ML to identify symmetries and integrability of physical systems

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UNIVERSITÄT
MÜNCHEN

Our purpose in theoretical physics is not to describe the world as we find it, but to explain - in terms of a few fundamental principles - why the world is the way it is.

Steven Weinberg

Can ML achieve this? [requiring explainable AI]

If yes, which NEW physics can we reveal?

Which problems?

Theoretical physics problems made for ML: understanding high-dimensional data

Lots of high-dimensional problems in string theory:

- Sampling String Vacua with RL and genetic algorithms
  see Gary Shiu's talk on Thursday for some of our work
- Numerical CY metrics
- …

**Today: How to extract domain knowledge/biases with ML
(e.g. what are the symmetries of a system)**

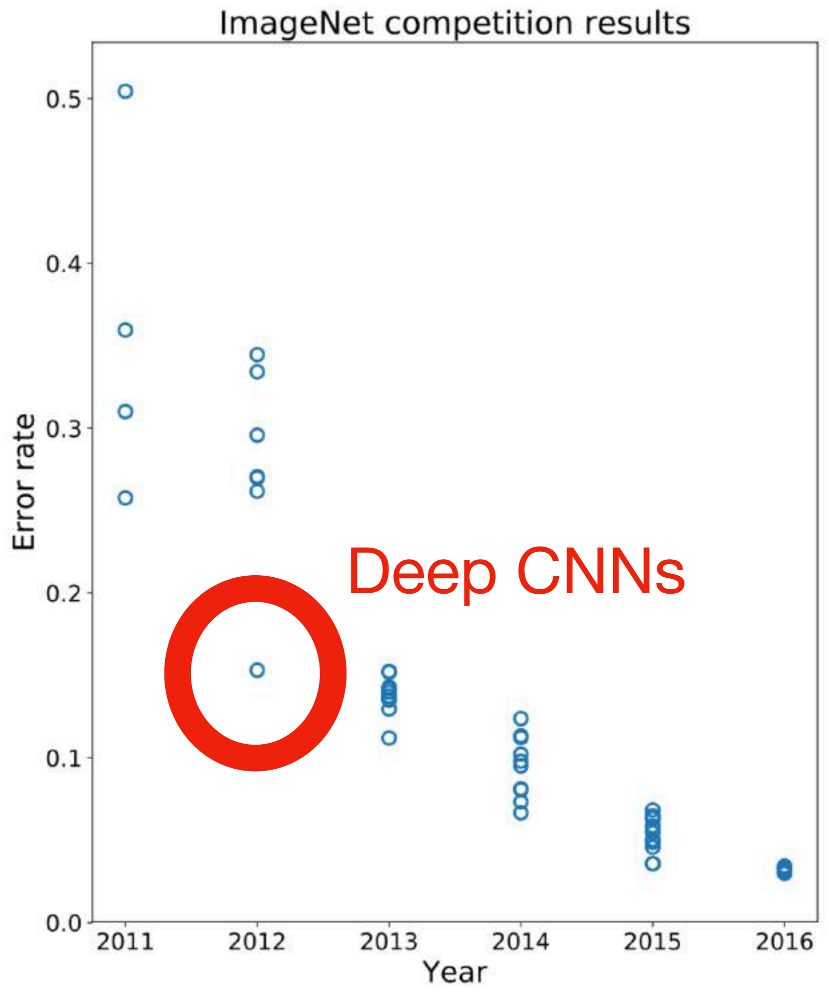
Why high-dimensional data? Large function space of possible solutions

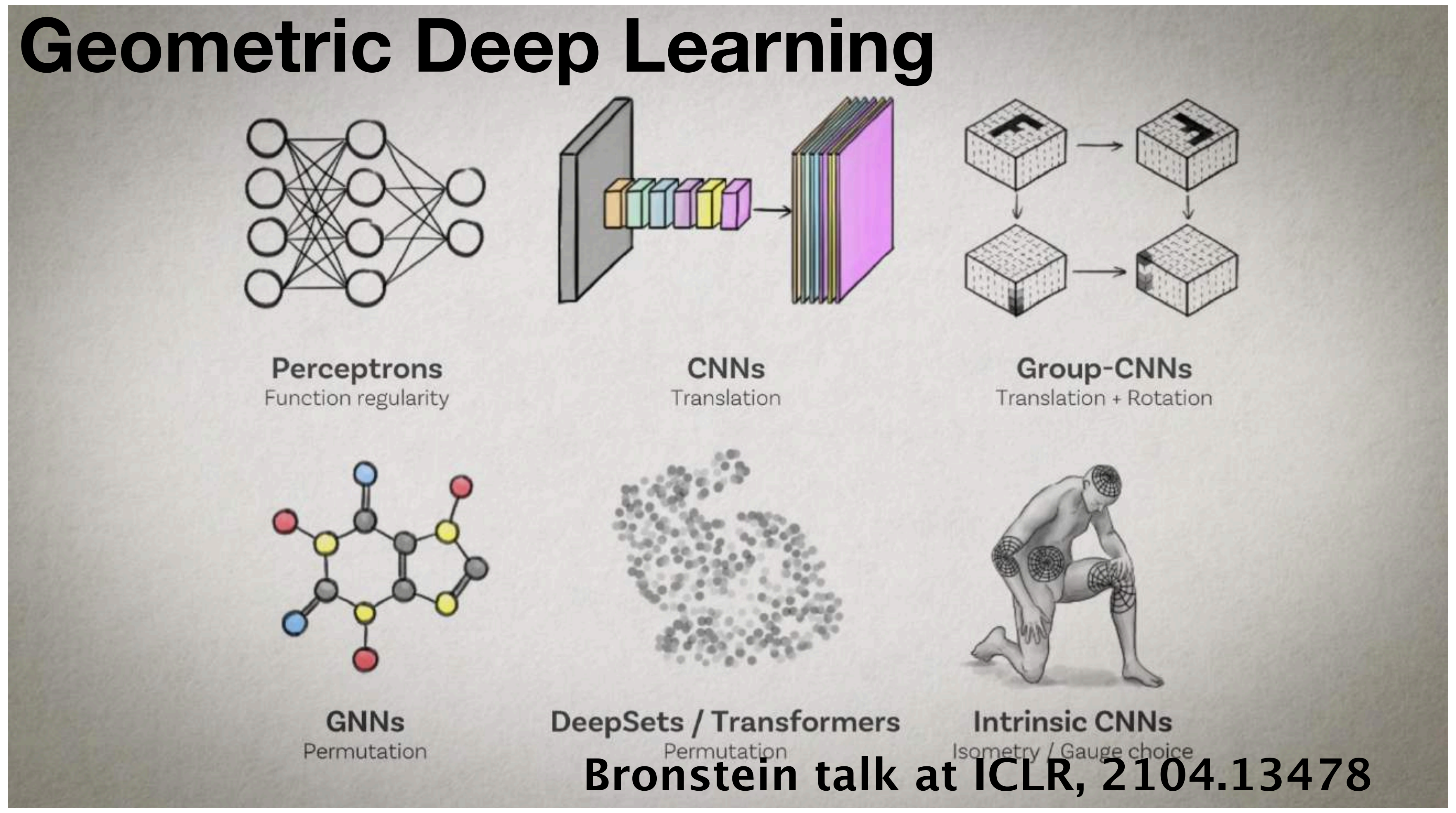
Why functional biases in ML?

ML can overcome curses of dimensionality when using symmetries

- Efficient functional biases can overcome this curse of dimensionality, e.g. utilising symmetries of your data

Translation invariance: CNNs





- Such functional biases (e.g. symmetries) are at the heart of all physics models

Finding symmetries and integrable structures of physical systems

and based on (2104.14444, 2103.07475, 2003.13679), in collaboration with:

Marc Syvaeri

Dieter Lüst

What to do when we do not have domain knowledge?

Can we use AI to identify the correct domain knowledge?

Underlying questions:

Are we missing mathematical/physical structures?

Can we find such structures with ML and then use them?

See also: Tegmark et al. (lots of works)

In Chemistry pre 1869?

Period ↓ / Group →	1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
			*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb		
			**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No		

Learning atoms for materials discovery

Quan Zhou, Peizhe Tang, Shenxiu Liu, Jinbo Pan, Qimin Yan, and Shou-Cheng Zhang
+ See all authors and affiliations

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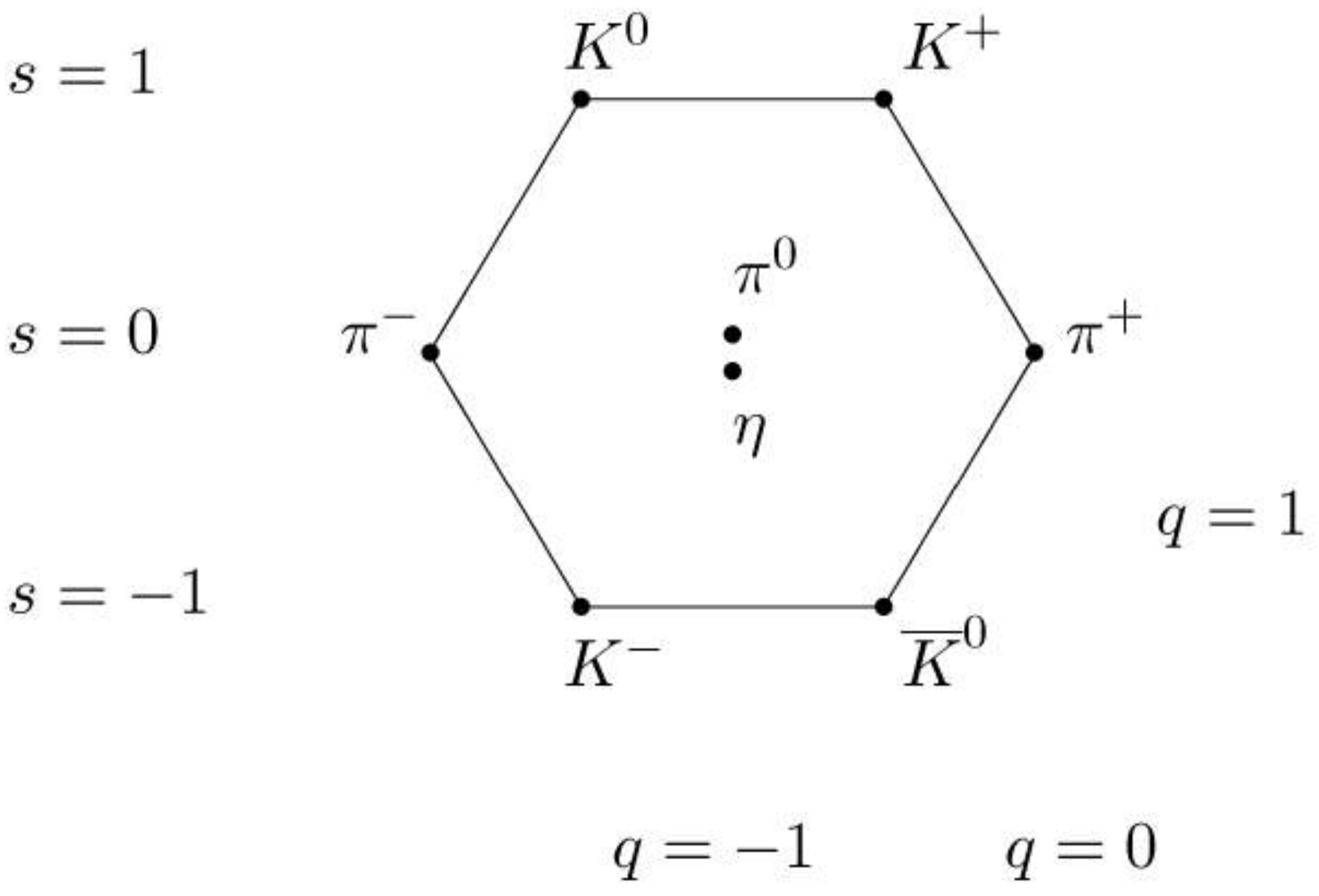
Contributed by Shou-Cheng Zhang, June 4, 2018 (sent for review February 2, 2018; reviewed by Xi Dai and Stuart P. Parkin)

