Physics-Informed-Neural-Networks (PINNs) for the Wigner-Fokker-Planck model of open quantum systems

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Introduction

Question: How can we quantify the agreement of a physical model with experimental data?
Answer: For example, by means of

$$D_o - O(y(p)) = \varepsilon(p), \quad J(p) = ||O(y(p)) - D_o||_q^q \tag{1}$$

D_o : Experimental Data of a given observable quantity
y: Predictive Model (either mathematical or computational)
O: Observable to be predicted by the model
$p \in P$: Parameter of our predictive model (scalar, vector, function...) in a space P
$\varepsilon(p)$: error (in experimental measurement, in theoretical model, in its computation...)
$J(p)$: Error Functional adequate for our problem; $q = 2$, or Wasserstein in Machine Learning, etc.
Approaches:

- Forward Modelling: Given D_o, y, and p, compare the prediction $O(y(p))$ against D_o.
- Inverse Modelling: Given D_o and y, infer p_0 that minimizes $J(p)$, without overfitting below experimental measurement error. There might be multiple local minimizers p_0's.

Physics-Informed-Neural-Networks (PINNs): an Intro

Data Science & Machine Learning: Main advantage is that one develops a computational model $y(p)$ that can predict future events, based on knowledge of data D, by fitting a large number of parameters, represented by a vector p. Choice of parameters is performed by minimizing a functional

$$J_{\mathrm{data}}(p) = ||D_o - O(y(p))||. \tag{2}$$

Seminal idea for **Physics-Informed**-Neural-Networks (M. Raissi, P. Perdikaris, G.E. Karniadakis, [3] *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, JCP 378, 2019): If a physical "law" is already known for the problem,

$$F(y) = 0 \tag{3}$$

consider as well, in the minimization problem for the parameters, the residual

$$F(y(p)) = R(p), \quad J_{\mathrm{phys}}(p) = ||R(p)||, \tag{4}$$

in respecting the satisfaction of a "physical law" known in advance:

$$J(p) = J_{\mathrm{data}}(p) + J_{\mathrm{phys}}(p) \tag{5}$$

Moral: A good model fits the data **and** also satisfies the Physics of the problem.
Key: role of automatic differentiation in deep learning. Differs from Wang et al, 17

Brief literature review (non-exhaustive) on Machine Learning in Computational Physics:

Previous work used Machine Learning as black-box tools

- Physics-informed ML: "Wang et al., A comprehensive physics-informed machine learning framework for predictive turbulence modeling, 2017"
- Examples of machine learning for prediction of physical systems:
  - Y. Zhu, N. Zabaras, Bayesian deep convolutional encoder-decoder networks for surrogate modeling and uncertainty quantification, 2018, arXiv:1801. 06879.
  - T. Hagge et al. Solving differential equations with unknown constitutive relations as recurrent neural networks, 2017, arXiv:1710.02242.
  - R. Tripathy et al. Deep UQ: learning deep neural network surrogate models for high dimensional uncertainty quantification, 2018, arXiv:1802.00850.

Brief literature review (non-exhaustive) on Machine Learning in Computational Physics:

- Raissi et al. 2019: revisit activation and loss functions for the differential operator. Open black-box by understanding automatic diff. in deep learning.
- Use automatic diff. as in deep learning, to physics-inform neural networks by differentiation w.r.t. space-time coords. Regularization & lets use simple feed-forward neural network architecture & training with small data.
- Lin et al. Why does deep & cheap learning work so well? J. Stat. Phys. 2017
- Builds upon
  - Psichogios et al. A hybrid neural network-first principles approach to process modeling, AIChE J. 38 (1992) 1499–1511.
  - I.E. Lagaris, A. Likas, D.I. Fotiadis, Artificial neural networks for solving ordinary and partial differential equations, IEEE Trans. Neural Netw. 9 (1998)
  - R. Kondor, N-body networks: a covariant hierarchical neural network architecture for learning atomic potentials, 2018, arXiv:1803 .01588.
  - R. Kondor, S. Trivedi, On the generalization of equivariance and convolution in neural networks to the action of compact groups, 2018, arXiv
  - M. Hirn, S. Mallat, N. Poilvert, Wavelet scattering regression of quantum chemical energies, Multiscale Model. Simul. 15 (2017) 827–863.
  - S. Mallat, Understanding deep convolutional networks, Philos. Trans. R. Soc. A 374 (2016) 20150203.

Machine Learning for open quantum systems

Previous work on this line has been developed in the papers below:

- Deep Reinforcement Learning for Quantum State Preparation with Weak Nonlinear Measurements. Riccardo Porotti, Antoine Essig, Benjamin Huard, and Florian Marquard. Quantum 6, 747 (2022)
- Ettore Canonici, Stefano Martina, Riccardo Mengoni, Daniele Ottaviani, and Filippo Caruso, "Machine Learning based Noise Characterization and Correction on Neutral Atoms NISQ Devices", Advanced Quantum Technologies 7 1, 2300192 (2024).
- Bjorn Annby-Andersson, Faraj Bakhshinezhad, Debankur Bhattacharyya, Guilherme De Sousa, Christopher Jarzynski, Peter Samuelsson, and Patrick P. Potts, "Quantum Fokker-Planck Master Equation for Continuous Feedback Control", Physical Review Letters 129 5, 050401 (2022).

