

Quantum Dynamics with Time-Dependent Neural Quantum States

A. Romero-Ros^{1,2,*}, J. Rozalén Sarmiento^{1,2}, A. Ríos^{1,2}

¹Departament de Física Quàntica i Astrofísica (FQA), Universitat de Barcelona (UB), c. Martí i Franquès, 1, 08028 Barcelona, Spain.

²Institut de Ciències del Cosmos (ICCUB), Universitat de Barcelona (UB), c. Martí i Franquès, 1, 08028 Barcelona, Spain.

*E-mail: alejandro.romero.ros@fqa.ub.edu



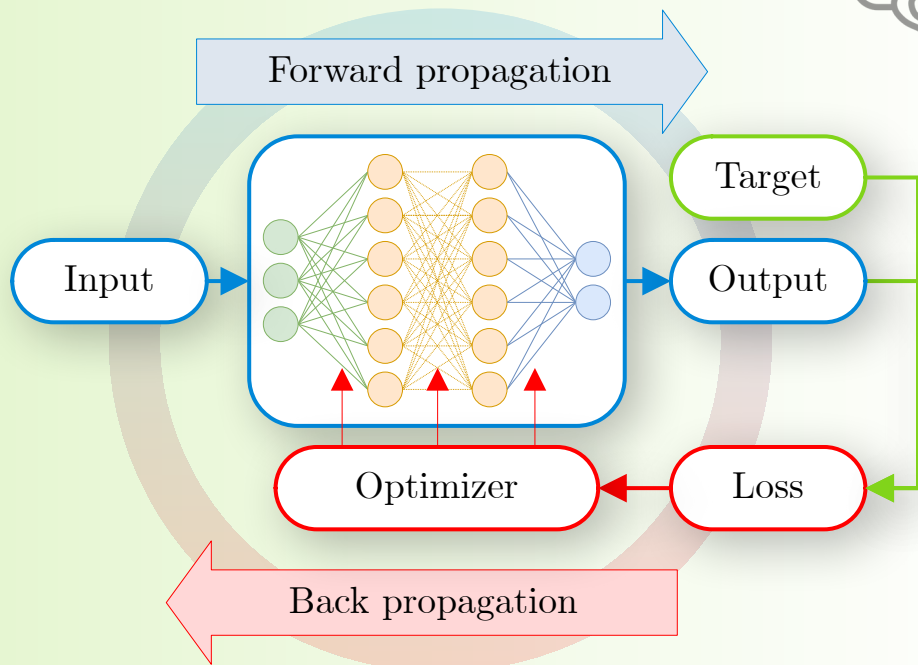
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Classical Neural Networks (train)

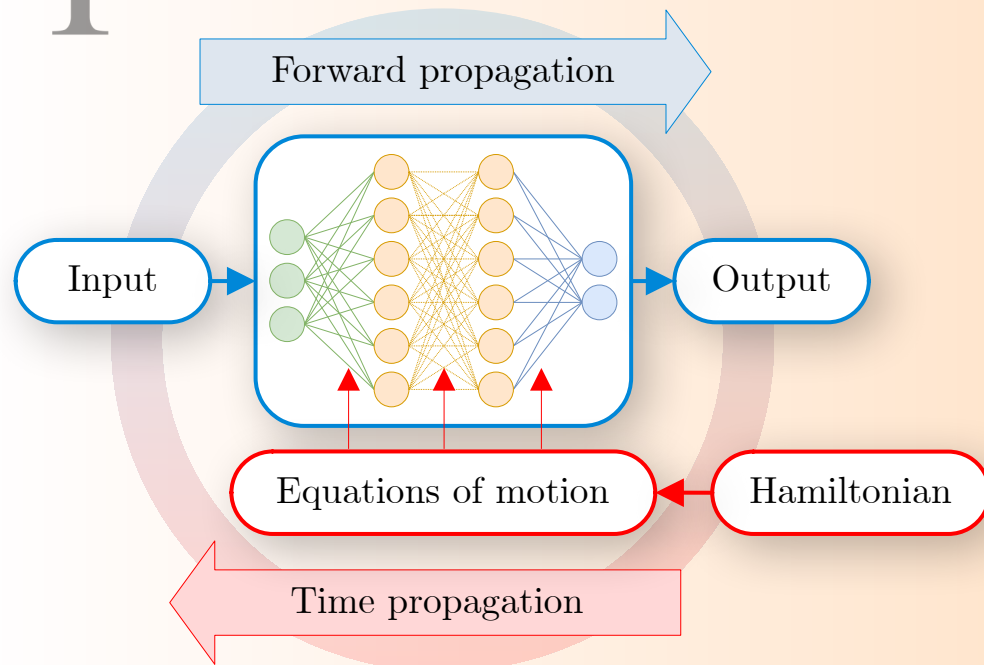


- Gradient Descent Optimizers

Parameters updated via
Optimizers driven by the Loss



Neural Quantum States (evolve)



- Time-dependent Variational Principle

Parameters updated via
Equations of Motion driven by the Hamiltonian

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NEURAL QUANTUM STATES (NQS)

