Qualcomm

Equivariance III: Literature, Applications and Beyond

Gabriele Cesa

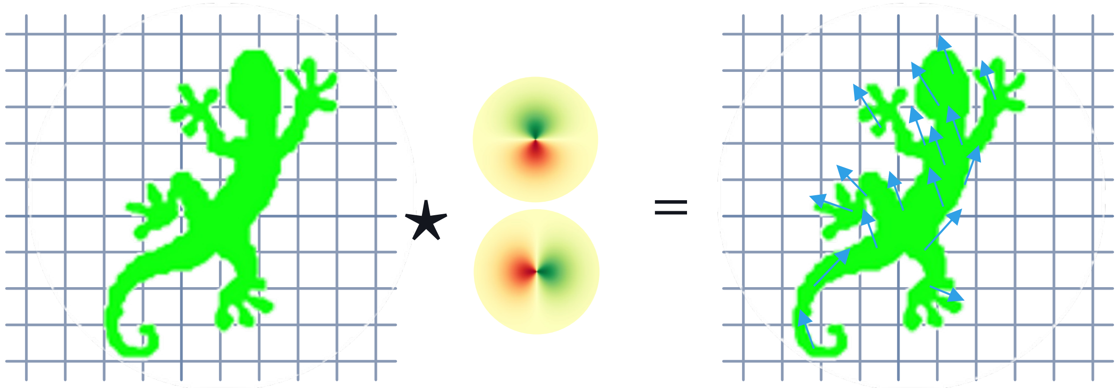
Senior Engineer, Qualcomm AI Research*

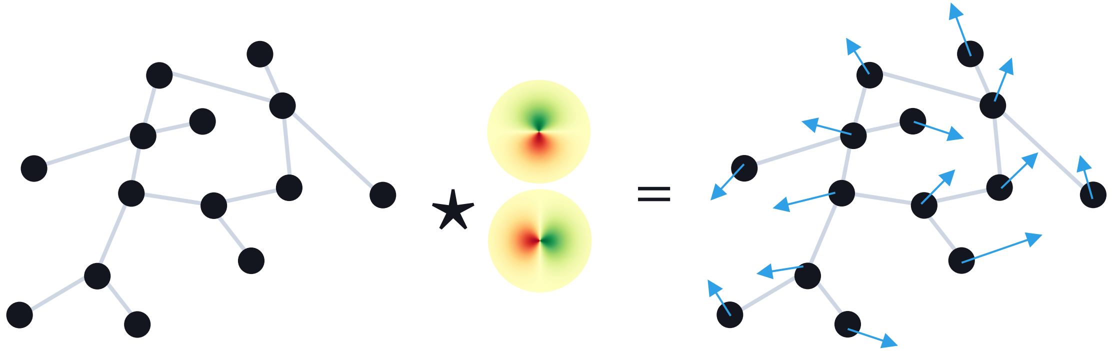
University of Amsterdam, AMLab

14/06/2024

*Qualcomm AI Research is an initiative of Qualcomm Technologies, Inc.

Convolution and Message Passing





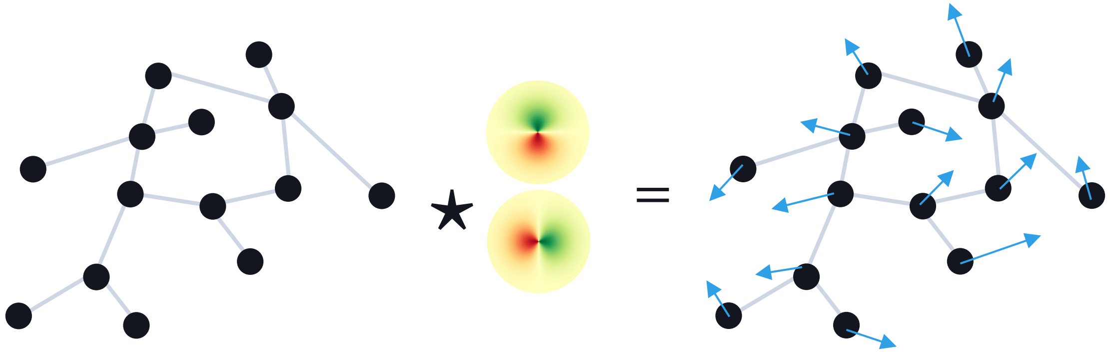
$$[\kappa \star f](y) = \sum_{x \in \mathbb{Z}^n} \kappa(x - y)\ f(x)$$

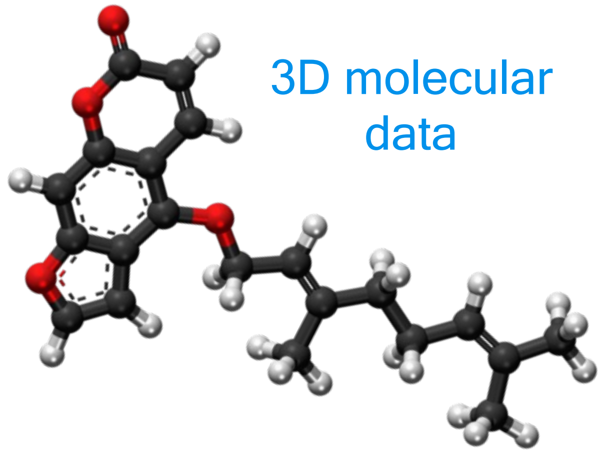
$$[\kappa \star f](i) = \sum_{j \in N_i} \kappa\left(x_i - x_j\right)\ f_j$$

