

PDO-eS²CNNs: Partial Differential Operator Based Equivariant Spherical CNNs

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Abstract

Partial differential operators (PDOs) are widely used in physics and engineering to describe the behavior of systems. In this paper, we propose a novel framework for spherical CNNs based on PDOs. The proposed framework is able to handle arbitrary spherical functions and is invariant to rotations. We show that the proposed framework can be used to solve a wide range of problems, including image classification, object detection, and scene reconstruction. The proposed framework is implemented in a software package called PDO-eS²CNNs, which is available at <https://github.com/zshen1999/PDO-eS2CNNs>.

Introduction

Partial differential operators (PDOs) are widely used in physics and engineering to describe the behavior of systems. In this paper, we propose a novel framework for spherical CNNs based on PDOs. The proposed framework is able to handle arbitrary spherical functions and is invariant to rotations. We show that the proposed framework can be used to solve a wide range of problems, including image classification, object detection, and scene reconstruction. The proposed framework is implemented in a software package called PDO-eS²CNNs, which is available at <https://github.com/zshen1999/PDO-eS2CNNs>.

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\mathcal{S}^2 α, β, γ R P $\bar{P} \cdot SO(2)$ A_R $C^1(SO(3))$ $\pi_{\tilde{R}}^S[s], \pi_{\tilde{R}}^{SO}[so]$ \tilde{U}_p \bar{s} $\partial/\partial x_i^{(A)}$ $\nabla_x^{(A)}, (\nabla_x^{(A)})^2$ Ψ, Φ f_P D_P, \hat{D}_P $\tilde{\chi}^{(A)}, \tilde{\Psi}, \tilde{\Phi}$	$R \in SO(3), \quad R = Z(\alpha_R)Y(\beta_R)Z(\gamma_R)$ $P \in \mathcal{S}^2, \quad P(\alpha, \beta) = Z(\alpha)Y(\beta)n$ $\{\bar{P}Z(\gamma) \gamma \in [0, 2\pi)\}, \quad SO(2)$ $Z(\gamma_R)$ $SO(3)$ $\tilde{R} \quad s, \quad so$ $\tilde{U}_p = \varphi_P(U_P) \subset \mathbb{R}^2$ \mathbb{R}^3 s $A \in SO(2)$ \mathfrak{fi} \mathfrak{fi} $f_P = \bar{s} \cdot \varphi_P^{-1}$ $\chi^{(A)}, \Psi, \Phi$	$SO(2), SO(3)$ $Z(\alpha), Y(\beta)$ $n = (0, 0, 1)^T$ \bar{P} $E \simeq F$ $C^1(\mathcal{S}^2)$ s, so U_P φ_P $H(\cdot, \cdot; \boldsymbol{w})$ $\nabla_x[f], \nabla_x^2[f]$ $\chi^{(A)}$ $\boldsymbol{I}, \boldsymbol{F}$ $O(\cdot)$ $\hat{\nabla}_x[f], \hat{\nabla}_x^2[f]$ C_N	z, y P E F \mathcal{S}^2 $s \in C^1(\mathcal{S}^2), \quad so \in C^1(SO(3))$ \mathcal{S}^2 P U_P \tilde{U}_P \boldsymbol{w} \mathbf{H} f \mathfrak{fi} $\mathbf{4}$ \mathfrak{fi} $\nabla_x[f], \quad \nabla_x^2[f]$ N
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\mathfrak{fi}
 \mathfrak{fi}
 \mathbf{K}
 $SO(\cdot)$

Related Work

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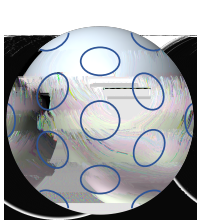
Prior Knowledge

