VARIATIONAL NEURAL NETWORK ANSATZ FOR STEADY-STATES IN OPEN QUANTUM SYSTEMS

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OPEN QUANTUM SYSTEMS

Describe the interaction of a quantum system $H$ with its environment

- Out of Equilibrium phenomena
- Reservoir Engineering
- Dissipative phase transitions

Reservoir

Semiconductor Micropillars

Superconducting circuits

Quantum Biology

N. Carlon Zambon et Al.
arXiv:1812.06163

A. A. Houck et Al.
Nat Phys 8, 292 (2012)

N. Lambert et Al.
Nat Phys 9, 10 (2013)
Schroedinger’s Equation \rightarrow Lindblad Master Eq.

Describe the interaction of a quantum system $H$ with its environment.

**The State**

$|\psi\rangle \in \mathcal{H}_{\text{sys}} \otimes \mathcal{H}_{\text{E}} \implies \hat{\rho} = \text{Tr}_E[|\psi\rangle \langle \psi|]$

**The Master Equation**

$$\frac{\partial \hat{\rho}}{\partial t} = -i \left[ \hat{H}, \hat{\rho} \right] + \sum_{j=1}^{N_{\text{channels}}} \left( \hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2} \left\{ \hat{L}_j^\dagger \hat{L}_j, \hat{\rho} \right\} \right)$$

**Coherent Evolution**

**Incoherent Evolution**

Rewritten as a linear super-operatorial equation

$$\partial_t \hat{\rho} = \mathcal{L} \hat{\rho}$$

We are usually interested in the steady-state

$$\hat{\rho}_{ss} = \lim_{t \to \infty} e^{\mathcal{L}t} \hat{\rho} \quad \mathcal{L} \hat{\rho}_{ss} = 0 \quad \partial_t \hat{\rho}_{ss} = 0$$

[HP Breuer, F Petruccione, The theory of quantum system (2012)]
THE DIMENSIONAL CURSE

For N lattices of N sites, the Hilbert space has an exponentially big dimension \( \dim \mathcal{H} \approx l^N \)

Numerical Techniques try to reduce this size with physical insight (e.g. MPS/MPOs, Cluster Mean Field..)

Neural Networks are low-dimensional approximations of high-dimensional functions...

\[
|\psi\rangle = \begin{pmatrix}
\psi(\uparrow\uparrow \ldots \uparrow) \\
\psi(\downarrow\uparrow \ldots \uparrow) \\
\psi(\uparrow\downarrow \ldots \uparrow) \\
\psi(\downarrow\downarrow \ldots \uparrow) \\
\vdots \\
\psi(\downarrow\downarrow \ldots \downarrow)
\end{pmatrix}
\]

[G. Carleo and M. Troyer, Science (2017)]
THE DIMENSIONAL CURSE

FOR N SPINS, THE HILBERT SPACE HAS AN EXPONENTIALLY BIG DIMENSION

\[ \dim \rho = \dim \mathcal{H} \otimes \mathcal{H} = 2^{2N} \]

\[ \hat{\rho} = \sum_{\sigma_1, \ldots, \sigma_N, \tilde{\sigma}_1, \ldots, \tilde{\sigma}_N} \rho(\sigma_1, \ldots, \sigma_N, \tilde{\sigma}_1, \ldots, \tilde{\sigma}_N) |\sigma_1, \ldots, \sigma_N \rangle \langle \sigma_1, \ldots, \sigma_N| \]

HIGH-DIMENSIONAL FUNCTION

4 ARTICLES CAME OUT IN A WEEK WITH SIMILAR PROPOSALS

F.V, A. Biella, N. Regnault and C. Ciuti \ ARXIV:1902.10104

M.J. Hartmann and G. Carleo \ ARXIV:1902.05131

A. Nagy and V. Savona \ ARXIV:1902.09483

N. Yoshioka and R. Hamazaki \ ARXIV:1902.07006

BUT \( \hat{\rho} \) IS POSITIVE-SEMIDEFINITE AND HERMITIAN. WE WANT TO ENFORCE THOSE PROPERTIES.

[G. Carleo and M. Troyer, Science (2017)]
**NEURAL DENSITY MATRIX**

Drawing inspiration from RBMs (Restricted Boltzmann Machines)...

[Diagram showing the neural density matrix with neurons and weights]

**TRACING OUT THE HIDDEN LAYER GIVES A WELL-DEFINED PROBABILITY DISTRIBUTION**

\[ p(\sigma) = \sum_h e^{-E(\sigma, h)} \]

[G. Torlai and R. Melko, PRL (2018)]
NEURAL DENSITY MATRIX

Drawing inspiration from RBMs (Restricted Boltzmann Machines)...

**Tracing out the hidden layer gives a well-defined probability distribution**

\[ p(\sigma) = \sum_{h} e^{-E(\sigma, h)} \]

**Double the «hidden» variables**

\[ p(\sigma, a) = \sum_{h} e^{-E(\sigma, a, h)} \]

[G. Torlai and R. Melko, PRL (2018)]
**NEURAL DENSITY MATRIX**

Drawing inspiration from RBMs (Restricted Boltzmann Machines)...

