PDO-eS^{2}CNNs: Partial Differential Operator Based Equivariant Spherical CNNs

Zhengyang Shen , Tiancheng Shen , Zhouchen Lin , Jinwen Ma

Abstract

Introduction

$\mathbb{R}^2$

$\mathcal{S}^2$		$SO(2), SO(3)$	
α, β, γ		$Z(\alpha), Y(\beta)$	z y
R	$R \in SO(3)$ $R = Z(\alpha_R)Y(\beta_R)Z(\gamma_R)$	$n = (0,0,1)^T$	
P	$P \in \mathcal{S}^2$, $P(\alpha, \beta) = Z(\alpha)Y(\beta)n$	$\bar{P}$	P
$\bar{P} \cdot SO(2)$	$\{\bar{P}Z(\gamma) \vert \gamma \in [0, 2\pi)\}$, $SO(2)$	$E \simeq F$	E F
A_R	$Z(\gamma_R)$	$C^1(\mathcal{S}^2)$	$\mathcal{S}^2$
$C^1(SO(3))$	$SO(3)$	s, so	$s \in C^1(\mathcal{S}^2)$ $so \in C^1(SO(3))$
$\pi^S_{\widetilde{R}}[s], \pi^{SO}_{\widetilde{R}}[so]$	$\widetilde{R}$ s so	U_P	$\mathcal{S}^2$ P
$\widetilde{U}_p$	$\widetilde{U}_p = \varphi_P(U_P) \subset \mathbb{R}^2$	φ_P	U_P $\widetilde{U}_P$
$\bar{s}$	$\mathbb{R}^3$ s	$H(\cdot, \cdot; \boldsymbol{w})$	$\boldsymbol{w}$
$\partial/\partial x_i^{(A)}$	$A \in SO(2)$	$\nabla_x[f], \nabla_x^2[f]$	f
$\nabla_x^{(A)}, (\nabla_x^{(A)})^2$	fi	$\chi^{(A)}$	fi
Ψ, Φ	fi	$\boldsymbol{I}, \boldsymbol{F}$	
f_P	$f_P = \bar{s} \cdot \varphi_P{}^{1}$	$O(\cdot)$	fi
$D_P, \hat{D}_P$		$\hat{\nabla}_x[f], \hat{\nabla}_x^2[f]$	$\nabla_x[f]$ $\nabla_x^2[f]$
$\widetilde{\chi}^{(A)}, \widetilde{\Psi}, \widetilde{\Phi}$	$\chi^{(A)}, \Psi$ Φ	C_N	N

$SO(\ )$

Related Work

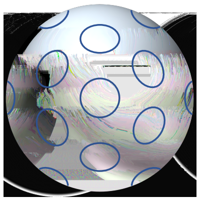
$SO(\ )$

Prior Knowledge

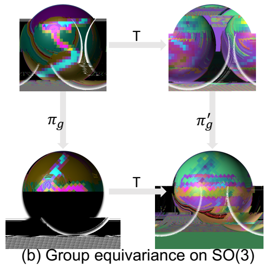
Parameterization of $\mathcal{S}^2$ and $SO(\ )$

$\mathcal{S}^2$ $SO(\ )$

$$\mathcal{S}^2 = \{(\ _1,\ _2,\ _3) \vert \Vert\ \Vert_2 = \ \},$$
$$SO(\ ) = \{R \in \mathbb{R}^3 \vert R^T R = I,\ (R) = \ \}.$$



(a) $S^2 \simeq SO(3)/SO( )$



(b) Group equivariance on SO(3)

$\mathcal{S}^2 \simeq SO( )/SO( )$. $SO( )$

ed $SO( )$. f

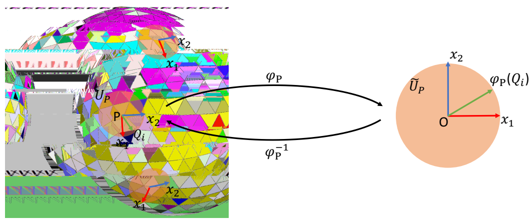
$g \in SO( )$ T

fi T

$SO( )$.

