How can we learn mathematical structures of physical systems? String compactifications as a tool

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As physics students we learn formalisms/algorithms to describe dynamical systems

As physicists we develop and teach formalisms/algorithms to describe dynamical systems



but why? What makes these formalisms/algorithms special?

This makes such formalisms susceptible for optimisation.

$$\dot{q} = \frac{\partial H}{\partial p}$$

They are efficient in describing these systems.

<u>Today:</u> How can we leverage this efficiency to find mathematical structures by formulating appropriate optimisation problems?

... before delving into it, let's talk a bit about why we should care in the long-term, e.g.:

- theories? (cf. talks on generalised symmetries)
- How should we describe dynamics with little supersymmetry? (cf. talks on understanding N=1 moduli spaces)
- How should we describe the scattering of particles?

• Are there new mathematical structures to be discovered in our favourite field

What do we mean with an efficient description? Simple dynamical system

Simulation

such a system.

 We can measure how well we approximate such a system.

How?

Data: We can simulate such systems. E.g. solve your EOM with an appropriate numerical solver.

Model to predict the next time step.

$$(\dot{p}, \dot{q}) = M$$

We can try to predict the dynamics of



 $A(p,q,\theta)$

model parameters



. . . .

Battaglia et al 2016 (1612.00222)



Why is this exciting? **Mathematical structures via automatic differentiation**

Isn't this the bread and butter fitting and designing models which has been done for centuries?

NO, using automatic differentiation we can search for different mathematical structures and demonstrate their efficiency.



Simulation

Greydanus et al. 2019 Cranmer et al. 2020

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Model



Learning model for dynamics **Hamiltonian Neural Networks**

Physics Bias helps for predictions!



HNNs are more efficient than baseline NNs.

Physics Bias: enforce energy conservation





Greydanus et al. 2019 Cranmer et al. 2020 . . .



Krippendorf, Syvaeri (ICLR simDL workshop, 2104.14444)



Conserved quantities Introducing further 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 I IIDWIG

$$\dot{p} = -\frac{\partial H}{\partial q}$$
$$\dot{q} = \frac{\partial H}{\partial P}$$

$$\begin{array}{c} \underset{\text{hic}}{\rightarrow}, \mathbf{P}_{\text{other}}, \mathbf{Q}_{\text{other}}) \\ \text{onian Network} \end{array} \longrightarrow \left(\begin{array}{c} \dot{\mathbf{p}} = -\frac{\partial \mathcal{H}_{\phi}}{\partial \mathbf{q}}, \dot{\mathbf{q}} = \frac{\partial \mathcal{H}_{\phi}}{\partial \mathbf{p}} \\ \text{(Output)} \end{array} \right)$$









Benefits from Physicists' Bias

Conserved quantities interpretable:

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

 $L = -1.1q_{x_1}p_{y_1} + 0.9q_{x_1}p_{y_2} + 0.9q_{x_2}p_{y_1} - 1.0q_{x_2}p_{y_2} + 1.0q_{y_1}p_{x_1} - 0.$

Using learned conserved quantities helps in predicting trajectories.

> More sophisticated symbolic regression very active area of research [e.g. PYSR, Transformer (Large Language Models)]

$$.9q_{y_1}p_{x_2} - 0.9q_{y_2}p_{x_1} + 1.0q_{y_2}p_{x_2}$$



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:

$$F_k = \operatorname{tr}(L^k)$$

(additional condition for $\{F_k, F_i\} = 0$)

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:

$$F_{1} = 2 \lambda$$

$$F_{2} = 2\lambda^{2} + 4H$$

$$F_{3} = 2\lambda^{3} + 12\lambda H$$
 $\lambda...$ spectral parameter

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

. . .