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

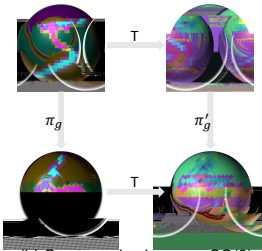
$$\mathcal{S}^2, \quad SO(\cdot)$$

$$\mathcal{S}^2 = \{(\cdot_1, \cdot_2, \cdot_3) | \| \cdot \|_2 = \cdot\},$$

$$SO(\cdot) = \{R \in \mathbb{R}^3 | R^T R = I, \det(R) = \cdot\}.$$



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



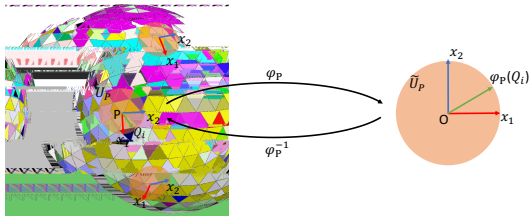
(b) Group equivariance on $SO(3)$

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

$$\begin{array}{ccc} \text{ed } SO(2) & \xrightarrow{f} & \\ g \in SO(2) & \text{fi} & T \end{array}$$

$$R \in SO(3)$$

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



$$U_P \subset \mathcal{S}^2 \quad P \in \mathcal{S}^2, \quad \tilde{U}_P \subset \mathbb{R}^2 \quad \varphi_P$$

$$\varphi_P(P) = \frac{U_P}{\varphi_P} \quad \tilde{U}_P = \varphi_P(U_P) \subset \mathbb{R}^2$$

$$\varphi_P^{-1}(\cdot_1, \cdot_2) = \bar{P} \left(\cdot_1, \cdot_2, \sqrt{-|\cdot|^2} \right)^T.$$

$$\varphi_P : \mathbb{R}^2 \rightarrow \mathbb{R}^3 \quad P \in \mathcal{S}^2$$

$$\varphi_P : \mathbb{R}^2 \rightarrow \mathbb{R}^3 \quad U_P,$$

$$\varphi_P \in C^\infty(\mathcal{S}^2), \quad \mathbb{R}^3,$$

$$\varphi_P \in C^\infty(\mathbb{R}^3).$$

$$\partial^2/\partial_i\partial_j(\cdot, \cdot) = \partial/\partial_i$$

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

$$\frac{\partial}{\partial_i}(P) = \frac{\partial}{\partial_i}[\cdot \cdot \varphi_P^{-1}](\cdot),$$

$$\frac{\partial^2}{\partial_i\partial_j}(P) = \frac{\partial^2}{\partial_i\partial_j}[\cdot \cdot \varphi_P^{-1}](\cdot).$$

Rotated Parameterized Differential Operators

H

fi

H

$$H(\cdot, \cdot) = \cdot_1 + \cdot_2 + \cdot_3 + \cdot_4^2 + \cdot_5 + \cdot_6^2,$$

[.]

$$\partial/\partial_1 \quad \quad \quad \partial/\partial_2 \quad \quad \quad H(\partial/\partial_1, \partial/\partial_2 \, w) =$$

$$H(\cdot, \cdot) = \cdot^2 + \cdot \quad \quad \quad H(\partial/\partial_1, \partial/\partial_2 \, w) =$$

$$\partial^2/\partial_1^2 + \partial^2/\partial_1\partial_2 \quad \quad \quad \times \quad \quad \quad A \in$$

$$SO(\cdot),$$

$$\chi^{(A)} = H \left(\frac{\partial}{\partial_1^{(A)}}, \frac{\partial}{\partial_2^{(A)}} \, w \right), \quad \mathbf{4}$$

$$\left(\frac{\partial}{\partial_1^{(A)}}, \frac{\partial}{\partial_2^{(A)}} \right)^T = A^{-1} \left(\frac{\partial}{\partial_1}, \frac{\partial}{\partial_2} \right)^T.$$