$|\Psi\rangle = \Psi(\vec{r}, \vec{p}, \vec{\sigma})$
 A NQS is a wavefunction ansatz parametrized by the weights and biases of an artificial neural network (NN).
 The architecture of the NN needs to be able to efficiently capture the relevant symmetries and global constraints of the system under consideration.^[1]
 The time-dependent variational principle allows to compute the equations of motion of the NN parameters that determine the dynamics of the wavefunction.^[2]

EQUATIONS OF MOTION

Given the Lagrangian $L(\vec{r}, \vec{p}, \vec{\sigma}) = \frac{(\Psi|\hat{H}|\Psi)}{(\Psi|\Psi)}$, the minimization of the action $\delta S[\vec{r}, \vec{p}, \vec{\sigma}] = 0$, yields the following equations of motion:

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial \vec{p}} \cdot \frac{\partial}{\partial \vec{r}} \right) \left(\frac{\partial}{\partial \vec{p}} \cdot \frac{\partial}{\partial \vec{r}} \right) \Psi = - \left(\frac{\partial}{\partial \vec{p}} \cdot \frac{\partial}{\partial \vec{r}} \right) \Psi$$

with $\vec{r} = \frac{\partial}{\partial \vec{p}}$, $\vec{p} = -\frac{\partial}{\partial \vec{r}}$

$$A_{\vec{r},\vec{p}} = \frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \left(\frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \right) \Psi = \frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \left(\frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \right) \Psi$$

$$B_{\vec{r},\vec{p}} = \frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \left(\frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \right) \Psi = \frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \left(\frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \right) \Psi$$

$$F_{\vec{r},\vec{p}} = \frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \left(\frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \right) \Psi = \frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \left(\frac{\partial}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} \right) \Psi$$

MOTIVATION

Neural Quantum States (NQS) leverage the power of machine learning to approximate quantum wavefunctions as parametrized neural networks.

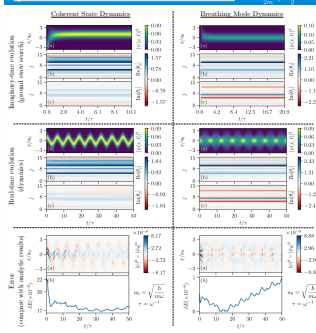
NQS offer a scalable framework for solving many-body problems beyond the reach of traditional methods – from spin systems^[3] to quantum density^[4].

In this poster, we present an introduction to NQS by solving two Quantum Harmonic Oscillator examples.

TIME-DEPENDENT VARIATIONAL PRINCIPLE

The variational manifold $\mathcal{M}$ contains all the possible trial states $|\Psi\rangle$.
 Our goal is to time-evolve the parameters $\theta(t)$ so that $|\Psi_{\text{exact}}\rangle$ reaches the target state $e^{-iHt}|\Psi_0\rangle$ through changes $\delta\theta$ within the manifold $\mathcal{M}$.

QUANTUM HARMONIC OSCILLATOR DYNAMICS



METHODS

NN architecture
 In our case, $|\Psi\rangle$ belongs to the equations of motion real $\vec{r} = -\vec{S}^{-1} \cdot \vec{p}$, where $\vec{S} = -\vec{p}^T \cdot \vec{r}$ is the so-called "symplectic tensor".^[5]
 In general, $\vec{S}$ is ill-conditioned. To invert it, we regularize it with a diagonal shift: $\vec{S} \leftarrow \vec{S} + \lambda \mathbb{I}$, with $\lambda \in \mathbb{C}$ and $|\lambda| \ll 1$.
 The equations of motion are integrated using a 4th order Runge-Kutta method.
 The NN is implemented using PyTorch^[6].

CONCLUSIONS

- NQS do not require learning new training.
- NQS evolve in time through the parameters of a NN.
- The equations of motion of the parameters can be integrated using traditional methods.
- Numerical instabilities are an important problem to be addressed.
- For simple systems, small architecture (<100 parameters) are enough to capture quantum dynamics.

ACKNOWLEDGMENTS

This work has been supported by the Spanish Ministerio de Ciencia e Innovación (MCIN) through the project PID2020-113586GB-I00 (MCIN/AEI/10.13039/501100011033) and the project PID2020-113586GB-I00 (MCIN/AEI/10.13039/501100011033).



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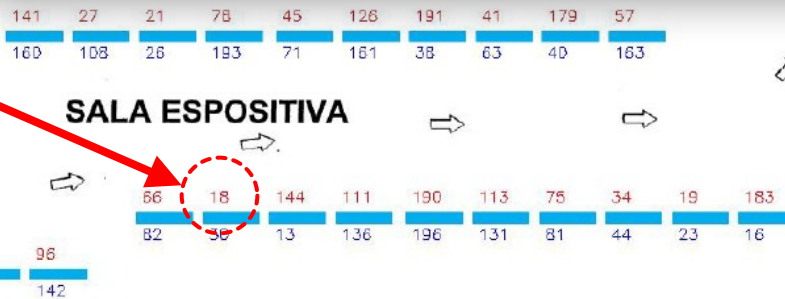
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SALA ESPOSITIVA



THANK YOU!