Geometric Deep Learning

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Part VII: Convolutions

A note on terminology

Caveat: Convolution operation

$$(f \star g)(t) = \int_0^T f(\tau) g(T - \tau)\,,$$

but in ML we call *cross-correlation* convolution

$$(f \star g)(t) = \int_0^T f(\tau) g(\tau)\,.$$

Grids vs Graphs

What makes the geometric domain of a grid different from that of a graph?

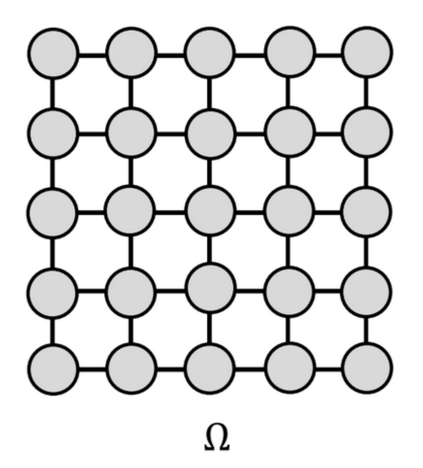

Image: Bronstein et al. (2021)

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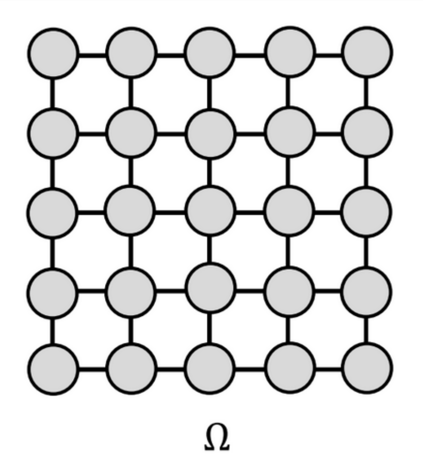
The symmetry group. Each node has well-defined top/bottom/left/right neighbour $\implies$ not *permutation-invariant*



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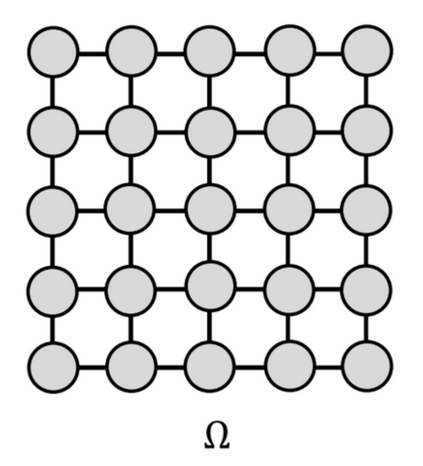

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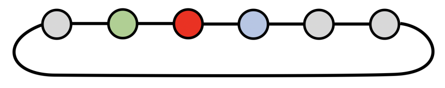
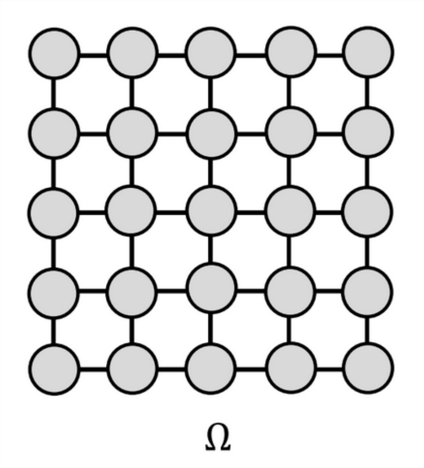
For simplicity: limit to one dimension





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Formal setup

Let $G = C(n)$ be the cyclic group of order n, and $\Omega = 1, \ldots, n$ be the domain of sequences of length n with periodic boundary conditions

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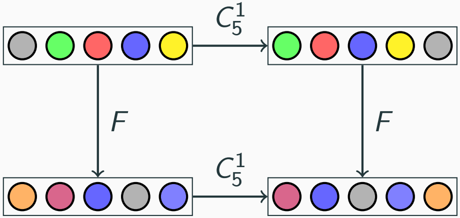
What are linear equivariant mappings?

