d_{21}	0	0	0	d_{22}	0
a ₃₁	0	0	0	a ₃₂	0	0	0	a ₃₃ _

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$$\begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 1 & & & \\ & & & -1 & & & \\ & & & & -i & & \\ & & & & -i & & \\ \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} & & & \\ a_{21} & a_{22} & a_{23} & & & \\ a_{31} & a_{32} & a_{33} & & & \\ & & & b_{11} & b_{12} & & \\ & & & b_{21} & b_{22} & & \\ & & & & c_{11} & c_{12} & \\ & & & & c_{21} & c_{22} & \\ & & & & d_{11} & d_{12} & \\ & & & & d_{21} & d_{22} & \\ \end{bmatrix}$$

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 \rightsquigarrow 6 components of $\mathcal{E}^{\sigma} \cap \mathcal{M}_2$



Consider $\mathcal{M}_r = \{W \in \mathbb{R}^{n \times n} \mid \text{rank}(W) \leq r\}$ and $\sigma \in \mathcal{S}_n$ represented by $P_{\sigma} \in \mathbb{R}^{n \times n}$.

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Lemma: A matrix $W \in \mathbb{R}^{n \times n}$ is σ -equivariant iff each block is a (possily non-square) circulant matrix.

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 $\#(\mathbb{Z}/1\mathbb{Z})^{\times} = 1, \ \#(\mathbb{Z}/2\mathbb{Z})^{\times} = 1, \ \#(\mathbb{Z}/4\mathbb{Z})^{\times} = 2$

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Theorem: The irreducible components of $\mathcal{E}^{\sigma} \cap \mathcal{M}_r$ over \mathbb{C} are in 1-to-1 correspondence with the integer solutions $(r_{m,u})$ of

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The component indexed by $(r_{m,u})$ is

$$\cong \prod_{m\in\mathbb{Z}_{>0}} \prod_{u\in(\mathbb{Z}/m\mathbb{Z})^\times} \{A\in\mathbb{C}^{d_m\times d_m}\mid \mathrm{rank}(A)\leq r_{m,u}\}.$$

Equivariance over $\mathbb R$

Consider $\mathcal{M}_r = \{W \in \mathbb{R}^{n \times n} \mid \text{rank}(W) \leq r\}$ and $\sigma \in \mathcal{S}_n$.

To diagonalize P_{σ} , we need a complex base change!

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This new basis can be scaled to become orthonormal!

Example: to diagonalize
$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$
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$$ightharpoonup rac{1}{2} egin{bmatrix} 1 & \sqrt{2} & 1 & 0 \ 1 & 0 & -1 & -\sqrt{2} \ 1 & -\sqrt{2} & 1 & 0 \ 1 & 0 & -1 & \sqrt{2} \ \end{pmatrix} \in O_4(\mathbb{R})$$

$$P=P_{\sigma}$$
 after $O_{9}(\mathbb{R})$ -base change

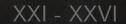
$$W = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ & & b_{11} & b_{12} \\ & & b_{21} & b_{22} \\ & & & c_1 & -c_2 & d_1 & -d_2 \\ & & & c_2 & c_1 & d_2 & d_1 \\ & & & e_1 & -e_2 & f_1 & -f_2 \\ & & & e_2 & e_1 & f_2 & f_1 \end{bmatrix}$$

There are 4 ways how W can have rank 2:

$$W = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ & & b_{11} & b_{12} \\ & & b_{21} & b_{22} \\ & & & c_1 & -c_2 & d_1 & -d_2 \\ & & & c_2 & c_1 & d_2 & d_1 \\ & & & e_1 & -e_2 & f_1 & -f_2 \\ & & & e_2 & e_1 & f_2 & f_1 \end{bmatrix}$$

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There are $\frac{4}{4}$ ways how W can have rank 2:

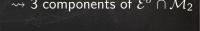
• One of the diagonal blocks has rank 2; \longrightarrow 3 components of $\mathcal{E}^{\sigma} \cap \mathcal{M}_2$ other blocks are 0

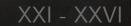


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- Two first 2 blocks have rank 1; last block is 0





running example

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

$$b_{11} & b_{12}$$

$$b_{21} & b_{22}$$

$$c_1 & -c_2 & d_1 & -d_2 \\ c_2 & c_1 & d_2 & d_1 \\ e_1 & -e_2 & f_1 & -f_2 \\ e_2 & e_1 & f_2 & f_1 \end{bmatrix}$$

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 \Rightarrow we can list all irreducible components of $\mathcal{E}^{\sigma} \cap \mathcal{M}_r$, parametrize them via autoencoders, understand their algebraic properties such as dimension, degree, ...



Which of these 4 components is best ??

$$W = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ & & b_{11} & b_{12} \\ & & & c_1 & -c_2 & d_1 & -d_2 \\ & & & c_2 & c_1 & d_2 & d_1 \\ & & & e_1 & -e_2 & f_1 & -f_2 \\ & & & e_2 & e_1 & f_2 & f_1 \end{bmatrix}$$

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Lemma: Given a sufficient amount of training data that is sufficiently generic, training a network with function space $\mathcal M$ using the squared-error loss means to solve an optimization problem of the form

 $\min_{W \in \mathcal{M}} \|W - U\|_F^2$, where U is a generic matrix encoding the data.

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- 2. $\mathsf{EDdeg}(\mathcal{X} \times \mathcal{Y}) = \mathsf{EDdeg}(\mathcal{X}) \cdot \mathsf{EDdeg}(\mathcal{Y})$
- 3. EDdeg $(\mathcal{X}_{s,d}) = \binom{d}{s}$, where $\mathcal{X}_{s,d}$ is either the space of $d \times d$ matrices of rank $\leq s$ or of $2d \times 2d$ matrices of rank $\leq 2s$ that consist of $\begin{bmatrix} a & -b \\ b & a \end{bmatrix}$ submatrices

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There are 4 ways how W can have rank 2:

- One of the diagonal blocks has rank 2;
 with EDdeg 3, 1, and 2, respectively.
- Two first 2 blocks have rank 1;
 with EDdeg 3 ⋅ 2 = 6.

 \leadsto 3 components of $\mathcal{E}^{\sigma}\cap\mathcal{M}_2$

 \leadsto 1 component of $\mathcal{E}^{\sigma} \cap \mathcal{M}_2$



Data science requires us to rethink the schism between mathematical disciplines!

> differential geometry ⇒ algebraic geometry ⇒

data science ⇒

Paul Breiding, Kathlén Kohn and Bernd Sturmfels

Metric Algebraic Geometry

5.2 Optimal Transport and Independence Models . . 5.3 Wasserstein meets Segre-Veronese

6.1 Plane Curves

7.3 Offset Discriminant.....

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