Deep Learning Beyond Loss Curves

A tutorial on statistical rigour and informed design in ML

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Quantum Information Theory and Quantum Optics Theory Groups ICFO

2nd Machine Learning Methods for Complex and Quantum Systems (ML2026)

CONTENT

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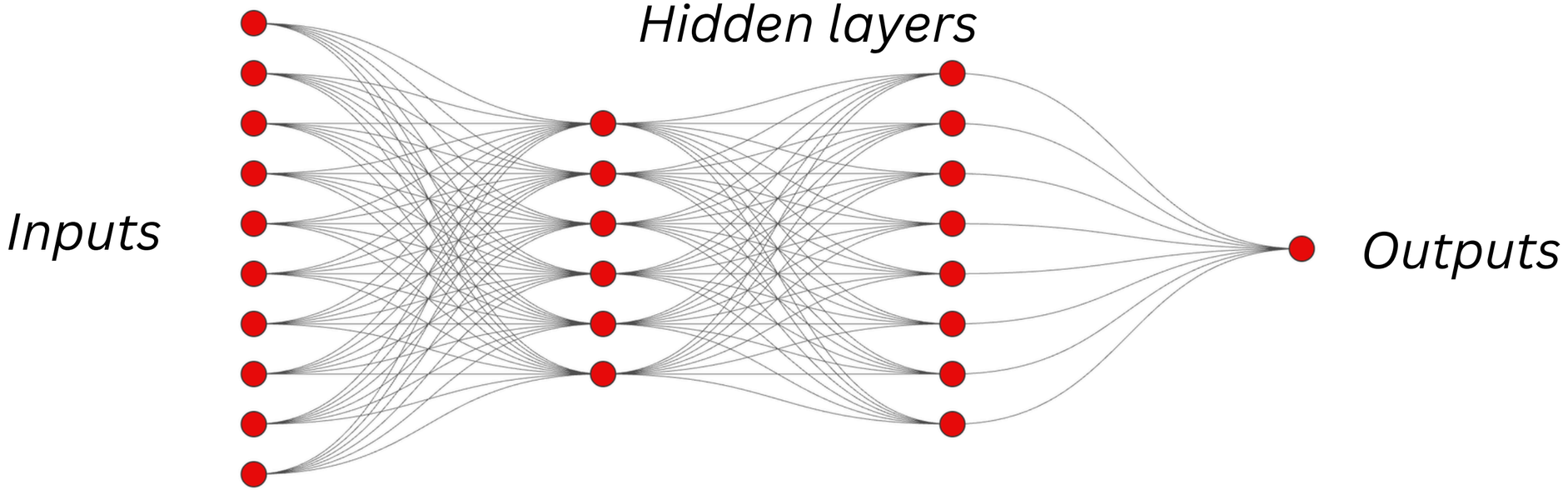
Neural Network Anatomy

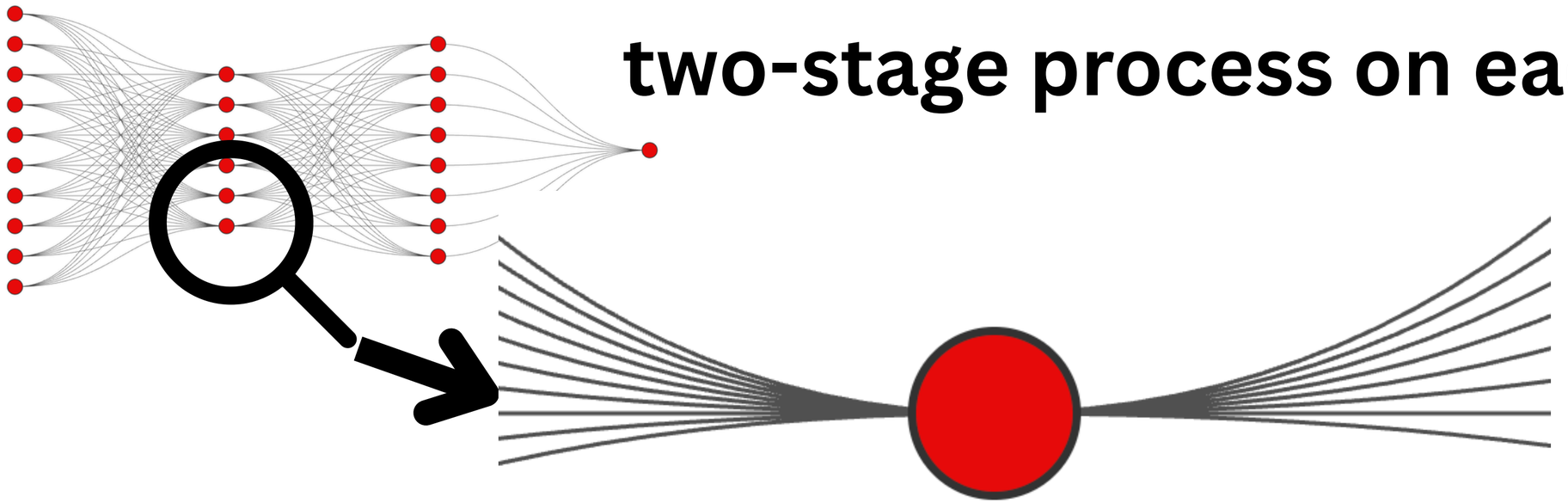
- A neural network is just a tunable non-linear function:



- Read from left to right tells us information flow

- Within a given neuron, there is is a non-linear “*activation function*”

Neuron Anatomy



two-stage process on each layer

1. Linear transformation $z \leftarrow \mathbf{W}z + b$

2. Non-linear activation e.g. *sigmoid* $\sigma(z) = \frac{1}{1 + e^{z}}$

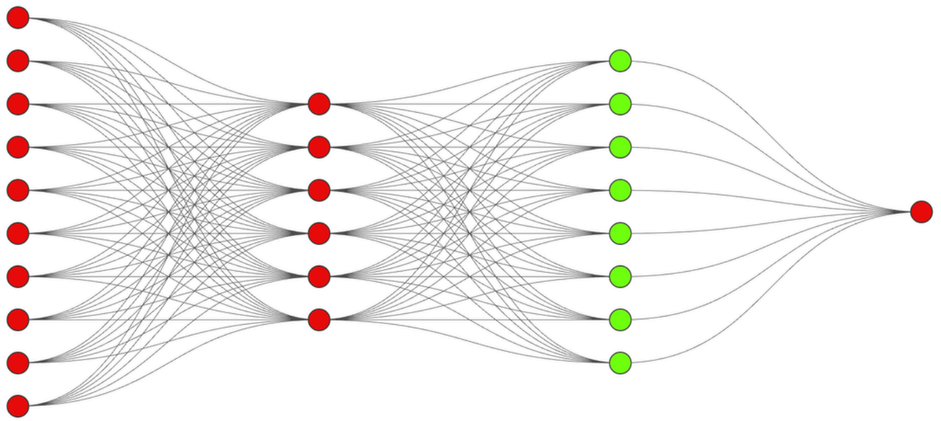
- W: Weight matrix
- b: bias
- z: latent vector

Neural Network Anatomy

- A full layer's transoformation is

$$h^{(l)}(\mathbf{z}) = \sigma\Big(\sum_{i=1}^{N_l}\sum_{j=1}^{N_{l-1}} \mathbf{W}_{i,j}^{(l)}\mathbf{z}_j + \sum_{i=1}^{N_l} \mathbf{b}_i^{(l)}\Big).$$

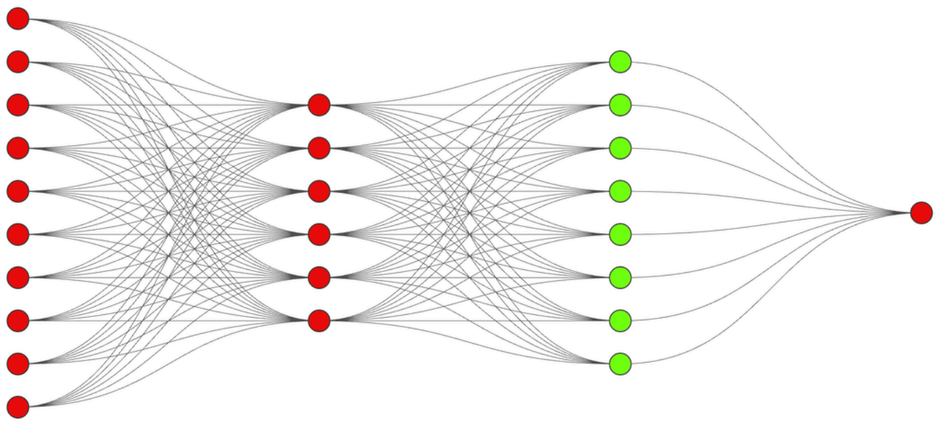
- e.g. layer two into three has 6 x 8 weight matrix



Neural Network Anatomy

- Variational paramters are any paramters we can tune

$$\boldsymbol{\theta} = \{\mathbf{W}^{(l)}, \mathbf{b}^{(l)} | l = 1, \ldots, L\}.$$



Neural Network Anatomy

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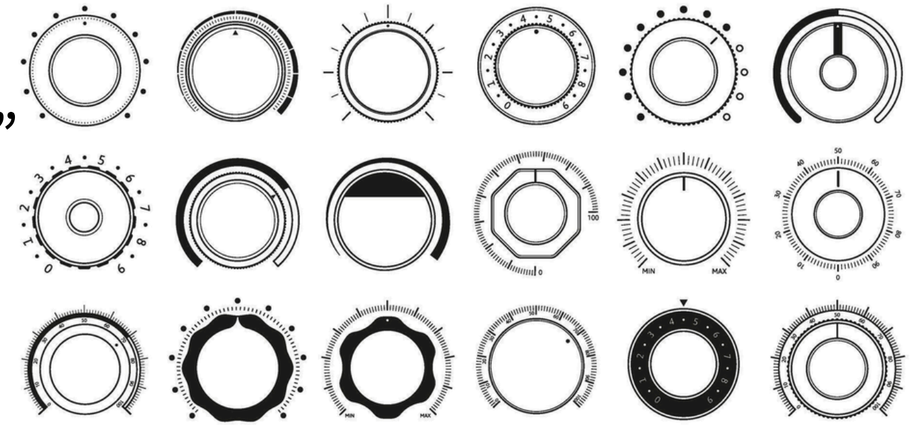
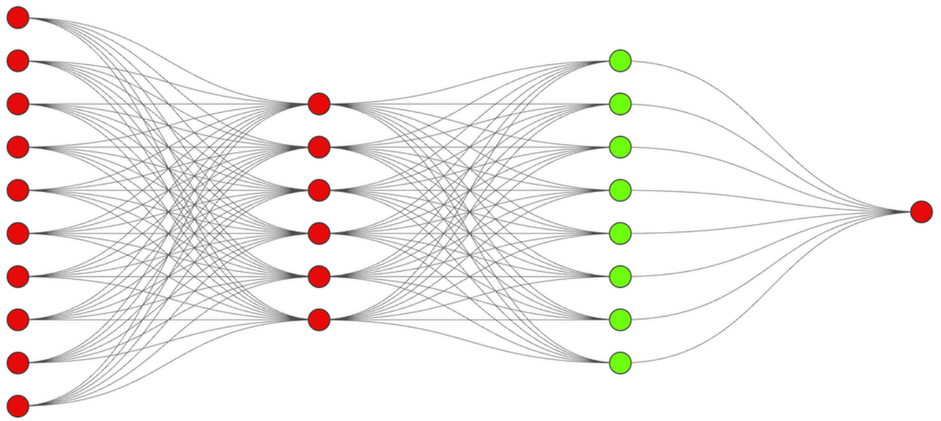
“bunch of dials and knobs we can tune”

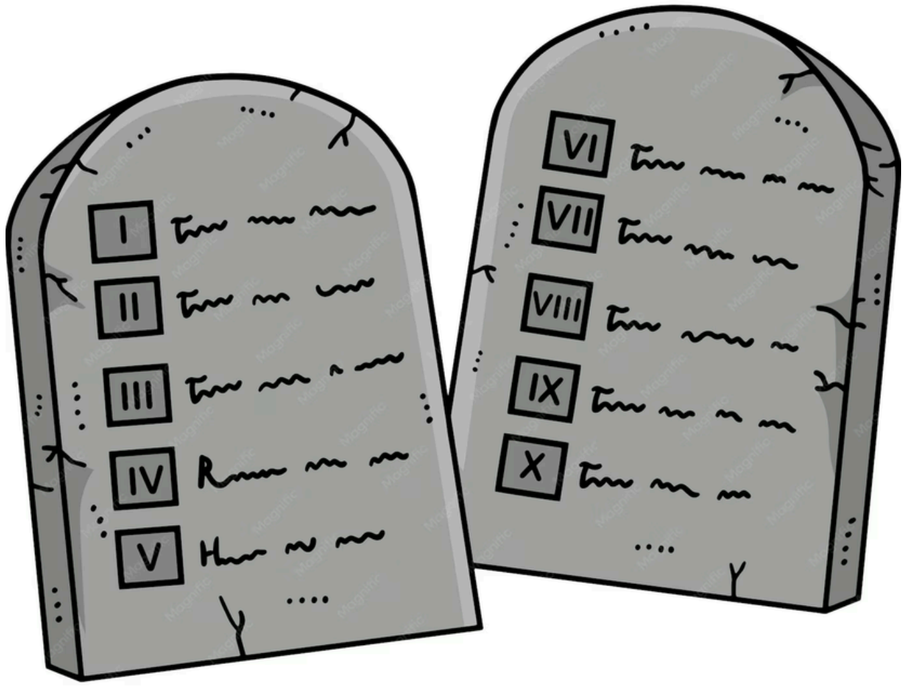




Universal Approximation Theorem

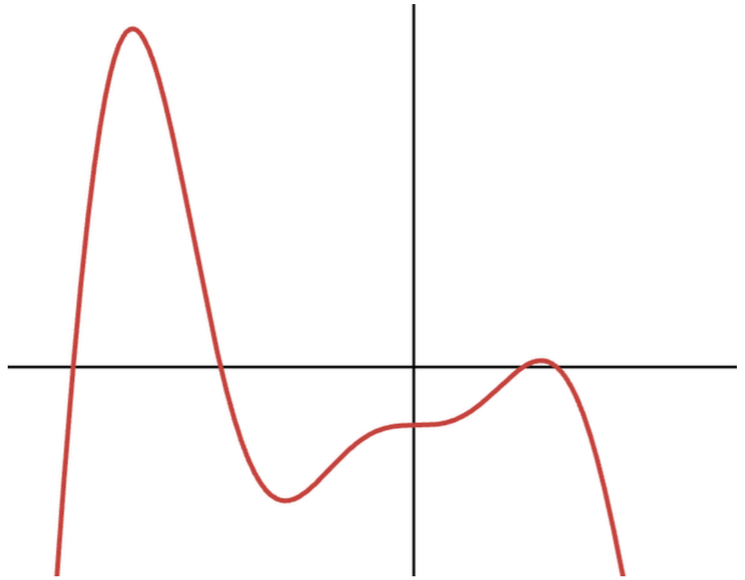
- Any continuous function on a compact domain can be approximated to an arbitrary level of accuracy with a sufficiently deep neural network.

- Central idea of deep learning!!



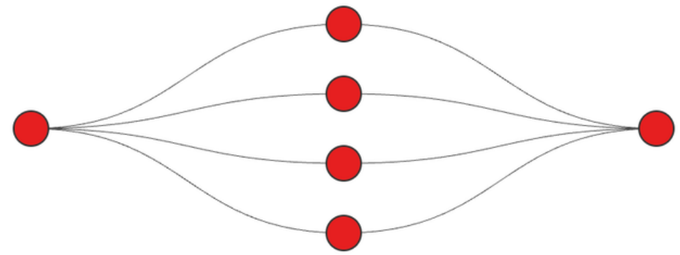
A First Example

$$g(x) = x^2 \sin(\pi x) - \frac{1}{2 + \cos(x)}$$



- Our goal is to find a set of *optimal* parameters $\boldsymbol{\theta}^* = \{\boldsymbol{W}^{(1)*}, \boldsymbol{b}^*, \boldsymbol{W}^{(2)*}\},$
- When we find them, we have a *good* approximation

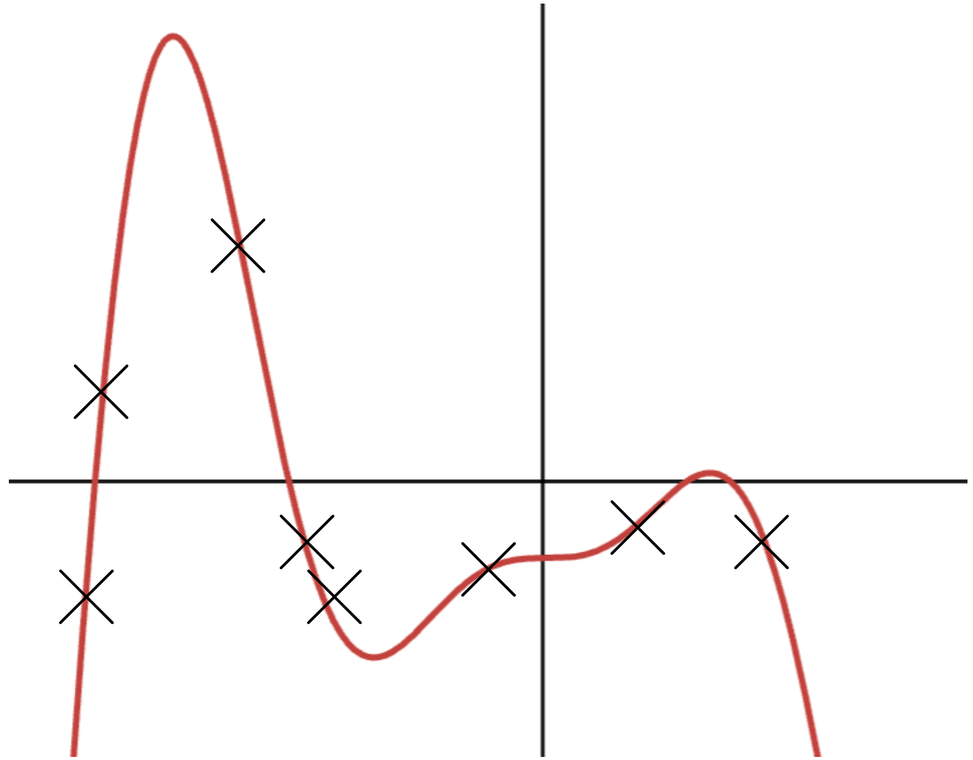
$$|f_\theta(x) - g(x)| \to 0$$



A First Example

- To tune parameters, we need a *dataset*

$$\mathcal{D} = \{x_i, g(x_i)\}_{i=1}^{K}$$



- We also need a measure of approximation quality - “*Loss function*”

