Theoretical Physicists' Biases Meet Machine Learning

Using and finding functional bias in ML for mathematical physics systems

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

29.10.2021, IAIFI Colloquium

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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?

Content

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

I. Efficient solutions to PDEs (in mathematical physics) with ML

Key: Using domain knowledge/bias in ML ansatz

Example: Numerical Calabi-Yau metrics

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

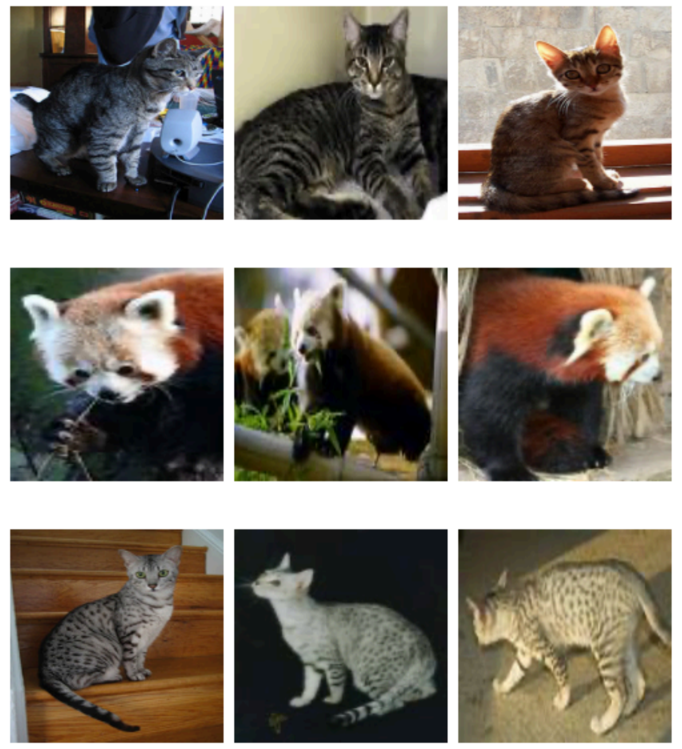
Why high-dimensional data? Large function space of possible solutions

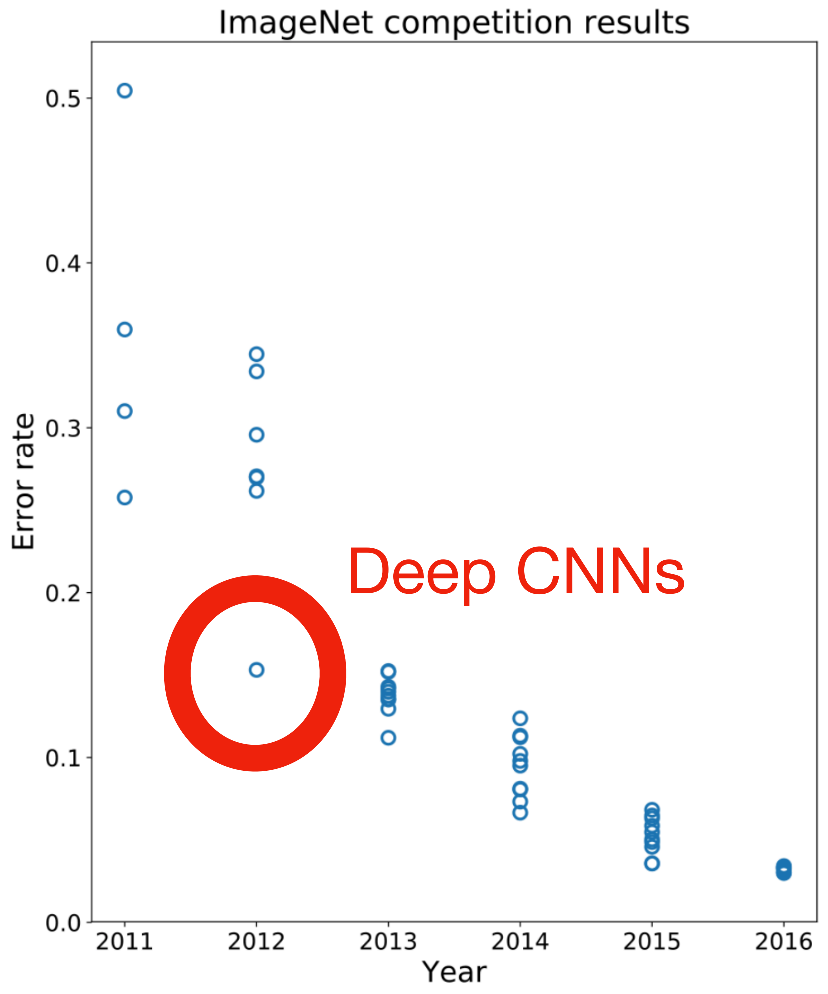
Why ML and physics?

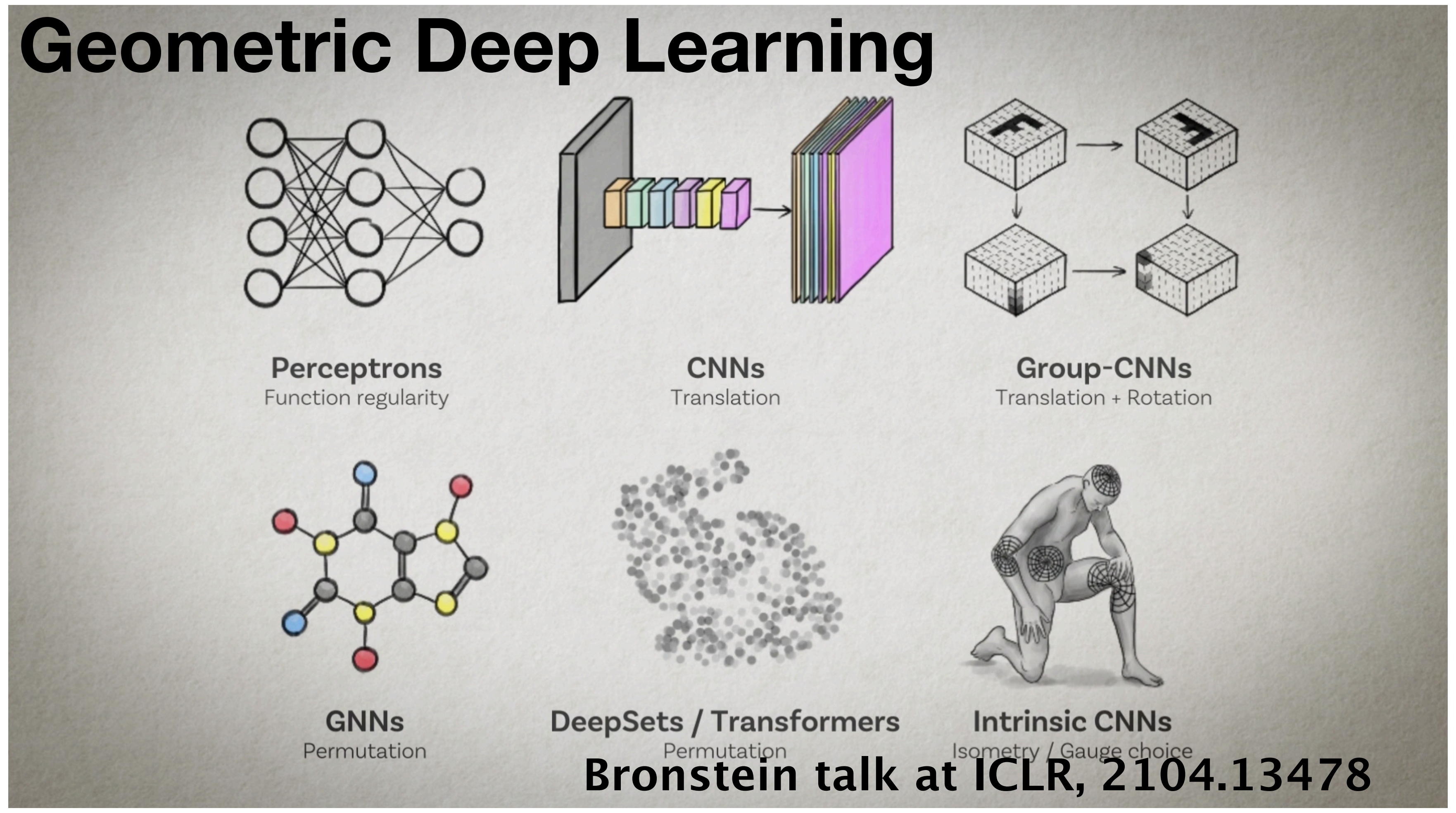
ML can overcome curses of dimensionality

- 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

Moduli dependent Calabi-Yau and SU(3)-structure metrics from Machine Learning

based on (2012.04656), in collaboration with:

Lara Anderson

Mathis Gerdes

James Gray

Nikhil Raghuram

Fabian Ruehle

Finding symmetries and integrable structures of physical systems

and based on (2104.14444, 2103.07475,
2003.13679, 2002.05169),
in collaboration with:

Philip Betzler

Marc Syvaeri

Dieter Lüst

How to improve our knowledge of EFTs in string theory with the metric (non-holomorphic quantities)?

Metrics with ML

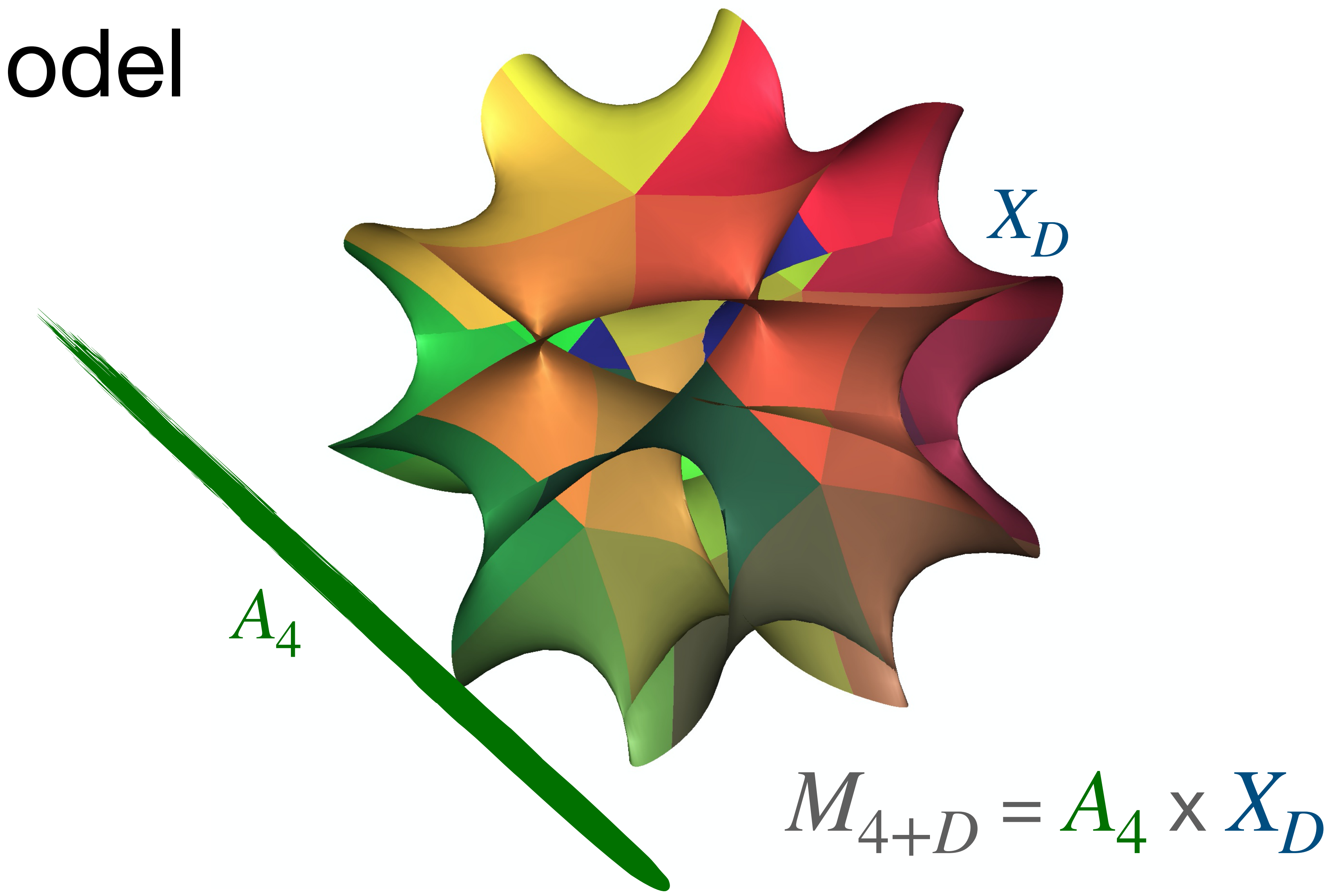
See also: Douglas et al 2012.04797, and Jejjala et al 2012.15821

Metrics matter

- The metric is key in any extra-dimensional physics model

$$S = \int_{M_{4+D}} d^{4+D}x \sqrt{-\det g_{4+D}}\; R(g_{4+D})$$

combined metric



- String compactifications are no exception to this. For instance:
  1. Matter kinetic terms (soft-terms, cf. 0906.3297)
  2. Moduli potential (D3-brane inflation [probing directly CY-moduli space])
  3. Massive string spectrum

Signatures of Quantum Gravity

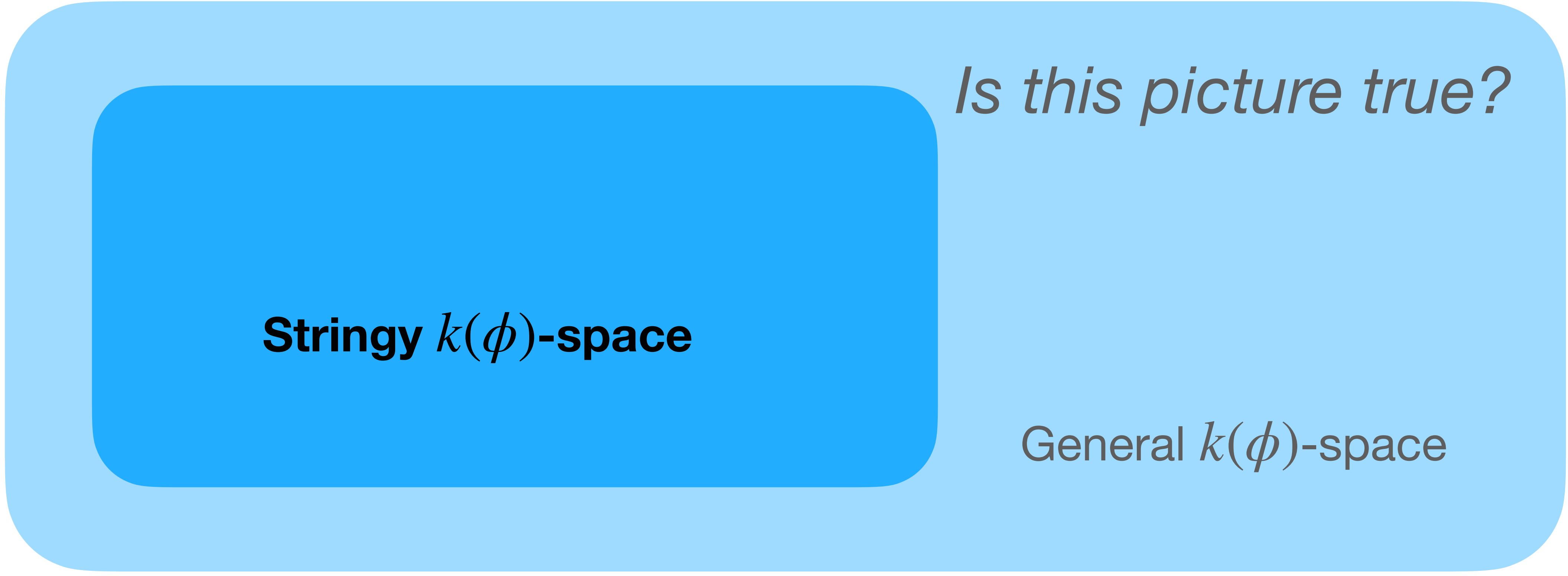
Metrics in the EFT

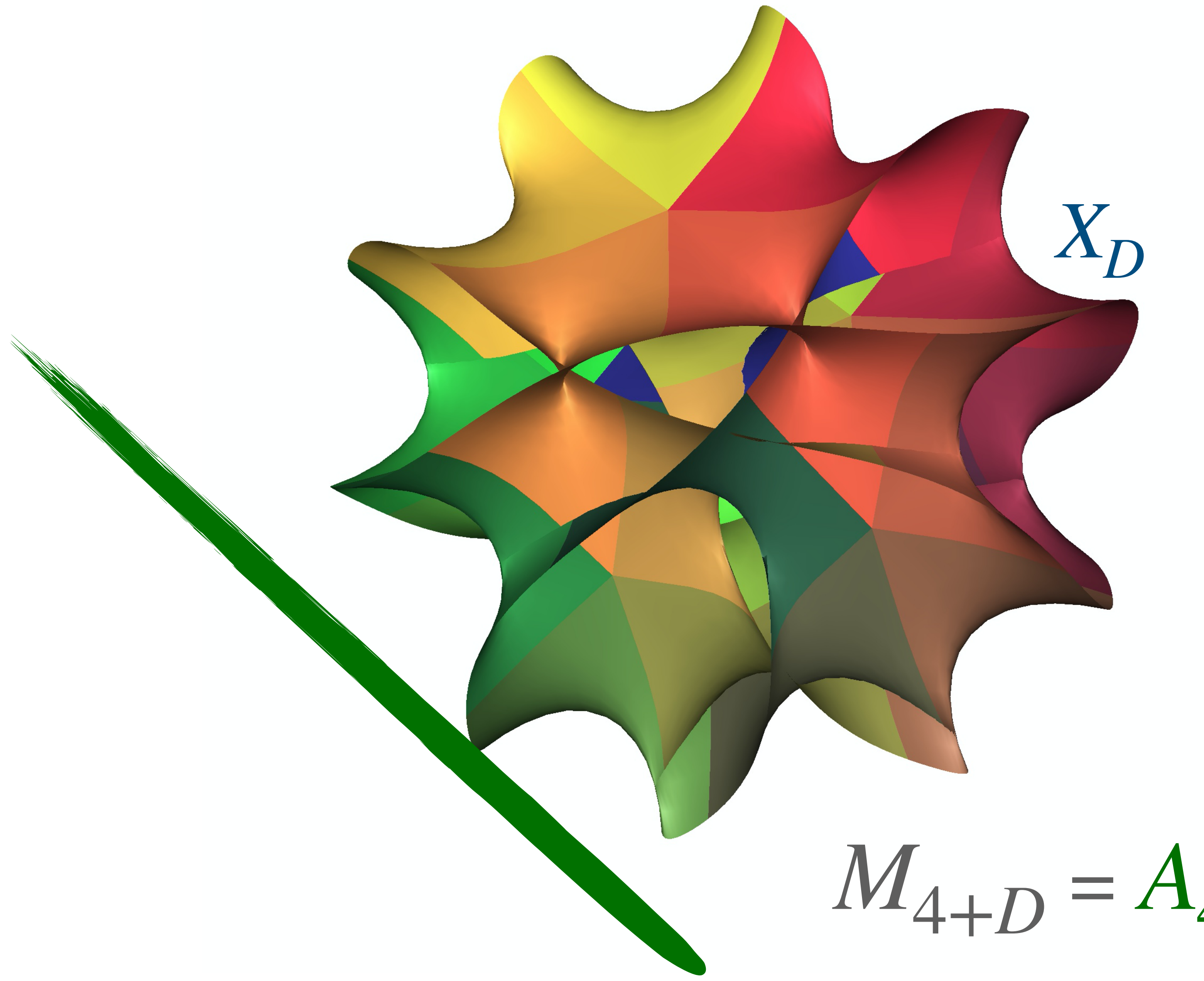
How to distinguish these signatures from some bottom-up BSM model?

Characteristic features in the EFTs of theories with extra dimensions?

$$\mathscr{L}_{\text{moduli}} = k(\phi)(\partial\phi)^2 + V(\phi)$$

Understand the string theory EFT better





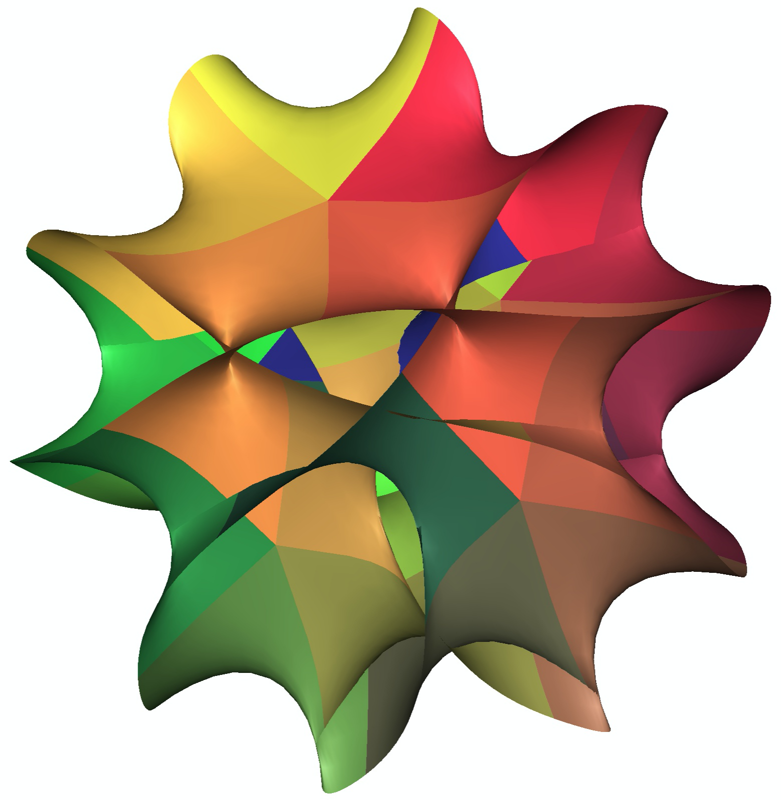
$$M_{4+D} = A_4 \times X_D$$

$$S = \int_{M_{4+D}} d^{4+D}x \sqrt{-\det g_{4+D}}\; R(g_{4+D})$$

combined metric

Which Metrics?

6D metrics relevant for string theory



- String Theory EOM for 4D $\mathcal{N} = 1$ Minkowski vacua require a Ricci-flat Kähler metric (Candelas, Horowitz, Strominger, Witten 1985)
- Which compact spaces do exist with a Ricci-flat Kähler metric?

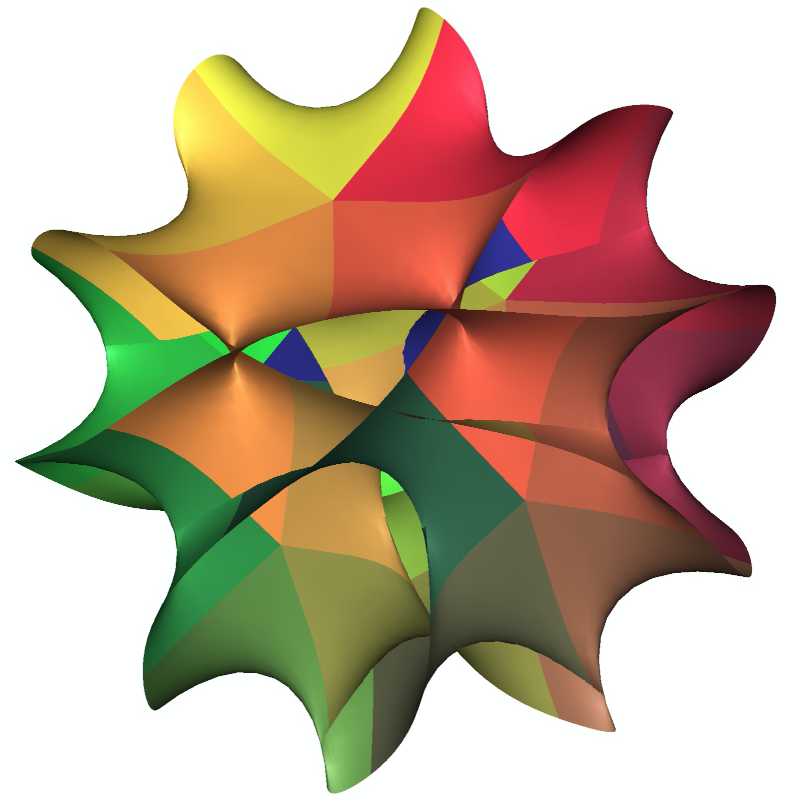
  Calabi-Yau manifolds
  (Example today: Quintic hypersurface in $\mathbb{P}^4$)

- Yau (1977) showed the existence of such a unique Ricci-flat Kähler metric, but without explicit constructions.
- One definition of CY-threefold: complex threefold admitting a nowhere vanishing real two-form J, and a complex three form Ω such that:

$$J \wedge \Omega = 0, \; J \wedge J \wedge J = \frac{3i}{4} \Omega \wedge \bar{\Omega}, \; dJ = 0, \; d\Omega = 0$$

Which Metrics?

