Geometric Deep Learning

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7.11.2024

Part V: Invariance through group smoothing

Label function invariant under group action

Invariant function class

Assume we want to learn a function f^* with

$$\forall x \in \mathcal{X}, g \in G: \ f^*(g.x) = f^*(x)$$

$\implies$ Function is constant within each orbit.

Example

$G = \mathbb{Z}/4\mathbb{Z} = C(4)$ cyclic group, acting as 90° rotations:

f^* () $=$ f^* () $=$ f^* ()

$=$ f^* () $=$ "airplane"

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How can we construct a hypothesis class that respects this constraint?

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Group smoothing operator

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Let $f : \mathcal{X} \longrightarrow \mathcal{Y}$, and G be a finite group with an action $.$ on $\mathcal{X}$. Define **group smoothing** through

$$\Sigma_G f(x) := |G|^{-1} \sum_{g \in G} f(g.x) \,.$$

$\implies$ Average over all elements within an orbit.

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Acts as identity on invariant functions:

$\Sigma_G f^* = f^*$.

$\implies$ Σ_G is a prjection.

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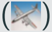
$\Sigma_G f\,($  $) = \frac{1}{4}\Big(f\,($  $) + f\,($  $)$

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Invariant hypothesis class through group smoothing

Smoothed hypothesis class

Let $\mathcal{F} \subset \{f : \mathcal{X} \longrightarrow \mathcal{Y}\}$ be a hypothesis class, define

$$\Sigma_G \mathcal{F} \coloneqq \{\Sigma_G f : f \in \mathcal{F}\}$$

Example

$\mathcal{X} = \{\text{space of } 3 \times 3 \text{ images}\}$,
$\mathcal{F} = \{\text{linear functions}\} = \mathbb{R}^{3\times 3}$
$\Sigma_G \mathcal{F} = ?$

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$$\Sigma_G f(\boldsymbol{x}) = 0.25 \sum_{g \in G} \langle \boldsymbol{f}, P_g \boldsymbol{x} \rangle ,$$

where P_g: permutation matrix corresponding to rotation.

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Rotation-invariant 3×3 linear functions

Original Basis

The 3×3 linear functions are generated by a basis

$\mathcal{F} = \mathrm{span}\{$ , , ,
, , ,
, ,  $\}$

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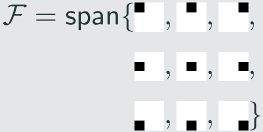
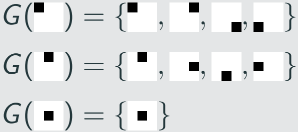


Orbits

Basis vectors fall intro three orbits



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$$\mathcal{F} = \operatorname{span}\left\{ \begin{bmatrix}1&0&0\\0&0&0\\0&0&0\end{bmatrix}, \begin{bmatrix}0&1&0\\0&0&0\\0&0&0\end{bmatrix}, \begin{bmatrix}0&0&1\\0&0&0\\0&0&0\end{bmatrix}, \begin{bmatrix}0&0&0\\1&0&0\\0&0&0\end{bmatrix}, \begin{bmatrix}0&0&0\\0&1&0\\0&0&0\end{bmatrix}, \begin{bmatrix}0&0&0\\0&0&1\\0&0&0\end{bmatrix}, \begin{bmatrix}0&0&0\\0&0&0\\1&0&0\end{bmatrix}, \begin{bmatrix}0&0&0\\0&0&0\\0&1&0\end{bmatrix}, \begin{bmatrix}0&0&0\\0&0&0\\0&0&1\end{bmatrix} \right\}$$

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Reduced Basis

The rotation-invariant functions have a three-dimensional basis

$$\Sigma_G \mathcal{F} = \operatorname{span}\left\{ \begin{bmatrix}1&0&1\\0&0&0\\1&0&1\end{bmatrix}, \begin{bmatrix}0&1&0\\1&0&1\\0&1&0\end{bmatrix}, \begin{bmatrix}0&0&0\\0&1&0\\0&0&0\end{bmatrix} \right\}$$

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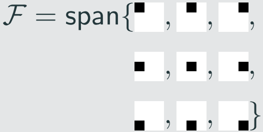

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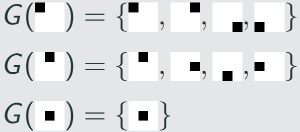

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The rotation-invariant functions have a three-dimensional basis

