TENSOR FIELD NETWORK (AND OTHER CONVNET GENERALISATIONS)

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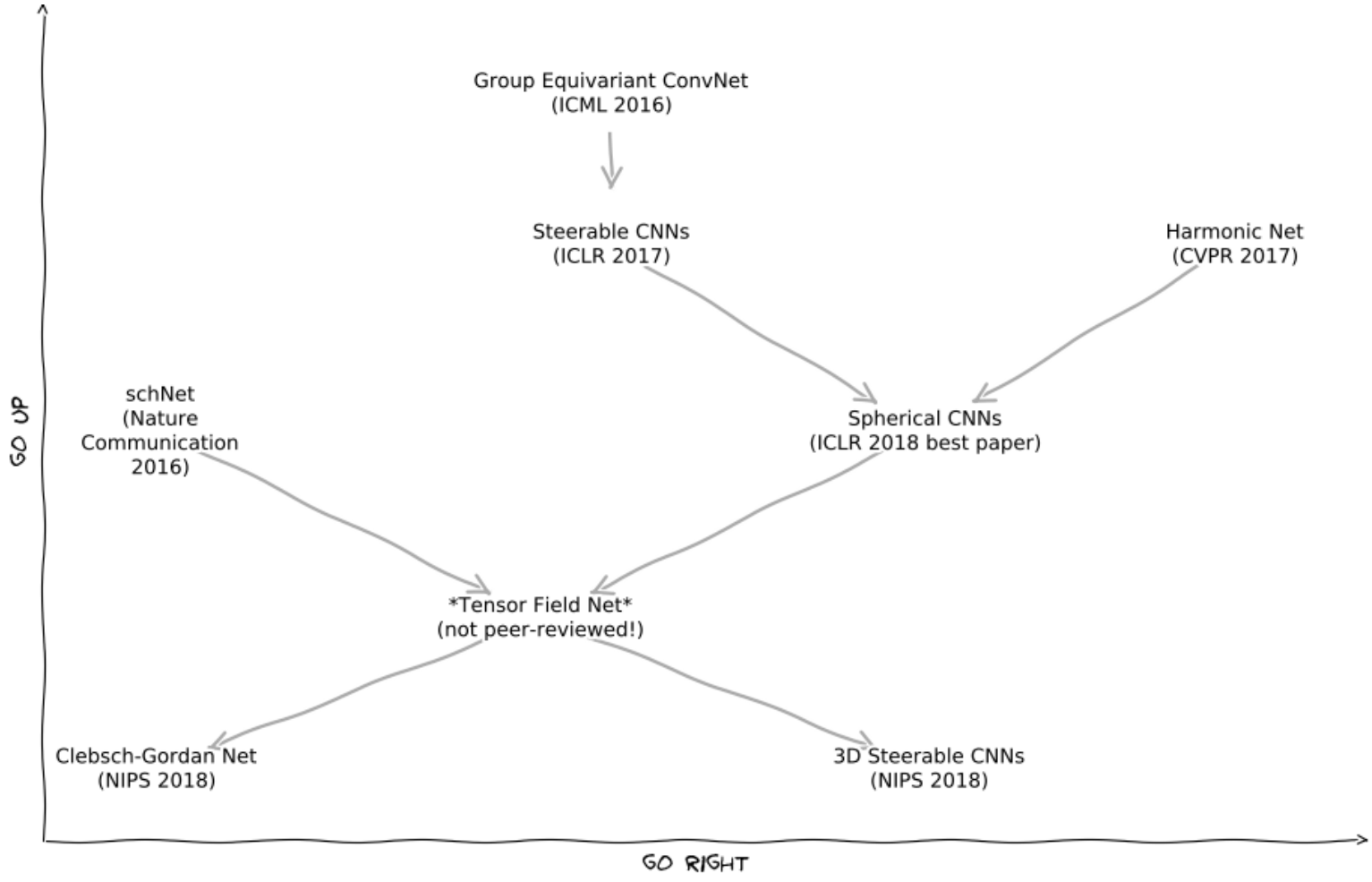
OVERVIEW



PRE-CONVNET (1960-1987)

PRE-CONVNET - LINEAR/FULLY CONNECTED/~~DENSE/PERCEPTRON~~ LAYER

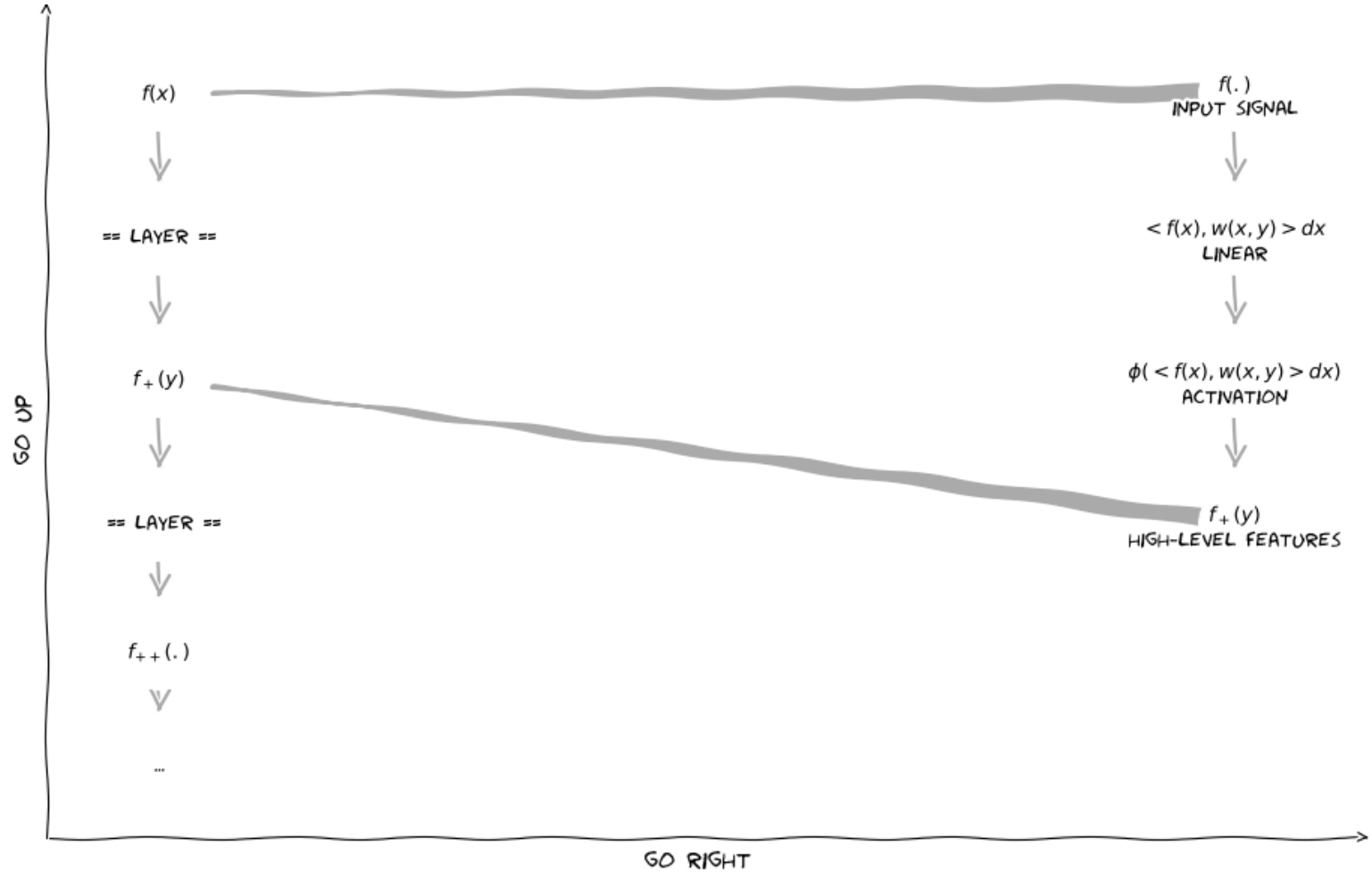
In pursuing of unbounded representation/approximation power

$$f_+(y) = \Phi\Big(f(x)\Big) \qquad = \phi\Big(\sum_{x \in \text{domain}} f(x)w(x, y)\Big)$$

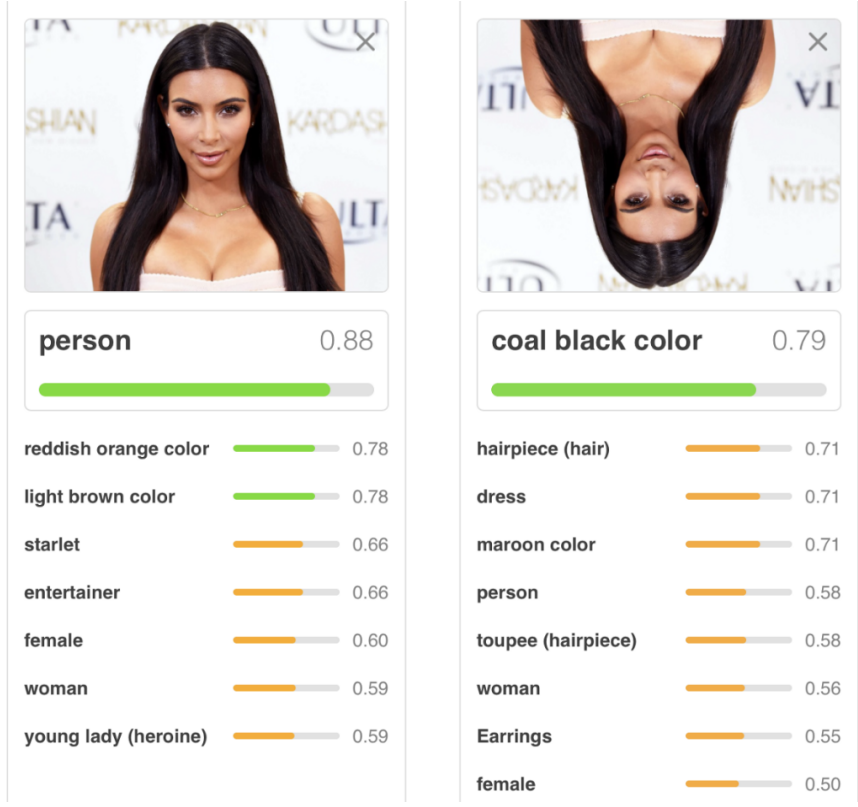
$$= \phi\Big(< f(x), w(x, y) >_x\Big)$$

(w are weight of neurons)

PRE-CONVNET - LINEAR/FULLY CONNECTED LAYER



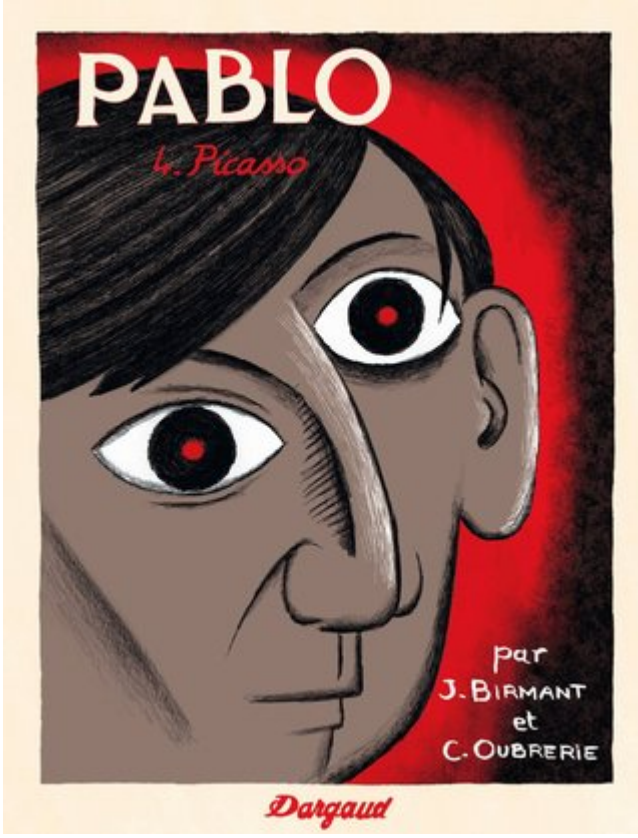
PRE-CONVNET - LINEAR/FULLY CONNECTED LAYER



[*] Image courtesy https://www.quora.com/What-is-the-difference-between-equivariance-and-invariance-in-Convolution-neural-networks (https://www.quora.com/What-is-the-difference-between-equivariance-and-invariance-in-Convolution-neural-networks)

INVARIANT LAYER / BAG-OF-WORDS?

- Don't do this



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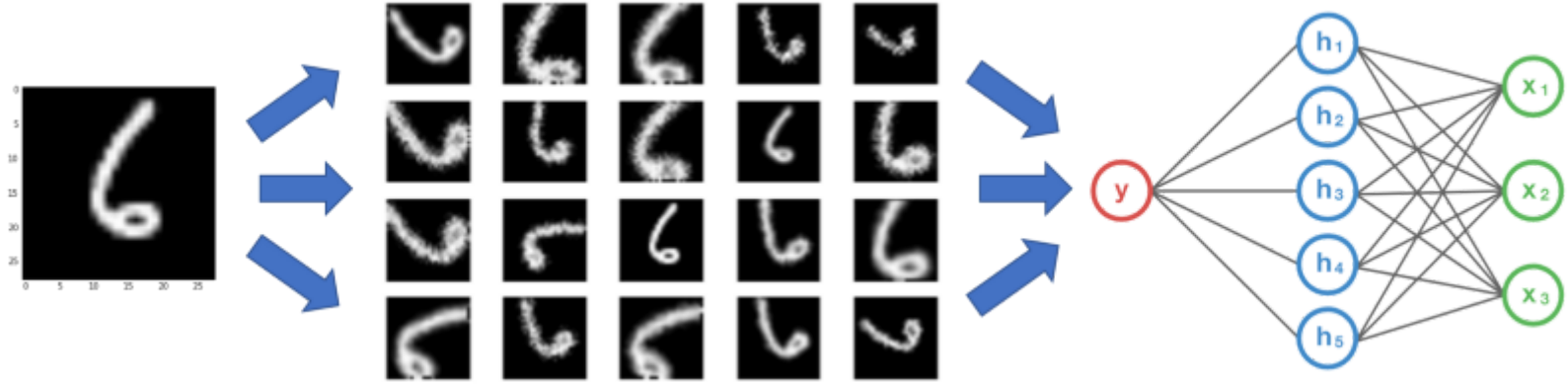
[*] Image Courtesy: https://www.amazon.ca/Pablo-Art-Masters-Julie-Birmant/dp/1906838941 (https://www.amazon.ca/Pablo-Art-Masters-Julie-Birmant/dp/1906838941)

DATA AUGMENTATION

- Good catch



DATA AUGMENTATION

- Too slow in practice
    - In **convex case** SGD "theoretically probably" converges equally fast
    - otherwise it "kind of works" but with much less efficiency