6D metrics relevant for string theory



- The metric is given as $ig_{a\bar{b}} = J_{a\bar{b}}$
- Simplest examples: complete intersection manifolds in projective spaces
- Quintic hypersurface in $\mathbb{P}^4$:

$$p_\psi(\vec{z}) = \sum_{i=0}^{d+1} z_i^{d+2} + \psi \prod_{i=0}^{d+1} z_i = 0$$

- Holomorphic (3,0) form (Candelas et al):

$$\Omega = \frac{1}{\partial p_\psi(\vec{z})/\partial z_b} \bigwedge_{\substack{c=1,\ldots,d \\ c \neq a,b}} dz_c \qquad \text{on patch with } (z_a = 1)$$

Quintic hypersurface in $\mathbb{P}^4$:

$$p_\psi(\vec{z}) = \sum_{i=0}^{d+1} z_i^{d+2} + \psi \prod_{i=0}^{d+1} z_i = 0$$

Algebraic metrics:

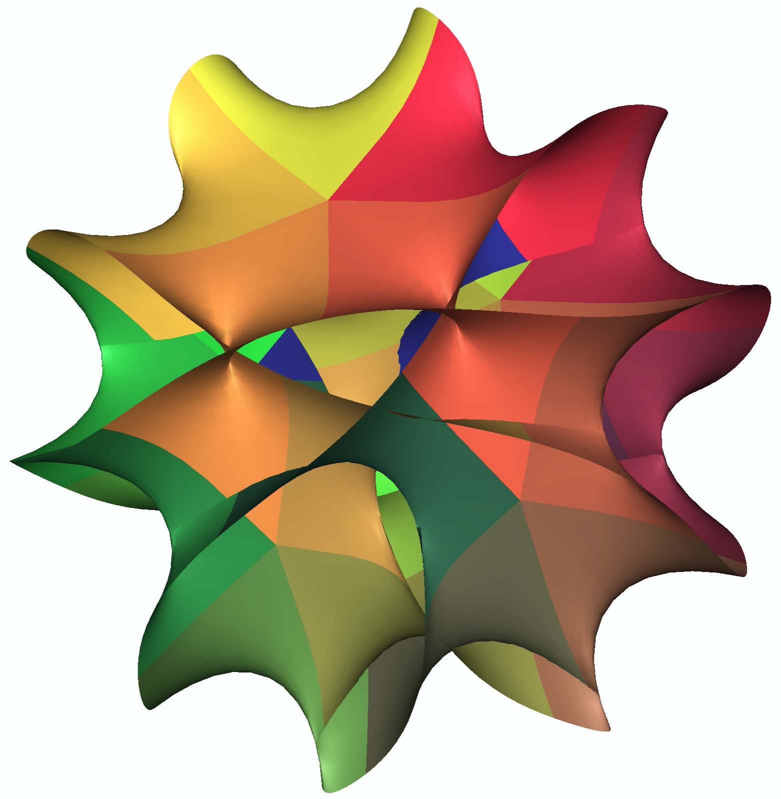
$$K = 1/2\pi \ln(\mathbf{k})$$

$$\mathbf{k} = \sum_{\alpha,\bar{\beta}=0}^{N_k} s_\alpha(\vec{z})\ H_{\alpha\bar{\beta}}\ \bar{s}_{\bar{\beta}}(\bar{\vec{z}})$$

$$g_{a\bar{b}} = \partial_a \bar{\partial}_{\bar{b}} K = \frac{1}{2\pi} \frac{\mathbf{k}\mathbf{k}_{a\bar{b}} - \mathbf{k}_a \mathbf{k}_{\bar{b}}}{\mathbf{k}^2}$$

Which Metrics?

Functional bias: algebraic metrics



- Idea: Generalised Fubini Study metrics can approximate the metric of our choice

$$K = 1/2\pi \ln(\mathbf{k}), \;\; \mathbf{k} = \sum_{\alpha,\bar{\beta}=0}^{N_k} s_\alpha(\vec{z}) \; H_{\alpha\bar{\beta}} \; \bar{s}_{\bar{\beta}}(\bar{\vec{z}})$$

$$g_{a\bar{b}} = \partial_a \bar{\partial}_{\bar{b}} K = \frac{1}{2\pi} \frac{\mathbf{k}\mathbf{k}_{a\bar{b}} - \mathbf{k}_a \mathbf{k}_{\bar{b}}}{\mathbf{k}^2}$$

- Embedding into larger projective space (Kodaira embedding): $s_\alpha(\vec{z})$ polynomials in z_a.
- These metrics provide "basis" of Kähler metrics on X. (Tian: such Kähler potentials are dense in the space of Kähler potentials)

Quintic hypersurface in $\mathbb{P}^4$:

$$p_\psi(\vec{z}) = \sum_{i=0}^{d+1} z_i^{d+2} + \psi \prod_{i=0}^{d+1} z_i = 0$$

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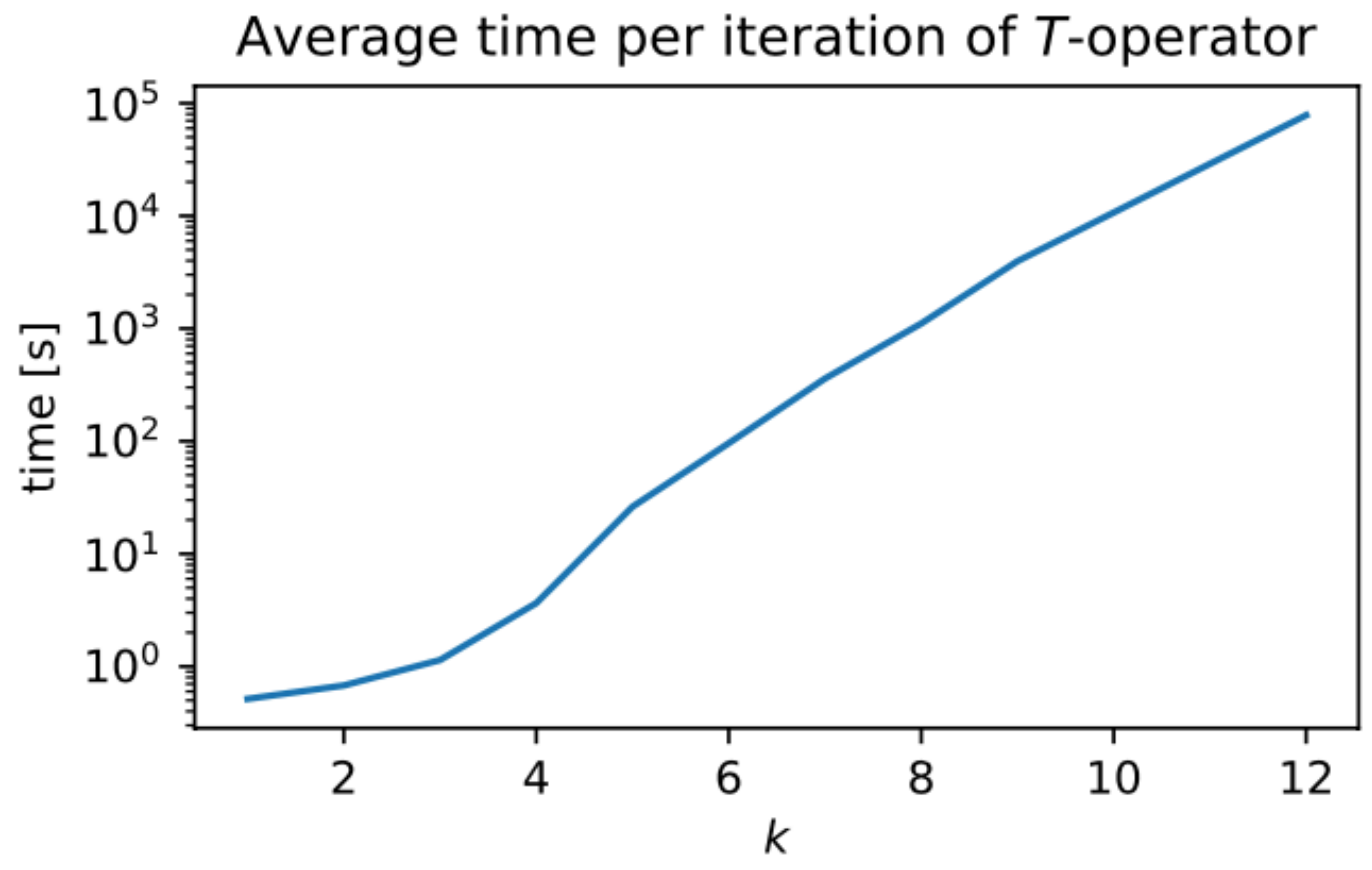
Metrics are hard without ML

6D metrics relevant for string theory

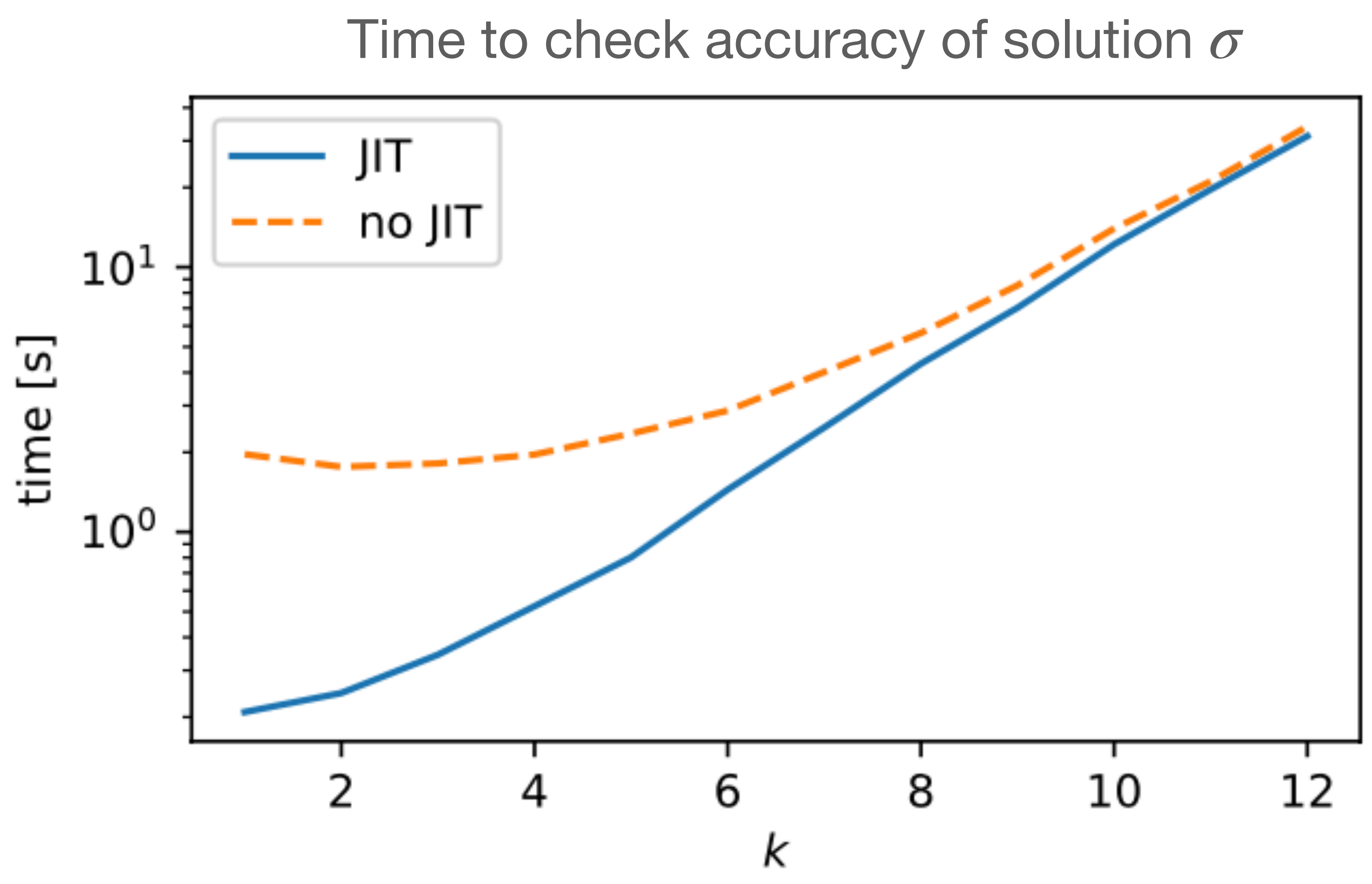
- Finite distance methods "fail" (Headrick, Wiseman 2009)
- Spectral methods simplify, but they are currently inefficient:
    1. Single point in moduli space
    2. High accuracies become expensive

  (Donaldson, Braun, Belidze, Douglas, Ovrut, Karp, Cui, Gray, Lukic, Ashmore, He; Kachru, Tripathy, Zimet; Headrick and Nasar)

- How about non-Kähler solutions?
- Target on a practical level: metric with reasonable accuracy for one string compactification ~ O(1 day) [impossible with non ML algorithms]



k ~ accuracy of spectral resolution



Can Machine Learning help?

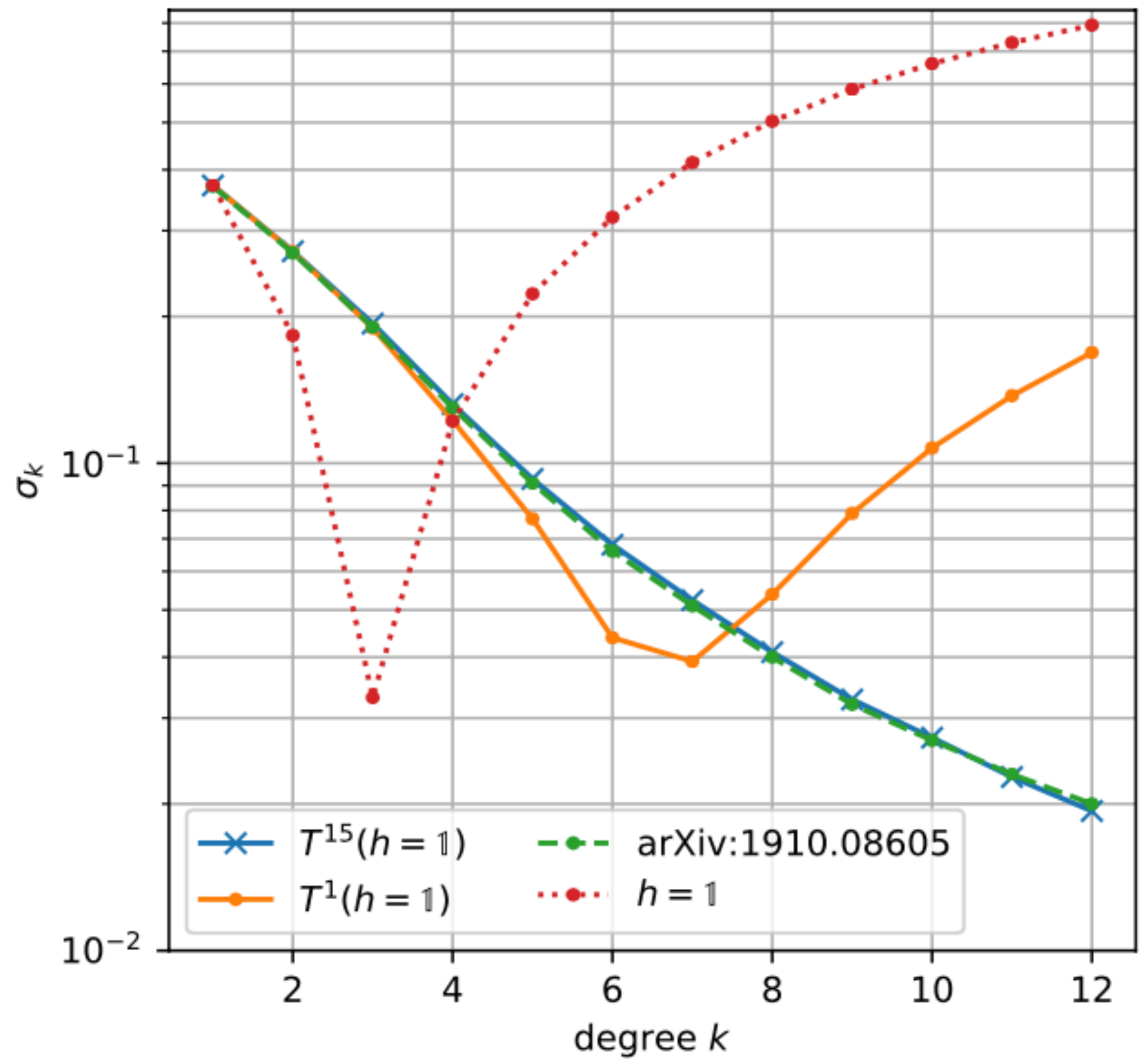
Which metric?

What is the optimisation problem

$$J \wedge J \wedge J \sim \det g$$

$$\Omega = \frac{1}{\partial p_\psi(\vec{z})/\partial z_b} \bigwedge_{\substack{c=1,\dots,d \\ c \neq a,b}} dz_c$$

Monge-Ampere Loss (different metrics)



1. Ricci-flatness: (Induced FS is not Ricci-flat):

   Ricci tensor: $R_{i\bar{j}} = -\partial_i \bar{\partial}_{\bar{j}} \log \det g$

   Cheaper alternative (less derivatives) via Monge-Ampere equation:

$$J \wedge J \wedge J = \kappa\, \Omega \wedge \bar{\Omega} \qquad \rightarrow \quad \mathscr{L}_{\mathrm{MA}} = \frac{1}{\int_X \Omega \wedge \bar{\Omega}} \int_X \left| 1 - \frac{1}{\kappa} \frac{J^3}{\Omega \wedge \bar{\Omega}} \right|$$

2. Kählerity:

$$dJ = 0 \quad \leftrightarrow \quad g_{i\bar{j},k}\, dz_i \wedge d\bar{z}_{\bar{j}} \wedge dz_k = 0 = g_{i\bar{j},\bar{k}}\, dz_i \wedge d\bar{z}_{\bar{j}} \wedge d\bar{z}_{\bar{k}}$$

$$c_{ijk} = g_{i\bar{j},k} - g_{k\bar{j},i} = 0 \qquad \rightarrow \quad \mathscr{L}_{\mathrm{dJ}} = \sum_{i,j,k} ||\mathrm{Re}(c_{ijk})||_n + ||\mathrm{Im}(c_{ijk})||_n$$

3. Well defined across different coordinate patches:

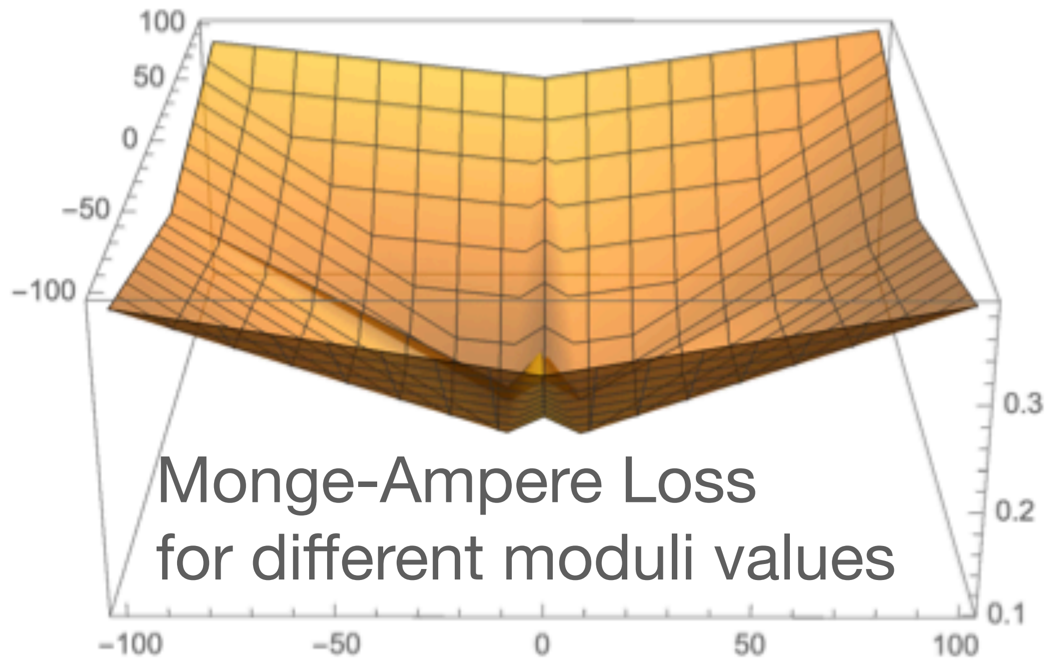
$$g^{(j)} = T_{ij} \cdot g^{(i)} \cdot T_{ij}^\dagger, \quad T_{ij} = \partial \vec{z}^{(i)} / \partial \vec{z}^{(j)} \quad \rightarrow \quad \mathscr{L}_{\text{Transition}} = \frac{1}{d} \sum_{k,j} \left|\left| g_{\mathrm{NN}}^{(k)}(\vec{z}) - T_{jk}(\vec{z}) \cdot g_{\mathrm{NN}}^{(j)}(\vec{z}) \cdot T_{jk}^\dagger(\bar{\vec{z}}) \right|\right|_n$$

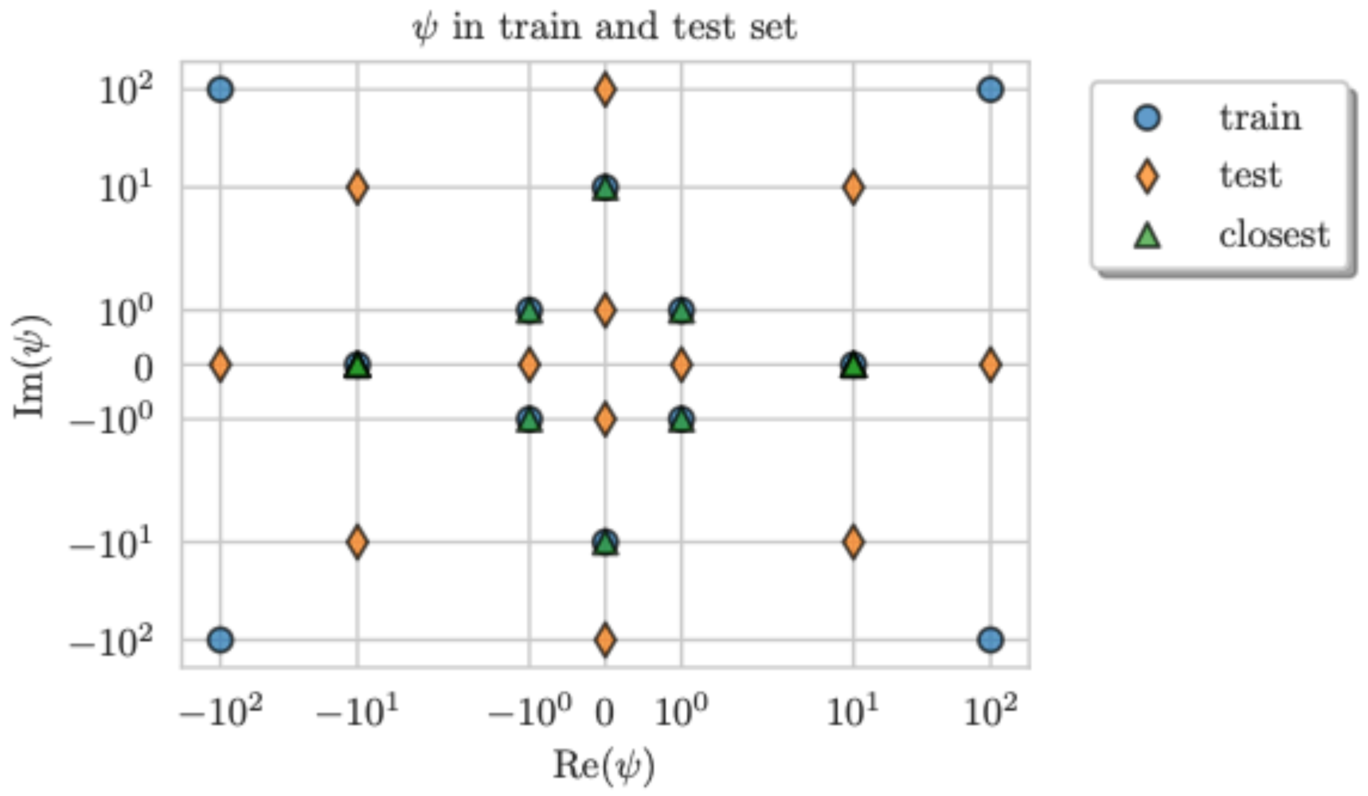
Our experiments

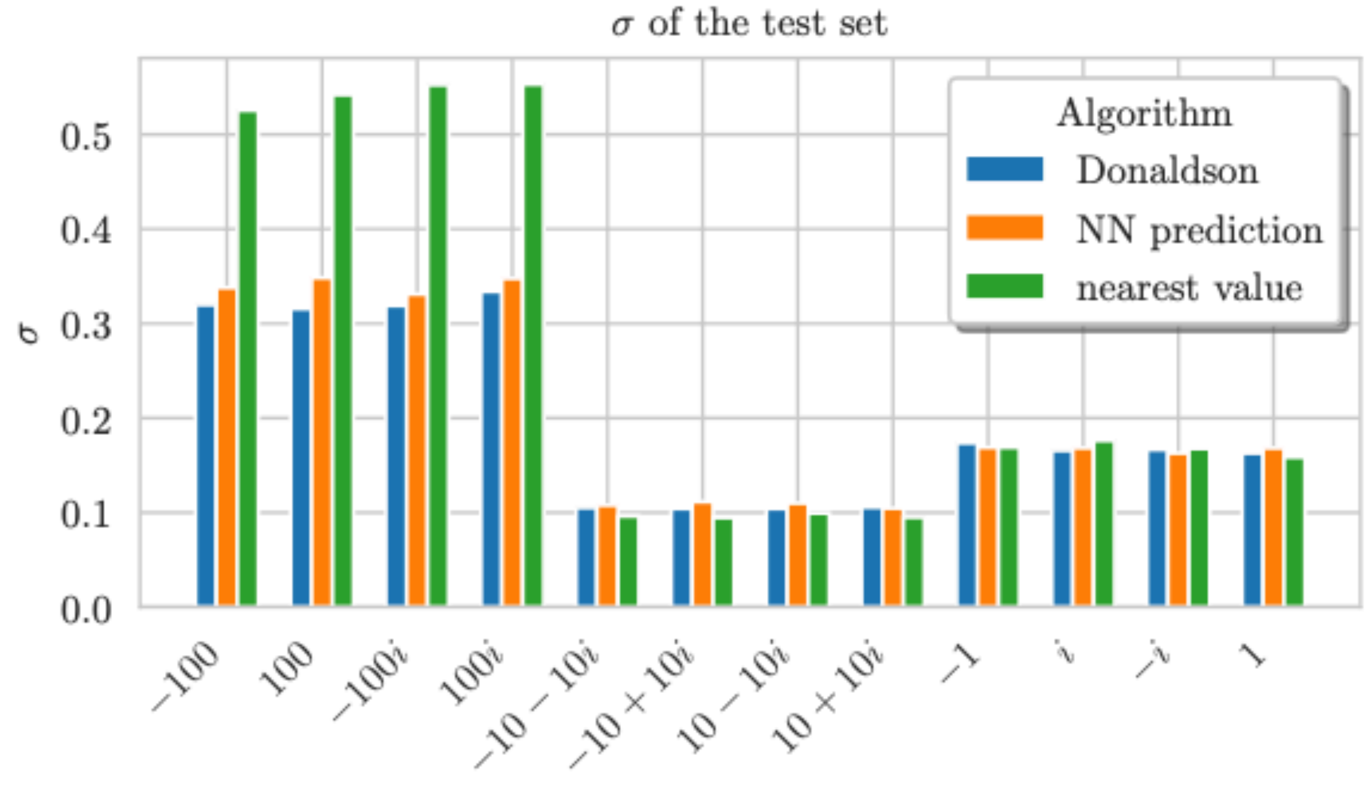
Overview on what we get to work

- Supervised learning of Kähler potential (data from running spectral algorithms)
  Improvement: moduli dependence of metric
- Unsupervised learning of Kähler potential (using energy functionals measuring deviation from Ricci-flatness)
  Improvement: moduli dependence of metric and efficiency (no running of spectral methods)
- Unsupervised learning of metric directly (perturbation of Fubini study metric)
- Metric networks to go beyond Calabi-Yau: here SU(3) structure manifolds, i.e. more general string backgrounds