$\Longrightarrow$ **Rotation-invariance reduced dimensionality by a factor of 3**

G-smoothing is an orthogonal projection

Group action as permutation

Reminder: For a one-dimensional signal $x \in \mathcal{X}(\Omega, \mathbb{R})$ over a finite domain Ω, the group action is given through:

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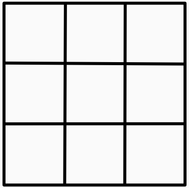

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4	5	6
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$$x = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{pmatrix}$$

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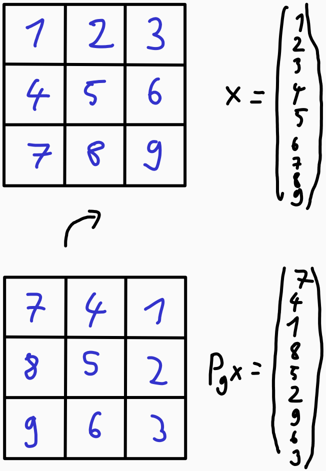

G-smoothing is an orthogonal projection

$$
\begin{aligned}
|G|\langle \Sigma_G \mathbf{x}, \mathbf{y}\rangle &= \langle \sum_{g\in G} P_g \mathbf{x}, \mathbf{y}\rangle && \text{(def.)}\\
&= \sum_{g\in G} \langle P_g \mathbf{x}, \mathbf{y}\rangle && \text{(linearity)}\\
&= \sum_{g\in G} \langle \mathbf{x}, P_g^{\mathsf{T}} \mathbf{y}\rangle && \text{(adjoint)}\\
&= \sum_{g\in G} \langle \mathbf{x}, P_{g^{-1}} \mathbf{y}\rangle && (P_g^{\mathsf{T}} = P_g^{-1})\\
&= \sum_{g'\in G} \langle \mathbf{x}, P_{g'} \mathbf{y}\rangle && \text{(change of var.)}\\
&= \langle \mathbf{x}, \sum_{g'\in G} P_{g'} \mathbf{y}\rangle = |G|\langle \mathbf{x}, \Sigma_G \mathbf{y}\rangle
\end{aligned}
$$

G-smoothing is an orthogonal projection

Σ_G is self-adjoint: $\langle \Sigma_G f, g \rangle = \langle f, \Sigma_G g \rangle$
This property allows to decompose inner products

$$
\begin{aligned}
\langle f, g \rangle &= \langle \Sigma_G f + (I - \Sigma_G) f, \Sigma_G g + (I - \Sigma_G) g \rangle \\
&= \langle \Sigma_G f, \Sigma_G g \rangle + \langle \Sigma_G f, (I - \Sigma_G) g \rangle + \langle (I - \Sigma_G) f, \Sigma_G g \rangle + \langle (I - \Sigma_G) f, (I - \Sigma_G) g \rangle \\
&= \langle \Sigma_G f, \Sigma_G g \rangle + \langle f, (\Sigma_G - \Sigma_G^2) g \rangle + \langle (\Sigma_G - \Sigma_G^2) f, g \rangle + \langle (I - \Sigma_G) f, (I - \Sigma_G) g \rangle \\
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&= \langle \Sigma_G f, \Sigma_G g \rangle + \langle (I - \Sigma_G) f, (I - \Sigma_G) g \rangle
\end{aligned}
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and Euclidian distances

$$
\|f - g\|^2 = \|\Sigma_G f - \Sigma_G g\|^2 + \|(I - \Sigma_G) f - (I - \Sigma_G) g\|^2
$$

G-smoothing cannot increase L_2 error

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\|f - f^*\|^2 &= \|\Sigma_G f - \Sigma_G f^*\|^2 + \|(I - \Sigma_G)f - (I - \Sigma_G)f^*\|^2 \\
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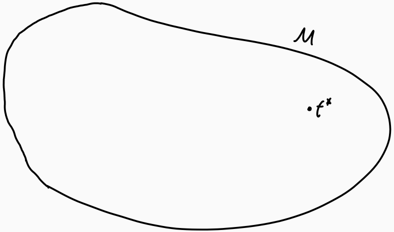

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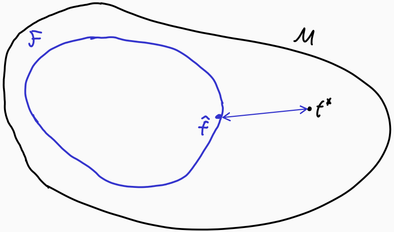