However, to our knowledge, nobody has applied PINNs to study the Wigner-Fokker-Planck model for open quantum systems such as collisional electron transport in semiconductors yet.

Overview

We want to solve the Wigner-Fokker-Planck (WFP) equation, under a harmonic potential, via a Physics Informed Neural Network (PINN).

This equation is used for open quantum systems to model the interaction between a quantum (sub-)system and its environment [4].

- WFP is a kinetic/diffusive model for open quantum systems
- Applications in semiconductors, computational electronics, quantum optics, quantum computing and information science, etc.
- Diffusion operator represents part of the noise (together with a friction term) introduced by the environment over the (sub-)system with which it interacts

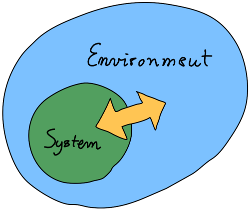


Figure: Open Quantum System

Wigner Fokker Planck Equation

Describes the time evolution of a quasi-probability Wigner function $w(x, k, t)$, which is the Wigner transform of the density matrix $\widehat{\rho}$ [2]

The Wigner-Fokker-Planck model is defined as an Initial Value Problem in the form

$$w_t + k \cdot \nabla_x w + \Theta_\hbar[V](w) = Q_{\hbar,FP}(w)$$
$$x, k \in \mathbb{R}^d, t \in \mathbb{R}^+, \quad w(t = 0, x, k) = w_0(x, k)$$

$Q_{\hbar,FP}(w)$: Quantum Fokker-Planck operator. Models the interaction of the quantum system and its environment.

$\Theta_\hbar[V](w)$: Pseudo-differential integral operator. Takes into account the non-local action of the Potential. [4]

Under a harmonic potential, this will look like a **convection-diffusion** problem, simpler than fluid models such as Navier-Stokes!

We will have a "quantum fluid" over a quantum phase space, where there is a flow of quantum information under diffusion and friction due to environment noise.

Where is our data coming from?

Using a Monte-Carlo-based (Euler-Maruyama) solver for WFP under a harmonic potential [1], we generated data from the initial condition to the steady state.

Computational Methods for Wigner-Fokker-Planck modeling of open quantum systems

31ST INTERNATIONAL MATERIALS RESEARCH CONGRESS 2023 Cancún, México

Arash Edrisi (Ph. D. student), Hamza Patwa (undergrad), JAME

Monte Carlo (MC) methods for Wigner-Fokker-Planck models under a harmonic potential

- Code benchmark: Stochastic modeling of WFP for harmonic potentials with Coherent State IC
- Implementation: Euler-Maruyama method for Stochastic Differential Equations
- Further work: More accurate time evolution methods such as Runge-Kutta 2
- *Work in progress: Study of Empirical Pseudo-potential Methods (Chelikowsky, Cohen) for (conduction/valence) band-structure of semiconductor materials (Si, Ge, etc.).*
- *Future Work: quantum computing methods for these eigenvalue calculations for Materials*
- Related view paper: ‘Noisy intermediate-scale quantum (NISQ) algorithms’, Bharti et al., 2021

Pseudocode:

- Initialize
- Define Variables
- $q^1 = zero[1,M]$
- $p^1 = zero[1,M]$
- $N = 10^4$
- $M = 10^4$
- $D_{qq} = 1$
- $D_{pp} = 1$
- $\mu = 0$
- $\Delta t = 0.01$
- for $(j = 1; j < M; j++)$

  {

  $q_j^1 = normrnd(\mu, D_{qq})$

  $p_j^1 = normrnd(\mu, D_{pp})$

  }

  end
- for $(i = 1; i < N; i++)$

  {

  $for\ (k = 1; k < M; k++)$

  {

  $$\vec{\varepsilon} = \begin{bmatrix} q \\ p \end{bmatrix} = \begin{bmatrix} normrnd(\mu, D_{qq}) \\ normrnd(\mu, D_{pp}) \end{bmatrix}$$

  $$\vec{\alpha} = \begin{bmatrix} p_k^i \\ -q_k^i - p_k^i \end{bmatrix}$$

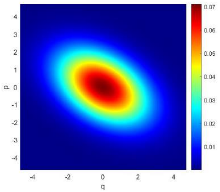
  $$\begin{bmatrix} q_k^{i+1} \\ p_k^{i+1} \end{bmatrix} = \begin{bmatrix} q_k^i \\ p_k^i \end{bmatrix} + \vec{\alpha}\Delta t + \vec{\varepsilon}\Delta t$$

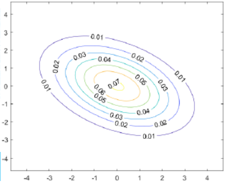
  }

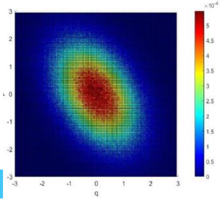
  end

  }

  end







Where is our data coming from?