$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{K}\sum_{i=1}^{K} |g(x_i) - f(x_i;\boldsymbol{\theta})|^2$$

A First Example

- We vary parameters when *training* the network with gradient information:

$$\theta \leftarrow \theta - \alpha \nabla_\theta L$$

$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{K} \sum_{i=1}^{K} |g(x_i) - f(x_i; \boldsymbol{\theta})|^2$$

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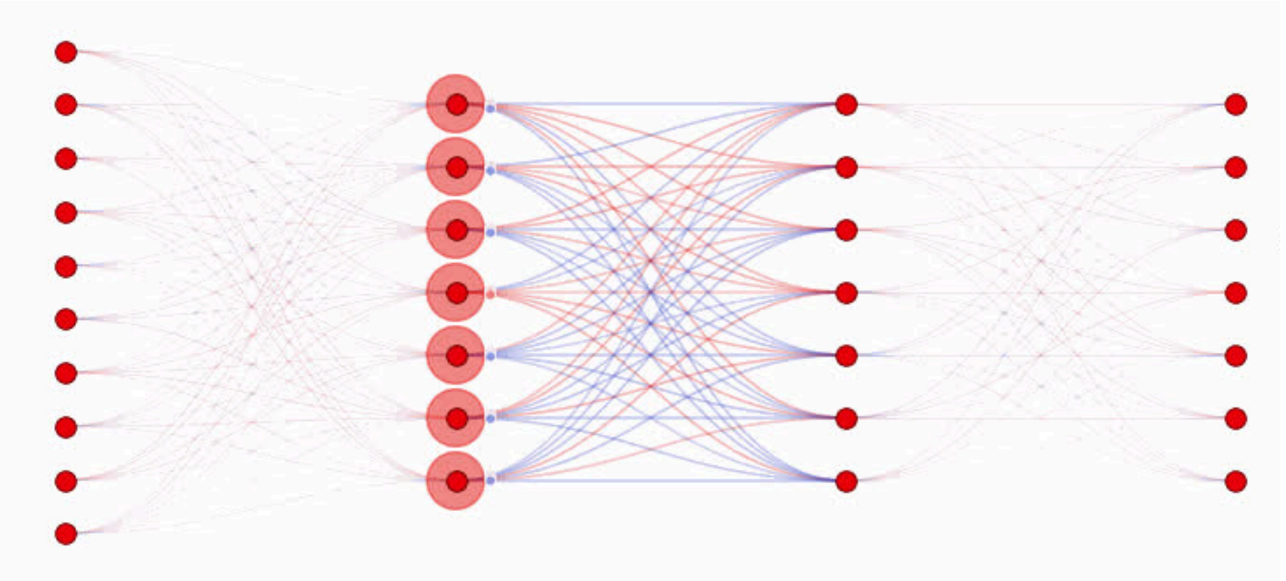
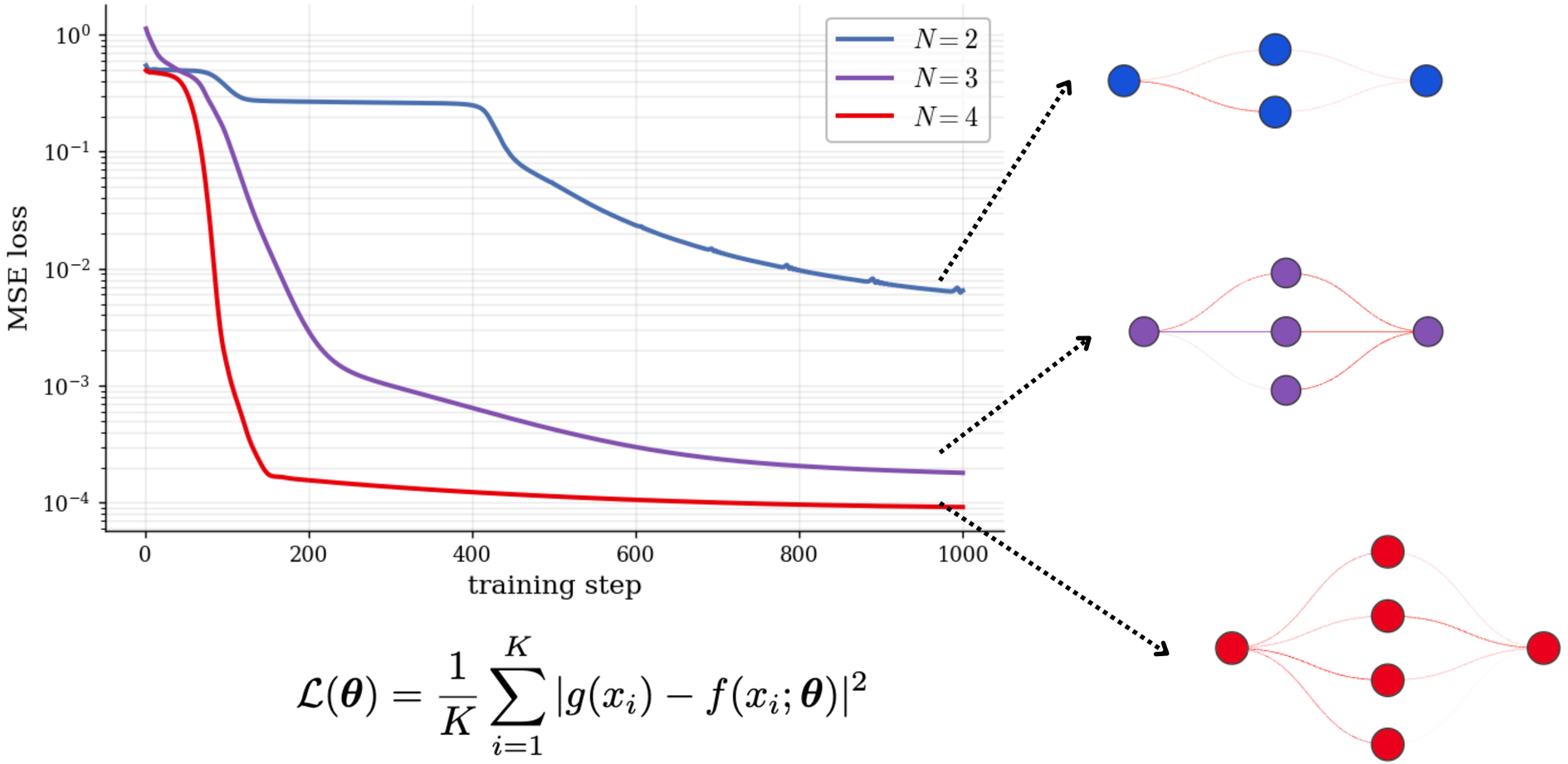
Input



$$\mathcal{L}(\theta)$$

A First Example

- After training



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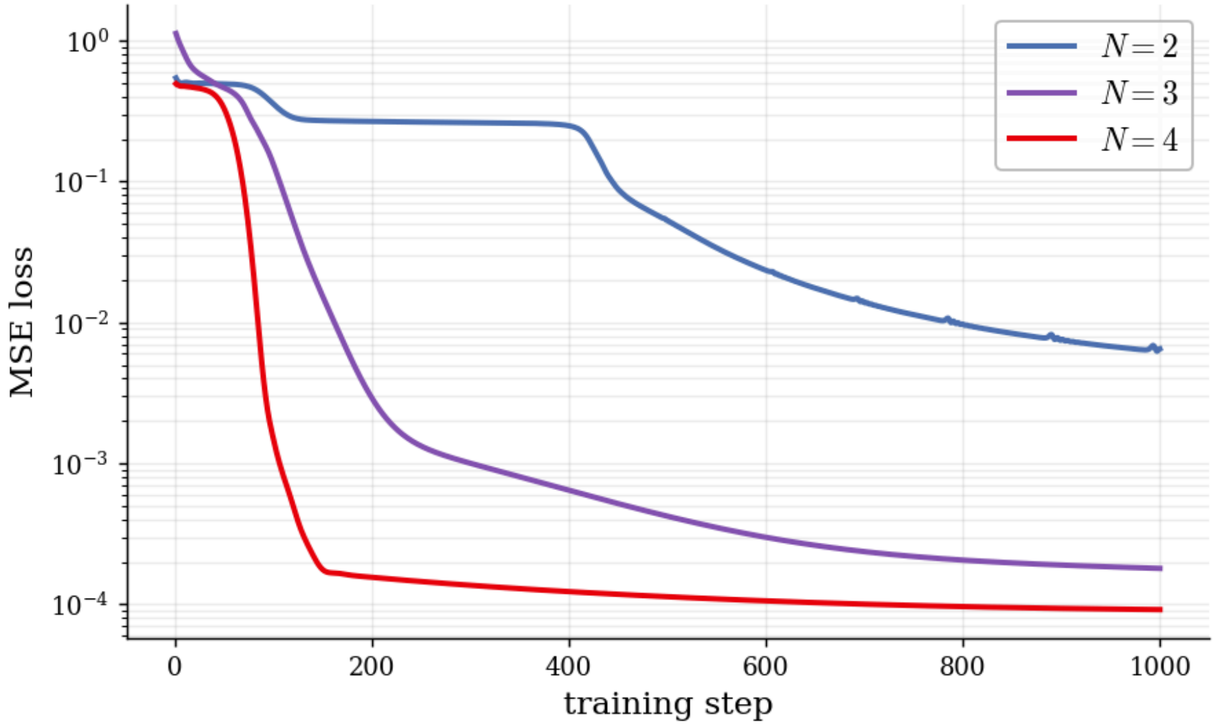
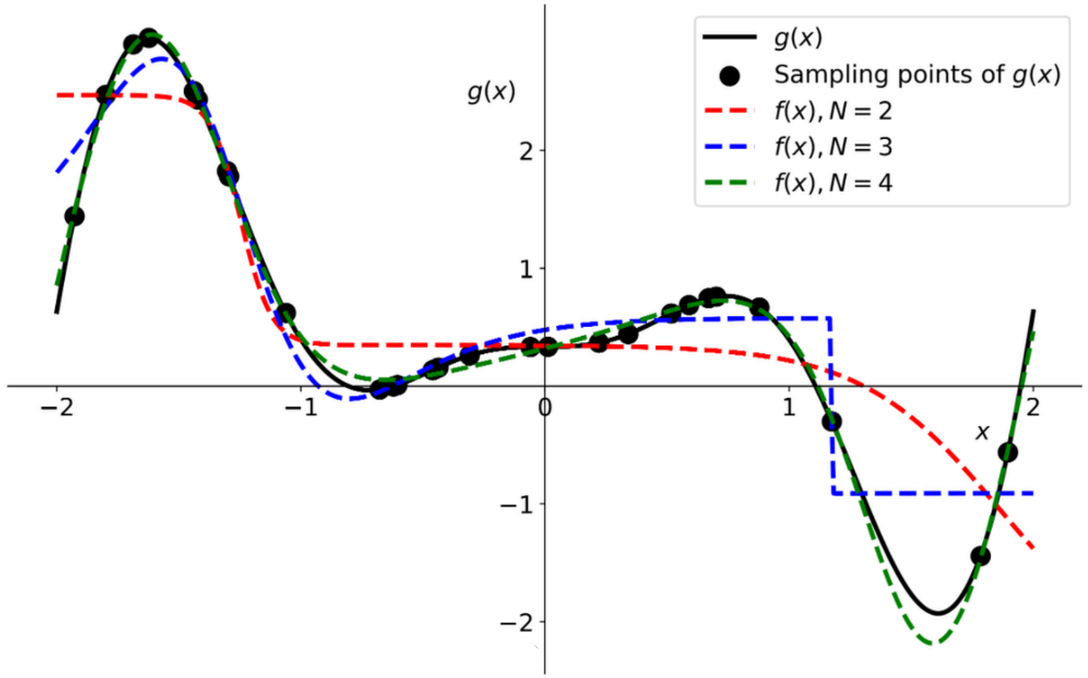




$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{K}\sum_{i=1}^{K} |g(x_i) - f(x_i;\boldsymbol{\theta})|^2$$

$$g(x) = x^2\sin(\pi x) - \frac{1}{2+\cos(x)}$$

Neural Network Anatomy and Training

1. **Forward Pass**

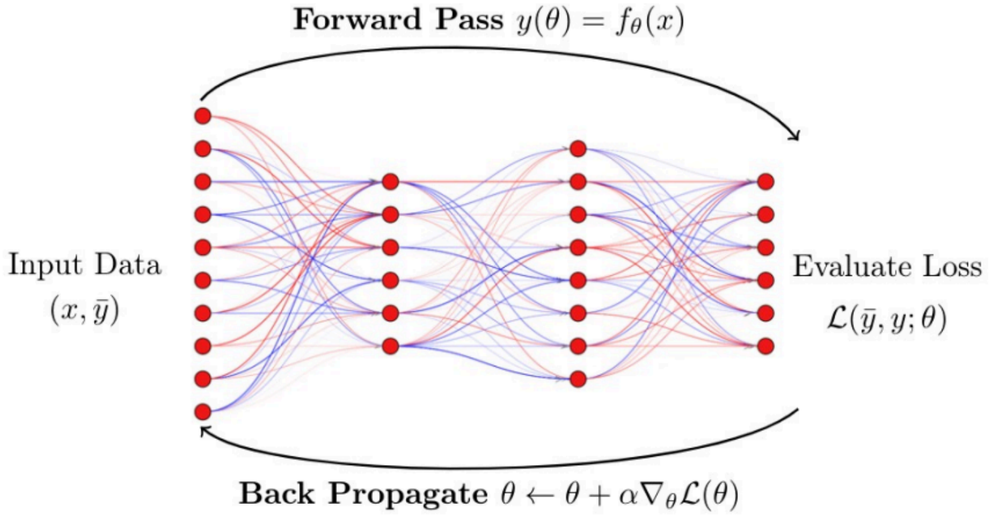
$$\bar{\vec{y}}_i^{(j)} = f_{\vec{\theta}_t}(\vec{x}_i^{(j)})$$

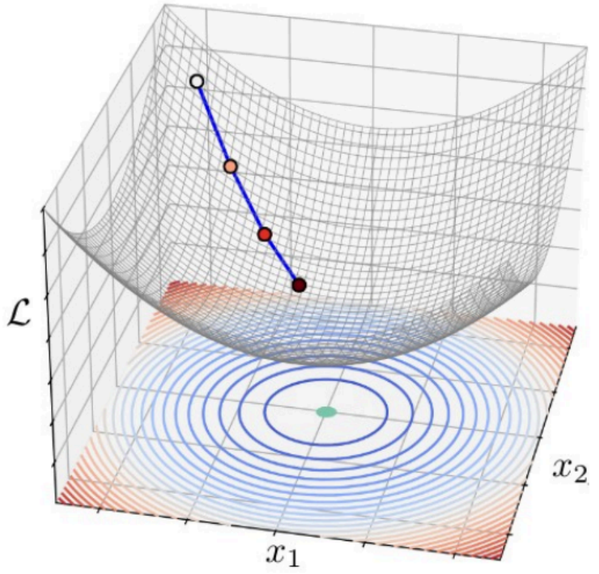
2. **Loss calculation**

$$\mathcal{L}^{(j)}(\vec{\theta}_t) = \frac{1}{N_{\mathcal{D}^{(j)}}} \sum_{i=1}^{N_{\mathcal{D}^{(j)}}} \mathcal{L}_i(\vec{y}_i^{(j)}, \bar{\vec{y}}_i^{(j)})$$

3. **Backpropagation**

$$\vec{\theta}_{t+1} \leftarrow \vec{\theta}_t - \eta \frac{\partial \mathcal{L}^{(j)}(\vec{\theta}_t)}{\partial \vec{\theta}_t}.$$





Seems simple enough right?...

- What about on more complicated functions?

$$g : \mathbb{R}^n \rightarrow \mathbb{R}^m$$

- Or say.... wavefunctions...?

$$|\psi\rangle \in \mathcal{H}$$

- Can we say a network is training well and learning a function correctly based on loss function alone?

Beyond the loss curve

- Loss is going down, is my model actually “good”?
- I “tweaked it” and loss improved… did it really, or did I just get lucky?
- Which network should I use?

