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

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Abstract

Introduction

$\mathcal{S}^2$		$SO(2), SO(3)$	
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	$P \in \mathcal{S}^2$ $P(\alpha,\beta) = Z(\alpha)Y(\beta)n$	$\bar{P}$	v P
$\bar{P} \cdot SO(2)$	$\{\bar{P}Z(\gamma) \mid \gamma \in [0, 2\pi)\}$ $SO(2)$	$E \simeq F$	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	$H(\cdot, \cdot; \boldsymbol{w})$	$\boldsymbol{w}$
$\partial/\partial x_i^{(A)}$	$A \in SO(2)$	$\nabla_x[f], \nabla_x^2[f]$	H 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
$D_P, \hat{D}_P$	v v	$\hat{\nabla}_x[f], \hat{\nabla}_x^2[f]$	$\nabla_x[f]$ $\nabla_x^2[f]$
$\widetilde{\chi}^{(A)}, \widetilde{\Psi}, \widetilde{\Phi}$	$\chi^{(A)}, \Psi$ Φ	C_N	N

C fi
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C
v v $SO(3)$

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Related Work

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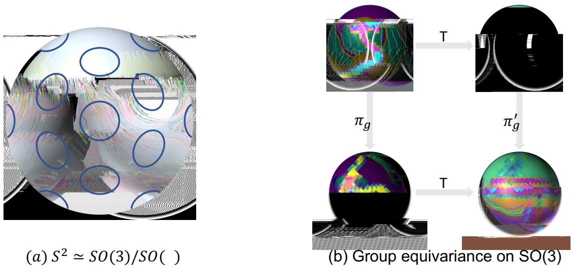
Prior Knowledge

Parameterization of $\mathcal{S}^2$ and $SO(3)$

$\mathcal{S}^2$ $SO(3)$
v

$$\mathcal{S}^2 = \{(\ _1,\ _2,\ _3) \mid \|\ \|_2 = 1\},$$
$$SO(3) = \{R \in \mathbb{R}^3 \mid R^T R = I, \det(R) = 1\}.$$



(a) $\mathcal{S}^2 \simeq SO(3)/SO(\ )$ (b) Group equivariance on SO(3)

$\mathcal{S}^2 \simeq SO(3)/SO(2)$ $SO(3)$ v
v G v
$SO(3)$
$g \in SO(3)$ T
v fi T

Rn $R \in SO(3)$ $SO(3)$

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

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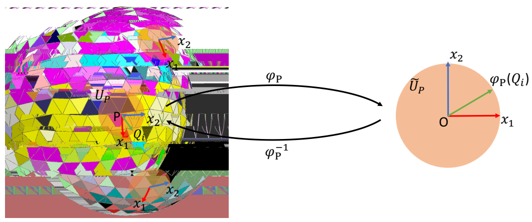

$P \in \mathcal{S}^2$ $U_P \subset \mathcal{S}^2$ $\widetilde{U}_P \subset \mathbb{R}^2$ φ_P v 3

U_P $\widetilde{U}_P = \varphi_P(U_P) \subset \mathbb{R}^2$ $\varphi_P(P) = 0$ φ_P v

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

$P \in \mathcal{S}^2$ 1 2 U_P φ_P fi v v

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

$\cdot \varphi_P^{-1} \in C^\infty(\mathbb{R}^2)$ $\forall P \in \mathcal{S}^2$

$$\frac{\partial}{\partial \ _i}[\ ](P) = \frac{\partial}{\partial \ _i}\left[\ \cdot \varphi_P^{-1}\right](0),$$

$$\frac{\partial^2}{\partial \ _i \partial \ _j}[\ ](P) = \frac{\partial^2}{\partial \ _i \partial \ _j}\left[\ \cdot \varphi_P^{-1}\right](0).$$

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Rotated Parameterized Differential Operators

H v fi H 2 v

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

$[\cdot]$

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

$$\chi^{(A)} = H\left(\frac{\partial}{\partial \ _1^{(A)}}, \frac{\partial}{\partial \ _2^{(A)}}; \boldsymbol{w}\right), \quad 4$$

$$\left(\frac{\partial}{\partial \ _1^{(A)}}, \frac{\partial}{\partial \ _2^{(A)}}\right)^T = A^{-1}\left(\frac{\partial}{\partial \ _1}, \frac{\partial}{\partial \ _2}\right)^T. \quad 5$$

5

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

$\nabla_x = (\partial/\partial \ _1, \partial/\partial \ _2)^T$ 5 v 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 4 $\chi^{(A)}$ $\partial/\partial \ _1^{(A)}$ $\partial/\partial \ _2^{(A)}$ $\partial/\partial \ _1$ $\partial/\partial \ _2$ 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 v v fi

C $\chi^{(A)}$ C B v C C C

Equivariant Differential Operators

fi v $\chi^{(A)}$ fi

fi $SO(3)$ $\forall R \in SO(3)$

$$[\ ](R) = [\ ](P_R, A_R) = \chi^{(A_R)}[\ ](P_R).$$

fi $SO(3)$

fi $SO(3)$ $\forall R \in SO(3)$

$$\begin{aligned}[\ ](R) &= [\ ](P_R, A_R)\\ &= \int_{SO(2)} \chi_A^{(A_R)}[\ ](P_R, A_R A) d\nu(A),\end{aligned}$$

