

# Neural Networks as Quantum States

NNs in Quantum Many-Body Problems

Deep Learning con Applicazioni

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# Introduction

## Neural Networks as Quantum States

- Quantum-many-body problems feature an exponential Hilbert-space growth
- Traditional variational ansätze reduce complexity sacrificing correlation and entanglement
- Neural-network quantum states can offer expressivity with a compact set of parameters

**Neural Networks can represent ground states for a many-body quantum system<sup>1</sup>**

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<sup>1</sup>Giuseppe Carleo, Matthias Troyer, Solving the quantum many-body problem with artificial neural networks. *Science* 355, 602-606 (2017)

# Project Outline

Find the Ground State

- Restricted Boltzmann Machine as a neural network
- Sample configurations from RBM
- Train RBM to find the ground state



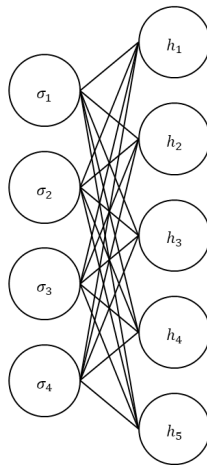
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# Restricted Boltzmann Machine

Generative Model

- Learns  $p(\vec{\sigma})$  of the input data  $\vec{\sigma}$
- Two layers:  $N$  visible and  $M$  hidden
- Parameters  $\mathcal{W}$ : weights  $W_{ij}$  and biases  $b_i, c_j$





# Restricted Boltzmann Machine

Probability Distribution

Internal Energy:

$$E(\vec{\sigma}, \vec{h}) = - \sum_i b_i \sigma_i - \sum_j c_j h_j - \sum_{i,j} w_{ij} \sigma_i h_j$$

Probability Distribution:

$$p(\vec{\sigma}, \vec{h}) = \frac{1}{Z} e^{-E(\vec{\sigma}, \vec{h})}$$

where  $Z$  is the partition function:

$$Z = \sum_{\vec{\sigma}, \vec{h}} e^{-E(\vec{\sigma}, \vec{h})}$$



# Restricted Boltzmann Machine

Application to Quantum States

Considering a spin configuration  $\vec{\sigma}$  and a set of parameters  $\mathcal{W}$ :

$$\psi(\vec{\sigma}, \mathcal{W}) = e^{\sum_i b_i \sigma_i + \sum_j c_j h_j + \sum_{i,j} w_{ij} \sigma_i h_j}$$

With no intra-layer connections:

$$\psi(\vec{\sigma}, \mathcal{W}) = e^{\sum_i b_i \sigma_i} \times \prod_{j=1}^M 2 \cosh \left[ c_j + \sum_i w_{ij} \sigma_i \right]$$

From the RBM we can sample configurations  $\vec{\sigma}$ .



# Training

Reinforcement Learning

Update parameters  $\mathcal{W}$  towards energy minimum.

$$E_0 \leq \frac{\langle \psi_{\mathcal{W}} | \hat{H} | \psi_{\mathcal{W}} \rangle}{\langle \psi_{\mathcal{W}} | \psi_{\mathcal{W}} \rangle}$$

The parameters  $\mathcal{W}$  are optimized using a gradient descent method:

- Variational Monte Carlo (VMC)<sup>2</sup>
- Stochastic Reconfiguration (SR)<sup>3</sup>

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<sup>2</sup>Moritz Reh, Markus Schmitt, Martin Gärtner, Optimizing design choices for neural quantum states, *Phys. Rev. B* 107, 195115 (2023)

<sup>3</sup>Becca F, Sorella S. *Quantum Monte Carlo Approaches for Correlated Systems*. Cambridge University Press; 2017



# Training

Variational Monte Carlo

We can compute the gradients:

$$\begin{aligned}\nabla_{\mathcal{W}}(E) &= \nabla_{\mathcal{W}}\langle E_{\text{loc}} \rangle \\ &= \langle E_{\text{loc}} \nabla_{\mathcal{W}} \log(p_{\psi}) \rangle \\ &= 2\Re [\langle E_{\text{loc}} \nabla_{\mathcal{W}} \log(\psi) \rangle - \langle E_{\text{loc}} \rangle \langle \nabla_{\mathcal{W}} \log(\psi) \rangle]\end{aligned}$$