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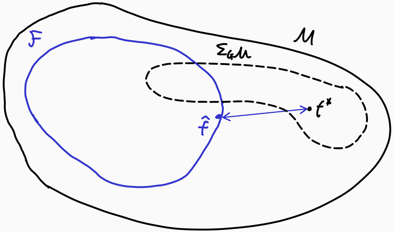

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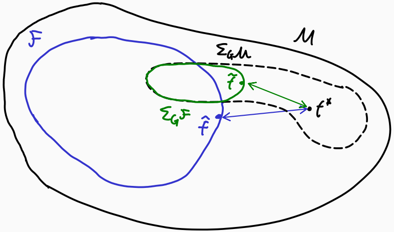

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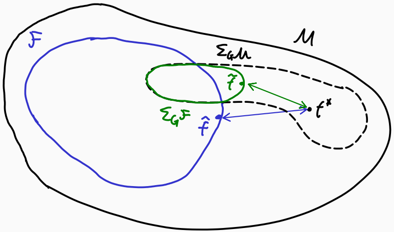

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$$\inf_{f \in \mathcal{F}} \|f - f^*\|^2 \geq \inf_{f \in \Sigma_G \mathcal{F}} \|f - f^*\|^2$$

If $\Sigma_G \mathcal{F} \subset \mathcal{F}$, we have equality.

G-smoothing of Lipschitz functions

Let $\mathcal{F}$ be the class of β-Lipschitz functions

and G act isometrically,

$|f(x)-f(x')| \leq \beta\|x-x'\|$ $\|g.x-g.x'\| = \|x-x'\|$.

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|\tilde{f}(x) - \tilde{f}(x')| &= \frac{1}{|G|}\left|\sum_g f(g.x) - \sum_g f(g.x')\right| \\
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&\leq \beta \min_h \left\|x - h.x'\right\|
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Isometric property is necessary?

Imagine $\Omega = \mathbb{R}^2$, $G = SO(2)$,

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g.\boldsymbol{x} = \begin{cases} \|\boldsymbol{x}\| = 1 : R_g \boldsymbol{x} \; R_g \text{ 2d-rotation} \\ \|\boldsymbol{x}\| \neq 1 : \boldsymbol{x} \end{cases}
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What is the "smoothed" version of $f(x, y) = x$?

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A non-continuous function

$\Sigma_G f(1, 1) = 0$, $\Sigma_G f(1, 1+\epsilon) = 1$

Sample complexity with G-smoothing

Ridge Regression

Using a G-invariant kernel ridge regression, the generalization error of learning a Lipshitz, G-invariant function f^* satisfies

$$\mathbb{E}[(f*(X) - \hat{f}(X))^2] < \mathcal{O}((|G|n)^{-1/d}) \,,$$

for d-dimensions.

Bietti, Venturi, and Bruna. (2021). "On the Sample Complexity of Learning under Geometric Stability"

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for d-dimensions.

- Group size $|G|$ could be exponential in d, $|G| \sim \alpha^d$, does not prevent $n^{-1/d}$
- Implementation very inefficient for large $|G|$

Bietti, Venturi, and Bruna. (2021). "On the Sample Complexity of Learning under Geometric Stability"

Part VI: Group Representations

Group Representations: Linear Group Actions

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Group Representation

A d-dimensional representation of a group G is a mapping

$$R : G \longrightarrow \mathrm{GL}(d) \subset \mathbb{R}^{d \times d}$$

that preserves the group structure (group *homomophism*)

$$\forall g, h \in G : R(g \circ h) = R(g)R(h)$$

Implies group action

$$\forall g \in G, v \in \mathbb{R}^d : g.v \mapsto R(g)v$$

Some examples of group representations

Given a group G, can you think of a 1-dimensional representation?