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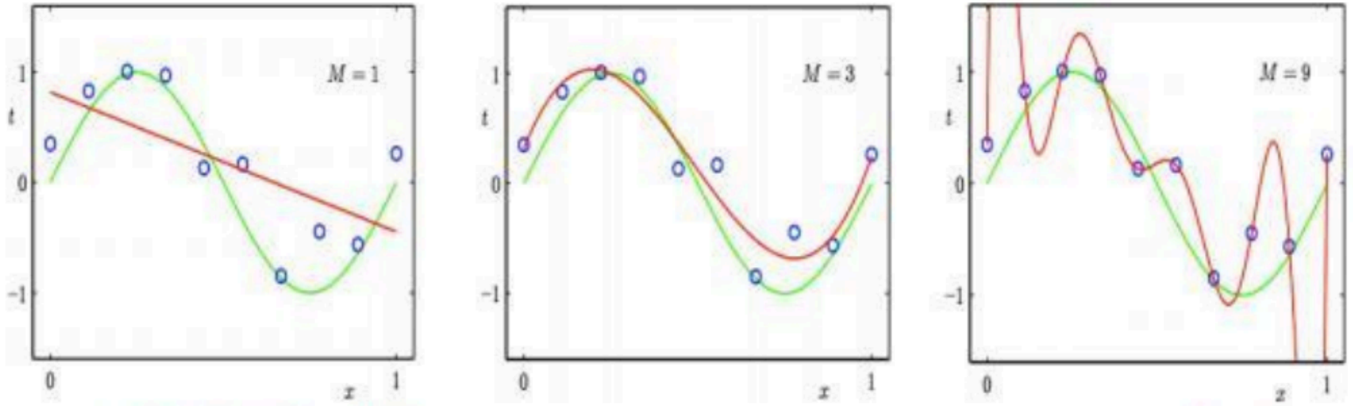
Overfitting Problem

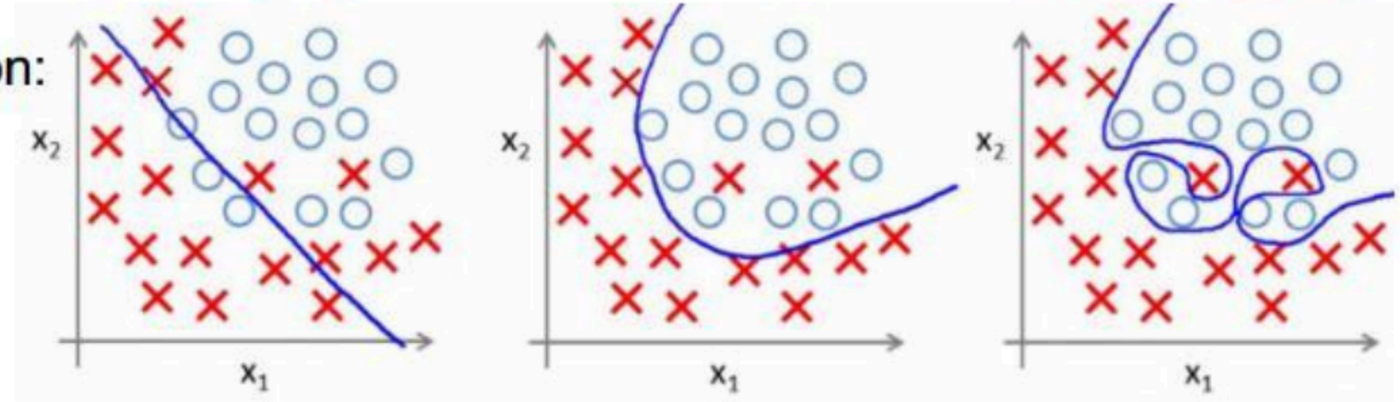
Regression:



predictor too inflexible:
cannot capture pattern

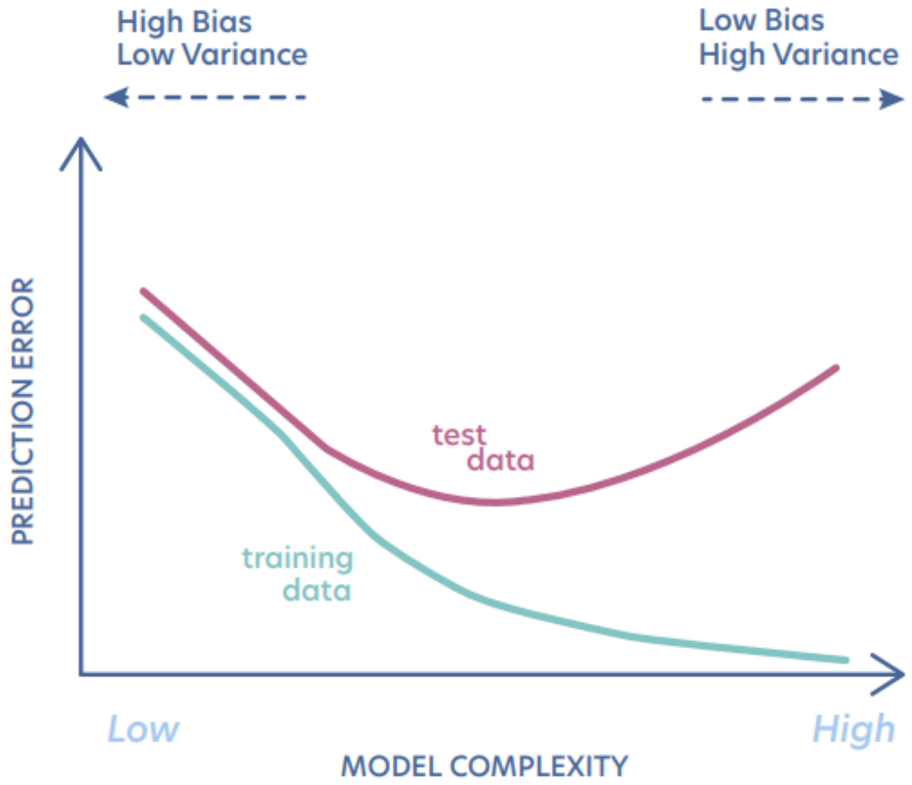
predictor too flexible:
fits noise in the data

Classification:



Overfitting Problem

- Prevent overfitting by splitting data into training, validation and testing sets



- Detect it by seeing error decrease on train set *only*...

Overfitting Problem

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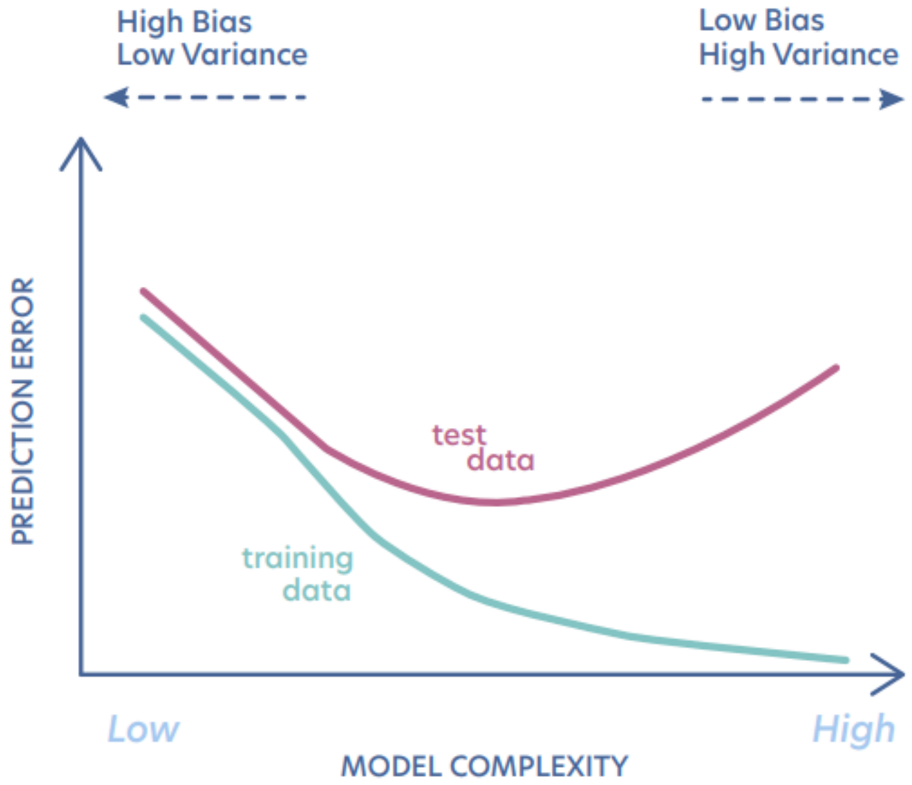
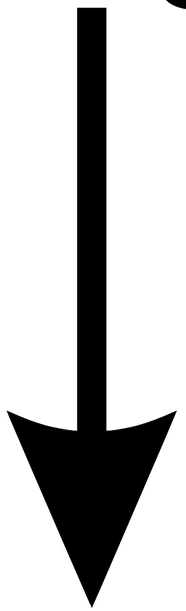


- Detect it by seeing error decrease on train set *only*...
- This happens because networks can learn the trend *and the noise*... *effectively memorising training data*

Overfitting Problem



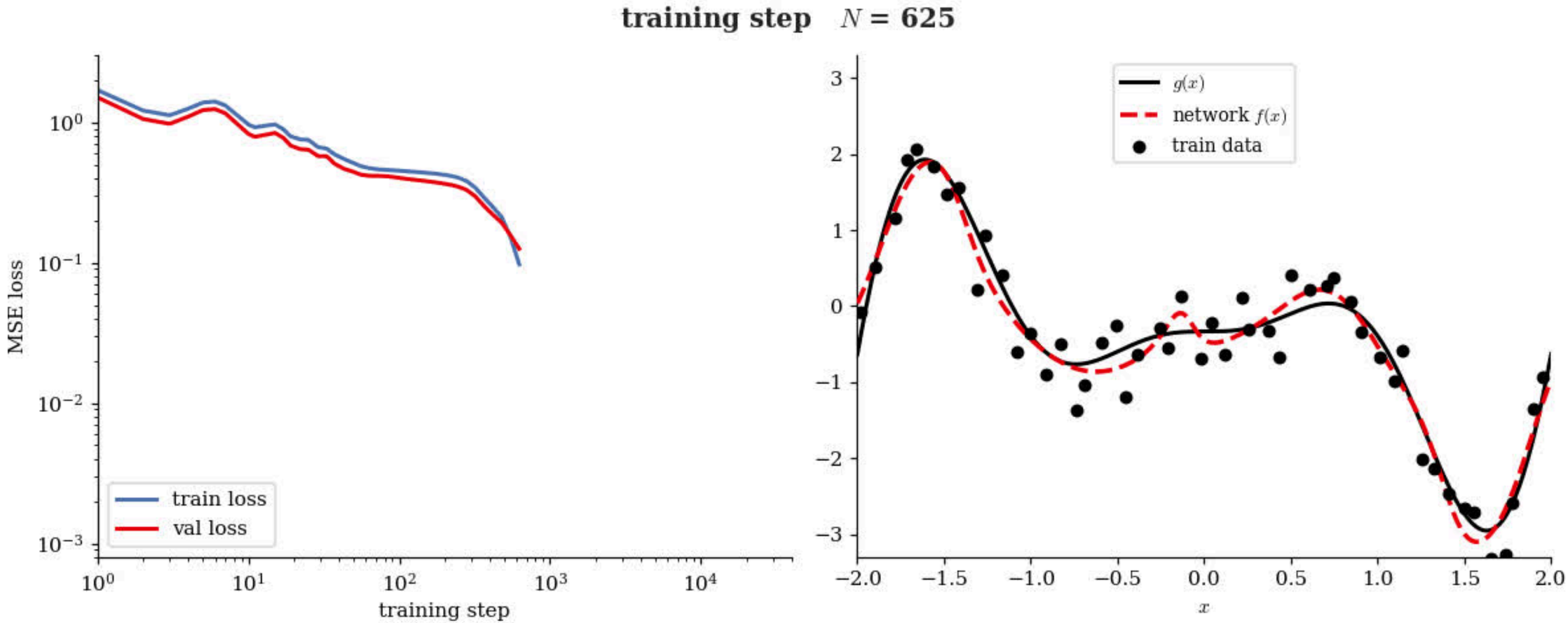
3 solutions...

1 Regularisation

- Any term that penalises complexity, so driving the loss down no longer rewards memorising... $R = |\theta|$
- Creates composite loss functions...

$$\mathcal{L} = \mathcal{L}_{data} + \lambda R$$

2 Early stopping



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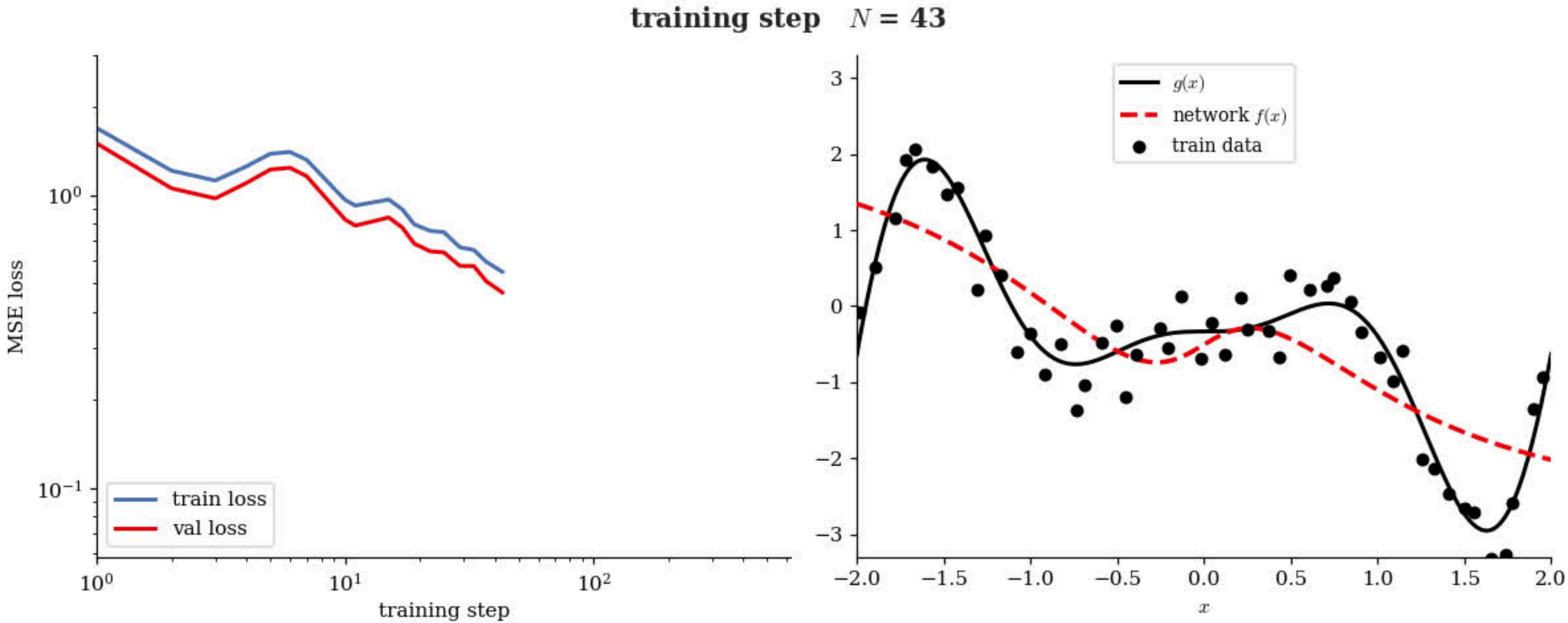
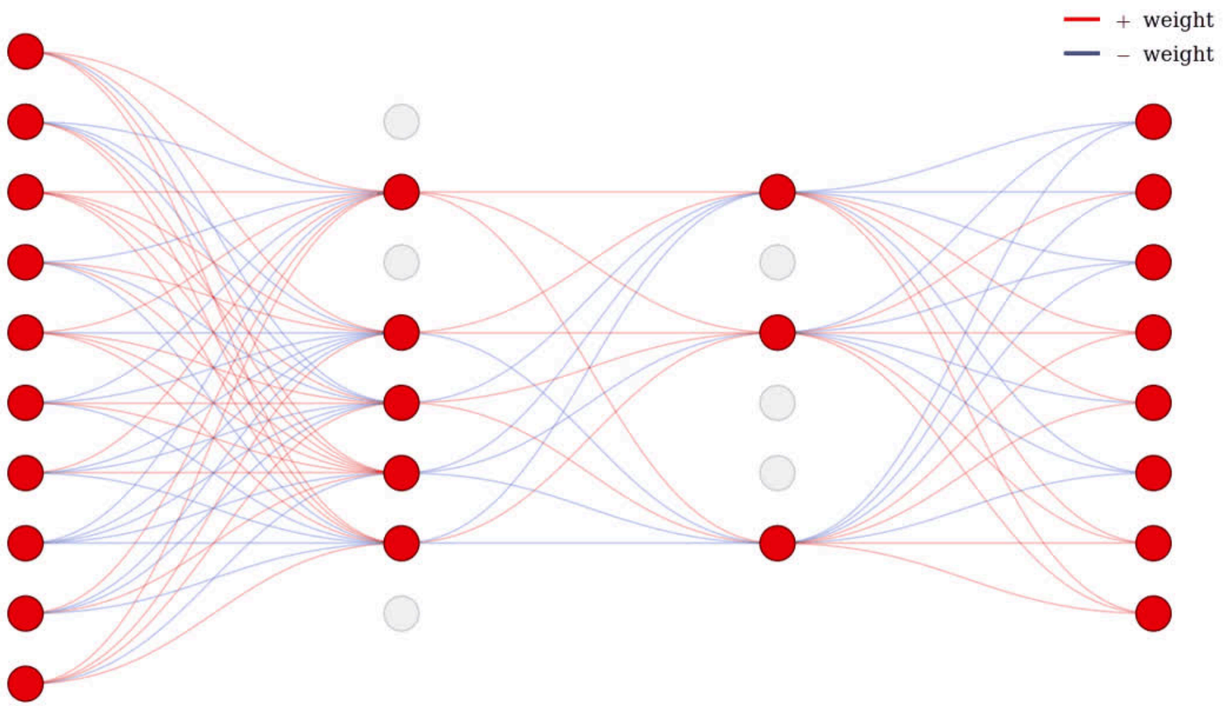


3 Dropout



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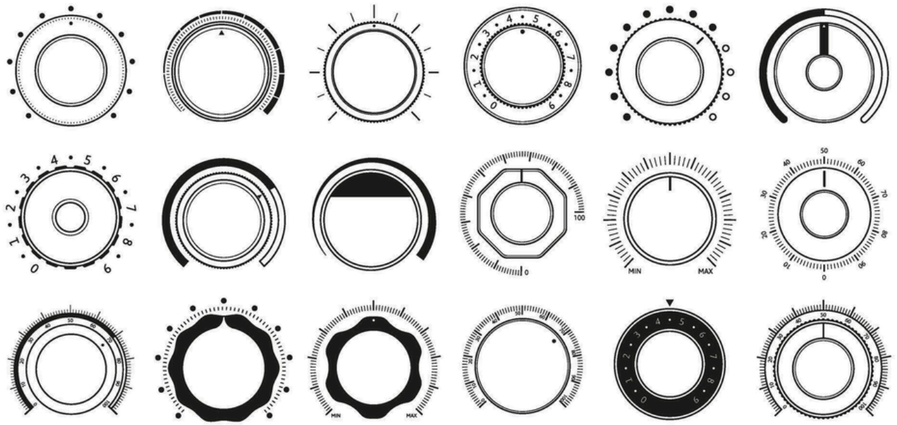
- Randomly switch off sets of parameters during training

Hyperparameters...