$R \in SO( )$

$$R = Z(\alpha_R)Y(\beta_R)Z(\gamma_R),$$



$P \in \mathcal{S}^2$, φ_P $U_P \subset \mathcal{S}^2$ $\widetilde{U}_P \subset \mathbb{R}^2$

U_P $\widetilde{U}_P = \varphi_P(U_P) \subset \mathbb{R}^2$ $\varphi_P(P) =$ φ_P

$$\varphi_P^{-1}(\ _1,\ _2) = \bar{P}\left(\ _1,\ _2, \sqrt{\ - |\ |^2}\right)^T.$$

$P \in \mathcal{S}^2$ 1 2 U_P, φ_P fi

$\in C^\infty(\mathcal{S}^2)$ fi $\mathbb{R}^3$, $\in C^\infty(\mathbb{R}^3)$ $\partial/\partial\ _i$ $\partial^2/\partial\ _i\partial\ _j$ $(\ , \ = \ , \ )$ $\cdot\, \varphi_P^{-1} \in C^\infty(\mathbb{R}^2)$ $\forall P \in \mathcal{S}^2$,

$$\frac{\partial}{\partial\ _i}(P) = \frac{\partial}{\partial\ _i}\left[\ \cdot \varphi_P^{-1}\right](\ ),$$
$$\frac{\partial^2}{\partial\ _i\partial\ _j}(P) = \frac{\partial^2}{\partial\ _i\partial\ _j}\left[\ \cdot \varphi_P^{-1}\right](\ ).$$

fi

fi fi fi fi

Rotated Parameterized Differential Operators

H fi H

$$H(\ ,\ \boldsymbol{w}) = \ _1 + \ _2 + \ _3 + \ _4\ ^2 + \ _5 + \ _6\ ^2,$$

$[\cdot]$

$\boldsymbol{w}$ $\partial/\partial\ _1$ $= \partial/\partial\ _2$ $H(\partial/\partial\ _1, \partial/\partial\ _2\ \boldsymbol{w})$ $H(\ ,\ \boldsymbol{w}) = \ ^2 +$ $H(\partial/\partial\ _1, \partial/\partial\ _2\ \boldsymbol{w}) = \partial^2/\partial\ _1^2 + \partial^2/\partial\ _1\partial\ _2$ $\times$ $A \in SO(\ )$,

$$\chi^{(A)} = H\left(\frac{\partial}{\partial\ _1^{(A)}}, \frac{\partial}{\partial\ _2^{(A)}}\ \boldsymbol{w}\right),$$

$$\left(\frac{\partial}{\partial\ _1^{(A)}}, \frac{\partial}{\partial\ _2^{(A)}}\right)^T = A^{-1}\left(\frac{\partial}{\partial\ _1}, \frac{\partial}{\partial\ _2}\right)^T.$$

$$\nabla_x^{(A)} = A^{-1}\nabla_x,$$

$\nabla_x = (\partial/\partial\ _1, \partial/\partial\ _2)^T$ fi Z,

$$\left(\nabla_x^{(A)}\right)^2 = \begin{bmatrix} \frac{\partial}{\partial x_1^{(A)}}\frac{\partial}{\partial x_1^{(A)}} & \frac{\partial}{\partial x_1^{(A)}}\frac{\partial}{\partial x_2^{(A)}} \\ \frac{\partial}{\partial x_1^{(A)}}\frac{\partial}{\partial x_2^{(A)}} & \frac{\partial}{\partial x_2^{(A)}}\frac{\partial}{\partial x_2^{(A)}} \end{bmatrix} = A^{-1}\begin{bmatrix} \frac{\partial^2}{\partial x_1^2} & \frac{\partial^2}{\partial x_1 \partial x_2} \\ \frac{\partial^2}{\partial x_1 \partial x_2} & \frac{\partial^2}{\partial x_2^2} \end{bmatrix} A = A^{-1}\nabla_x^2 A.$$

fi $\chi^{(A)}$ $\partial/\partial\ _1^{(A)}$ $\partial/\partial\ _2^{(A)}$ $\partial/\partial\ _1$ $\partial/\partial\ _2$ fi,

$$\begin{aligned} ^{(A)} &= w_1 + (w_2; w_3)\nabla_x^{(A)} + \left\langle \begin{bmatrix} w_4 & \frac{w_5}{2} \\ \frac{w_5}{2} & w_6 \end{bmatrix}; \left(\nabla_x^{(A)}\right)^2 \right\rangle \\ &= w_1 + (w_2; w_3)A^{-1}\nabla_x + \left\langle \begin{bmatrix} w_4 & \frac{w_5}{2} \\ \frac{w_5}{2} & w_6 \end{bmatrix}; A^{-1}\nabla_x^2 A \right\rangle \\ &= w_1 + (w_2; w_3)A^{-1}\nabla_x + \left\langle A\begin{bmatrix} w_4 & \frac{w_5}{2} \\ \frac{w_5}{2} & w_6 \end{bmatrix}A^{-1}; \nabla_x^2 \right\rangle; \end{aligned}$$

$\langle \cdot, \cdot \rangle$ $\chi^{(A)}$ $\boldsymbol{w}$, fi

fi

$\chi^{(A)}$

Equivariant Differential Operators

fi Ψ Φ, $\chi^{(A)}$ fi,

Ψ

fi $SO( )$ $\forall R \in SO( )$,

$$\Psi \quad (R) = \Psi \quad (P_R, A_R) = \chi^{(A_R)} \quad (P_R).$$

Φ

fi $SO( )$

fi $SO( )$ $\forall R \in SO( )$,

$$\Phi \quad (R) = \Phi \quad (P_R, A_R)$$
$$= \int_{SO(2)} \chi_A^{(A_R)} \quad (P_R, A_R A) d\nu(A),$$