Krippendorf, Lüst, Syvaeri 2021

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 Human interaction using domain knowledge

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

$$\mathscr{L}_{L} = \sum_{i,j} \min_{k} \left(||c_{ijk}\dot{L} - \dot{x}_{k}||^{2}, ||\dot{L}_{ij}||^{2} \right) + \sum_{k} \min_{ij} \left(||c_{ijk}\dot{L}_{ij} - \dot{x}_{k}||^{2} \right), \quad c_{ijk} = \frac{\sum_{batch} \dot{L}_{ij}}{\sum_{batch} \dot{x}_{k}}$$
$$\mathscr{L}_{LM} = \sum_{i,j} \min_{k} \left(||\tilde{c}_{ijk}[L, M]_{ij} - f_{k}||^{2}, ||[L, M]_{ij}||^{2} \right) + \sum_{k} \min_{ij} \left(||\tilde{c}_{ijk}[L, M]_{ij} - f_{k}||^{2} \right), \quad \tilde{c}_{ijk} = \frac{\sum_{batch} [L, M]_{ij}}{\sum_{batch} f_{k}}$$

• Avoiding mode collapse:

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

• Total loss:

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

• Aim: Method to find new Lax pairs with unsupervised learning (i.e. not requiring prior knowledge of a Lax pair)

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

Ansatz and Training

- Samples: points in phase space
- "complexity" of eom), e.g. for harmonic oscillator:

$$L_{ij}(p,q) = a_{ij} + b_{ij}q + c_i$$
$$M_{ij}(p,q) = d_{ij} + e_{ij}q + f_i$$
$$a_k = \sigma \left(a_k - \sum_{j \neq k} a_j \right)$$

enabling the network to single out individual components

Network ansatz: simple functions in terms of the variables/fields (guided by

ijP $p_{ij}p$ $\operatorname{Softmax}(\overrightarrow{a_k}) \cdot \overrightarrow{v}$ adding more parameters for better convergence

Applications Harmonic Oscillator

• Harmonic Oscillator:

 $H = \frac{1}{2}p^2 + \frac{\omega^2}{2}q^2;$

• Lax Pair:

 $L = \begin{pmatrix} 0.437 \ q & -0.07 \\ -0.666 \ p & -0.43 \end{pmatrix}$

• 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:

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

$$\dot{q} = p$$
, $\dot{p} = -\omega^2 q$

$$\begin{pmatrix} 0.73 & p \\ 437 & q \end{pmatrix}, \quad M = \begin{pmatrix} 0.001 & 0.329 \\ -3.043 & -0.001 \end{pmatrix}$$

Applications **Further systems**

Korteweg-de Vries (waves in shallow water):

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

• Heisenberg magnet:

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

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

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

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

$$\begin{aligned} A_x &= \begin{pmatrix} -1.7\phi & 1.7\phi + 1.0 \\ 1.7\phi + 1.0 & -1.7\phi \end{pmatrix}, \\ A_t &= \begin{pmatrix} 5.0\phi^2 + 1.7\phi'' & -5.0\phi^2 - 1.7\phi'' - 0.5 \\ -5.0\phi^2 - 1.7\phi'' - 0.5 & 5.0\phi^2 + 1.7\phi'' \end{pmatrix} \end{aligned}$$

$$\begin{split} A_{x} &= - \ \mathrm{i} \ \vec{\sigma} \vec{S} + 0.3 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ A_{t} &= \begin{pmatrix} 2 \ \mathrm{i} \ S_{z} & 2 \ \mathrm{i} \ S_{x} + 2S_{y} \\ 2 \ \mathrm{i} \ S_{x} - 2S_{y} & - \ \mathrm{i} \ S_{z} \end{pmatrix} \\ &+ \begin{pmatrix} \mathrm{i} \ S'_{y}S_{x} - \ \mathrm{i} \ S'_{x}S_{y} & -S'_{z}S_{x} + S'_{x}S_{z} + \ \mathrm{i} \ (S'_{z}S_{y} - S'_{y}S_{x}) & - \ \mathrm{i} \ S'_{y}S_{x} + \ \mathrm{i} \ S'_{x}S_{y} \\ &= 2 \ \mathrm{i} \ \vec{\sigma} \vec{S} + \ \mathrm{i} \ \epsilon_{ijk}\sigma_{i}S_{j}S'_{k} \ , \end{split}$$

see also recent work Lal, Majumder, Sobko 2304.07247





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





Summary: Learning 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,
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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)

We can do this with ML!