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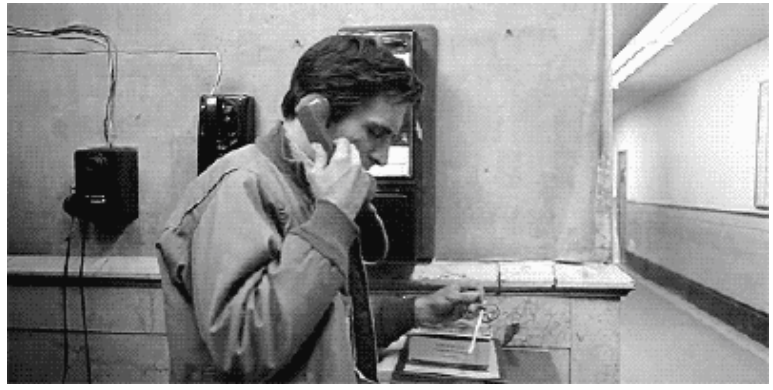
- Time & space complexity increase exponentially with the dimensionality of augmentation



2D translation

DATA AUGMENTATION

- Time & space complexity increase exponentially with the dimensionality of augmentation

2D translation x 1D rotation, no gravity

DATA AUGMENTATION

- Time & space complexity increase exponentially with the dimensionality of augmentation

2D translation × 1D rotation, gravity perpendicular to domain

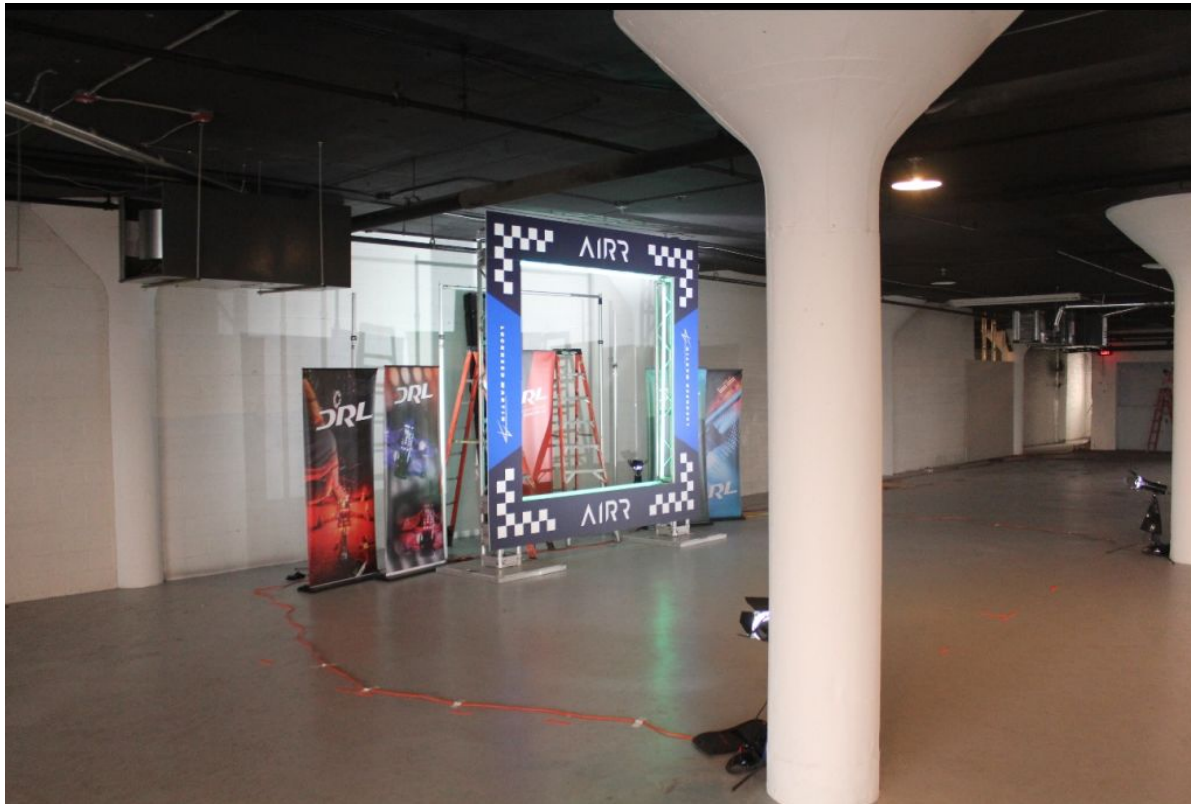
DATA AUGMENTATION

- Time & space complexity increase exponentially with the dimensionality of augmentation

3D rotation

DATA AUGMENTATION

- Time & space complexity increase exponentially with the dimensionality of augmentation

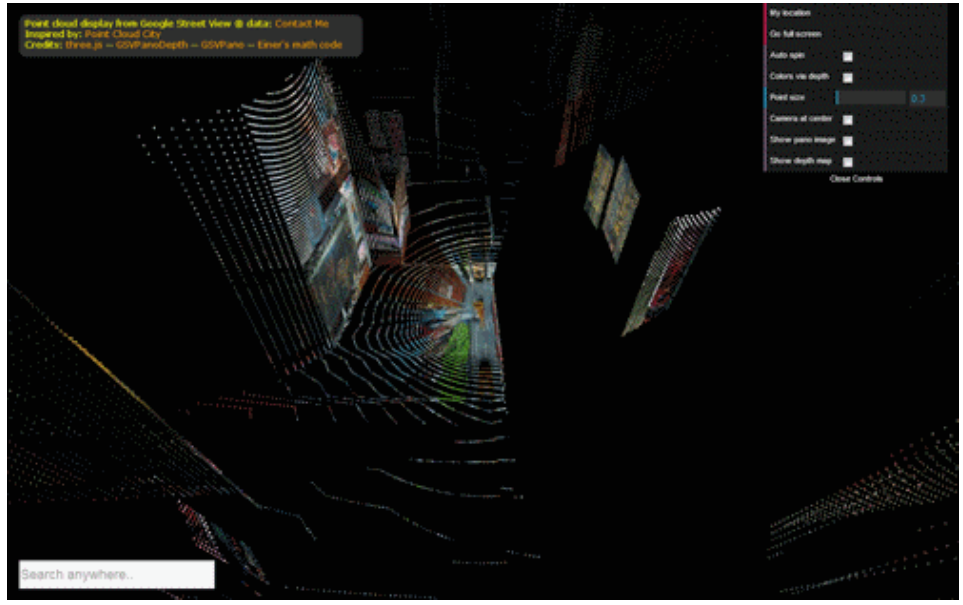


4D affine transformations

[*] Image Courtesy: AIRR https://thedroneracingleague.com/airr/ (https://thedroneracingleague.com/airr/)

DATA AUGMENTATION

- Time & space complexity increase exponentially with the dimensionality of augmentation



3D translation × 3D rotation

DATA AUGMENTATION

- Time & space complexity increase exponentially with the dimensionality of augmentation

IAS and TAS

Rules of Thumb: Increase your IAS at from MSL by 2% (or 1.8%) per 1000ft increase to obtain the Gross TAS:

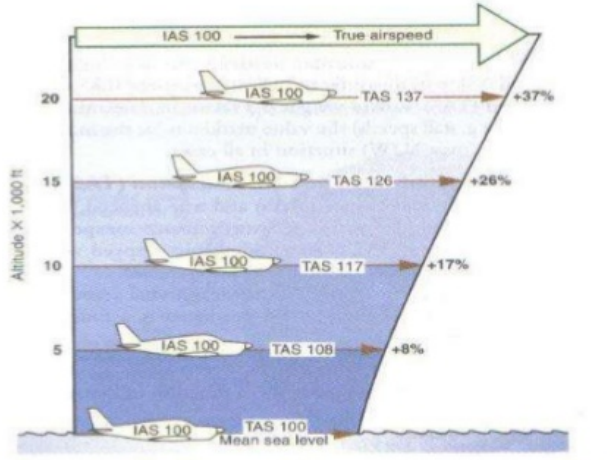


Figure 25-52 **With IAS constant, TAS increases with increase in altitude**

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Air pressure depending on translation

DATA AUGMENTATION

How about a better idea?

- Instead of augmenting, we hard-bake such prior knowledge into the network to yield identical result!

Augmentation types	**Answer**
2d translation	ConvNet
others	**G-ConvNet**
- 2d translation + 90° rotation	Group Equivariant CNNs
- 2d translation + rotation	Harmonic Net
- 3d rotation	Spherical CNNs
- 3d translation + rotation	Tensor Field Net

Let's do a hello-world experiment on MNIST dataset:

... for which each image can be augmented until all cases are covered

START LEARNING!

2 LAYERS ONLY

1. Highway only bypassing Linear/FC/~~Dense/Perceptron~~
    - Designed to break symmetry at saddle points*
    - WITHOUT initialisation (all weights start with 0)
    - 10x10 => 10x10 => ReLU
2. Plain old Linear/FC
    - 10x10 => one-hot 1~10 => ReLU

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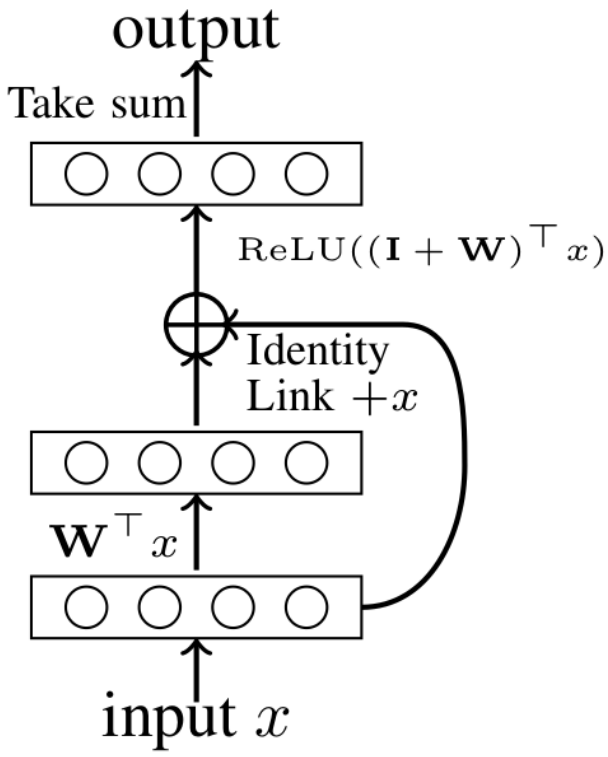
[*] Y. Li and Y. Yuan, “Convergence Analysis of Two-layer Neural Networks with ReLU Activation” NIPS 2017, pp. 1–11.

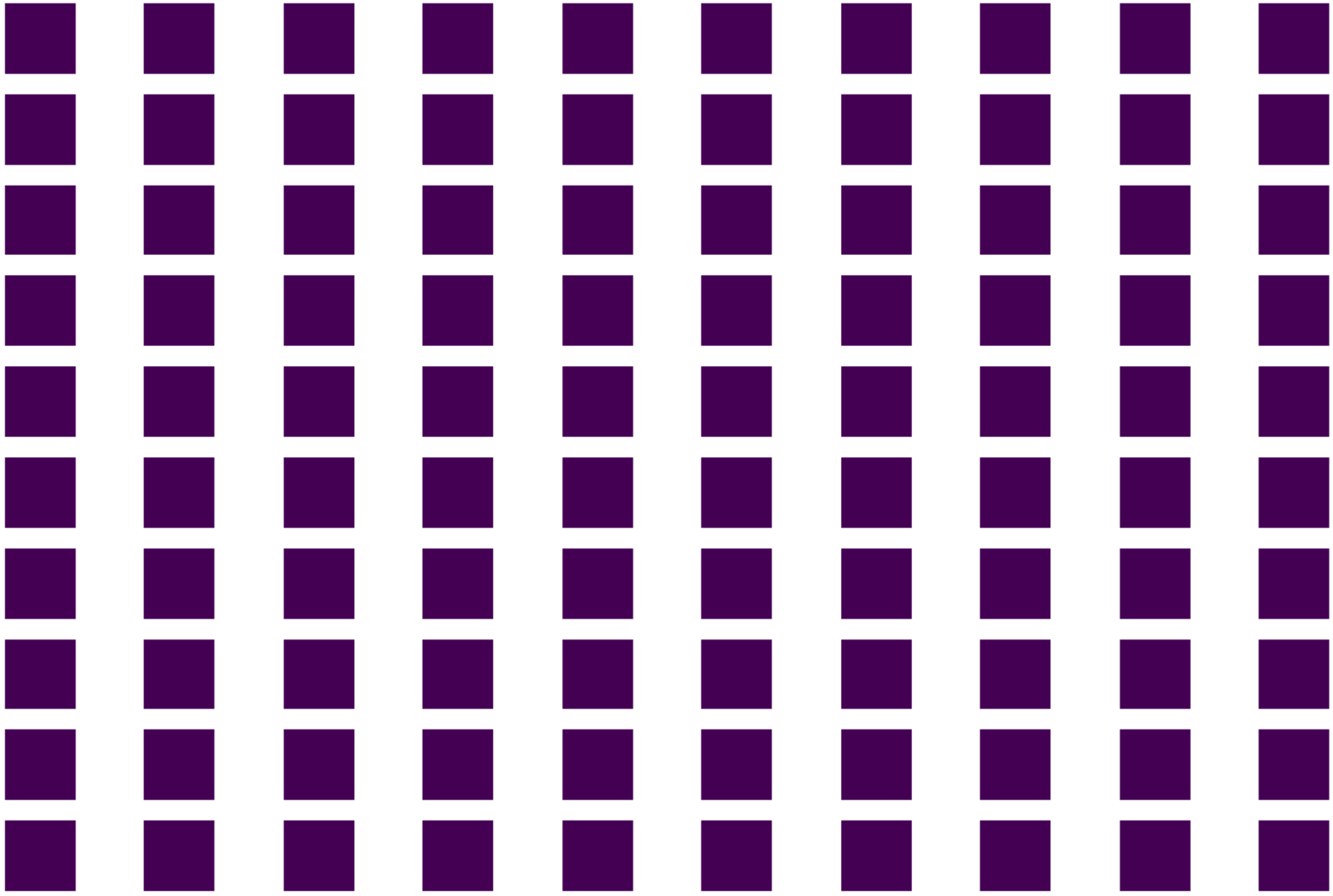
START LEARNING!