Some examples of group representations

Trivial representation

Given a group G, can you think of a 1-dimensional representation?

$$G \ni g \mapsto 1$$

Some examples of group representations

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$$G \ni g \mapsto 1$$

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$$r_\theta \mapsto \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

Permutation group

The permutation group $S(n)$ can be represented in $\mathbb{R}^n$ with permutation matrices, e.g.,

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Note: Transforming adjacency matrices is *not* a group representation: $g.A = P(g)AP(g)^T$

Representing Translations

A simple group action for two-dimensional translations $T_2 := (\mathbb{R}^2, +)$:

$$\boldsymbol{t} \in T_2, \boldsymbol{s} \in \mathbb{R}^2; (\boldsymbol{t}, \boldsymbol{s}) \mapsto \boldsymbol{t} + \boldsymbol{s}\,.$$

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$$(u, v) \mapsto \begin{pmatrix} \exp(u) & 0 \\ 0 & \exp(v) \end{pmatrix}$$

Composition:

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does not match desired group action

Embed group action into larger space to enable linear representation

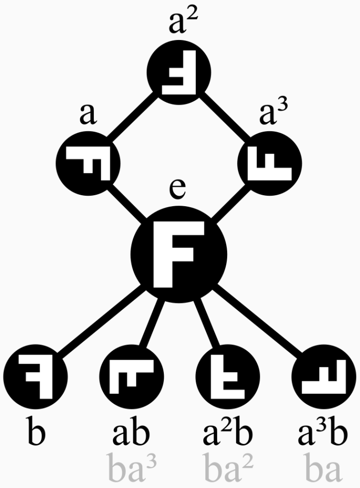
Expand target space to $\mathbb{R}^2 \times \{1\} \subset \mathbb{R}^3$.

$$(u, v) \mapsto \begin{pmatrix} 1 & 0 & u \\ 0 & 1 & v \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & u \\ 0 & 1 & v \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ 1 \end{pmatrix} = \begin{pmatrix} x + u \\ y + v \\ 1 \end{pmatrix}$$

Constructing representations of D4

- Observation: Specifying representation of generator is enough.
- For D4: rotation by 90° a, horizontal flip b
- $D_4 = \{e, a, a^2, a^3, b, ab, a^2b, a^3b\}$



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Constructing representations of D4: Necessariy Conditions

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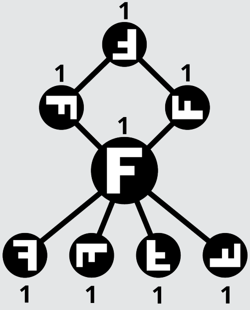
Note: Eigenvalues might be complex, so $\lambda \in 1, -1, i, -i$, $\mu \in 1, -1$

Constructing one-dimensional representations of D4

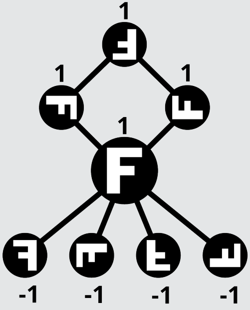
Candidates

$A = (\lambda), B = (\mu)$, real matrices $\implies \lambda \in 1, -1$.

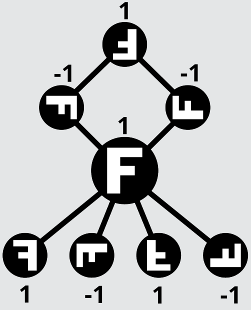
A1: $A = 1, B = 1$



A2: $A = 1, B = -1$



B1: $A = -1, B = 1$



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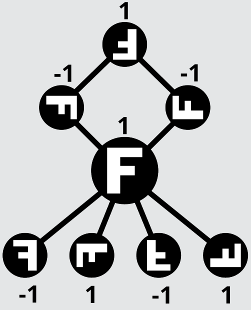

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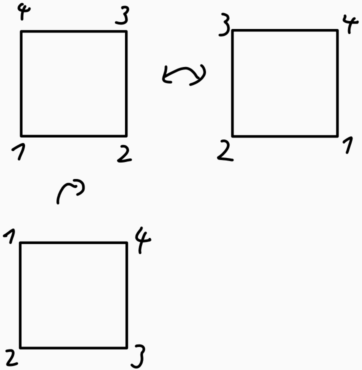

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$$R(a) = \begin{pmatrix} \cos 90 & -\sin 90 \\ \sin 90 & \cos 90 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

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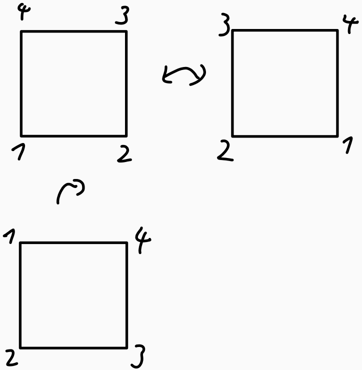

In $\mathbb{C}$, we can diagonalize this representation

This representation uses the complex Eigenvalues $i, -i$.