$$\kappa(g.x) = \rho_{out}(g)\kappa(x)\rho_{in}(g)^T$$

Steerability Constraint

Tensor Field Networks

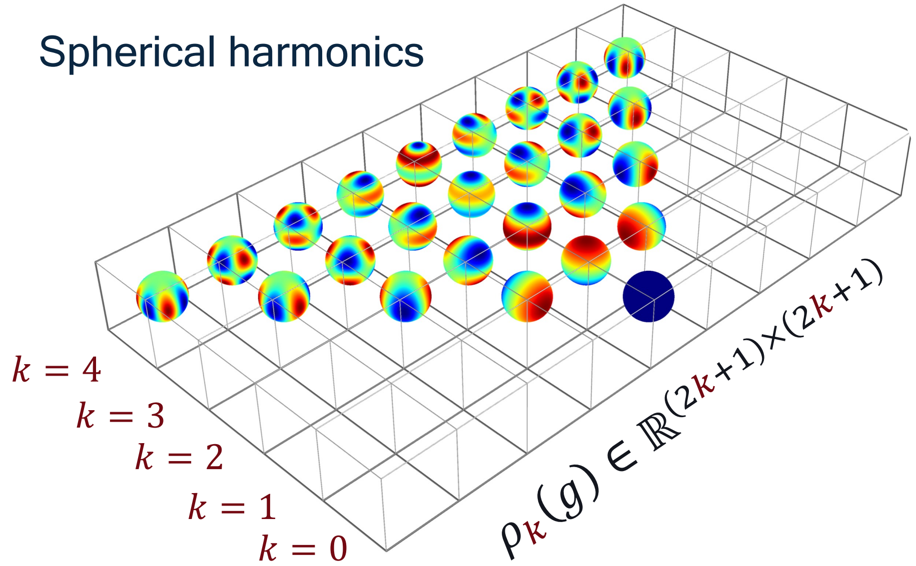




source: Jynto, CC0, Wikimedia Commons

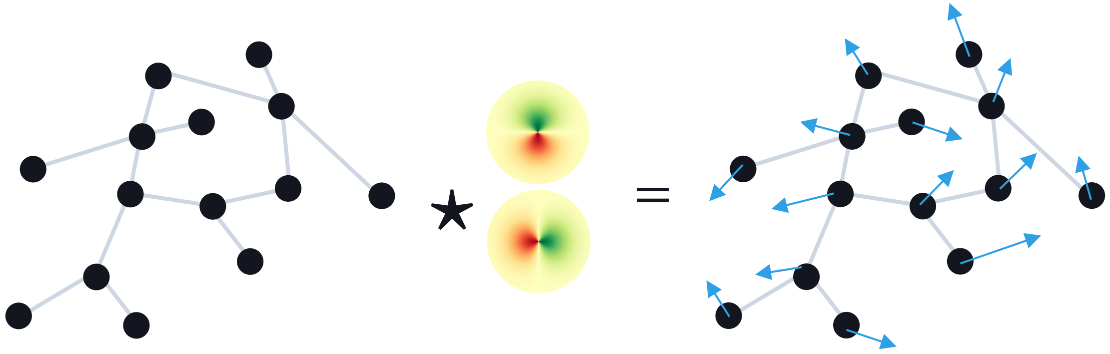
$$[\kappa \star f](i) = \sum_{j \in N_i} \kappa(x_i - x_j)\ f_j$$

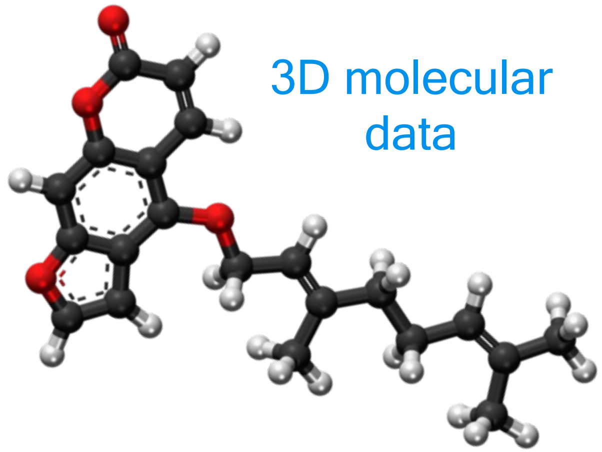
- $SE(3) = (\mathbb{R}^n, +) \rtimes SO(3)$
- **Norm Non-Linearity:** $f_k(x) \mapsto \sigma(|f_k(x)|_2^2)\ f_k(x)$



Nathaniel Thomas, Tess Smidt, Steven Kearnes, Lusann Yang, Li Li, Kai Kohlhoff, and Patrick Riley. Tensor field networks: Rotation-and translation-equivariant neural networks for 3d point clouds. (2018)