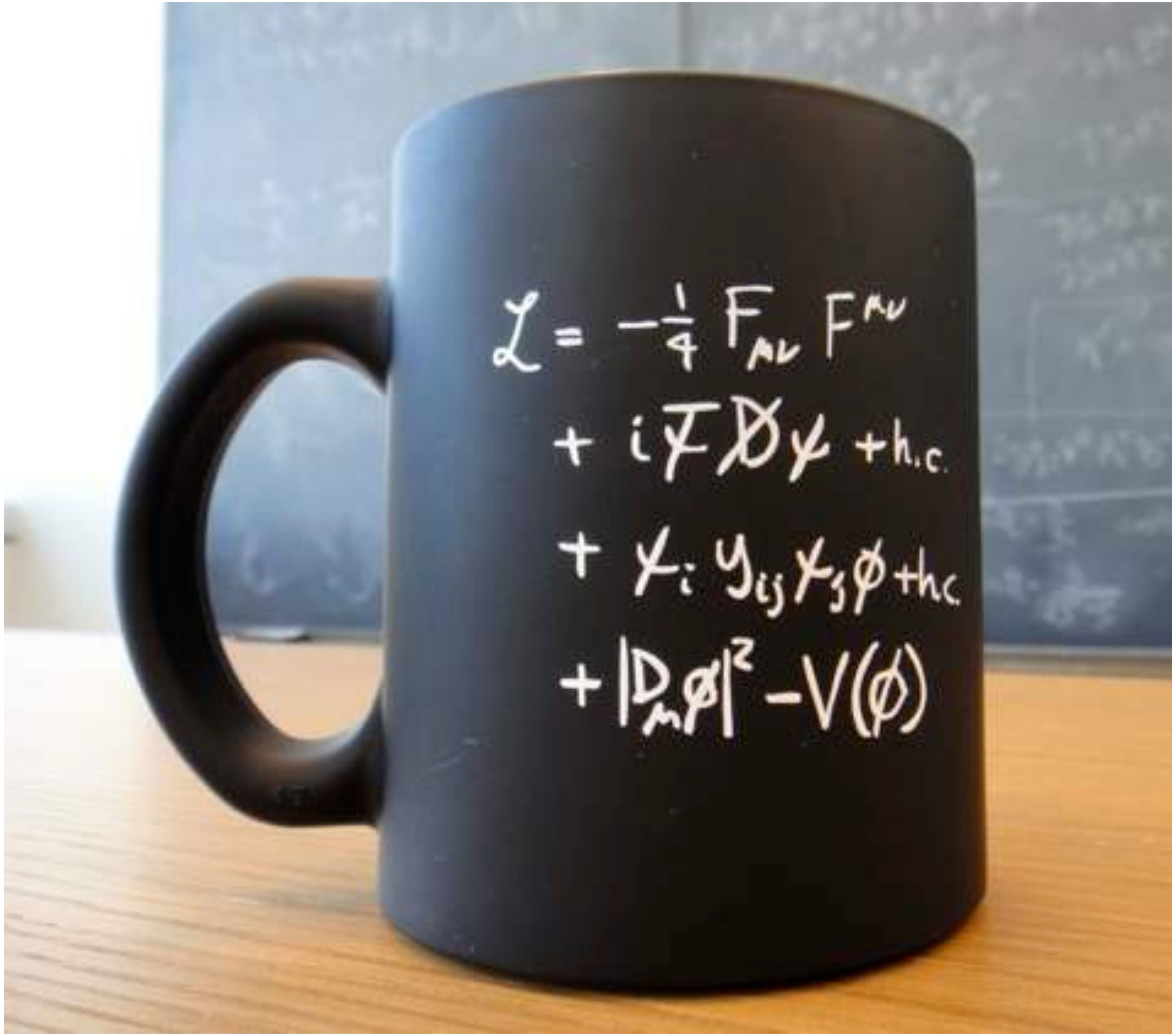
Article | Figures & SI | Info & Metrics | PDF

Significance

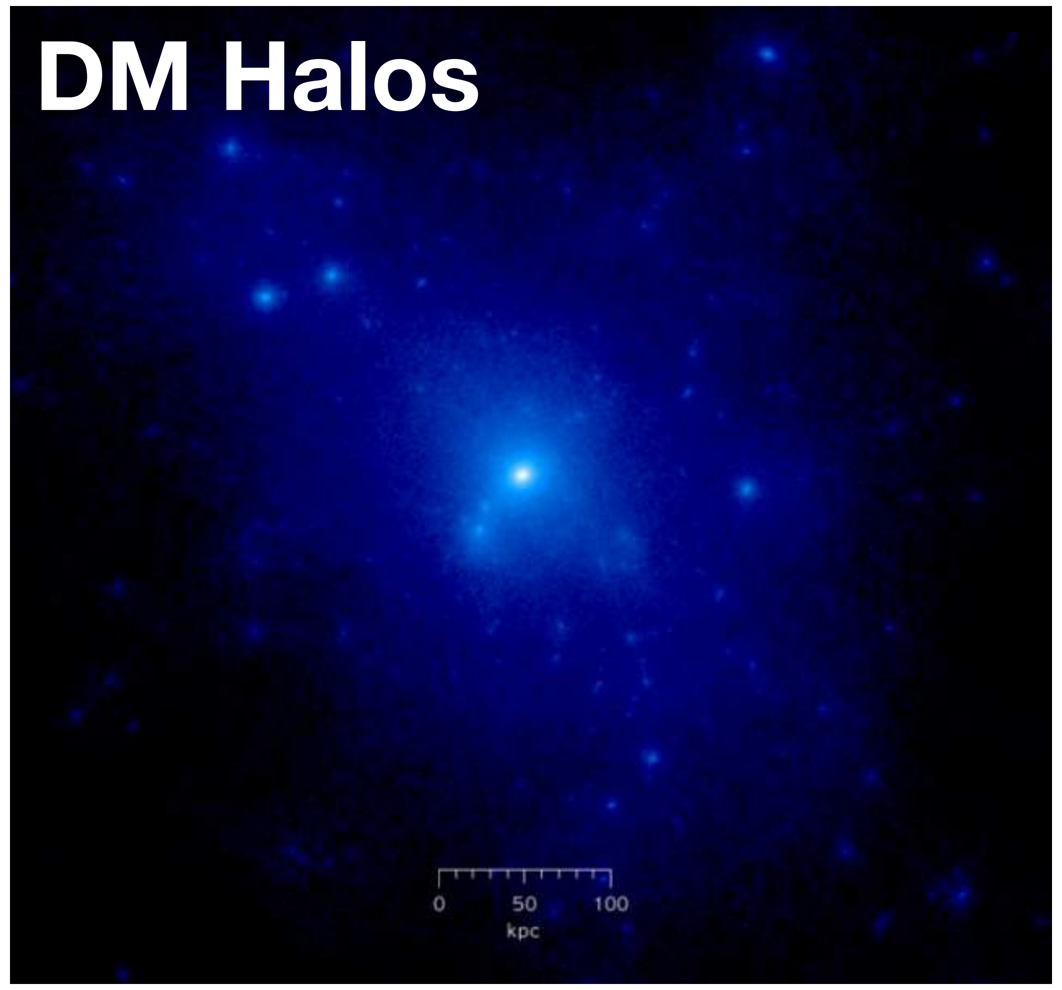
Motivated by the recent achievements of artificial intelligence (AI) in linguistics, we design AI to learn properties of atoms from materials data on its own. Our work realizes knowledge representation of atoms via computers and could serve as a foundational step toward materials discovery and design fully based on machine learning.

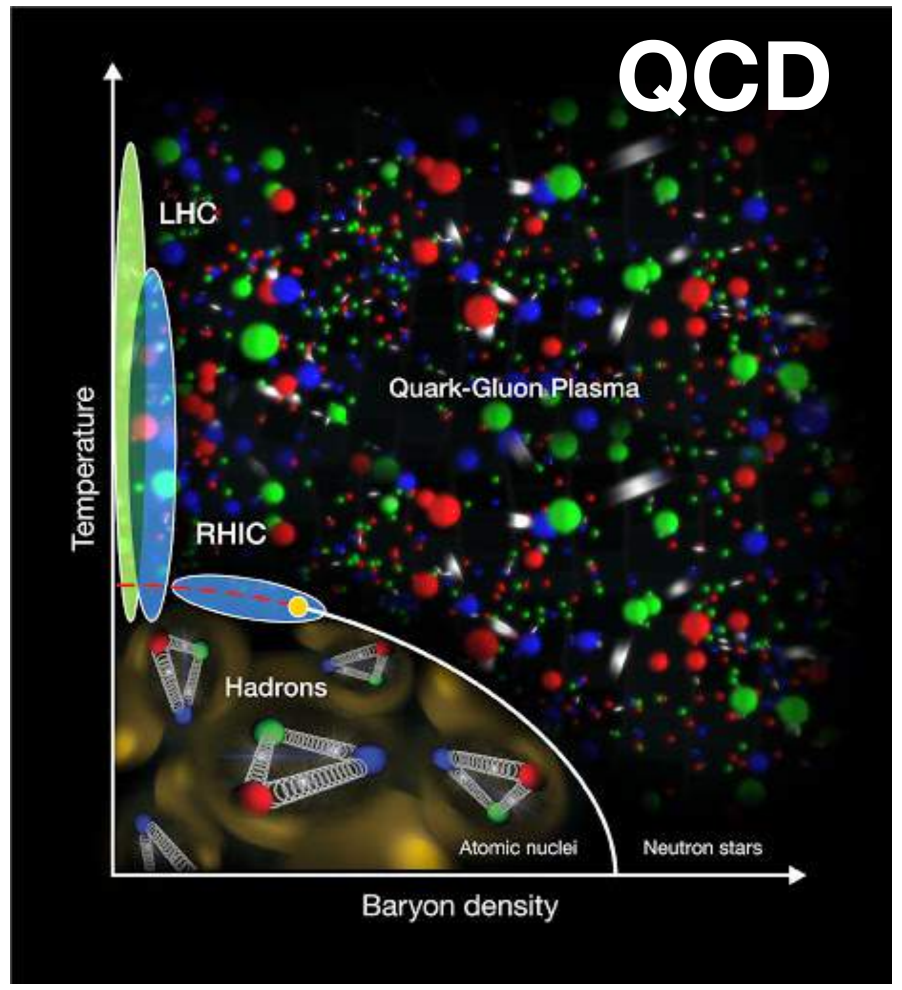
In Particle Physics pre ~ 60s/70s?



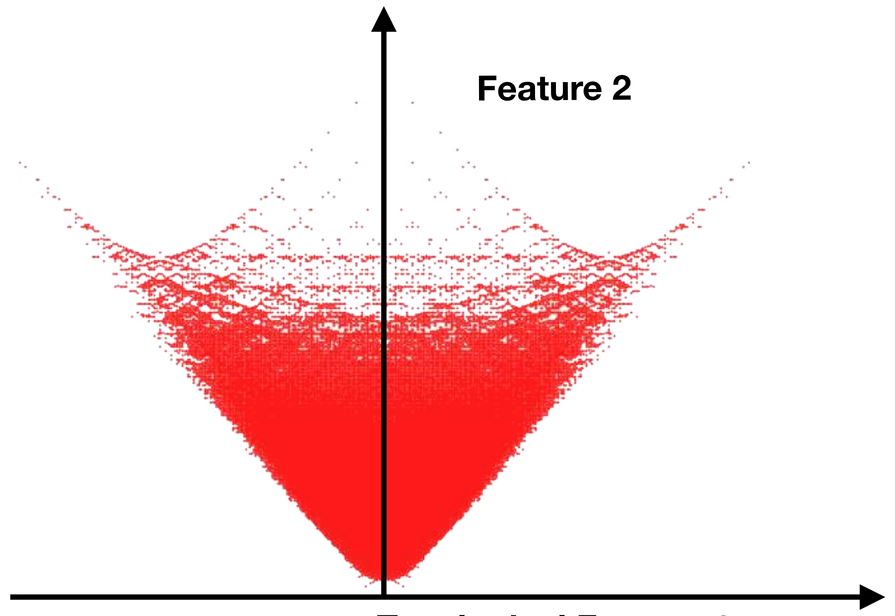


Which tools do we need to make such discoveries with ML in the 2020s?

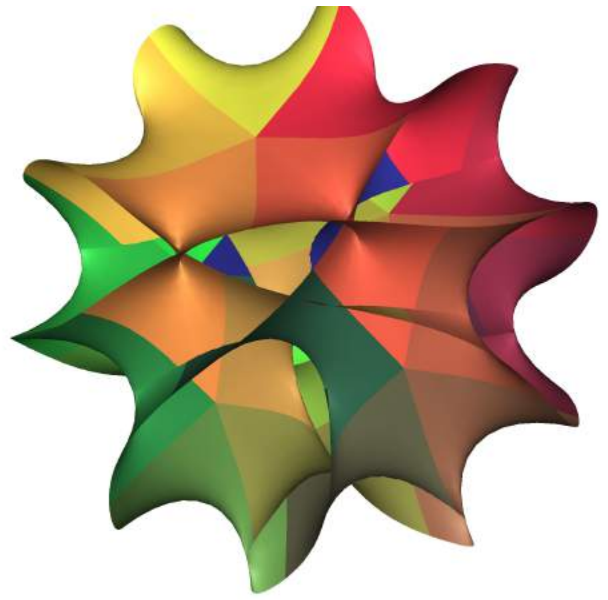




Pattern in Calabi-Yau data



CY-metrics



Finding mathematical structures to describe systems more efficiently

Our approach: Symmetries, Dualities, and Integrability

Why care for ML systems? Symmetries, dualities and integrability are standard structures used in physical systems which make your life easier (parameter inference, predictions from functional bias)
→ good functional bias