- A hyperparameter is any part of a model we can tweak that is not touched by backpropagation
    - Learning rate
    - Network shape
    - Choice of activation function
    - Encoding of input data
    - Choice of Optimiser



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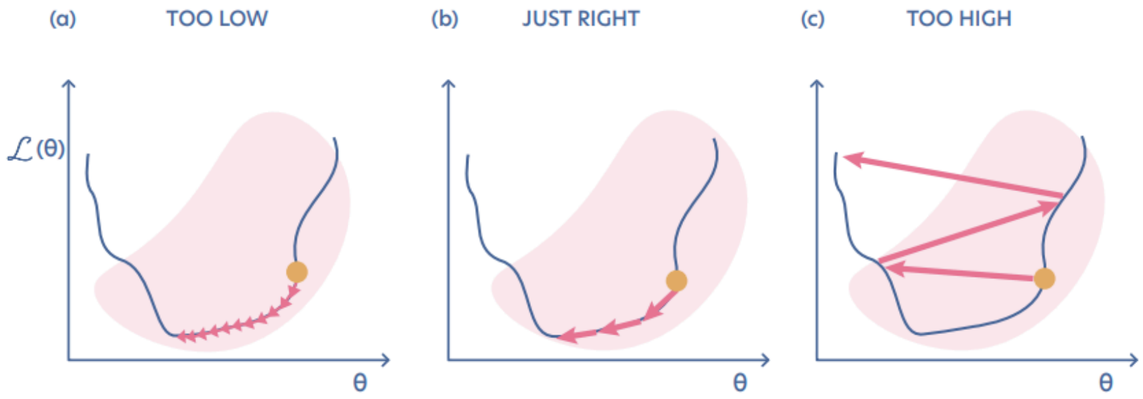

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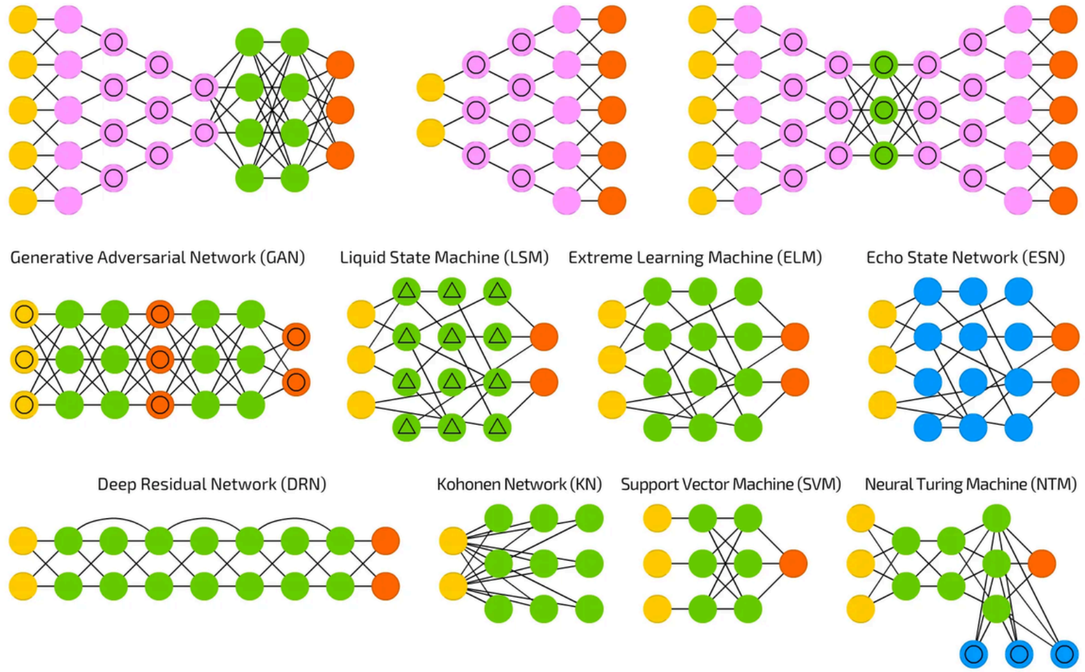

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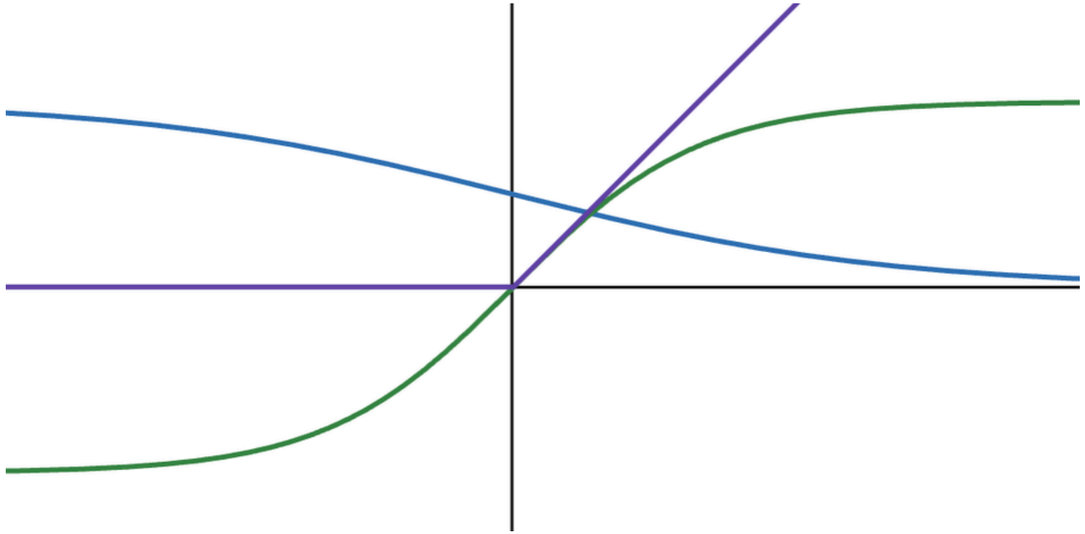

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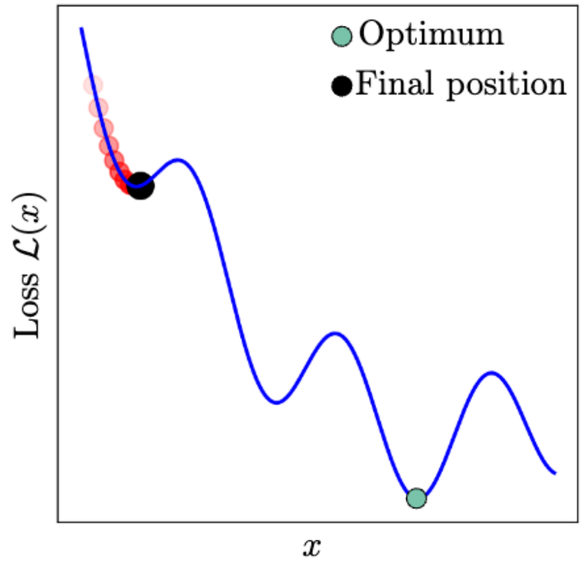
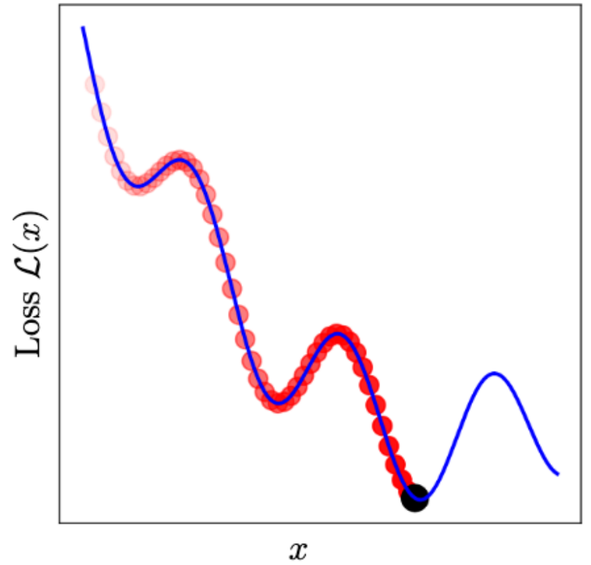
    (vanilla, momentum, ADAM, SPFS, Kron, Spring, KFAC...)



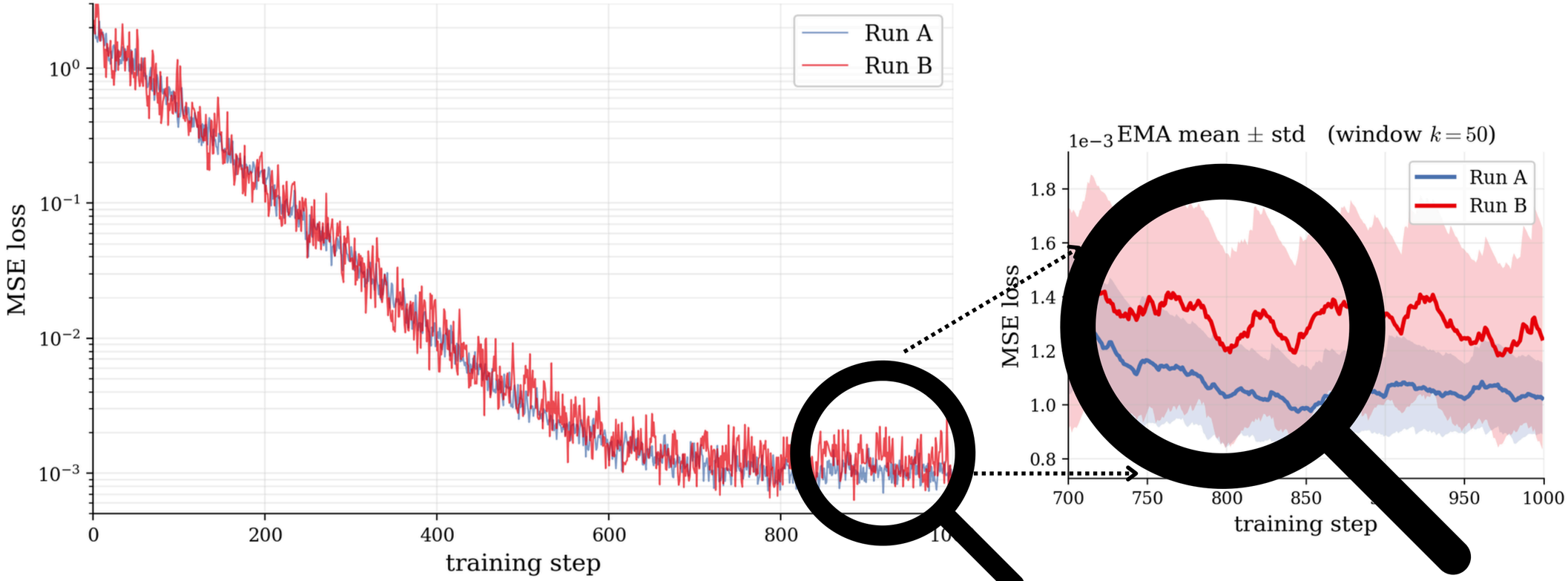


Data-driven Network Design

- Suppose we have two reasonable looking loss curves, A and B, both with reasonable loss curves, which is better?

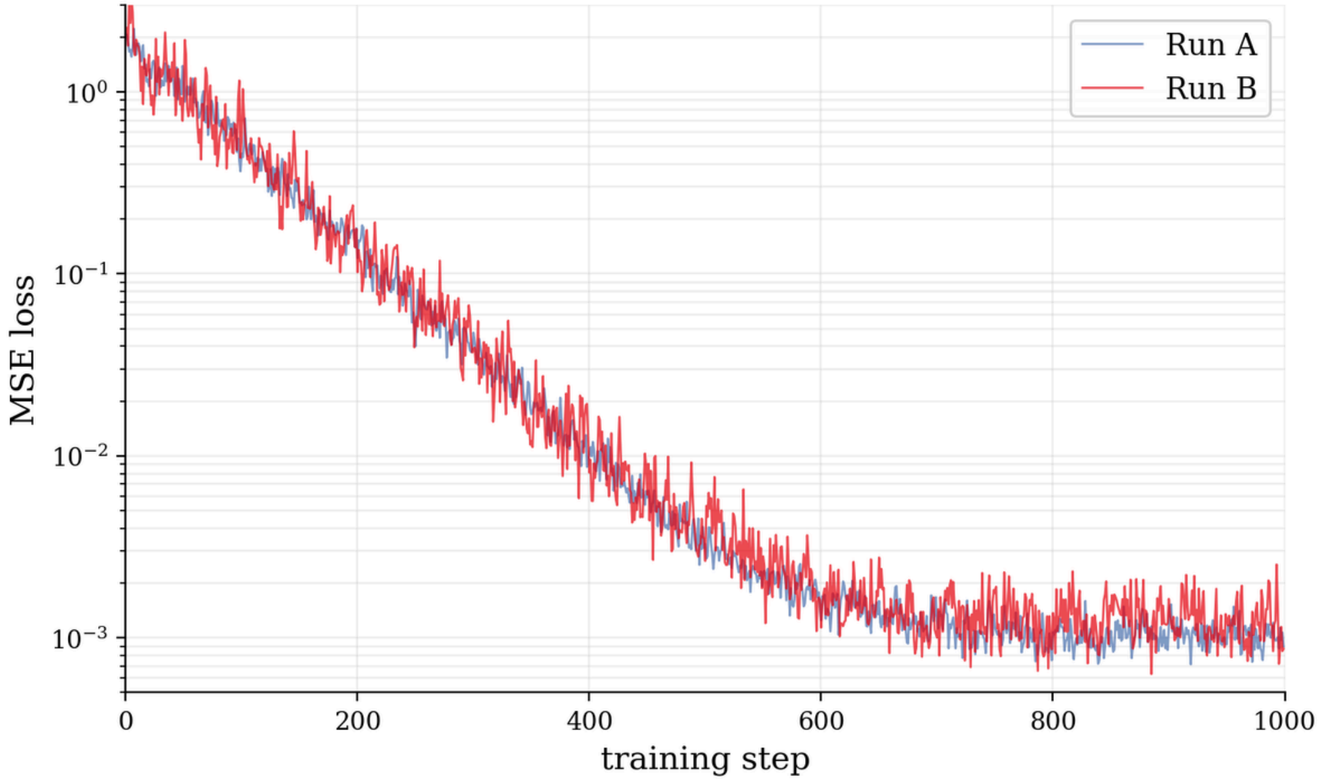
Data-driven Network Design

- Suppose we have two reasonable looking loss curves, A and B, both with reasonable loss curves, which is better?
  - Avoid comparing two runs by their final-step loss due to minibatch noise

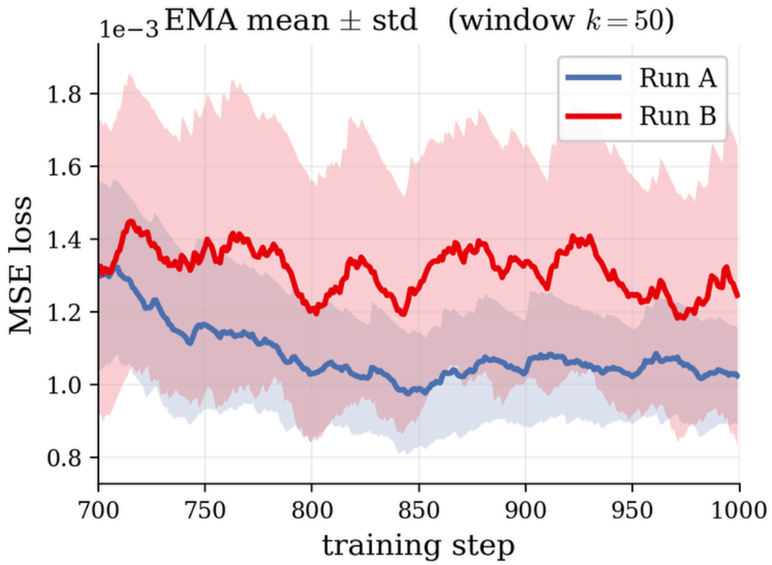


Data-driven Network Design

- Suppose we have two reasonable looking loss curves, A and B, both with reasonable loss curves, which is better?
  - Better to compute the **average loss over a window** of K later steps



$$\hat{L} = \frac{1}{K} \sum_{t=T-K+1}^{T} \mathcal{L}(\boldsymbol{\theta}_t), \qquad T_0 \leq T - K + 1,$$



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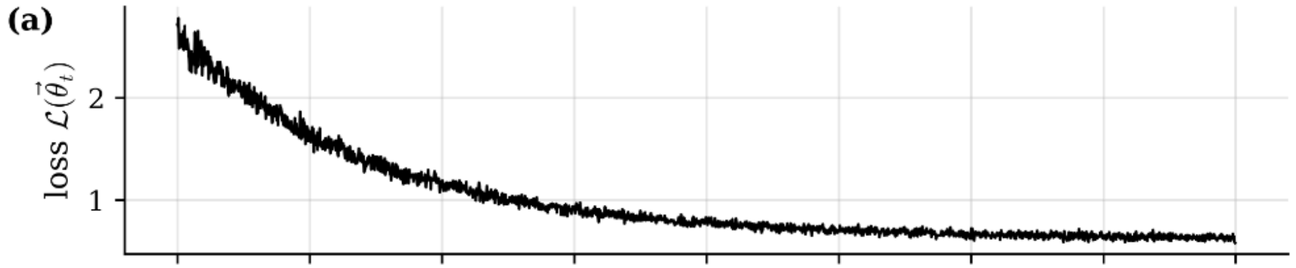
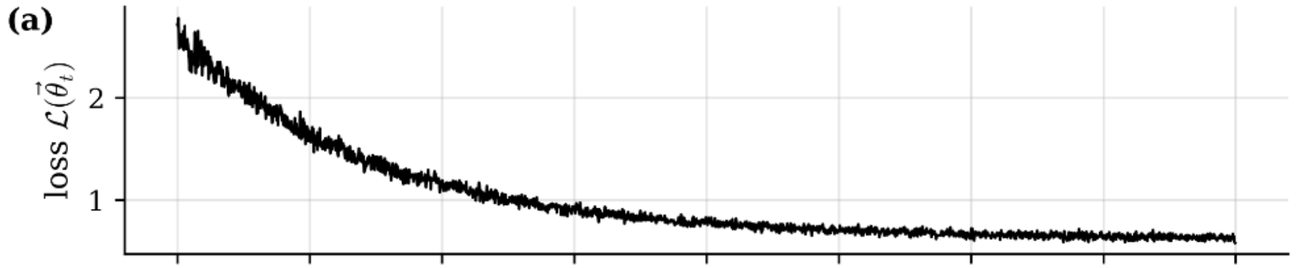


- Good idea to monitor the gradient *norm* during training steps $g_t = ||\nabla_\theta||_2$

Data-driven Network Design



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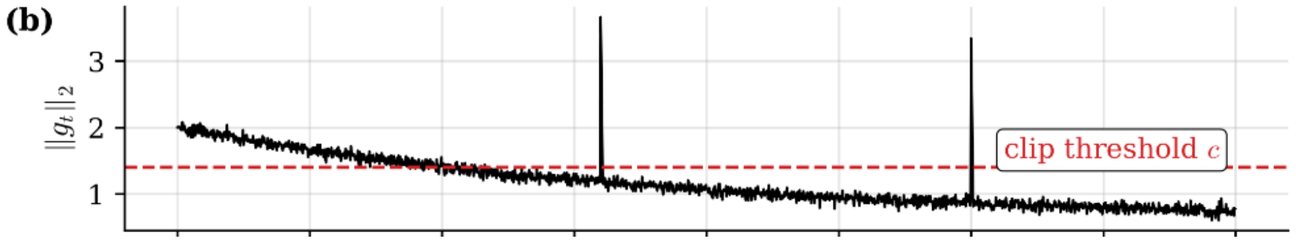
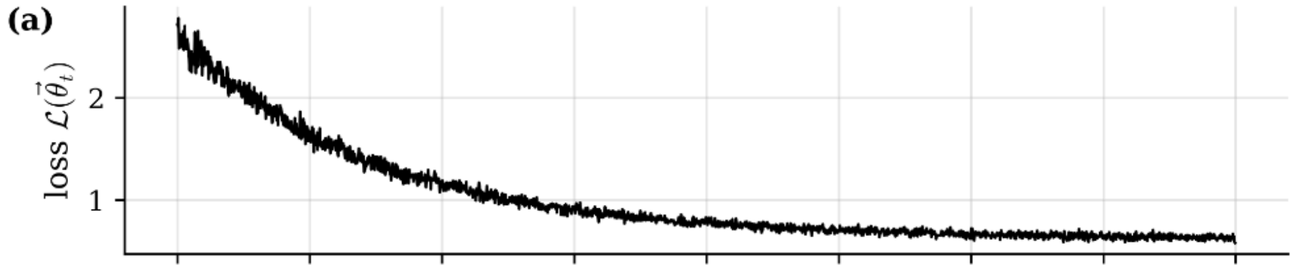