We want $CF\boldsymbol{a} = FC\boldsymbol{a}$,

C shift-matrix, $\boldsymbol{a}$ activations/inputs, F equivariant mapping



Eigendecomposition of shift-matrices

The regular representation of $C(n)$ is given by circulant matrices

$$C_n^k := \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \ddots & 1 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}^k$$

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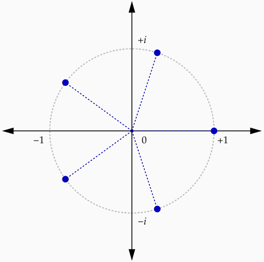

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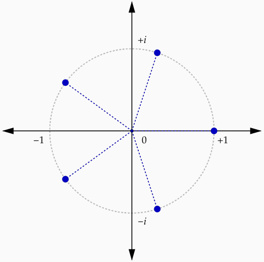

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- $\implies C_n^k = J^{-1}DJ$ for *diagonal* D with entries $\psi_\cdot^n$

Gaussian elimination

To find J, we can solve

$$(C_n^1 - \exp(2\pi ik/n)I)\mathbf{v} = 0$$

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$$\begin{array}{cl}
\begin{pmatrix}
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\end{pmatrix}
&
\left|\begin{array}{l}
\cdot\, \psi_n^{n-k} \\
\\
\\
\\
\text{-row } 1
\end{array}\right.
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Resolving the Eigenvectors

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Set $v_n = 1$, we can start solving:

$$-\psi_n^k v_{n-1} + 1 = 0 \qquad \Longrightarrow \qquad \psi_n^{-k} = v_{n-1}$$

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The Fourier Basis

Therefore, the kth eigenvector is given by:

$$\boldsymbol{v}_k = (\psi_n^{n-k}, \psi_n^{n-2k}, \ldots, \psi_n^{k}, 1)^\mathsf{T} \,.$$

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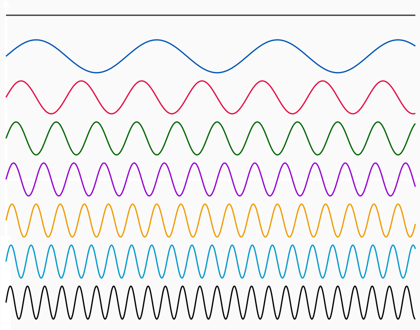
Let $J = [\boldsymbol{v}_0, \ldots, \boldsymbol{v}_{n-1}]^{\mathsf{T}}$, u an arbitrary vector. Change-of-basis results in **discrete Fourier transform**

$$\begin{aligned}(Ju)_k = \langle v_k, u \rangle &= \sum_t \exp(2\pi i \tfrac{k}{n} \cdot t) u_t \\ &= \sum_t \cos(2\pi \tfrac{k}{n} \cdot t) u_t + i \sin(2\pi \tfrac{k}{n} \cdot t) u_t\end{aligned}$$



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Fourier-transform diagonalizes *all* shifts simultaneously:

$$C_n^1 = J^{-1} D J \implies C_n^k = J^{-1} D^k J$$

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Thus, we can use arbitrary combinations

$$F = \sum \alpha_k C_n^k = J^{-1} (\sum \alpha_k D^k) J$$

$$\begin{pmatrix} \alpha_0 & \alpha_1 & \alpha_2 & \cdots \\ \alpha_{n-1} & \alpha_0 & \alpha_1 & \cdots \\ \alpha_{n-2} & \alpha_{n-1} & \alpha_0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \\ \alpha_1 & \alpha_2 & \alpha_3 & \cdots \end{pmatrix}$$

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Then

$$F C_n^1 \boldsymbol{x} = C_n^1 F \boldsymbol{x} \,,$$

so *any* convolution commutes with the shift operator.