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = 0.5 \begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix} \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix}$$

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This is just two times B1 stacked on the diagonal!

Representations can be concatenated

Let A and B be two representations of G with dimension d_A and d_B. Then $A \oplus B$, the *direct sum* of A and B, defined through

$$(A \oplus B)(g) = \begin{pmatrix} A(g) & 0 \\ 0 & B(g) \end{pmatrix} \in \mathrm{GL}(d_A + d_B)\,,$$

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Example

Describing a spinning particle.

- Velocity: E (**vector**)
- Mass: A1 (**scalar**)
- Spin: A2 (**pseudoscalar**)

Full system: $E \oplus A1 \oplus A2$

Representations are preserved under change of basis

Let $J \in \mathrm{GL}(d)$, and R be a d-dimensional representation of group G.
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In particular $A \oplus B$ and $B \oplus A$ are equivalent.

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A representation is called **reducible** if it has a non-trivial *invariant subspace*:

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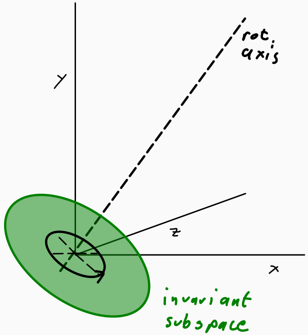

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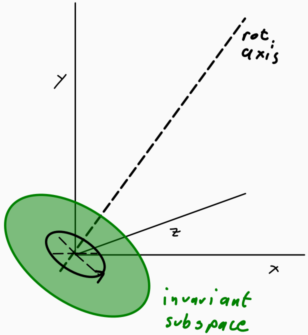

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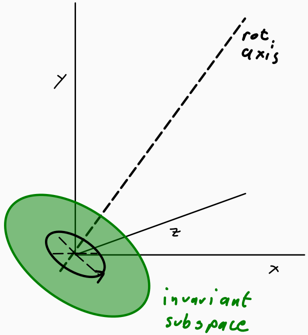

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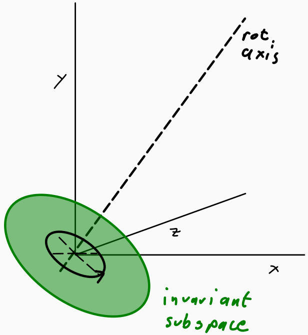

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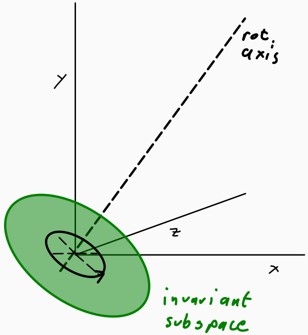

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- For finite groups these are equivalent (Maschke's theorem).

The number of irreps is limited by the group size

A result in group theory ("Main theorem"[1]) tells us that the set of all irreducible representations (**irreps**) $R_1, \ldots, R_k$ of a group G fulfills

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$\implies$ We found *all* irreps.

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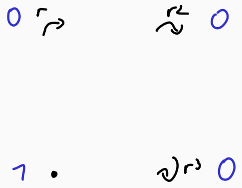

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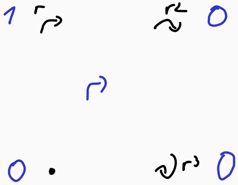

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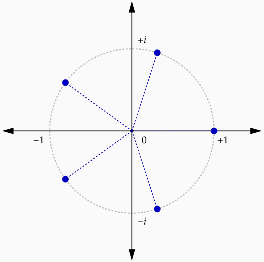
Roots of unit $\sqrt[n]{1}$



Summary

- Representations are linear group actions $g.v = R(g)v$, $R(g) \in \mathrm{GL}(d)$
- Can be built up from *irreducible representations*
- *Regular representation* acts on the group itself

References

[1] Michael Artin. **Algebra, 2nd edition.** Pearson, 2010.

[2] Alberto Bietti, Luca Venturi, and Joan Bruna. **"On the Sample Complexity of Learning under Geometric Stability".** In: *Advances in Neural Information Processing Systems*. Ed. by M. Ranzato et al. Vol. 34. Curran Associates, Inc., 2021, pp. 18673–18684.