- We sometimes get spikes…

Data-driven Network Design



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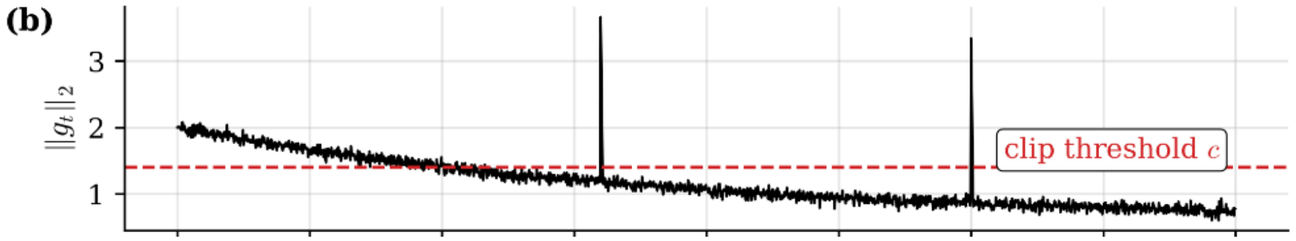
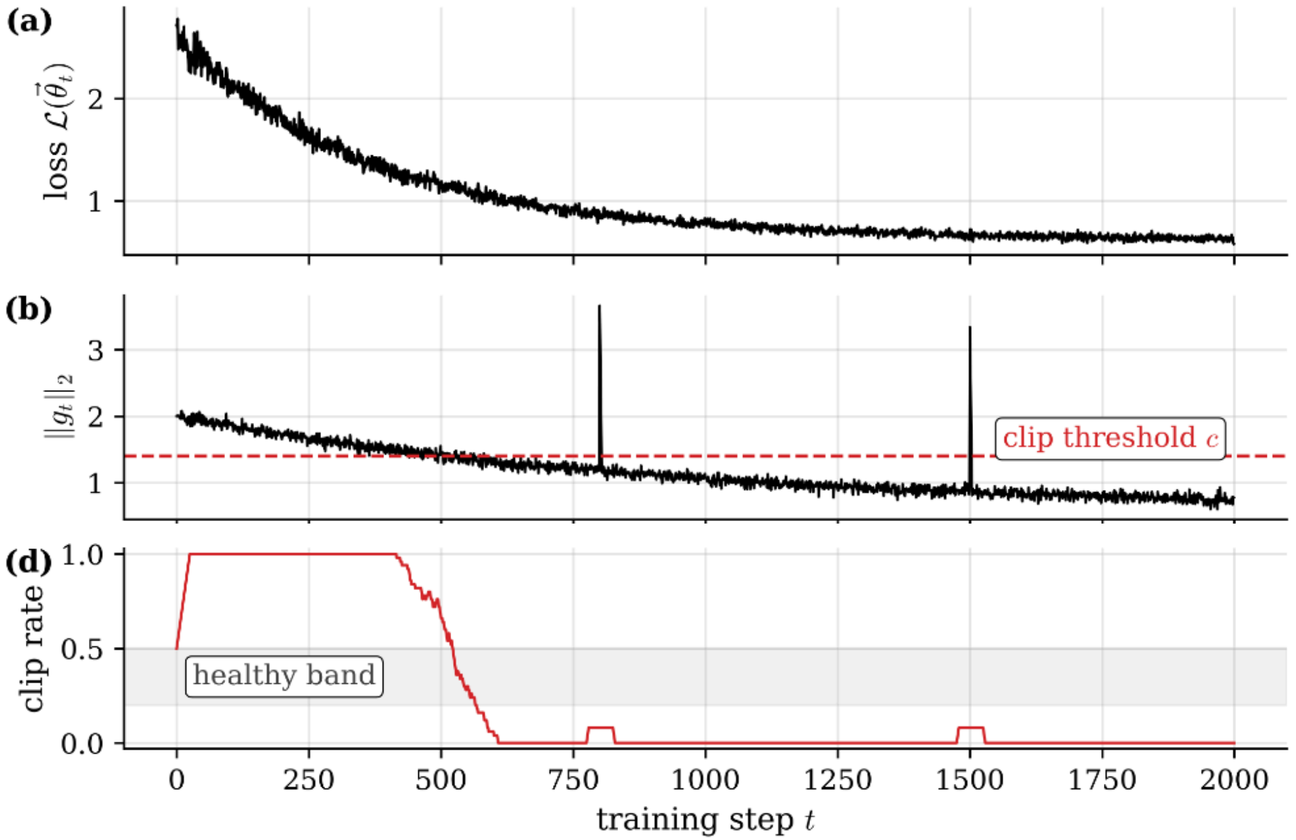


- We sometimes get spikes...

- These can affect update steps $\theta \leftarrow \theta - \alpha \nabla_\theta L$

Data-driven Network Design

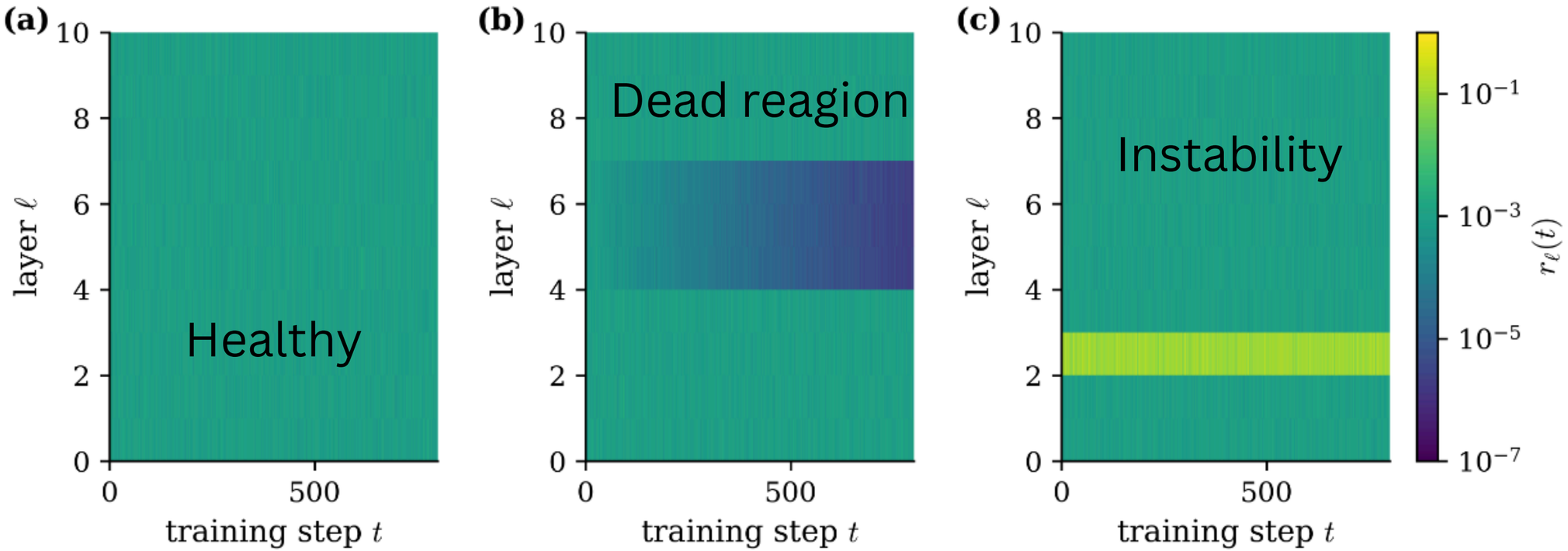
- **Gradient Clipping** can regularise *step-size*



- Careful not to under- or over-clip!

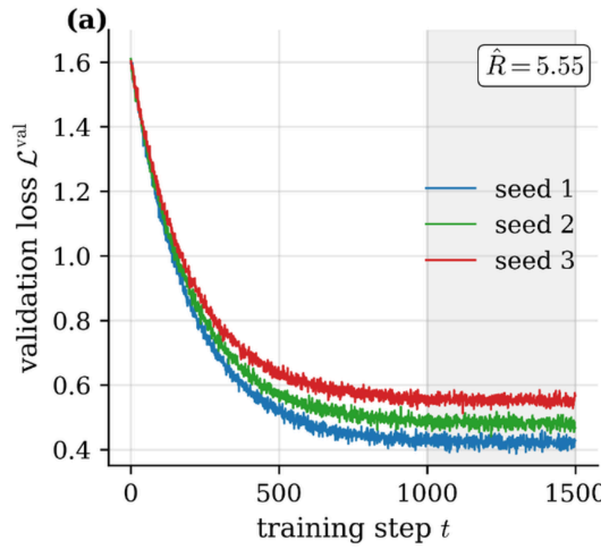
Data-driven Network Design

Per-layer update-to-weight ratio



Luck vs Progress

- To claim one *architecture* is better than another, we want to see it outperforming on many random seeds.
- How can we tell if one model is more or less responsive to seed-luck?
  - Using the tail window of length M from each seed



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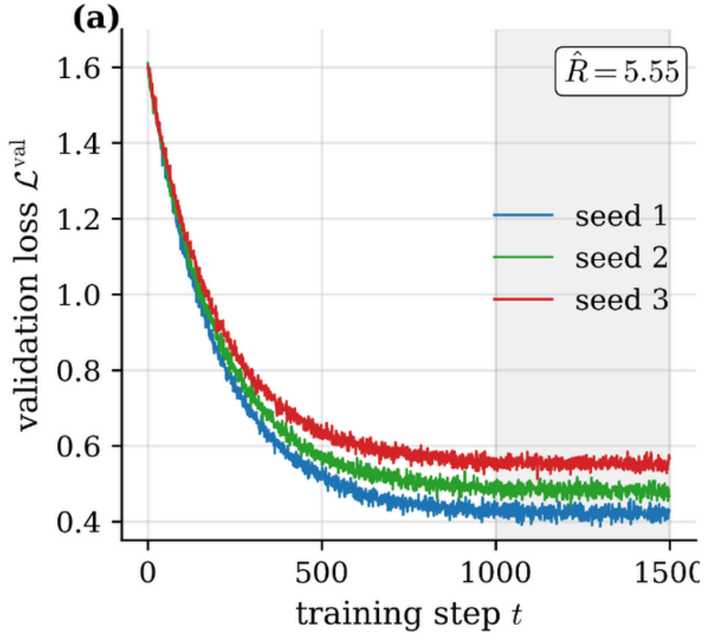

- Compute Gelman-Rubin Metric
  - (we will do this in the practical!)

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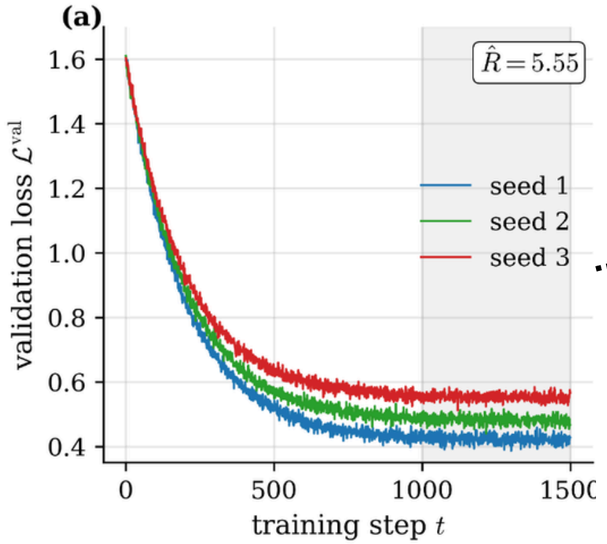
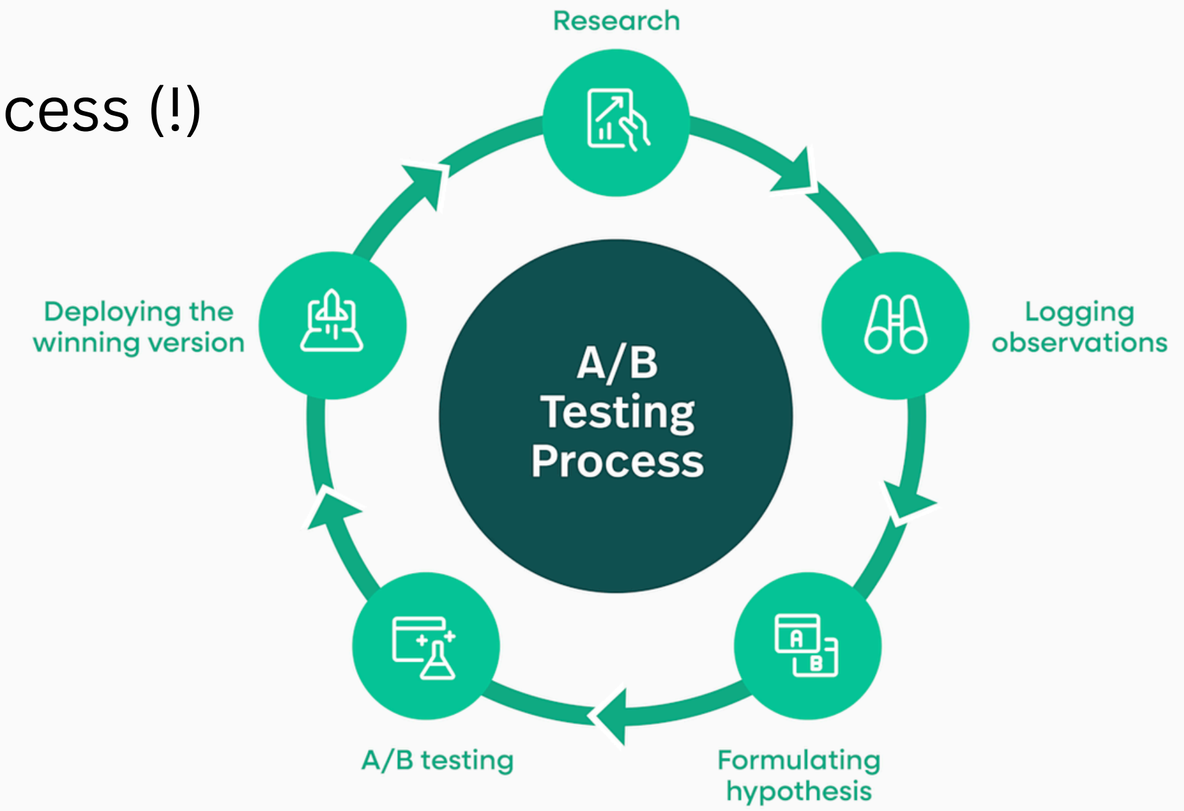
  - Using the tail window of length M from each seed



$$\hat{L}_m \qquad s_m^2 \qquad W = \frac{1}{M} \sum_{m=1}^{M} s_m^2,$$

Agentic Architecture Search

- Tests are good gates for coding agents to find architectures
- This can automate the tuning process (!)



Data-driven Network Design

- Learning rate
- EMA-windows
- Gradient clipping
- Update ratios
- Seed safety

} Shown (very!) briefly today

- Batch norm
- Data encoding
- Layer norms
- Types of optimizer
- Layer eigen-spectra
- Effective step-sizes

} Not shown but worth understanding (!)

Data-driven Network Design

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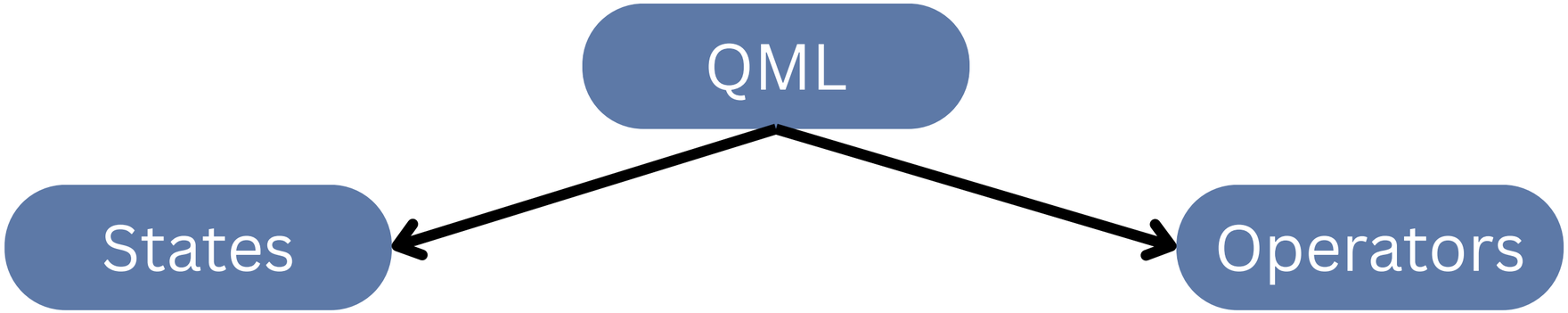
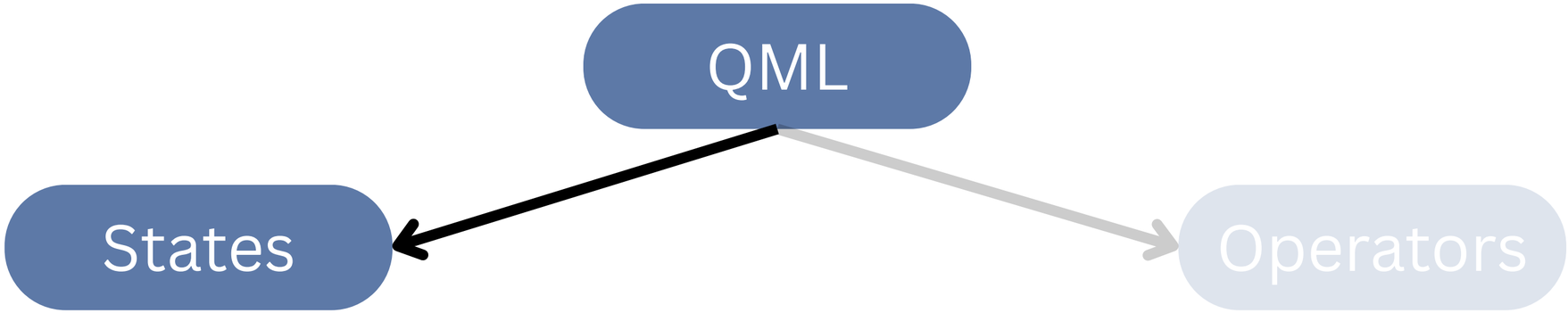
CONTENT