And consequently update the parameters:

$$\Delta \mathcal{W} = -\eta \nabla_{\mathcal{W}}(E)$$





# Training

## Stochastic Reconfiguration

Parameters evolution in the variational space:

$$\Delta \mathcal{W} = -\eta \mathbf{S}^{-1} \vec{F}$$

where  $\mathbf{S}^{-1}$  is the pseudo-inverse of the covariance matrix:

$$\mathbf{S}_{ij} = \langle O_i^* O_j \rangle - \langle O_i^* \rangle \langle O_j \rangle$$

and  $\vec{F}$  is the force vector:

$$F_i = \langle O_i^* E_{\text{loc}} \rangle - \langle O_i^* \rangle \langle E_{\text{loc}} \rangle$$

where  $O_i$  are the local operators defined as:

$$O_i = \frac{\partial \log (\psi (\vec{\sigma}, \mathcal{W}))}{\partial W_{ij}}$$

# Code Implementation

- RBM
- Sampler
- Hamiltonian
- Optimizers



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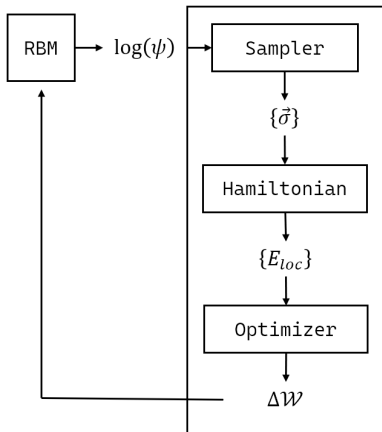


# Code Implementation

## Code Structure

nnqs/

- nnqs.py -> RBM
- hamiltonian.py -> Ising1D
- optimizer.py -> MRT2,  
GibbsSampler
- sampler.py -> VMC, SR





## Code Implementation

### RBM

Custom `tf.module` implementing the RBM.

Weights and biases are initialized randomly as complex values:

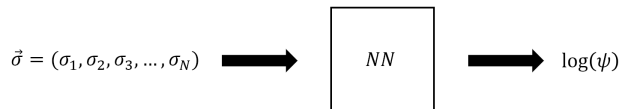
```
self.W = tf.Variable(  
    tf.random.normal([self.N_visible, self.N_hidden], dtype=tf.complex64)  
)  
self.b = tf.Variable(tf.random.normal([self.N_visible], dtype=tf.complex64))  
self.c = tf.Variable(tf.random.normal([self.N_hidden], dtype=tf.complex64))
```

$$\psi(\vec{\sigma}, \mathcal{W}) = e^{\sum_i b_i \sigma_i} \times \prod_{j=1}^M 2 \cosh \left[ c_j + \sum_i W_{ij} \sigma_i \right]$$



# Code Implementation

RBM - Logarithm of the Wave Function



$$\log(\psi) = \sum_i b_i \sigma_i + \sum_{j=1}^M \log \left[ 2 \cosh \left( c_j + \sum_i w_{ij} \sigma_i \right) \right]$$



# Code Implementation

RBM - Logarithm of the Wave Function

```
sum_visible = tf.reduce_sum(  
    a * spins, axis=1  
)  
w_h = b + tf.matmul(spins, W)  
sum_hidden = tf.reduce_sum(  
    tf.math.log(2.0 * (  
        tf.math.cosh(b + tf.matmul(spins, W))  
    )), axis=1  
)  
return sum_visible + sum_hidden
```

$$\sum_i b_i \sigma_i$$
$$\sum_{j=1}^M \log \left[ 2 \cosh \left( c_j + \sum_i W_{ij} \sigma_i \right) \right]$$



# Code Implementation

## Sampler

Samples configurations from the RBM.

- **Metropolis-Hastings** MCMC using *TensorFlow Probability*
- **Gibbs sampling** Double-step method to sample visible and hidden variables<sup>4</sup>

Provides batches of configurations. Example:

```
>>> sam.sample(rbm)
<tf.Tensor: shape=(5, 4), dtype=float32, numpy=
array([[0., 0., 0., 0.],
       [1., 1., 1., 0.],
       [0., 0., 1., 0.],
       [0., 0., 0., 0.],
       [0., 0., 0., 1.]], dtype=float32)>
```

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<sup>4</sup>Francesco D'Angelo, Lucas Böttcher, Learning the Ising model with generative neural networks, *Phys. Rev. Research* 2, 023266 (2020)



# Code Implementation

Hamiltonian - 1D Ising

Simple 1D Ising Hamiltonian:

$$H = -J \sum_i \sigma_i \sigma_{i+1} - h \sum_i \sigma_i$$

Provides `local_energy(samples)` which computes  $E_{\text{loc}}$  for each configuration  $\vec{\sigma}$ .