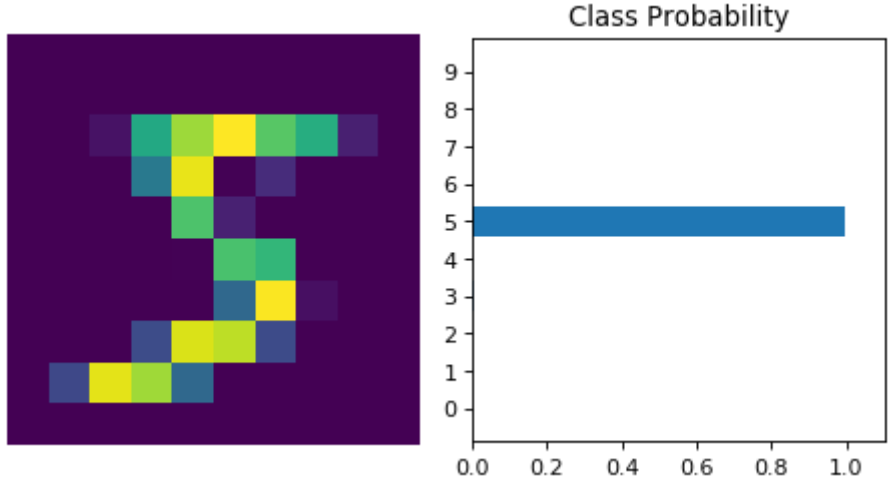
), with identity mapping (right)

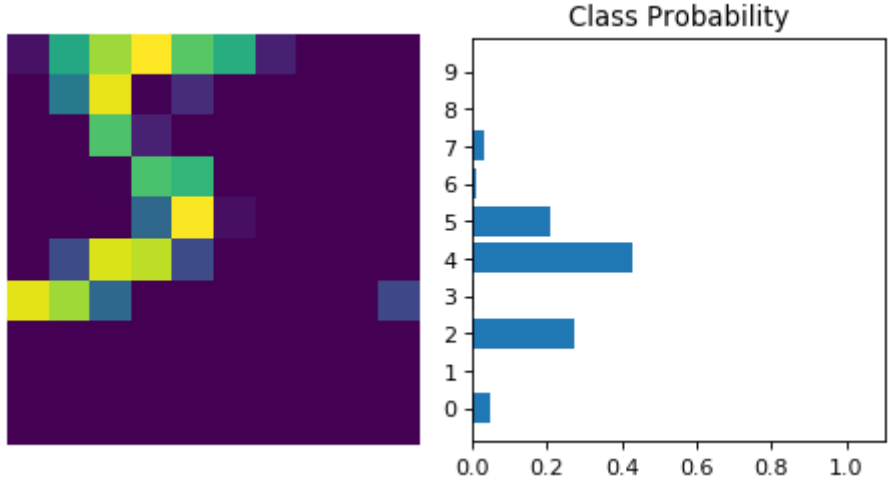
[*] Y. Li and Y. Yuan, “Convergence Analysis of Two-layer Neural Networks with ReLU Activation” NIPS 2017, pp. 1–11.

Weight map before training

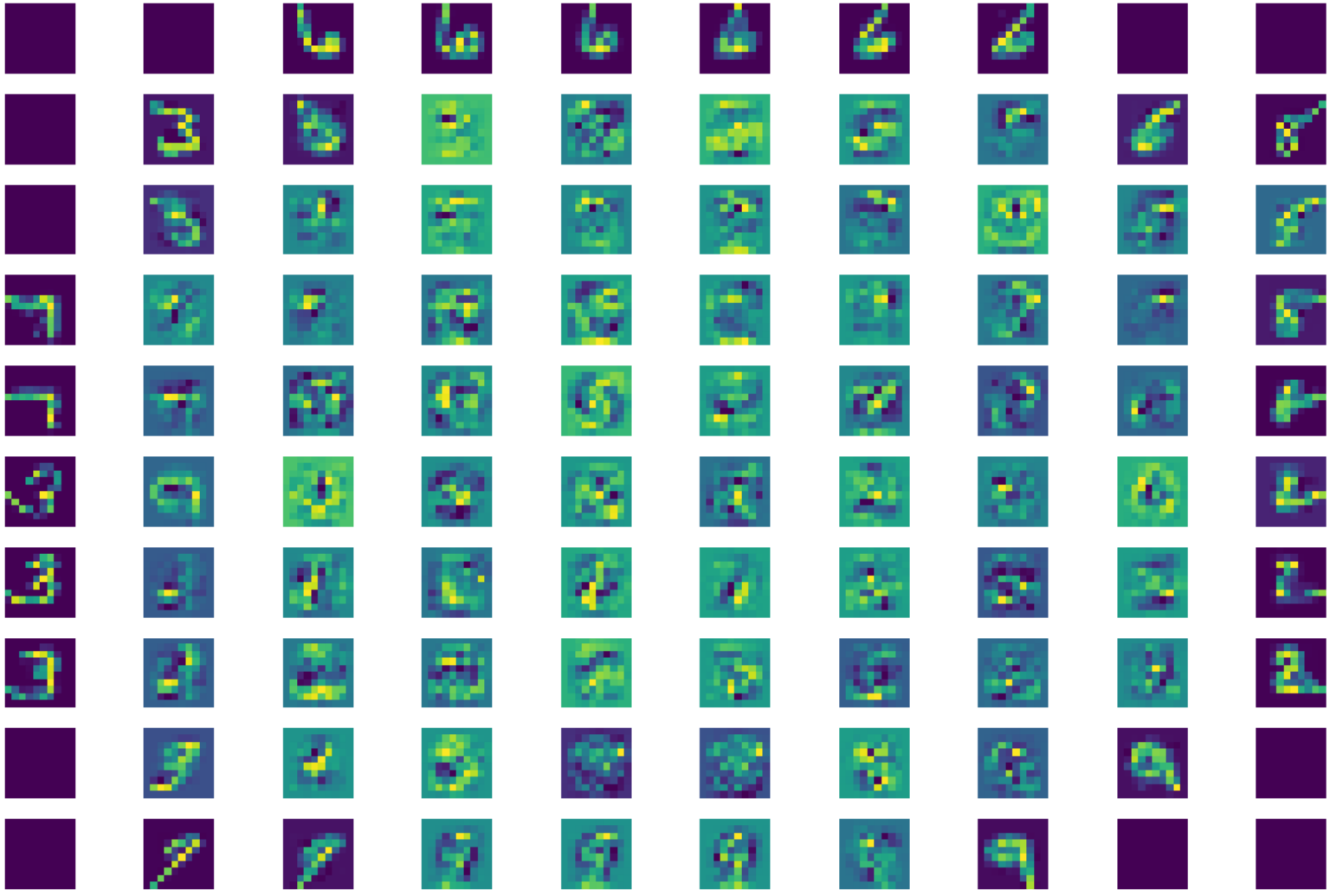


Trained on raw MNIST dataset

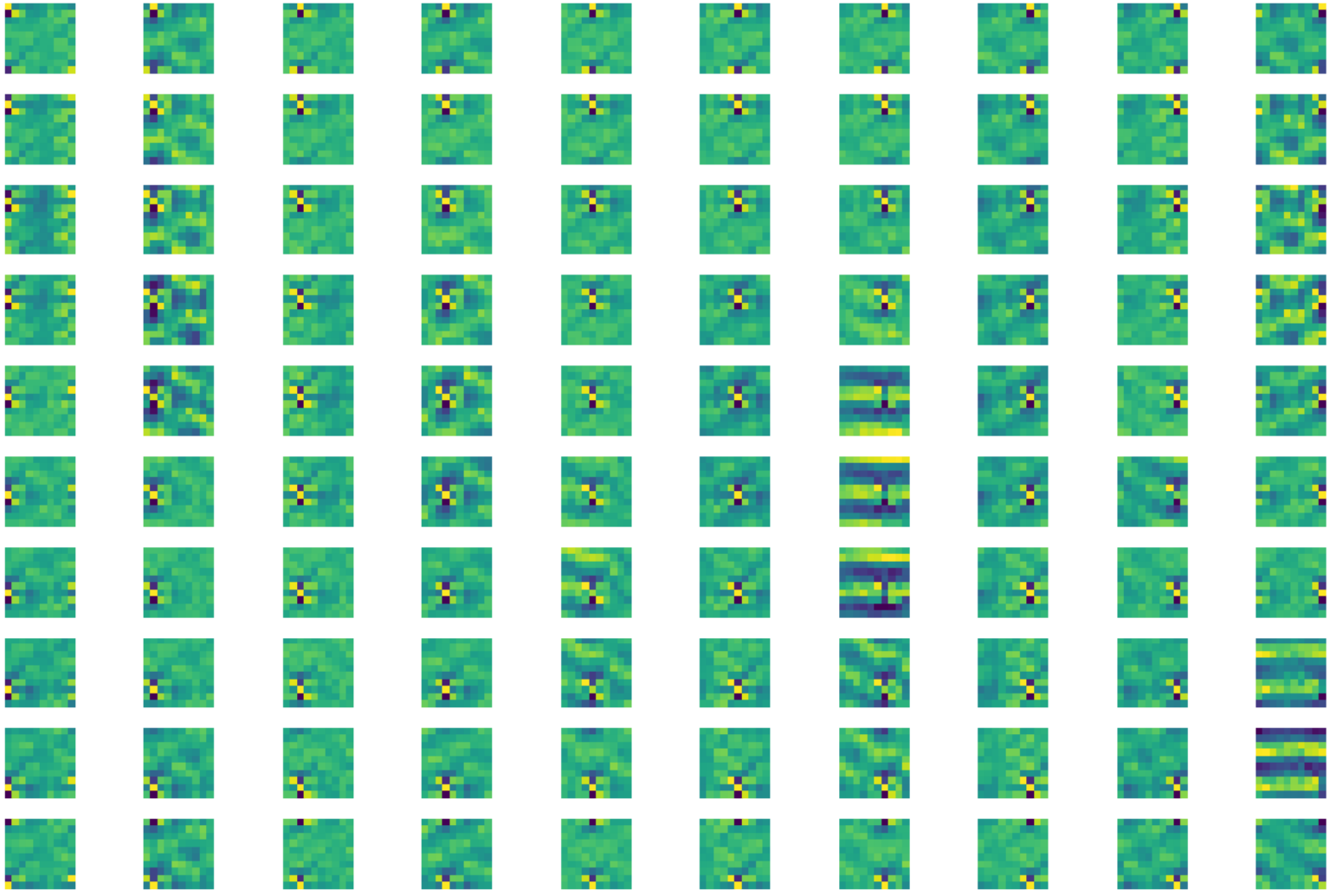




Weight map after training on raw MNIST dataset

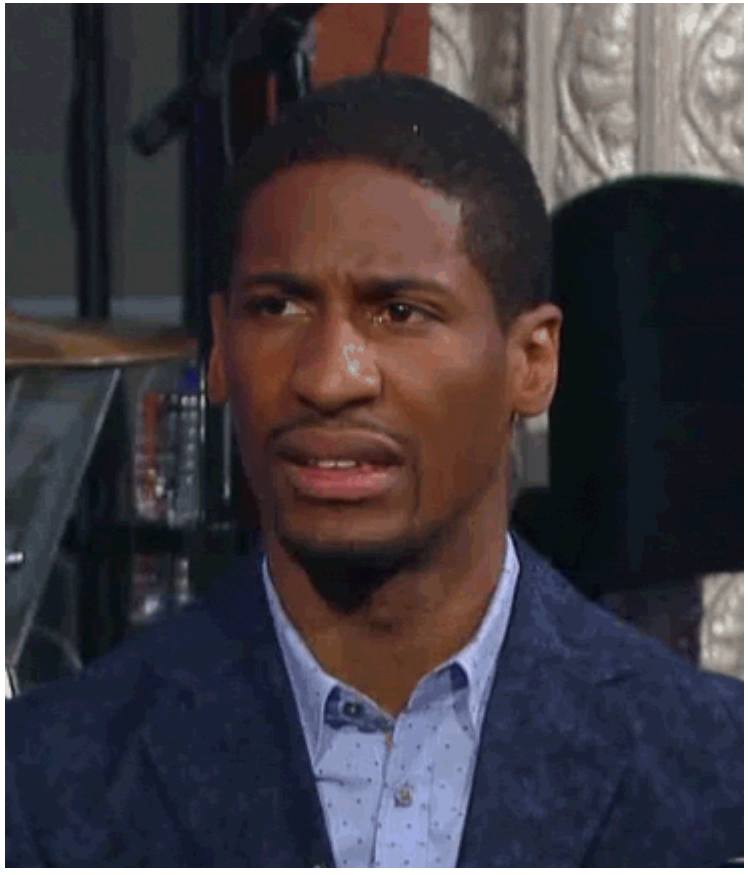


Weight map after training on AUGMENTED MNIST dataset



DATA AUGMENTATION

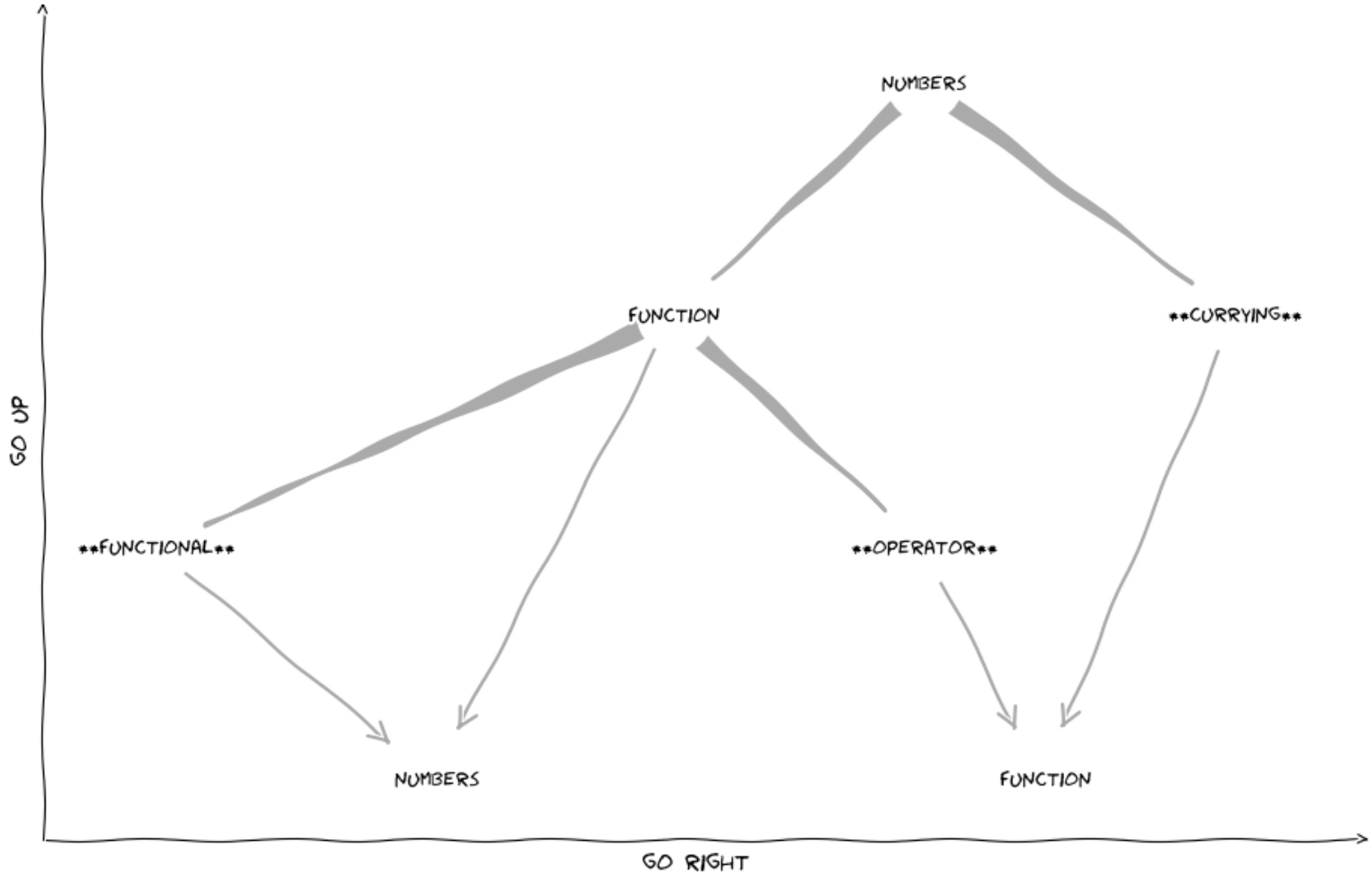
- How did this happen? (you probably want to try this on neural-ODE)



DATA AUGMENTATION

- Form a group $\left\{A_{ug}, U_{ga}, G_{au}. . . . . .\right\}$, sometimes not commutative/Abelian
- $\subset$ unary operator : Signal $\Longrightarrow$ Signal (making it a group action)
- $\subset$ **higher-order function**

DATA AUGMENTATION



DATA AUGMENTATION $\Longrightarrow$ G-CONVNET

Lemma: If the augmentation group $\{A_{ug}\}$ satisifes:

- **Transitivity**: for any pair of points x, y and any function f, we can always find an augmentation that can transform value f(x) to point y
- **Group Equivariance**: applying an augmentation A_{ug} on the input has the same effect as applying an augmentation U_{ga} from the same group on the output

Then a fully connected layer:

$$f_+(y) =< f(x), w(x, y) >_x$$

collapses to a group convolution (**G-conv**) layer:

$$f_+(y) =< A_{ug} \circ f(x), w_0(x) >_x$$

Looks familiar?

$$\text{conv}(f(-\Delta), w_0(\Delta)) = \text{corr}(f(\Delta), w_0(\Delta)) =< f(\Delta + x), w_0(x) >_x$$

DATA AUGMENTATION $\Longrightarrow$ G-CONVNET

$$f_+(y) =< A_{ug} \circ f(x), w_0(x) >_x$$

In short:

A CONVNET LAYER IS JUST AN AUGMENTED LINEAR/FULLY-CONNECTED LAYER!