Non-Linear Message Passing

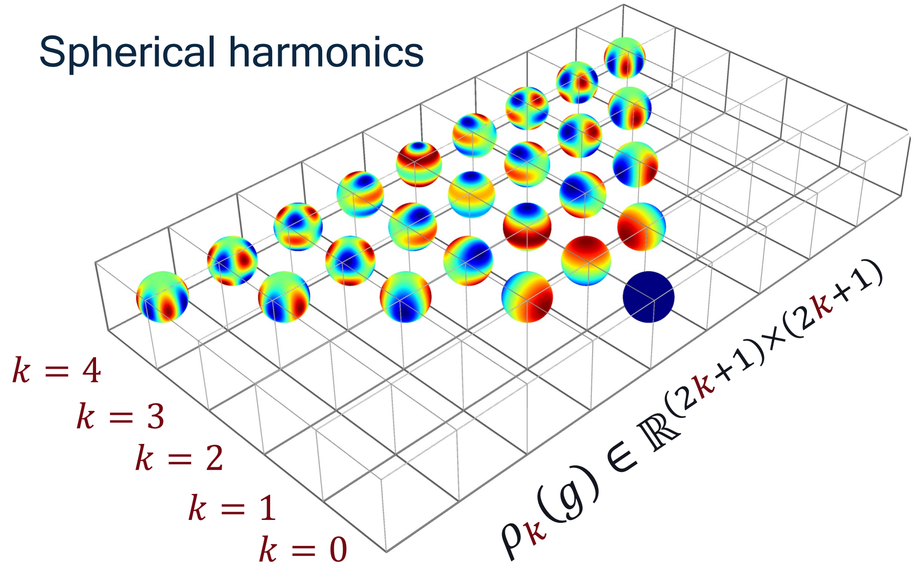




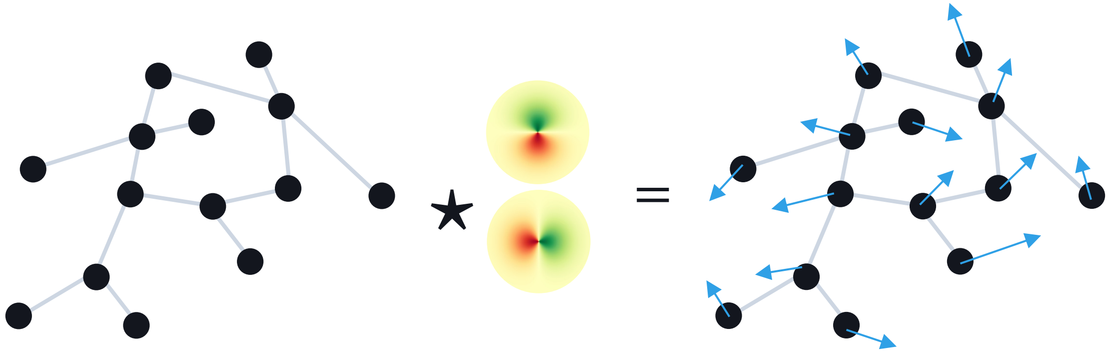
source: Jynto, CC0, Wikimedia Commons

$$m(i) = \sum_{j \in N_i} \phi\left(x_i - x_j, f_i, f_j\right)$$

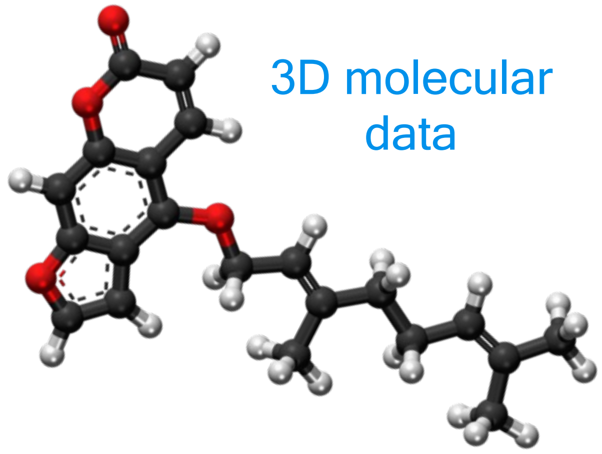
- $SE(3) = (\mathbb{R}^n, +) \rtimes SO(3)$



Non-Linear Message Passing



3D molecular data



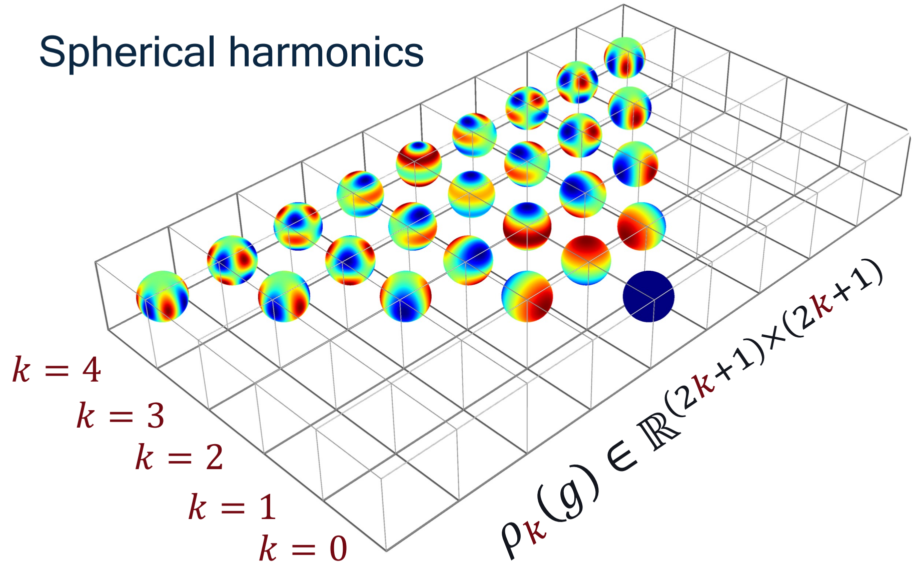
source: [Jynto, CC0, Wikimedia Commons]

$$m(i) = \sum_{j \in N_i} m_L(i,j)$$

$$m_l(i,j) = \sigma\big(\kappa_l(x_i - x_j)\, m_{l-1}(i,j)\big)$$
$$m_0(i,j) = (f_i, f_j)$$

- $E(3) = (\mathbb{R}^n, +) \rtimes O(3)$
- **Gated Non-Linearity:** $f(x), f_g(x) \mapsto \sigma\big(f_g(x)\big)\, f(x)$

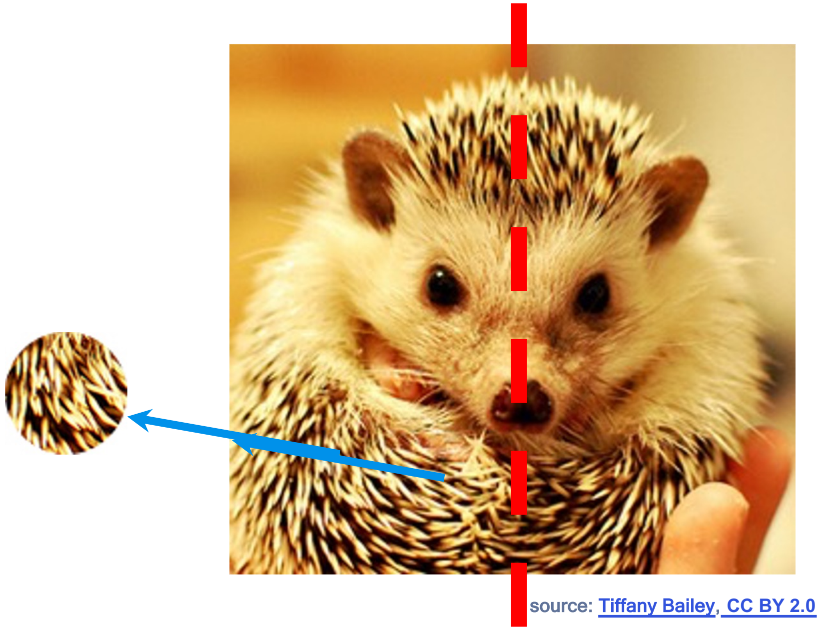
Spherical harmonics



Johannes Brandstetter, Rob Hesselink, Elise van der Pol, Erik J. Bekkers, and Max Welling. Geometric and Physical Quantities improve E(3) Equivariant Message Passing. *International Conference on Learning Representations (ICLR). 2021.*