# Code Implementation

## Optimizers

Leverage `tf.GradientTape` to compute gradients of  $\log(\psi)$

```
with tf.GradientTape() as tape:  
    log_psi = self.wave_function.log_psi(samples)  
grad_log_psi = tape.jacobian(log_psi, self.wave_function.trainable_variables)
```

VMC and SR methods obtain parameters update in different ways.

Update the parameters of the wave function in the same way:

```
for grad_val, var in grads_vars:  
    var.assign_sub(self.learning_rate * grad_val)
```



# Code Implementation

Optimizers - VMC

$$\nabla_{\mathcal{W}}(E) = 2\Re[\langle E_{\text{loc}} \nabla_{\mathcal{W}} \log(\psi) \rangle - \langle E_{\text{loc}} \rangle \langle \nabla_{\mathcal{W}} \log(\psi) \rangle]$$

```
mean_energy = tf.reduce_mean(local_energies)
for grad_i in grad_log_psi:
    loc_grad = e_loc * grad_i
    grad_energy = tf.reduce_mean(loc_grad, axis=0)
    grad_log_psi_mean = tf.reduce_mean(grad_i, axis=0)

    vmc_grad = 2.0 * tf.math.real(
        grad_energy - mean_energy * grad_log_psi_mean
    )
    gradients.append(vmc_grad)
```



# Code Implementation

Optimizers - Stochastic Reconfiguration

The SR approach computes the variational increments as follows:

```
# compute covariance matrix / QGT
O_mean = tf.reduce_mean(O, axis=0)
O_centered = O - O_mean
O_0 = tf.matmul(
    O_centered, O_centered, transpose_a=True
)
S = O_0 / norm
```

$$S_{ij} = \langle O_i^* O_j \rangle - \langle O_i^* \rangle \langle O_j \rangle$$



# Code Implementation

Optimizers - Stochastic Reconfiguration

$$F = \langle E_{\text{loc}} \nabla_{\mathcal{W}} \log(\psi) \rangle - \langle E_{\text{loc}} \rangle \langle \nabla_{\mathcal{W}} \log(\psi) \rangle$$

```
# compute force vector
```

```
mean_energy = tf.reduce_mean(local_energies)
```

```
F_vec = (  
    tf.reduce_mean(local_energies * 0, axis=0) - mean_energy * 0_mean  
)
```



# Code Implementation

Optimizers - Stochastic Reconfiguration

$$\Delta \mathcal{W} = S^{-1} F$$

```
# solve for delta
P = tf.shape(S)[0]
S_reg = S + self.epsilon * tf.eye(P, dtype=S.dtype)
# dW = S^{-1} F
gradients = tf.linalg.solve(S_reg, tf.expand_dims(F_vec, 1))
```

# Results



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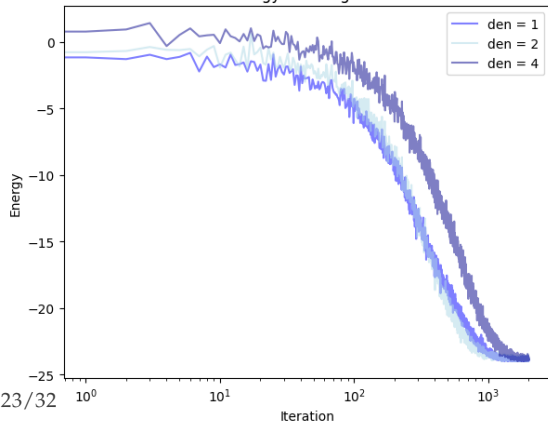