Supervised Learning of Metrics:



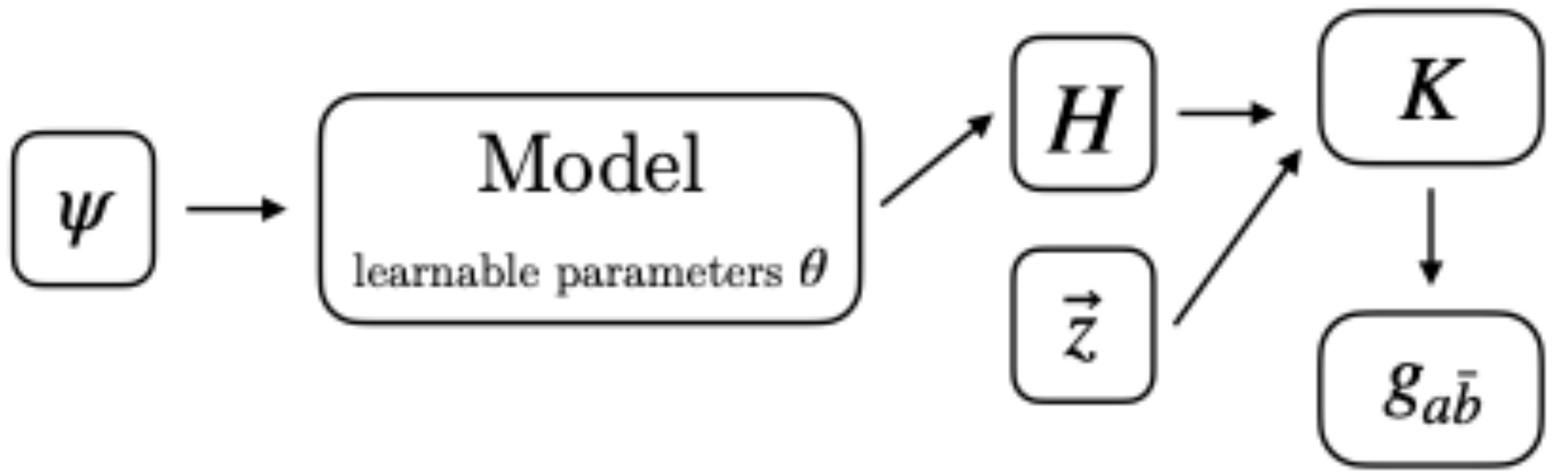




Improved results outside training domain

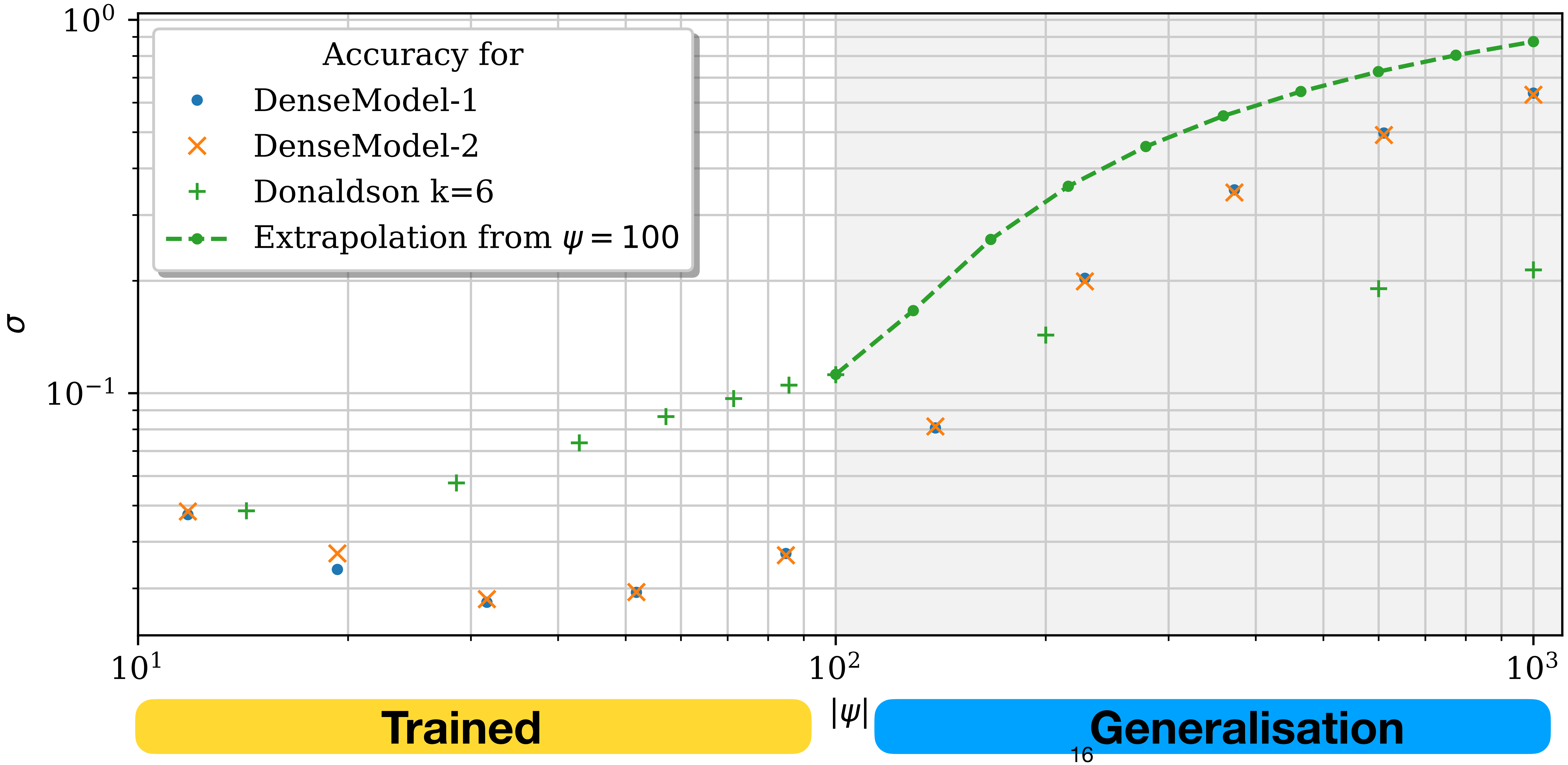
Learning H

Optimising with σ (no Donaldson)



- k=6 (42025 components in H), sampling fast and always using new points

$$\sigma = \frac{1}{\int_X \Omega \wedge \bar{\Omega}} \int_X \left| 1 - \frac{1}{\kappa} \frac{J^3}{\Omega \wedge \bar{\Omega}} \right|$$



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Quintic hypersurface in $\mathbb{P}^4$:

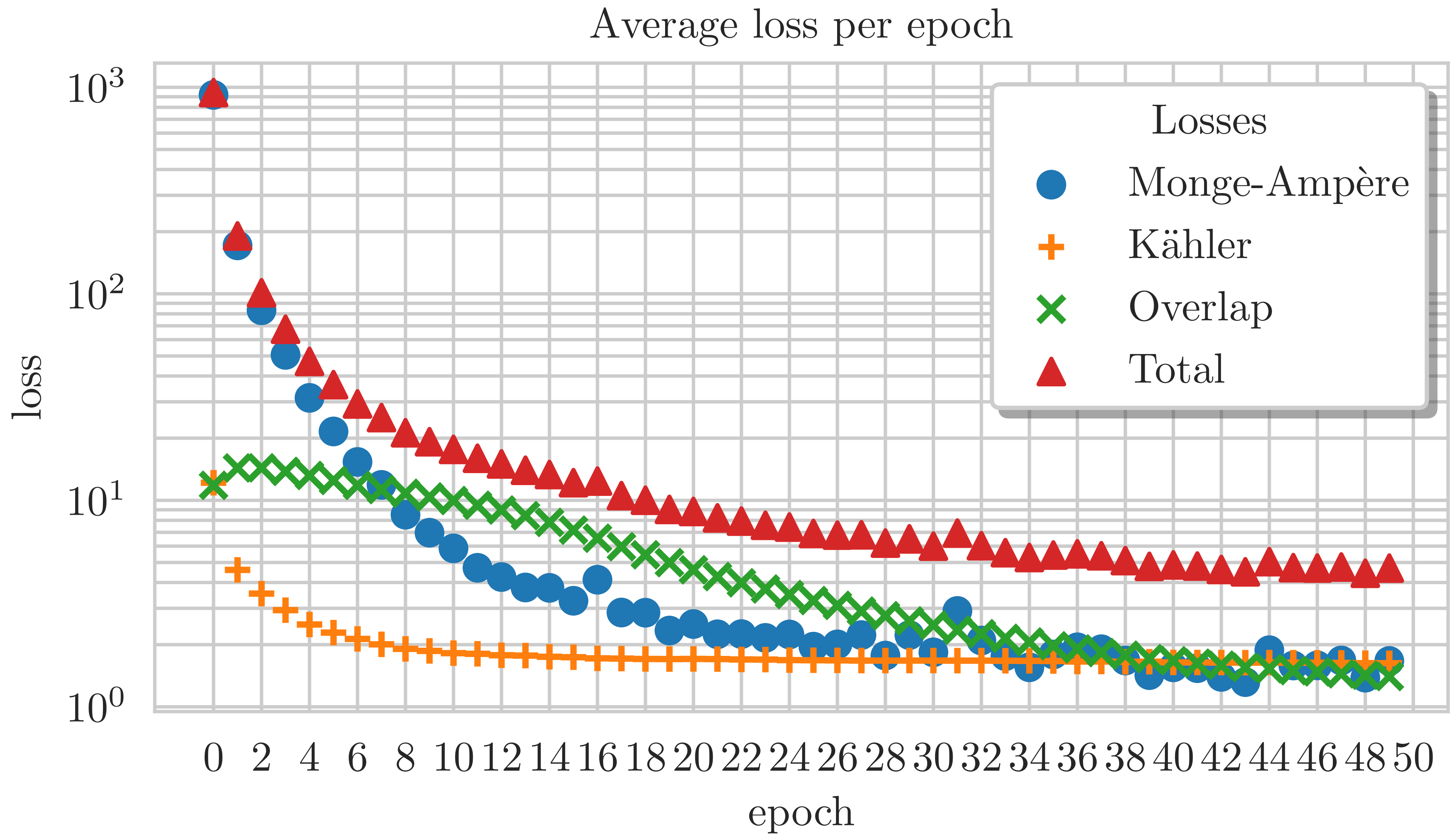
$$p_\psi(\vec{z}) = \sum_{i=0}^{d+1} z_i^{d+2} + \psi \prod_{i=0}^{d+1} z_i = 0$$

Beyond Calabi-Yau Metrics with ML

Anderson, Gerdes, Gray, Krippendorf, Raghuram, Ruehle 2020

- Approach of learning metric directly allows to search for metrics with different properties
- Philosophy: modified loss functions, additionally learned outputs.
- Augment the landscape of metrics to G2 and SU(3) structure manifolds? Phenomenologically necessary, otherwise missing large parts of string theory constructions; unexplored mathematical structures.
- Example SU(3) structure manifolds (simple example works)

modification of loss: $dJ(g) = 0 \rightarrow dJ(g) = W_4 \wedge J(g)$



	Donaldson, Headrick & Nassar	Kähler potential	Metric Directly
Fixed point in Moduli Space	✔	✔	✔
Moduli Dependence	✗ (interpolation)	✔	✔
Non Kähler	✗	✗	✔
Analytic	✗	✗	✗

Neural networks for differential equations

Going beyond CY metrics

- Can NN give efficient approximations to PDE solutions?
- Motivation beyond universal approximation scheme (NN can be shown to give good and accurate predictions to PDEs):
  - Solutions to high-dimensional Schrödinger equations (Rupp, Tkatchenko, Müller, von Lilienfeld 2012, …)
  - Black-Scholes PDE (Grohs, Hornung, Jentzen, von Wurstemberger 2018, …)
  - Approximation rates of NNs to solutions of PDEs (Kutyniok, Petersen, Raslan, Schneider 2019, …)
  - SimDL workshop at ICLR 2021

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	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

PNAS July 10, 2018 115 (28) E6411-E6417; first published June 26, 2018; https://doi.org/10.1073/pnas.1801181115

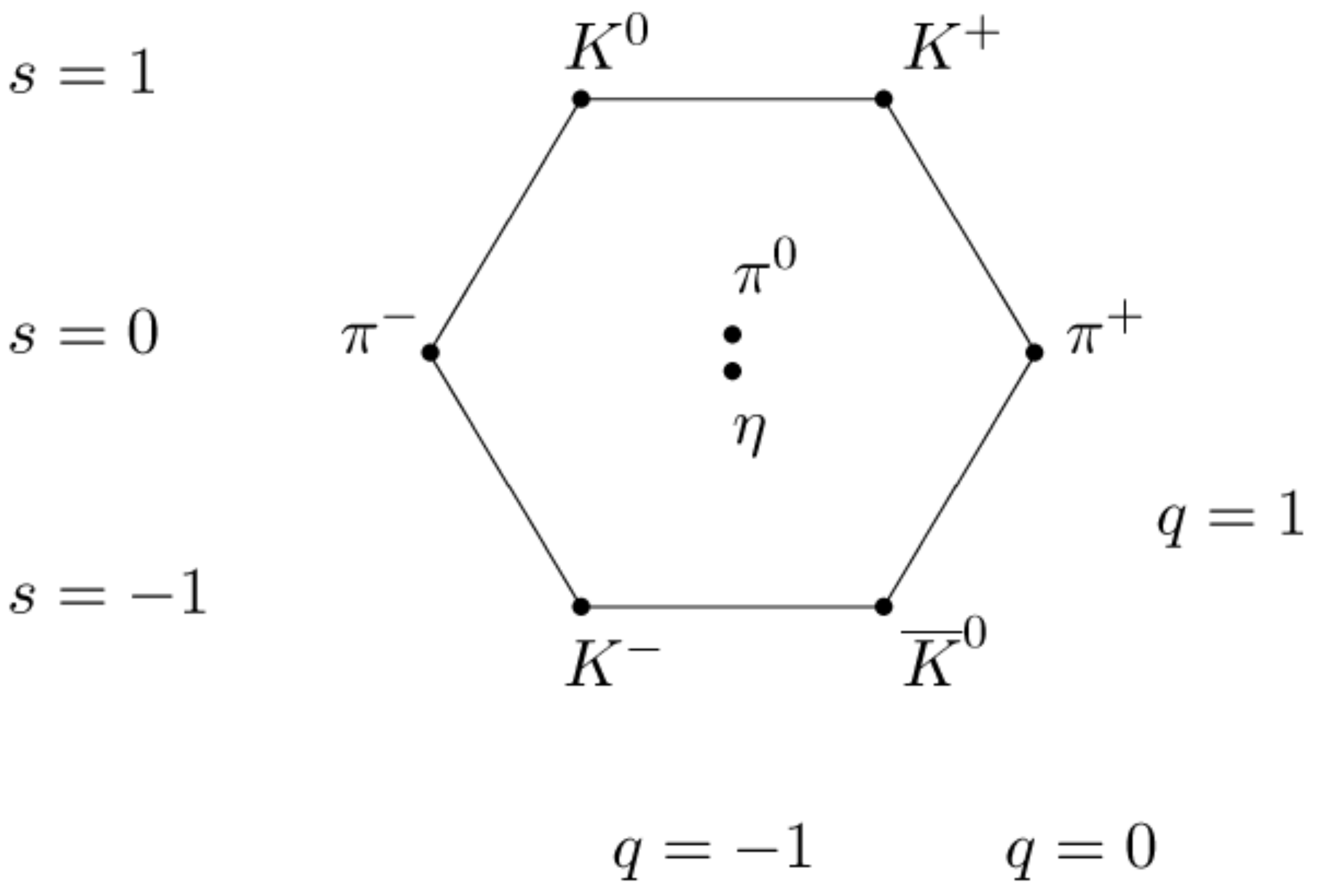
Contributed by Shou-Cheng Zhang, June 4, 2018 (sent for review February 2, 2018; reviewed by Xi Dai and Stuart P. Parkin)

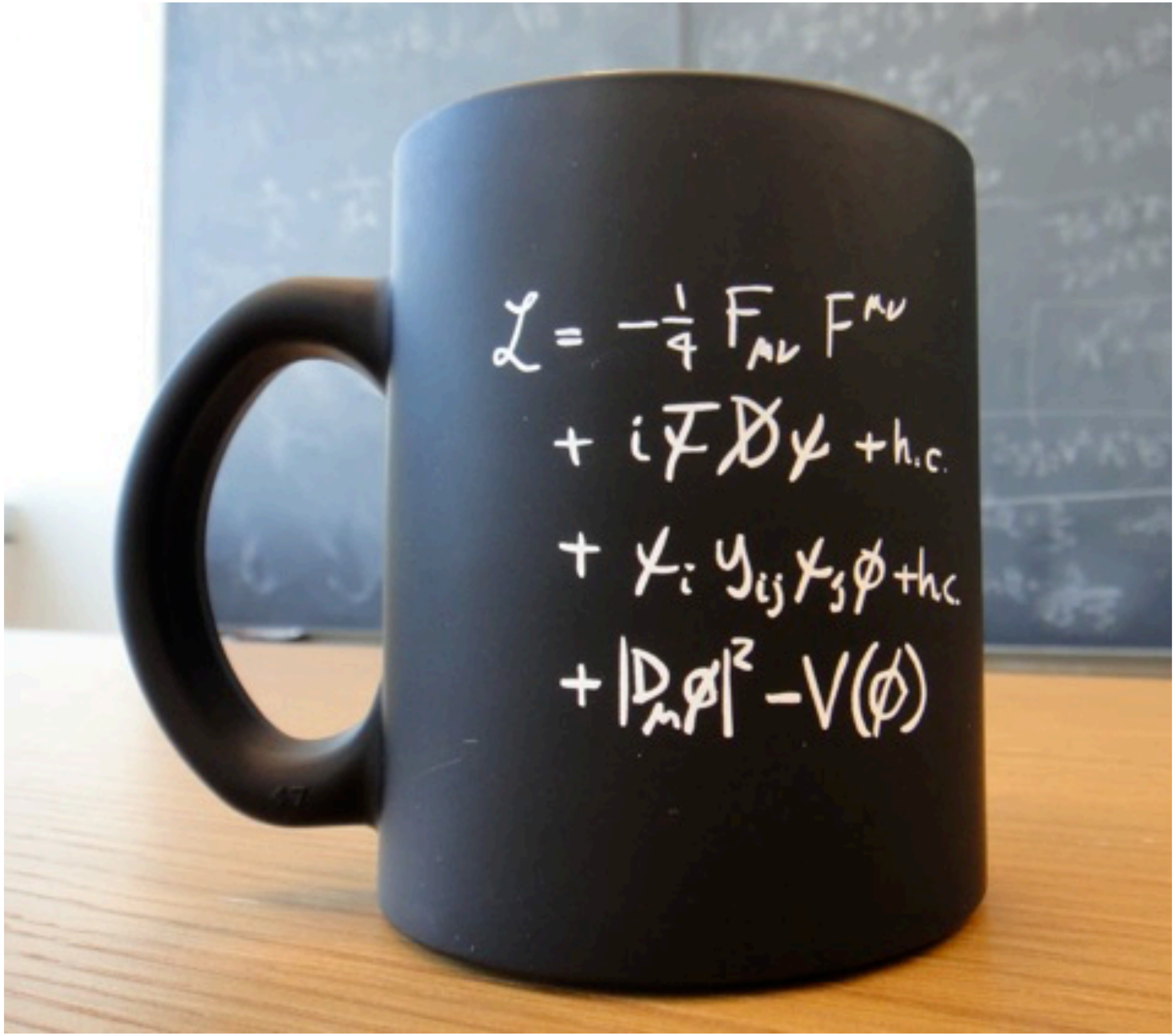
Article | Figures & SI | Info & Metrics | PDF

Significance

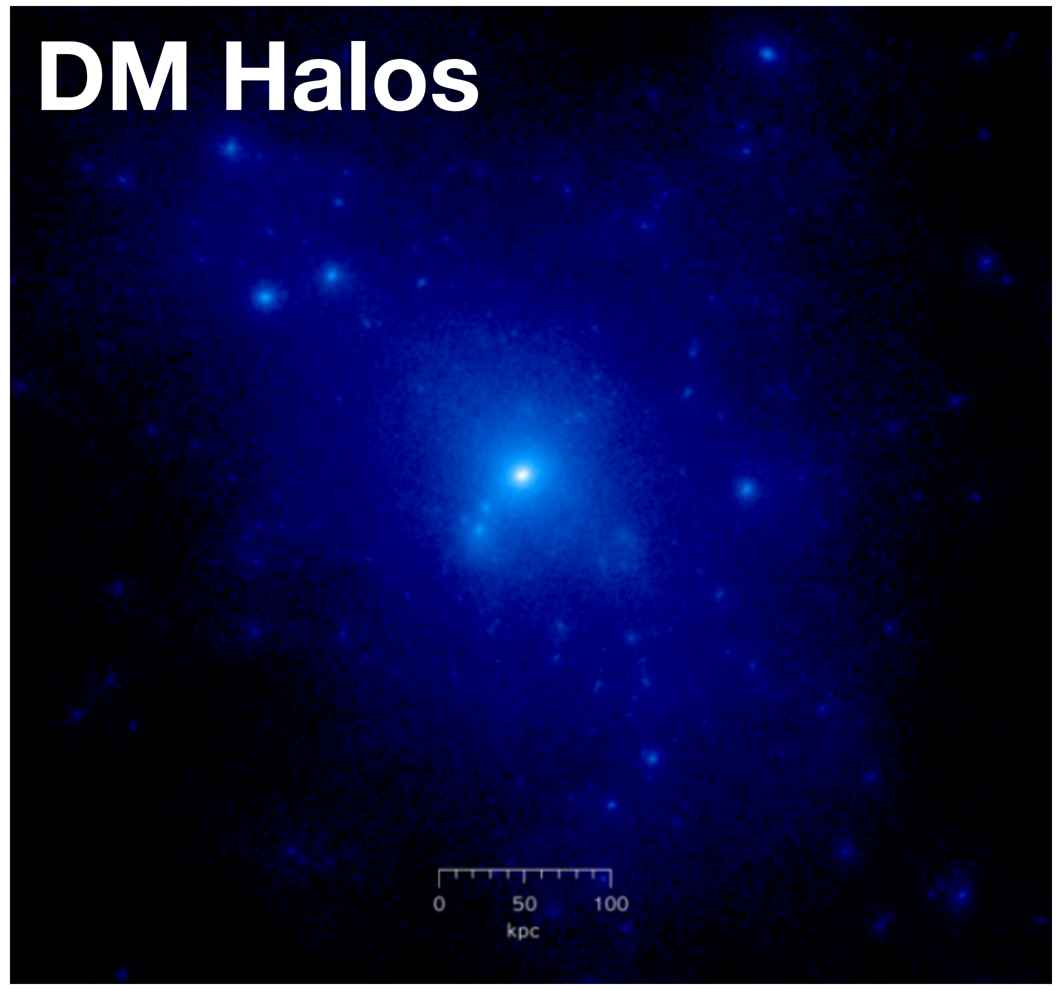
Motivated by the recent achievements of artificial intelligence (AI) in linguistics, we design AI to learn properties of atoms from materials data on its own. Our work realizes knowledge representation of atoms via computers and could serve as a foundational step toward materials discovery and design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

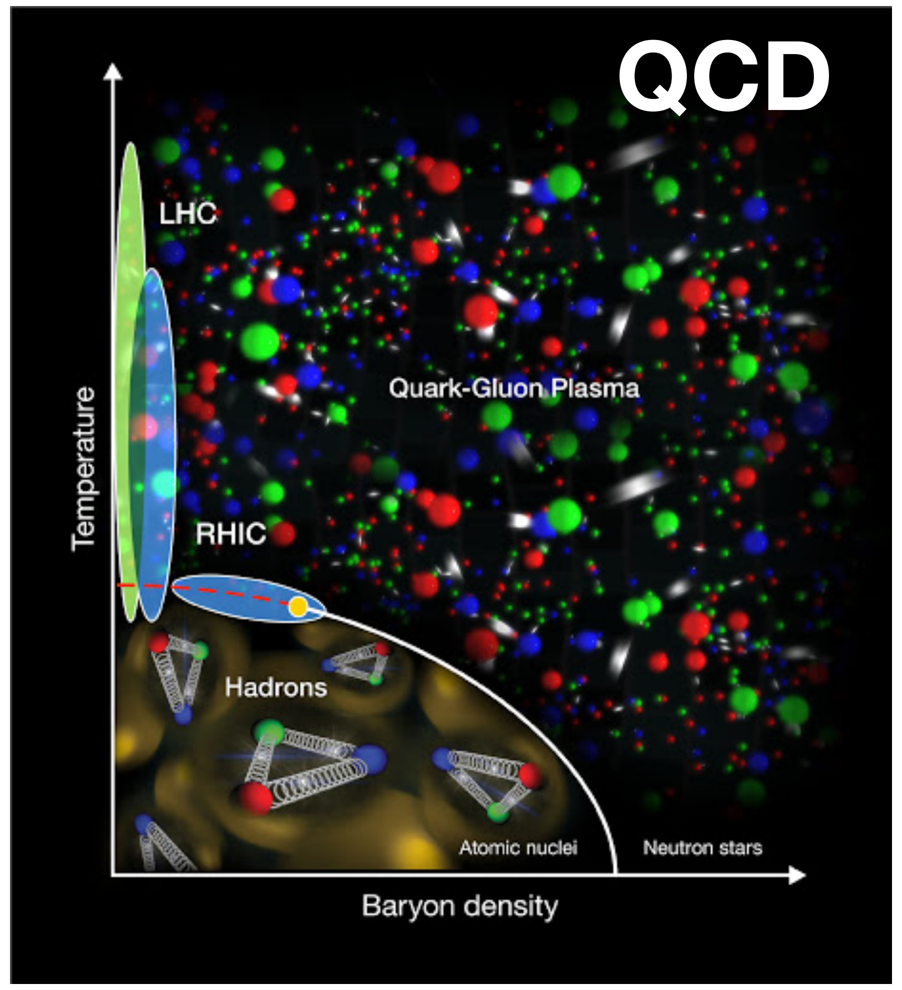
In Particle Physics pre ~ 60s/70s?



