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

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joint work with

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Algebra & Geometry $\Rightarrow$ Neural Network Theory

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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?

Algebra & Geometry ⇒ Neural Network Theory

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Algebraic settings:

network architecture		
activation	**network structure**	**loss**

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identity		
ReLU		
polynomial		

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activation	**network structure**	**loss**
identity	fully-connected	
ReLU	convolutional	
polynomial	group equivariant	

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identity	fully-connected	squared-error loss	= Euclidean dist
ReLU	convolutional	Wasserstein distance	= polyhedral dist.
polynomial	group equivariant	cross-entropy	$\cong$ KL divergence

Algebra & Geometry ⇒ Neural Network Theory

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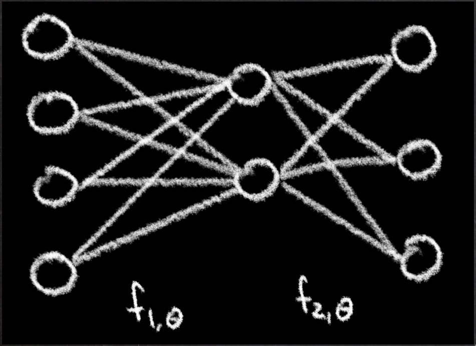
Linear Fully-Connected Networks

activation = identity & network structure = fully-connected



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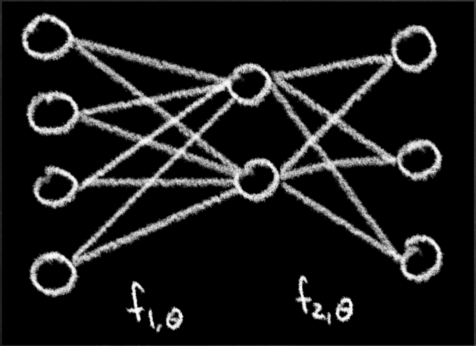

This network parametrizes linear maps:

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

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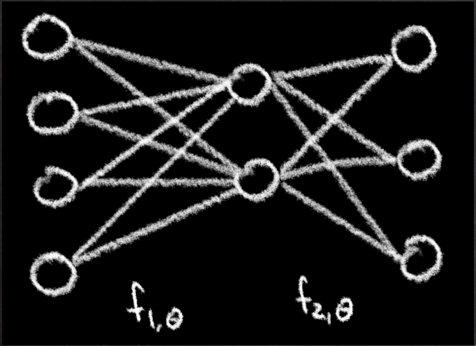

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Its function space is

$$\mathcal{M}_2 = \{W \in \mathbb{R}^{3\times 4} \mid \operatorname{rank}(W) \leq 2\}.$$

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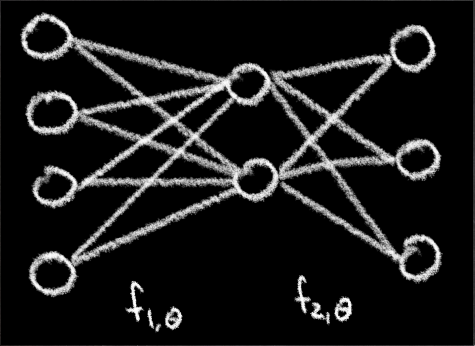

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In general: $\mu : \mathbb{R}^{k_1\times k_0} \times \mathbb{R}^{k_2\times k_1} \times \ldots \times \mathbb{R}^{k_L\times k_{L-1}} \longrightarrow \mathbb{R}^{k_L\times k_0},$

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

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

Linear Group-Equivariant Networks

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}
a_{31}	a_{32}	a_{33}

$\in \mathbb{R}^9$.