$$\begin{pmatrix} \alpha_0 & \alpha_1 & \alpha_2 & \dots \\ \alpha_{n-1} & \alpha_0 & \alpha_1 & \dots \\ \alpha_{n-2} & \alpha_{n-1} & \alpha_0 & \dots \\ \vdots & \vdots & \vdots & \ddots \\ \alpha_1 & \alpha_2 & \alpha_3 & \dots \end{pmatrix}$$

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Shift-equivariant functions are convolutions

Assume the converse; for matrix F:

$$\forall \boldsymbol{x} : FC_n^1\boldsymbol{x} = C_n^1F\boldsymbol{x} \Leftrightarrow FJ^{-1}DJ\boldsymbol{x} = J^{-1}DJF\boldsymbol{x}$$

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Set $F = J^{-1}F'J$, and $\boldsymbol{x} = J^{-1}\boldsymbol{y}$, then

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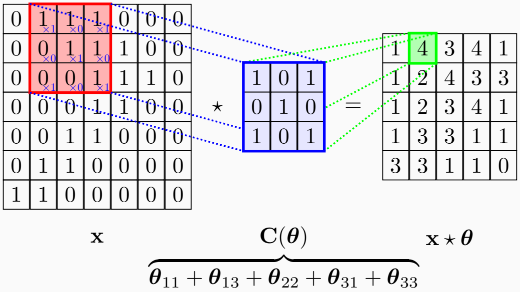
Pick $\boldsymbol{x} = \hat{e}_1$:

$$F'(d_{11}, 0, \ldots)^{\mathsf{T}} = D(f_{11}, f_{21}, \ldots)^{\mathsf{T}} \Leftrightarrow (f_{11}d_{11}, 0 \ldots)^{\mathsf{T}} = (d_{11}f_{11}, d_{22}f_{21}, \ldots)^{\mathsf{T}} \tag{1}$$

Thus, equality requires $f_{21}, f_{32} \ldots = 0$

Every convolution is shift-equivariant, and any shift-equivariant linear function is a convolution

Recap



Interpretation: Given some filter F, we apply *all* possible group-elements (shift) and record all corresponding responses.

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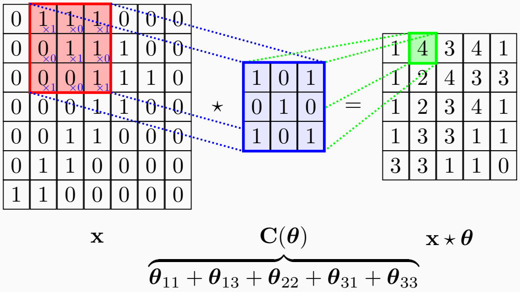

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Can we generalize this to arbitrary groups?

Image: Bronstein et al. (2021)

Part VIII: Steerable Kernels

A first construction for an equivariant linear layer

Standard linear layer

Select a filter $f \in \mathcal{X}(\Omega, \mathcal{C})$, output is given by inner product

$$f(x) = \int_{\Omega} \langle f(\omega), x(\omega) \rangle \mathrm{d}\omega \, .$$

Stacking c filters defines the layer with c output channels.

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Equivariant linear layer

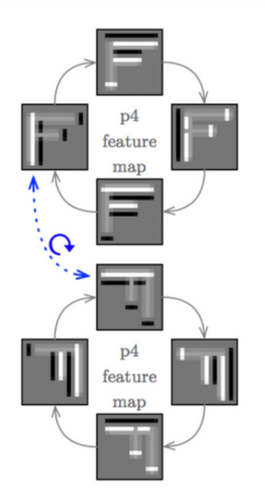
Let R be a representation of the action of G on $\mathcal{X}$. Then, for any filter f and group element g, define

$$f_g(x) = \int_{\Omega} \langle g.f(\omega), x(\omega) \rangle \mathrm{d}\omega \,.$$

Stack all such activations, resulting in $|G|c$ output channels.