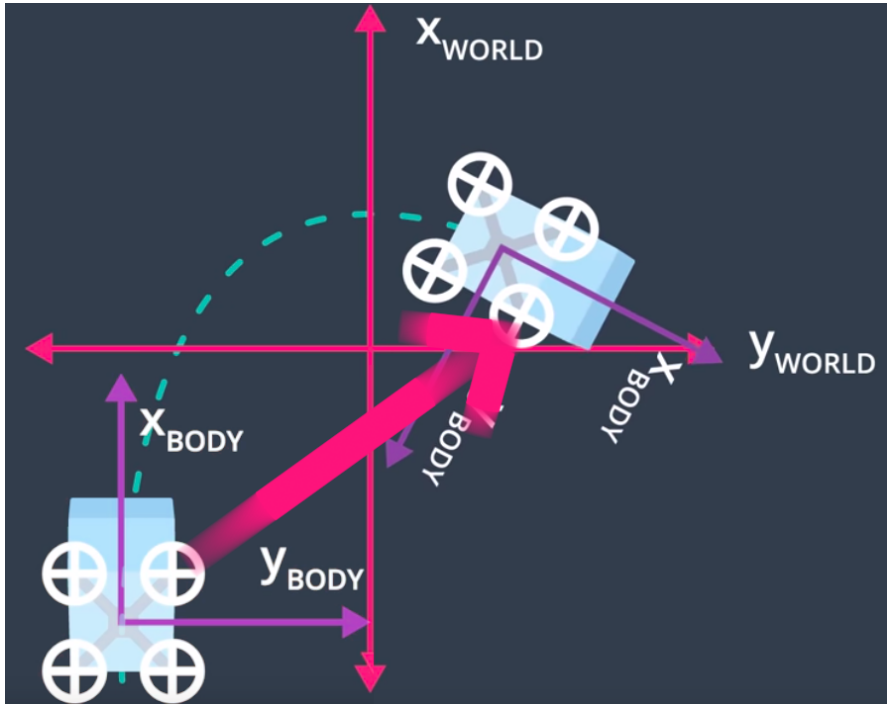
DATA AUGMENTATION - TRANSITIVITY

Transitivity: for any pair of points x, y and any function f, we can always find an augmentation that can transform value f(x) to point y

$$\forall x : f(x) = \left(A_{ug} \circ f\right)(x_0)$$

DATA AUGMENTATION - TRANSITIVITY

- Effectively means the augmentation group is the 'carriage' to move reference frame around the observer



[*] Image courtesy: udacity.com

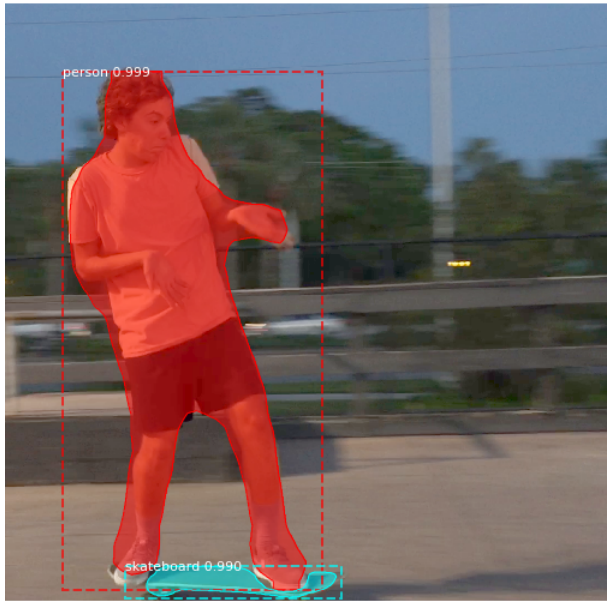
DATA AUGMENTATION - EQUIVARIANCE

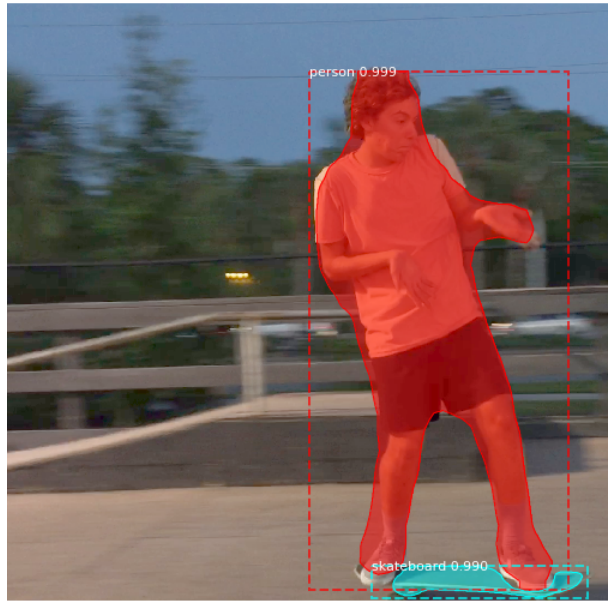
Plain old **Equivariance**: applying an augmentation A_{ug} on the input has the same effect as applying A_{ug} on the output

$$A_{ug} \circ f_{+}(y) =< A_{ug} \circ f(x), w(x, y) >_{x}$$

DATA AUGMENTATION - EQUIVARIANCE

- example: SQL prediate pushdown
- example: first input & final output of Masked-CNN & Autoencoder (& maybe Style Transfer)





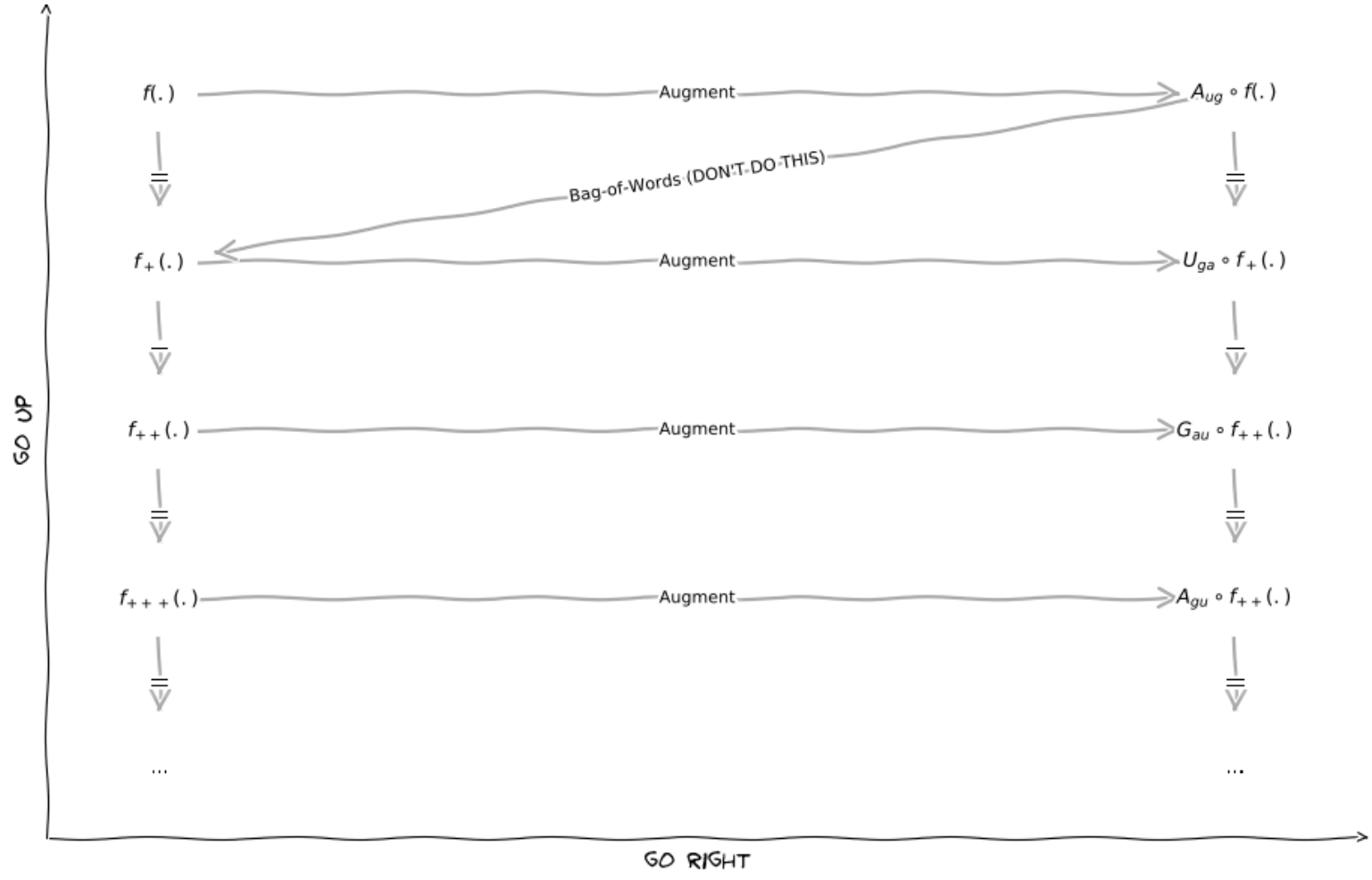
DATA AUGMENTATION - GROUP EQUIVARIANCE

Group Equivariance: applying an augmentation A_{ug} on the input has the same effect as applying an augmentation **U_{ga} from the same group** on the output

$$U_{ga} \circ f_{+}(y) =< A_{ug} \circ f(x), w(x, y) >_{x}$$

- Relaxed a bit comparing to Plain old equivariance
- Effectively means that the architecture of the first layer can be carried over to the subsequent layers with little changes, applied on high-level features

DATA AUGMENTATION - GROUP EQUIVARIANCE



DATA AUGMENTATION $\Longrightarrow$ G-CONVNET - PROOF

- **Transitivity**:

$$\forall x : f(x) = \left(\bar{A}_{ug} \circ f\right)(x_0)$$

- **Group equivariance**

$$U_{ga} \circ f_+(y) =< A_{ug} \circ f(x), w(x, y) >_x$$

Combining all together:

$$f_+(y) = \left(\bar{U}_{ga} \circ f_+\right)(y_0) =< \bar{A}_{ug} \circ f(x), w(x, y_0) >_x =< \bar{A}_{ug} \circ f(x), w_0(x) >_x$$

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[*] More rigorous proof: R. Kondor and S. Trivedi, “On the Generalization of Equivariance and Convolution in Neural Networks to the Action of Compact Groups” 2018

G-CONVNET

$$f_+(y) =< A_{ug} \circ f(x), w_0(x) >_x$$

- this implies bijection/isomorphism $y \longleftrightarrow A_{ug}$
- ... and high-level features usually have more dimensions $\{x\} \subset \{y\}$

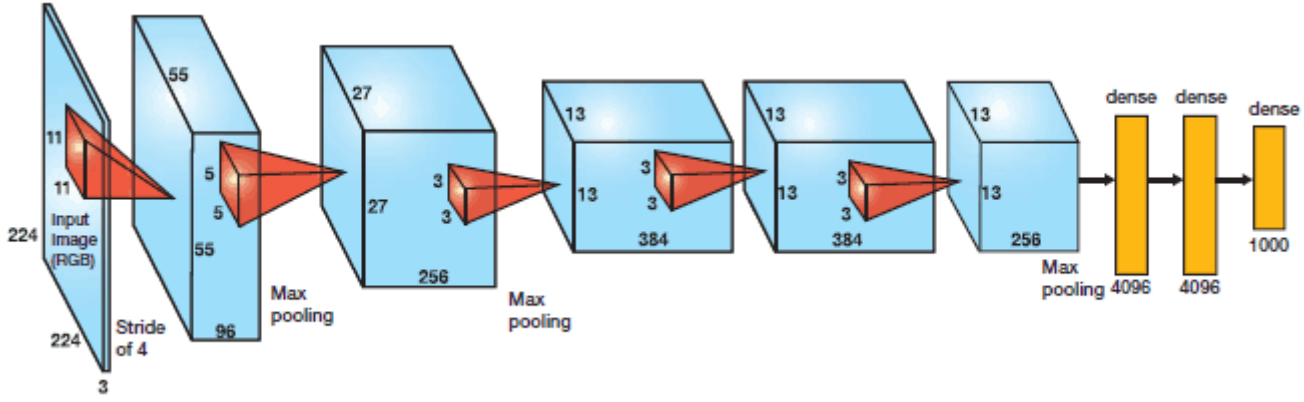
All of the followings are concrete subclasses:

Augmentation types	**Answer**
2d translation	ConvNet
others	**G-ConvNet**
- 2d translation + 90° rotation	Group Equivariant CNNs
- 2d translation + rotation	Harmonic Net
- 3d rotation	Spherical CNNs
- 3d translation + rotation	Tensor Field Net