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

$$\nabla_x = (\partial/\partial_1, \partial/\partial_2)^T$$

Z

$$\left(\nabla_x^{(A)} \right)^2 = \left[\begin{array}{cc} \frac{\partial}{\partial x_1^{(A)}} \frac{\partial}{\partial x_1^{(A)}} & \frac{\partial}{\partial x_1^{(A)}} \frac{\partial}{\partial x_2^{(A)}} \\ \frac{\partial}{\partial x_1^{(A)}} \frac{\partial}{\partial x_2^{(A)}} & \frac{\partial}{\partial x_2^{(A)}} \frac{\partial}{\partial x_2^{(A)}} \end{array} \right]$$

$$= A^{-1} \left[\begin{array}{cc} \frac{\partial^2}{\partial x_1^2} & \frac{\partial^2}{\partial x_1 \partial x_2} \\ \frac{\partial^2}{\partial x_1 \partial x_2} & \frac{\partial^2}{\partial x_2^2} \end{array} \right] A = A^{-1} \nabla_x^2 A.$$

$$\mathbf{4}, \chi^{(A)} \quad \quad \quad \partial/\partial_1^{(A)}$$

$$\partial/\partial_2^{(A)} \quad \quad \quad \partial/\partial_1$$

$$^{(A)} = W_1 + (W_2; W_3) \nabla_x^{(A)} + \left\langle \left[\begin{array}{cc} W_4 & \frac{w_5}{2} \\ \frac{w_5}{2} & W_6 \end{array} \right]; \left(\nabla_x^{(A)} \right)^2 \right\rangle$$

$$= W_1 + (W_2; W_3) A^{-1} \nabla_x + \left\langle \left[\begin{array}{cc} W_4 & \frac{w_5}{2} \\ \frac{w_5}{2} & W_6 \end{array} \right]; A^{-1} \nabla_x^2 A \right\rangle$$

$$= W_1 + (W_2; W_3) A^{-1} \nabla_x + \left\langle A \left[\begin{array}{cc} W_4 & \frac{w_5}{2} \\ \frac{w_5}{2} & W_6 \end{array} \right] A^{-1}; \nabla_x^2 \right\rangle;$$

$\langle \cdot, \cdot \rangle$

$\chi^{(A)}$

w_i

fi

fi

$\chi^{(A)}$

Equivariant Differential Operators

fi

Ψ

Φ

$\chi^{(A)}$

fi

$$\begin{aligned} & \Psi \\ & \text{fi} \quad SO(\cdot) \quad \forall R \in SO(\cdot), \\ & \Psi(R) = \Psi(P_R, A_R) = \chi^{(A_R)}(P_R). \\ & \Phi \\ & \text{fi} \quad SO(\cdot) \quad \forall R \in SO(\cdot), \\ & \Phi(R) = \Phi(P_R, A_R) \\ & = \int_{SO(2)} \chi_A^{(A_R)}(P_R, A_R A) d\nu(A), \\ & \nu \quad SO(\cdot) \quad \chi_A^{(A_R)} \\ & A \\ & w_A \\ & A_R A \\ & \chi_A^{(A_R)} \\ & \Psi \\ & \Phi, \\ & \tilde{R} \in SO(\cdot) \end{aligned}$$

Theorem 1 *If $\varphi \in C^\infty(S^2)$ and $\psi \in C^\infty(SO(3))$, $\forall R \in SO(3)$, we have*

$$\begin{aligned}\Psi\left[\pi_{\tilde{R}}^S\right] &= \pi_{\tilde{R}}^{SO} \Psi, \\ \Phi\left[\pi_{\tilde{R}}^{SO}\right] &= \pi_{\tilde{R}}^{SO} \Phi\end{aligned}$$

Equivariant Network Architectures

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

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

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

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

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

$$\pi_{\tilde{R}}^S \quad \text{fi} \quad T \quad SO(\quad), \quad \Psi \quad \Phi \quad \times \quad w$$

Implementation

Icosahedral Spherical Mesh

Estimation of Partial Derivatives

$$\begin{aligned}
 & \mathbf{I} \\
 & \Omega \subset \mathcal{S}^2, \quad \mathbf{I}(P) = \\
 & (P), \forall P \in \Omega, \\
 & P \in \Omega, \quad Q_i(= , , \cdots ,) \\
 & \varphi_P \\
 & \tilde{U}_P \subset \mathbb{R}^2, \quad Q_i \in \Omega, \\
 & P, \quad \varphi_P(P) = \\
 & \varphi_P(Q_i) = (i_1, i_2), \quad \forall = , , \cdots , \\
 & \left(i_1, i_2, \sqrt{-\frac{2}{i_1} - \frac{2}{i_2}} \right)^T = \bar{P}^{-1} Q_i. \\
 & f_P = \varphi_P^{-1}, \quad f_P() = (P) = \mathbf{I}(P), \\
 & f_P(i_1, i_2) = (Q_i) = \mathbf{I}(Q_i), \quad \forall = , , \cdots ,
 \end{aligned}$$