Formally equivalent to defining an RBM in the bigger space, summing over the hidden space and then

$$\psi(\vec{\sigma}, \vec{a}) \in \mathcal{H}_s \otimes \mathcal{H}_a \implies \rho(\vec{\sigma}, \vec{\sigma}') = \sum_{a \in \mathcal{H}_a} [\psi(\vec{\sigma}, \vec{a}) \psi^*(\vec{\sigma}', \vec{a})]$$

Can be generalized to FFNN!

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[G. Torlai and R. Melko, PRL (2018)]
OUT OF EQUILIBRIUM: FINDING THE STEADY STATE

We have a variational ansatz (where $v$ are the variational parameters)

$$\rho_v(\sigma, \sigma')$$

I want to find the steady state

$$\frac{d\rho_{ss}}{dt} = \mathcal{L}\rho_{ss} = 0$$

We need a variational principle: I define the `Cost Function`

$$\mathcal{C}(v) = \frac{\|d\hat{\rho}_v/dt\|_2^2}{\|\hat{\rho}_v\|_2^2} = \frac{\text{Tr}[\hat{\rho}_v^\dagger \mathcal{L}^\dagger \mathcal{L}\hat{\rho}_v]}{\text{Tr}[\hat{\rho}_v^\dagger \hat{\rho}_v]}$$

Which has the nice properties:

$$\mathcal{C}(\nu_{ss}) = 0 \iff \hat{\rho}_{\nu_{ss}} = \hat{\rho}_{ss}$$

$$\mathcal{C}(\nu) \geq 0$$

[H. Weimer, PRL (2015)]

DIFFERENT COST FUNCTIONS ARE POSSIBLE!
SEE POSTER OF A. NAGY FOR A DIFFERENT ONE
**Out Of Equilibrium: Finding the Steady State III**

We recasted the problem of finding the steady state $\rho_{ss}$ to a minimization problem for $C(v)$

So we could perform a gradient-descent like minimization: $v \rightarrow v - \nabla_v C(v)$

But there’s a problem! Local Minimas! ⇒ **Natural Gradient Descent**

But there’s a problem! Computing the Cost Fun ⇒ **Sampling**

$$C(v) = \frac{\text{Tr}[\hat{\rho}_v L^\dagger L \hat{\rho}_v]}{\text{Tr}[\hat{\rho}_v \hat{\rho}_v]} = \sum_{\sigma, \tilde{\sigma}} p_v(\sigma, \tilde{\sigma}) C^{\text{Loc}}(v, \sigma, \tilde{\sigma}),$$

$$p_v(\sigma, \tilde{\sigma}) = \frac{|p_v(\sigma, \tilde{\sigma})|^2}{\sum_{\sigma, \tilde{\sigma}} p_v(\sigma, \tilde{\sigma})}$$

This is a probability distribution ⇒ I can sample it! (and the gradient)
RESULTS FOR DRIVEN-DISSIPATIVE QUANTUM ISING MODEL

The Hamiltonian is
\[ H = \frac{V}{4} \sum_{\langle j,l \rangle} \hat{\sigma}_j^z \hat{\sigma}_l^z + \frac{g}{2} \sum_j \hat{\sigma}_j^x \]

With de-exitation jump operators \( L_j = \sigma_j^- \)

We study the magnetizations \( m^{(\alpha)} = \frac{1}{N} \sum_i \sigma_i^{(\alpha)} \)

For a chain of \( N=16 \) sites (PBC)

Observables are sampled like:
\[ \langle \hat{m}^{(\alpha)} \rangle = \frac{\text{Tr} \left[ \hat{\rho} \hat{m}^{(\alpha)} \right]}{\text{Tr} [\hat{\rho}]} = \sum_\sigma p_\nu^{\text{obs}} (\sigma) \sum_{\tilde{\sigma}} \frac{\rho_\nu (\sigma, \tilde{\sigma}) m^{(\alpha)} (\tilde{\sigma}, \sigma)}{\rho_\nu (\sigma, \sigma)} , \]
A full scan in the transverse field gives:
CONCLUSIONS

• Density Matrices can be approximated with Neural Networks
• Variational Monte Carlo can be remapped to machine learning procedures
• We can solve the exponential growth problem

Perspectives:
• Try different topologies, layers to enforce simmetries...
• Test different cost functions
• [Also investigate Neural Network encodings for Digital Quantum Algorithm applications]
AKNOWLEDGEMENTS

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QUESTIONS?
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CODE?
Will soon be available on GitHub. If you want to have a look now drop me an email.

COLLABORATE?
I am finalizing a framework written in Julia to perform MonteCarlo simulations using Neural Network ansatzes. If you would like to collaborate and/or help, I would love an hand.