Example: P4 symmetry

- 90° rotations, translations
- rotated input rotated in rotated output, and **cyclic shift** in feature maps
- translated input results in translated output



The resulting operation is equivariant

Let $h \in G$ be a group element. Then, for a single filter f we have

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- Change of variables $\omega \to h^{-1}\omega =: \omega'$ assumes $\mathrm{d}\omega = \mathrm{d}\omega'$ (otherwise, we shouldn't call G a symmetry of Ω).

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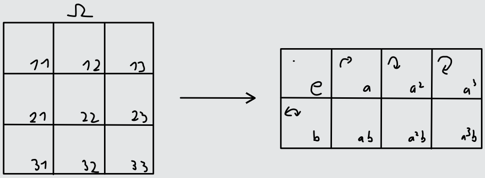
$\implies$ Collect $\mathbf{f}_G(x) = (f_g(x))_{g \in G} \in \mathbb{R}^{|G|}$, then $\mathbf{f}_G(h.x) = P_h^{-1}\mathbf{f}_G(x)$.

$\implies$ $\mathbf{f}_G$ transforms according to the regular representation.

Group-convolution maps signals to signals over the group itself

$$\mathbf{f}_G : \mathcal{X}(\Omega, \mathcal{C}) \longrightarrow \mathcal{X}(G, \mathcal{C})$$

D4-Convolution



T2-Convolution

Original (image) domain: $\Omega \cong (\mathbb{Z}/n\mathbb{Z})^2$

Translation group:

$T_2(n) \cong C(n)^2 \cong (\mathbb{Z}/n\mathbb{Z})^2$

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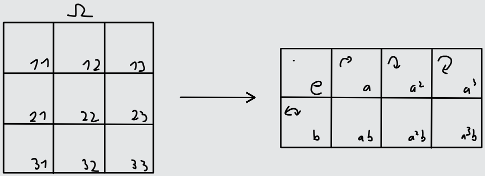

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This construction requires the output to have $c|G|$ channels, which becomes infeasible for large groups.

Steerable Kernels

Steerable Mapping (Intertwiner)

Let G be a group, Ω, Ψ two geometric domains. A linear mapping L from $\mathcal{X}(\Omega, \mathcal{C})$ to $\mathcal{X}(\Omega', \mathcal{C}')$ is called (linearly) **steerable** if there exist group actions (representations) μ, ν such that

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$$\begin{tikzcd}
\boxed{\mathcal{X}(\Omega, \mathcal{C})} \arrow[r, "\mu(g)"] \arrow[d, "L"] & \boxed{\mathcal{X}(\Omega, \mathcal{C})} \arrow[d, "L"] \\
\boxed{\mathcal{X}(\Omega', \mathcal{C}')} \arrow[r, "\nu(g)"] & \boxed{\mathcal{X}(\Omega', \mathcal{C}')}
\end{tikzcd}$$

Steerable Kernels

Steerable Mapping (Intertwiner)

Let G be a group, Ω, Ψ two geometric domains. A linear mapping L from $\mathcal{X}(\Omega, \mathcal{C})$ to $\mathcal{X}(\Omega', \mathcal{C}')$ is called (linearly) **steerable** if there exist group actions (representations) μ, ν such that

$$\forall x \in \mathcal{X}(\Omega, \mathcal{C}), g \in G: \ \nu(g).L(x) = L(\mu(g).x)$$

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Note: If ν is the trivial representation, then L is *invariant* ($\nu(g) = \mathrm{id}$).

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Equivariance implies invariant mapping

Invariance of weights

For $\nu(g) \in \mathrm{GL}(m)$, $\mu(g) \in \mathrm{GL}(n)$

$$
\begin{aligned}
& \forall g, x : \; \nu(g).L(x) = L(\mu(g).x) \\
\Leftrightarrow\; & \forall g : \; \nu(g) \circ L = L \circ \mu(g)
\end{aligned}
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The weight matrix L is invariant under this particular group action.