CONTENT

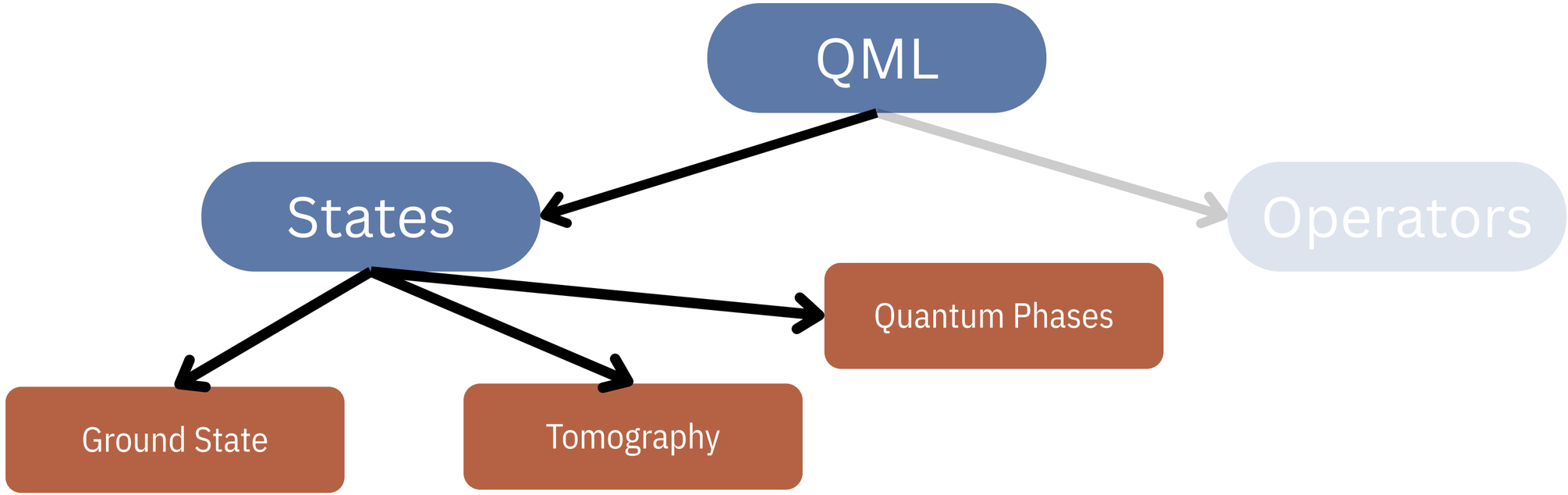
Quantum Machine Learning - Top Down View



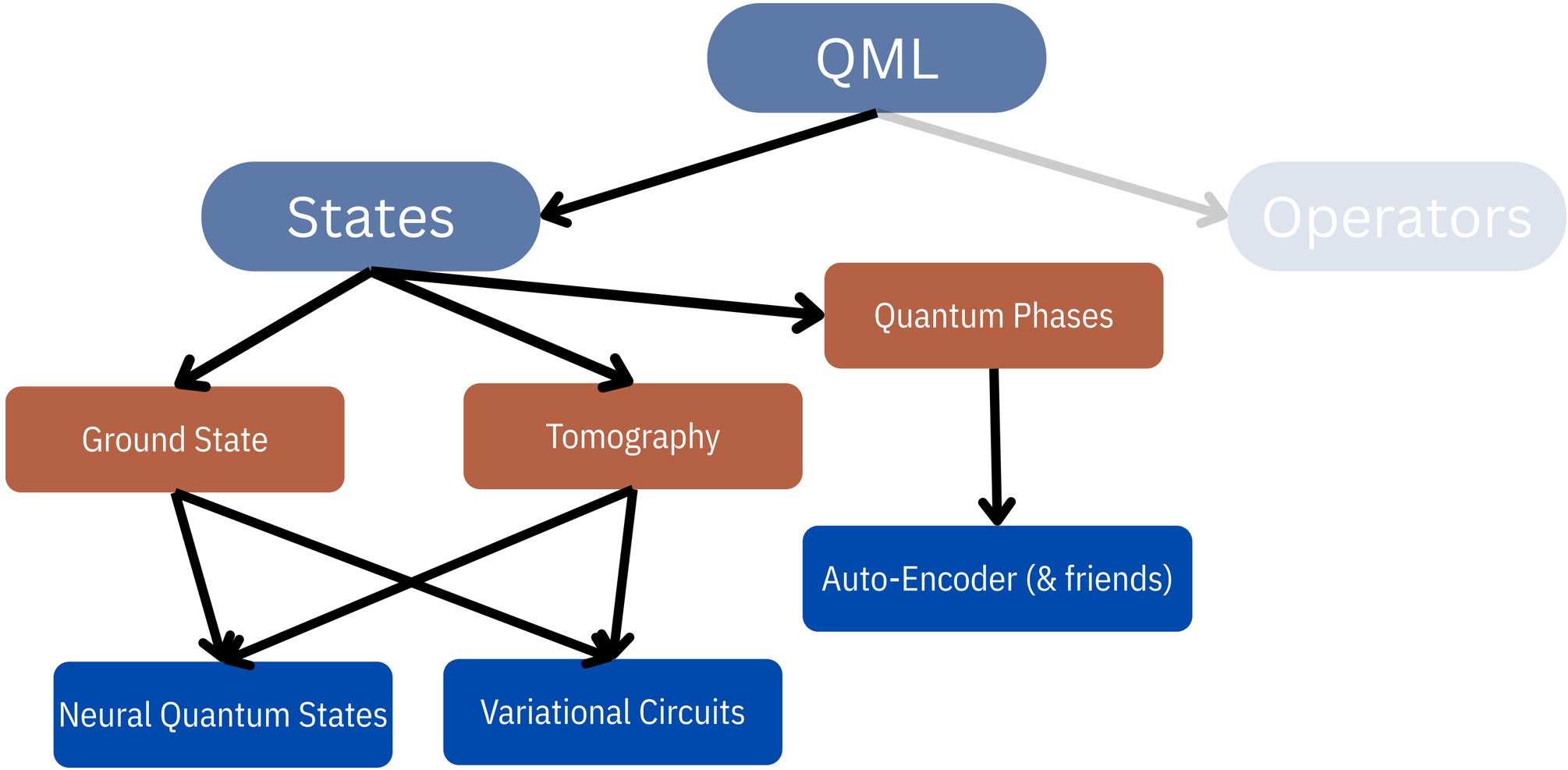
Quantum Machine Learning - Top Down View



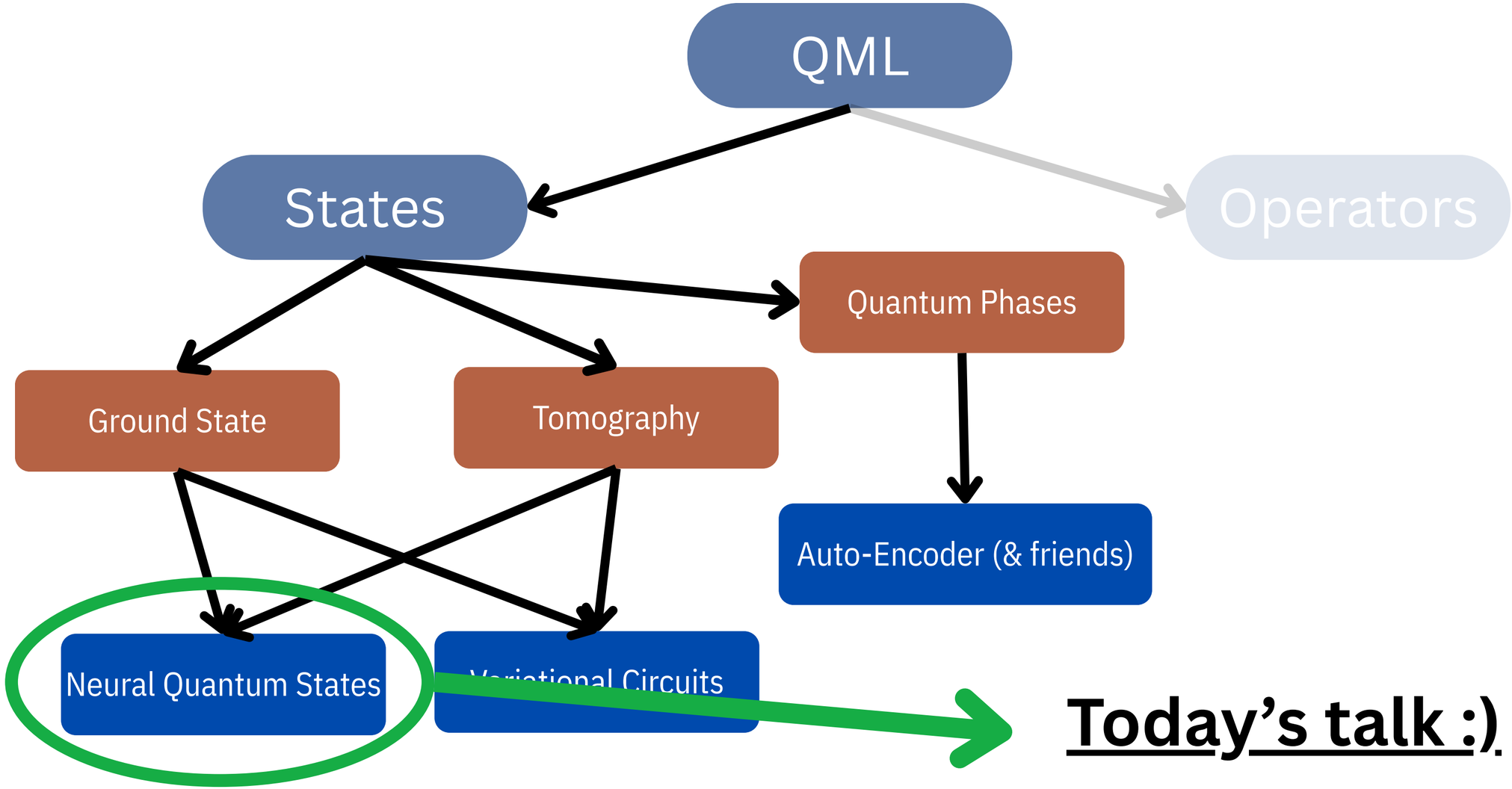
Quantum Machine Learning - Top Down View



Quantum Machine Learning - Top Down View

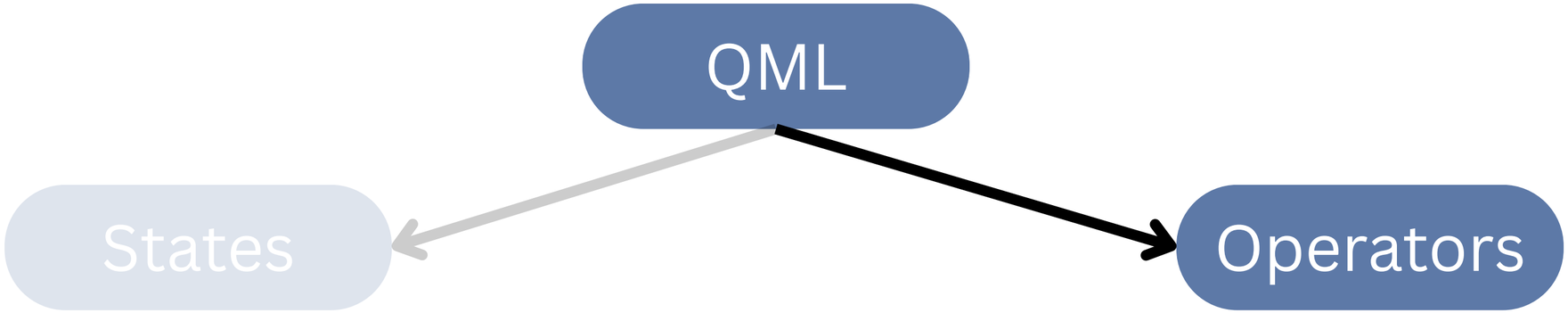


Quantum Machine Learning - Top Down View

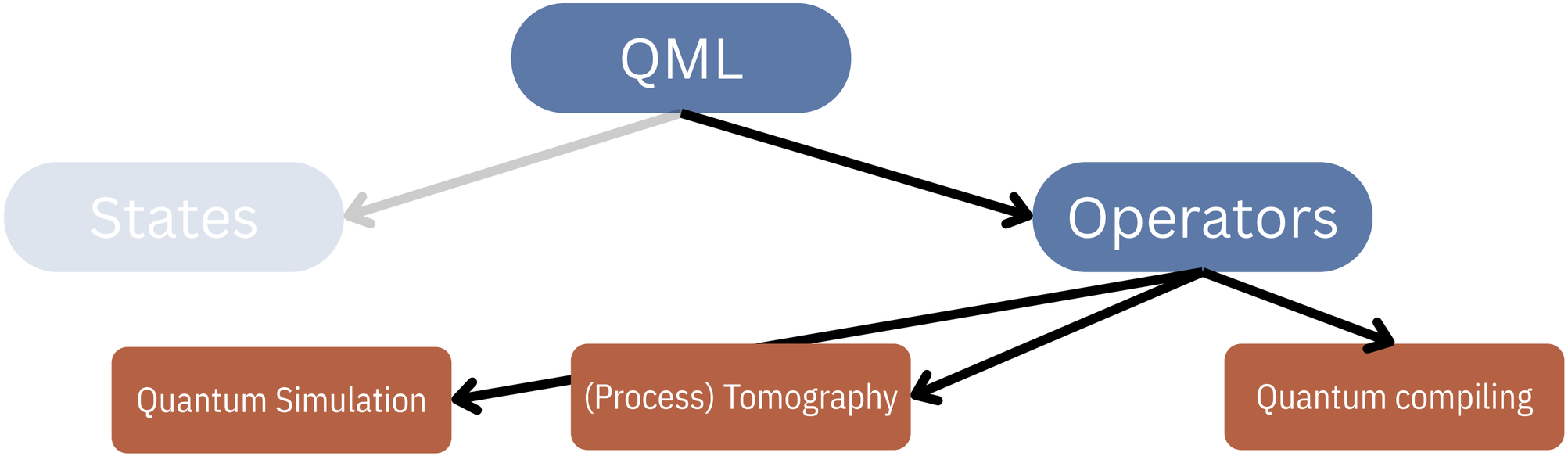


Today's talk :)

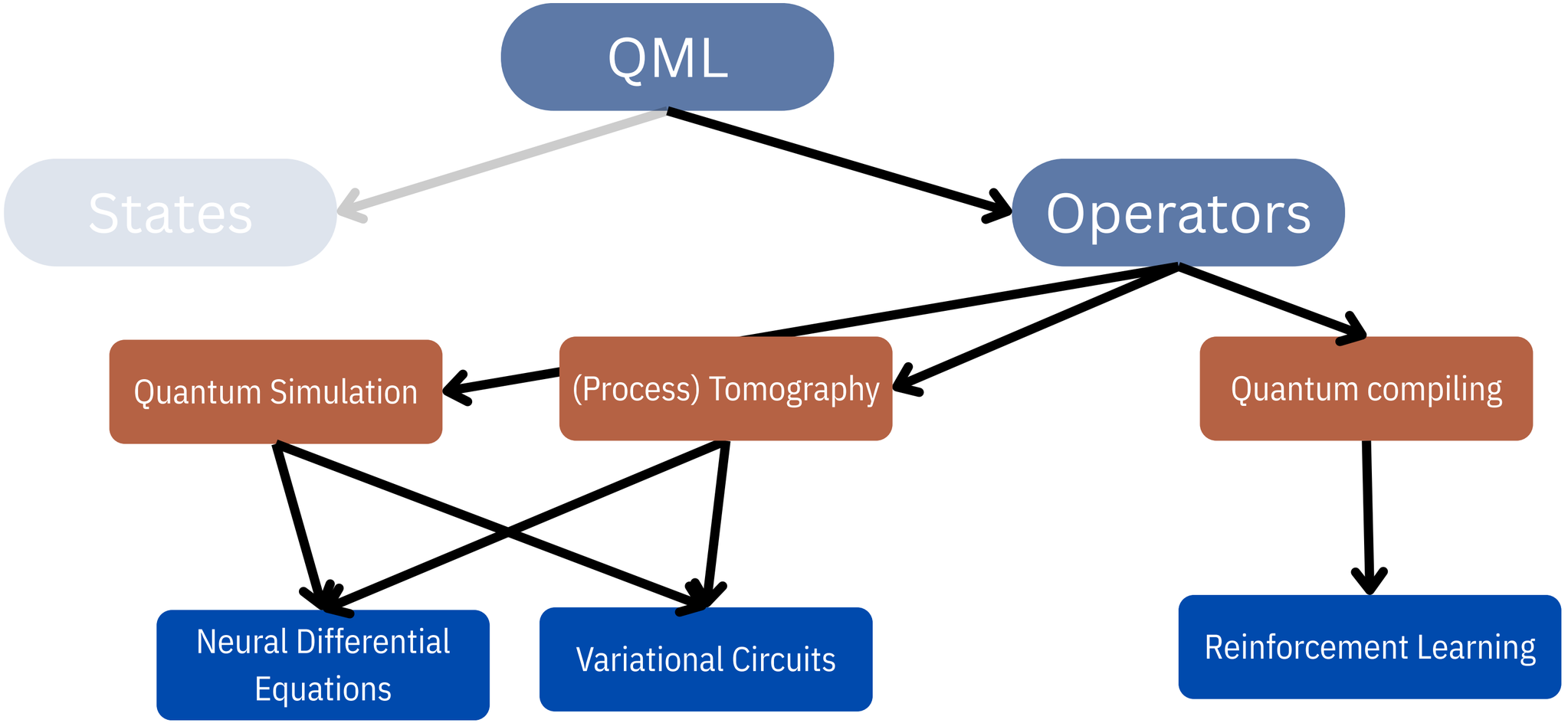
Quantum Machine Learning - Top Down View



Quantum Machine Learning - Top Down View



Quantum Machine Learning - Top Down View



NQS PART I

- Definitions
- Computing observables

WHAT DOES A WAVEFUNCTION DO ANYWAYS?

The Quantum Many-Body Problem

- Consider an *N*-qubit quantum state

$$|\psi(t)\rangle = \sum_{b_1,\ldots,b_N=0}^{1} c_{b_1,\ldots,b_N}(t)|b_1,\ldots,b_N\rangle$$

- Exponential number of coefficients to keep track of here

- Representing states and dynamics quickly becomes intractible with N...