We get analytic and verifiable results. (see also review Gukov, Halverson, Ruehle)

Key insight: formulate this search as an optimisation problem. Generate data and solve it.



Human vs. LLM (2021 \rightarrow 2024) Scalability of scientific analysis from toy examples

- What is known about relevant mathematical structures for problem X? LLMs, graduate student, postdoc, professor
- Setting up the optimisation problem? LLMs, graduate student, postdoc, professor
- Implementing the code? LLMs, unexperienced coder, experienced coder



ChatGPT 4 ~

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You

 $\langle \rangle$

I am interested in integrable systems. Which mathematical structures are useful to describe such systems?



ChatGPT

Integrable systems are fascinating objects in mathematical physics and dynamical systems theory, showcasing a blend of algebraic, geometric, and analytical techniques. They are distinguished by their ability to be solved exactly in terms of integrals and often exhibit rich, complex behaviors that are, nonetheless, highly predictable. Several mathematical structures are particularly useful for describing and analyzing integrable systems:



Message ChatGPT...

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1. Lie Groups and Lie Algebras: These provide a framework for understanding the symmetries and associated Lie algebras help in the study of infinitesimal transformations, which play a crucial

ChatGPT can make mistakes. Consider checking important information.

LLMs can do some simple calculations, simple coding, and give some overview. NNs are extremely good function approximators.

What can we get out of Al numerical tools?

Which target for scaling up?

Cosmological constant How can we get hierarchies? Which mathematical structures to address hierarchies? Which *conjectures* can we proof for classes of models?

Roadmap: theoretical ways to address the CC

- Pick an interesting benchmark to develop customised ML methods, demonstrate capabilities and compare with human explorations:
 - Benchmark 1: IIB flux vacua. Different types of construction for $|W_0| \ll 1$? P(phenomenology|UV-data) searches]
 - Benchmark 2: mathematically proven statements about IIB flux vacua [exciting interface with LLMs in automated theorem proving]
- but we can be very explicit about the EFT.

[talk about our work by Andreas Schachner, interface with BSM experimental

Many compactifications and combinatorial choices, reasonable level of sophistication,



Systematically exploring model space Few \rightarrow Many $\rightarrow \infty$ -parameters: enhancing our analysis of EFTs

	Example	Method
Few parameter models	V(a,b)	Analytic
Models with scalable number of field	V(a i) I=1,…,N, N>>1	Analytic (often statistical physics) [Bousso/Polchinski, Douglas/Denef et al.,]
Models approximating any possible model	V _{NN} (x)	ML (NNs are universal approximations)





- Many parameter models
- NN models

Our target: exploration with numerical model building



Space of all models







Which BSM physics does string theory predict? **Problem: Analyse physics for many string compactifications**



Many physics models: As many as $10^{272,000}$ vacua [Taylor et al.: 1511.03209]

<u>Example</u>: Which model has a particular scale of supersymmetry breaking $|W_0^{\text{target}}|$?

How to solve this problem?

Design optimisation problem and find solution, e.g.:

- Evolutionary algorithms (genetic algorithms)

• ...

$$P_{\mathrm{NN},\theta}(\Delta \overline{N}_{\mathrm{flux}} | \overline{N}_{\mathrm{flux}})$$

<u>Result on "toy" model:</u> Learning a strategy can be more efficient in finding solutions than "standard" Monte Carlo.

Krippendorf, Kroepsch, Syvaeri: 2107.04039 Cole, Krippendorf, Schachner, Shiu: 2111.11466 (Neurips Physics Workshop) Krippendorf, Vall Camell: 2209.15433



Which BSM physics does string theory predict? Is there structure in the solutions? Yes

How are our solutions arranged in \overrightarrow{N} -space?