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Group averaging

Can reuse our group-averaging to construct equivariant weights from arbitrary weights $\tilde{L}$:

$$L = \sum_{g \in G} \nu(g)^{-1} \, \tilde{L} \, \mu(g)$$

Convolutions through weight-sharing

Let $\mu(k) = C_3^k, \nu(k) = C_3^k$, select $\tilde{L} = \delta_{11}$.
Group action:

$$(C_3^1)^{-1} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} C_3^1$$

Convolutions through weight-sharing

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$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

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Group action:

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \color{red}{1} & \color{red}{0} & \color{red}{0} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & \color{red}{1} & 0 \\ 0 & \color{red}{0} & 1 \\ 1 & \color{red}{0} & 0 \end{pmatrix}$$

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$$(C_3^1)^{-1} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} C_3^1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

In general: Move to the right by k places, then move down k places.

Convolutions through weight-sharing

In total, we get the following nine group-averages (color indicates original matrix):

$$\begin{pmatrix} \color{blue}{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 0 & \color{orange}{1} & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & 0 & \color{red}{1} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ \color{red}{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 \\ 0 & \color{blue}{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \color{orange}{1} \\ 1 & 0 & 0 \end{pmatrix}$$

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In total, we get the following nine group-averages (color indicates original matrix):

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Three distinct matrices $\rightarrow$ three orbits that serve as basis vectors

Steerable Filter Banks

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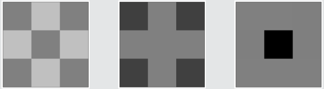
In general, generate all orbits and orthogonalize (e.g., Gram-Schmidt)

The same strategy also works for trivial (invariant) representation of D4

Trivial Representation A1

We have already seen this: rotation-invariant linear functions



What about non-trivial representations?

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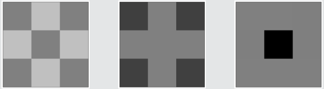

What about non-trivial representations?

Constructing a basis for D4's B1 representation

B1

a: rotate 90°, b: flip along y-axis.

B1 is a 1-dimensional representation with

$$\nu(a) = -1, \quad \nu(b) = 1$$

Smoothing

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$$\underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{E_{11}} + \underbrace{(-1)}_{\nu(a)} \cdot \underbrace{\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{R(a)E_{11}}$$

$$+ \underbrace{(1)}_{\nu(a^2)} \cdot \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{R(a^2)E_{11}} + \dots$$

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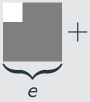

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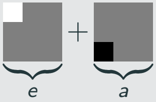

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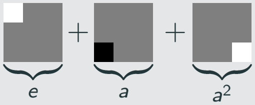

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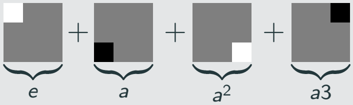

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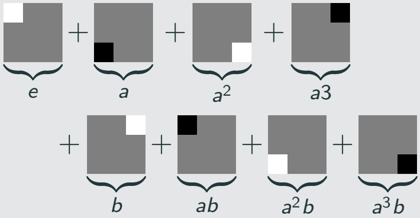

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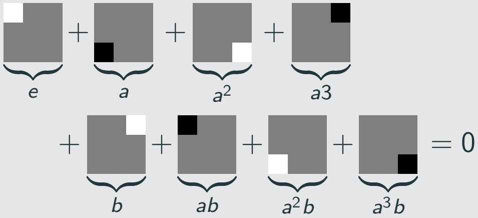

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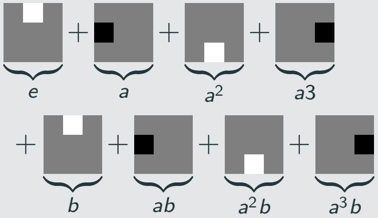

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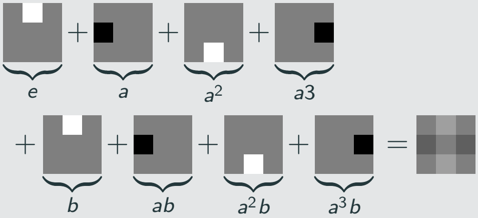