Symmetries from embedding layer

Krippendorf, Syvaeri 2020

Krippendorf, Syvaeri 2020

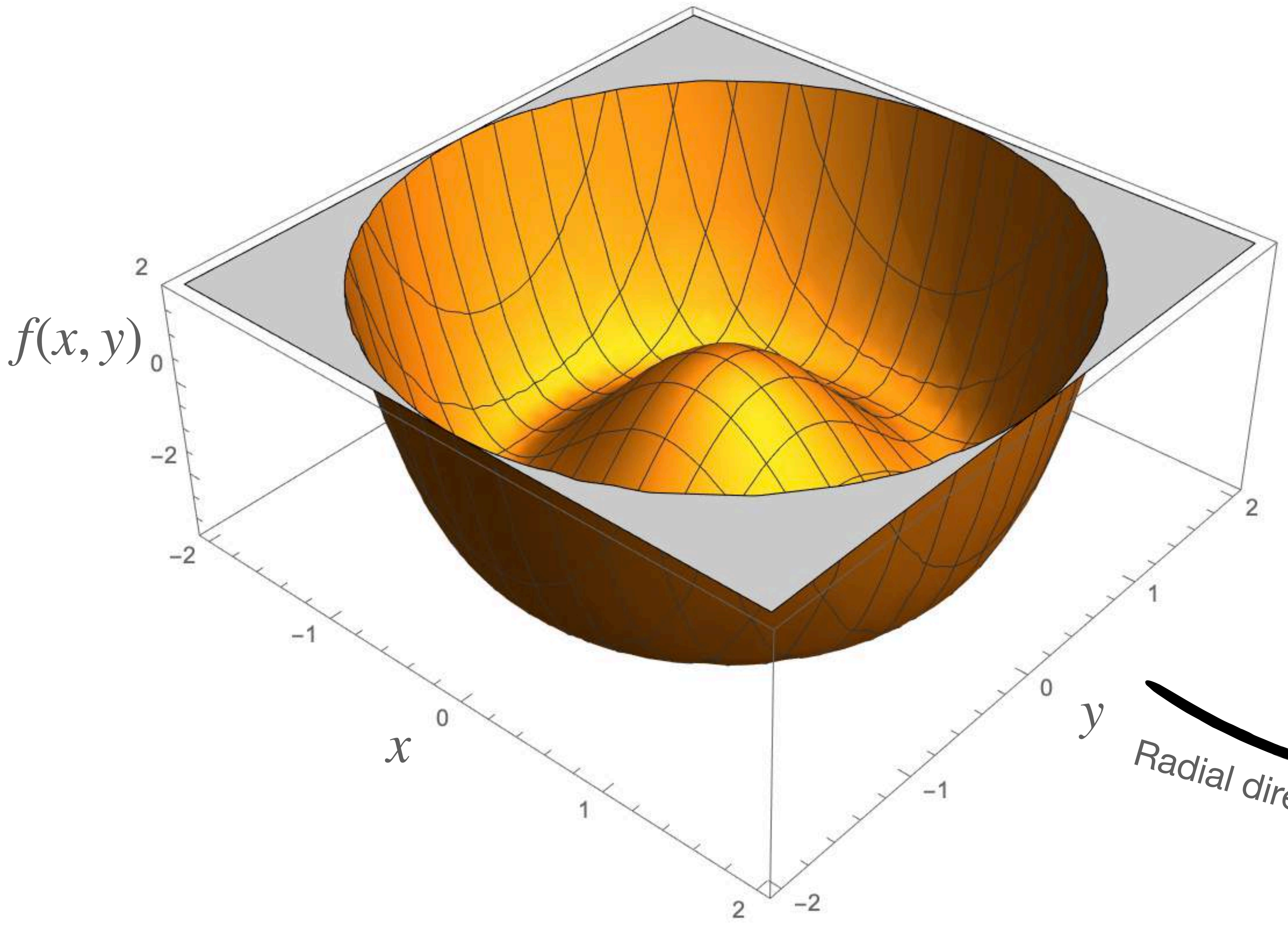
How to search for symmetries?

The problem

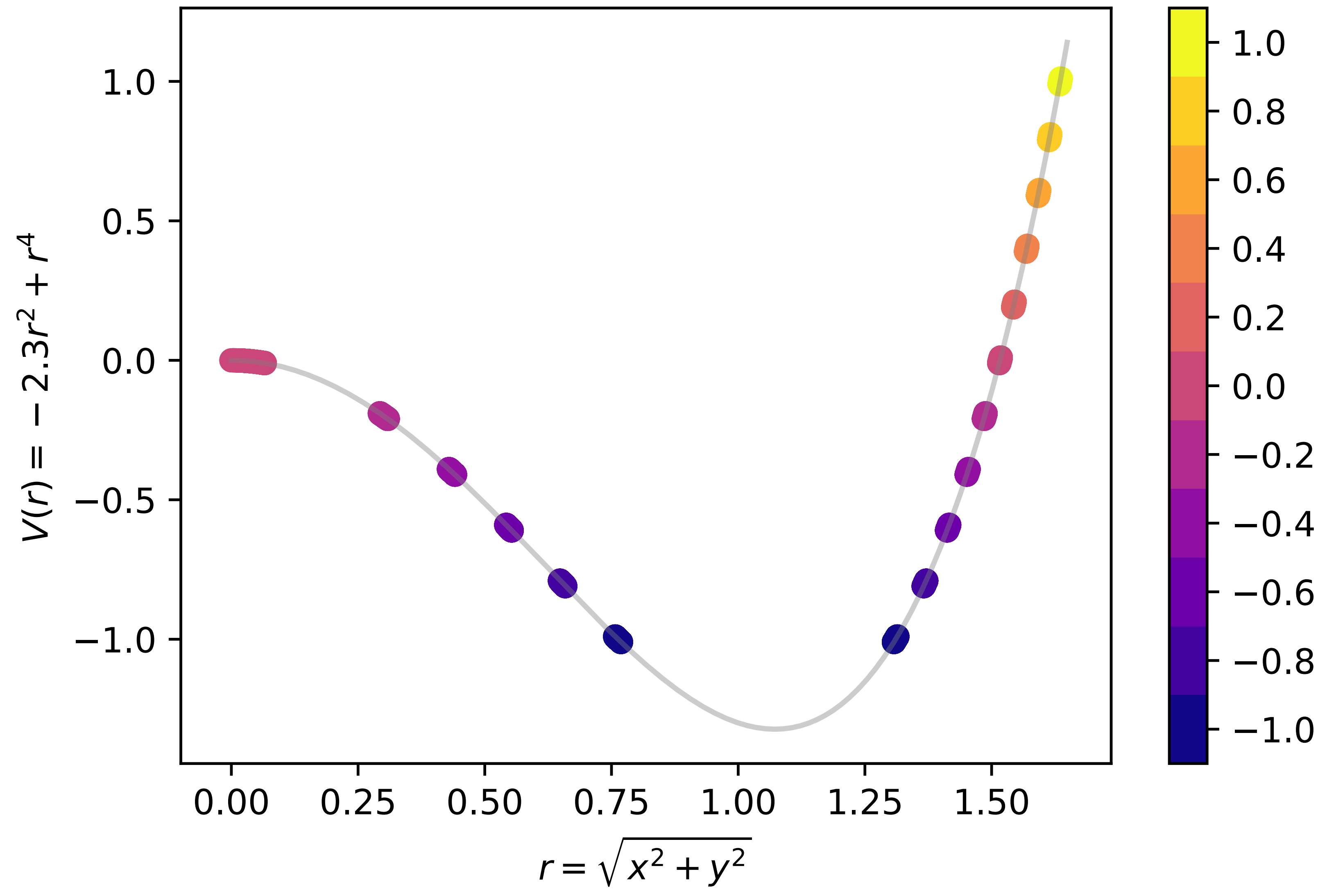
1. How to find invariances?

$$f(\phi) = f(\tilde{\phi})$$

2. Which symmetry is behind such an invariance?



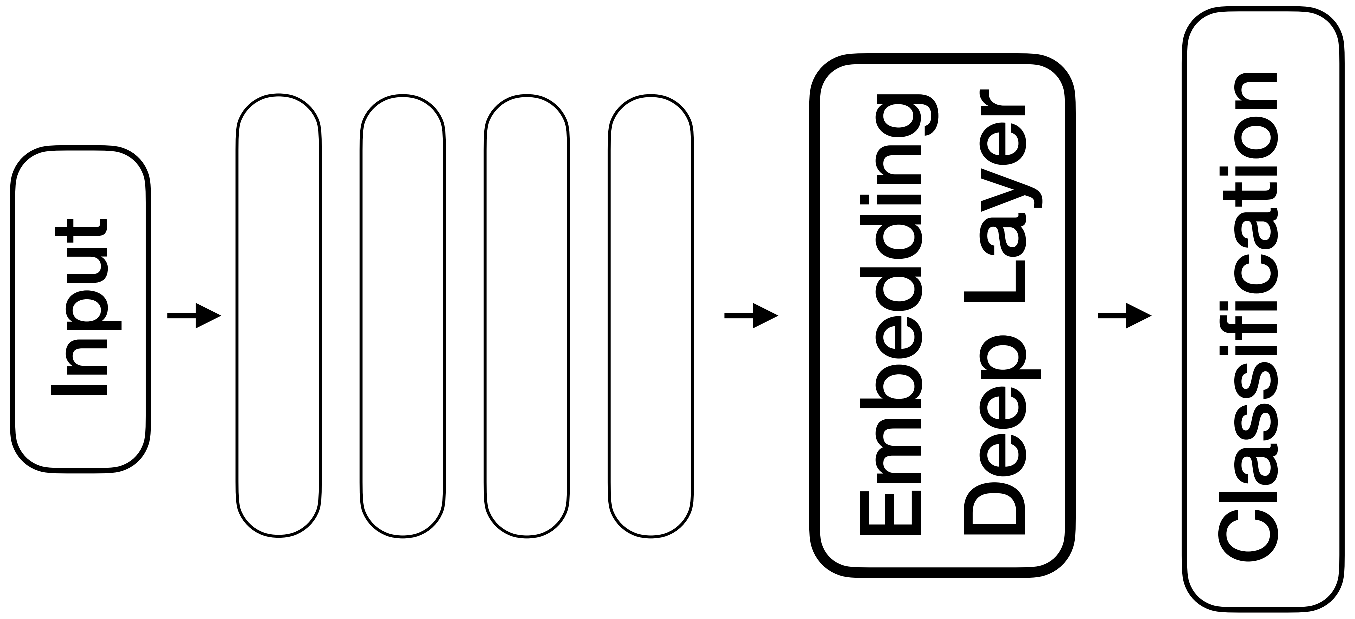
Radial direction



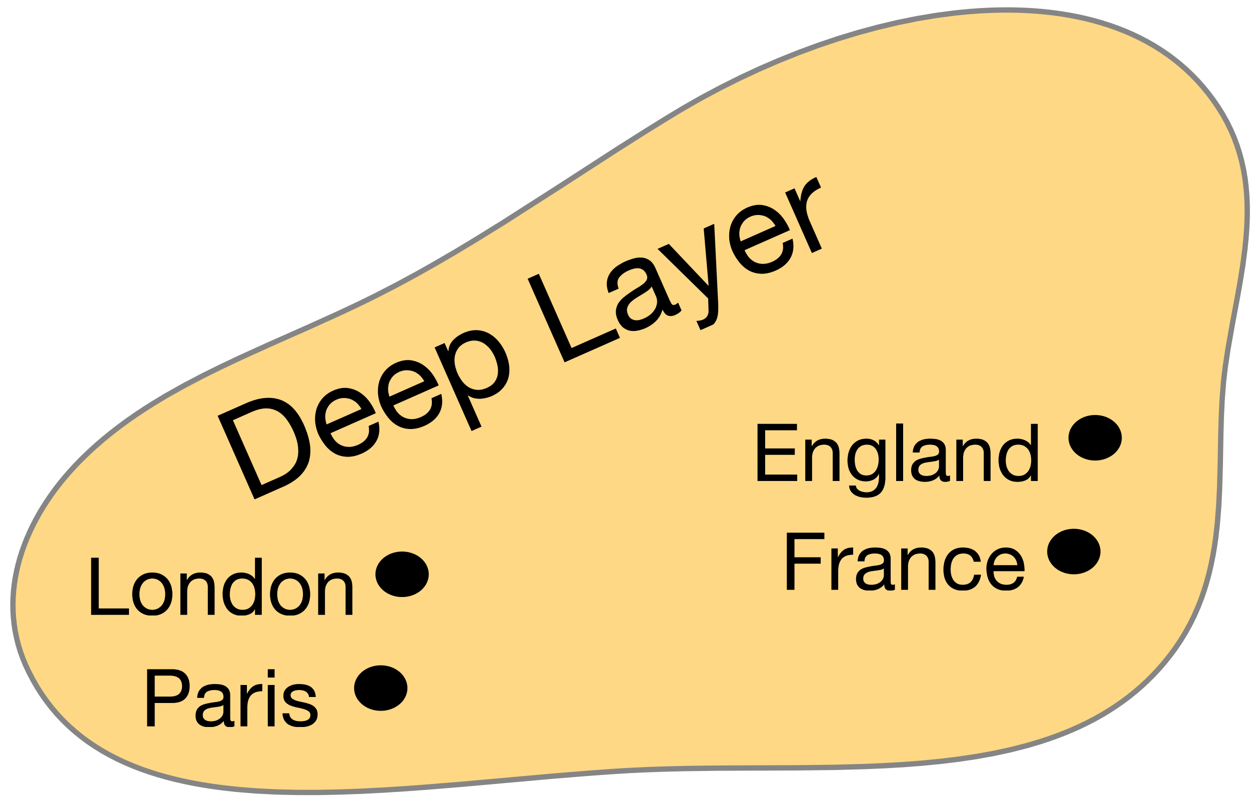
How to search for symmetries?