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Consider the clockwise rotation by 90°:

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

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

example cont'd

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is represented by the permutation matrix

$$P_\sigma = \left[\begin{array}{c|c|c} \begin{matrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{matrix} & 0 & 0 \\ \hline 0 & \begin{matrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{matrix} & 0 \\ \hline 0 & 0 & 1 \end{array}\right]$$

example cont'd

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$W \in \mathbb{R}^{9\times 9}$

is equivariant under σ

$\Leftrightarrow$

$W \cdot P_\sigma = P_\sigma \cdot W.$

example cont'd

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$W \in \mathbb{R}^{9\times 9}$
is invariant under σ
$\Leftrightarrow$
$W \cdot P_\sigma = W$.

example cont'd

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

$$W = \left[\begin{array}{cccc|cccc|c}
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \beta_1 & \beta_2 & \beta_3 & \beta_4 & \varepsilon_3 \\
\alpha_4 & \alpha_1 & \alpha_2 & \alpha_3 & \beta_4 & \beta_1 & \beta_2 & \beta_3 & \varepsilon_3 \\
\alpha_3 & \alpha_4 & \alpha_1 & \alpha_2 & \beta_3 & \beta_4 & \beta_1 & \beta_2 & \varepsilon_3 \\
\alpha_2 & \alpha_3 & \alpha_4 & \alpha_1 & \beta_2 & \beta_3 & \beta_4 & \beta_1 & \varepsilon_3 \\
\hline
\gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \delta_1 & \delta_2 & \delta_3 & \delta_4 & \varepsilon_4 \\
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\hline
\varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_5
\end{array}\right].$$

example cont'd

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The linear space $\mathcal{E}^\sigma$ of σ-equivariant $W \in \mathbb{R}^{9\times 9}$

example cont'd

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The linear space $\mathcal{E}^\sigma$ of σ-equivariant $W \in \mathbb{R}^{9\times 9}$ intersected with the function space $\mathcal{M}_2 = \{W \in \mathbb{R}^{9\times 9} \mid \mathrm{rank}(W) \leq 2\}$ of our autoencoder is an algebraic variety with

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

takeaway message

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

takeaway message

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

Any neural network can parametrize at most one of the real irreducible components of $\mathcal{E}^\sigma \cap \mathcal{M}_2$.

example cont'd

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

Invariance

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

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Decompose $\sigma = \pi_1 \circ \pi_2 \circ \ldots \circ \pi_k$ into disjoint cycles.

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Lemma: The linear space $\mathcal{I}^\sigma$ of σ-invariant $W \in \mathbb{R}^{m \times n}$ consists of all matrices W whose columns indexed by π_i are equal, for all $i = 1, 2, \ldots, k$.

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

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What are all ways to parametrize $I^\sigma \cap \mathcal{M}_r$ with autoencoders?

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

Decompose $\sigma = \pi_1 \circ \pi_2 \circ \ldots \circ \pi_k$ into disjoint cycles.

Lemma: The linear space $\mathcal{I}^\sigma$ of σ-invariant $W \in \mathbb{R}^{m\times n}$ consists of all matrices W whose columns indexed by π_i are equal, for all $i = 1, 2, \ldots, k$. Hence, $\mathcal{I}^\sigma \cap \mathcal{M}_r \cong \{W \in \mathbb{R}^{m\times k} \mid \mathrm{rank}(W) \leq r\}$ is an irreducible variety.

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

What are all ways to parametrize $I^\sigma \cap \mathcal{M}_r$ with autoencoders?

Lemma: $\{(A, B) \in \mathbb{R}^{m\times k} \times \mathbb{R}^{k\times n} \mid \mathrm{rank}(AB) = k, AB \in \mathcal{I}^\sigma\} =$

Invariance

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

Decompose $\sigma = \pi_1 \circ \pi_2 \circ \ldots \circ \pi_k$ into disjoint cycles.

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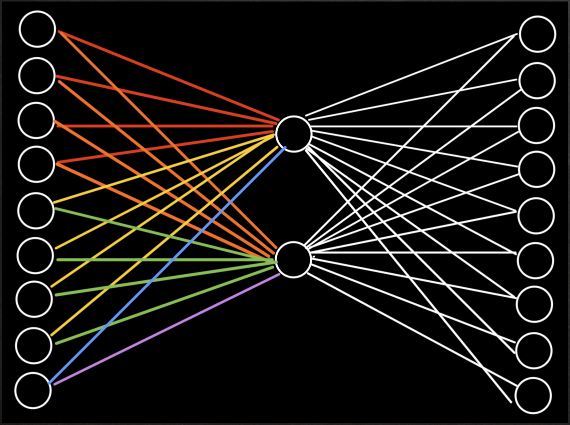
$\{A \in \mathbb{R}^{m\times k} \mid \mathrm{rank}(A) = k\} \times \{B \in \mathbb{R}^{k\times n} \mid \text{columns indexed by } \pi_i \text{ are equal}\}$