One-dimensional representations of D4

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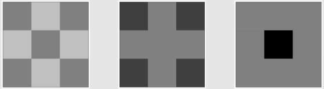
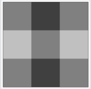


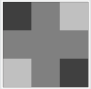
B1

Rotation sign, reflection inv:



B2

Rotation, reflection sign:



T. S. Cohen and Welling. (2016). *Steerable CNNs*

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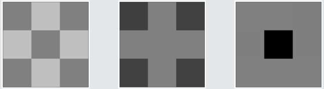

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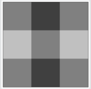

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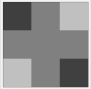
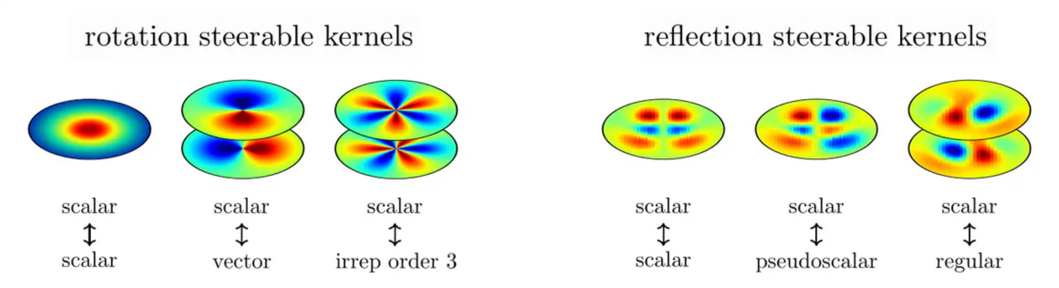


What about A2? (rotation invariant, reflection sign-change)

T. S. Cohen and Welling. (2016). *Steerable CNNs*

Steerable kernels for SO(2)



Homogenous spaces

Definition (Transitive Action)

A group action is called **transitive** iff

$$\forall x, y \in \Omega : \exists g \in G \text{ s. t. } x = gy\,.$$

T. Cohen, Geiger, and Weiler. (2019). "A general theory of equivariant cnns on homogeneous spaces"

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Theorem (Convolutions are all you need)

An equivariant map can always be written as a convolution-like integral

T. Cohen, Geiger, and Weiler. (2019). "A general theory of equivariant cnns on homogeneous spaces"

Part IX: Scale Separation

Can we just use any convolution operation?

Parameter Cost

A generic convolution on an $n \times n$ image with c input and d output channels requires

$$c \times n \times n \times d \text{ parameters}.$$

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Scales quadratically with input size.

Group-smoothing

For a single linear layer, a "global" convolution is just *group smoothing*.

Downsampling

Rescale the input to be small enough that we can easily handle it.

Loses detail information

Rigid

Local Patches

Use very sparse filter matrices so that only local neighbourhoods interact.

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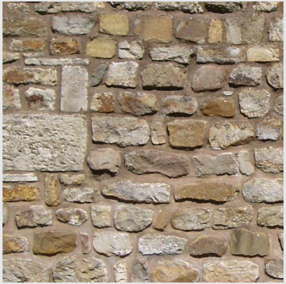
Cannot capture global structure

Scale separation prior

Sometimes, coarse scales are sufficient


Sometimes, local patches are sufficient



Deformation Stability

- Let G be translations, a subgroup of the diffeomorphisms $\tau : \Omega \longrightarrow \Omega$.
- Define $c(\tau) := \sup \|\nabla \cdot \tau(u)\|$. For $g \in G$ we have $c(g) = 0$; c measures the distance to the group
- We want **deformation stability**: $\|f(x) - f(\tau.x)\| \leq c(\tau)$.