ν $SO( )$. $\chi_A^{(A_R)}$,

A

$\boldsymbol{w}_A$

$A_R A$

$\chi_A^{(A_R)}$

Ψ

Φ,

$\widetilde{R} \in SO( )$

Theorem 1 *If* $\in C^\infty(\mathcal{S}^2)$ *and* $\in C^\infty(SO( ))$, $\forall \widetilde{R} \in SO( )$, *we have*

$$\Psi \left[\pi_{\widetilde{R}}^{S} \quad \right] = \pi_{\widetilde{R}}^{SO} \Psi \quad ,$$
$$\Phi \left[\pi_{\widetilde{R}}^{SO} \quad \right] = \pi_{\widetilde{R}}^{SO} \Phi \quad .$$

Equivariant Network Architectures

Ψ Φ,

fi Ψ

fi Φ

$\sigma(\cdot)$, ReLU

$$T \quad = \Phi^{(L)} \left[\cdots \sigma \left(\Phi^{(1)} \sigma(\Psi \quad) \right) \right].$$

Theorem 2 *If* $\in C^\infty(\mathcal{S}^2)$, $\forall \widetilde{R} \in SO( )$, *we have*

$$T \left[\pi_{\widetilde{R}}^{S} \quad \right] = \pi_{\widetilde{R}}^{SO} T \quad .$$

$\widetilde{R}$

$\pi_{\widetilde{R}}^{S}$ T

fi T

$SO( )$,

Ψ Φ

$\times$

$\boldsymbol{w}$

Implementation

Icosahedral Spherical Mesh

fi

fi

H

Estimation of Partial Derivatives

$\boldsymbol{I}$

$\Omega \subset \mathcal{S}^2$, $\boldsymbol{I}(P) = (P), \forall P \in \Omega$,

$P \in \Omega$

φ_P P $Q_i(= , , \cdots ,)$

$\widetilde{U}_P \subset \mathbb{R}^2$, $Q_i \in \Omega$

P $\varphi_P(P) =$,

$\varphi_P(Q_i) = (\ _{i1}, \ _{i2})$, $\forall = , , \cdots , ,$

$$\left(\ _{i1}, \ _{i2}, \sqrt{ \ - \ _{i1}^2 - \ _{i2}^2} \right)^T = \bar{P}^{-1} Q_i.$$

$f_P = \ ^- \cdot \varphi_P^{-1}$, $f_P(\ ) = (P) = \boldsymbol{I}(P)$

$f_P(\ _{i1}, \ _{i2}) = (Q_i) = \boldsymbol{I}(Q_i)$.

f_P $\forall =$ $, , \cdots , ,$

$$f_P(x_{i1}, x_{i2}) = f_P(0,0) + x_{i1} \frac{\partial f_P}{\partial x_1} + x_{i2} \frac{\partial f_P}{\partial x_2} + \frac{1}{2} x_{i1}^2 \frac{\partial^2 f_P}{\partial x_1^2}$$
$$+ x_{i1} x_{i2} \frac{\partial^2 f_P}{\partial x_1 \partial x_2} + \frac{1}{2} x_{i2}^2 \frac{\partial^2 f_P}{\partial x_2^2} + O(\rho_i^3)$$

$(\ , \ )$,

$\rho_i = \sqrt{ \ _{i1}^2 + \ _{i2}^2}$.

$$\begin{bmatrix} \vdots \\ f_P(x_{i1}, x_{i2}) - f_P(0) \\ \vdots \end{bmatrix} \approx \begin{bmatrix} \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{i1} & x_{i2} & \frac{x_{i1}^2}{2} & x_{i1} x_{i2} & \frac{x_{i2}^2}{2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} D_P,$$

D_P

$$D_P = \left(\frac{\partial f_P}{\partial \ _1}, \frac{\partial f_P}{\partial \ _2}, \frac{\partial^2 f_P}{\partial \ _1^2}, \frac{\partial^2 f_P}{\partial \ _1 \ _2}, \frac{\partial^2 f_P}{\partial \ _2^2} \right)^T \Bigg|_{x_1 = x_2 = 0}.$$

P,

3×3

$F_P \approx V_P D_P$, D_P

$$D_P = {}_{D} \|V_P D - F_P\|_2 = (V_P^T V_P)^{-1} V_P^T F_P.$$

$\partial/\partial\ _1, \partial/\partial\ _2$,

Discretization of $SO(\ )$

$A \in SO(\ )$ $SO(\ )$. fi, $SO(\ )$ N C_N, $C_N = \{e = A_0, A_1, \cdots, A_{N-1}\}$,

$$A_i = \begin{bmatrix} \frac{2\ i}{N} & -\ \frac{2\ i}{N} \\ \frac{2\ i}{N} & \frac{2\ i}{N} \end{bmatrix}.$$