$\Rightarrow$ σ induces weight sharing on the encoder!

running example

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



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

Equivariance

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

Equivariance

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

Idea: Let $T \in \mathrm{GL}_n$.
W is P_σ-equivariant iff $T^{-1}WT$ is $T^{-1}P_\sigma T$-equivariant.

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

Idea: Let $T \in \mathrm{GL}_n$.
W is P_σ-equivariant iff $T^{-1}WT$ is $T^{-1}P_\sigma T$-equivariant.

This base change also preserves rank!

running example

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

$P = P_\sigma$

$$\left[\begin{array}{cccc|cccc|c} 0 & 0 & 0 & 1 & & & & & \\ 1 & 0 & 0 & 0 & & & & & \\ 0 & 1 & 0 & 0 & & 0 & & & 0 \\ 0 & 0 & 1 & 0 & & & & & \\ \hline & & & & 0 & 0 & 0 & 1 & \\ & & & & 1 & 0 & 0 & 0 & \\ & & 0 & & 0 & 1 & 0 & 0 & 0 \\ & & & & 0 & 0 & 1 & 0 & \\ \hline & & 0 & & & & 0 & & 1 \end{array}\right]$$

P-equivariant matrices

$$\left[\begin{array}{cccc|cccc|c} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \beta_1 & \beta_2 & \beta_3 & \beta_4 & \varepsilon_3 \\ \alpha_4 & \alpha_1 & \alpha_2 & \alpha_3 & \beta_4 & \beta_1 & \beta_2 & \beta_3 & \varepsilon_3 \\ \alpha_3 & \alpha_4 & \alpha_1 & \alpha_2 & \beta_3 & \beta_4 & \beta_1 & \beta_2 & \varepsilon_3 \\ \alpha_2 & \alpha_3 & \alpha_4 & \alpha_1 & \beta_2 & \beta_3 & \beta_4 & \beta_1 & \varepsilon_3 \\ \hline \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \delta_1 & \delta_2 & \delta_3 & \delta_4 & \varepsilon_4 \\ \gamma_4 & \gamma_1 & \gamma_2 & \gamma_3 & \delta_4 & \delta_1 & \delta_2 & \delta_3 & \varepsilon_4 \\ \gamma_3 & \gamma_4 & \gamma_1 & \gamma_2 & \delta_3 & \delta_4 & \delta_1 & \delta_2 & \varepsilon_4 \\ \gamma_2 & \gamma_3 & \gamma_4 & \gamma_1 & \delta_2 & \delta_3 & \delta_4 & \delta_1 & \varepsilon_4 \\ \hline \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_5 \end{array}\right]$$

running example

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

P = diagonalization of P_σ

$$\left[\begin{array}{cccc|cccc|c} 1 & 0 & 0 & 0 & & & & & \\ 0 & i & 0 & 0 & & 0 & & & 0 \\ 0 & 0 & -1 & 0 & & & & & \\ 0 & 0 & 0 & -i & & & & & \\ \hline & & & & 1 & 0 & 0 & 0 & \\ & 0 & & & 0 & i & 0 & 0 & 0 \\ & & & & 0 & 0 & -1 & 0 & \\ & & & & 0 & 0 & 0 & -i & \\ \hline & 0 & & & & 0 & & & 1 \end{array}\right]$$