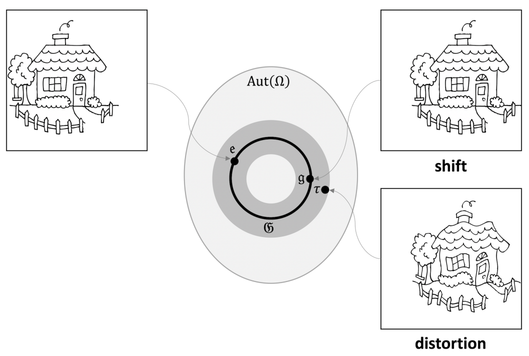
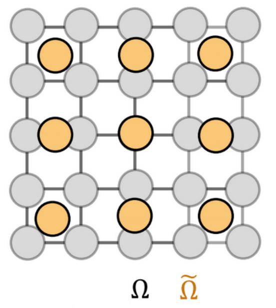


Image: Bronstein et al. (2021)

Multiresolution analysis

- Decompose signal $x \in \mathcal{X}(\Omega)$ into a lower resolution version $\tilde{x} \in \mathcal{X}(\tilde{\Omega})$ and residuals.



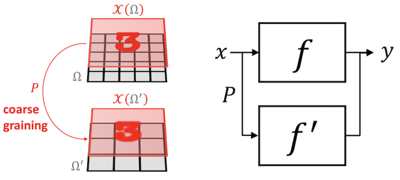
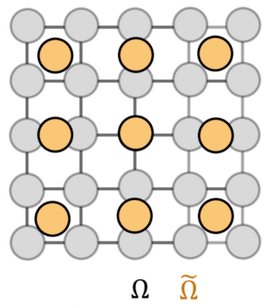
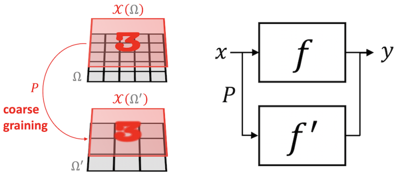


Image: Bronstein et al. (2021),

Multiresolution analysis

- Decompose signal $x \in \mathcal{X}(\Omega)$ into a lower resolution version $\tilde{x} \in \mathcal{X}(\tilde{\Omega})$ and residuals.
- (Wavelet) filters localized in space





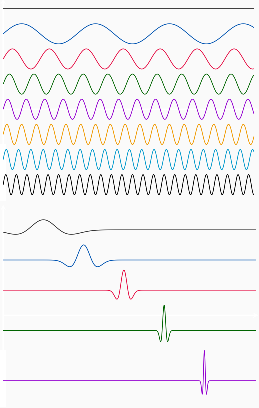
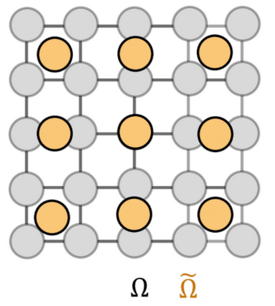
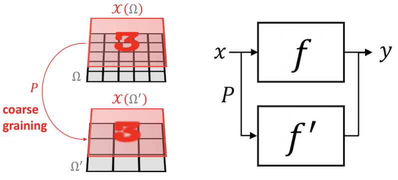


Image: Bronstein et al. (2021),

Multiresolution analysis

- Decompose signal $x \in \mathcal{X}(\Omega)$ into a lower resolution version $\tilde{x} \in \mathcal{X}(\tilde{\Omega})$ and residuals.
- (Wavelet) filters localized in space
- Exhibit deformation stability[1]





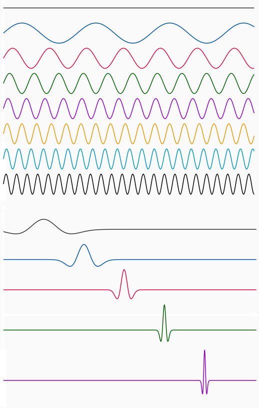


Image: Bronstein et al. (2021), [1]Mallat. (2010)

Compositionality

- The *deep* in deep learning
- Multiple layers of *local* connectivity can accumulate a *global* receptive field
- $\Rightarrow$ **The GDL Blueprint**

Image: Zeiler. (2014)