ν $SO(2)$ $\chi_A^{(A_R)}$

A

$\boldsymbol{w}_A$

v $A_R A$

$\chi_A^{(A_R)}$

v v

v

$\widetilde{R} \in SO(3)$

Theorem 1 *If* $\in C^\infty(\mathcal{S}^2)$ *and* $\in C^\infty(SO(3))$, $\forall \widetilde{R} \in SO(3)$, *we have*

$$\left[\pi^{S}_{\widetilde{R}}[\ ]\right] = \pi^{SO}_{\widetilde{R}}[\ [\ ]],$$

$$\left[\pi^{SO}_{\widetilde{R}}[\ ]\right] = \pi^{SO}_{\widetilde{R}}[\ [\ ]].$$

Equivariant Network Architectures

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$\sigma(\cdot)$ U

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

Theorem 2 *If* $\in C^\infty(\mathcal{S}^2)$, $\forall \widetilde{R} \in SO(3)$, *we have*

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

$\widetilde{R}$

$\pi^{S}_{\widetilde{R}}$ T

v fi T

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v $SO(3)$

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Implementation

Icosahedral Spherical Mesh

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Estimation of Partial Derivatives

v $\boldsymbol{I}$

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

v v $P \in$

φ_P P $Q_i(= 1, 2, \cdots,)$

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

P $\varphi_P(P) = 0$

$\varphi_P(Q_i) = (\ _{i1},\ _{i2})$ $\forall = 1, 2, \cdots,$

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

$f_P = \cdot \varphi_P^{-1}$ $f_P(0) = (P) = \boldsymbol{I}(P)$

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

f_P v $\forall =$ $1, 2, \cdots,$

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

v v v v $(0,0)$

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

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

D_P v v

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

P

3×3 v C

v $F_P \approx$
$V_P D_P$ D_P

$$\hat{D}_P = \arg\min_D \|V_P D - F_P\|_2 = (V_P^T V_P)^{-1} V_P^T F_P.$$

v v

B

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

Discretization of $SO(2)$

$A \in SO(2)$
$SO(2)$ fi
$SO(2)$ N
C_N $C_N = \{e = A_0, A_1, \cdots, A_{N-1}\}$

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

C $\forall P \in$
$= 0, 1, \cdots, N-1$

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

v v $\boldsymbol{I}$
v $\widetilde{\ }[\boldsymbol{I}]$
N fi
$A \in SO(2)$ $\forall P \in$
$= 0, 1, \cdots, N-1$

$$\widetilde{\ }[\boldsymbol{F}](P,) = \frac{\nu(SO(2))}{N} \sum_{j=0}^{N-1} \widetilde{\chi}_{Z_j}^{(Z_i)} [\boldsymbol{F}](P, \bigcirc\ ),$$

$\boldsymbol{F}$ N
$\in$
$C^\infty(SO(3))$ $\boldsymbol{F}(P,) = \ (P, A_i)$ $\bigcirc$
N
C v
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C v
v v

Equivariance Error Analysis

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

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

$$\widetilde{\ } \left[\pi_{\widetilde{R}}^{S}[\boldsymbol{I}]\right] = \pi_{\widetilde{R}}^{SO} \left[\widetilde{\ }[\boldsymbol{I}]\right] + O(\rho), \qquad 4$$

$$\widetilde{\ } \left[\pi_{\widetilde{R}}^{SO}[\boldsymbol{F}]\right] = \pi_{\widetilde{R}}^{SO} \left[\widetilde{\ }[\boldsymbol{F}]\right] + O(\rho) + O\left(\frac{1}{N^2}\right), \qquad 5$$

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.

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Experiments

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Spherical MNIST Classification

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v 99.44%
90.14%
v
H U C v
fi
v C

v H v

45 v v v
45 fi
v v v v v

					#
C C	✓	96	94	95	5
U G C	✗	99.23	35.60	94.92	
H U C	✗	99.45	29.84	97.05	5
PDO-eS^{2}CNN	✓	99.44 ± 0.06	90.14 ± 0.58	98.93 ± 0.08	
C C G	✗	94.4			
C K v	✓	96.4	**96**	96.6	
C C	✓	99.43	69.99	99.31	
PDO-eS^{2}CNN	✓	**99.60 ± 0.04**	94.25 ± 0.29	**99.45 ± 0.05**	

v

			#
U C	5 55	5 U	
U G C H U	5 5 5		5 5
PDO-eS^{2}CNN	**60.4 ± 1.0**	**44.6 ± 0.4**	

		#
C C C	5.96 ± 0.48	
PDO-eS^{2}CNN	**3.78 ± 0.07**	

v 5 U

fi

v 5 69.99% B C v v v 60 C v fi

Atomization Energy Prediction

B v v i i 5 23 5 H C fi 5 v v

C C C v v fi fi v v C C v

Omnidirectional Image Segmentation

v v G B 13 v 5 fi v v v U

fi fi C C H U fi H U v 5 fi

Conclusions

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Acknowledgements

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C G K C *ICLR*

C K B G v C v C *ICML*

C G v C v *ICML* v

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