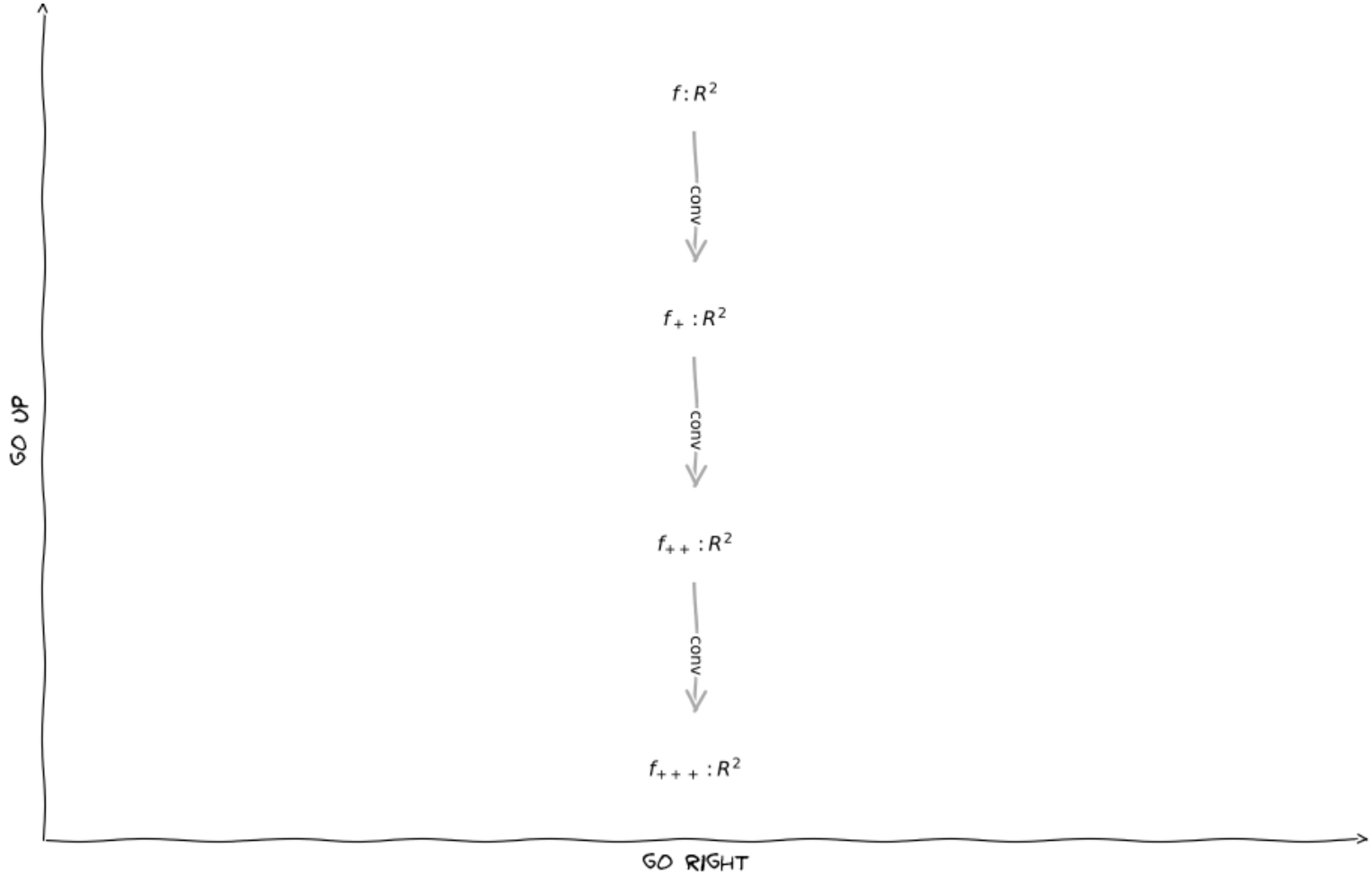
CONVNET

-	Input f(x)	High-level $f_+(y)$, $f_{++}(z)$, ...	Augmentation A_{ug}, U_{ga}, ...
domain	R^2	R^2	R^2 (translation only)

- First of its kind but not the last
- A rare case when high-level feature domain {y} = {x}, in all other cases {y} ⊃ {x}



CONVNET



GROUP EQUIVARIANT CNNS (ICML 2016*)

-	Input f(x)	High-level $f_+(y)$, $f_{++}(z)$, ...	Augmentation A_{ug}, U_{ga}, ...
domain	R^2	$R^2 \times p4$	$R^2 \times p4$ (translation, rotation $\pm 90^\circ$)

- change looks trivial

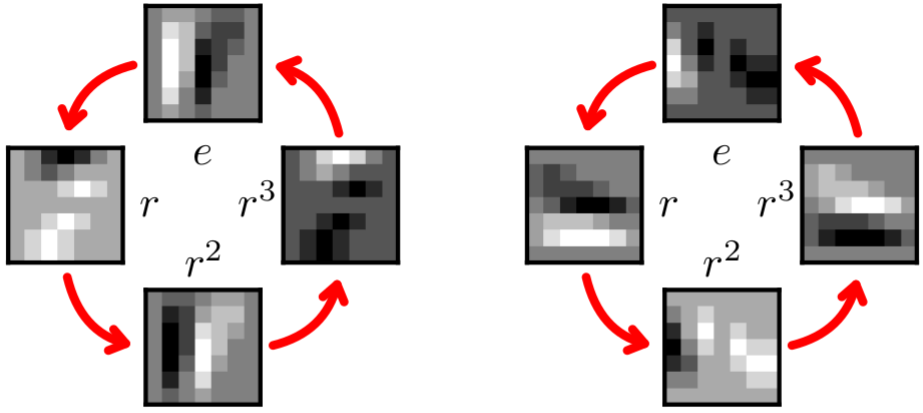
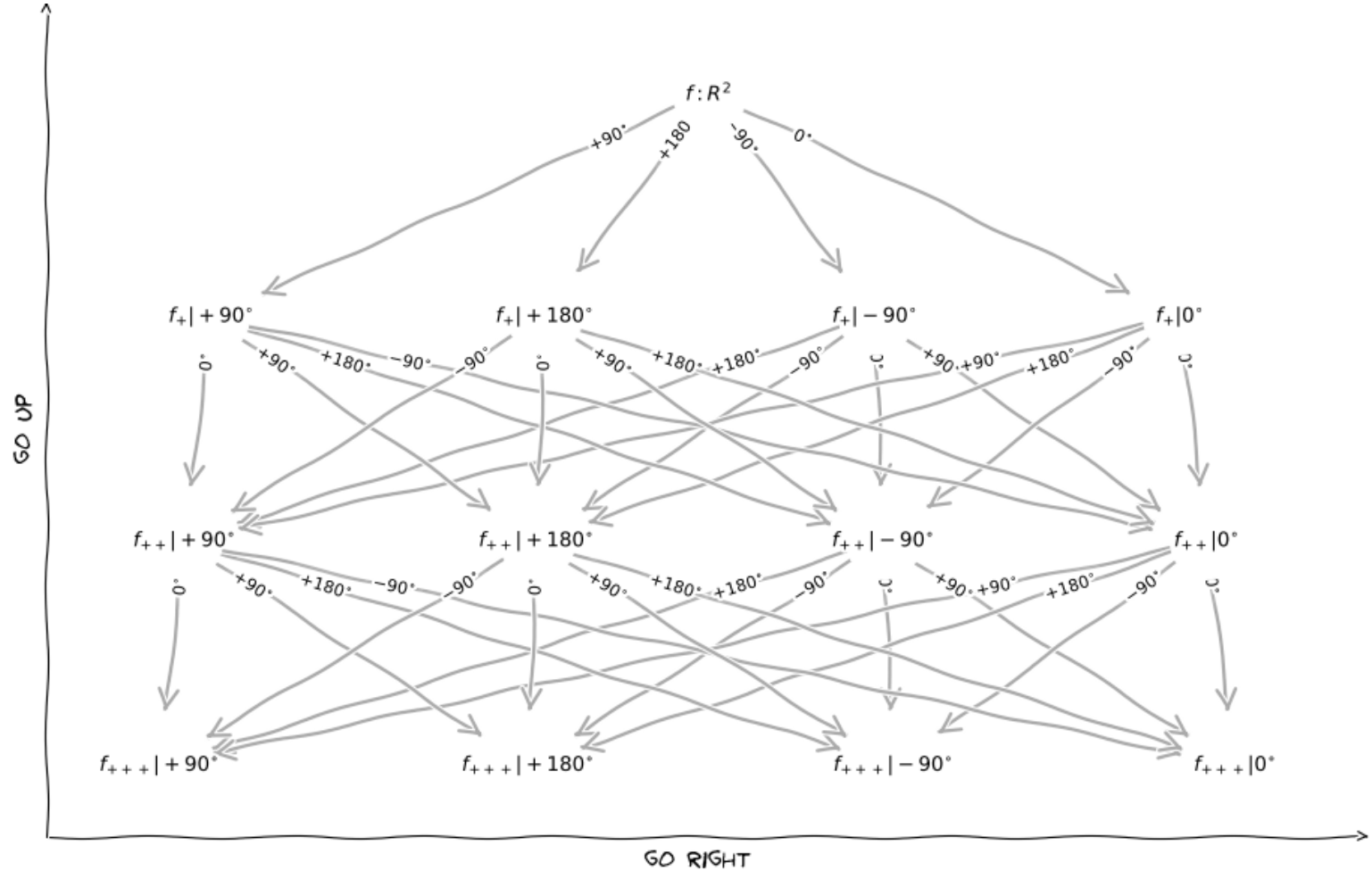


Figure 1. A p4 feature map and its rotation by r.

[*] T. S. Cohen and M. Welling, “Group Equivariant Convolutional Networks,” ICML 2016.

GROUP EQUIVARIANT CNNS (ICML 2016*)



GROUP EQUIVARIANT CNNS (ICML 2016*) - ALTERNATIVELY

-	Input f(x)	High-level $f_+(y)$, $f_{++}(z)$, ...	Augmentation A_{ug}, U_{ga}, ...
domain	R^2	$R^2 \times p4m$	$R^2 \times p4m$ (translation, rotation $\pm 90^\circ$, flipping)

- Size of filter bank start to become annoying, but still acceptable.

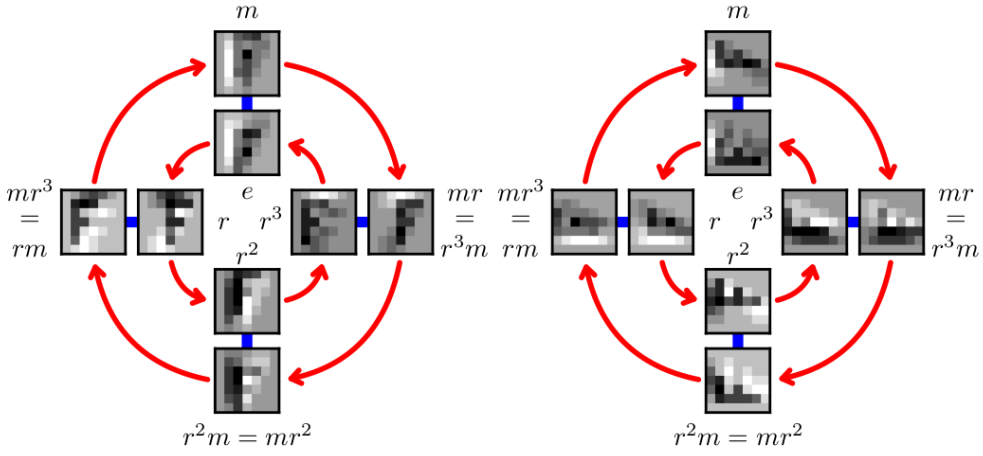


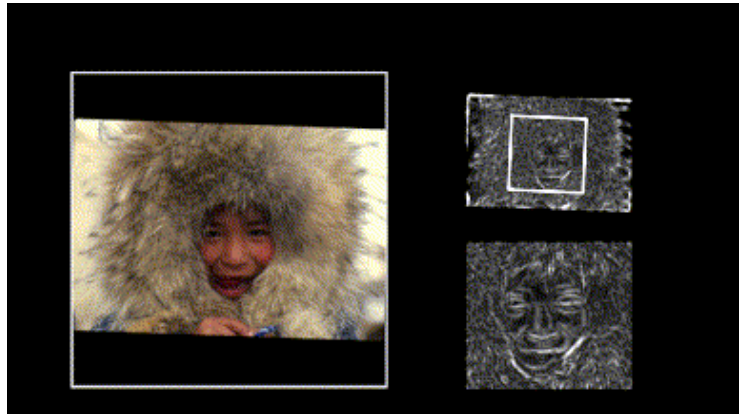
Figure 2. A p4m feature map and its rotation by r.

[*] T. S. Cohen and M. Welling, “Group Equivariant Convolutional Networks,” ICML 2016.

HARMONIC NET (CVPR 2017*)

-	Input f(x)	High-level $f_+(y)$, $f_{++}(z)$, ...	Augmentation A_{ug}, U_{ga}, ...
domain	R^2	O(2)	$O(2) \cong R^2 \times SO(2)$ (translation, arbitrary rotation)

- Size of the filter bank become intolerably big, can't take it any more
- First algorithm to use **spectral decomposition as a weight compressor**



[*] D. E. Worrall, S. J. Garbin, D. Turmukhambetov, and G. J. Brostow, “Harmonic Networks: Deep Translation and Rotation Equivariance” CVPR 2017, vol. 2017–Jan, pp. 7168–7177.

GOING SPECTRAL

- function is like infinite-dimension vector
- Spectral decomposition for functions is like eigen-decomposition for vectors

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orthonormal basis: given a function domain $X \longrightarrow C$, there may exist a (likely infinite) series of bases $u_1, u_2, \ldots$ that are both:

- **complete**: linear combination can approximate arbitrary function on the domain

$$f(.) = \sum_{\forall m} \phi_m u_m(.) = \begin{bmatrix} \phi_1, \phi_2, \ldots \end{bmatrix} \begin{bmatrix} u_1(.) \\ u_2(.) \\ \ldots \end{bmatrix}$$

- ... and **orthonormal**: have unit norms and orthogonal to each other

$$< u_m(.), u_n(.) >= I_{mn} \text{ (Kronecker delta)}$$

- ... which implies:

$$\phi_m = \hat{f}(m) =< f(.), u_m(.) > \quad \text{(GFT)}$$

GOING SPECTRAL - WHAT'S THE POINT?

It makes a few things easier:

- Convolution theorem still works in most cases! a.k.a. **G-conv theorem**

$$\hat{f}_+(m) = \langle \hat{A}_{ug}(m) \circ \hat{f}(m), \hat{w}_0(m) \rangle_m$$

(This makes dot product and G-conv much faster)

- Most G-ConvNet features are smooth on all dimensions

(This means low-frequency coefficients can compress high-dimension filter banks)

G-CONV THEOREM - PROOF

$$f_+(y) = \langle A_{ug} \circ f(x), w_0(x) \rangle_x$$

$$= \sum_m \sum_n \hat{A}_{ug} \circ \hat{f}(m) w_0(j) \langle u_m(.), u_n(.) \rangle$$

(orthonormal) $$= \sum_m \hat{A}_{ug} \circ \hat{f}(m) w_0(m)$$

(GFT) $$= \sum_m \langle A_{ug} \circ f(x), u_m(x) \rangle_x \cdot \langle w_0(x), u_m(x) \rangle_x$$

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[*] More rigorous proof for SO(3) case: T. S. Cohen, M. Geiger, J. Koehler, and M. Welling, “Spherical CNNs,” no. 3, pp. 1–15, 2018.