# Results

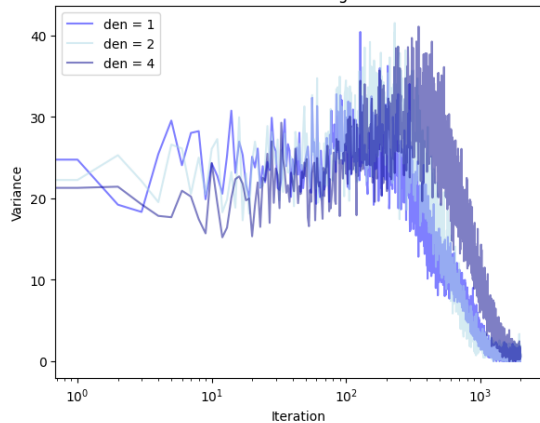
1D Ising Model - 16 spins

Using  $J = 1.0$  and  $h = 0.5$

Energy Convergence



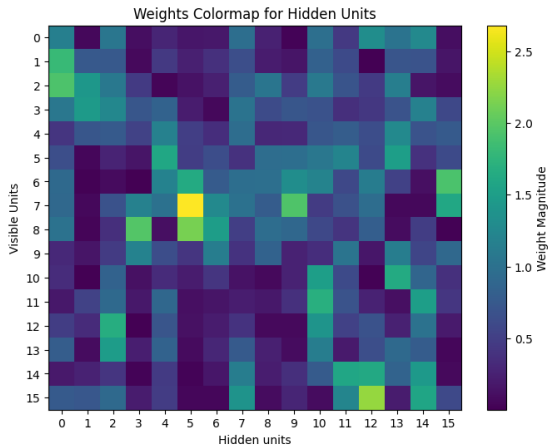
Variance Convergence





# Results

Weights for  $den = 1$

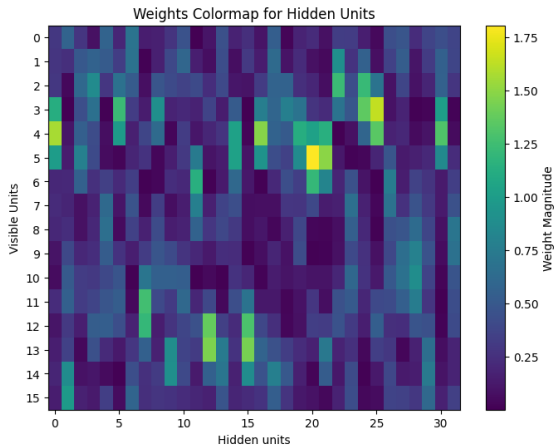






# Results

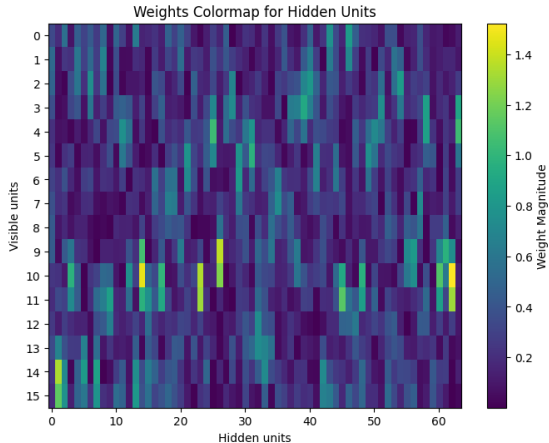
Weights for  $den = 2$





# Results

Weights for  $den = 4$

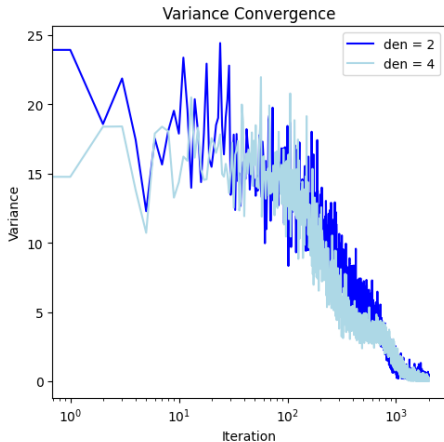
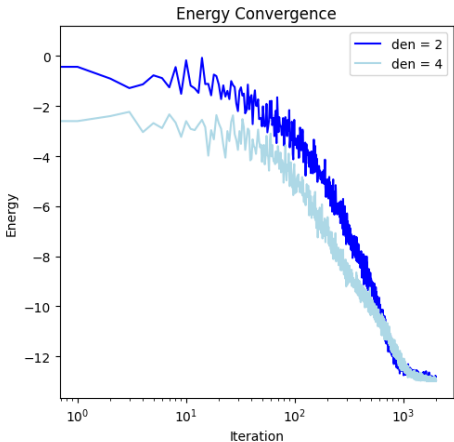