Local Symmetries

- Reflection symmetry in the class
- Rotational symmetry in the *local* patterns



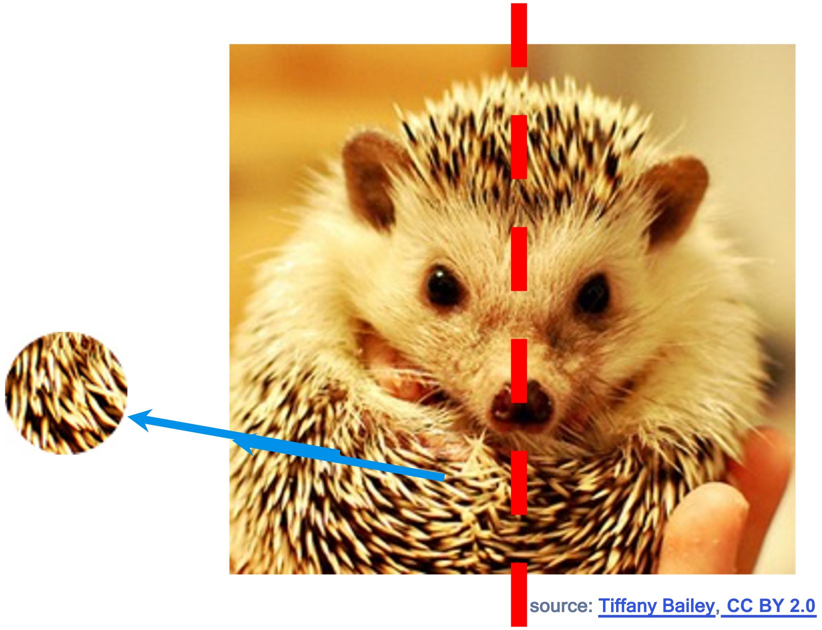
source: Tiffany Bailey, CC BY 2.0

Maurice Weiler* and Gabriele Cesa*.
General E(2)-Equivariant Steerable CNNs,
Neural Information Processing Systems (NeurIPS), 2019

Local Symmetries

- Reflection symmetry in the class
- Rotational symmetry in the *local* patterns

source: MikeLynch, CC BY-SA 3.0



source: Tiffany Bailey, CC BY 2.0

Maurice Weiler* and Gabriele Cesa*.
General E(2)-Equivariant Steerable CNNs,
Neural Information Processing Systems (NeurIPS), 2019

Group Restriction

- Model the loss of symmetries at larger scales by relaxing the equivariance constraint at different depths:
  - exploit more symmetries in the first layers
  - restrict later to the symmetries of your output

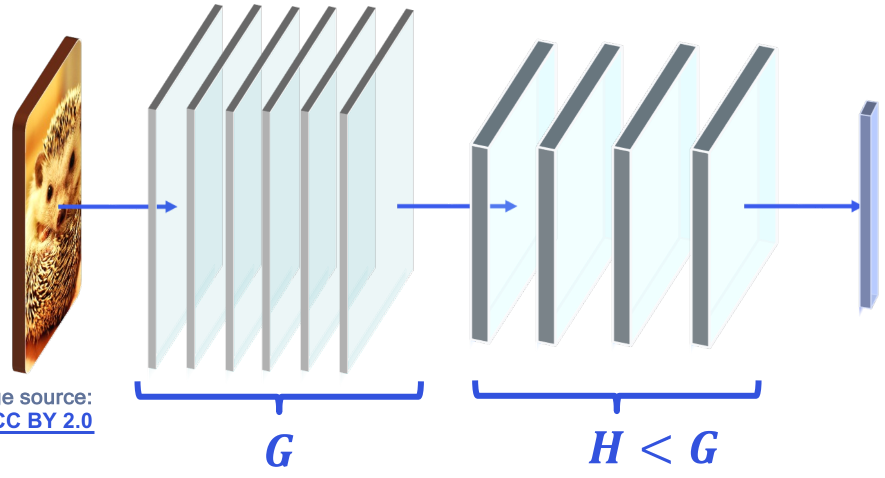


Image source:
Tiffany Bailey, CC BY 2.0

Maurice Weiler* and Gabriele Cesa*.
General E(2)-Equivariant Steerable CNNs,
Neural Information Processing Systems (NeurIPS), 2019