G-CONV THEOREM - PROOF

If luckily A_{ug} is linear:

(bijectory) $$\hat{f}_+(n) = \sum_m \left\langle < A_{ug}(y) \circ f(x), u_m(x) >_x \;\middle|\; u_n(y) \right\rangle_y \cdot <$$

(linear) $$= \sum_m < u_n(y), A_{ug}(y) >_y \circ < f(x), u_m(x) >_x \cdot <$$

$$=< A_{ug}(n) \circ \hat{f}(m), w_0(m) >_m$$

(IFF A_{ug} is distance-preserving) $$=< \hat{f}(m), A_{ug}^{-1}(n) \circ w_0(m) >_m$$

HARMONIC NET (CVPR 2017*)

-	Input f(x)	High-level $f_+(y)$, $f_{++}(z)$, ...	Augmentation A_{ug}, U_{ga}, ...
domain	R^2	O(2)	$O(2) \cong R^2 \times SO(2)$ (translation, arbitrary rotation)

- $u_m(x) \longleftarrow e^{mx}$ (2D Fourier series, x is a complex number)
- GFT ⟵ FFT (with Gaussian resampling)
- number of coefficients ⟵ 2: $m \in 0, 1$

[*] D. E. Worrall, S. J. Garbin, D. Turmukhambetov, and G. J. Brostow, “Harmonic Networks: Deep Translation and Rotation Equivariance” CVPR 2017, vol. 2017–Jan, pp. 7168–7177.

HARMONIC NET (CVPR 2017*)

Orthonormal bases (without radial):

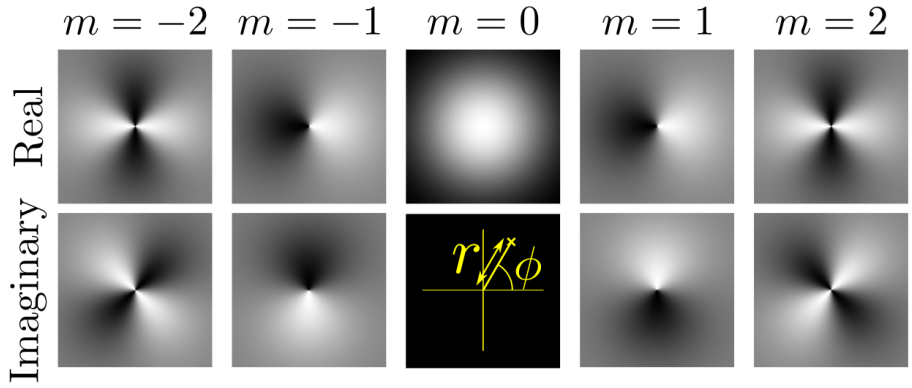
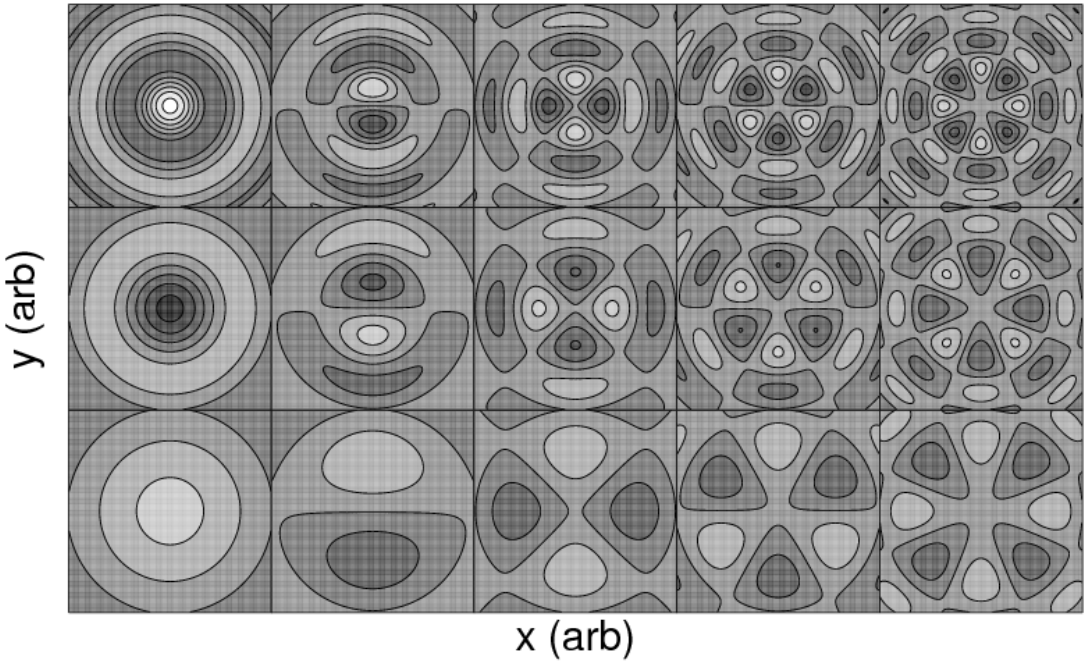


Figure 2. Real and imaginary parts of the complex Gaussian filter $\mathbf{W}_m(r,\phi';e^{-r^2},0) = e^{-r^2}e^{im\phi}$, for some rotation orders. As a simple example, we have set $R(r) = e^{-r^2}$ and $\beta = 0$, but in general we learn these quantities. Cross-correlation, of a feature map of rotation order n with one of these filters of rotation order m, results in a feature map of rotation order $m+n$. Note the negative rotation order filters have flipped imaginary parts compared to the positive orders.

[*] D. E. Worrall, S. J. Garbin, D. Turmukhambetov, and G. J. Brostow, “Harmonic Networks: Deep Translation and Rotation Equivariance” CVPR 2017, vol. 2017–Jan, pp. 7168–7177.

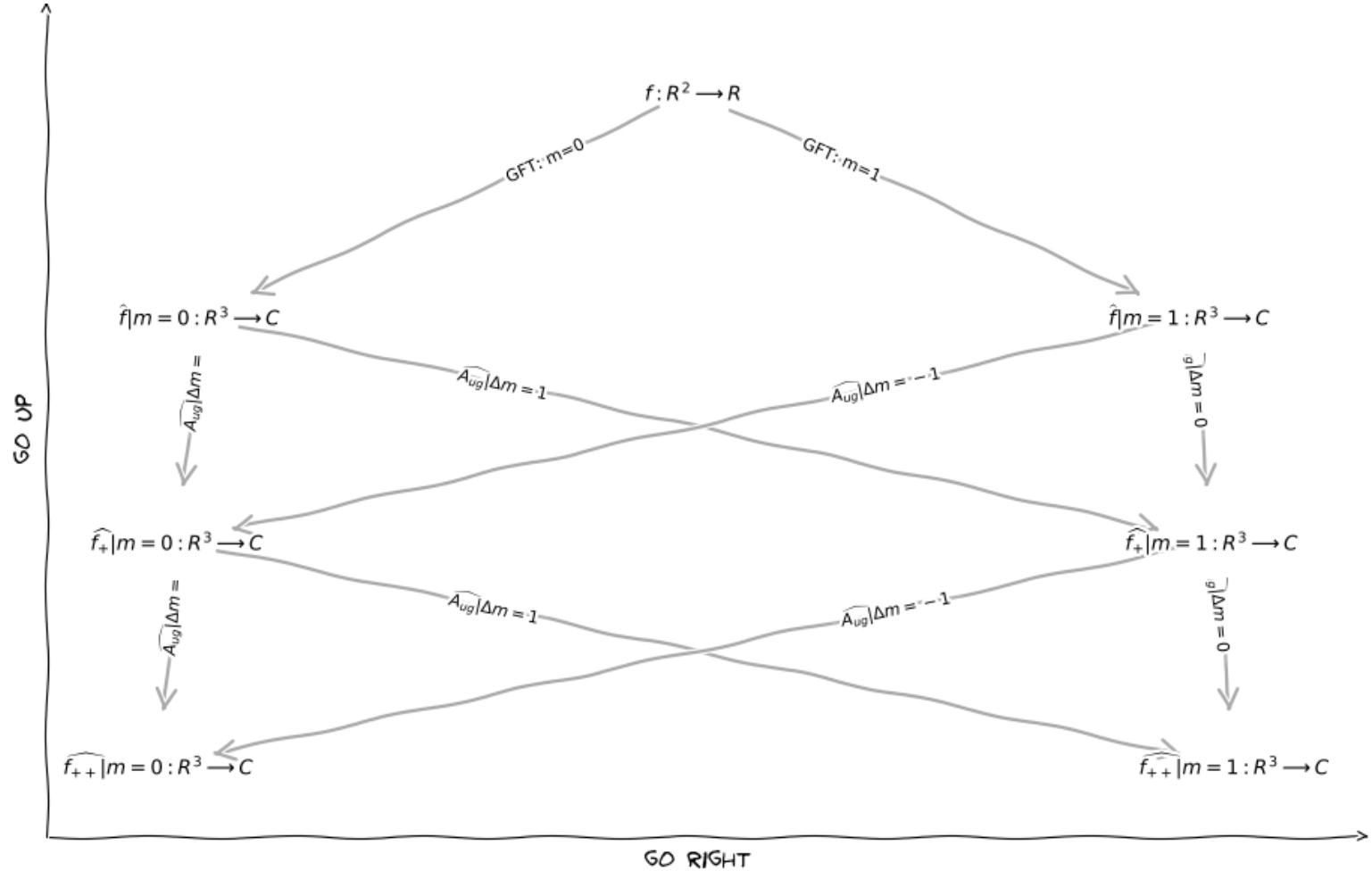
HARMONIC NET (CVPR 2017*)

Orthonormal bases (with radial):



[*] Image courtesy: C. E. Coleman-Smith, H. Petersen, and R. L. Wolpert, “Classification of initial state granularity via 2d Fourier Expansion” Apr. 2012.

HARMONIC NET (CVPR 2017*)



SPHERICAL CNNS (ICLR 2018* BEST PAPER)

You can use many cameras for situation awareness

[*] Image Courtesy: https://www.tesla.com/en_CA/autopilot (https://www.tesla.com/en_CA/autopilot)

SPHERICAL CNNS (ICLR 2018* BEST PAPER)

... Or you can use few fisheye camera(s)

[*] Image courtesy: DJI-X https://www.halfchrome.com/dji-360-drone/ (https://www.halfchrome.com/dji-360-drone/)

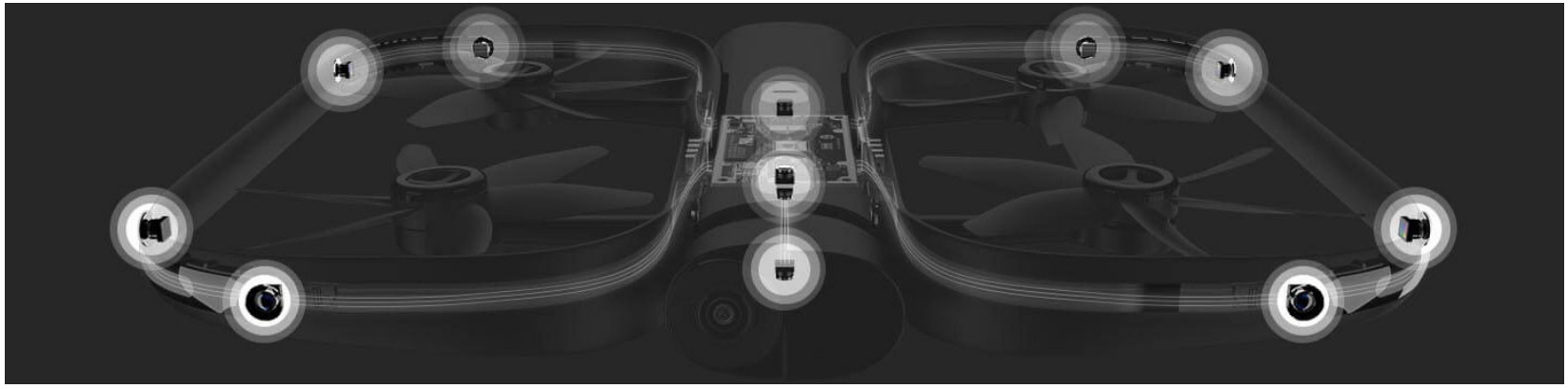
SPHERICAL CNNS (ICLR 2018* BEST PAPER)

Instead ...

[*] Image Courtesy: Skydio R1 https://www.skydio.com/technology/ (https://www.skydio.com/technology/)

SPHERICAL CNNS (ICLR 2018* BEST PAPER)

Instead ...



[*] Image Courtesy: Skydio R1 https://www.skydio.com/technology/ (https://www.skydio.com/technology/)

SPHERICAL CNNS (ICLR 2018* BEST PAPER)

-	Input f(x)	High-level $f_{+}(y)$, $f_{++}(z)$, ...	Augmentation A_{ug}, U_{ga}, ...
domain	S^2	SO(3)	SO(3) ≅ SU(2) (3d rotation)

- $u_m(x) \longleftarrow D_m(x)$ (Wigner-D function, x is an Euler-angle tuple or quaternion)
  - collapses to spherical harmonics on the first layer
- GFT ⟵ SO(3) FFT
- number of coefficients ≤ 25: $l \in [0, 4]$ (increasing beyond that contributes little to accuracy)

[*] T. S. Cohen, M. Geiger, J. Koehler, and M. Welling, “Spherical CNNs,” no. 3, pp. 1–15, 2018.

SPHERICAL CNNS (ICLR 2018* BEST PAPER)