Embedding in deep layer

Feed-forward network



We need: group input with the same meaning together



Word2Vec does it:
(England - London = Paris - France)

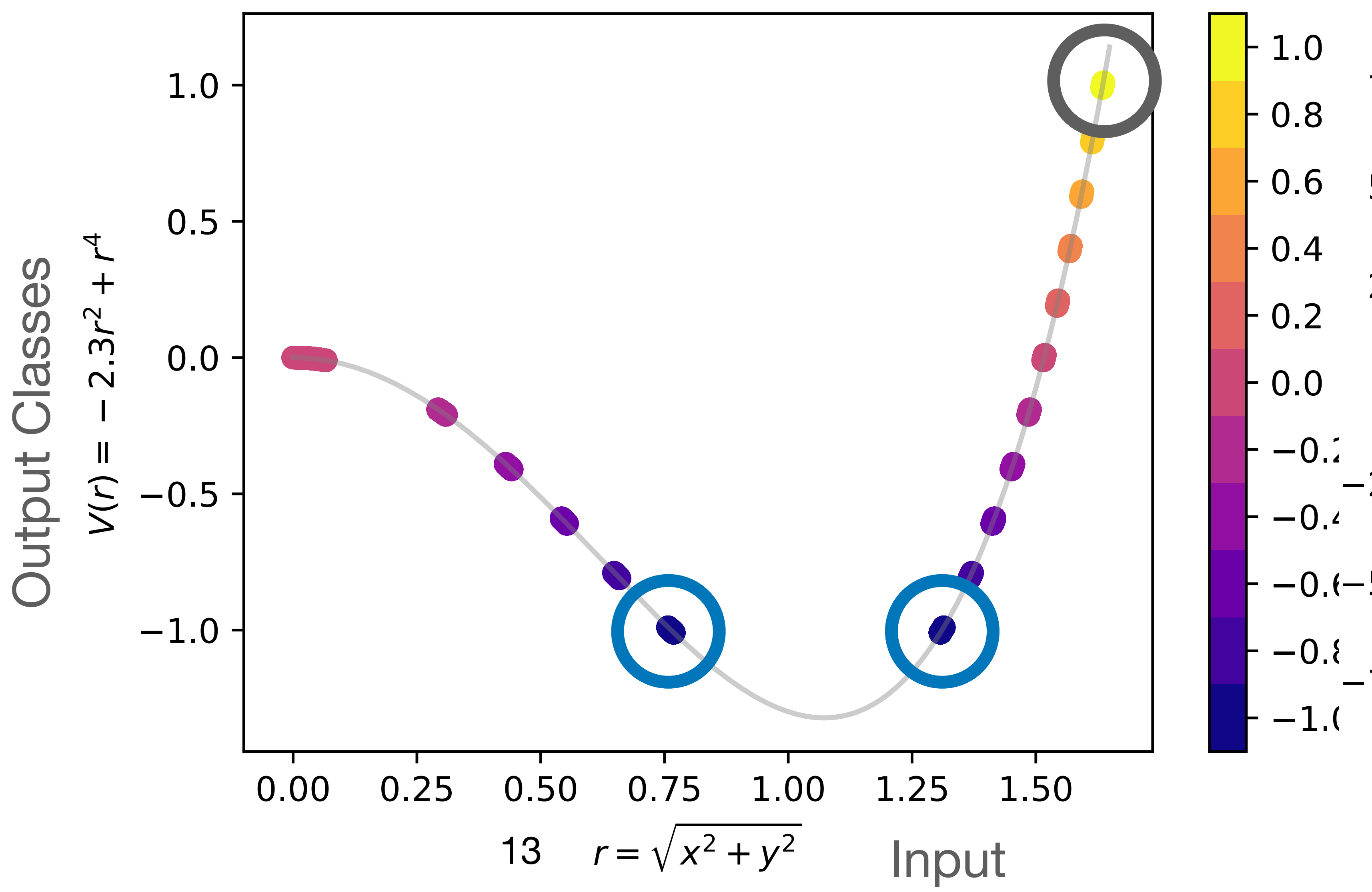
[1301.3781, used for re-discovering periodic table 1807.05617, classifying scents of molecules 1910.10685]

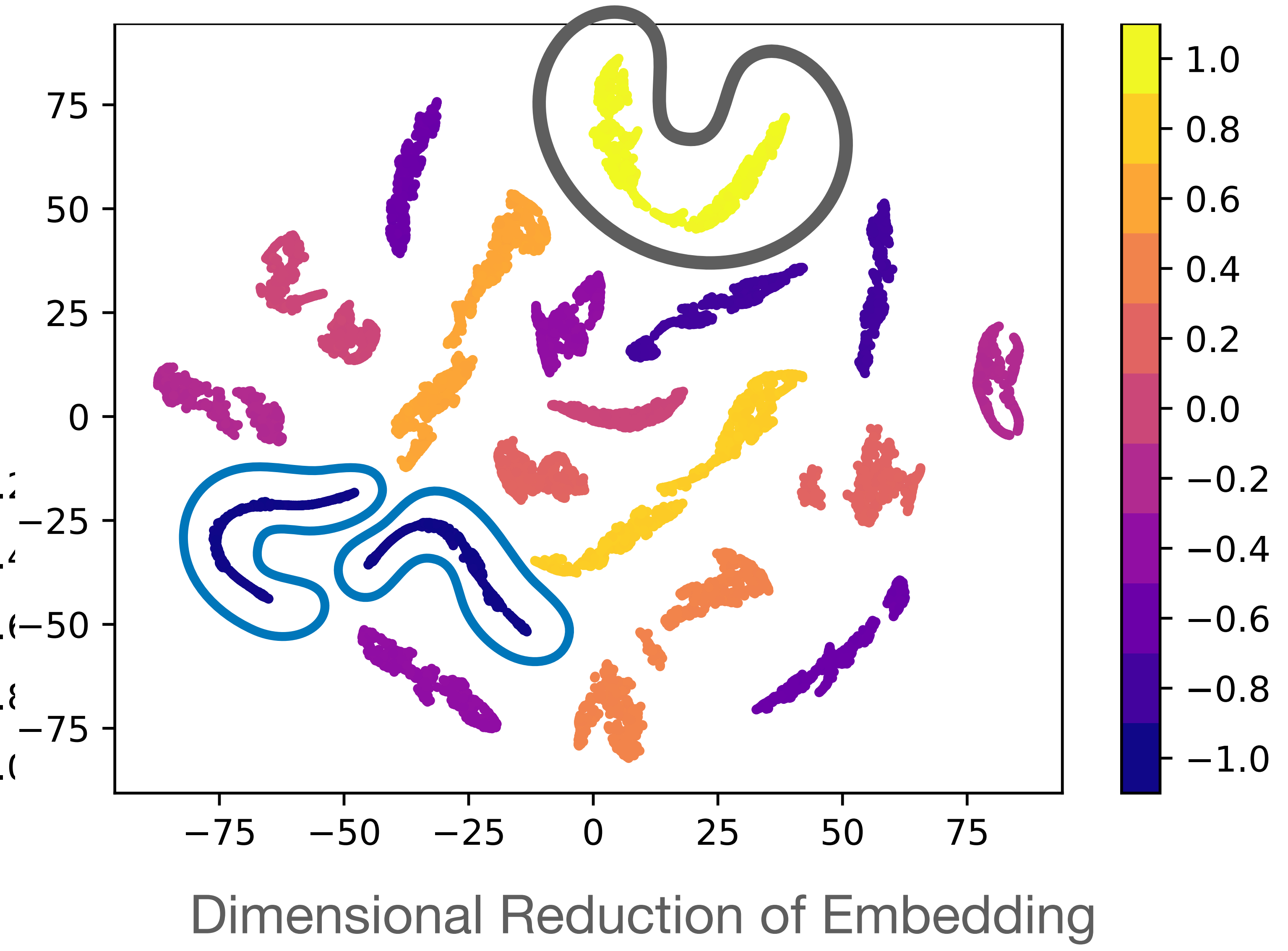
Can we search for symmetries in this way?

Yes!

Examples: SO(2), SU(2), discrete symmetries (CICY)

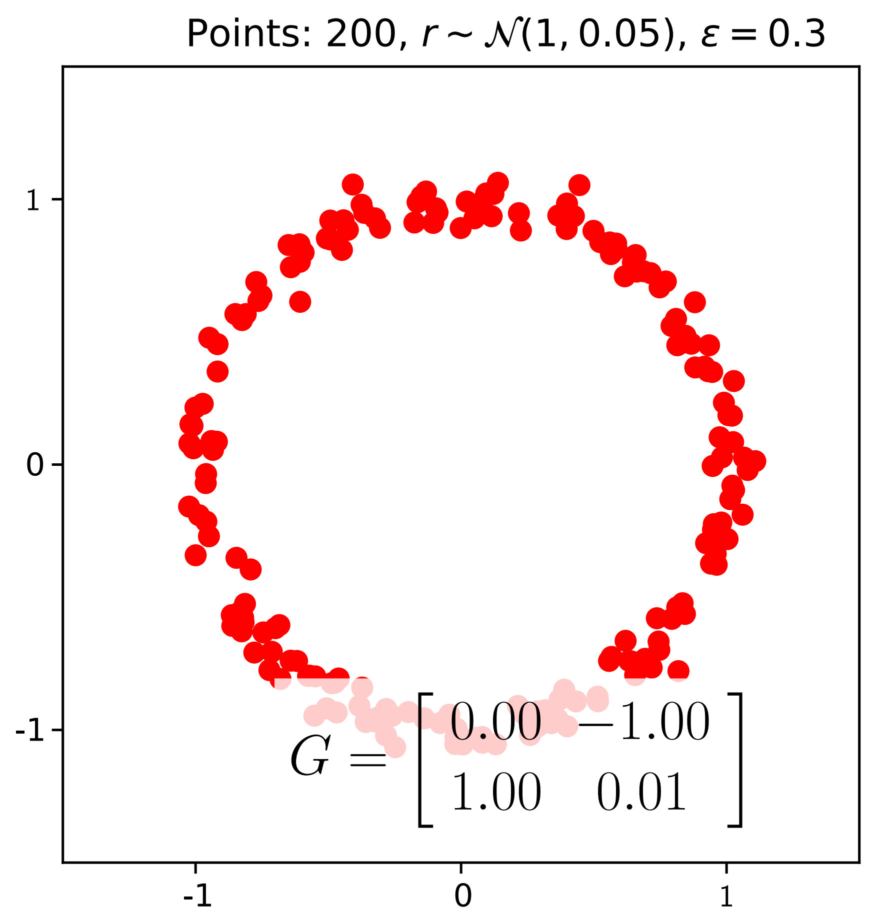
Krippendorff, Syvaeri 2020





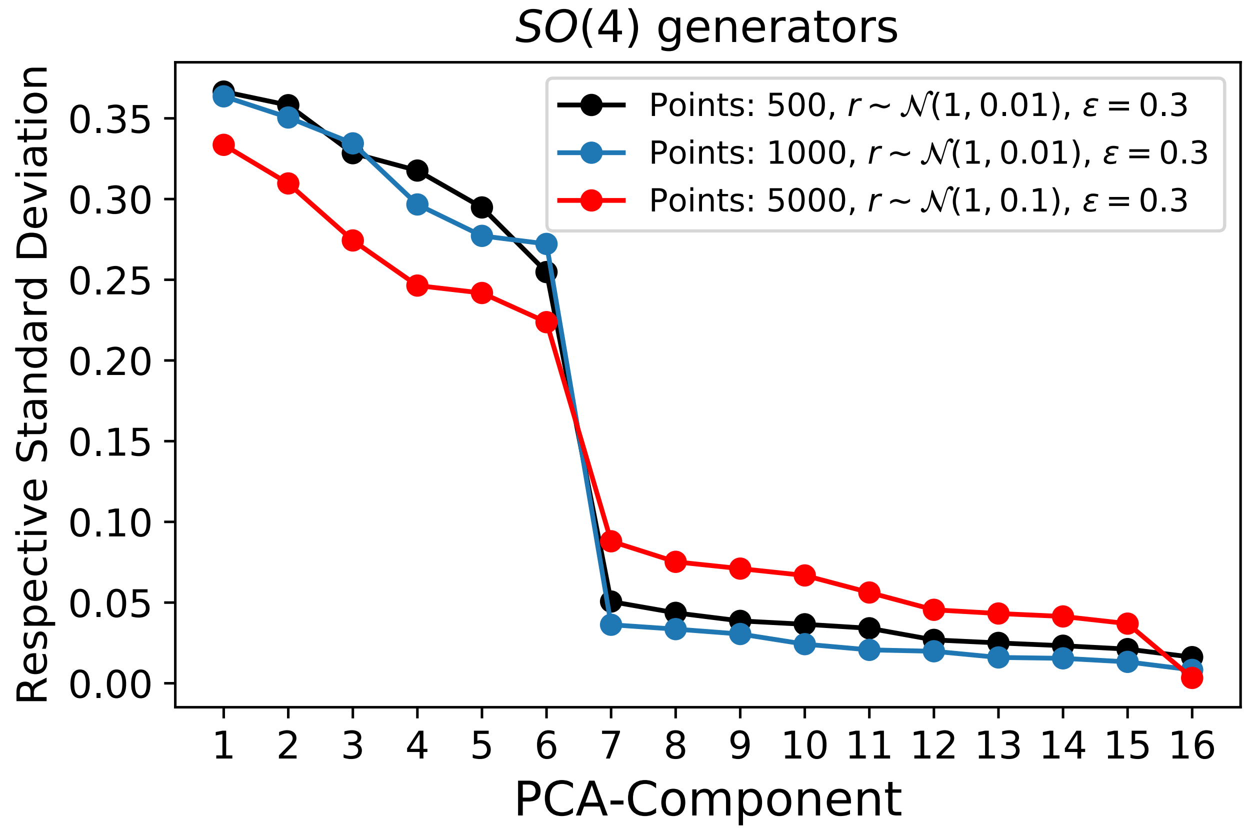
How to determine the symmetry?

Connected points in input space:



Which symmetry?

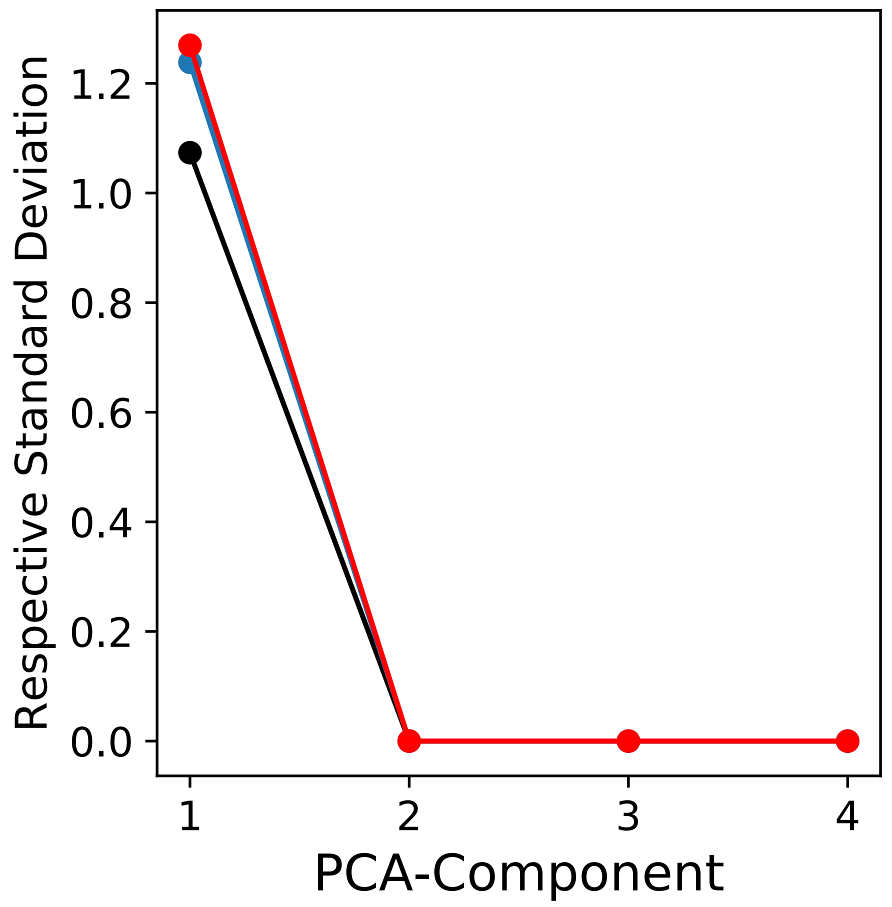
Other Examples?