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

$$\rho_i = \sqrt{\frac{2}{i_1} + \frac{2}{i_2}}$$

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

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

$$V_P D_{P_i} \approx F_P \approx D_P$$

$$D_P = \frac{1}{D} \|\mathbf{V}_P D - F_P\|_2 = (\mathbf{V}_P^T \mathbf{V}_P)^{-1} \mathbf{V}_P^T F_P.$$

$$\frac{\partial}{\partial \theta_1}, \frac{\partial}{\partial \theta_2}$$

Discretization of $SO(\cdot)$

$$A \in SO(\cdot)$$

$$C_N = \{e = A_0, A_1, \cdots, A_{N-1}\},$$

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

$$\forall P \in \Omega$$

$$\tilde{\Psi}[\mathbf{I}](P;l) = \sim^{(A_i)}[\mathbf{I}](P)$$

$$= \left(w_1 + (w_2, w_3) A_i^{-1} \hat{\nabla}_x + \left\langle A_i \begin{bmatrix} \frac{w_4}{2} & \frac{w_5}{2} \\ \frac{w_5}{2} & w_6 \end{bmatrix} A_i^{-1}, \hat{\nabla}_x^2 \right\rangle \right) [f_P](0)$$

$$= w_1 f_P(0) + (w_2, w_3) A_i^{-1} \hat{\nabla}_x [f_P](0)$$

$$+ \left\langle A_i \begin{bmatrix} \frac{w_4}{2} & \frac{w_5}{2} \\ \frac{w_5}{2} & w_6 \end{bmatrix} A_i^{-1}, \hat{\nabla}_x^2 [f_P](0) \right\rangle;$$

$$A \in SO(\cdot)$$

$$\forall P \in \Omega$$

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

$$\mathbf{F} \in C^\infty(SO(\cdot)), \mathbf{F}(P, \cdot) = (P, A_i), \bigcirc \in \mathbb{H}^N$$

$$\tilde{\Psi}, \tilde{\Phi}$$

Equivariance Error Analysis

$$\Psi, \Phi$$

$$O(\rho_1) = O(\rho_2) = \dots =$$

$$O(\rho_m)$$

$$O(\rho_i) = O(\rho)$$

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

$$\tilde{\Psi} \left[\pi_{\tilde{R}}^S \mathbf{I} \right] = \pi_{\tilde{R}}^{SO} \left[\tilde{\Psi} \mathbf{I} \right] + O(\rho),$$

$$\tilde{\Phi} \left[\pi_{\tilde{R}}^{SO} \mathbf{F} \right] = \pi_{\tilde{R}}^{SO} \left[\tilde{\Phi} \mathbf{F} \right] + O(\rho) + O\left(\frac{1}{N^2}\right),$$

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

$$\mathbf{H}$$

$$\rho_i$$

Experiments

Spherical MNIST Classification

$$\mathbf{H}$$

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$$\mathbf{H}$$

$$\mathbf{H}$$

Acknowledgements

The diagram shows a 2D lattice with points arranged in a grid. A central point is labeled 'K'. To its right is a point labeled 'K + fi'. Above 'K' is a point labeled 'K + fi'. To the left of 'K' is a point labeled 'K - fi'. Below 'K' is a point labeled 'K - fi'. The lattice is bounded by a dashed line on the right and a solid line on the left. The top and bottom boundaries are also indicated by dashed lines.

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 | 4 | 4 4

A word cloud of computer science and machine learning conferences. The words are arranged in a circular pattern, with some appearing multiple times. The conferences listed include: ECCV, IJCAI, The Astrophysical Journal, ICML, ICLR, NeurIPS, The American Mathematical Monthly, NeurIPS, Astronomy and Computing, NeurIPS, and ICML.

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NeurIPS
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NeurIPS
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ICCV
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IJ-CAI
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