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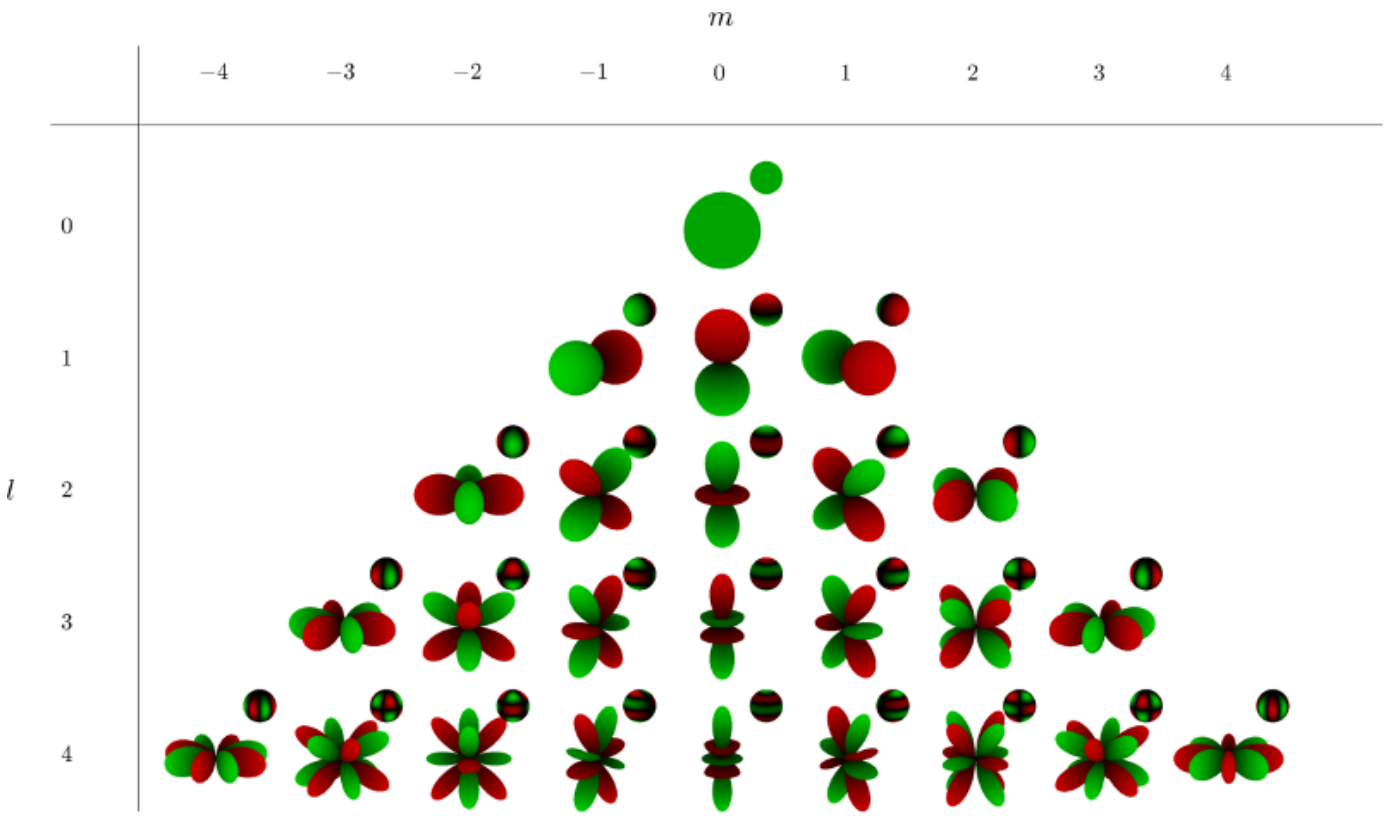
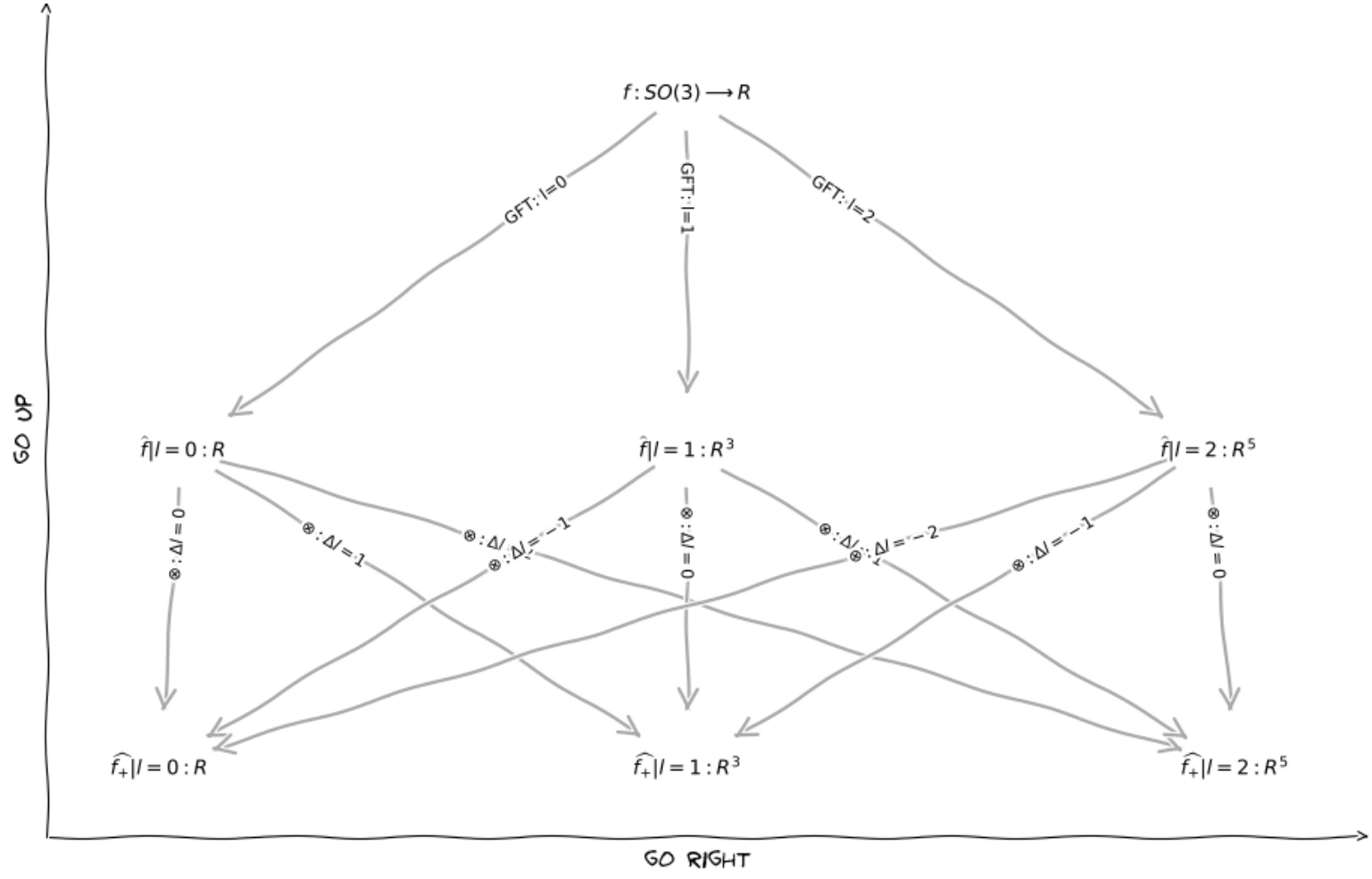


[*] T. S. Cohen, M. Geiger, J. Koehler, and M. Welling, “Spherical CNNs,” no. 3, pp. 1–15, 2018.

SPHERICAL CNNS (ICLR 2018* BEST PAPER)

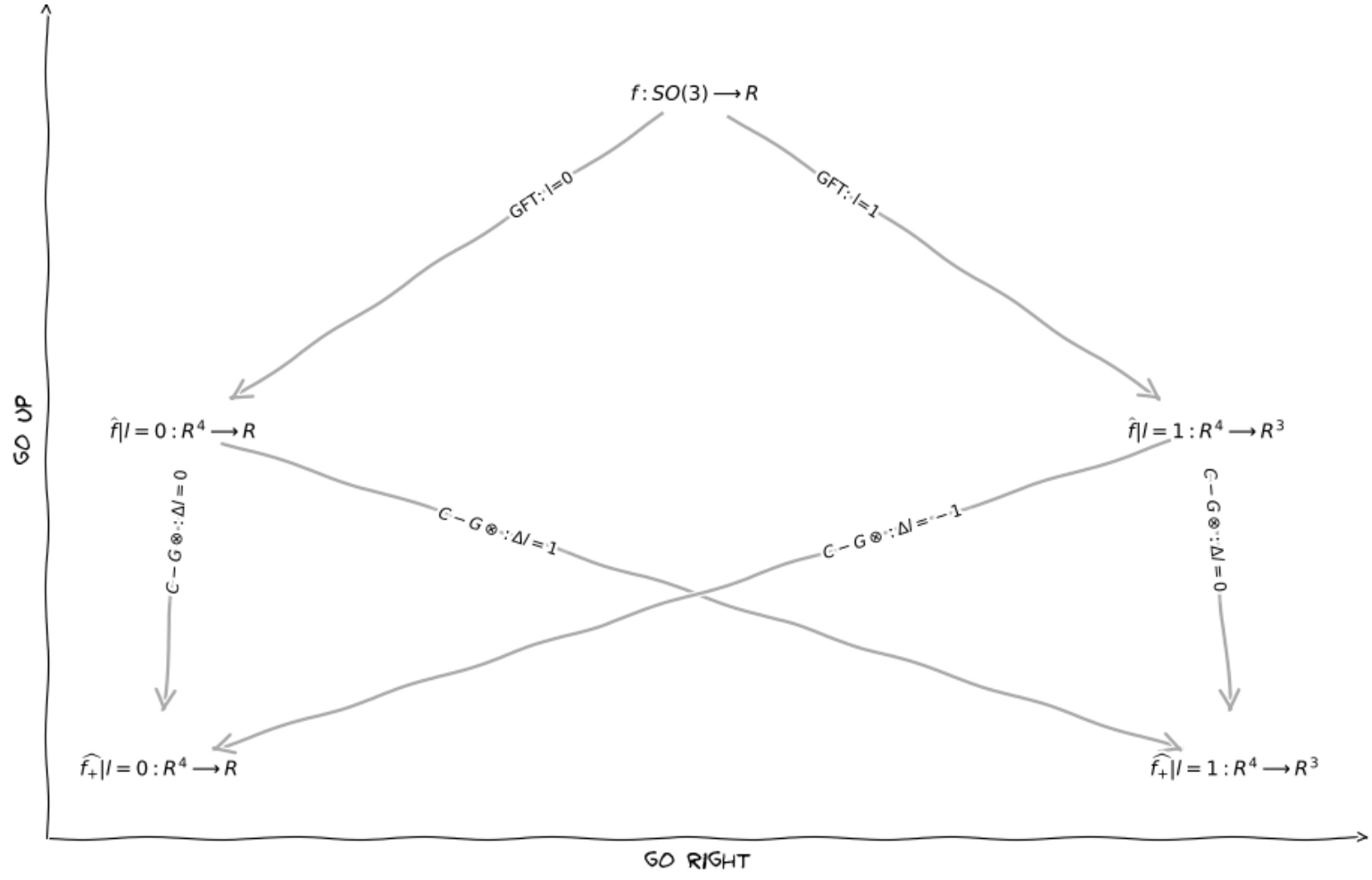


TENSOR FIELD NETWORK (NOT PEER REVIEWED!)

-	Input f(x)	High-level $f_{+}(y)$, $f_{++}(z)$, ...	Augmentation A_{ug}, U_{ga}, ...
domain	R^3	O(3)	$O(3) \cong R^3 x SO(3)$ (3d translation & rotation)

- $u_m(x) \longleftarrow D_m(x)$ (Wigner-D function, x is an Euler-angle tuple or quaternion)
  - collapses to spherical harmonics on the first layer
- GFT $\longleftarrow$ SO(3) FFT
- number of coefficients $\longleftarrow$ 4: $l \in 0, 1$
- C-G transformation is used to accelerate G-conv in frequency space
  - which was not needed in Spherical CNNs due to lack of radial component

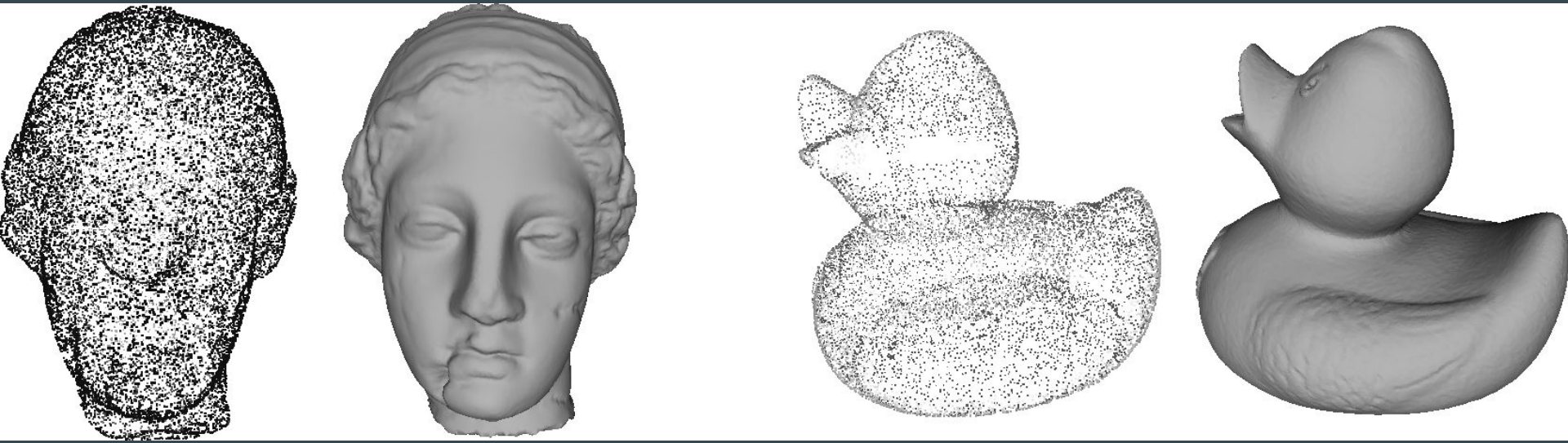
TENSOR FIELD NETWORK (NOT PEER REVIEWED!)