Algorithm 1 Euler–Maruyama for the Wigner–Fokker–Planck equation (harmonic potential)

Define:
$L \leftarrow 1.0$
$\sigma_q \leftarrow \frac{L}{\sqrt{2}}$
$\sigma_p \leftarrow \frac{1}{\sqrt{2}L}$
$\delta_t \leftarrow 0.01$
$Total\_Time \leftarrow 50.$
$NumOfTimeStep \leftarrow \text{round}\{\frac{Total\_Time}{\delta_t}\}$
$NumOfParticles \leftarrow 10^4$
$\mu_1 \leftarrow 0.$
$\mu_2 \leftarrow 0.$
$\mu \leftarrow \begin{bmatrix}\mu_1 & \mu_2\end{bmatrix}$
$D_{qq} = 1., \quad D_{pp} = 1.$
$\gamma = 1.$
$D \leftarrow \begin{bmatrix} D_{qq} & 0 \\ 0 & D_{pp} \end{bmatrix}$
Arrays Initialization:
$q \leftarrow \text{zeros}[NumOfTimeStep,\ NumOfParticles]$
$p \leftarrow \text{zeros}[NumOfTimeStep,\ NumOfParticles]$
Initial Conditions:
$q[1,:] \leftarrow \text{normrnd}(\mu[1],\ \sigma_q,\ [1,\ NumOfParticles])$
$p[1,:] \leftarrow \text{normrnd}(\mu[2],\ \sigma_p,\ [1,\ NumOfParticles])$
Update:
for each $i \in NumOfTimeStep$ **do**
  for each $j \in NumOfParticles$ **do**
    $\epsilon \leftarrow \text{mvnrnd}(\mu,\ 2D\delta_t)$
    $q[i+1,\ j] \leftarrow q[i,j] + p[i,j]\delta_t + \epsilon[1]$
    $p[i+1,\ j] \leftarrow p[i,j] + (-q[i,j] - \gamma p[i,j])\delta_t + \epsilon[2]$
  end for
end for

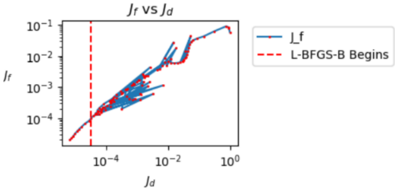
Figure: GitHub repository https://github.com/phjame/StochasticWFP (accessed on 29 February 2024), for the computational implementation of an Euler–Maruyama-based Monte Carlo solver for WFP under a harmonic potential

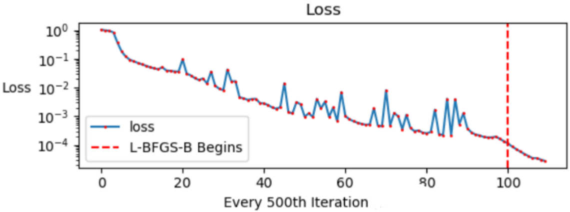
WFP PINN Latest Results

A Feed Forward Neural Network with 8 Hidden layers of 20 neurons. First trained using the Adam optimizer followed by L-BFGS-B. From the 1,320,000 data points, we trained using 6,600. Only 0.5% of total dataset.

Noiseless: Losses

Quantity of Interest	Error for Noiseless Training	Error for Noisy Training
Relative Error in L2-norm for Wigner function	0.002	0.002
D_{pq}(absolute)	0.004	0.004
D_{pp}(relative)	1.547%	1.536%
D_{qq}(relative)	0.662%	0.687%





We modified Raissi's repo for N-S (maziarraissi.github.io/PINNs) for WFP

Conclusions

- We have used Physics-Informed-Neural-Networks (PINNs) for "data-driven discovery of PDEs": the inverse problem for the diffusion matrix in the Wigner-Fokker-Planck equation under a harmonic potential.
- By modifying Raissi et al.'s repository, we have adapted their code for the data-driven discovery of the Navier-Stokes fluids problem to our "quantum-fluid" problem in phase space, the Wigner-Fokker-Planck equation, given the similarities in the math & physical interpretation of a flow transport under diffusion processes.
- Preliminary data indicates that parameters estimated to both fit the data and respect the quantum physics are found to be as close to the true values as Raissi et al. were for Navier Stokes (relative errors of order 1%): Sanity check
- So far our data is "synthetic". Later on, our data for this phenomenon could come from actual observables measured in an experimental lab:
  - Assuming that the noise in an open quantum system is Markovian, WFP is a good model (the Physics to be respected)
  - This data-driven discovery of PDEs could help estimate both diffusion and friction mechanisms of the problem: we could estimate quantitatively the noise introduced by the environment!
  - This could have interesting applications in the control and use of noise in open quantum systems: ground state preparation via Lindbladians, etc.

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Figure: Isaul Garcia (Physics Ph. D. student at Boston University; UTSA B. Physics), Jose Morales Escalante (UTSA Assistant Professor, Math and Physics & A. Depts.)

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