P-equivariant matrices

$$\left[\begin{array}{cccc|cccc|c} a_{11} & 0 & 0 & 0 & a_{12} & 0 & 0 & 0 & a_{13} \\ 0 & c_{11} & 0 & 0 & 0 & c_{12} & 0 & 0 & 0 \\ 0 & 0 & b_{11} & 0 & 0 & 0 & b_{12} & 0 & 0 \\ 0 & 0 & 0 & d_{11} & 0 & 0 & 0 & d_{12} & 0 \\ \hline a_{21} & 0 & 0 & 0 & a_{22} & 0 & 0 & 0 & a_{23} \\ 0 & c_{21} & 0 & 0 & 0 & c_{22} & 0 & 0 & 0 \\ 0 & 0 & b_{21} & 0 & 0 & 0 & b_{22} & 0 & 0 \\ 0 & 0 & 0 & d_{21} & 0 & 0 & 0 & d_{22} & 0 \\ \hline a_{31} & 0 & 0 & 0 & a_{32} & 0 & 0 & 0 & a_{33} \end{array}\right]$$

running example

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

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$$\begin{bmatrix} 1 &&&&&&&& \\ & 1 &&&&&&& \\ && 1 &&&&&& \\ &&& -1 &&&&& \\ &&&& -1 &&&& \\ &&&&& i &&& \\ &&&&&& i && \\ &&&&&&& -i & \\ &&&&&&&& -i \end{bmatrix}$$

P-equivariant matrices

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

running example

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

There are 10 ways how W can have rank 2:

running example

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

There are 10 ways how W can have rank 2:

- One of the diagonal blocks has rank 2; other blocks are 0

running example

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

There are 10 ways how W can have rank 2:

- One of the diagonal blocks has rank 2; other blocks are 0 $\rightsquigarrow$ 4 components of $\mathcal{E}^\sigma \cap \mathcal{M}_2$

running example

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

There are 10 ways how W can have rank 2:

- One of the diagonal blocks has rank 2; other blocks are 0 $\rightsquigarrow$ 4 components of $\mathcal{E}^\sigma \cap \mathcal{M}_2$
- Two distinct blocks have rank 1; other blocks are 0

running example

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

There are 10 ways how W can have rank 2:

- One of the diagonal blocks has rank 2; other blocks are 0 $\rightsquigarrow$ 4 components of $\mathcal{E}^\sigma \cap \mathcal{M}_2$
- Two distinct blocks have rank 1; other blocks are 0 $\rightsquigarrow$ 6 components of $\mathcal{E}^\sigma \cap \mathcal{M}_2$

Equivariance

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

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Chop W into blocks following the same pattern!

$$P_\sigma = \left[\begin{array}{cccc|cccc|c} 0&0&0&1 & & & & & \\ 1&0&0&0 & &0& & & 0\\ 0&1&0&0 & & & & & \\ 0&0&1&0 & & & & & \\ \hline & & & & 0&0&0&1 & \\ &0& & & 1&0&0&0 & 0\\ & & & & 0&1&0&0 & \\ & & & & 0&0&1&0 & \\ \hline &0& & & &0& & & 1 \end{array}\right] \qquad W = \left[\begin{array}{cccc|cccc|c} \alpha_1&\alpha_2&\alpha_3&\alpha_4 & \beta_1&\beta_2&\beta_3&\beta_4 & \varepsilon_3\\ \alpha_4&\alpha_1&\alpha_2&\alpha_3 & \beta_4&\beta_1&\beta_2&\beta_3 & \varepsilon_3\\ \alpha_3&\alpha_4&\alpha_1&\alpha_2 & \beta_3&\beta_4&\beta_1&\beta_2 & \varepsilon_3\\ \alpha_2&\alpha_3&\alpha_4&\alpha_1 & \beta_2&\beta_3&\beta_4&\beta_1 & \varepsilon_3\\ \hline \gamma_1&\gamma_2&\gamma_3&\gamma_4 & \delta_1&\delta_2&\delta_3&\delta_4 & \varepsilon_4\\ \gamma_4&\gamma_1&\gamma_2&\gamma_3 & \delta_4&\delta_1&\delta_2&\delta_3 & \varepsilon_4\\ \gamma_3&\gamma_4&\gamma_1&\gamma_2 & \delta_3&\delta_4&\delta_1&\delta_2 & \varepsilon_4\\ \gamma_2&\gamma_3&\gamma_4&\gamma_1 & \delta_2&\delta_3&\delta_4&\delta_1 & \varepsilon_4\\ \hline \varepsilon_1&\varepsilon_1&\varepsilon_1&\varepsilon_1 & \varepsilon_2&\varepsilon_2&\varepsilon_2&\varepsilon_2 & \varepsilon_5 \end{array}\right]$$