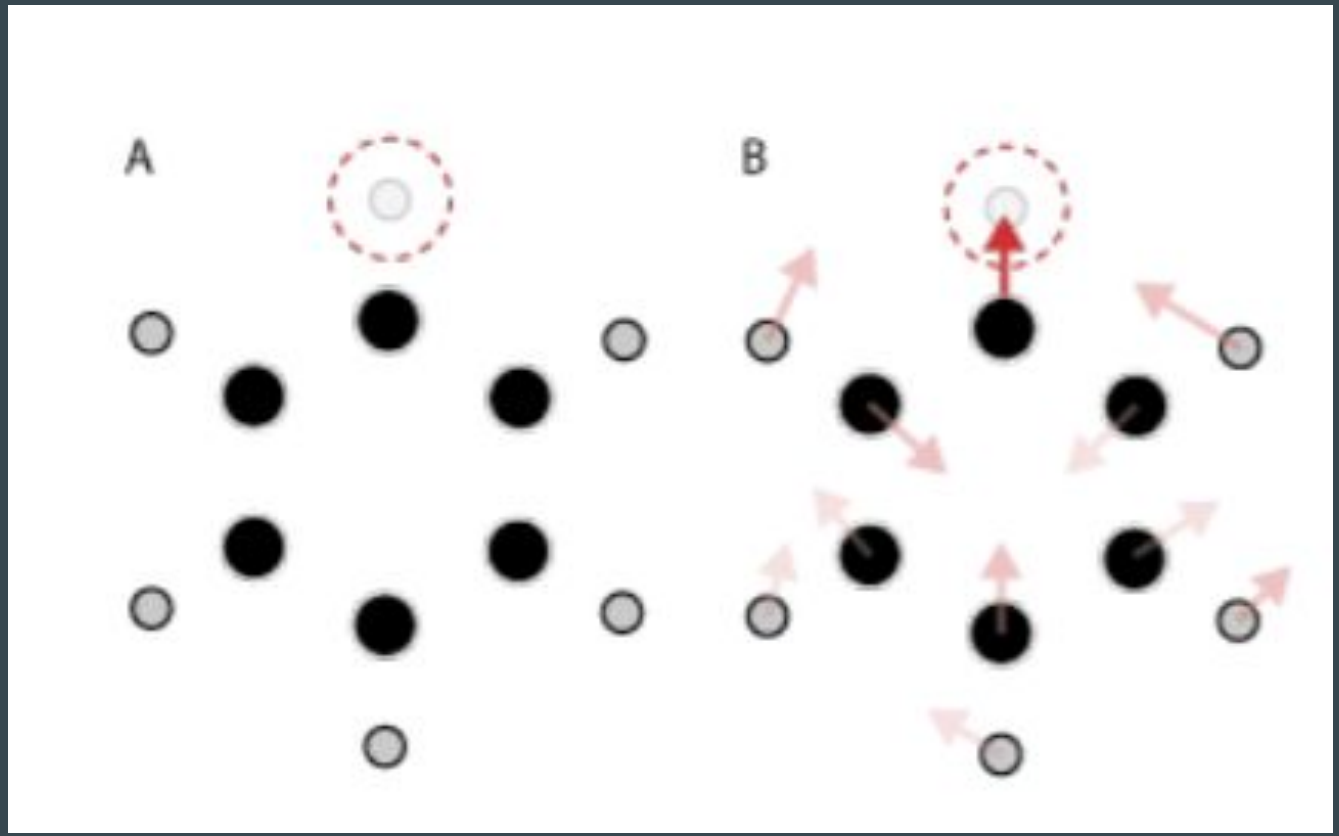
Tensor Field Networks

Chris Dryden, Peng Cheng

Point Cloud Networks

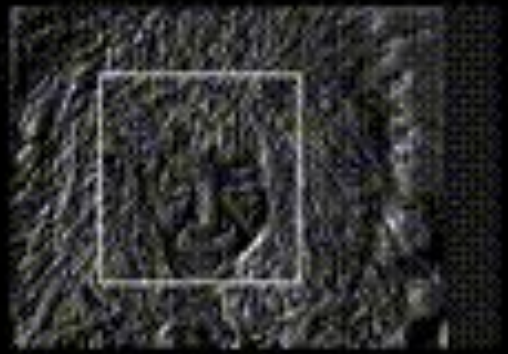


Chemical Point Cloud



Existing CNNs: Translation Equivariance

Input

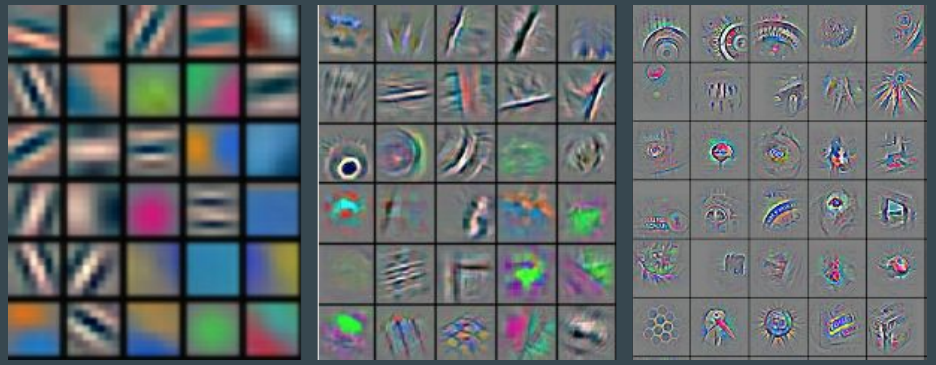


Features

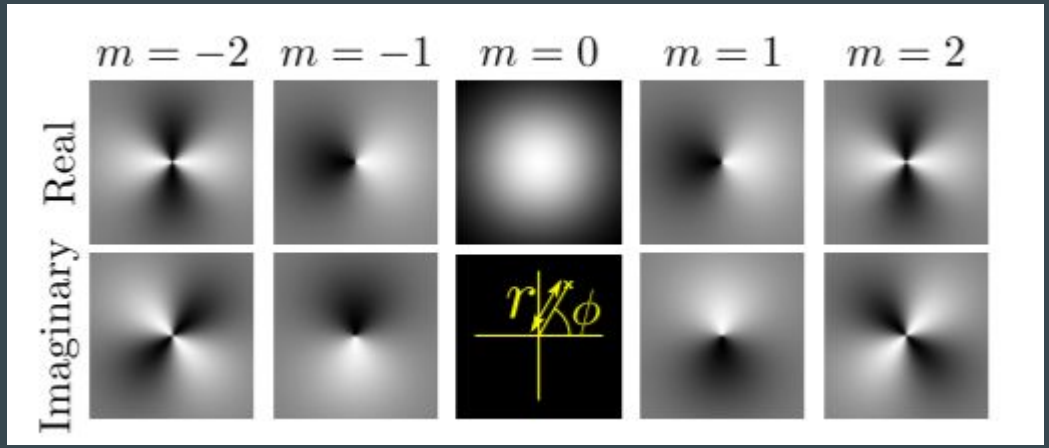
Windowed view

Harmonic Networks

Spatial Domain

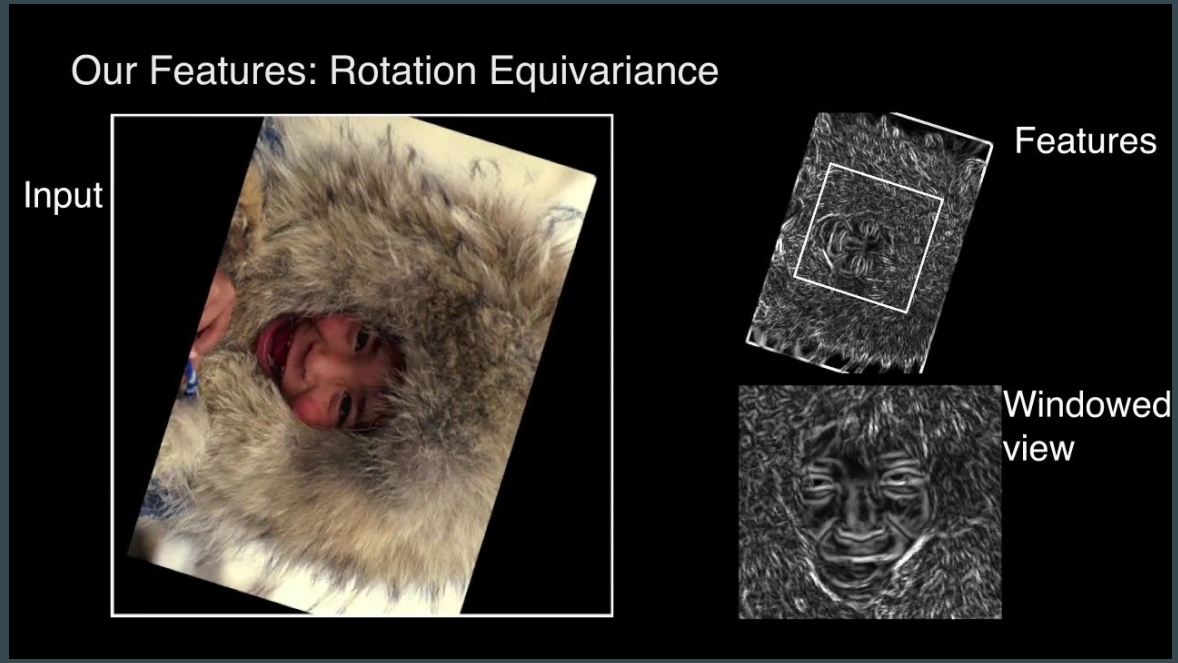


Frequency Domain



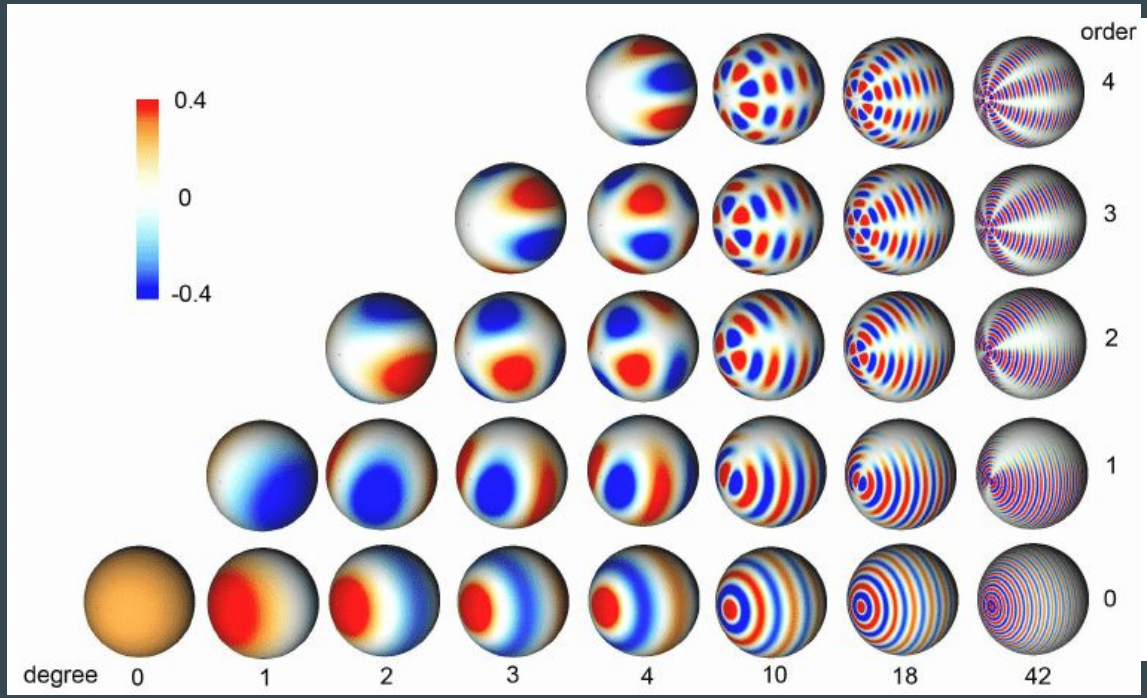
Harmonic Networks - Rotation Equivariance

Frequency Domain



Harmonic Networks - Spherical

Frequency Domain



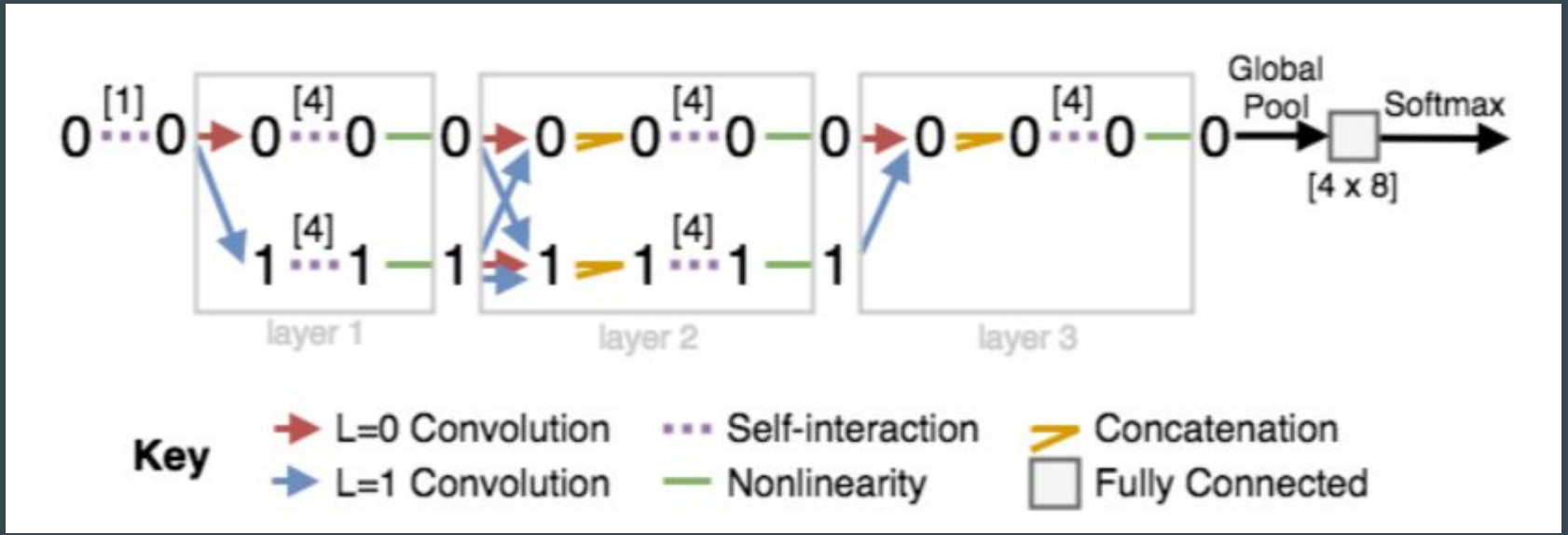
1	1	1
1	1	1
1	1	1

-1	-2	-1
0	0	0
1	2	1

1	1	1
1	1	1
1	1	1

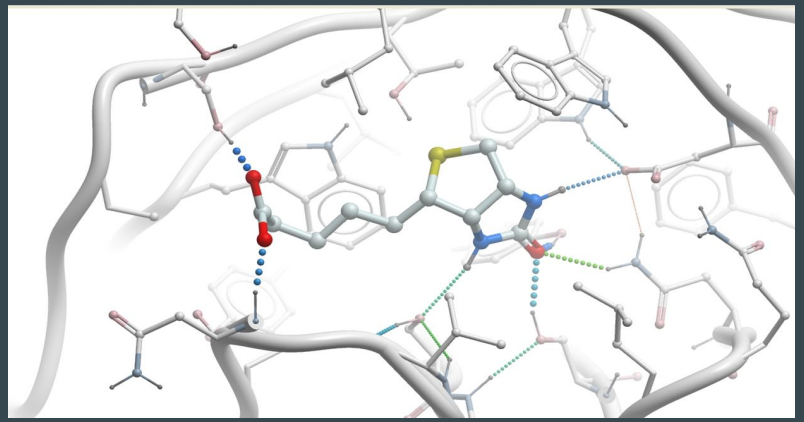
1	2	1
0	0	0
-1	-2	-1

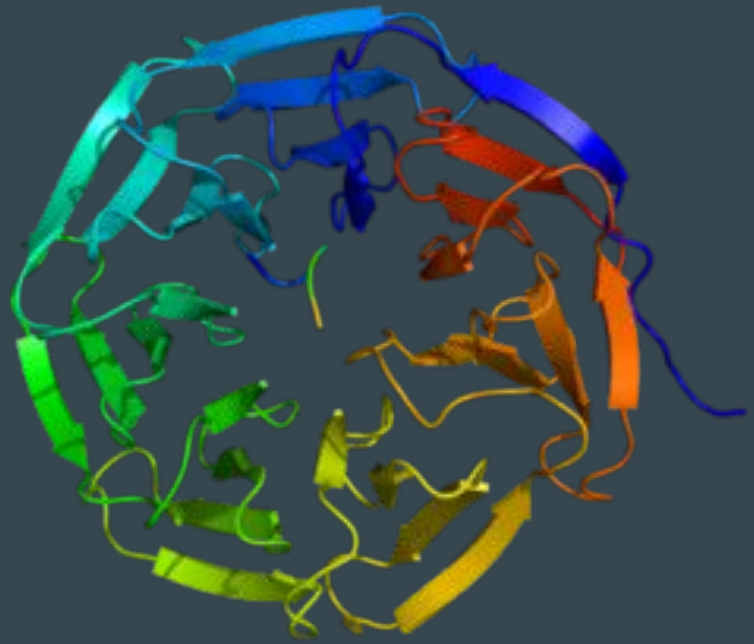
Tensor-Field Model



Current Applications

Scalable to size of a protein





WDR5

Discussion Points -

- Paper did not go in depth about the information stored in the points
  - More applications are possible. Would the chemical dataset work with chemical properties.
- Can it be applied to more traditional 3d-image sets?
  - Eg: Autonomous Driving
- Can we incorporate in this architecture other types of symmetries?
  - Ex: Mirror Symmetries, R-L Enantiomers
- Can this be applied to Neural-ODE's?