Part X: The GDL Blueprint

The GDL Blueprint

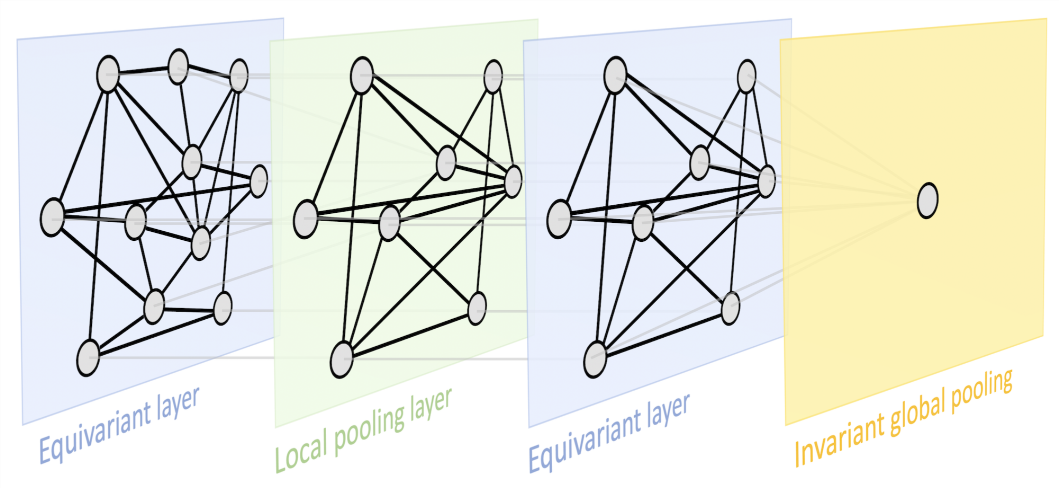


Image: Bronstein et al. (2021)

The GDL Blueprint

- Linear G-equivariant layer
  $B : \mathcal{X}(\Omega, \mathcal{C}) \longrightarrow \mathcal{X}(\Omega', \mathcal{C}')$ s.t.
  $g.B(x) = B(g.x)$
- Pointwise non-linearity
- Local pooling layer (coarsening)
  $P : \mathcal{X}(\Omega, \mathcal{C}) \longrightarrow \mathcal{X}(\Omega', \mathcal{C})$ s.t. $\Omega' \subset \Omega$
- G-invariant layer (global pooling)
  $A : \mathcal{X}(\Omega, \mathcal{C}) \longrightarrow \mathcal{Y}$ s.t. $A(x) = A(g.x)$

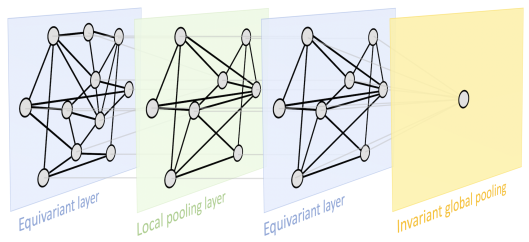


Image: Bronstein et al. (2021)

Many famous architectures follow this blueprint

Architecture	**Domain** Ω	**Group** G
CNN	Grid	Translation
LSTM	1D-Grid	Time translation
Spherical CNN	Sphere	Rotation SO(3)
Mesh CNN	Manifold	Gauge SO(2)
GNN	Graph	Permutation $S(n)$
Deep Sets	Set	Permutation $S(n)$
Transformer	Complete Graph	Permutation $S(n)$

References

[1] Michael M. Bronstein et al. **Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges.** 2021. arXiv: 2104.13478 [cs.LG]. URL: https://arxiv.org/abs/2104.13478.

[2] Taco Cohen, Mario Geiger, and Maurice Weiler. **"A general theory of equivariant cnns on homogeneous spaces".** In: *Advances in neural information processing systems* 32 (2019).

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[4] Stéphane Mallat. **"Recursive interferometric representation".** In: *Proc. of EUSICO conference, Danemark*. Vol. 3. 2010.

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