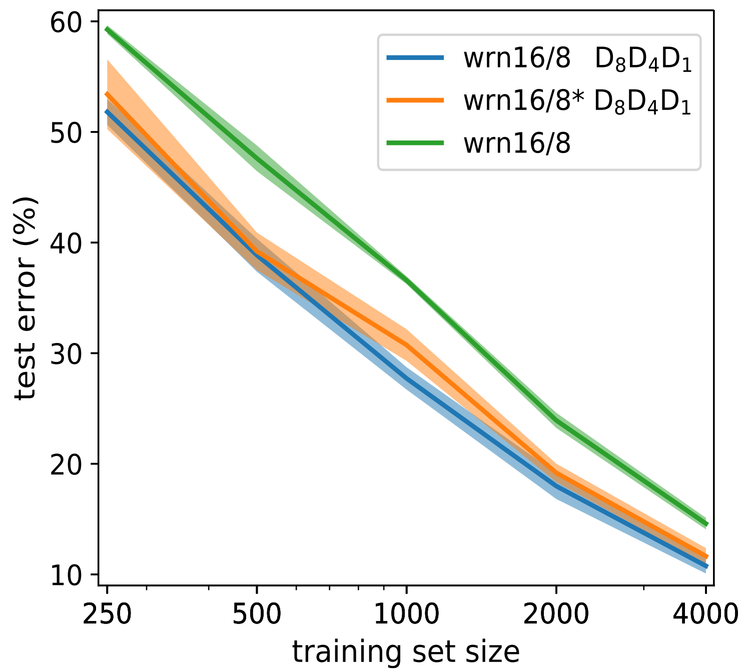
Experiments on Natural Images

model			CIFAR-10	CIFAR-100
wrn28/10	[30]		3.87	18.80
wrn28/10	$D_1\,D_1\,D_1$		3.36 ± 0.08	17.97 ± 0.11
wrn28/10*	$D_8\,D_4\,D_1$		3.32 ± 0.10	17.42 ± 0.38
wrn28/10	$C_8\,C_4\,C_1$		3.20 ± 0.04	16.47 ± 0.22
wrn28/10	$D_8\,D_4\,D_1$		3.13 ± 0.17	16.76 ± 0.40
wrn28/10	$D_8\,D_4\,D_4$		2.91 ± 0.13	16.22 ± 0.31
wrn28/10	[31]	AA	2.6 ± 0.1	17.1 ± 0.3
wrn28/10*	$D_8\,D_4\,D_1$	AA	2.39 ± 0.12	15.55 ± 0.13
wrn28/10	$D_8\,D_4\,D_1$	AA	2.05 ± 0.03	14.30 ± 0.09

AA = Auto Augment

model	group	#params	test error (%)
wrn16/8 [32]	-	11M	12.74 ± 0.23
wrn16/8*	$D_1\,D_1\,D_1$	5M	11.05 ± 0.45
wrn16/8	$D_1\,D_1\,D_1$	10M	11.17 ± 0.60
wrn16/8*	$D_8\,D_4\,D_1$	4.2M	10.57 ± 0.70
wrn16/8	$D_8\,D_4\,D_1$	12M	9.80 ± 0.40

STL - 10



Maurice Weiler* and Gabriele Cesa*.
General E(2)-Equivariant Steerable CNNs,
Neural Information Processing Systems (NeurIPS), 2019

Imperfect or Unknown symmetries

- Group Restriction: layer **adapted to the symmetries** manifested in the scale of **its field of view**
  - Still requires knowledge about these symmetries

- Can we learn the level of equivariance from data?

Finzi, M., Benton, G., and Wilson, A. G. Residual pathway priors for soft equivariance constraints. *Advances in Neural Information Processing Systems (NeurIPS) 2021.*

van der Ouderaa, T., Romero, D. W., and van der Wilk, M. Relaxing equivariance constraints with non-stationary continuous filters. Advances in Neural Information Processing Systems (NeurIPS), 2022

Wang, R., Walters, R., and Yu, R. Approximately equivariant networks for imperfectly symmetric dynamics. International Conference on Machine Learning (ICML), 2022

Romero, D. W. and Lohit, S. Learning partial equivariances from data. Advances in Neural Information Processing Systems (NeurIPS), 2022

Imperfect or Unknown symmetries

- Group Restriction: layer **adapted to the symmetries** manifested in the scale of **its field of view**
  - Still requires knowledge about these symmetries

- Can we learn the level of equivariance from data?

$$[\kappa \star f](y) = \sum_{x \in \mathbb{Z}^n} \kappa(x - y)\ f(x)$$

$$[\kappa \star f](g) = \int_{h \in G} \kappa(g^{-1} h)\ f(h) d\mu(h)$$

Finzi, M., Benton, G., and Wilson, A. G. Residual pathway priors for soft equivariance constraints. *Advances in Neural Information Processing Systems (NeurIPS) 2021.*

van der Ouderaa, T., Romero, D. W., and van der Wilk, M. Relaxing equivariance constraints with non-stationary continuous filters. Advances in Neural Information Processing Systems (NeurIPS), 2022

Wang, R., Walters, R., and Yu, R. Approximately equivariant networks for imperfectly symmetric dynamics. International Conference on Machine Learning (ICML), 2022

Romero, D. W. and Lohit, S. Learning partial equivariances from data. Advances in Neural Information Processing Systems (NeurIPS), 2022

Imperfect or Unknown symmetries

- Group Restriction: layer **adapted to the symmetries** manifested in the scale of **its field of view**
  - Still requires knowledge about these symmetries

- Can we learn the level of equivariance from data?

$$[\kappa \star f](y) = \sum_{x \in \mathbb{Z}^n} \kappa(x - y, x)\ f(x)$$

$$[\kappa \star f](g) = \int_{h \in G} \kappa(g^{-1} h, h)\ f(h) d\mu(h)$$

Finzi, M., Benton, G., and Wilson, A. G. Residual pathway priors for soft equivariance constraints. *Advances in Neural Information Processing Systems (NeurIPS) 2021.*

van der Ouderaa, T., Romero, D. W., and van der Wilk, M. Relaxing equivariance constraints with non-stationary continuous filters. Advances in Neural Information Processing Systems (NeurIPS), 2022

Wang, R., Walters, R., and Yu, R. Approximately equivariant networks for imperfectly symmetric dynamics. International Conference on Machine Learning (ICML), 2022

Romero, D. W. and Lohit, S. Learning partial equivariances from data. Advances in Neural Information Processing Systems (NeurIPS), 2022

Imperfect or Unknown symmetries

- Group Restriction: layer **adapted to the symmetries** manifested in the scale of **its field of view**
  - Still requires knowledge about these symmetries

- Can we learn the level of equivariance from data? (Veefkind and Cesa, 2024)

$$[\kappa \star f](g) = \int_{h \in G} \left[\int_{u \in G} \kappa(ug, uh) dP(u) \right] f(h) d\mu(h)$$

Finzi, M., Benton, G., and Wilson, A. G. Residual pathway priors for soft equivariance constraints. *Advances in Neural Information Processing Systems (NeurIPS) 2021.*

van der Ouderaa, T., Romero, D. W., and van der Wilk, M. Relaxing equivariance constraints with non-stationary continuous filters. Advances in Neural Information Processing Systems (NeurIPS), 2022

Wang, R., Walters, R., and Yu, R. Approximately equivariant networks for imperfectly symmetric dynamics. International Conference on Machine Learning (ICML), 2022

Romero, D. W. and Lohit, S. Learning partial equivariances from data. Advances in Neural Information Processing Systems (NeurIPS), 2022

Veefkind, L. and Cesa G. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. *International Conference on Machine Learning (ICML), 2024*

Beyond $\mathbb{R}^n$

- So far, Steerable CNNs only on $(\mathbb{R}^n, +) \rtimes G$
  - With compact rotation group $G < O(n)$