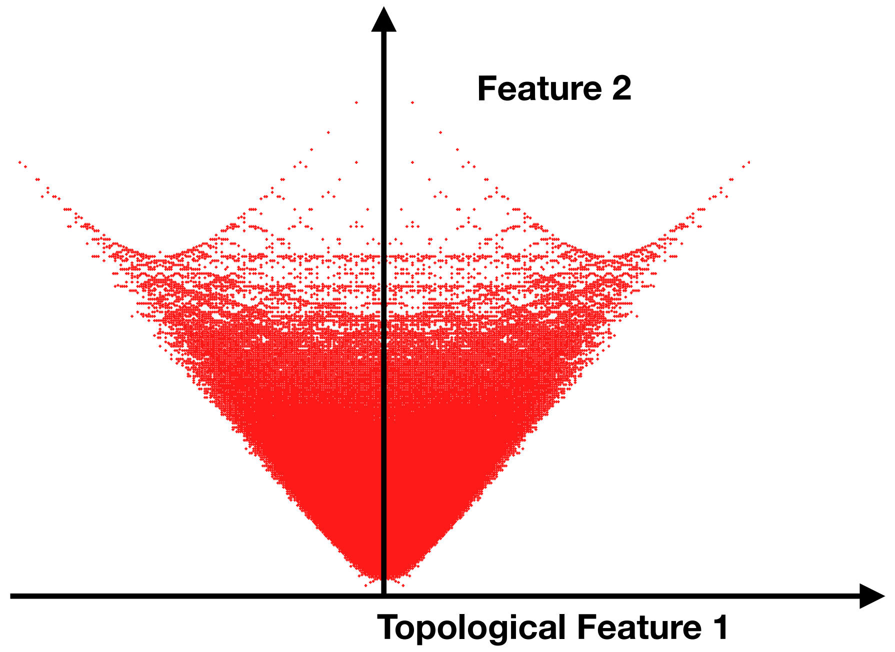


Which tools do we need to make such discoveries with ML in the 2020s?

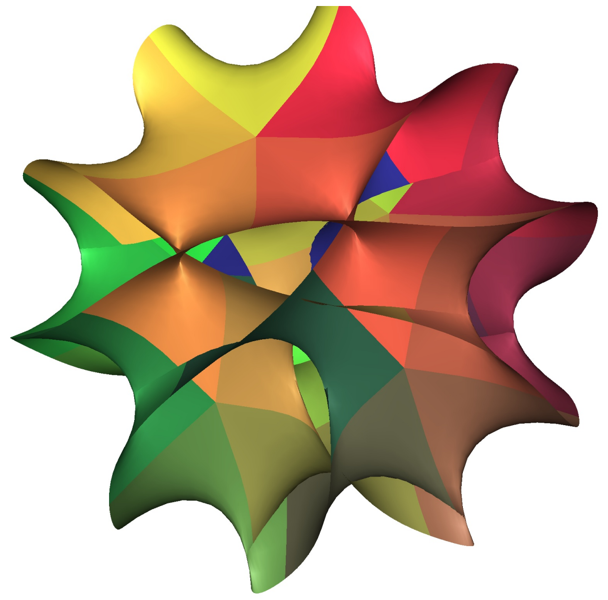




Pattern in Calabi-Yau data



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

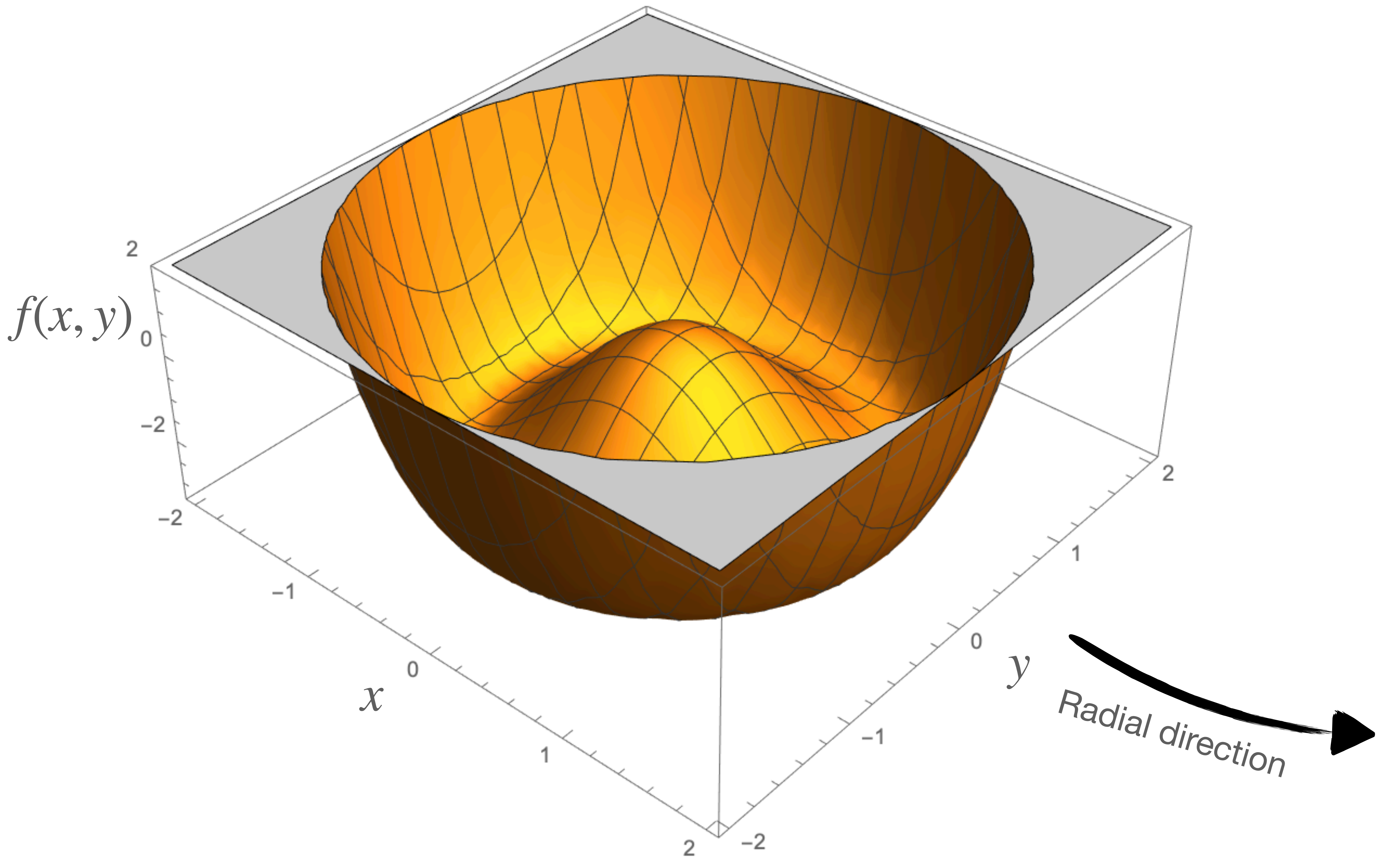
Symmetries from embedding layer

Krippendorf, Syvaeri 2020

Krippendorf, Syvaeri 2020

How to search for symmetries?

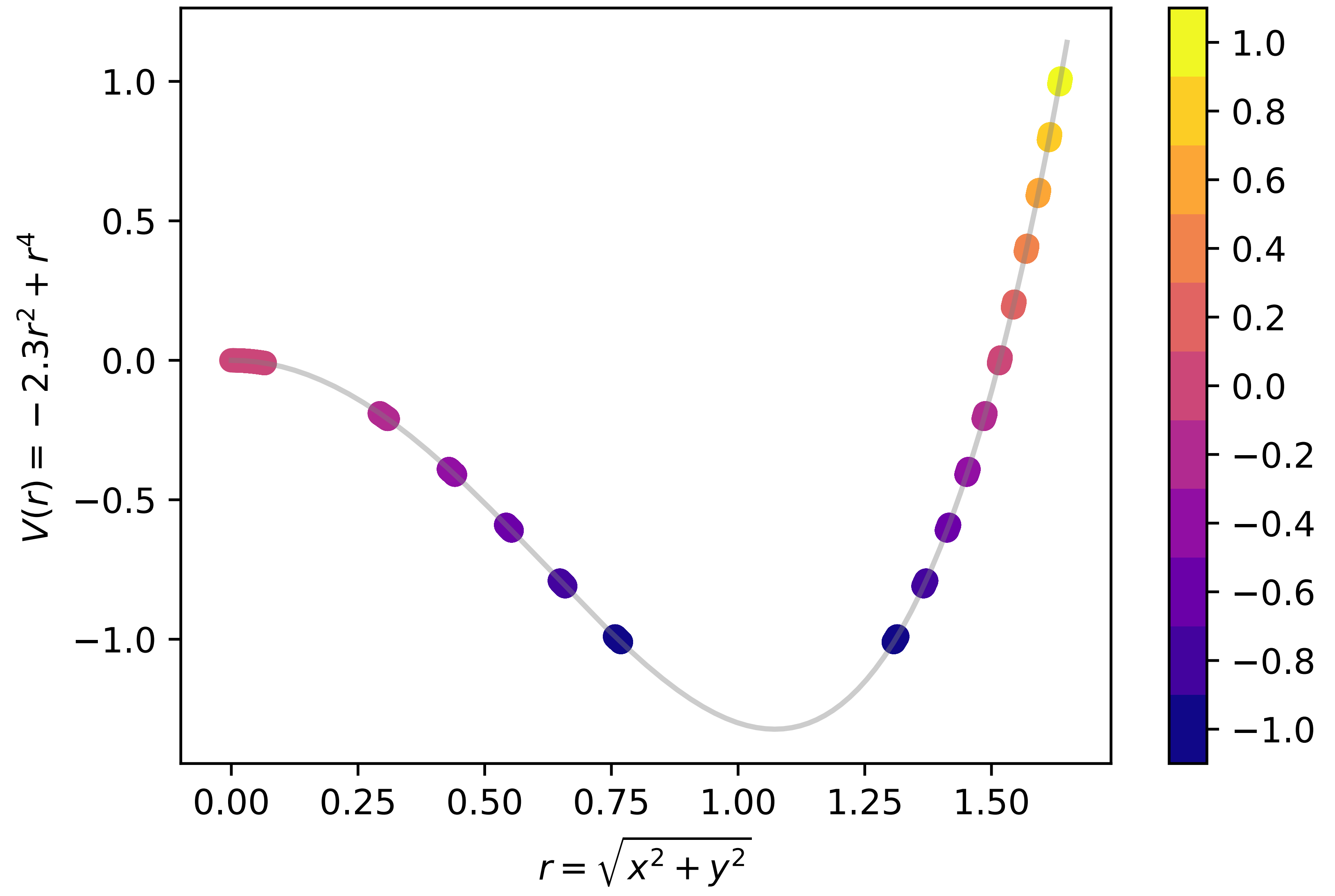
The problem



1. How to find invariances?

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

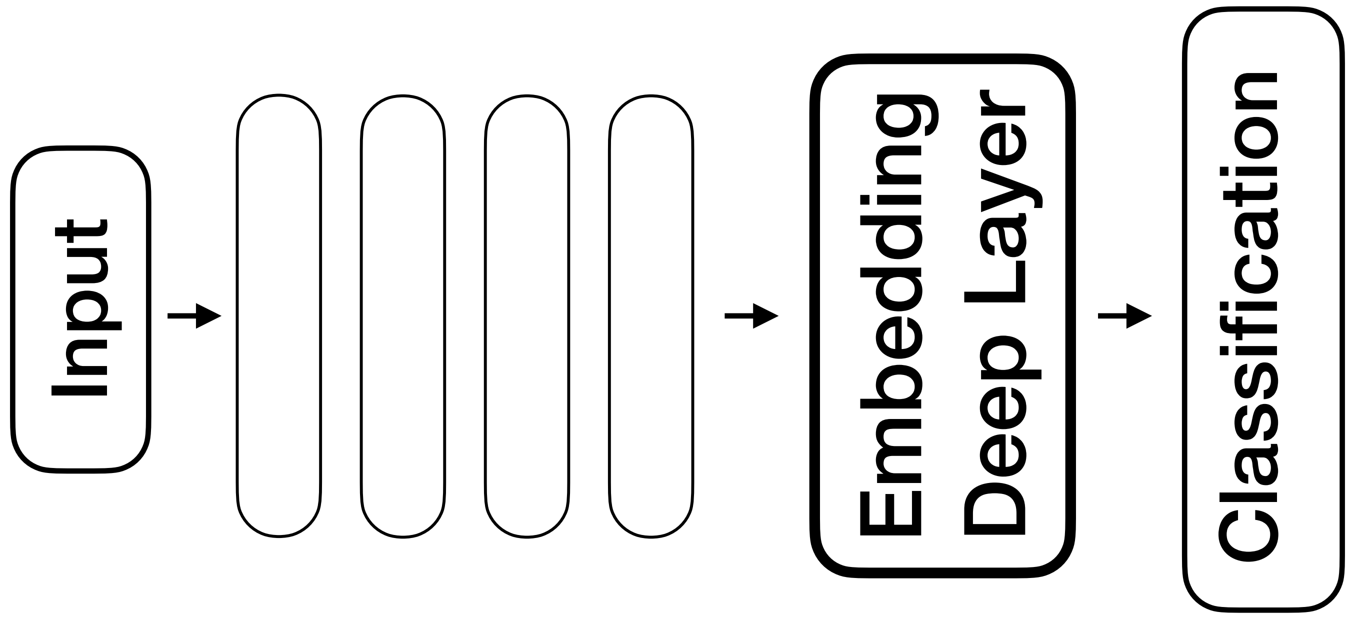
2. Which symmetry is behind such an invariance?



How to search for symmetries?

Embedding in deep layer

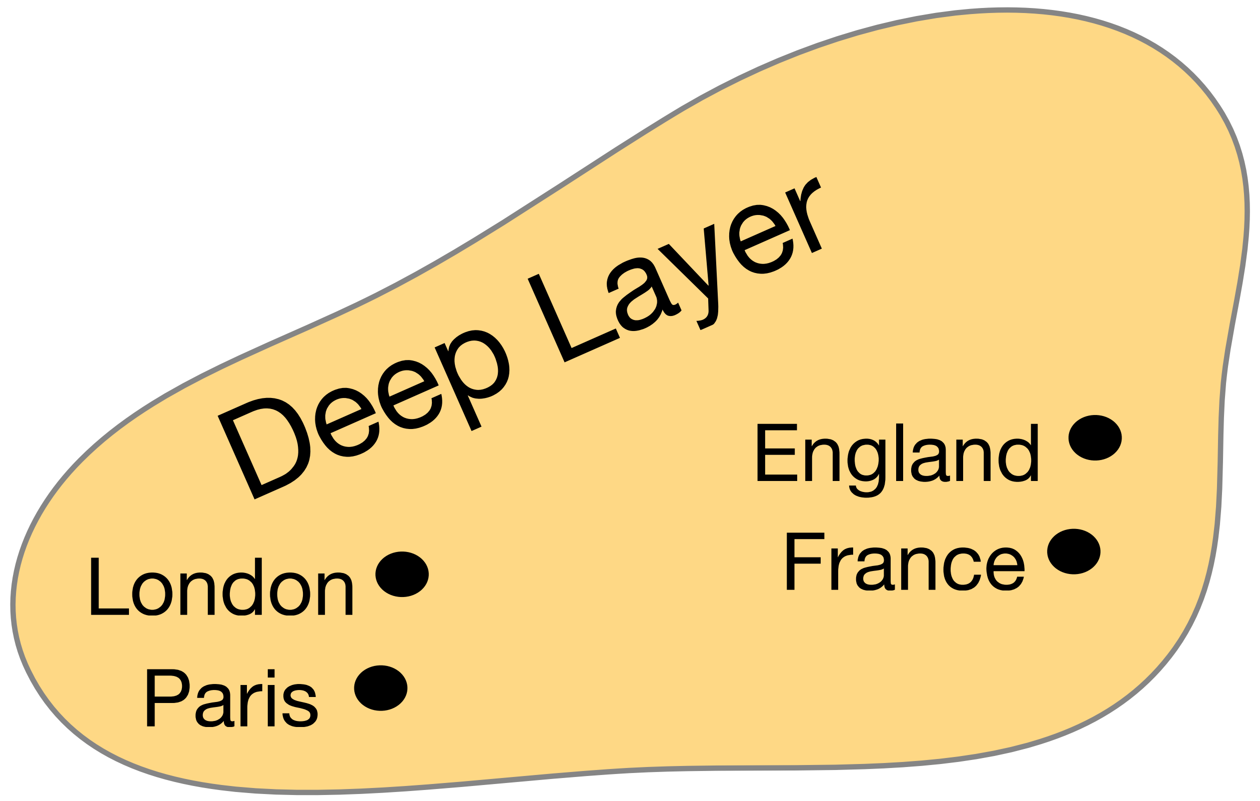
Feed-forward network



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]

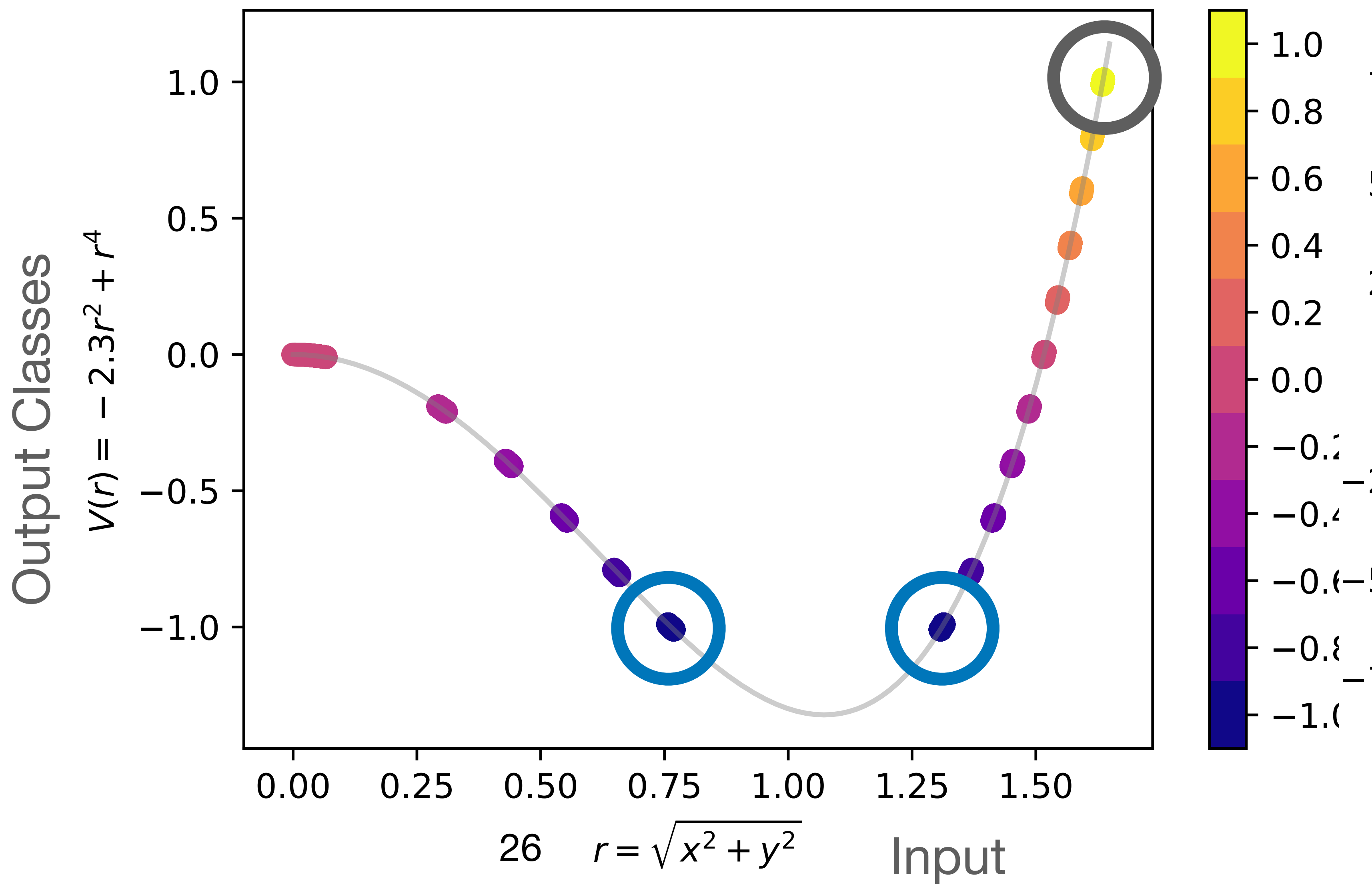


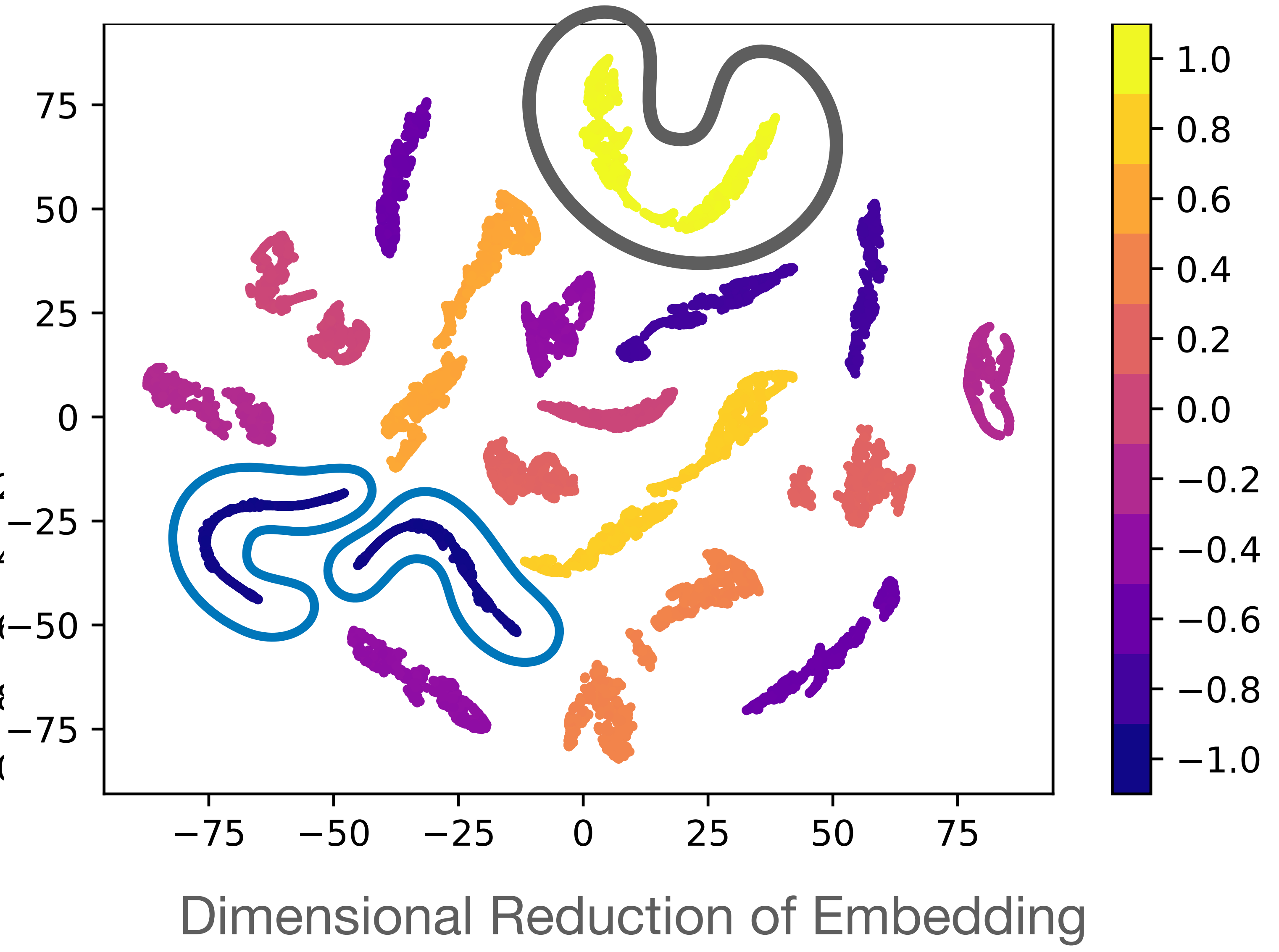
Can we search for symmetries in this way?

Yes!