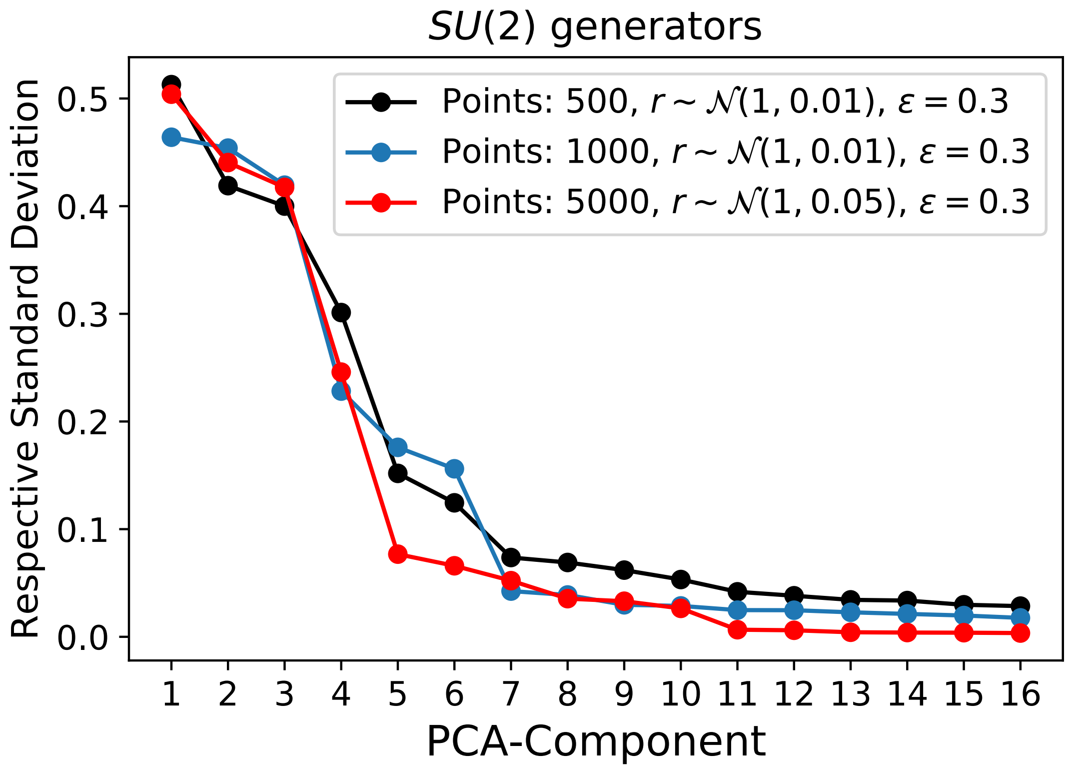


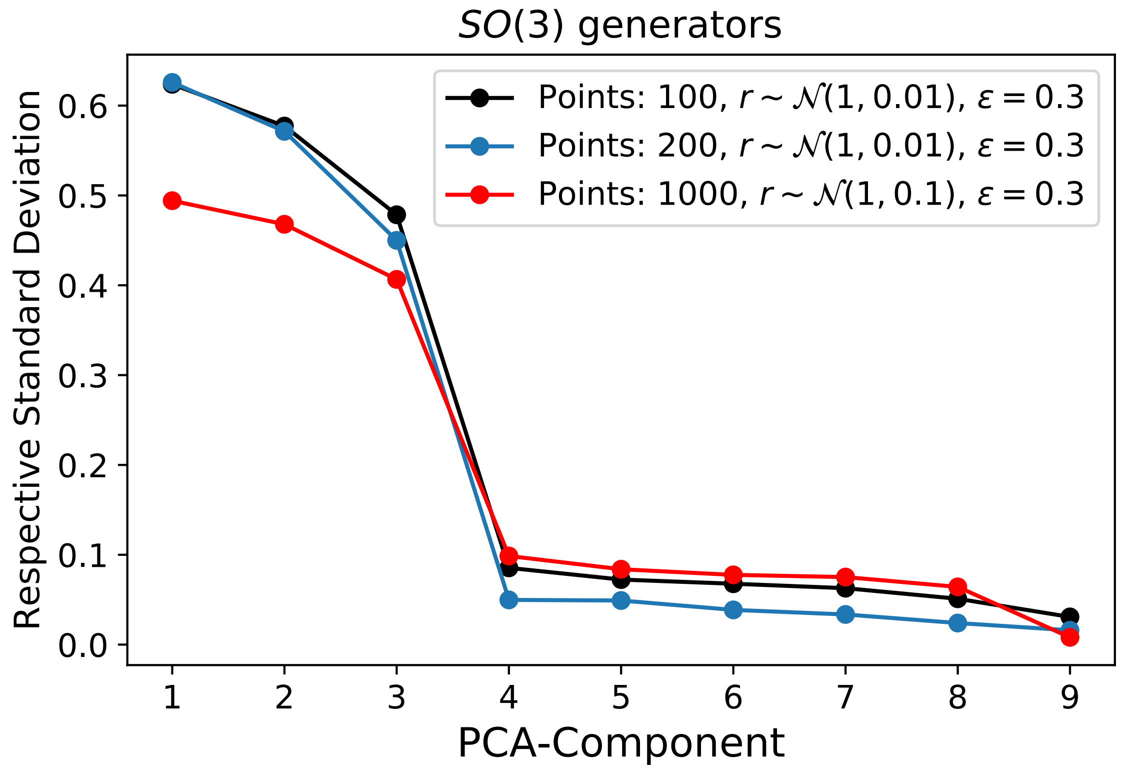
Determine generator connecting points in (sub)-space:

$$p' = p + \epsilon_a T^a p$$

Repeat multiple times (covering all sub-spaces) and perform PCA on generators:







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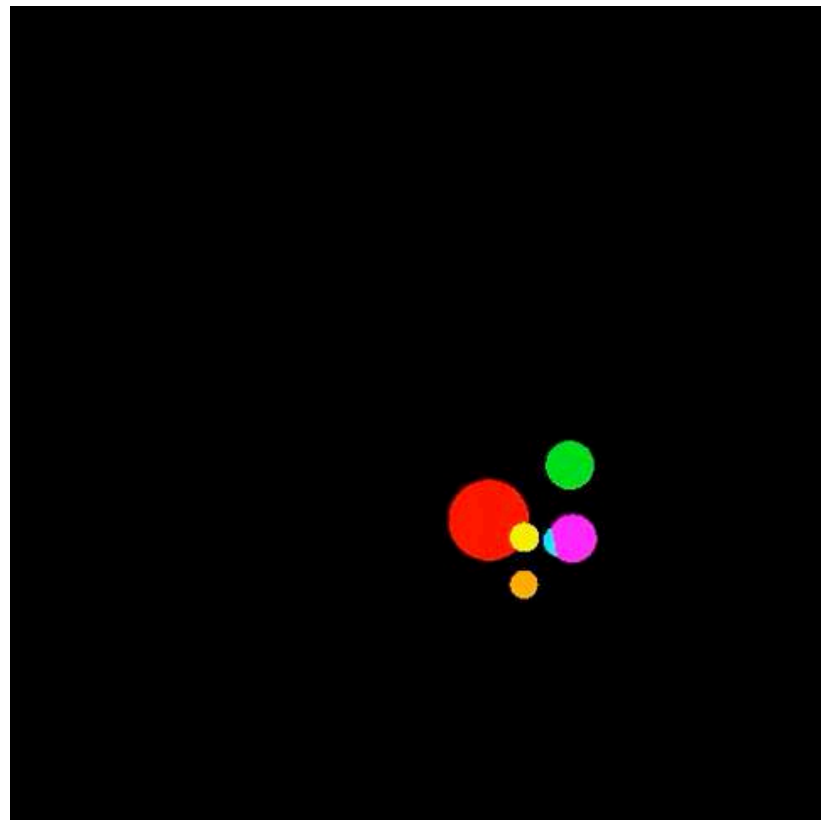
Symmetries from data (samples of phase space)

Krippendorf, Syvaeri (ICLR simDL workshop, 2104.14444)

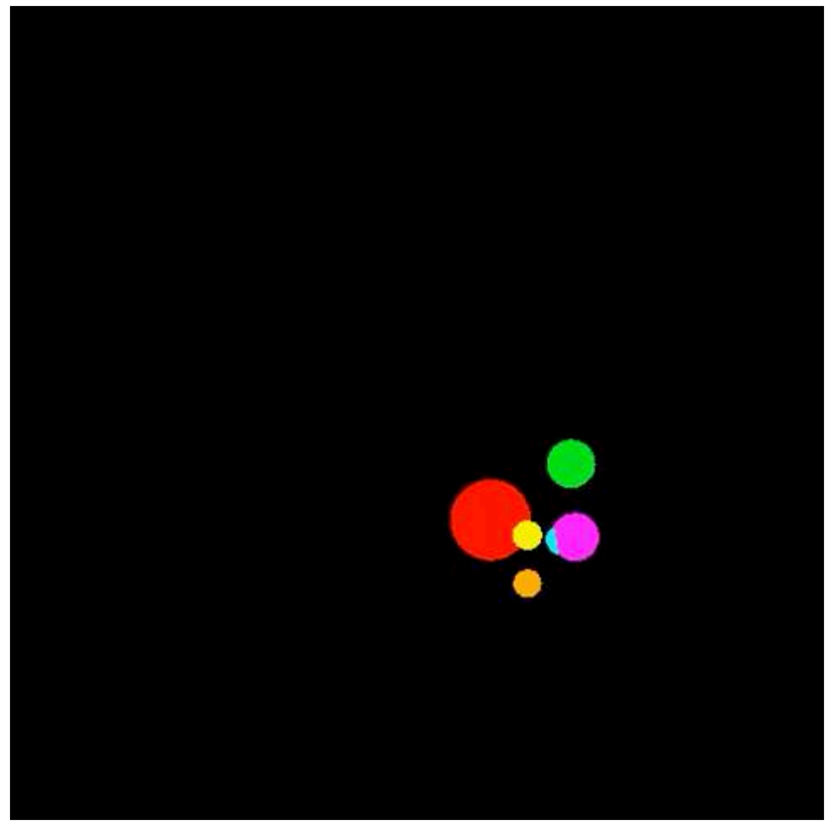
Simulations and physics bias

- The correct functional expressivity is key (vision: CNNs; geometric deep learning). Example for prediction of trajectories:

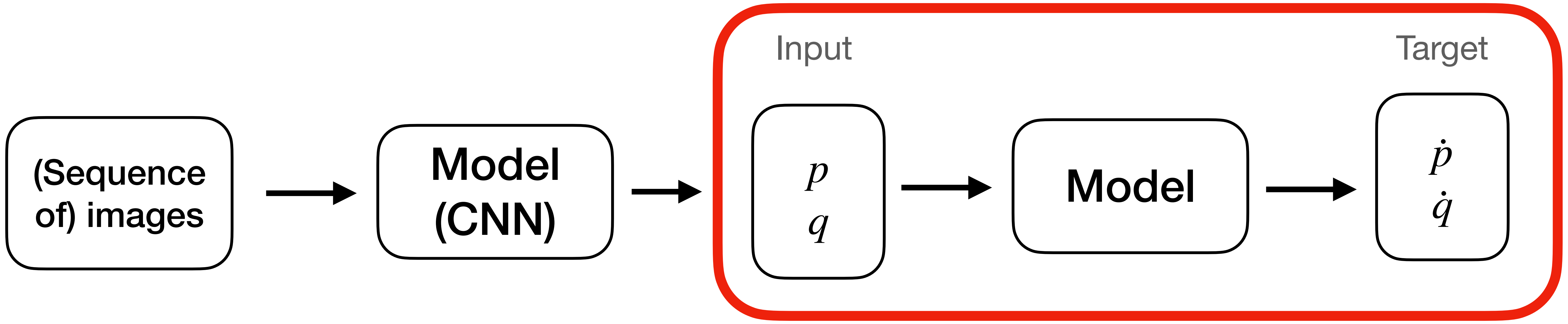
True



Model



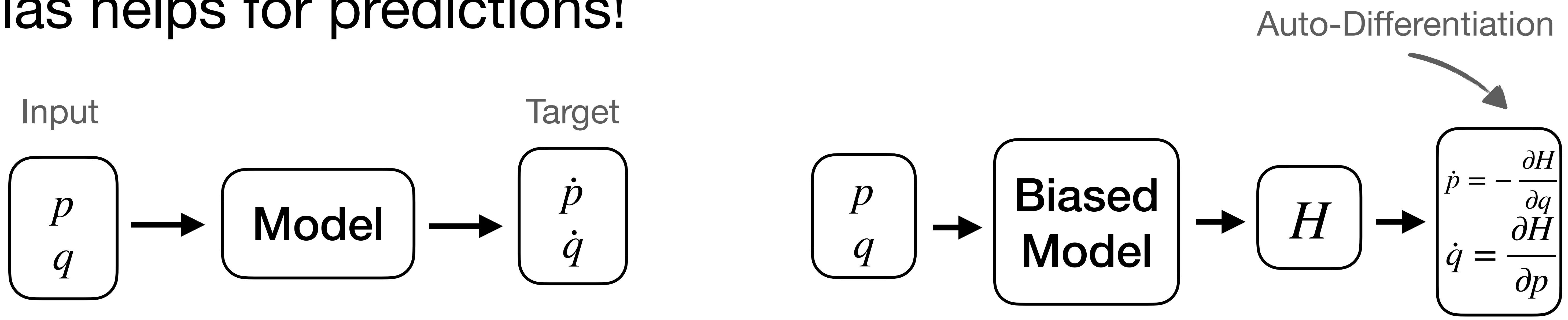
Battaglia et al 2016 (1612.00222)
….