- Can we build them over other spaces than $\mathbb{R}^n$?
  - theoretically yes, but…

Gauge Equivariant CNNs

- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$

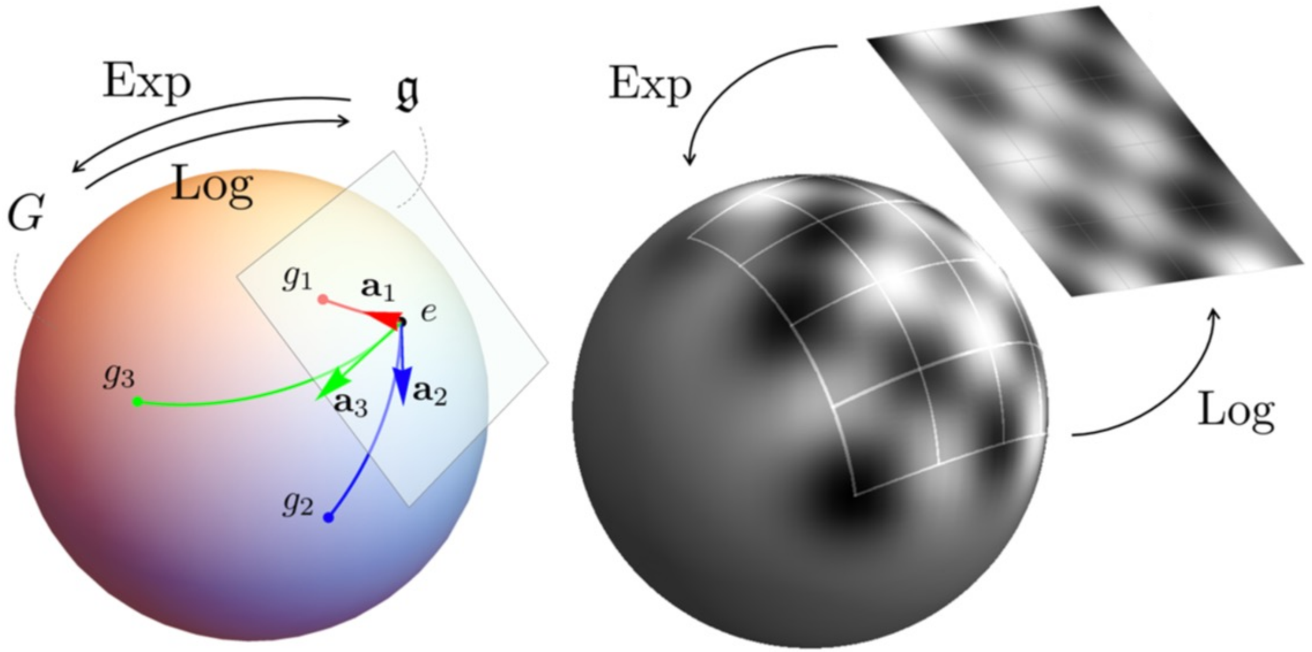


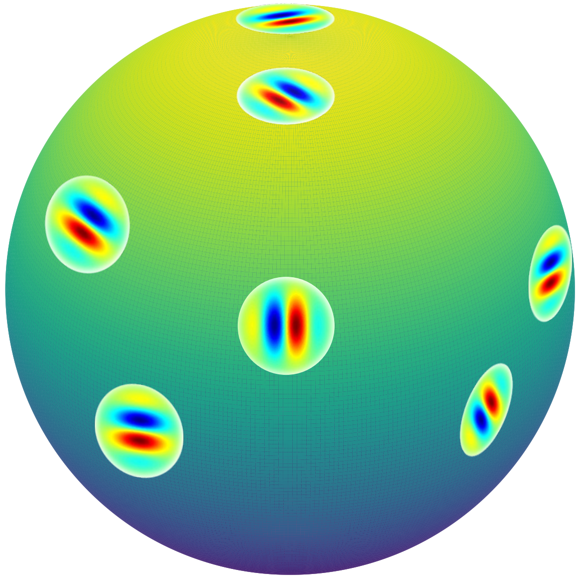
Image source: courtesy of Erik J Bekkers

Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$

- How do we orient filters?

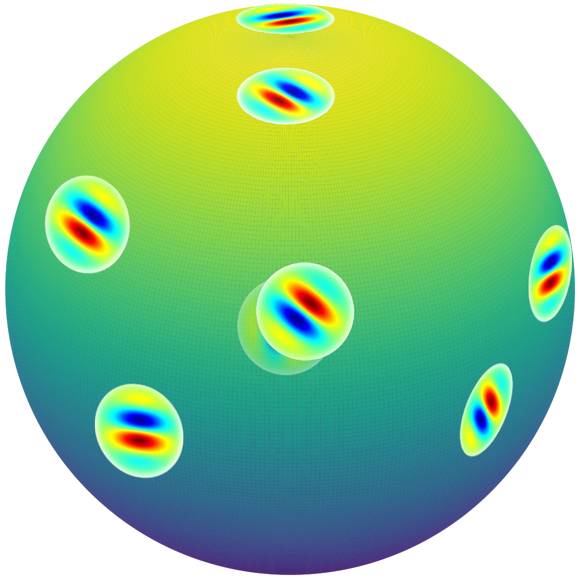


Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$

- How do we orient filters?

