ML and Physics Lec II: ML for Physics



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What is Physics?

• A Physical law:

$$\mathcal{S}_{\mathrm{i}} \xrightarrow{\mathscr{L}} \mathcal{S}_{\mathrm{f}} ,$$

- A restriction on the space of (mathematically) possible S
- How we make theories?
- The whole Process:
 - 1) Information from nature
 - 2) (Complicated) process of analysis by the physicist (intelligence)
 - 3) Making Models
 - 4) Prediction of new Phenomena
- In Brief: Data \Rightarrow Training (intelligence) \Rightarrow Predictions

The Physics Challenges

-) What are good representations of States \mathcal{S} and Laws \mathcal{L} ?
- The representations (S, \mathcal{L}) are usually (in practice and maybe in principle) effective
- 2) Assuming Universality of a given description, Applying it to different systems
 - Description of larger systems in term of smaller systems (Different Level of effectiveness)
 - Solving models
- 3 Relation of description with Previous Knowledge and Models

Two Paradigms for Programming



- Hard problems: a lot of computational steps (time) or/and memory
- Finite amount of resource

Two Computations



IF B > D THEN IF A > B THEN PRINT C * C ELSE IF C > A THEN IF D > C THEN IF B > C THEN PRINT B * C ELSE PRINT C * D END IF ELSE PRINT A * B END IF ELSE PRINT A * C IF A > D THEN PRINT A * D ELSE PRINT B * D END IF END IF END IF ELSE PRINT A * A END IF



Inverse problems and ML

- e.g. Discovery of Neptune from the perturbed trajectory of Uranus.
- Earth density from acoustic wave
- Tomographic reconstruction, i.e CT scan

An Inverse Problem

• Given the input x find the value of f(x) by:

$$f(x) = \sum_{k=0}^n J_k x^k$$

- The Inverse:
 - 1. given an output y_1 find the input x_1 such that $y_1 = f(x_1)$
 - 2. given some data $\{(x_1,y_1),(x_2,y_2),\dots\}$ find the function y=f(x), i.e. J_k

• Example:

$$y_i = \sum\limits_{k=1}^m J_{ik} x_k$$

• Very special cases: $(n=m,\det J\neq 0)$

$$x_k = \sum_{i=1}^m \left[J^{-1} \right]_{ki} y_i$$

- In many cases, the solution to the inverse problem is ill-posed.
- In general it is possible to define:

$$L\equiv\sum_{i=1}^n\left(y_i-\sum_{k=1}^mJ_{ik}x_k\right)^2=0$$

 $\bullet\,$ seek an x_k that minimizes L

Inverse Problem And ML

- \Rightarrow Optimization problem
- \Rightarrow Representing the map with an NN
- Estimation of parameters of the model based on observation
- Printing Vs Digit Recognition

Inverse Problems in Physics

- Knowing objects that cannot be measured directly
- Infering the cause from the results
- Determining physical laws and governing equations
- Determining physical constants
- All physics innovations are inverse problems

Scattering And Imaging

• Unknown Object



• The image is reconstructed from information of scattered waves

Inverse Scattering Problem

• Unknown Potential, Law,



• The potential is determined from information such as scattering amplitudes

Simulations and ML

- Use of computer simulations to generate samples of labeled training data $\{x_i,y_i\}$
- Learn fast neural network to generate the results of simulations.
- Data generation
- Learn the network once

Machine learning phases of matter^{1, 2}

- Large state space \rightarrow complexity
- Classification of phases
- Identify phases from state
- \Rightarrow neural-network classification
- Study of phase transitions and order parameters
- Classify The Ising Phases

¹nature.com/articles/nphys4035 ²nature.com/articles/nphys4037

String Theory And ML

- String Theory: First Prediction: 10d spacetime
- Don't Worry \Rightarrow $M^{10} = M^4 \times X^6$
- A lot of possibilities! \bigcirc
- Topology and geometry of compact dimensions (in addition of Branes and Fluxes)
- The problem is to select a manifold necessary for compaction of string theory so that it becomes the standard model of elementary particles
- \Rightarrow An inverse problem

2-D Manifolds



String Phenomenology to CY

- Classical vacuum of string theory on X^{10} preserves $\mathcal{N} = 1$ SUSY in M^4
- Killing Spinor \Rightarrow Covariant constant spinor \Rightarrow Ricci-Flat internal X⁶ space
- The gauge group/particle content of low energy theory depends on the topology of compact space
- Direct Problem: Find the resulting 4D theory from a given topology?

Calabi–Yau manifolds

$$d=1$$
 Torus $T^2=S^1 imes S^1$



4-torus:
$$T^4=\left(S^1
ight)^4$$

$$d = 3$$
 CY3: Unclassified, billions known



Complete Intersection Calabi-Yau

- $\bullet\,$ CY as Intersections of hypersurfaces in \mathbb{P}^n
- Configuration matrices:

$$\mathbf{K} = \begin{bmatrix} \mathbf{n}_1 & \mathbf{q}_1^1 & \mathbf{q}_1^2 & \dots & \mathbf{q}_1^K \\ \mathbf{n}_2 & \mathbf{q}_2^1 & \mathbf{q}_2^2 & \dots & \mathbf{q}_2^K \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{n}_m & \mathbf{q}_m^1 & \mathbf{q}_m^2 & \dots & \mathbf{q}_m^K \end{bmatrix}_{m \times K}$$

- Classifying the CICY matrices, checking redundancies and equivalences
- Obtained ~ 10^{10} configuration

Train The CYs

- Training data: $\{k_i, h(k_i)\}$ from very lengthy calculations
- Being Similar to SM as a label:



- Design the network \Rightarrow Probe the landscape, More than 90% accuracy
- Refer to HRD problem

The CY Landscape: from Geometry to Physics, to ML

Lecture Notes in Mathematics 2293

Yang-Hui He

The Calabi—Yau Landscape

From Geometry, to Physics, to Machine Learning



Machine-Learning the Classification of Spacetimes¹

 Petrov-Penrose Classification of Spacetimes

$$\begin{split} \Psi_0 &\equiv \mathrm{C}_{abcd} k^a m^b k^c m^d, \quad \Psi_1 \equiv \mathrm{C}_{abcd} k^a l^b k^c m^d \\ \Psi_2 &\equiv \mathrm{C}_{abcd} k^a m^b \bar{m}^c l^d \qquad \Psi_3 \equiv \mathrm{C}_{abcd} k^a l^b \bar{m}^c l^d \\ \Psi_4 &\equiv \mathrm{C}_{abcd} \bar{m}^a l^b \bar{m}^c l^d \end{split}$$

$$\Psi_0 - 4z\Psi_1 + 6z^2\Psi_2 - 4z^3\Psi_3 + z^4\Psi_4 = 0$$



• NNs: $\{\Psi_0, \Psi_1, \Psi_2, \Psi_3, \Psi_4\} \rightarrow$ Types



¹arXiv:2201.01644 , Y. He, J. Manuel P. Ipiña

Particle Physics

- Experiments such as CMS and ATLAS at the LHC generate petabytes of data per year.
- Features x_i in detector labeled y_i by particles or interactions \Rightarrow classification
- Signal and Background discrimination
- Jet Classification (heavy and light quarks, gluons, and W, Z, and H bosons)
- Fast Simulation: SM and BSM leads to which results
- Search for anomalies: classify SM and BSM events
- Neutrino physics, phase transitions of quantum chromodynamics, ...
- Many other applications^{1, 2}

¹arXiv:1807.02876

²arXiv:1806.11484

Cosmology And Astrophysics

- Gravitational lens finding
- Simulation
- Inverse problem: Interferometer Gravitational-Wave Observatory (LIGO) time series to the underlying waveform from a gravitational wave
- Data recorded on detectors \rightarrow gravitational wave
- Reconstruct the image of a black hole from data from array of telescopes (EHT)
- Classification of galaxies
- ...1

Other Applications

- Other examples of inverse problems in physics
- Inverse of boundary value problem
- Landscape of Theories e.g. Conformal Bootstrap, Space of Integrable Theories
- Quantum State Tomography¹: Reconstruct the density matrix of an unknown quantum state, through experimentally available measurements
- AdS/CFT correspondence: determining gravity theory, the inside (bulk), from the quantum field theory living on the boundary

¹arxiv:1703.05334

Wave Function of a Quantum Many-Body System

• The Quantum state

$$\left|\psi\right\rangle = \sum_{s_{1},\cdots,s_{N}}\psi\left(s_{1},\cdots,s_{N}
ight)\left|s_{1}
ight
angle\cdots\left|s_{N}
ight
angle$$

- The nonlinear function ψ transforms the input $(s_1, , s_N) = (0, 0, 1, 0, 1,)$ into output $\psi(0, 0, 1, 0, 1,)$.
- Minimize the energy function

$$\mathbf{E} = \frac{\langle \psi | \mathbf{H} | \psi \rangle}{\langle \psi | \psi \rangle}$$

• The ground state

The NN Quantum States

• Neural networks as a method of constructing quantum states

Represent the nonlinear state function as $|\Psi\rangle$ by

$$\Psi(\mathbf{q}) \equiv \mathbf{g}^{(L)} \left(\boldsymbol{\theta}^{(L)} \dots \mathbf{g}^{(2)} \left(\boldsymbol{\theta}^{(2)} \mathbf{g}^{(1)} \left(\boldsymbol{\theta}^{(1)} \mathbf{q} \right) \right) \right)$$

- An Energy Function
- \Rightarrow Optimization $\Rightarrow \theta^*$
- $\Rightarrow \Psi_{\theta^{\star}}(\mathbf{q})$

RBM and The Wave Function¹

• Restricted Boltzmann Machines:



• The Neural-Network Quantum States:

$$\Psi_{M}(\mathcal{S}; \mathcal{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

• Minimize the Energy Function

$$E(\mathcal{W}) = \left< \Psi_{M} | \mathcal{H} | \Psi_{M} \right> / \left< \Psi_{M} | \Psi_{M} \right>$$

• Exponential to polynomial complexity ¹Science 355, 602 (2017) 8.

DBM and The Wave Function¹

• Deep Boltzmann Machines:



$$\Psi_{\mathcal{W}}\left(\sigma^{z}\right) = \sum_{\{h,d\}} \exp\left[\sum_{i} a_{i}\sigma_{i}^{z} + \sum_{ij}\sigma_{i}^{z}W_{ij}h_{j} + \sum_{j}b_{j}h_{j} + \sum_{jk}h_{j}d_{k}W_{jk}' + \sum_{k}b_{k}'d_{k}\right]$$

¹Nat Commun 9, 5322 (2018).

Some Refrences

- 1 A high-bias, low-variance introduction to Machine Learning for physicists: arXiv:1803.08823
 - Introduction to the core concepts and tools of machine learning
 - Python Jupyter notebooks
- (2) Deep Learning and Physics; Akinori Tanaka, Akio Tomiya, and Koij Hashimoto, springer.com/book/10.1007/978-981-33-6108-9

Summery

- Technique and methods of ML are well adapted to physics
- Using ML in physics is rapidly expanding
- The range of problems vary from classical physics, to quantum theory, particle physics and string theory