Coefficients can themselves be functions…

- Consider an *N*-qubit quantum state

$$|\psi(t)\rangle = \sum_{b_1,\ldots,b_N=0}^{1} c_{b_1,\ldots,b_N}(t)|b_1,\ldots,b_N\rangle$$

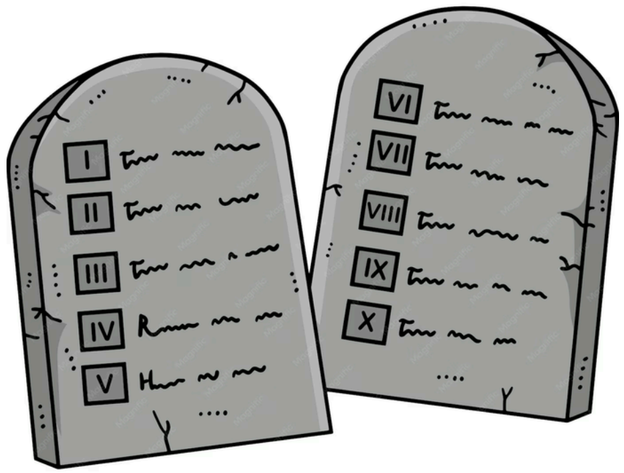
- Coefficient "function" $c : \{0,1\}^N \to \mathbb{C}$ receives a binary vector $\mathbf{b} \in \{0,1\}^N$ as input and spits out a complex number.

$$c(\mathbf{b}) \in \mathbb{C}$$

Neural Quantum States

- **Key idea:** use neural networks to approximate this function

$$\psi_\theta(\mathbf{b}) = \sqrt{p_\theta(\mathbf{b})} e^{i\phi_\theta(\mathbf{b})} \approx c(\mathbf{b})$$



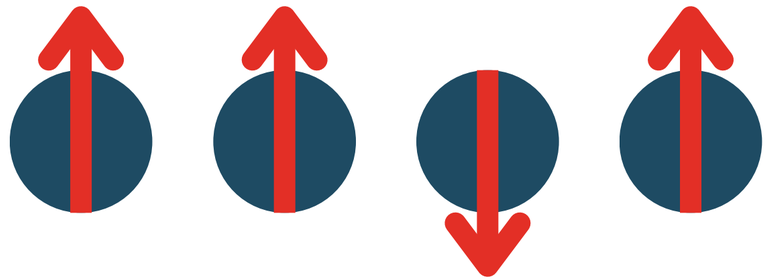
This works again thanks to the Universal Approximation Theorem - which says a large enough neural network can approximate *any* compact function given enough training and expressivity.

How does this work in practise?

Neural Quantum States

e.g. 4 quantum spin-1/2 chain (qubits)

$$|\psi\rangle = \sum_{j=\{0,1\}^4} c_{j_1,\ldots,l_4} |j_1, \ldots, j_4\rangle$$

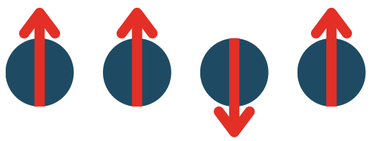


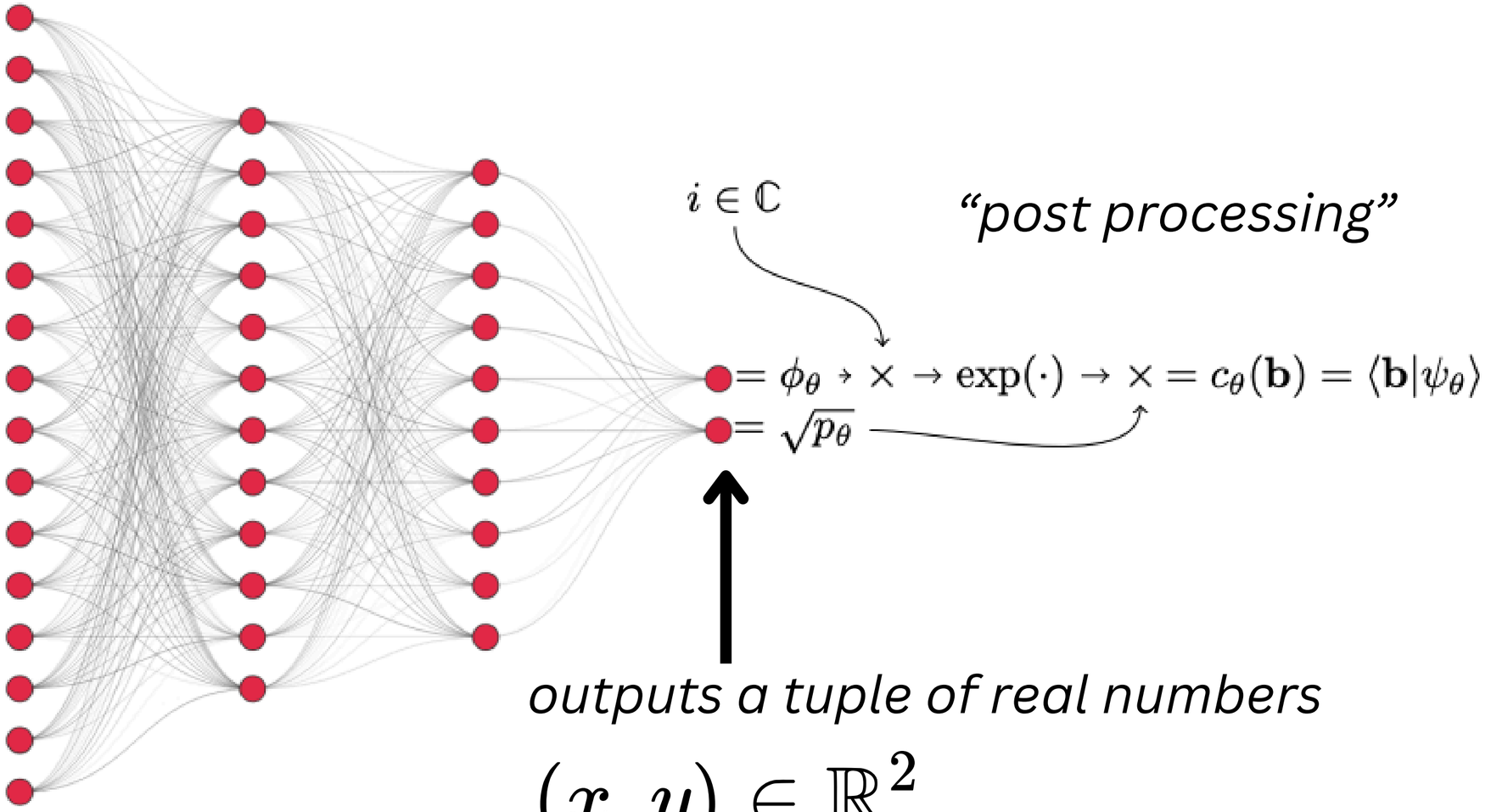
$$\psi_\theta(\mathbf{b}) = \sqrt{p_\theta(\mathbf{b})} e^{i\phi_\theta(\mathbf{b})} \approx c(\mathbf{b})$$

Neural Quantum States

16-bit binary number

$\mathbf{b} \in \{0, 1\}^{16}$





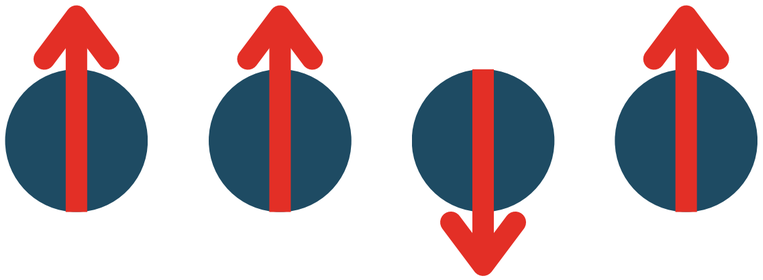
Neural Quantum States

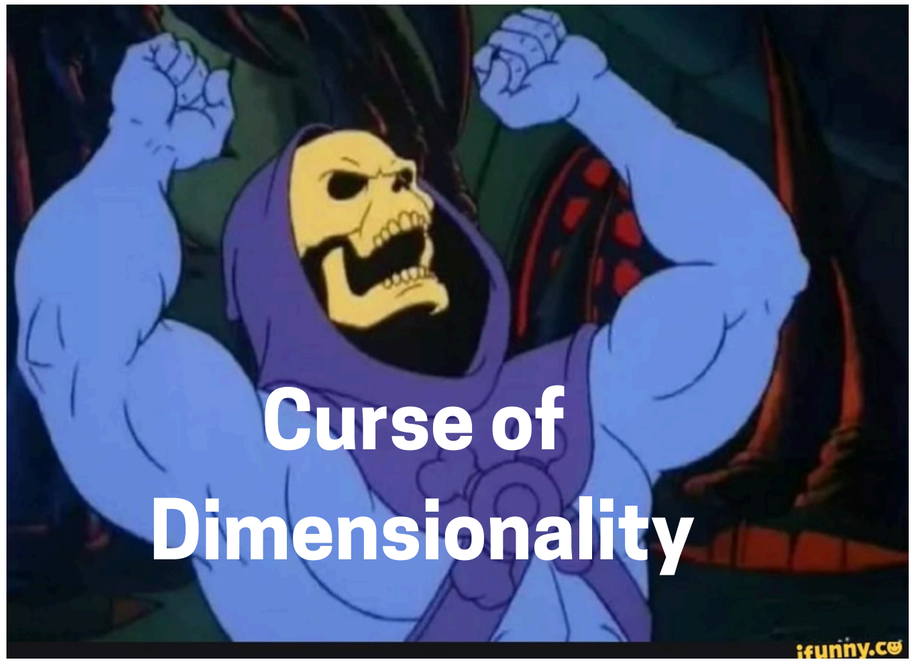
- Is this construction is at all useful?

- In order to know the complete description of

$$|\psi\rangle = \sum_{j=\{0,1\}^4} c_{j_1,\ldots,l_4} |j_1, \ldots, j_4\rangle$$

We need $t \sim \mathcal{O}(2^N)$ for N-bodies





Neural Quantum States

The postulates of quantum mechanics tell us that once we know a wavefunction, every observable quantity can be derived from it.

$$|\psi\rangle \rightarrow \mathbf{tr}(\hat{O}|\psi\rangle)$$

we are *actually* interested in when using a wave function is computing statistics of observables

Neural Quantum States

- One way to do this is with exact wave-functions, inner products, and the Born rule.

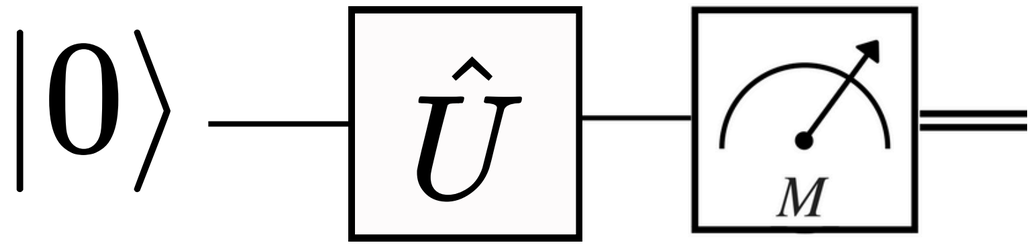
$$|\psi\rangle \in \mathcal{H} \qquad \hat{O} \in \beta(\mathcal{H}) \qquad \langle\ ,\ \rangle$$

Neural Quantum States

- One way to do this is with exact wave-functions, inner products, and the Born rule.

$$|\psi\rangle \in \mathcal{H} \qquad \hat{O} \in \beta(\mathcal{H}) \qquad \langle\ ,\ \rangle$$

$$p(m|\psi) = \mathrm{Tr}(\hat{O}|\psi\rangle\langle\psi|) = \langle\psi|\hat{O}|\psi\rangle$$



Neural Quantum States

- Another way is to employ the *Variational Monte Carlo* method
- VMC says to emulate wave-function statistics we need:

1. Efficiently generate amplitudes for any basis element

$$\langle \mathbf{b} | \psi \rangle$$

2. The ability to sample from the distribution

$$p\big(\mathbf{b}|\psi_\theta\big) = \frac{|\langle \mathbf{b}|\psi_\theta\rangle|^2}{\langle \psi_\theta|\psi_\theta\rangle}.$$

Computational mechanism for executing the Born rule

$$\langle \hat{H} \rangle_\psi \approx \sum_{\mathbf{b}} p(\mathbf{b}|\psi_\theta) \cdot \langle \mathbf{b}|\psi\rangle$$

Neural Quantum States

- VMC says to emulate wave-function statistics we need:

  1. Efficiently generate amplitudes for any basis element $\langle \mathbf{b} | \psi \rangle$

  2. The ability to sample from the distribution $p\left(\mathbf{b} | \psi_\theta\right) = \dfrac{|\langle \mathbf{b} | \psi_\theta \rangle|^2}{\langle \psi_\theta | \psi_\theta \rangle}.$

- With the two properties, we can sample any observable

This is because we can write down any observable in terms of these two quantities...

Neural Quantum States

$$\langle \hat{O} \rangle = \frac{\langle \psi_\theta | \hat{O} | \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle} = \sum_{\mathbf{b}} \left(\frac{|\langle \mathbf{b} | \psi_\theta \rangle|^2}{\sum_{\mathbf{b}''} |\langle \mathbf{b}'' | \psi_\theta \rangle|^2} \cdot \sum_{\mathbf{b}'} \frac{\langle \mathbf{b} | \psi_\theta \rangle}{\langle \mathbf{b}' | \psi_\theta \rangle} \langle \mathbf{b} | \hat{O} | \mathbf{b}' \rangle \right).$$

1

This is just the probability distribution

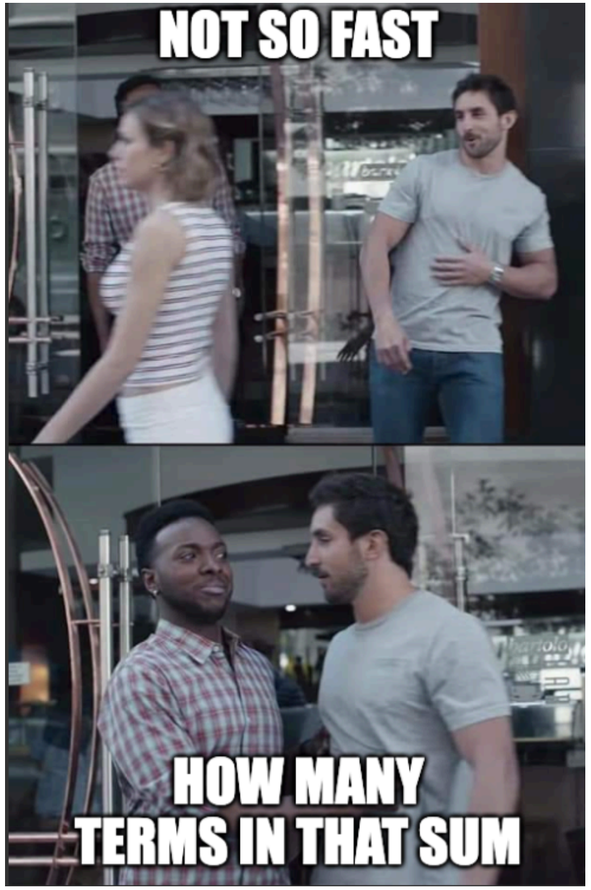
$$p\big(\mathbf{b}|\psi_\theta\big) = \frac{|\langle \mathbf{b} | \psi_\theta \rangle|^2}{\langle \psi_\theta | \psi_\theta \rangle}.$$

2

There are amplitudes times a matrix element in the computational basis

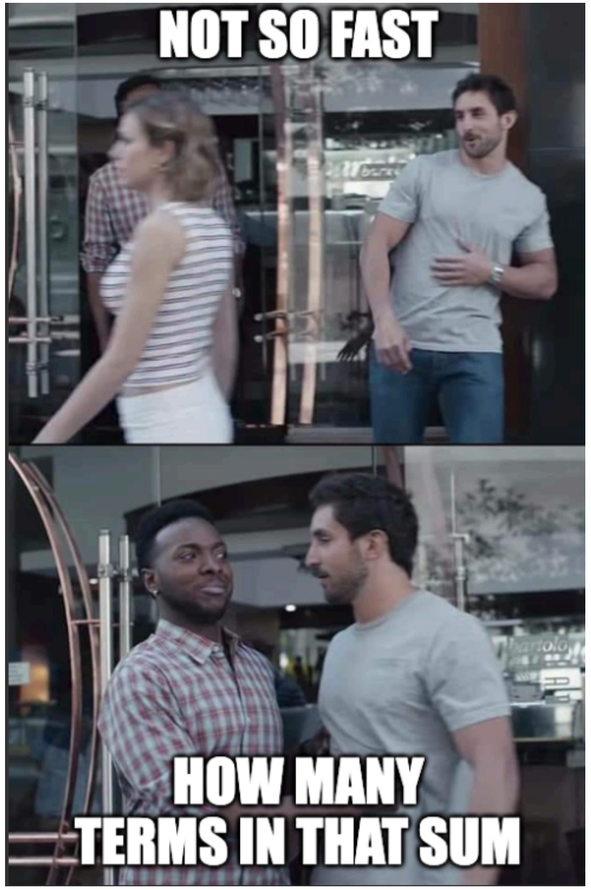
Neural Quantum States

$$\langle \hat{O} \rangle = \sum_{\mathbf{b}} \left(\frac{|\langle \mathbf{b} | \psi_\theta \rangle|^2}{\sum_{\mathbf{b}''} |\langle \mathbf{b}'' | \psi_\theta \rangle|^2} \cdot \sum_{\mathbf{b}'} \frac{\langle \mathbf{b} | \psi_\theta \rangle}{\langle \mathbf{b}' | \psi_\theta \rangle} \langle \mathbf{b} | \hat{O} | \mathbf{b}' \rangle \right).$$



Neural Quantum States

$$\langle \hat{O} \rangle = \sum_{\mathbf{b}} \left(\frac{|\langle \mathbf{b} | \psi_\theta \rangle|^2}{\sum_{\mathbf{b}''} |\langle \mathbf{b}'' | \psi_\theta \rangle|^2} \cdot \sum_{\mathbf{b}'} \frac{\langle \mathbf{b} | \psi_\theta \rangle}{\langle \mathbf{b}' | \psi_\theta \rangle} \langle \mathbf{b} | \hat{O} | \mathbf{b}' \rangle \right).$$



Neural Quantum States

Let’s make a *sparsity* assumption for the operator…

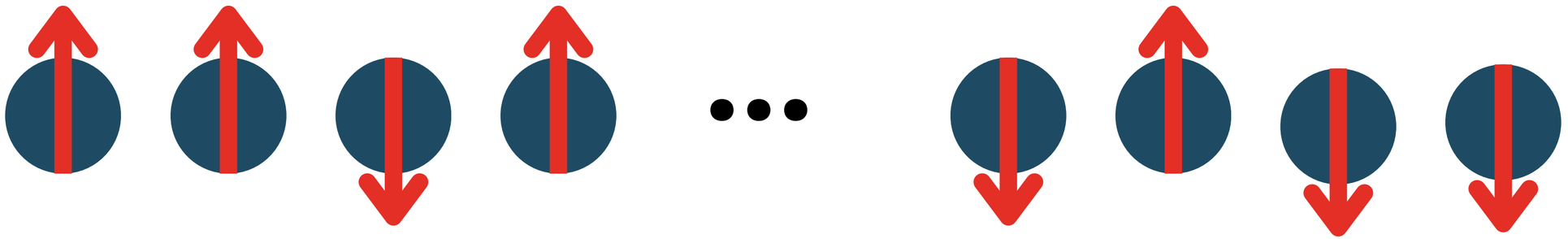
$$\langle \mathbf{b} | \hat{O} | \mathbf{b}' \rangle \neq 0$$

At most a polynomial number of bistrings should have non-zero amplitude w.r.t operator

Good or bad assumtion?