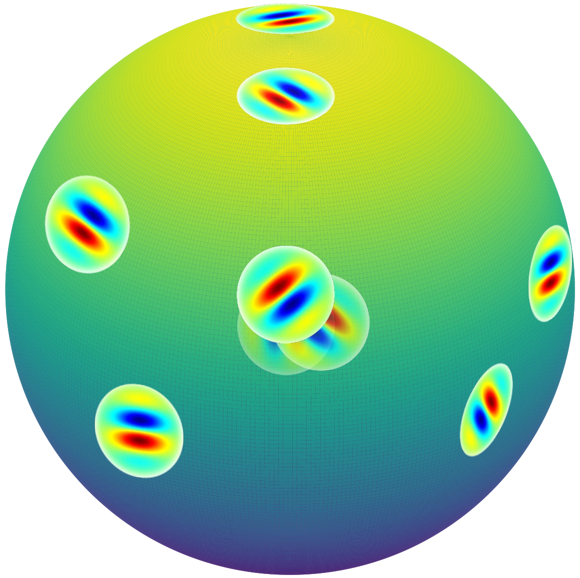


Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$

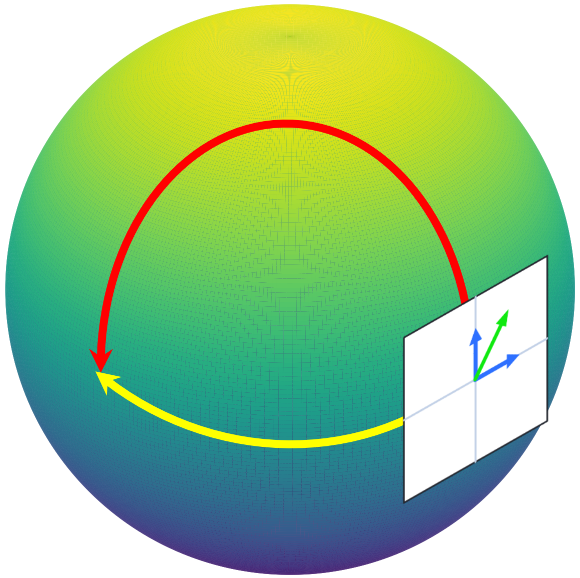
- How do we orient filters?



Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

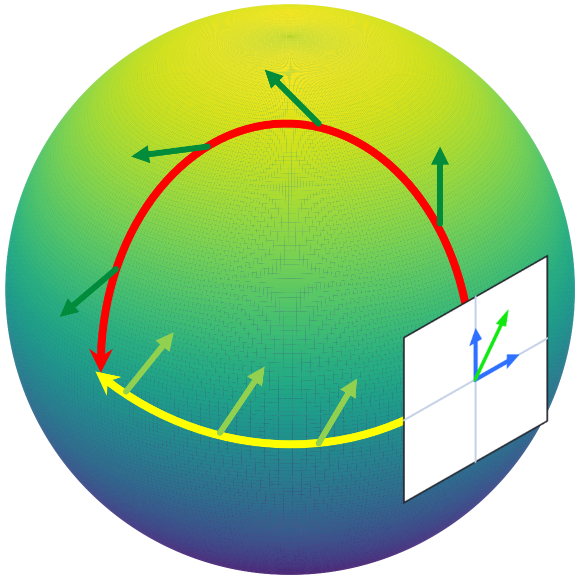
- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$



Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

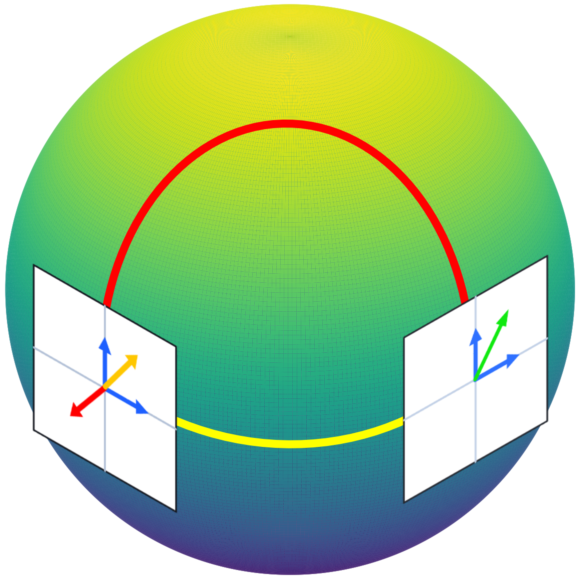
- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$



Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

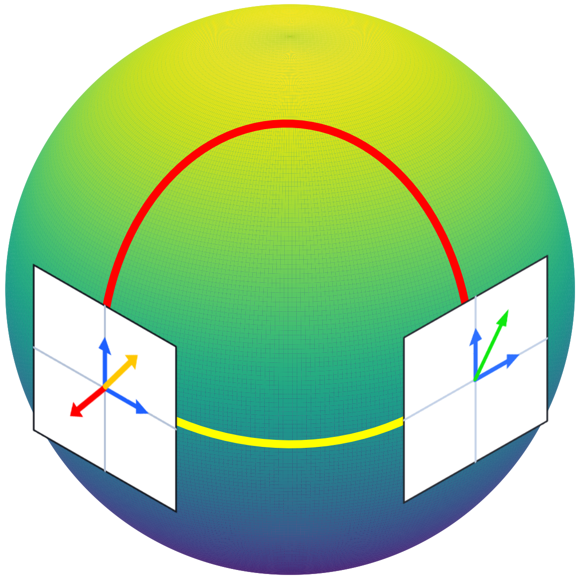
- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$