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

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$$P_\sigma = \left[\begin{array}{cccc|cccc|c} 0 & 0 & 0 & 1 & & & & & \\ 1 & 0 & 0 & 0 & & 0 & & & 0 \\ 0 & 1 & 0 & 0 & & & & & \\ 0 & 0 & 1 & 0 & & & & & \\ \hline & & & & 0 & 0 & 0 & 1 & \\ & 0 & & & 1 & 0 & 0 & 0 & 0 \\ & & & & 0 & 1 & 0 & 0 & \\ & & & & 0 & 0 & 1 & 0 & \\ \hline & 0 & & & & 0 & & & 1 \end{array}\right] \qquad W = \left[\begin{array}{cccc|cccc|c} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \beta_1 & \beta_2 & \beta_3 & \beta_4 & \varepsilon_3 \\ \alpha_4 & \alpha_1 & \alpha_2 & \alpha_3 & \beta_4 & \beta_1 & \beta_2 & \beta_3 & \varepsilon_3 \\ \alpha_3 & \alpha_4 & \alpha_1 & \alpha_2 & \beta_3 & \beta_4 & \beta_1 & \beta_2 & \varepsilon_3 \\ \alpha_2 & \alpha_3 & \alpha_4 & \alpha_1 & \beta_2 & \beta_3 & \beta_4 & \beta_1 & \varepsilon_3 \\ \hline \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \delta_1 & \delta_2 & \delta_3 & \delta_4 & \varepsilon_4 \\ \gamma_4 & \gamma_1 & \gamma_2 & \gamma_3 & \delta_4 & \delta_1 & \delta_2 & \delta_3 & \varepsilon_4 \\ \gamma_3 & \gamma_4 & \gamma_1 & \gamma_2 & \delta_3 & \delta_4 & \delta_1 & \delta_2 & \varepsilon_4 \\ \gamma_2 & \gamma_3 & \gamma_4 & \gamma_1 & \delta_2 & \delta_3 & \delta_4 & \delta_1 & \varepsilon_4 \\ \hline \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_5 \end{array}\right]$$

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

Equivariance

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

The decomposition $\sigma = \pi_1 \circ \ldots \circ \pi_k$ into disjoint cycles chops P_σ into blocks.
Chop W into blocks following the same pattern!

$$P_\sigma = \left[\begin{array}{cccc|cccc|c} 0 & 0 & 0 & 1 & & & & & \\ 1 & 0 & 0 & 0 & & 0 & & & 0 \\ 0 & 1 & 0 & 0 & & & & & \\ 0 & 0 & 1 & 0 & & & & & \\ \hline & & & & 0 & 0 & 0 & 1 & \\ & 0 & & & 1 & 0 & 0 & 0 & 0 \\ & & & & 0 & 1 & 0 & 0 & \\ & & & & 0 & 0 & 1 & 0 & \\ \hline & 0 & & & & 0 & & & 1 \end{array}\right] \qquad W = \left[\begin{array}{cccc|cccc|c} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \beta_1 & \beta_2 & \beta_3 & \beta_4 & \varepsilon_3 \\ \alpha_4 & \alpha_1 & \alpha_2 & \alpha_3 & \beta_4 & \beta_1 & \beta_2 & \beta_3 & \varepsilon_3 \\ \alpha_3 & \alpha_4 & \alpha_1 & \alpha_2 & \beta_3 & \beta_4 & \beta_1 & \beta_2 & \varepsilon_3 \\ \alpha_2 & \alpha_3 & \alpha_4 & \alpha_1 & \beta_2 & \beta_3 & \beta_4 & \beta_1 & \varepsilon_3 \\ \hline \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \delta_1 & \delta_2 & \delta_3 & \delta_4 & \varepsilon_4 \\ \gamma_4 & \gamma_1 & \gamma_2 & \gamma_3 & \delta_4 & \delta_1 & \delta_2 & \delta_3 & \varepsilon_4 \\ \gamma_3 & \gamma_4 & \gamma_1 & \gamma_2 & \delta_3 & \delta_4 & \delta_1 & \delta_2 & \varepsilon_4 \\ \gamma_2 & \gamma_3 & \gamma_4 & \gamma_1 & \delta_2 & \delta_3 & \delta_4 & \delta_1 & \varepsilon_4 \\ \hline \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_1 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_2 & \varepsilon_5 \end{array}\right]$$