$\forall P \in \Omega$ $=\ ,\ ,\cdots, N-\ ,$

$$\begin{aligned} &\widetilde{\Psi}[\boldsymbol{I}](P; i) = {}^{\sim(A_i)}[\boldsymbol{I}](P) \\ =&\left(w_1 + (w_2; w_3)A_i^{-1}\widehat{\nabla}_x + \left\langle A_i \begin{bmatrix} w_4 & \frac{w_5}{2} \\ \frac{w_5}{2} & w_6 \end{bmatrix} A_i^{-1}; \widehat{\nabla}_x^2 \right\rangle\right)[f_P](0) \\ =&w_1 f_P(0) + (w_2; w_3)A_i^{-1}\widehat{\nabla}_x[f_P](0) \\ &+ \left\langle A_i \begin{bmatrix} w_4 & \frac{w_5}{2} \\ \frac{w_5}{2} & w_6 \end{bmatrix} A_i^{-1}; \widehat{\nabla}_x^2 [f_P](0) \right\rangle; \end{aligned}$$

$\boldsymbol{I}$, $\widetilde{\Psi}\boldsymbol{I}$ N, fi $A \in SO(\ )$. $\forall P \in \Omega$ $=\ ,\ ,\cdots, N-\ ,$

$$\widetilde{\Phi}\,\boldsymbol{F}\,(P,\ ) = \frac{\nu(SO(\ ))}{N} \sum_{j=0}^{N-1} \widetilde{\chi}_{Z_j}^{(Z_i)}\ \boldsymbol{F}\,(P, \bigcirc\ ),$$

$\boldsymbol{F}$ N $\in$ $C^\infty(SO(\ ))$, $\boldsymbol{F}(P,\ ) = (P, A_i)$, $\bigcirc$ N $\widetilde{\Psi}$ $\widetilde{\Phi}$

Equivariance Error Analysis

Ψ Φ $O(\rho_1) = O(\rho_2) = \cdots = O(\rho_m)$ fi $O(\rho_i) = O(\rho)$

Theorem 3 $\forall \widetilde{R} \in SO(\ )$,

$$\begin{aligned} \widetilde{\Psi}\left[\pi_{\widetilde{R}}^{S}\,\boldsymbol{I}\,\right] &= \pi_{\widetilde{R}}^{SO}\left[\widetilde{\Psi}\,\boldsymbol{I}\,\right] + O(\rho), \\ \widetilde{\Phi}\left[\pi_{\widetilde{R}}^{SO}\,\boldsymbol{F}\,\right] &= \pi_{\widetilde{R}}^{SO}\left[\widetilde{\Phi}\,\boldsymbol{F}\,\right] + O(\rho) + O\left(\frac{}{N^2}\right), \end{aligned}$$

where transformations acting on discrete inputs and feature maps are defined as $\pi_{\widetilde{R}}^{S}\,\boldsymbol{I}\,(P) = \pi_{\widetilde{R}}^{S}\ (P)$ *and* $\pi_{\widetilde{R}}^{SO}\,\boldsymbol{F}\,(P,\ ) = \pi_{\widetilde{R}}^{SO}\ (P, A_i)$, *respectively.*

H, fi ρ,

Experiments

Spherical MNIST Classification

% %

H U fi

H

fi

					#
	✓				
	✗	.	.	.	
	✗	.	.	.	
PDO-eS²CNN	✓	. ± .	. ± .	. ± .	
K	✗	.			
	✓	.	96	.	
	✓	.	.	.	
PDO-eS²CNN	✓	**99.60 ± 0.04**	. ± .	**99.45 ± 0.05**	

			#
PDO-eS²CNN	**60.4 ± 1.0**	**44.6 ± 0.4**	

		#
	. ± .	
PDO-eS²CNN	**3.78 ± 0.07**	

. %

Omnidirectional Image Segmentation

Atomization Energy Prediction

Conclusions

Acknowledgements

References

ArXiv e-prints.

SIAM Journal on Numerical Analysis

Journal of the American Chemical Society

NeurIPS,

IEEE Signal Processing Magazine

ICLR

NeurIPS,

International Conference on 3D Vision (3DV)

ICLR

ICML,

ICML,

ECCV,

ICLR

ICRA,

Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition,

ECCV,

IJCAI,

The Astrophysical Journal

ICML,

ICLR

NeurIPS,

The American Mathematical Monthly

NeurIPS,

Astronomy and Computing

NeurIPS,

ICML,

K

NeurIPS,

NeurIPS,

ICCV,

IJ-CAI,