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

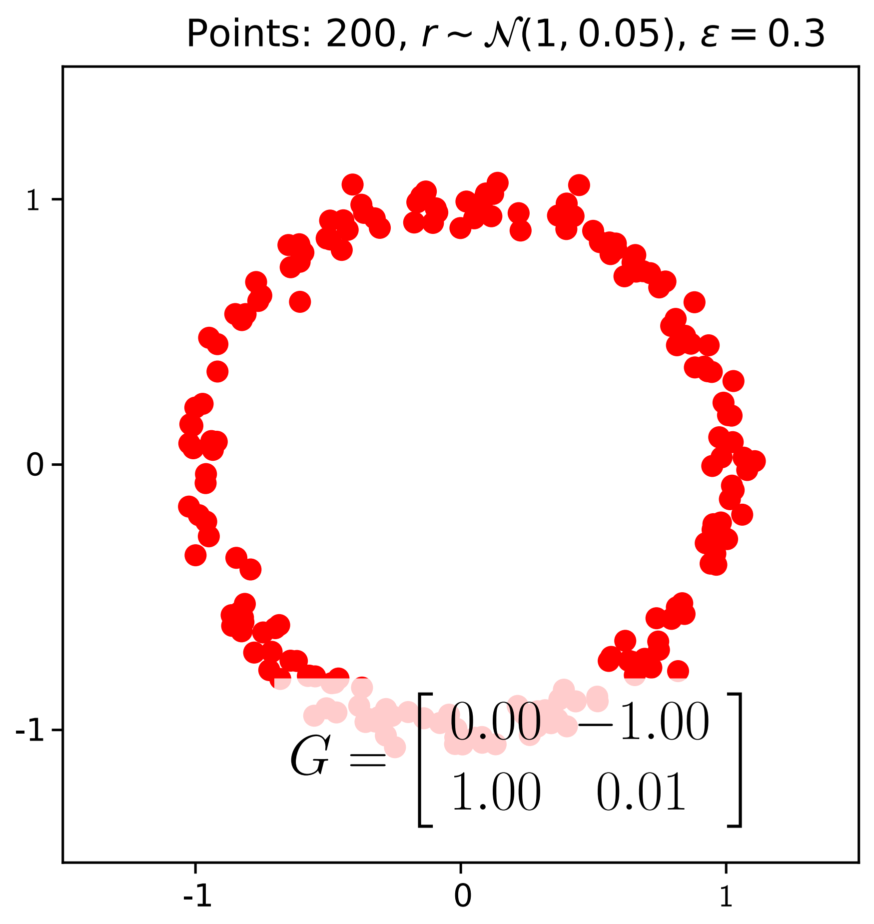
Krippendorf, Syvaeri 2020





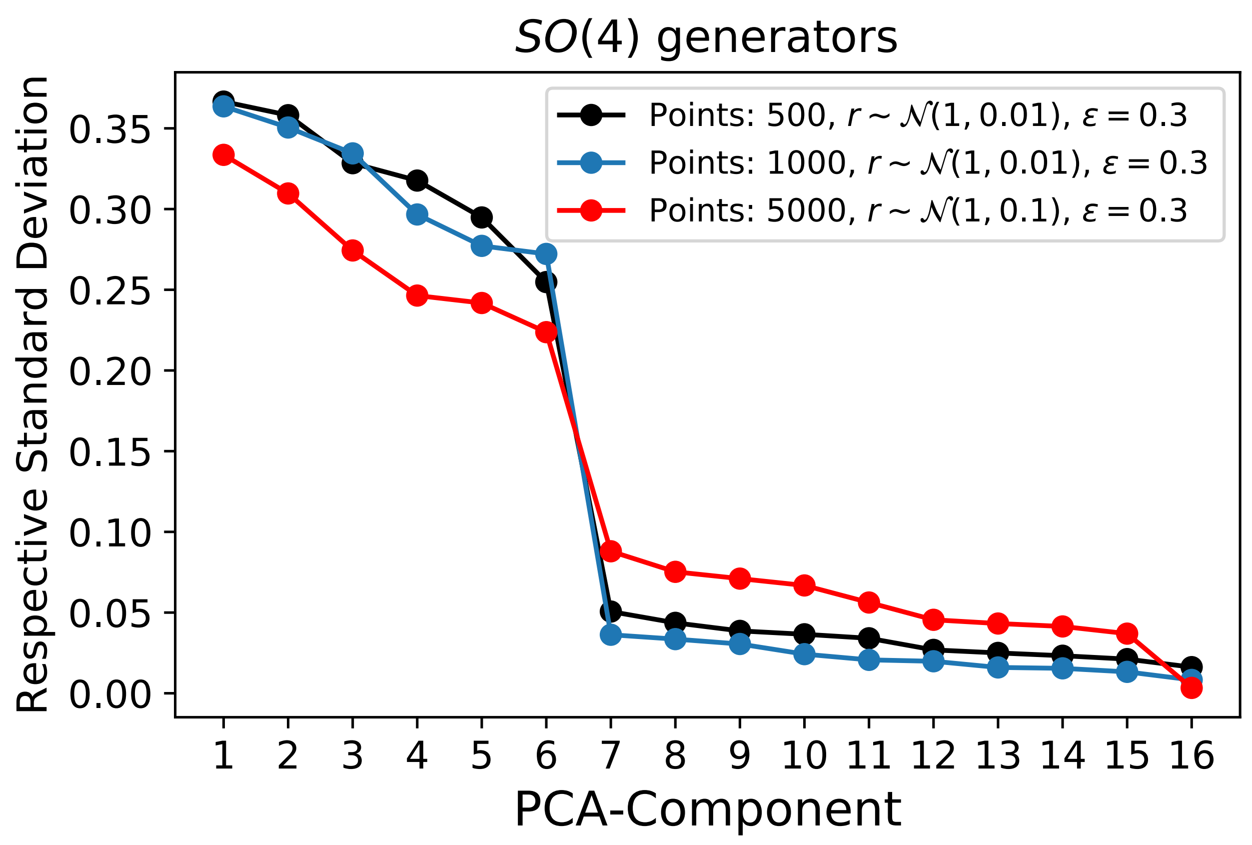
How to determine the symmetry?

Connected points in input space:



Which symmetry?

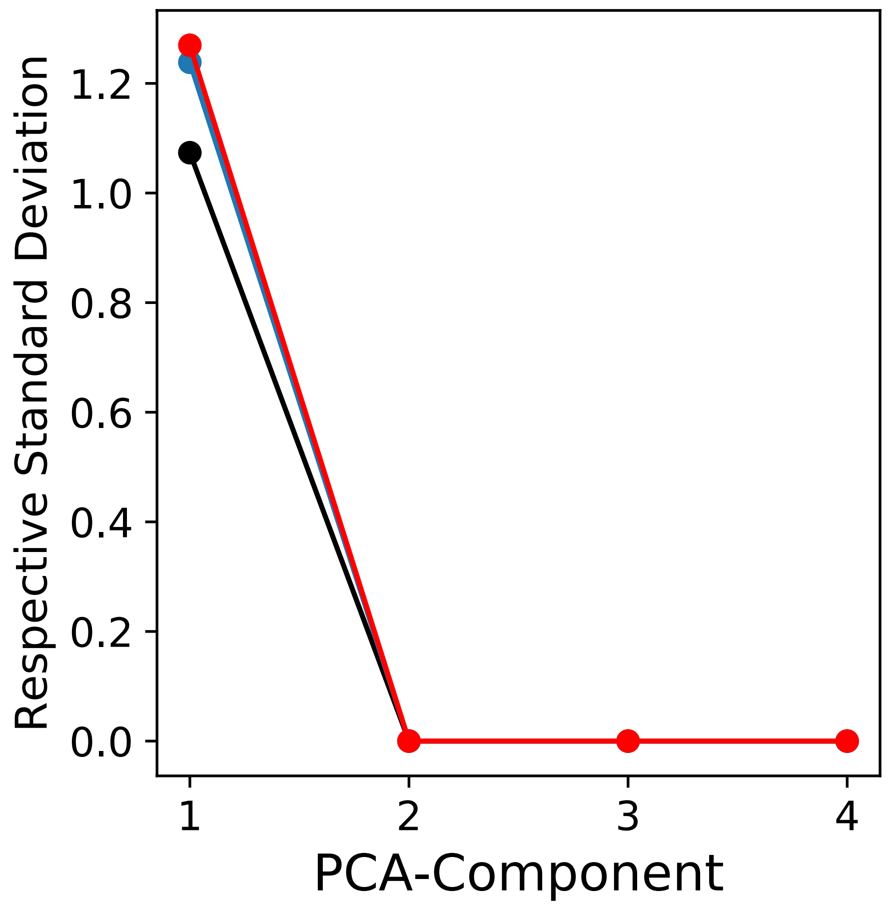
Other Examples?

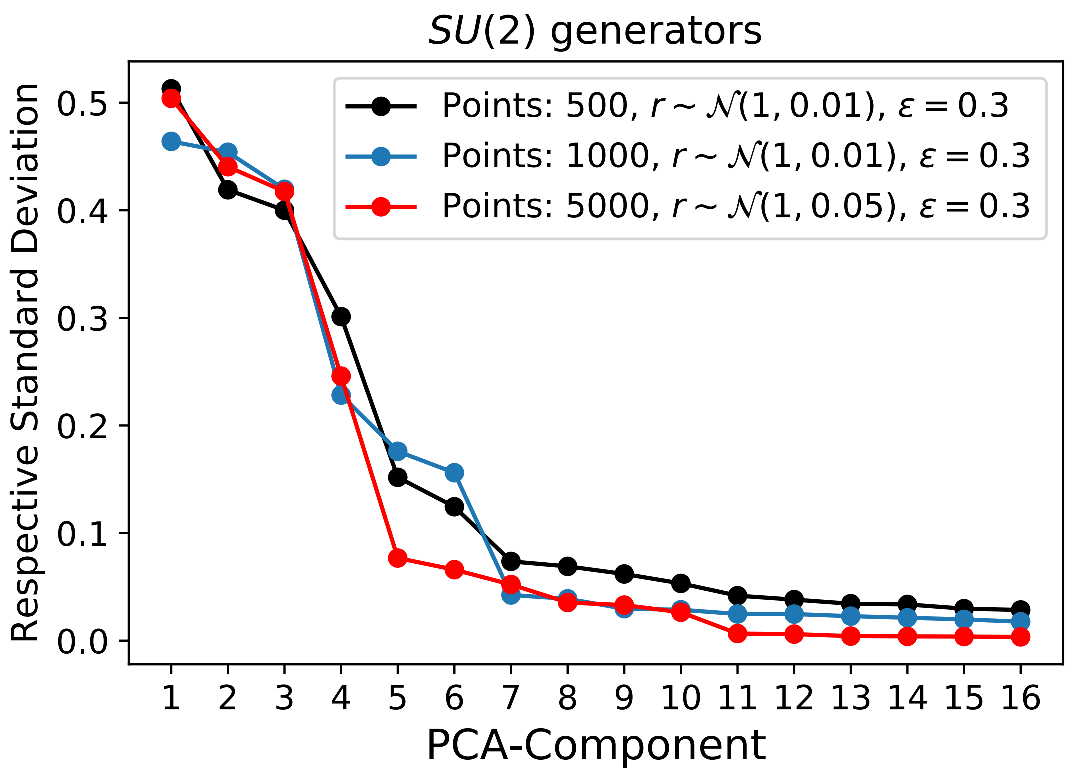


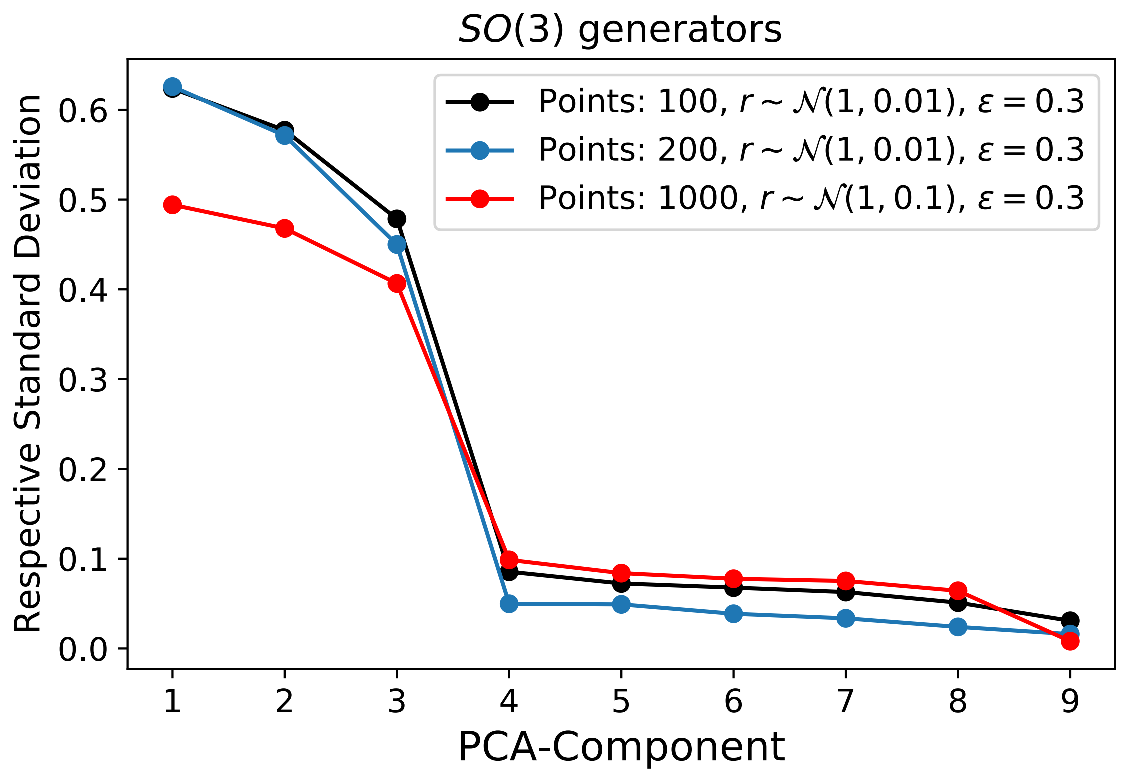
Determine generator connecting points in (sub)-space:

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

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







Krippendorf, Syvaeri 2020

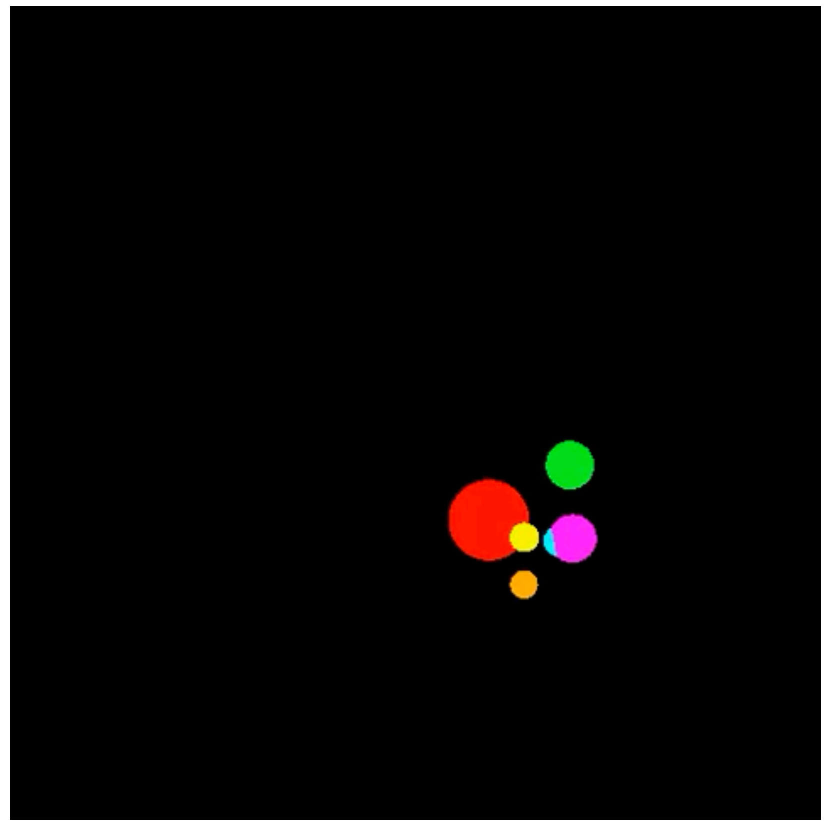
Symmetries from data (samples of phase space)

Krippendorf, Syvaeri (ICLR simDL workshop, 2104.14444)

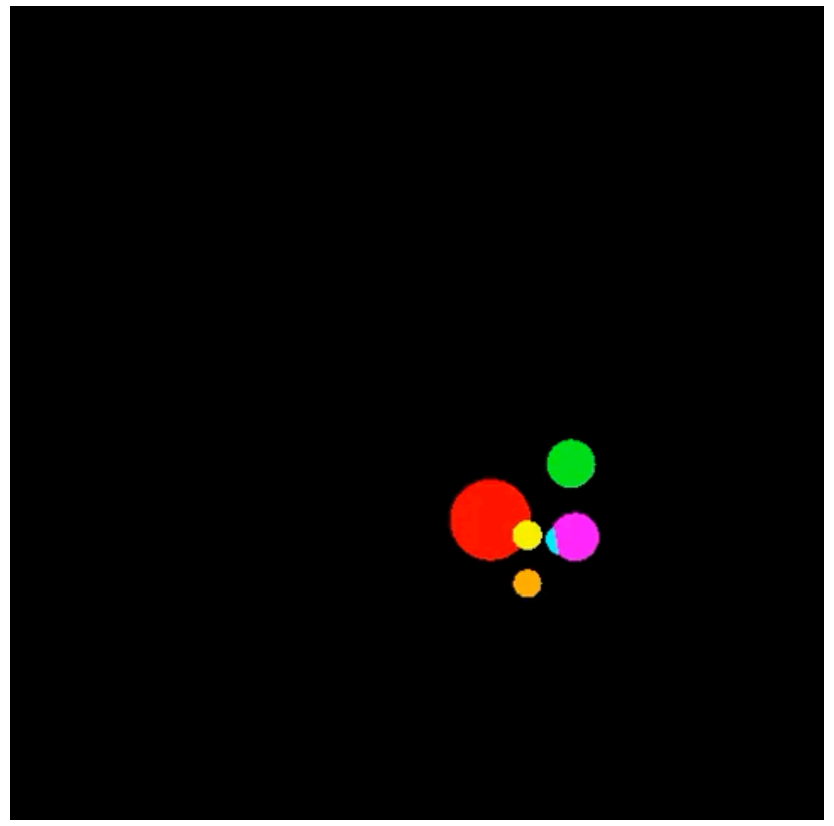
Simulations and physics bias

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

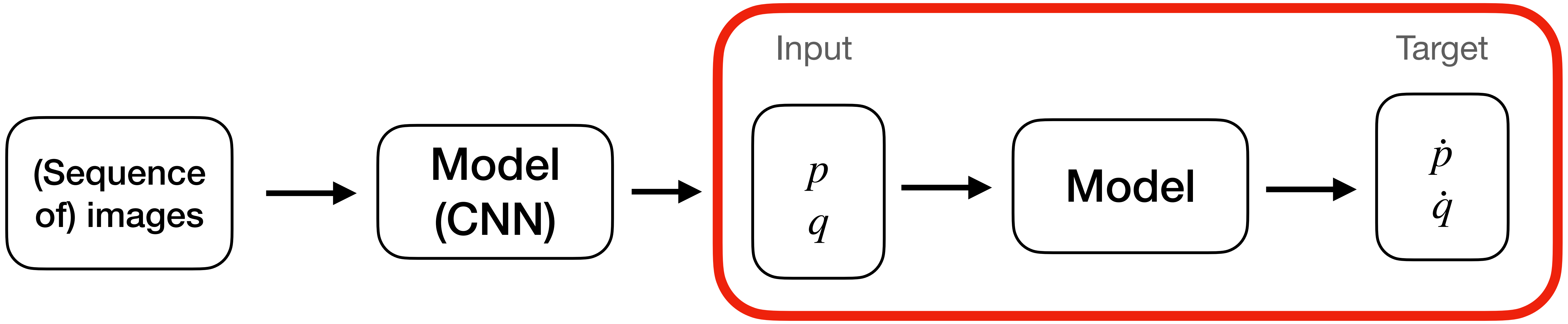
True



Model



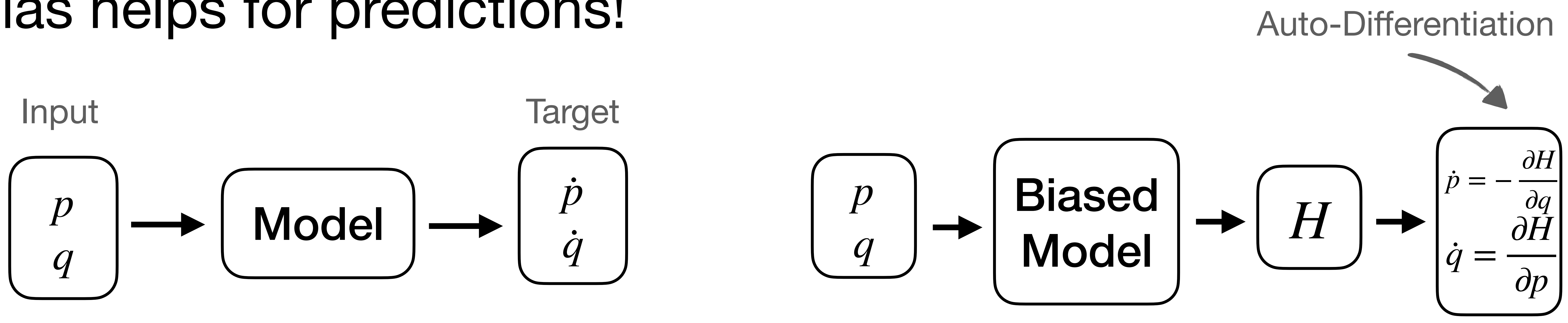
Battaglia et al 2016 (1612.00222)
....



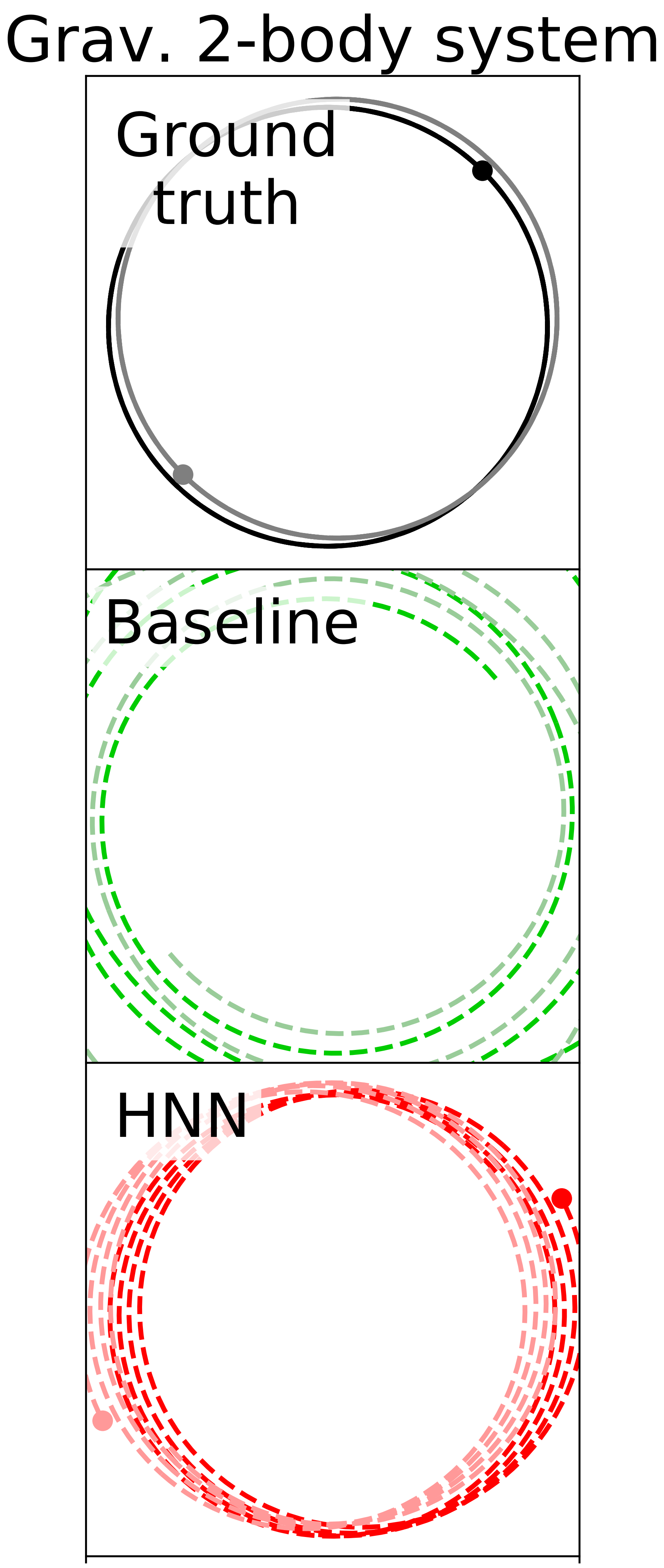
AI and Physics for Simulations

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?

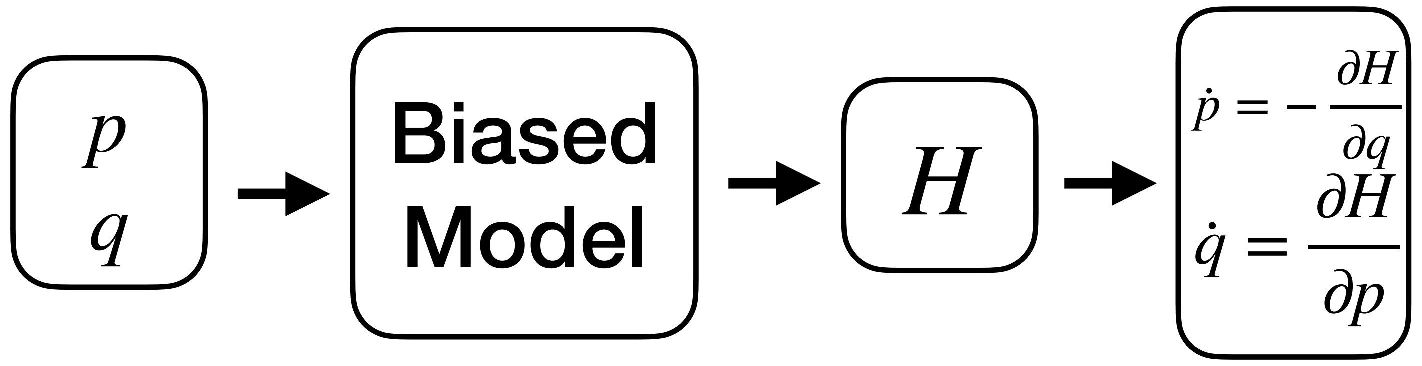
More structures from neural networks?