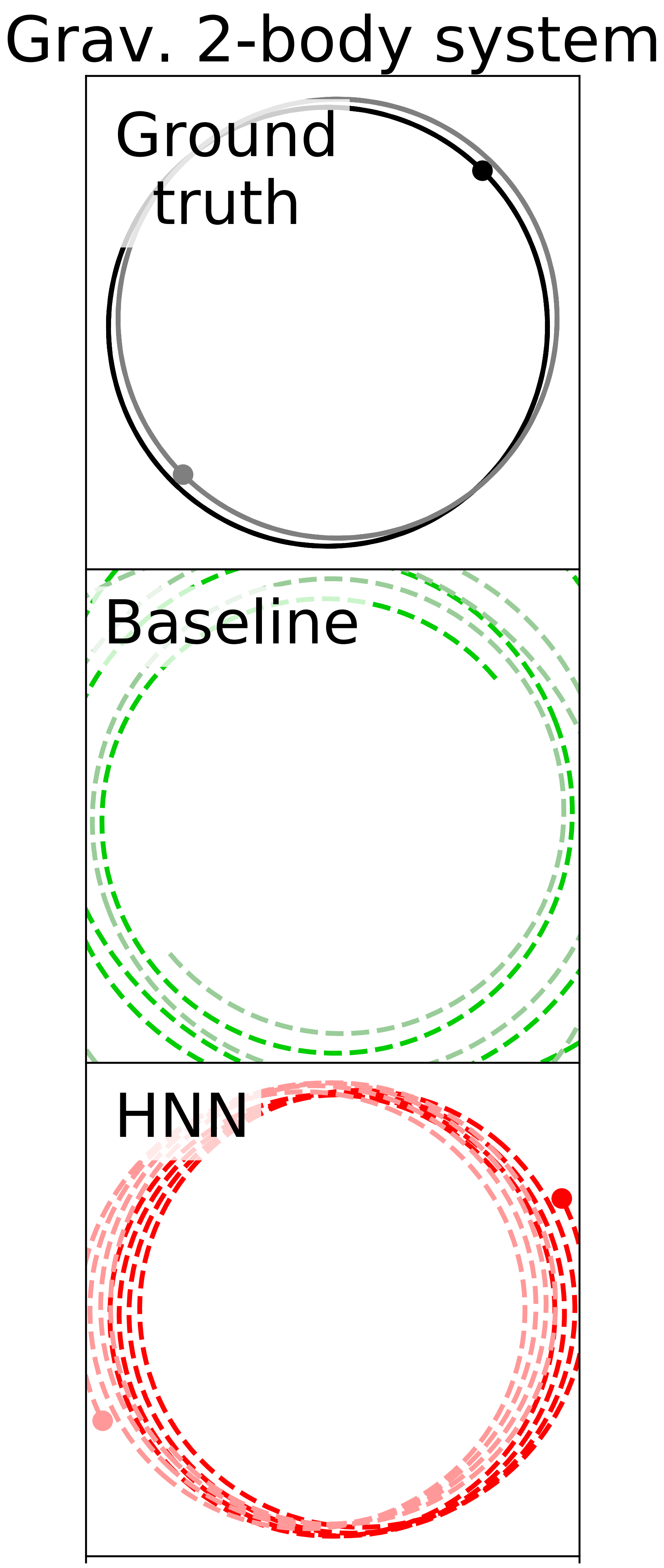


AI and Physics for Simulations

Greydanus et al. 2019
...

Physics Bias helps for predictions!





Physics Bias: enforce energy conservation

Krippendorf, Syvaeri (ICLR simDL workshop, 2104.14444)

Can we learn more structures from samples of phase space?

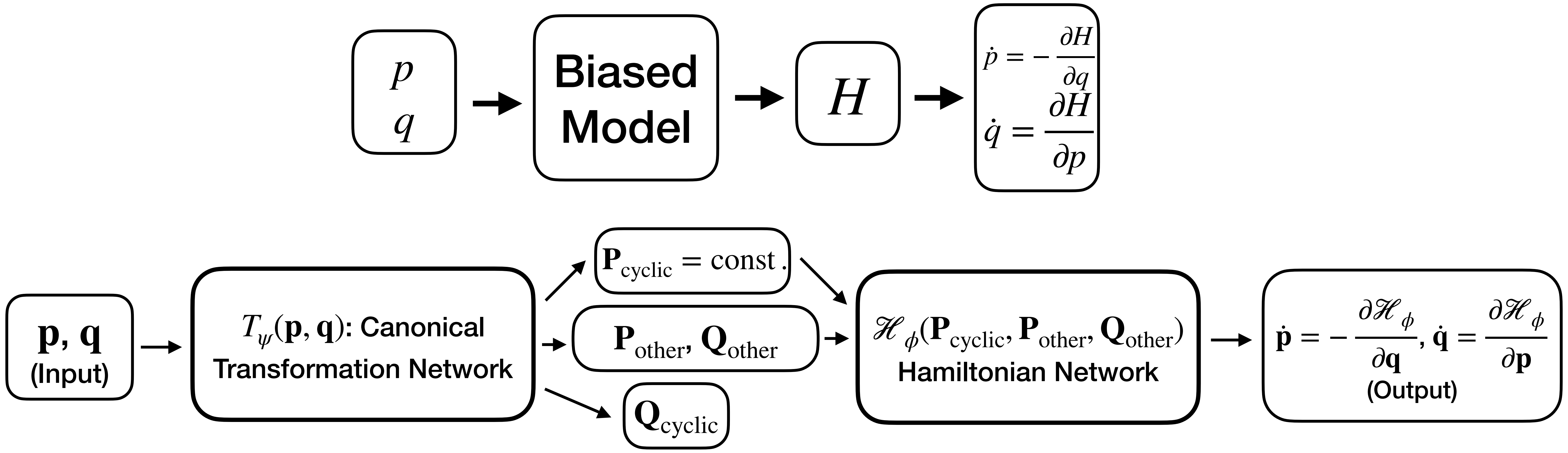
More structures from neural networks?

- If we can train NNs to find the Hamiltonian of a system, can we use it to learn other interesting structures?
- Symmetries of the system? E.g. via canonical transformations (cyclic coordinates reveal conserved quantities)
- How does this work? 2 key steps:
    1. Formulate your physics search problem as an optimisation problem.
    2. Make sure it's learnable for your architecture.
- Good news for analytic understanding of numerical approximations: most physics functions are simple (AI Feynman [Udrescu, Tegmark 1905.11481])
- Interesting **side effect**: quantify how much these structures help in predicting dynamics

AI for Simulations — Symmetries

Introducing physicists' bias

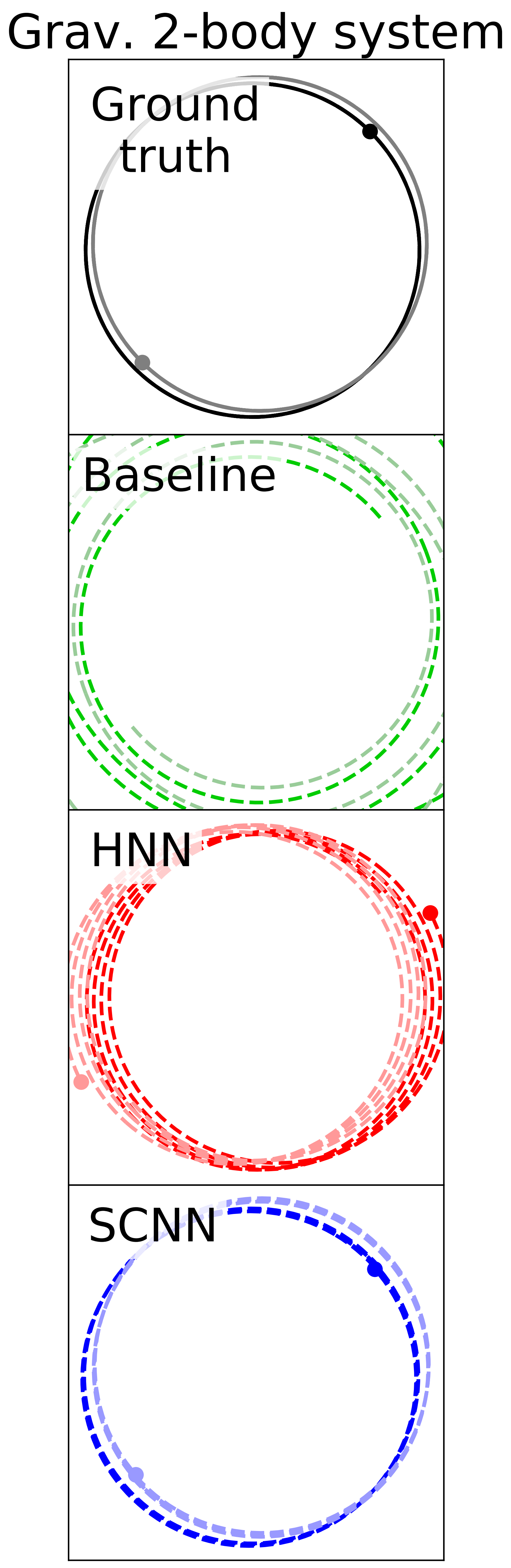
SCNNs: We cannot only learn the Hamiltonian but also the symmetries by enforcing canonical coordinates



Modified Losses:

$$0 = \dot{F}_k(p, q) = \{H(p, q), F_k(p, q)\}$$

Additional constraint on motion (not just energy conservation), i.e. motion takes place on hyper-surface in phase space

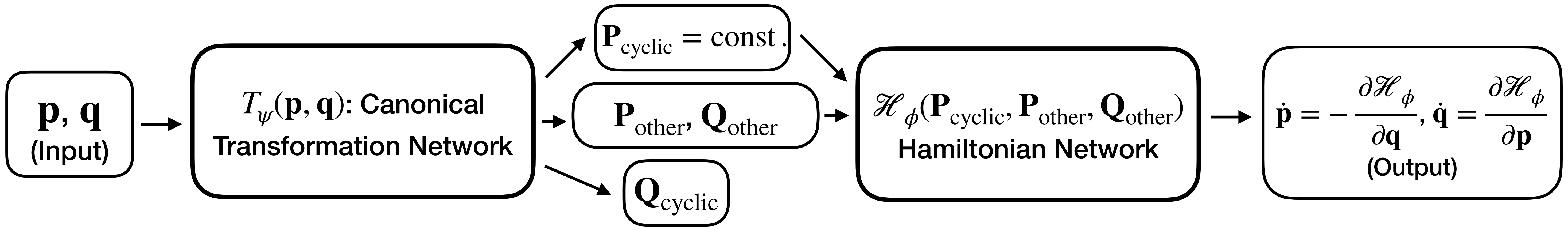


Krippendorf, Syvaeri 2104.14444

AI for Simulations — Symmetries

Introducing physicists' bias

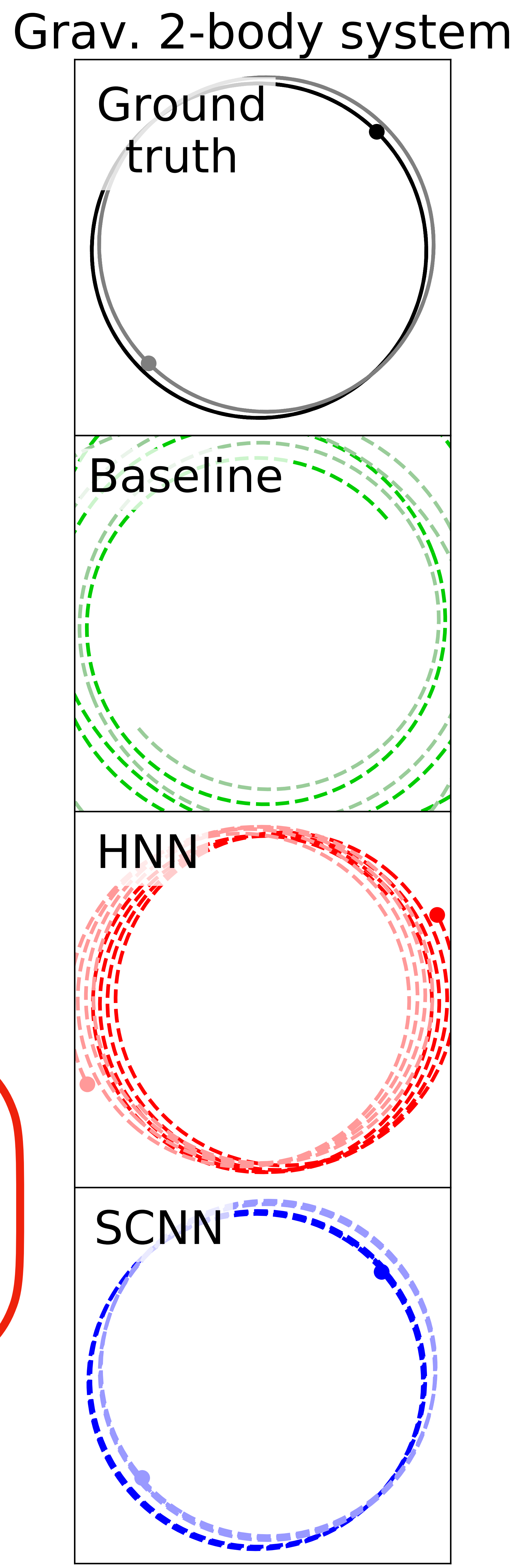
SCNNs: We cannot only learn the Hamiltonian but also the symmetries by enforcing canonical coordinates