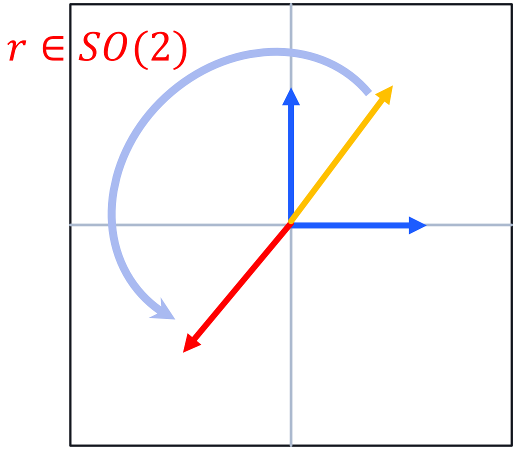


Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$

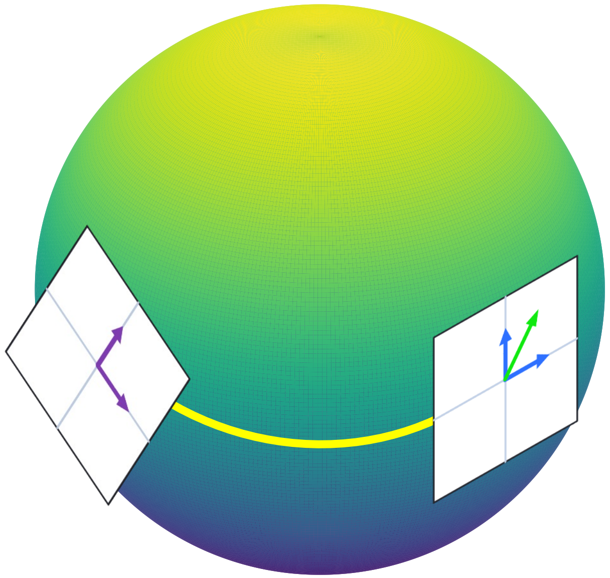




Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

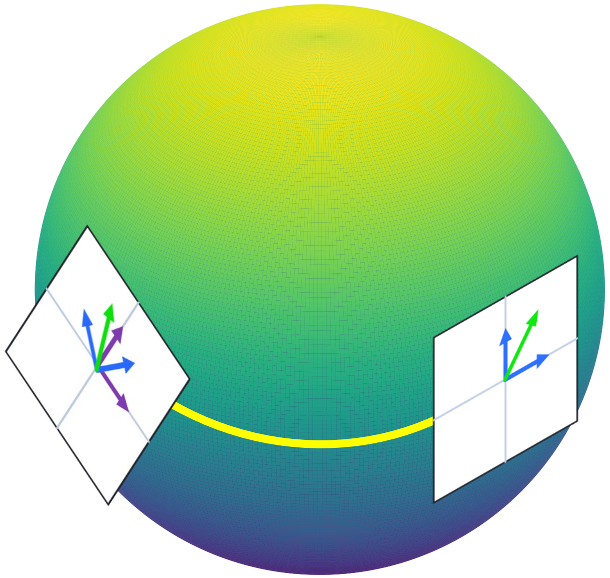
- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$

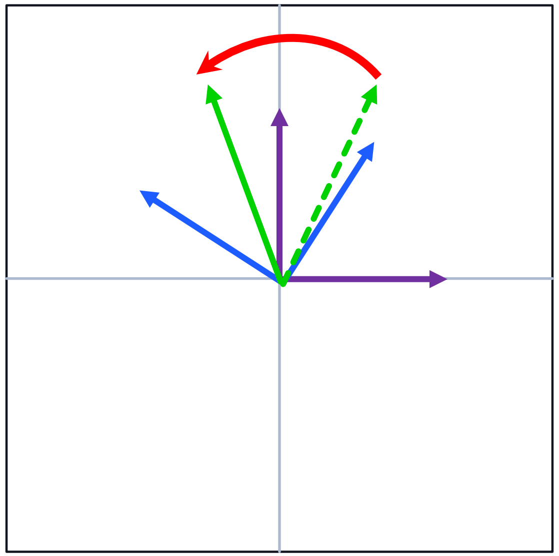


Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Gauge Equivariant CNNs

- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^n, +) \rtimes G$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$





Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

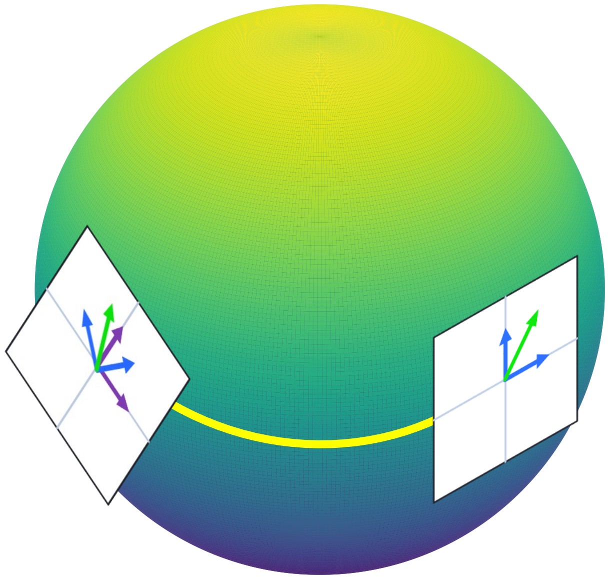
Gauge Equivariant CNNs

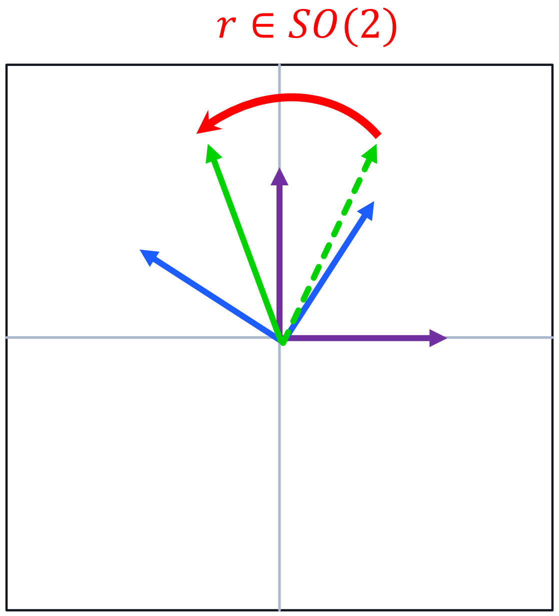
- Convolution on general manifold $\mathcal{M}$
- Leveraging a $(\mathbb{R}^2, +) \rtimes SO(2)$ **steerable convolution**
- On the **tangent space** $T_p\mathcal{M}$

$$[\kappa \star f](i) = \sum_{j \in N_i} \kappa(x_i - x_j)\, \rho(g_{ij})\, f_j$$

$$\kappa(g.x) = \rho_{out}(g)\kappa(x)\rho_{in}(g)^T$$

Steerability Constraint





Taco Cohen, Maurice Weiler, Berkay Kicanaoglu, and Max Welling. Gauge equivariant convolutional networks and the icosahedral CNN. International conference on Machine learning, 2019.
Weiler, M., P. Forré, E. Verlinde, and M. Welling. Coordinate Independent Convolutional Networks: Isometry and Gauge Equivariant Convolutions on Riemannian Manifolds. (2021).

Open Question: Scaling Models vs Inductive Biases

- SOTA models are huge foundational models
- **No inductive bias**
- Huge datasets
- Very expensive and expressive transformer architecture

- Do we still care about equivariance?

Thank you

Follow us on:

For more information, visit us at qualcomm.com & qualcomm.com/blog