# Results

1D Ising Model - 16 spins

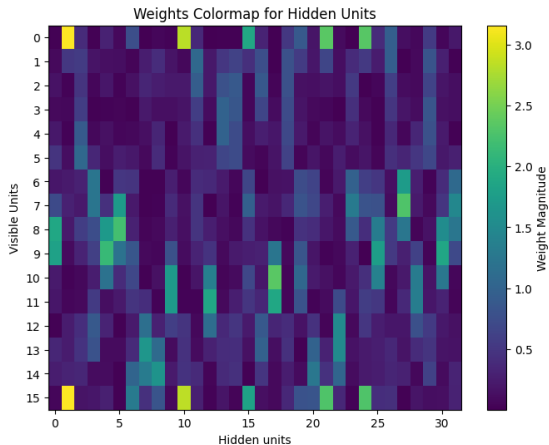
Using  $J = -1.0$  and  $h = 0.5$





# Results

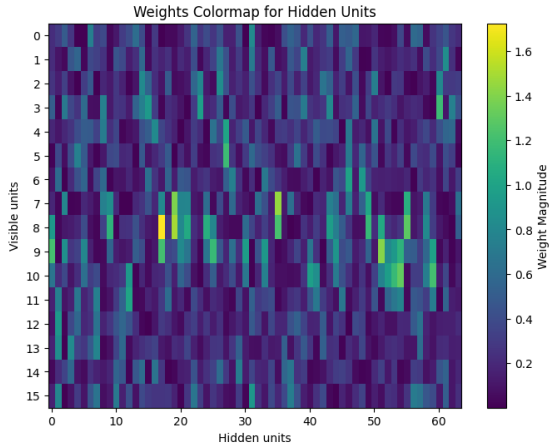
Weights for  $den = 2$





# Results

Weights for  $den = 4$





## Further Work

Optimization and Extensions

### Extensions

- Extend to 2D systems
- Other neural networks (FFNN, CNN)
- Unitary (and non) dynamics

### Optimization

- Efficient SR update (single parameter updates)
- Change tensor framework (JAX, ...)





### Other Projects

**NetKet:** The Machine-Learning toolbox for Quantum Physics





## References

-  Giuseppe Carleo, Matthias Troyer, Solving the quantum many-body problem with artificial neural networks. *Science* 355, 602-606 (2017).
-  Moritz Reh, Markus Schmitt, Martin Gärttner, Optimizing design choices for neural quantum states, *Phys. Rev. B* 107, 195115 (2023).
-  Becca F, Sorella S. *Quantum Monte Carlo Approaches for Correlated Systems*. Cambridge University Press; 2017.
-  Francesco D'Angelo, Lucas Böttcher, Learning the Ising model with generative neural networks, *Phys. Rev. Research* 2, 023266 (2020).



Thanks for your attention!



# Appendix



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## Appendix

### Probabilities for the RBM

Thanks to no intra-layer connections, we can factorize the joint probability:

$$p(\vec{\sigma} | \vec{h}) = \prod_i p(\sigma_i | \vec{h})$$

$$p(\vec{h} | \vec{\sigma}) = \prod_j p(h_j | \vec{\sigma})$$

where:

$$p(\sigma_i | h) = \sigma \left( b_i + \sum_j W_{ij} h_j \right)$$

$$p(h_j | \sigma) = \sigma \left( c_j + \sum_i W_{ij} \sigma_i \right)$$

where  $\sigma(x) = \frac{1}{1+e^{-x}}$  is the logistic or sigmoid function.



# Appendix

Local operators for the RBM

Explicit form of the partial derivatives of  $\log(\psi)$



## Appendix

### Metropolis-Hastings and MCMC sampling

Propose a single bit flip, and accept it with the Metropolis criterion:

$$\alpha = \min \left( 1, \frac{p(\sigma')}{p(\sigma)} \right)$$

where  $\sigma'$  is the proposed state and  $\sigma$  is the current state.

Uses the `tfp.mcmc` module for efficient sampling.

- Requires target  $\log(p)$
- Requires new state proposal



## Appendix

### Gibbs sampling

We can sample the visible and hidden variables in a double-step Gibbs sampling:

```
def sample(self, wave_function):  
    v = tf.cast(self.current_state, tf.float32)  
    for _ in range(self.k):  
        v_complex = tf.cast(v, wave_function.W.dtype)  
        v_W = tf.matmul(v_complex, wave_function.W)  
        p_h = tf.sigmoid(tf.math.real(wave_function.b + v_W))  
        h = tf.cast(tf.random.uniform(tf.shape(p_h), dtype=tf.float32) < p_h, tf.  
float32)  
        h_complex = tf.cast(h, wave_function.W.dtype)  
        h_Wt = tf.matmul(h_complex, tf.transpose(wave_function.W))  
        p_v = tf.sigmoid(tf.math.real(wave_function.a + h_Wt))  
        v = tf.cast(tf.random.uniform(tf.shape(p_v), dtype=tf.float32) < p_v, tf.  
float32)  
    self.current_state.assign(tf.cast(v, tf.int32))  
return v
```