Modified Losses for canonical coordinates:

- Hamilton equations: $\dot{P}_i(p,q) = -\dfrac{\partial H(p,q)}{\partial Q_i(p,q)} = 0$ and $\dot{Q}_i(p,q) = \dfrac{\partial H(p,q)}{\partial P_i(p,q)}$
- Poisson algebra: $\{P_i, Q_j\} = \delta_{ij}$ and $\{P_i, P_j\} = \{Q_i, Q_j\} = 0$

Additional Loss terms



Krippendorff, Syvaeri 2104.14444

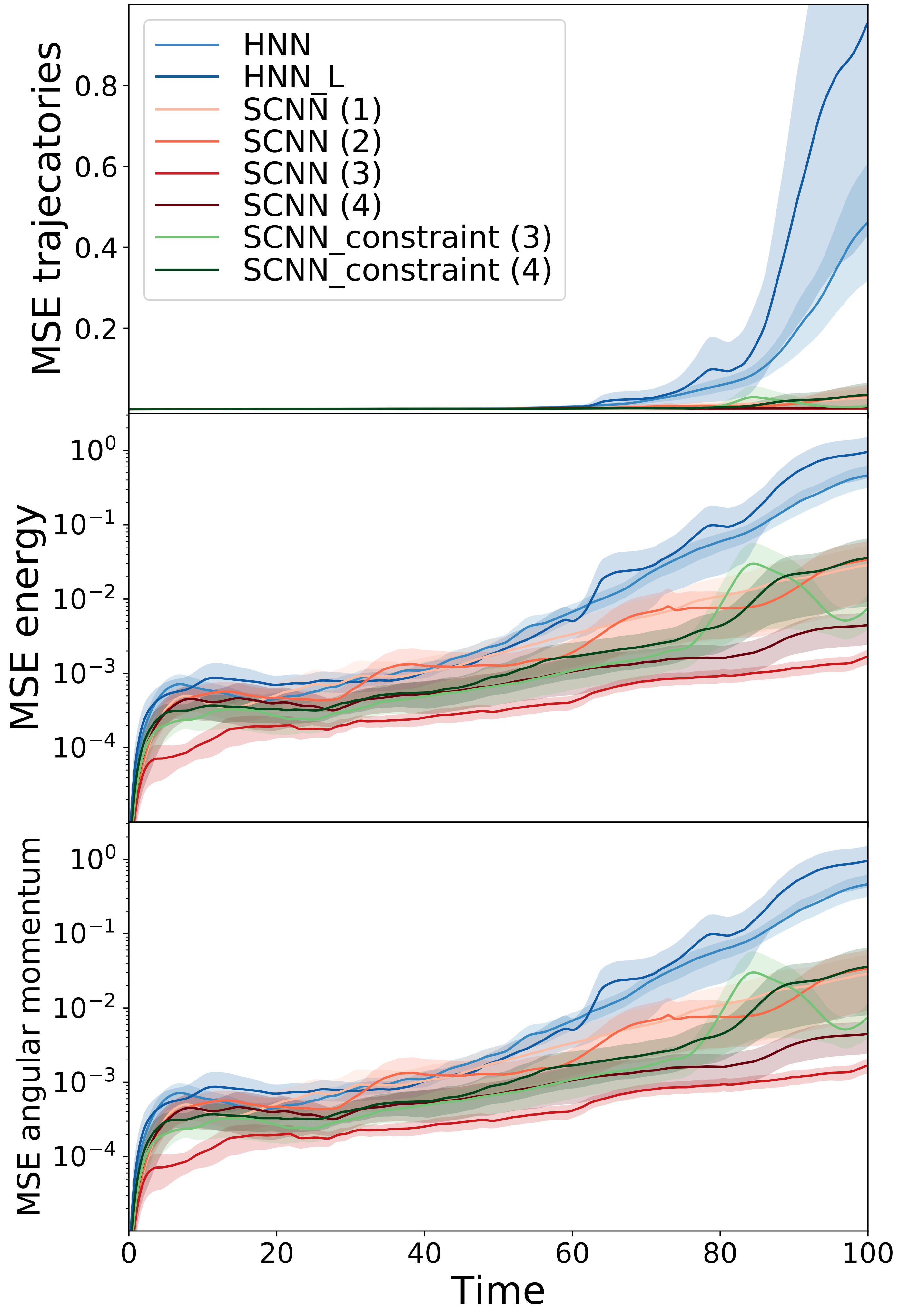
Benefits from Physicists' Bias

- Conserved quantities interpretable:

$$P_{c_1} = -4.2p_{x_1} - 4.2p_{x_2} - 1.3p_{y_1} - 1.3p_{y_2}\ ,\ P_{c_2} = -0.9p_{x_1} - 0.9p_{x_2} - 3.2p_{y_1} - 3.2p_{y_2}$$

$$L = -1.1q_{x_1}p_{y_1} + 0.9q_{x_1}p_{y_2} + 0.9q_{x_2}p_{y_1} - 1.0q_{x_2}p_{y_2} + 1.0q_{y_1}p_{x_1} - 0.9q_{y_1}p_{x_2} - 0.9q_{y_2}p_{x_1} + 1.0q_{y_2}p_{x_2}$$

- Using learned conserved quantities helps in predicting trajectories



Can we search for new mathematical/physical structures?

Symmetries → Integrability

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Integrability

A lightning overview

- Additional constraint F_k on motion:
$$0 = \dot{F}_k = \{H, F_k\}$$
How many F_k can there be?

- **System** (2n dimensional) **integrable** iff:
n independent, everywhere differentiable integrals of motion F_k (in involution).

- Alternatively search for **Lax pair**:
$$\dot{L} = [L, M]$$
s.t. eom are satisfied. Conserved quantities via:
$$F_k = \mathrm{tr}(L^k)$$
(additional condition for $\{F_k, F_j\} = 0$)

Example: Harmonic Oscillator

- Hamiltonian and EOM:
$$H = \frac{1}{2}p^2 + \frac{\omega^2}{2}q^2\,; \quad \dot{q} = p, \dot{p} = -\omega^2 q$$

- Lax pair:
$$L = a\begin{pmatrix} p & b\omega q \\ \frac{\omega}{b}q & -p \end{pmatrix}, \quad M = \begin{pmatrix} 0 & \frac{b}{2}\omega \\ -\frac{\omega}{2b} & 0 \end{pmatrix}$$

- Conserved quantities:
$$F_1 = 2\lambda$$
$$F_2 = 2\lambda^2 + 4H$$
$$F_3 = 2\lambda^3 + 12\lambda H$$
$$\dots$$

$\lambda\dots$ spectral parameter

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Integrability

Having a Lax pair formulation of integrability is very convenient, but

- inspiration is needed to find it,
- its structure is hardly transparent,
- it is not at all unique,
- the size of the matrices is not immediately related to the dimensionality of the system.

Therefore, the concept of Lax pairs does not provide a means to decide whether any given system is integrable (unless one is lucky to find a sufficiently large Lax pair).

Beisert: Lecture Notes on Integrability (p17)

Applications:
- Classical mechanics (e.g. planetary motion)
- Classical field theories (1+1 dimensions)
- Spin Chain Models
- D=4 N=4 SYM in the planar limit
- ...

We need some *deus ex machina* moment…

Nonlinear Sciences > Exactly Solvable and Integrable Systems

[Submitted on 12 Mar 2021]

Integrability ex machina

Sven Krippendorf, Dieter Lust, Marc Syvaeri

Formulating the search as optimisation

- **Aim: Method to find new Lax pairs with unsupervised learning (i.e. not requiring prior knowledge of a Lax pair)**
- Lax equation as loss:

$$\dot{L} = [L, M] \to \mathscr{L}_{\mathrm{Lax}} = \left| \dot{L} - [L, M] \right|^2$$

- Equivalence to EOM (e.g. $\dot{x}_i = f_i\left(x_i, \partial x_i, \ldots\right)$): L has to include x_i in some component (LHS of EOM), $[L, M]$ has to include RHS of EOM

$$\mathscr{L}_{\mathrm{L}} = \sum_{i,j} \min_k \left(||c_{ijk}\dot{L} - \dot{x}_k||^2, ||\dot{L}_{ij}||^2 \right) + \sum_k \min_{ij} \left(||c_{ijk}\dot{L}_{ij} - \dot{x}_k||^2 \right), \quad c_{ijk} = \frac{\sum_{batch} \dot{L}_{ij}}{\sum_{batch} \dot{x}_k}$$

$$\mathscr{L}_{\mathrm{LM}} = \sum_{i,j} \min_k \left(||\tilde{c}_{ijk}[L, M]_{ij} - f_k||^2, ||[L, M]_{ij}||^2 \right) + \sum_k \min_{ij} \left(||\tilde{c}_{ijk}[L, M]_{ij} - f_k||^2 \right), \quad \tilde{c}_{ijk} = \frac{\sum_{batch} [L, M]_{ij}}{\sum_{batch} f_k}$$

only fixed up to proportionality (loss function independent of refactor)

- Avoiding mode collapse:

$$\mathscr{L}_{\mathrm{MC}} = \max\left(1 - \sum \left|A_{ij}\right|, 0\right)$$

- Total loss:

$$\mathscr{L}_{\mathrm{Lax-pair}} = \alpha_1 \mathscr{L}_{\mathrm{Lax}} + \alpha_2 \mathscr{L}_{\mathrm{L}} + \alpha_3 \mathscr{L}_{\mathrm{LM}} + \alpha_4 \mathscr{L}_{\mathrm{MC}}$$

Applications

Harmonic Oscillator

- Harmonic Oscillator:

$$H = \frac{1}{2}p^2 + \frac{\omega^2}{2}q^2; \qquad \dot{q} = p \ , \qquad \dot{p} = -\,\omega^2 q$$

- Lax Pair:

$$L = \begin{pmatrix} 0.437\ q & -0.073\ p \\ -0.666\ p & -0.437\ q \end{pmatrix}, \quad M = \begin{pmatrix} 0.001 & 0.329 \\ -3.043 & -0.001 \end{pmatrix}$$

- Consistency check:

$$\frac{dL}{dt} = \begin{pmatrix} 0.437\ \dot{q} & -0.073\ \dot{p} \\ -0.666\ \dot{p} & -0.437\ \dot{q} \end{pmatrix} = \begin{pmatrix} 0.441\ p & 0.288\ q \\ 2.660\ q & -0.441\ p \end{pmatrix} = [L, M]$$

- Conserved quantities:

$$L^2 = \begin{pmatrix} 0.048618p^2 + 0.190969q^2 & 0 \\ 0 & 0.048618p^2 + 0.190969q^2 \end{pmatrix} \Rightarrow \mathrm{tr}L^2 \approx 0.2\ H$$

Applications

Further systems

- Korteweg-de Vries (waves in shallow water):

$$\dot{\phi}(x,t) + \phi'''(x,t) + 6\phi(x,t)\phi'(x,t) = 0$$

$$A_x = \begin{pmatrix} -1.7\phi & 1.7\phi + 1.0 \\ 1.7\phi + 1.0 & -1.7\phi \end{pmatrix},$$

$$A_t = \begin{pmatrix} 5.0\phi^2 + 1.7\phi'' & -5.0\phi^2 - 1.7\phi'' - 0.5 \\ -5.0\phi^2 - 1.7\phi'' - 0.5 & 5.0\phi^2 + 1.7\phi'' \end{pmatrix}$$

- Heisenberg magnet:

$H = \dfrac{1}{2}\displaystyle\int dx\, \overrightarrow{S}^2(x)$, $\overrightarrow{S} \in S^2$; constraint:
$\{S_a(x), S_b(y)\} = \epsilon_{abc} S_c(x) \delta(x-y)$

$$A_x = -\ \mathrm{i}\ \vec{\sigma}\vec{S} + 0.3 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\begin{aligned} A_t = &\begin{pmatrix} 2\ \mathrm{i}\ S_z & 2\ \mathrm{i}\ S_x + 2S_y \\ 2\ \mathrm{i}\ S_x - 2S_y & -\ \mathrm{i}\ S_z \end{pmatrix} \\ &+ \begin{pmatrix} \mathrm{i}\ S'_y S_x -\ \mathrm{i}\ S'_x S_y & -S'_z S_x + S'_x S_z +\ \mathrm{i}\ (S'_z S_y - S'_y S_x) \\ +S'_z S_x - S'_x S_z +\ \mathrm{i}\ (S'_z S_y - S'_y S_x) & -\ \mathrm{i}\ S'_y S_x +\ \mathrm{i}\ S'_x S_y \end{pmatrix} \\ =&2\ \mathrm{i}\ \vec{\sigma}\vec{S} +\ \mathrm{i}\ \epsilon_{ijk}\sigma_i S_j S'_k\ , \end{aligned}$$

- O(N) non-linear sigma models (Sine-Gordon equation and principal chiral model):

$$\mathscr{L} = -\,\mathrm{Tr}(J_\mu J^\mu)\ , \quad J_\mu = (\partial_\mu g) g^{-1}\ , \quad \mu = 0{,}1.$$