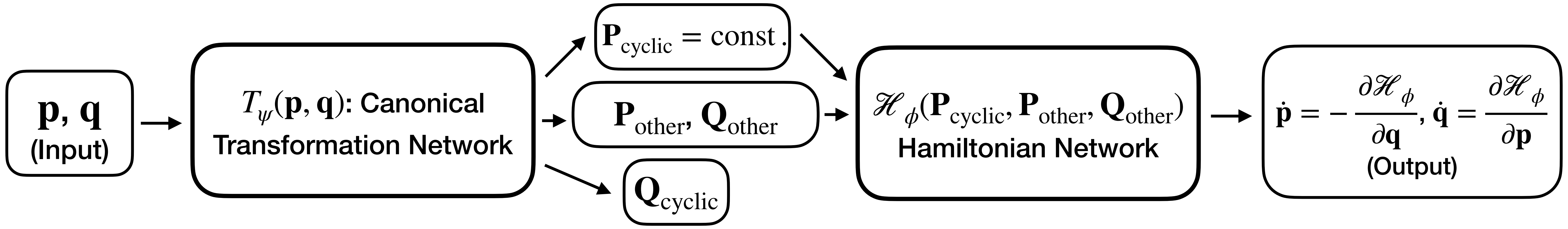
- If we can train NNs to find the Hamiltonian of a system, can we use it to learn other interesting structures?
- Symmetries of the system? E.g. via canonical transformations (cyclic coordinates reveal conserved quantities)
- How does this work? 2 key steps:
  1. Formulate your physics search problem 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

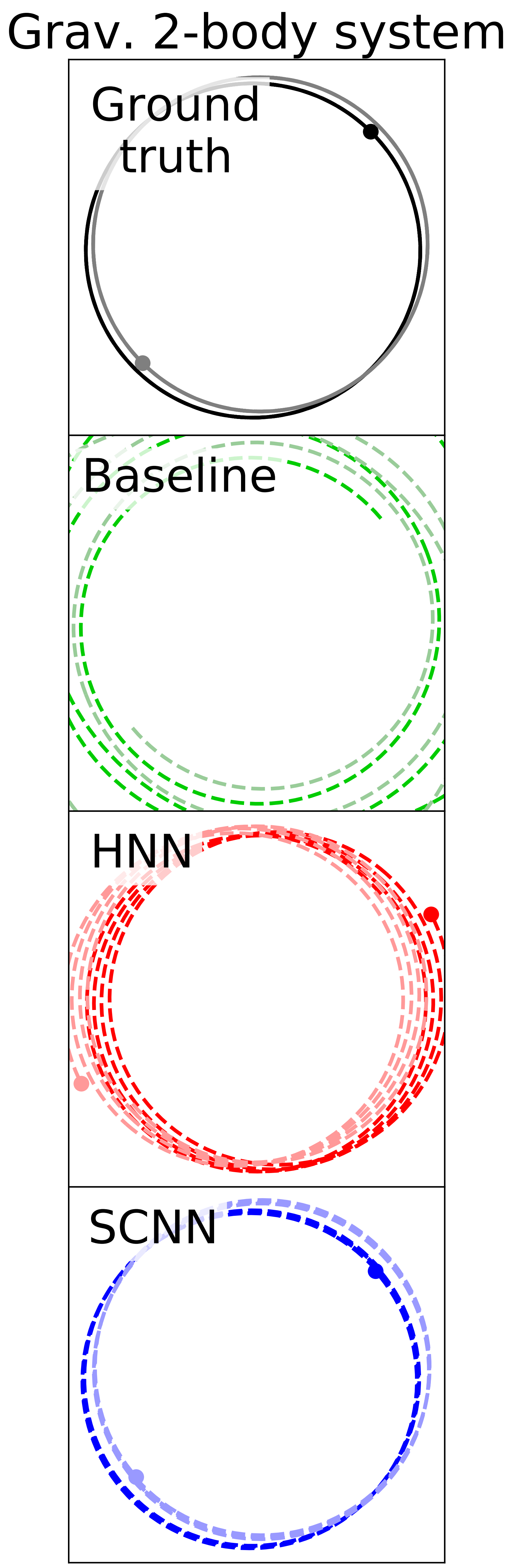




Modified Losses:

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

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

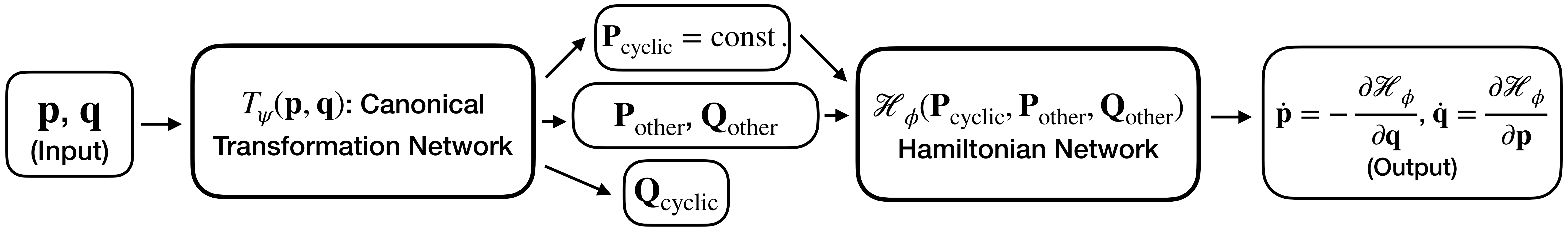


Krippendorf, Syvaeri 2104.14444

AI for Simulations — Symmetries

Introducing physicists' bias

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

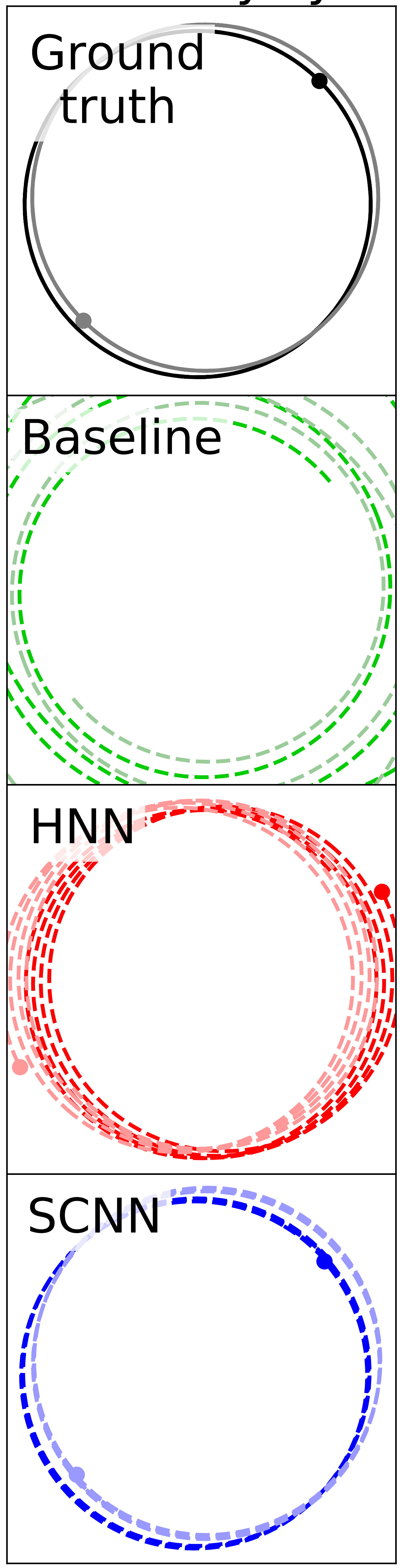


Modified Losses for canonical coordinates:

- 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

Grav. 2-body system



Krippendorf, Syvaeri 2104.14444

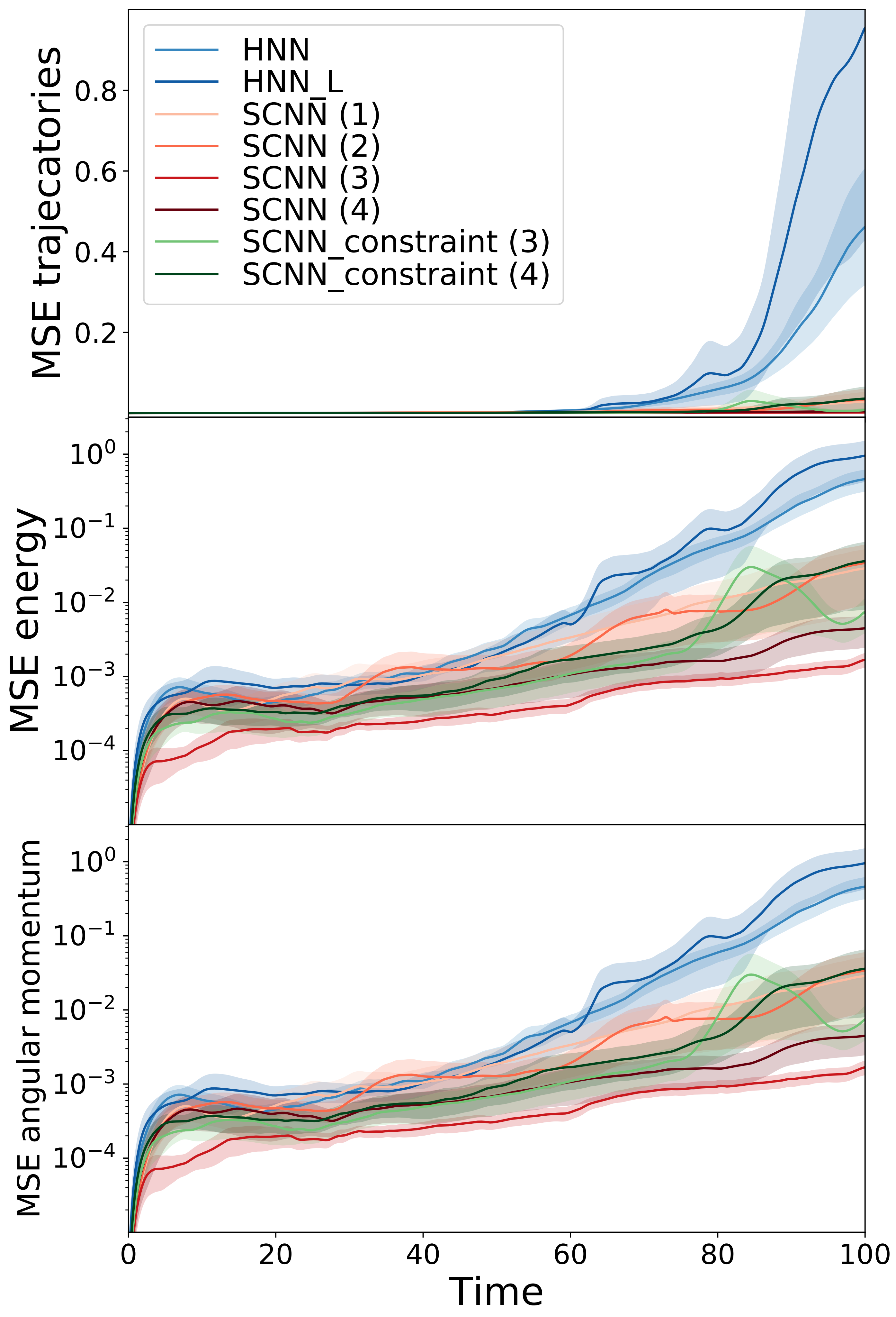
Benefits from Physicists' Bias

- 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

Krippendorf, Lüst, Syvaeri 2021

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:
  $$F_1 = 2\,\lambda$$
  $$F_2 = 2\lambda^2 + 4H$$
  $$F_3 = 2\lambda^3 + 12\lambda H$$
  $$\ldots$$

$\lambda\ldots$ spectral parameter

Krippendorf, Lüst, Syvaeri 2021

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:

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

- 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

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

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

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

- Avoiding mode collapse:

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

- Total loss:

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

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:

$$H = \frac{1}{2}\int dx\, \overrightarrow{S}^2(x)\ ,\quad \overrightarrow{S} \in S^2;\ \text{constraint:}$$

$$\{S_a(x), S_b(y)\} = \epsilon_{abc} S_c(x)\delta(x-y)$$

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

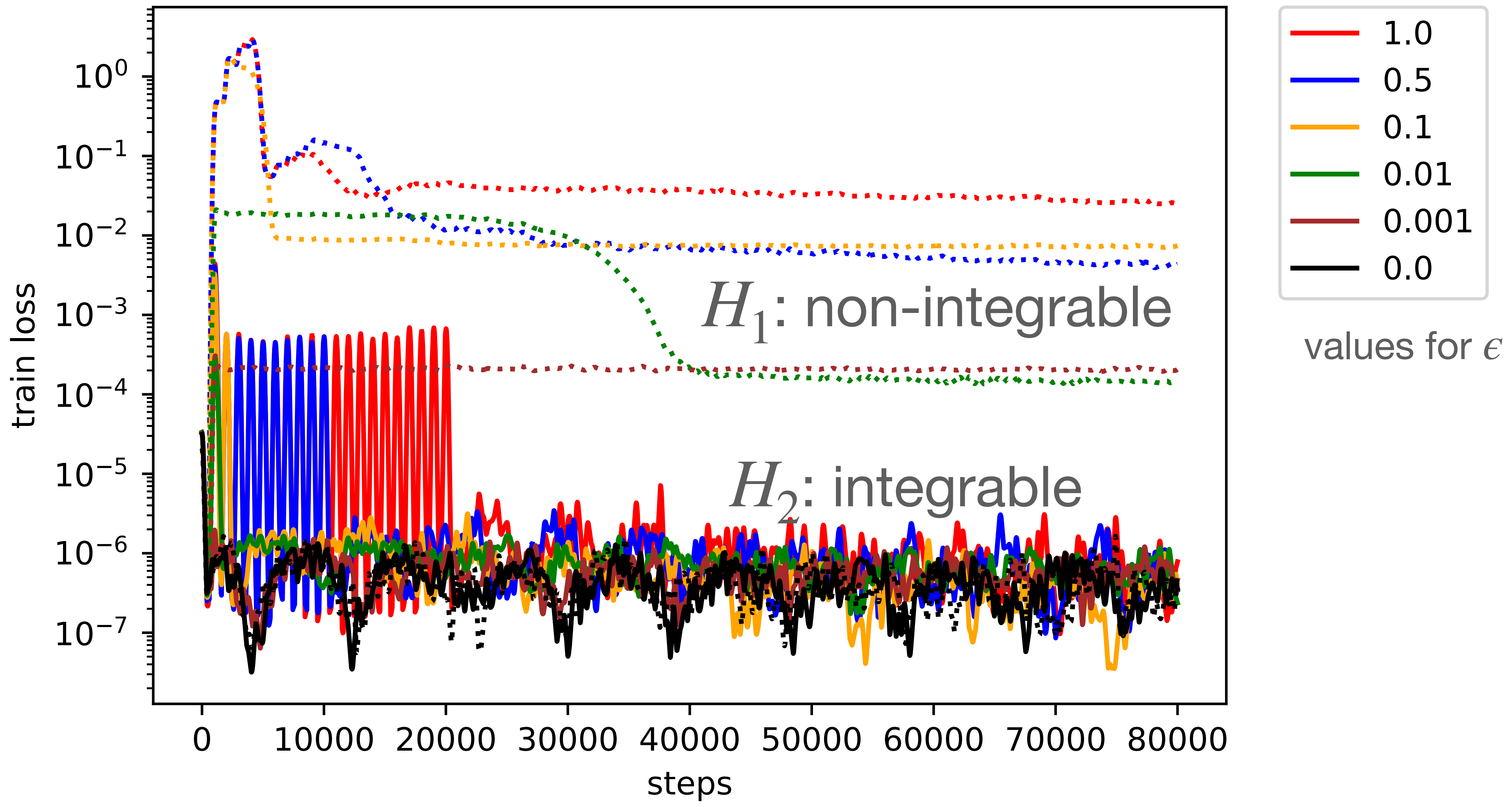
$$\begin{aligned} A_t =& \begin{pmatrix} 2\ \mathrm{i}\ S_z & 2\ \mathrm{i}\ S_x + 2S_y \\ 2\ \mathrm{i}\ S_x - 2S_y & -\ \mathrm{i}\ S_z \end{pmatrix} \\ &+ \begin{pmatrix} \mathrm{i}\ S'_y S_x -\ \mathrm{i}\ S'_x S_y & -S'_z S_x + S'_x S_z +\ \mathrm{i}\ (S'_z S_y - S'_y S_x) \\ +S'_z S_x - S'_x S_z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

- 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



Beyond symmetries, are there other structures in theoretical (particle) physics?

Dualities

Can they be useful in ML?
Can ML provide new perspectives on dualities?

2002.05169 with P. Betzler

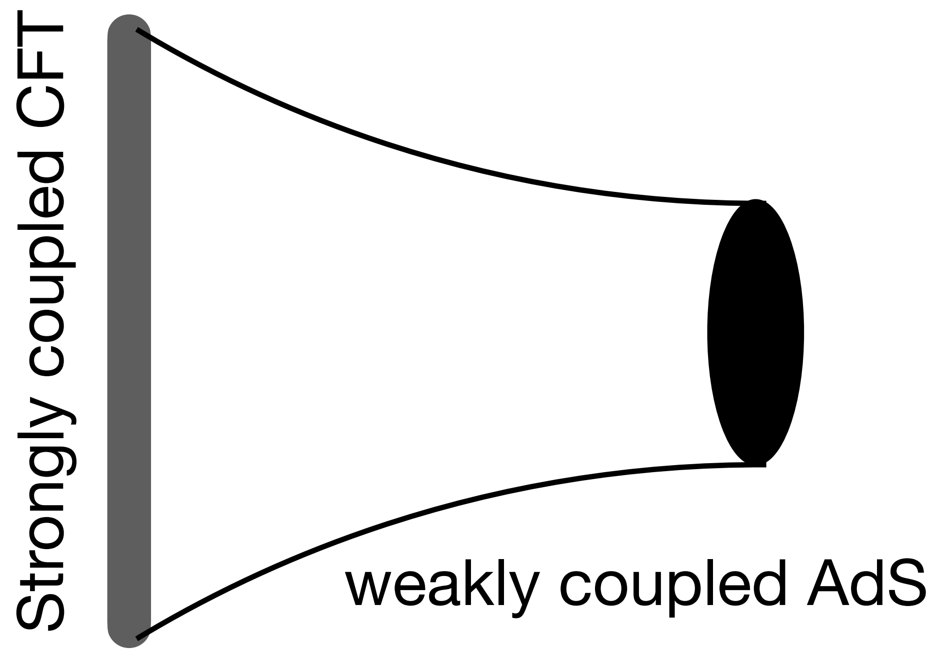
see also: Hashimoto et al. [2018-today]
DL and Holography

Dualities

2D Ising — Self-duality

Ordered rep. ↔ Disordered rep.

Holography



$$Z_{\mathrm{CFT}}(\phi) = Z_{\mathrm{AdS}}(\phi)$$

D-dim. field theory

D+1-dim. gravitational theory

Application: calculation of transport coefficients

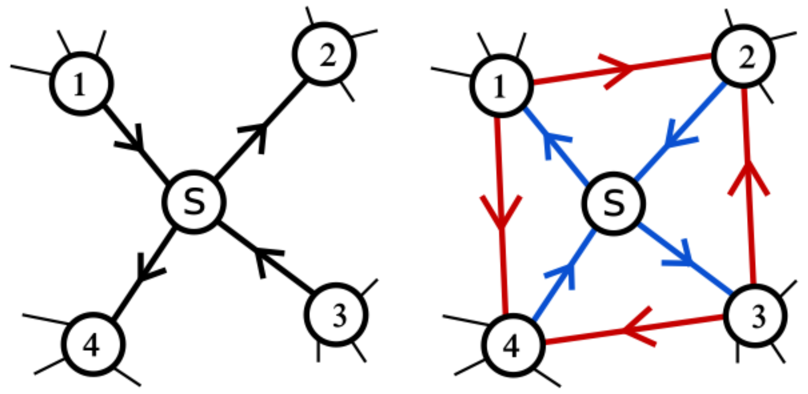
Field Theories

Electromagnetic Duality:

$$\vec{\mathbf{E}} \leftrightarrow \vec{\mathbf{B}}$$

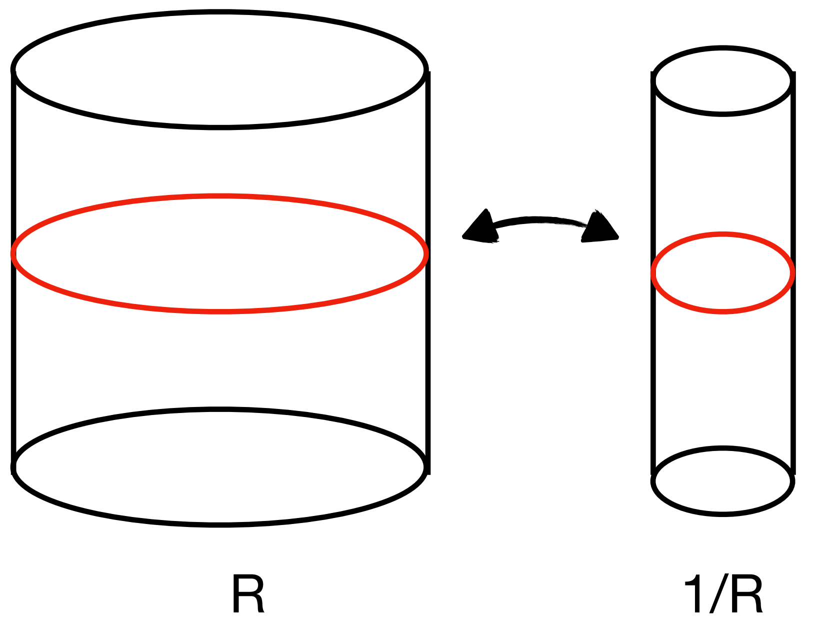
el. charges ↔ mag. monopoles

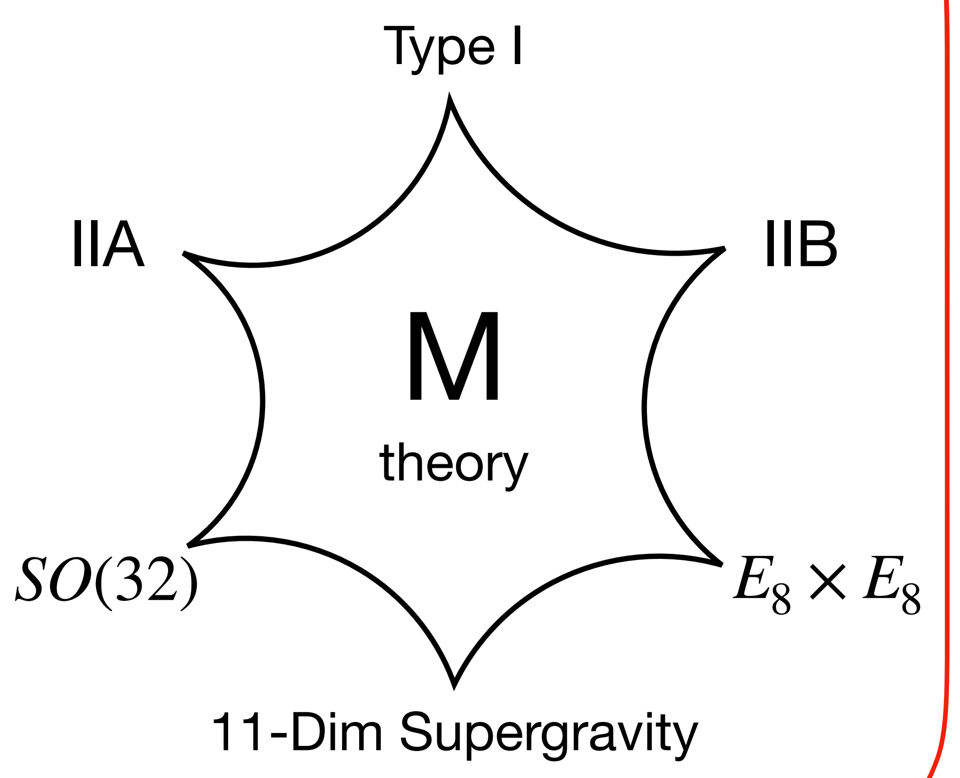
Seiberg Dualities in supersymmetric gauge theories:



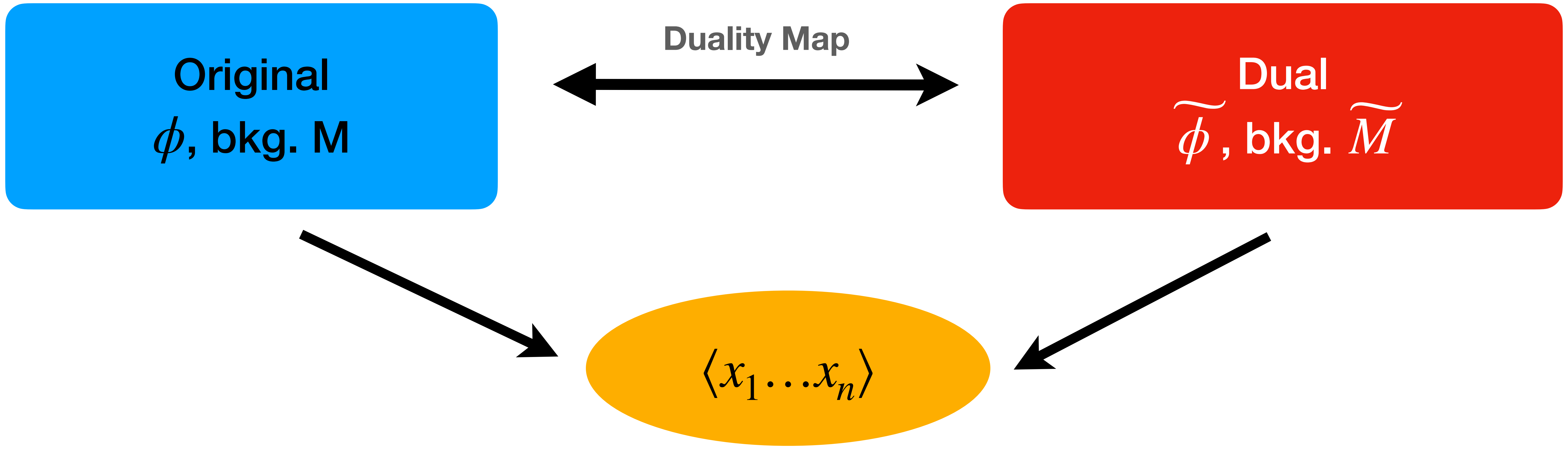
String Dualities

T-duality: winding & momentum strings

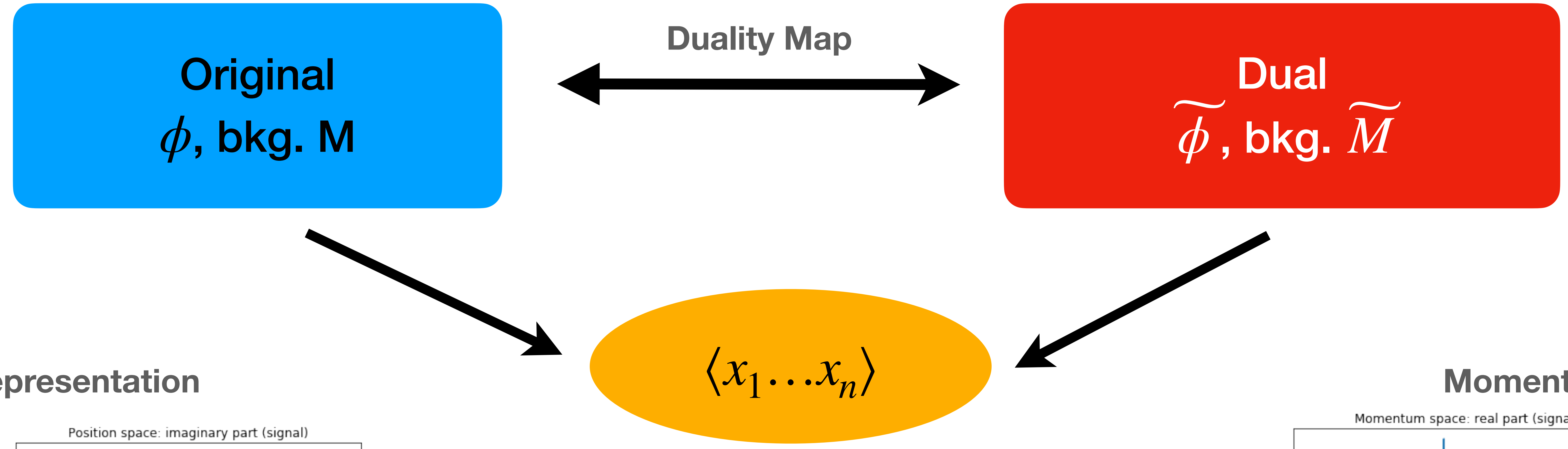




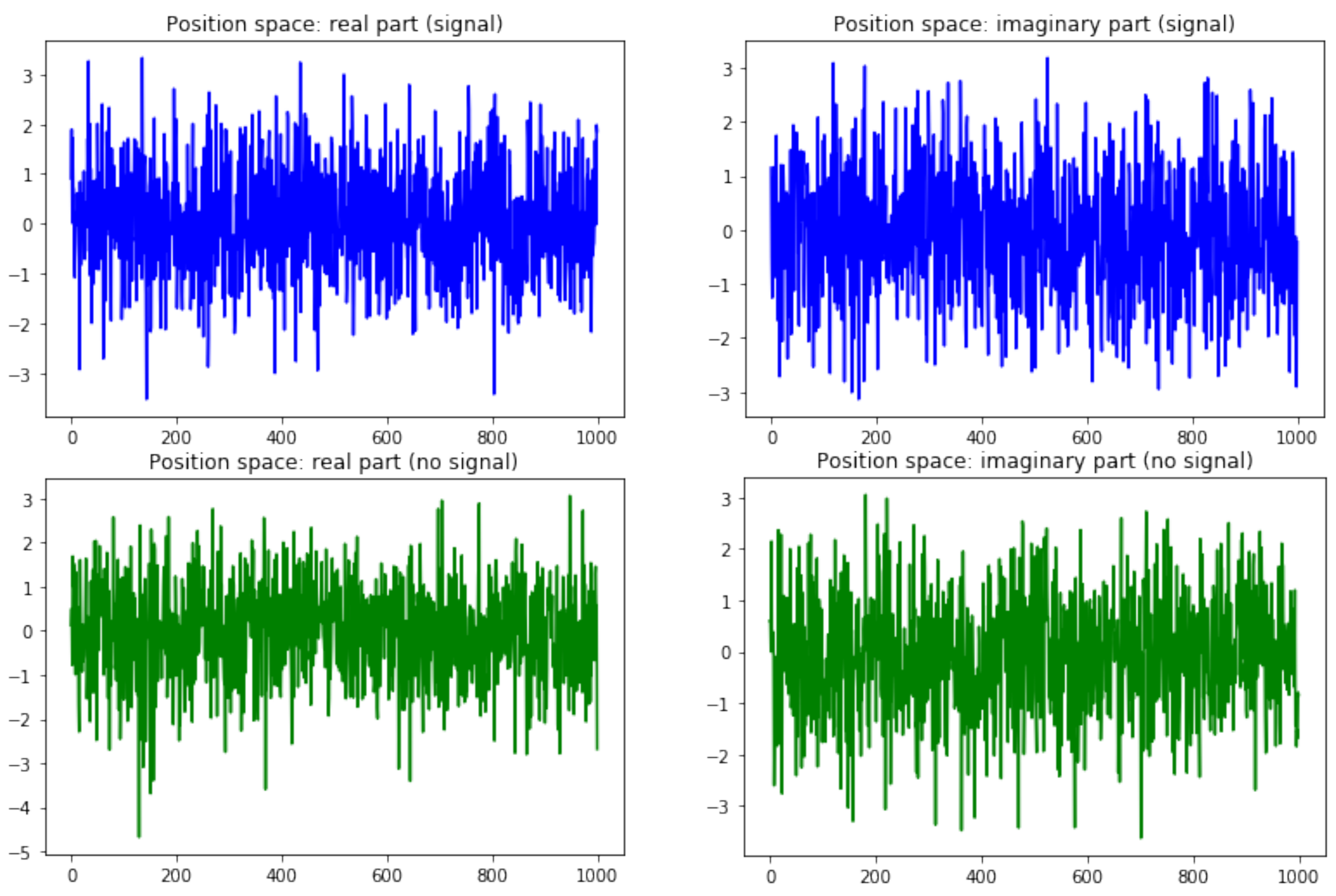
Essence of Dualities



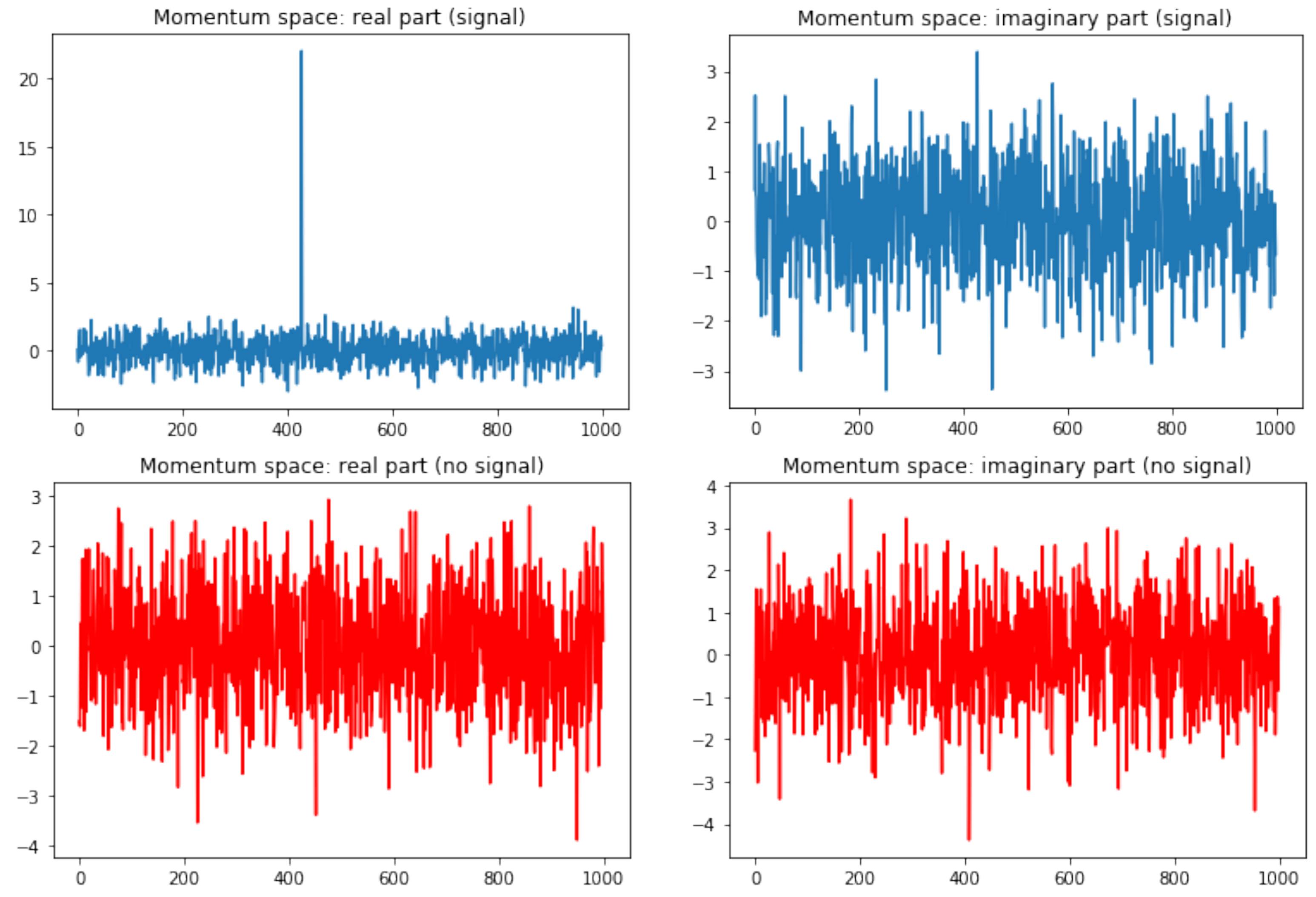
Essence of Dualities



Position space representation



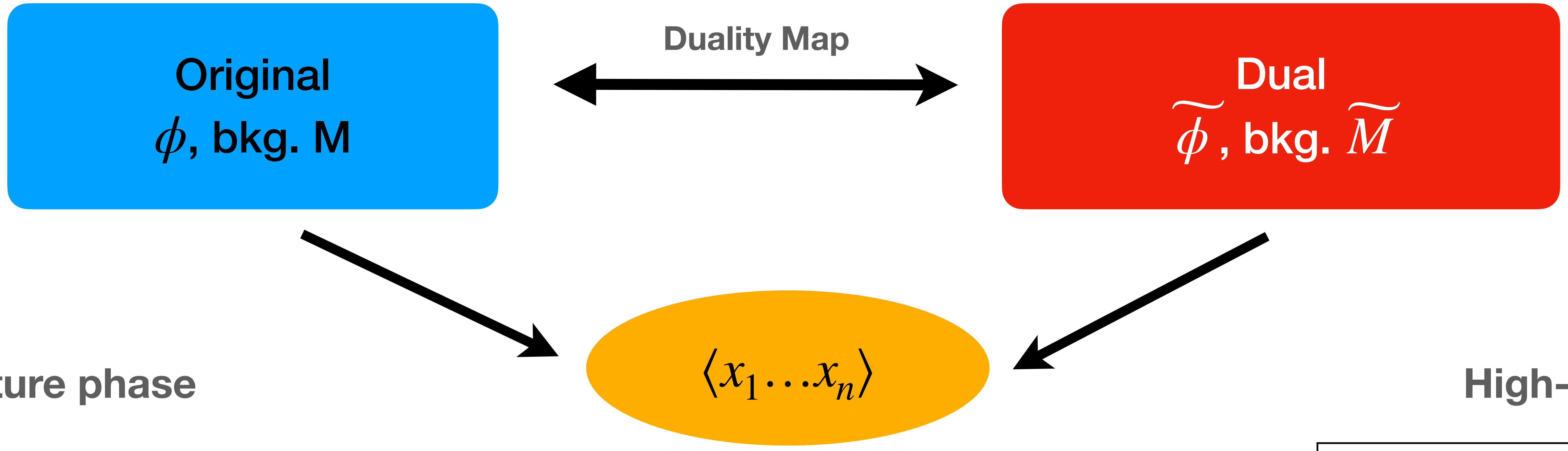
Momentum space representation



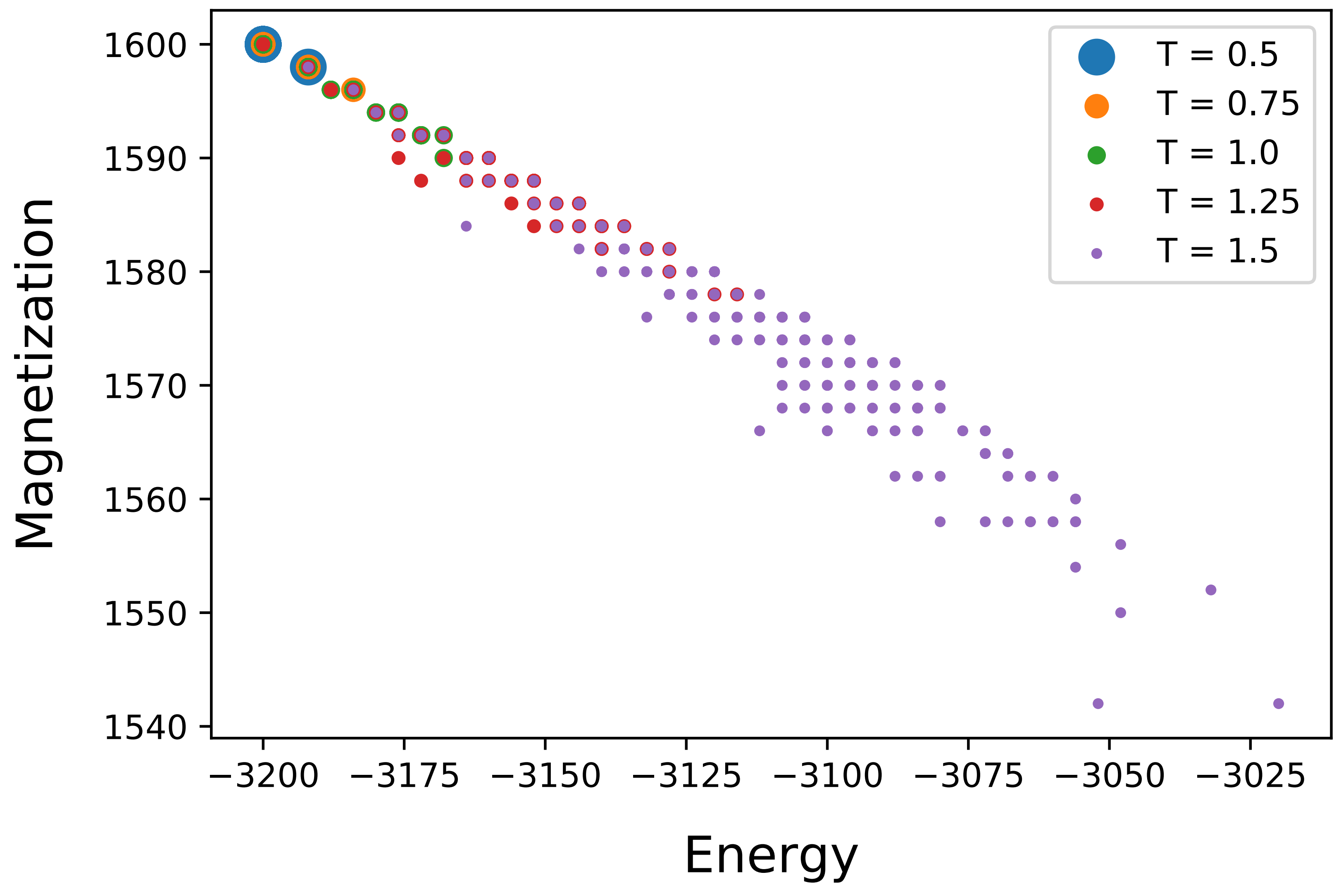
Is there a signal under noise?

Easy to answer in dual momentum space representation

Essence of Dualities



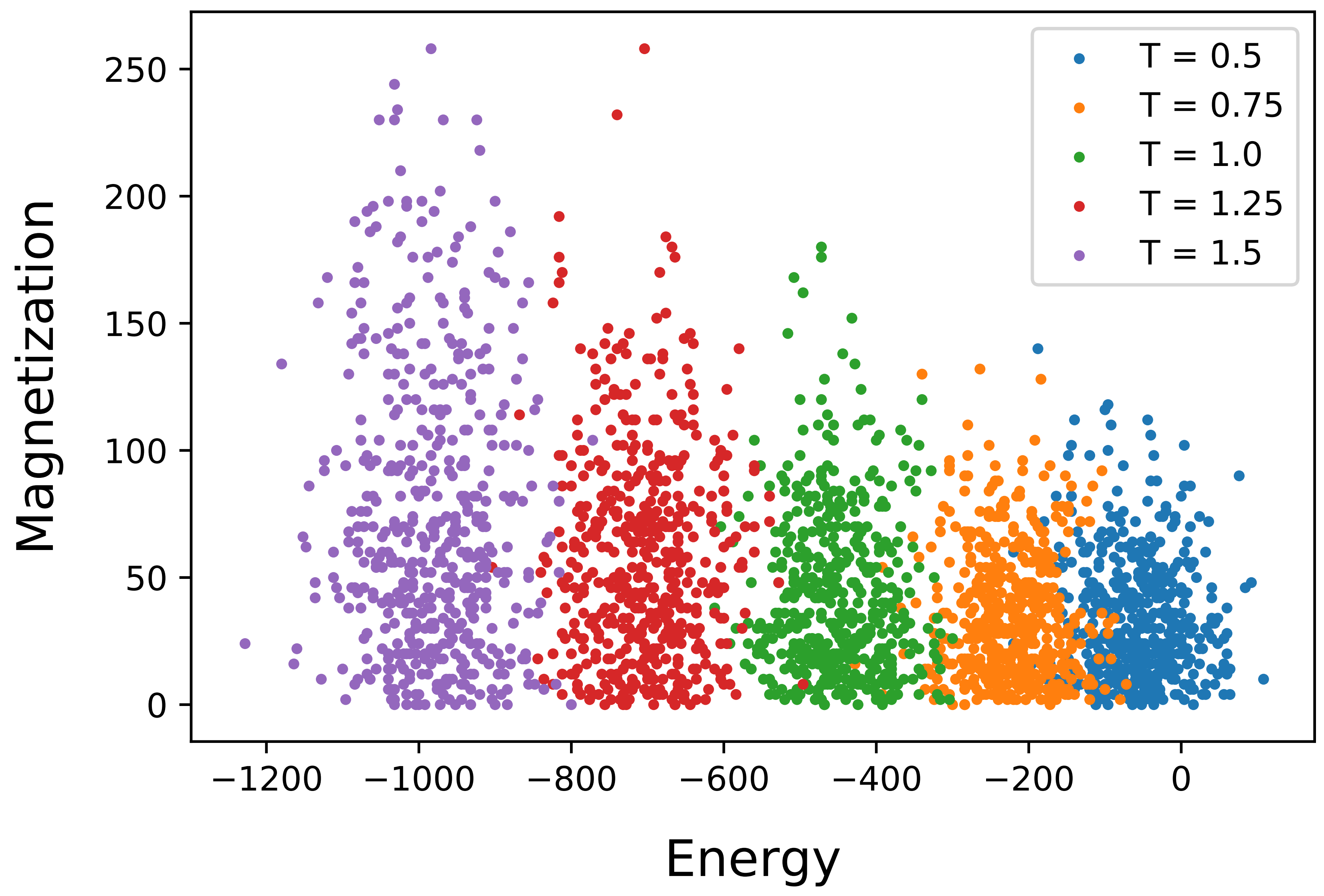
Low-temperature phase



Which temperature sample is drawn from?

Easy to answer in dual high temperature representation for 2D Ising

High-temperature phase

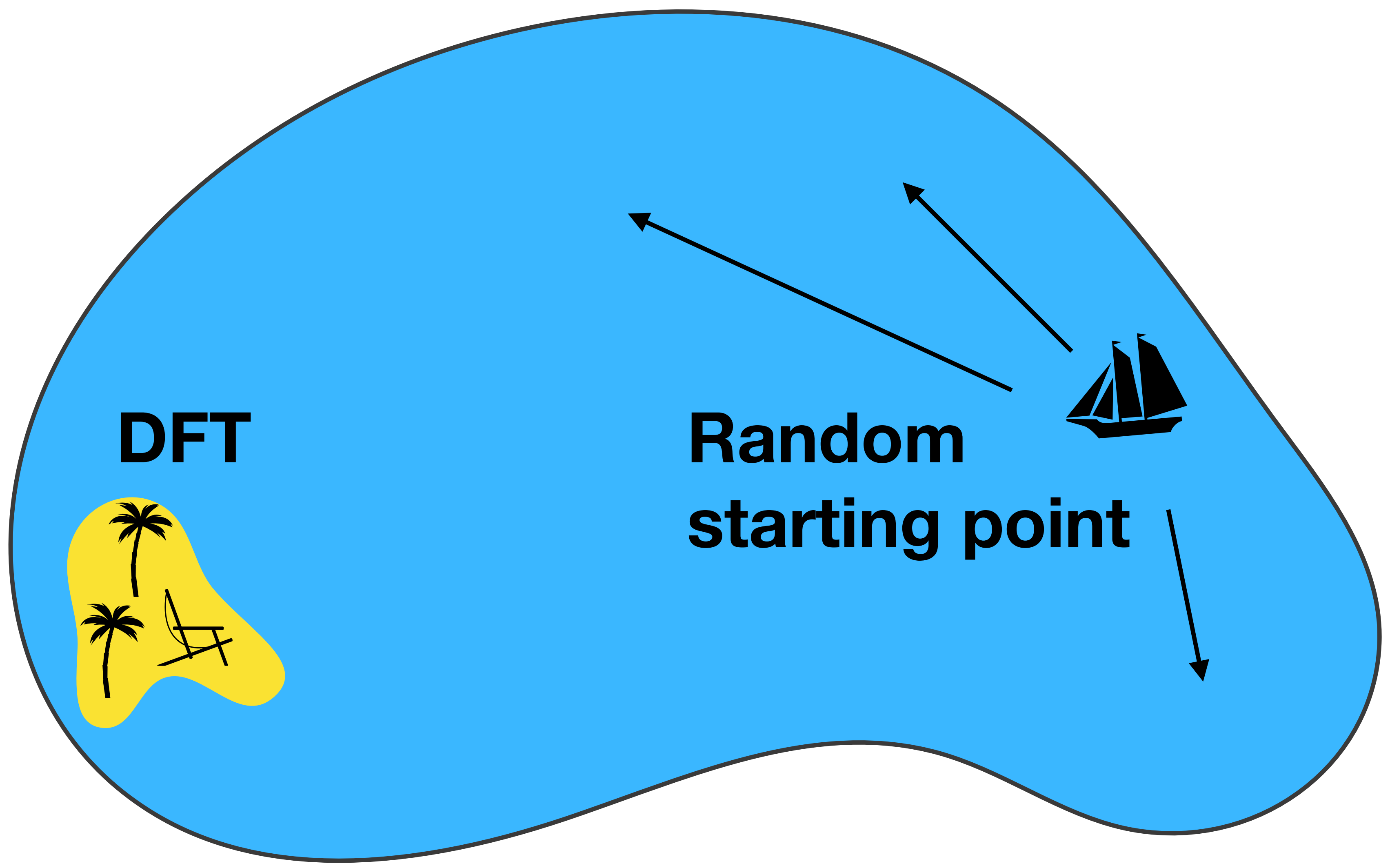


Betzler, Krippendorf 2020

Connecting Dualities and Machine Learning

Does a neural network use such transformations automatically?

No!



If not, how can we make use of such transformations?