Krippendorf, Kroepsch (Master student), Syvaeri (PhD student): 2107.04039 Cole, Krippendorf, Schachner, Shiu: 2111.11466 (Neurips Physics Workshop) Krippendorf, Vall Camell: 2209.15433

 $(\overline{N} \in \mathbb{Z}^8)$

Time evolution from RL

0

100

400

100

0

200 300

Timestep

200 300 400

Timestep

 Flux Correlation Heatmap A3C

 $r_1 = 100$ 0.05 0.24 0.03 0.02 0.15 0.00 -0.8

 $r_1 = 0.05$ 100 0.12 0.01 0.00 0.03 0.06 0.31 -0.6

 $r_1 = 0.24$ 0.12 100 0.06 0.75 0.29 0.22 0.04 -0.6

 $r_{1} = 0.03$ 0.01 0.06 10 0.04 0.7 0.04 0.05 -0.4

 $r_{1} = 0.02$ 0.00 0.75 0.04 0.7 0.04 0.05 -0.2

 $r_{1} = 0.02$ 0.00 0.75 0.04 100 0.14 0.38 0.01 -0.2

 $r_{1} = 0.02$ 0.03 0.22 0.04 100 0.09 0.03 -0.2

 $r_{1} = 0.15$ 0.06 0.22 0.04 0.33 0.09 100 0.00 -0.4

 $r_{1} = 0.00$ 0.31 0.04 0.33 0.09 100 0.00 -0.6

 $r_{1} = 0.00$

Components of \overrightarrow{N} show correlations.

- 0.020 Japer Martin

0.015

0.010

0.005

0.025

Can we characterise structures analytically via dimensional reduction?

Performed Principal Component Analysis on the output of flux vectors in \mathbb{Z}_8 .

<u>Robustness:</u> same structure with genetic algorithm (GA).

Hints that solution space is effectively lower-dimensional.

Distribution of samples generated by RL $(\overrightarrow{N} \in \mathbb{Z}^8)$



What do we need for many-moduli examples?

Easily obtain flux vacua relevant for our physics questions:

- Many geometries, different regions of moduli space
- Different questions (e.g. SUSY, non SUSY vacua)
- Many samples (statistics, dedicated search algorithms)

\rightarrow JAXvacua

See Andreas Schachner's talk

2306.06160

ace)

What can we say about W_0 using JAXvacua?

2307.15747: work with J. Ebelt (Master student), A. Schachner

What can we say about W_0 ?

 $W_0 = \sqrt{2/\pi} \ e^{K/2} \ W$

Universal behaviour

Looks Gaussian? (Near origin: Gaussian [Denef, Douglas, ...])



cf. Erik Plauschinn's talk

What can we say about W_0 ?

Gaussian distribution is a reasonable fit.

We observe deviations which now can be characterised.

Gaussian approximation \rightarrow Expectation for smallest value for $|W_0|$ for a given sample (interesting for dS in KKLT).

Standard deviation + $N_{\rm flux}$ + sample size relevant!

Benchmark for dedicated search algorithms.





Conclusions How can we learn mathematical structures?

- Formulate appropriate optimisation problem and solve it. This does not require knowing the mathematical structure apriori.
- Today examples where this allows to find symmetries and integrable structures (Lax pair/connection, symmetries)
- Why is it working? Using physics bias and appropriate mathematical structures is more efficient, i.e. mathematics is unreasonably effective and this can be used to find it [Wigner]
- Automatic differentiation and probabilistic programming are key. Numerically harder problems can be addressed as well using dedicated efforts with reasonable scaling of computational cost.
- Flux vacua benchmark: what can we obtain for models with many moduli?
- Which role will LLMs play? How quickly can we scale from toy tasks to larger tasks? What are foundation models for mathematical physics?





Thank you!

New Master of Physics degrees at LMU Munich and Cambridge

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https://mphildis.bigdata.cam.ac.uk/