Perturbations on integrable systems

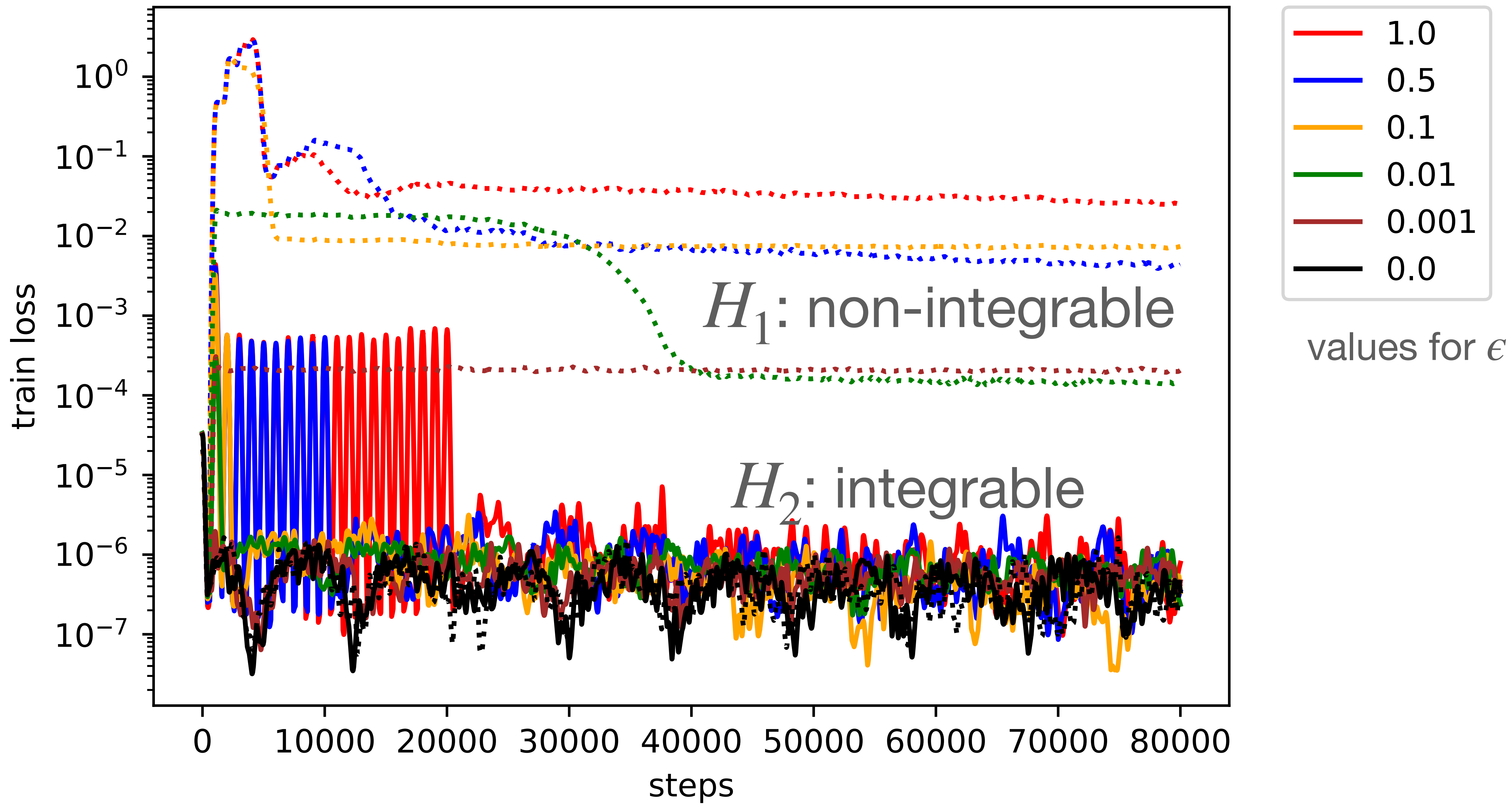
- Harmonic Oscillator:

$$H_0 = \frac{p_x^2 + p_y^2}{2m} + \omega^2 \left(q_x^2 + q_y^2 \right)$$

- Are the following perturbations integrable:

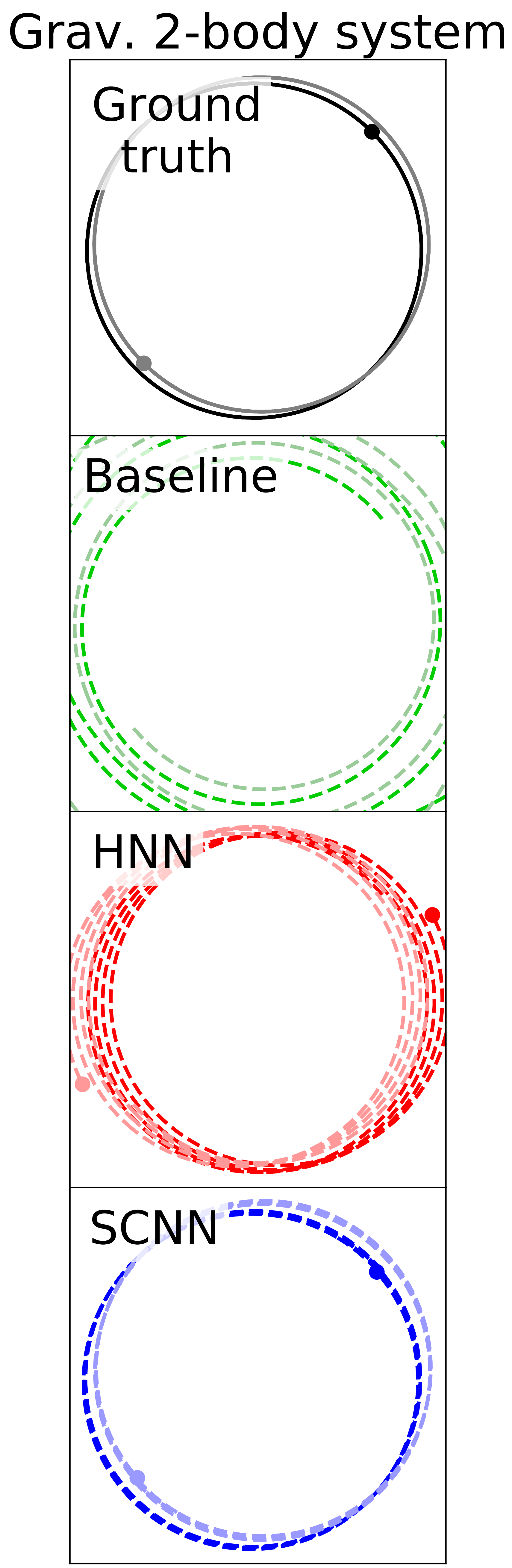
$$H_1 = \epsilon q_x^2 q_y^2, \quad H_2 = \epsilon q_x q_y$$

- Initialise network at known solution for unperturbed system and see how it reacts to samples from perturbed system



Conclusions and Outlook

Learning physics bias with ML



- Bias networks with physics knowledge for efficient results: (e.g. improving simulations with symmetry constraints)
- Finding the functional bias possible: Learning mathematical structures (e.g. metric, Hamiltonian, symmetries) is possible in an unsupervised way when “appropriate” loss functions can be identified:
  - Symmetries from embedding layer without prior knowledge
  - Symmetries from phase space samples
- Machinery for discovery of novel structures in integrability: Currently Lax pairs and connections for classical systems. Identify (some) integrable perturbations.

Thank you!

2104.14444: Simulations with Symmetry Control Neural Networks
2103.07475: Integrability
2003.13679: Symmetries from Embedding Layer

For talks at the interface of physics and ML: physicsmeetsml.org

Control via Symmetries

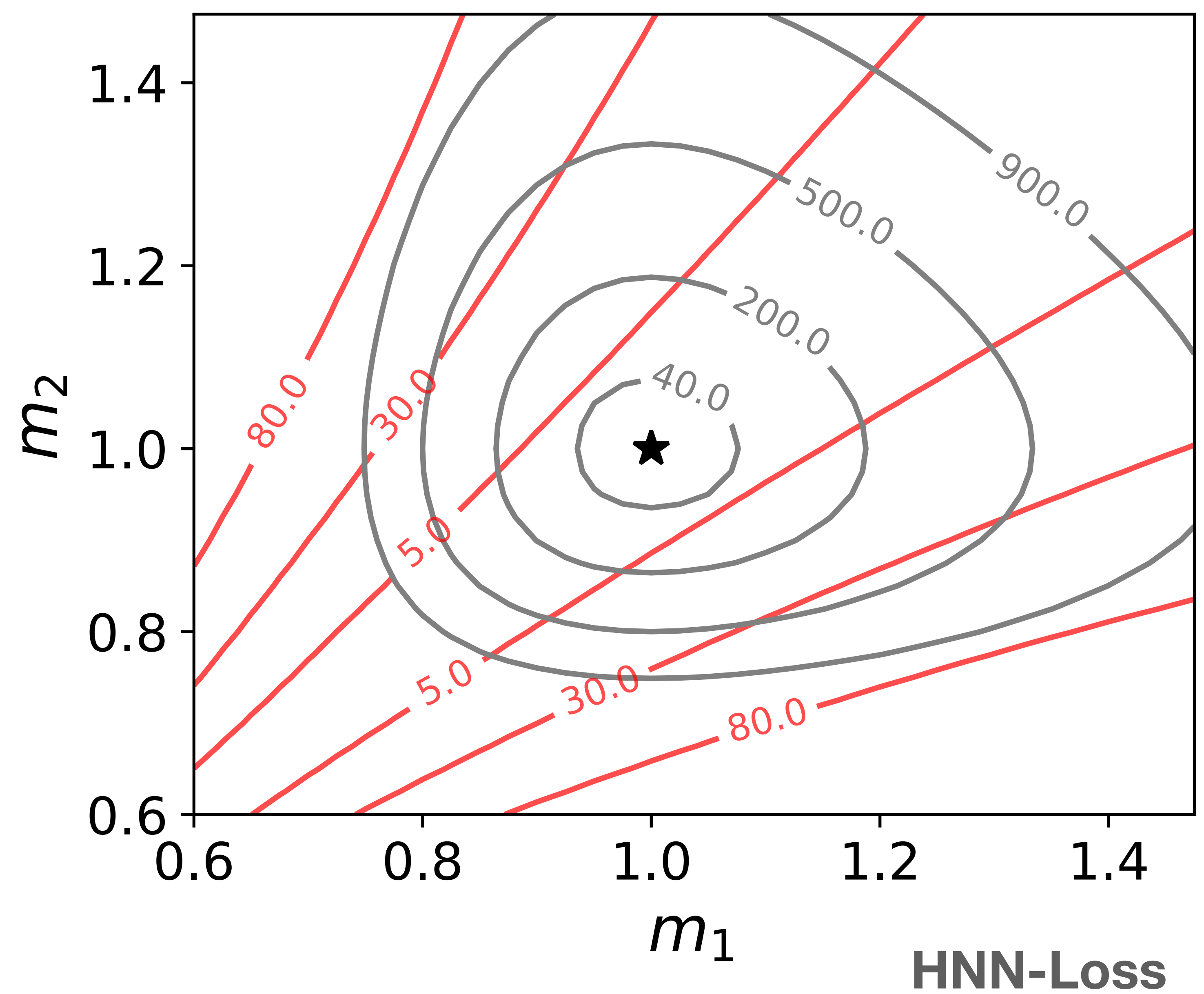
- Losses to ensure appropriate functional forms:

$$\mathscr{L}_{\text{HNN}} = \sum_{i=1}^{N\cdot d} \left\| \frac{\partial \mathscr{H}_\phi(\mathbf{P},\mathbf{Q})}{\partial p_i} - \frac{dq_i}{dt} \right\|_2 + \left\| \frac{\partial \mathscr{H}_\phi(\mathbf{P},\mathbf{Q})}{\partial q_i} + \frac{dp_i}{dt} \right\|_2$$

$$\mathscr{L}_{\text{Poisson}} = \sum_{i,j=1}^{N\cdot d} \left\| \{Q_i, P_j\} - \delta_{ij} \right\|_2 + \sum_{i,j>i}^{N\cdot d} \left\| \{P_i, P_j\} \right\|_2 + \left\| \{Q_i, Q_j\} \right\|_2$$

$$\mathscr{L}^{(n)}_{\text{HQP}} = \sum_{i=1}^{n} \left\| \frac{dP_i}{dt} \right\|_2 + \left\| \frac{dQ_i}{dt} - \frac{\partial \mathscr{H}_\phi(\mathbf{P},\mathbf{Q})}{\partial P_i} \right\|_2 + \beta \sum_{i=n+1}^{N\cdot d} \left\| \frac{dP_i}{dt} + \frac{\partial \mathscr{H}_\phi(\mathbf{P},\mathbf{Q})}{\partial Q_i} \right\|_2 + \left\| \frac{dQ_i}{dt} - \frac{\partial \mathscr{H}_\phi(\mathbf{P},\mathbf{Q})}{\partial P_i} \right\|_2$$

Effect of different loss components



HNN-Loss

Poisson-Loss

$\mathbf{p}, \mathbf{q}$ (Input) → $T_\psi(\mathbf{p},\mathbf{q})$: Canonical Transformation Network → $\mathbf{P}_{\text{cyclic}} = \text{const.}$; $\mathbf{P}_{\text{other}}, \mathbf{Q}_{\text{other}}$; $\mathbf{Q}_{\text{cyclic}}$ → $\mathscr{H}_\phi(\mathbf{P}_{\text{cyclic}}, \mathbf{P}_{\text{other}}, \mathbf{Q}_{\text{other}})$ Hamiltonian Network → $\dot{\mathbf{p}} = -\frac{\partial \mathscr{H}_\phi}{\partial \mathbf{q}}, \dot{\mathbf{q}} = \frac{\partial \mathscr{H}_\phi}{\partial \mathbf{p}}$ (Output)