Betzler, Krippendorf 2020

Connecting Dualities and Machine Learning

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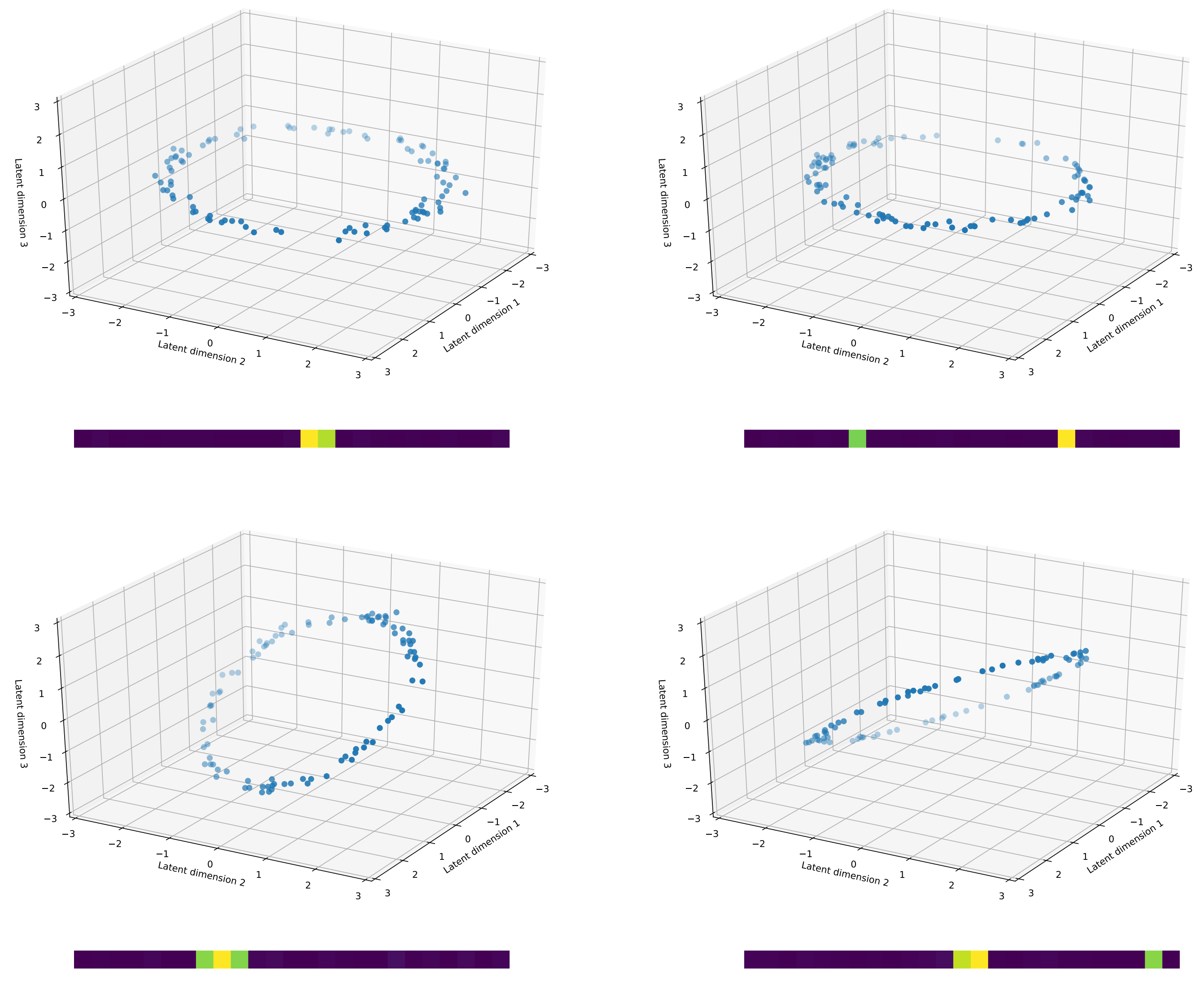
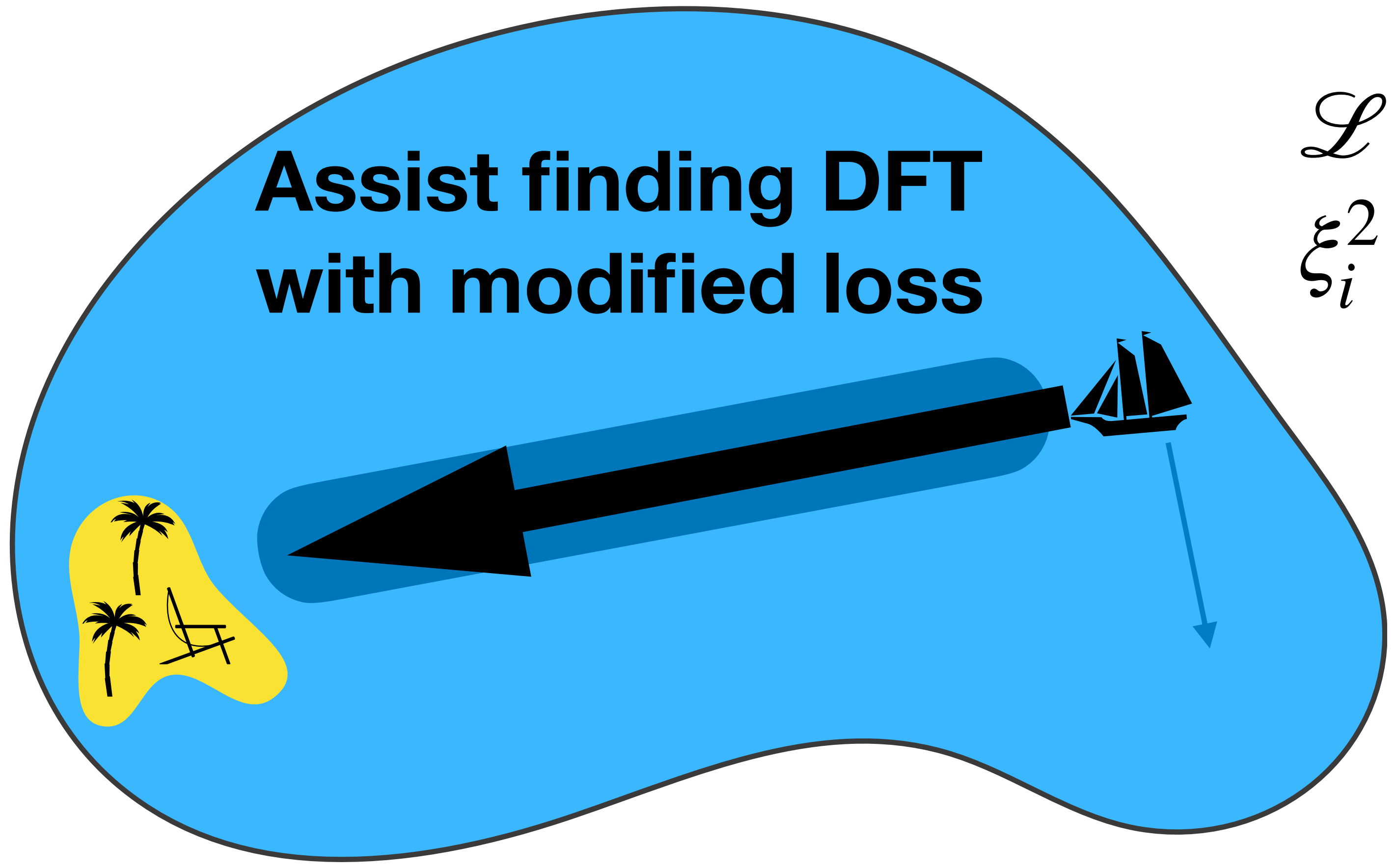


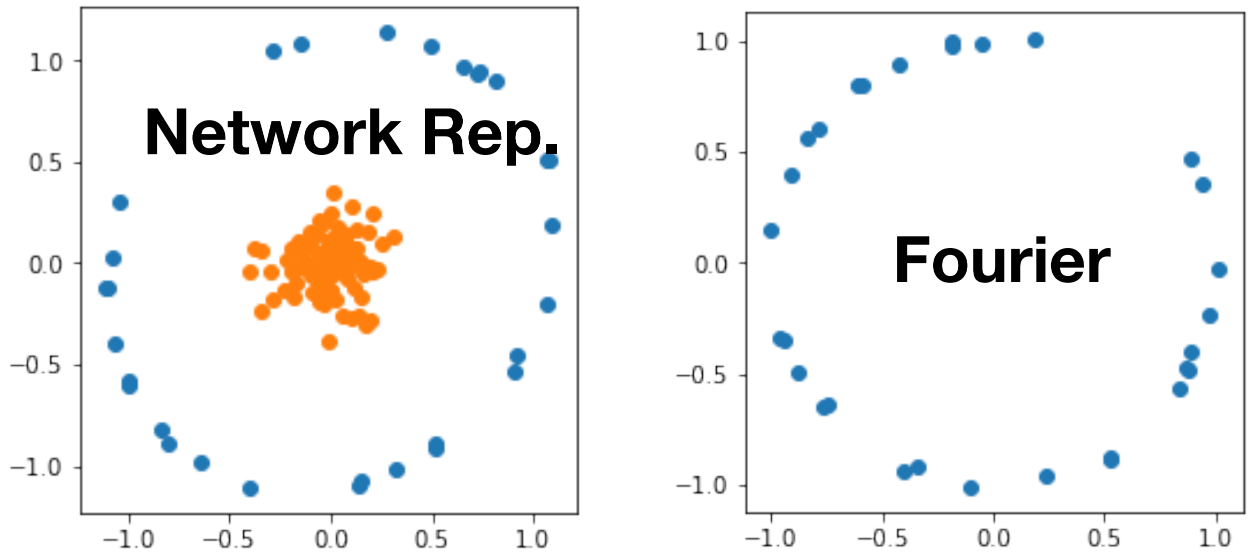
If not, how can we make use of such transformations?

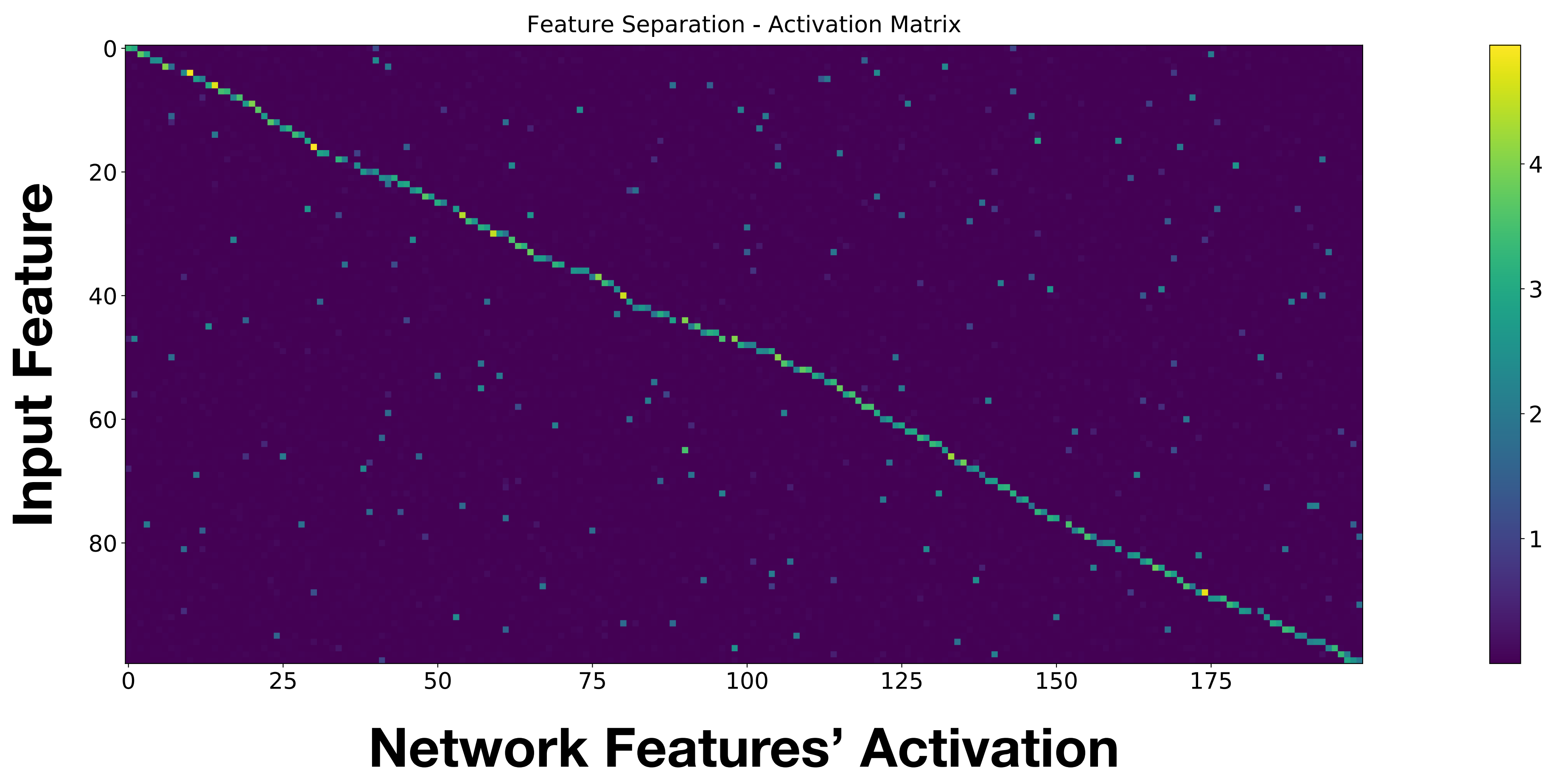
1) Latent loss to maximize distance between signal & noise:



$$\mathscr{L} = \max(0, \alpha - \xi_1^2 - \xi_2^2),$$

ξ_i^2 largest square values of outputs





Betzler, Krippendorf 2020

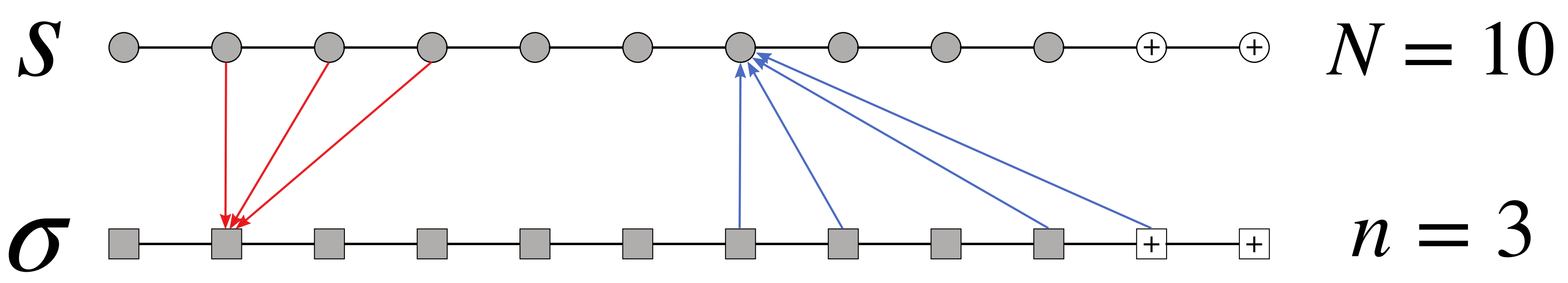
Connecting Dualities and Machine Learning

Does a neural network use such transformations automatically?

No!

1D Ising Model with multiple spin-interactions:
Feasible task: Energy
Hard inference task: Metastable state

If not, how can we make use of such transformations?

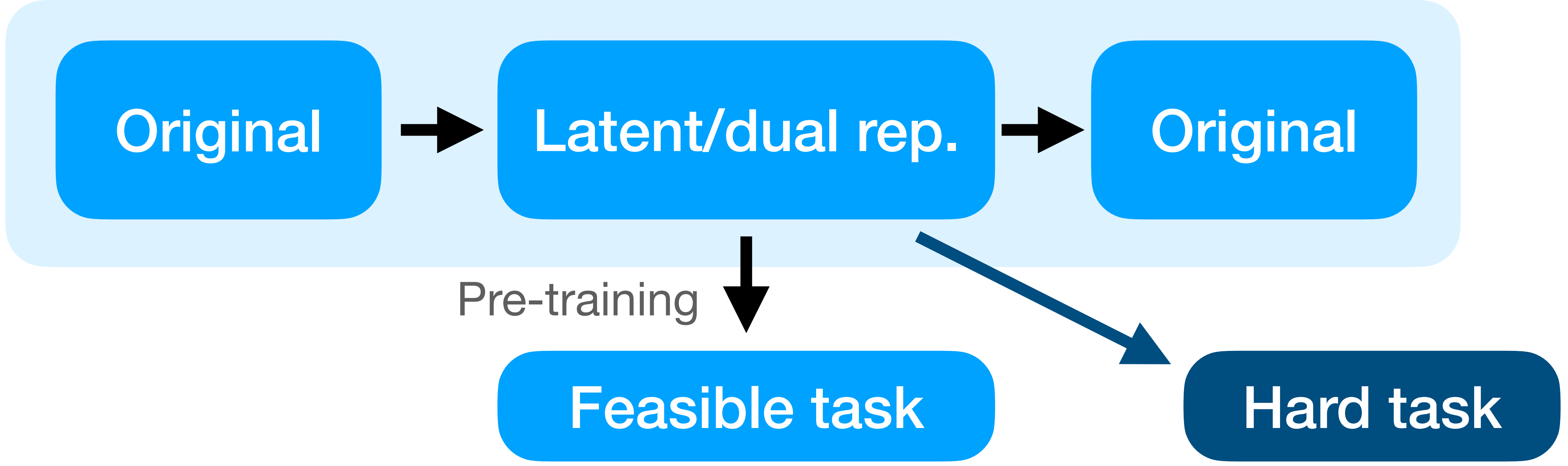


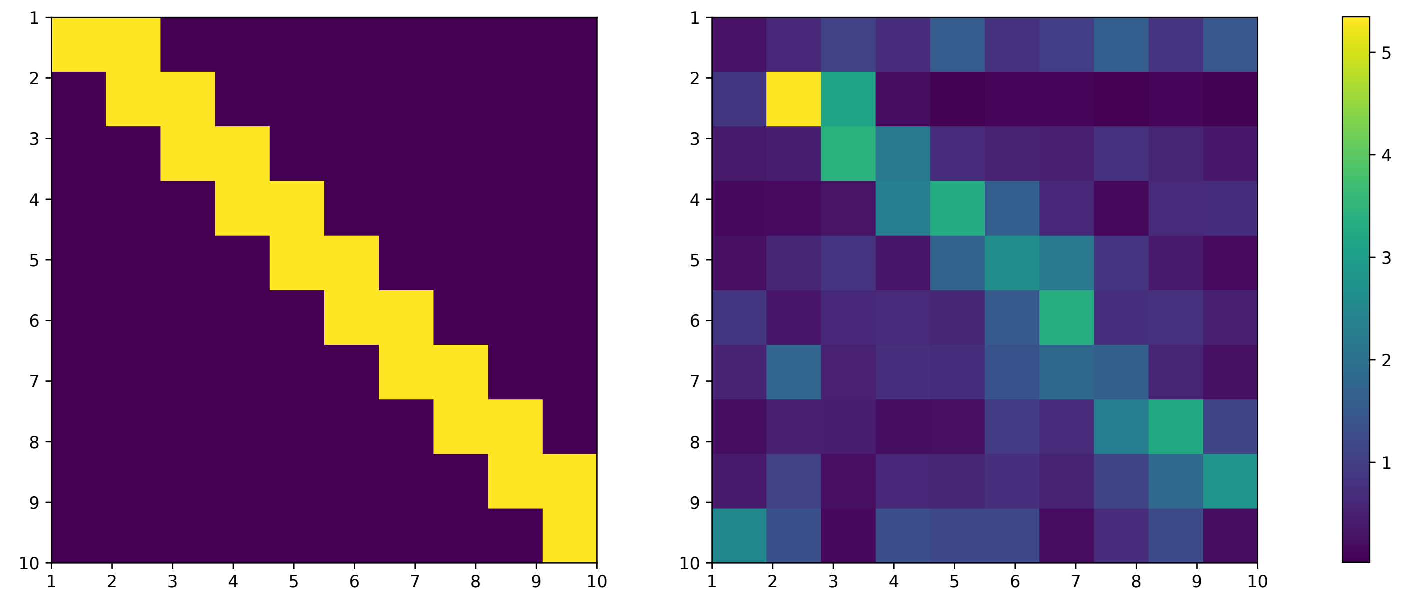
normal: $H(s) = -J \sum_{k=1}^{N-n+1} \prod_{l=0}^{n-1} s_{k+l} - B \sum_{k=1}^{N} s_k$ (here: $B = 0$)

dual: $H(\sigma) = -J \sum_{k=1}^{N-n+1} \sigma_k$ where $\sigma_k = \prod_{l=0}^{n-1} s_{k+l}$

2) Pre-training with medium hard inference task on latent dimension

Autoencoder





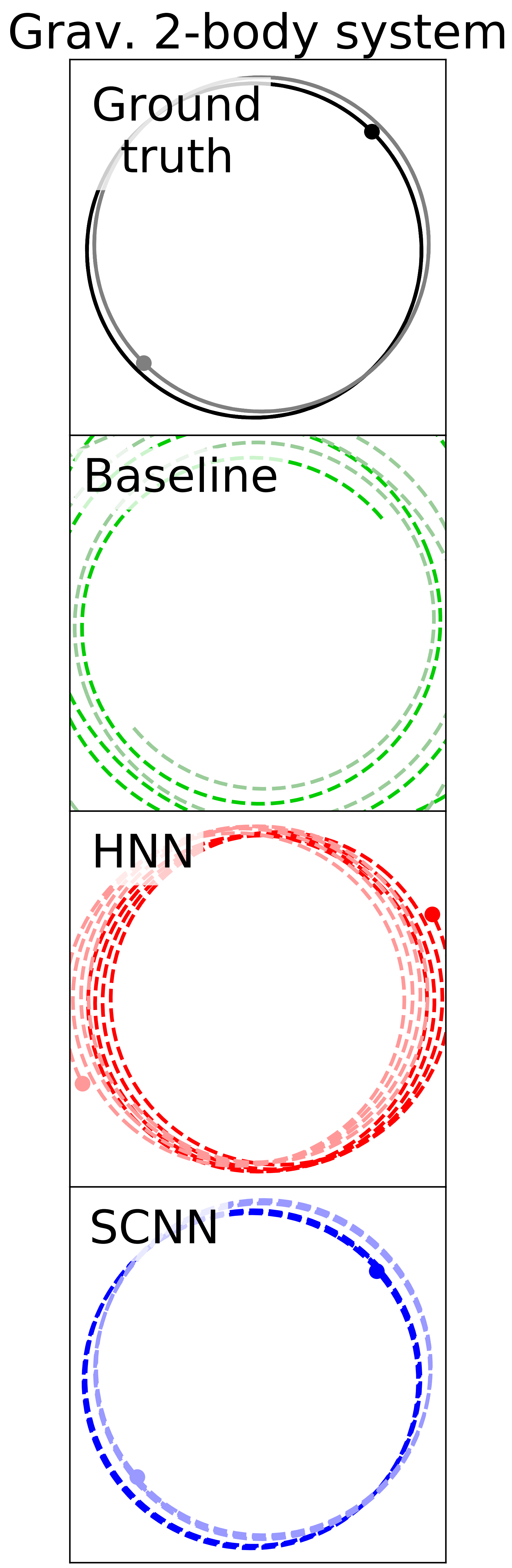
Actual Dual variables **Intermediate variables**

Betzler, Krippendorf 2020

Conclusions and Outlook

Learning and using physics bias with ML

- Bias networks with physics knowledge for efficient results:
  (e.g. numerical CY metrics, 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.
- Interpretation/enforcing of latent variables as variables of a dual theory (via appropriate losses)



Thank you!

2012.04656: Numerical CY-Metrics
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

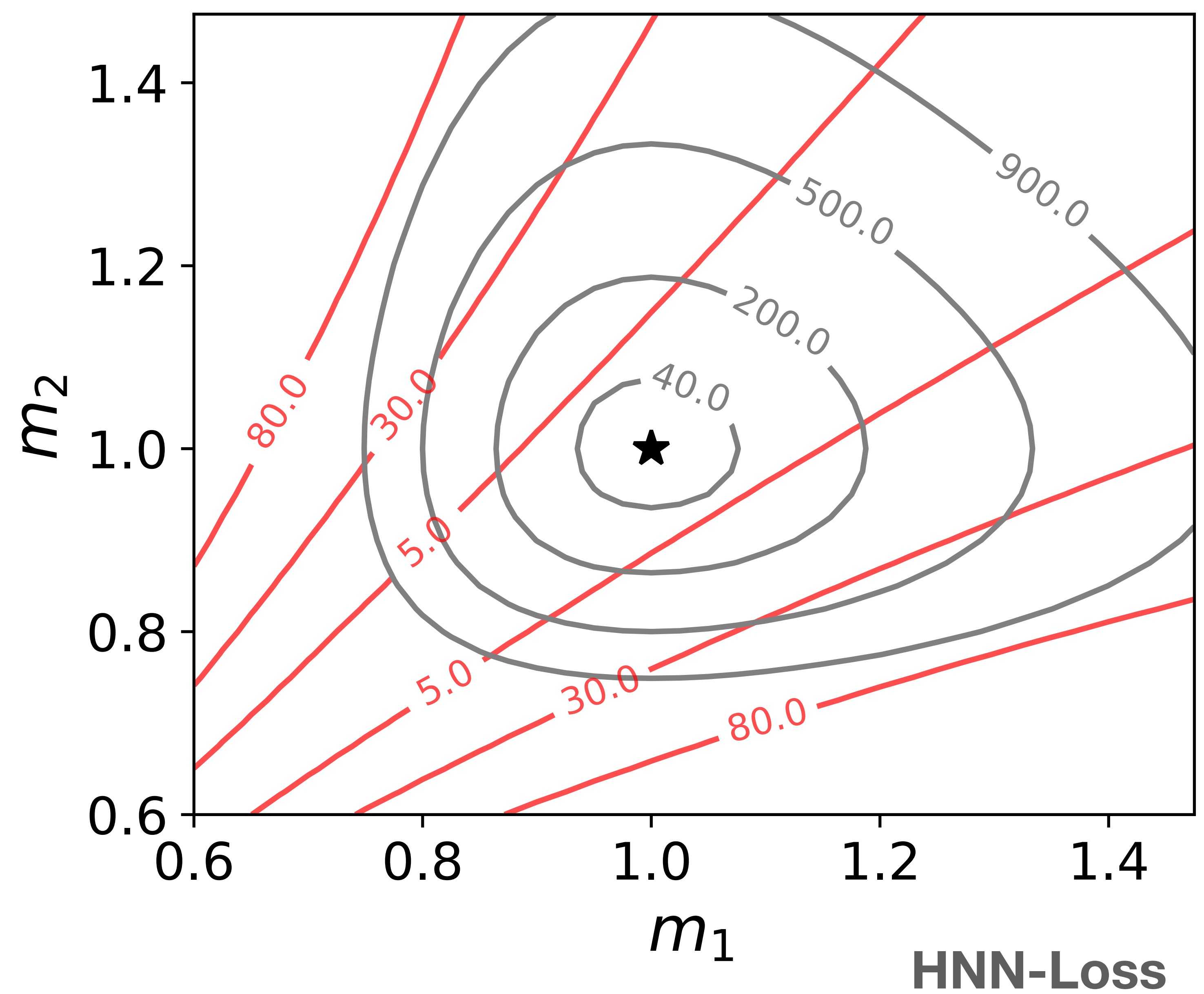
- Losses to ensure appropriate functional forms:

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

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

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

Effect of different loss components



HNN-Loss

Poisson-Loss