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

$$\begin{bmatrix} a & a & a \\ a & a & a \\ a & a & a \\ a & a & a \end{bmatrix}, \quad \begin{bmatrix} a & a & a \\ a & a & a \end{bmatrix}, \quad \begin{bmatrix} a & b & a & b \\ b & a & b & a \end{bmatrix}, \quad \ldots$$

Equivariance

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

Decompose $\sigma = \pi_1 \circ \ldots \circ \pi_k$ into disjoint cycles and let $\ell_j :=$ length(π_j).

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Diagonalize P_σ and sort the eigenvalues. This yields the diagonal matrix P.

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Lemma: A matrix $W \in \mathbb{R}^{n\times n}$ is P-equivariant iff its block diagonal with $\#(\mathbb{Z}/m\mathbb{Z})^\times$ many blocks of size $d_m \times d_m$, where $d_m := \#\{j$ such that $m|\ell_j\}$.

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

$\ell_1 = 4,\ \ell_2 = 4,\ \ell_3 = 1$

Equivariance

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

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

$\ell_1 = 4,\ \ell_2 = 4,\ \ell_3 = 1$

$d_1 = 3,\ d_2 = 2,\ d_3 = 0,\ d_4 = 2,\ d_5 = 0,\ \ldots$

Equivariance

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

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

$\ell_1 = 4,\ \ell_2 = 4,\ \ell_3 = 1$

$d_1 = 3,\ d_2 = 2,\ d_3 = 0,\ d_4 = 2,\ d_5 = 0,\ \ldots$

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

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

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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

$$\sum_{m\in\mathbb{Z}_{>0}} \sum_{u\in(\mathbb{Z}/m\mathbb{Z})^\times} r_{m,u} = r, \qquad \text{where } 0 \leq r_{m,u} \leq d_m.$$

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

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

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Example: to diagonalize $\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$, use base change $\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix}$

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$$\rightsquigarrow \frac{1}{2}\begin{bmatrix} 1 & \sqrt{2} & 1 & 0 \\ 1 & 0 & -1 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 & 0 \\ 1 & 0 & -1 & \sqrt{2} \end{bmatrix} \in O_4(\mathbb{R})$$

running example

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

$P = P_\sigma$ after $O_9(\mathbb{R})$-base change

$$\begin{bmatrix} 1 &&&&&&&& \\ & 1 &&&&&&& \\ && 1 &&&&&& \\ &&& -1 &&&&& \\ &&&& -1 &&&& \\ &&&&& 0 & 1 && \\ &&&&& -1 & 0 && \\ &&&&&&& 0 & 1 \\ &&&&&&& -1 & 0 \end{bmatrix}$$

P-equivariant matrices

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

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

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In general: After the $O_n(\mathbb{R})$-base change, the σ-equivariant matrices become block diagonal:

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parametrize them via autoencoders,
understand their algebraic properties such as dimension, degree, ...

Which of these 4 components is best ??

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- One of the diagonal blocks has rank 2; other blocks are 0 $\rightsquigarrow$ 3 components of $\mathcal{E}^\sigma \cap \mathcal{M}_2$
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Euclidean distance degree

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

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

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3. $\mathrm{EDdeg}(\mathcal{X}_{s,d}) = \binom{d}{s}$, 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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- One of the diagonal blocks has rank 2; $\rightsquigarrow$ 3 components of $\mathcal{E}^\sigma \cap \mathcal{M}_2$
  with EDdeg 3, 1, and 2, respectively.
- Two first 2 blocks have rank 1; $\rightsquigarrow$ 1 component of $\mathcal{E}^\sigma \cap \mathcal{M}_2$
  with EDdeg $3 \cdot 2 = 6$.

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

Springer Nature