Neural Quantum States

$$|\psi(t)\rangle = \sum_{b_1,\ldots,b_N=0}^{1} c_{b_1,\ldots,b_N}(t)|b_1,\ldots,b_N\rangle$$



Which kinds of operators satisfy

$$\langle \mathbf{b}|\hat{O}|\mathbf{b}'\rangle \neq 0 \sim \mathcal{O}(\mathrm{Poly}(n))?$$

Neural Quantum States

$$\langle \hat{O} \rangle = \sum_{\mathbf{b}} p(\mathbf{b}|\psi_\theta) \sum_{\mathbf{b}'} \frac{\langle \mathbf{b}|\psi_\theta\rangle}{\langle \mathbf{b}'|\psi_\theta\rangle} \langle \mathbf{b}|\hat{O}|\mathbf{b}'\rangle \approx \langle O^{\mathrm{loc}}(\mathbf{b};\theta)\rangle_{\mathbf{b}}$$

Efficient sampling

Sparse

Sampling some bitstrings, $\{\mathbf{s}_1, \ldots, \mathbf{s}_M\} \sim p(\mathbf{b}|\psi_\theta)$

We can estimate observables by the arithmetic mean

$$\langle \hat{O} \rangle \approx \frac{1}{M} \sum_{j=1}^{M} \langle O^{\mathrm{loc}}(\mathbf{s}_j;\theta)\rangle.$$

Neural Quantum States

$$\langle \hat{O} \rangle \approx \frac{1}{M} \sum_{j=1}^{M} \langle O^{\mathrm{loc}}(\mathbf{s}_j; \theta) \rangle.$$

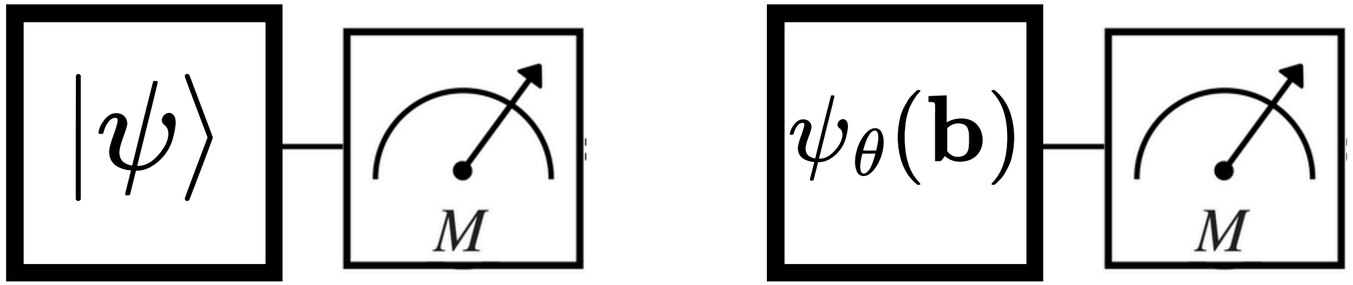
Error in sampling this way...

$$\epsilon = \sqrt{\sigma^2 / M},$$

NB: This is known and controllable - simply change the number of samples!

Neural Quantum States

Representing a given state



Algorithm 7 Estimating Local Observables with a NQS

Input: a NQS $\psi_\theta : \{0,1\}^N \to \mathbb{C}$ and a set of random Binary bitstrings $\mathbf{B} = \{\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_M\}$
for each $\mathbf{b}$ in $\mathbf{B}$ **do**
    Forward pass $\psi_\theta(\mathbf{b}) = \langle \mathbf{b}|\psi_\theta\rangle$ ▷ Should be efficient
    Compute $\langle O^{\text{loc}}(\mathbf{b};\theta)\rangle$ ▷ See Eq. (4.103), $\hat{O}$ inputted therefore efficient
end for
Return $\langle \hat{O}\rangle \approx \frac{1}{M}\sum_{\mathbf{b}\in\mathbf{B}} \langle O^{\text{loc}}(\mathbf{b};\theta)\rangle$

NQS Part II

- Variational Princinple
- Training with Energy Gradients
- Zero Variance Principle

Neural Quantum States

The variational principle applies to neural quantum states

Box 4: Variational Principle

For any normalised wavefunction, $|\psi\rangle$, the variational principle states that

$$E_{gs} \leq \langle\psi|\hat{H}|\psi\rangle\,. \tag{4.56}$$

That is, all states of a quantum system with Hamiltonian H overestimate the ground-state energy except for the ground state itself, $|\psi_{gs}\rangle$. Variational methods seek to find a tight upper bound to this.

Neural Quantum States

Using a neural network as a map from a binary bitstring (the index) to an amplitude will still be an upper bound for the ground state energy

$$E(\theta) = \frac{\langle \psi_\theta | \hat{H} | \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle} \geq E_{gs}$$

Thanks to Monte Carlo sampling,

$$E(\theta) = \langle \hat{H} \rangle \approx \sum_{\mathbf{b}} p\left(\mathbf{b} | \psi_\theta\right) \langle H^{\mathrm{loc}}(\mathbf{b}; \theta) \rangle_{\mathbf{b}}$$

Neural Quantum States

To create a training loop that solves $\min_{\theta} \frac{\langle \psi_\theta | \hat{H} | \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle},$

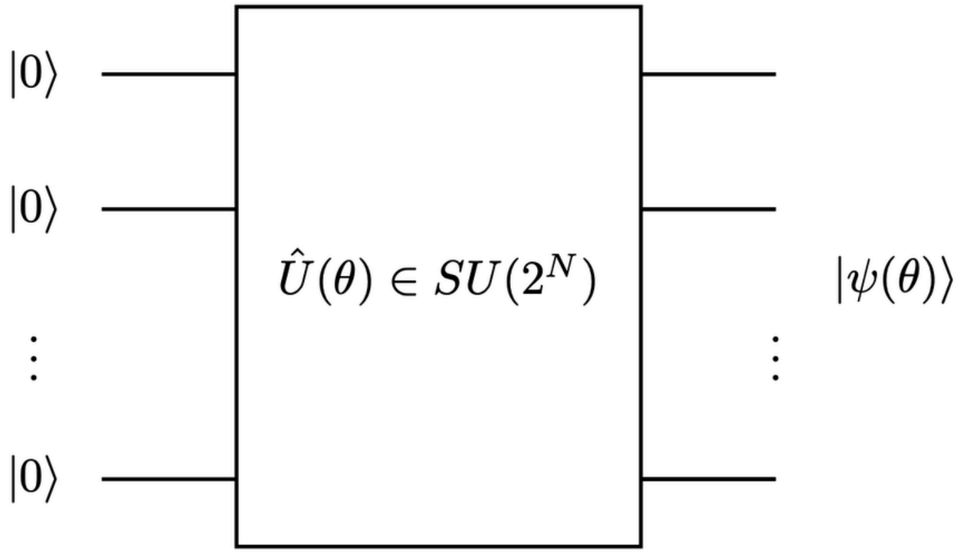
We need to show that our estimate of the system's energy is differentiable if we want to do gradient based updates

$$\theta \leftarrow \theta - \eta \nabla_\theta E(\theta), \qquad E(\theta) = \frac{\langle \psi_\theta | \hat{H} | \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle}$$

Neural Quantum States

How is this **different from** a **variational quantum eigensolver**??

All variational **params** in a VQE are ***real***



this is because the **state** is constructed **from** a parametric **circuit**

Neural Quantum States

How is this different from VQE?

In NQS, we have a neural representation of a wave-function rather than access to it as the output of some unitary process....

Complex numbers now form an integral part of the computational graph...

$$E(\psi_\theta) : \mathbb{C} \rightarrow \mathbb{R}$$

Neural Quantum States

- We now want to find states of *minimal energy*...
- Back propagation through a complex-to-real function

Remember complex analysis?

- A function is *holomorphic* when

$$\frac{\partial}{\partial z^*} f(z, z^*) = 0.$$

f is not a function of the conjugate

- We need a key assumption that the wave-function is *holomorphic*

$$\frac{\partial \psi_\theta}{\partial \theta^*} = 0.$$

Remember complex analysis?

- We need a key assumption that the wave-function is *holomorphic*

$$\frac{\partial \psi_\theta}{\partial \theta^*} = 0.$$

- Reasonable assumption - components of a complex neural network can easily be made holomorphic by ensuring the activation functions and sums over layers are taken over θ (not the conjugate)

Neural Quantum States

We can derive the following:

$$\frac{\partial E(\theta)}{\partial \theta^*} = \mathbb{E}_{x\sim p_\theta(x)}\left[\left(\partial_\theta \log \psi_\theta(x)\right)\left(H^{\mathrm{loc}} - \mathbb{E}_{x\sim p_\theta(x)}[H^{\mathrm{loc}}(x)]\right)\right].$$

All that remains is to conjugate

Hence, our model should be the logarithm of the amplitudes

Neural Quantum States

We can derive the following:

$$\frac{\partial E(\theta)}{\partial \theta^*} = \mathbb{E}_{x\sim p_\theta(x)}\left[\left(\partial_\theta \log \psi_\theta(x)\right)\left(H^{\mathrm{loc}} - \mathbb{E}_{x\sim p_\theta(x)}[H^{\mathrm{loc}}(x)]\right)\right].$$

All that remains is to conjugate

(and to write code)

Neural Quantum States

Since this gradient is based on expectation under distributions, we can approximate it with batches of samples $x \sim p_\theta(x)$

$$\partial_{\theta^*} E(\theta) \approx \frac{1}{N} \sum_{i=1}^{M} (\partial_\theta \log \psi_\theta(x_i)) \left(H^{\mathrm{loc}}(x_i) - \frac{1}{N} \sum_{j=1}^{M} H^{\mathrm{loc}}(x_j) \right),$$

Zero-Variance Principle

- Variance of local energy vanishes if (and only if!) we have an eigenstate

$$H^{\mathrm{loc}}(x) = \frac{\langle x|\hat{H}|\psi_\theta\rangle}{\langle x|\psi_\theta\rangle} = \frac{E_n \langle x|\psi_\theta\rangle}{\langle x|\psi_\theta\rangle} = E_n$$

- We can see that

$$\mathrm{Var}_{p_\theta}\left[H^{\mathrm{loc}}\right] = \frac{\langle \psi_\theta|(\hat{H} - E_0)^2|\psi_\theta\rangle}{\langle \psi_\theta|\psi_\theta\rangle} = 0$$

- **Variance is a measure of how close to**

CONTENT

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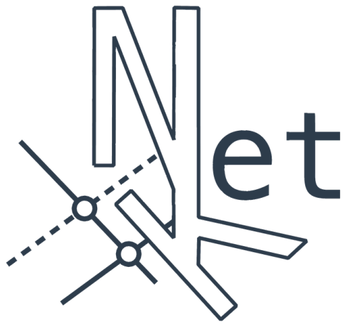
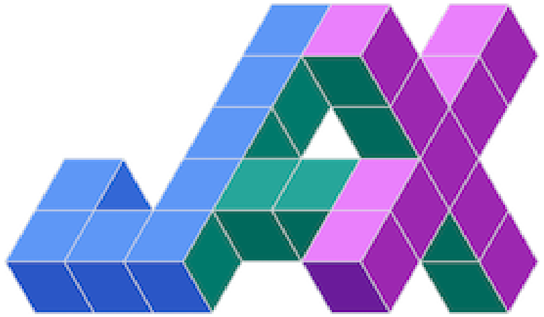
The NetKet package



Built on



Open source package developed by group of Filipo Vicentini

NQS Ground state search - Ising Model

Consider states of a 1D spin-1/2 chain with Ising Hamiltonian

$$\hat{H} = J \sum_j \sigma_j^{(x)} \sigma_{j+1}^{(x)} - h \sum_j \sigma_j^{(z)}$$

NQS Ground state search - Ising Model

Consider states of a 1D spin-1/2 chain with Ising Hamiltonian

$$\hat{H} = J \sum_j \sigma_j^{(x)} \sigma_{j+1}^{(x)} - h \sum_j \sigma_j^{(z)}$$

With reference state found by exact diagonalisation

$$\langle \mathbf{b} | \hat{H} | \mathbf{b}' \rangle \in \mathbb{C}^{2^n \times 2^n} \sim \mathcal{O}(4^n)$$

NQS Ground state search - Ising Model

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With reference state found by exact diagonalisation

$$\langle \mathbf{b} | \hat{H} | \mathbf{b}' \rangle \in \mathbb{C}^{2^n \times 2^n} \sim \mathcal{O}(4^n)$$

(so we can check an exact
numerical result for small systems)

NQS Ground state search - Ising Model

Consider states of a 1D spin-1/2 chain with Ising Hamiltonian

$$\hat{H} = J \sum_j \sigma_j^{(x)} \sigma_{j+1}^{(x)} - h \sum_j \sigma_j^{(z)}$$

To go beyond the curse of dimensionality we need to look for variational approximations with a *polynomial* scaling for the number of bodies

Let’s look at three example models

NQS Ground state search - Ising Model

Normalised Mean Field Ansatz $\langle \sigma_1^z, \dots, \sigma_N^z | \psi_{mf} \rangle = \prod_{i=1}^{N} \Phi(Z_i)$

Polar representation of the wavefunction

$$\Phi(\sigma_z) = \sqrt{A(\sigma^z)} e^{i\phi(\sigma^z)}$$

$$A : \{0,1\}^n \to \mathbb{R}_+$$

To simplify our lives

NQS Ground state search - Ising Model

Normalised Mean Field Ansatz $\langle \sigma_1^z, \ldots, \sigma_N^z | \psi_{mf} \rangle = \prod_{i=1}^{N} \Phi(Z_i)$

Polar representation of the wavefunction

$$\Phi(\sigma_z) = \sqrt{A(\sigma^z)} e^{i\phi(\sigma^z)}$$

$$A : \{0,1\}^n \to \mathbb{R}_+ \qquad A(\sigma^z;\theta) = \frac{1}{1 - e^{-\theta\sigma_z}}$$

To simplify our lives $\phi = 0$

e.g. in 2D, Onsager's solution is known and real so we can safely assume this here

NQS Ground state search - Ising Model

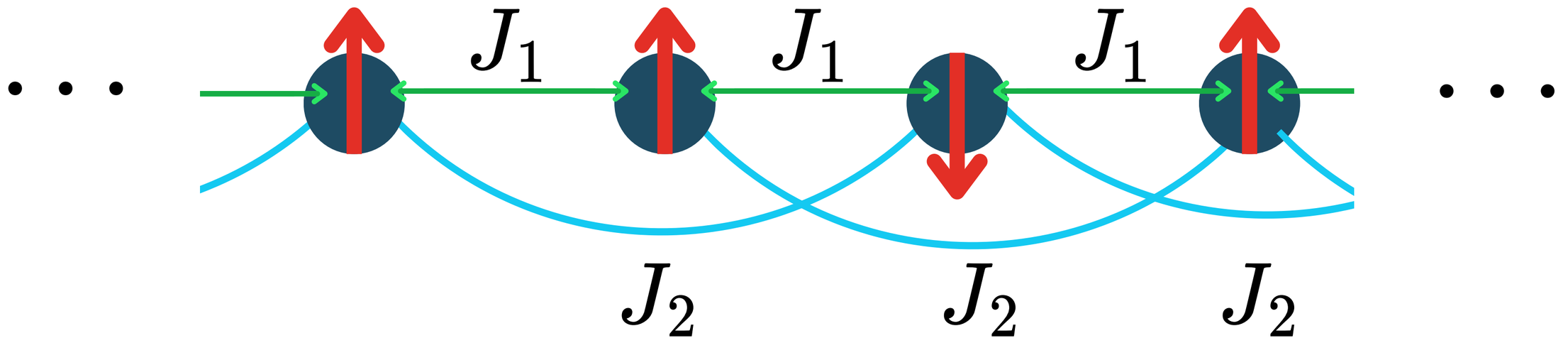
Jastrow Ansatz

$$\langle \sigma_1^z, \dots, \sigma_N^z | \Psi_{\text{jas}} \rangle = e^{\sum_i J_1 \sigma_i^z \sigma_{i+1}^z + J_2 \sigma_i^z \sigma_{i+2}^z}$$

NQS Ground state search - Ising Model

Jastrow Ansatz

$$\langle \sigma_1^z, \dots, \sigma_N^z | \Psi_{\text{jas}} \rangle = e^{\sum_i J_1 \sigma_i^z \sigma_{i+1}^z + J_2 \sigma_i^z \sigma_{i+2}^z}$$



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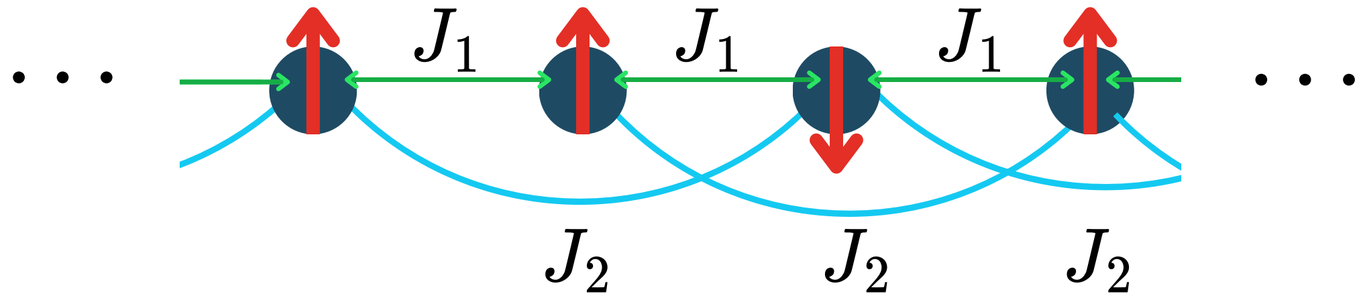
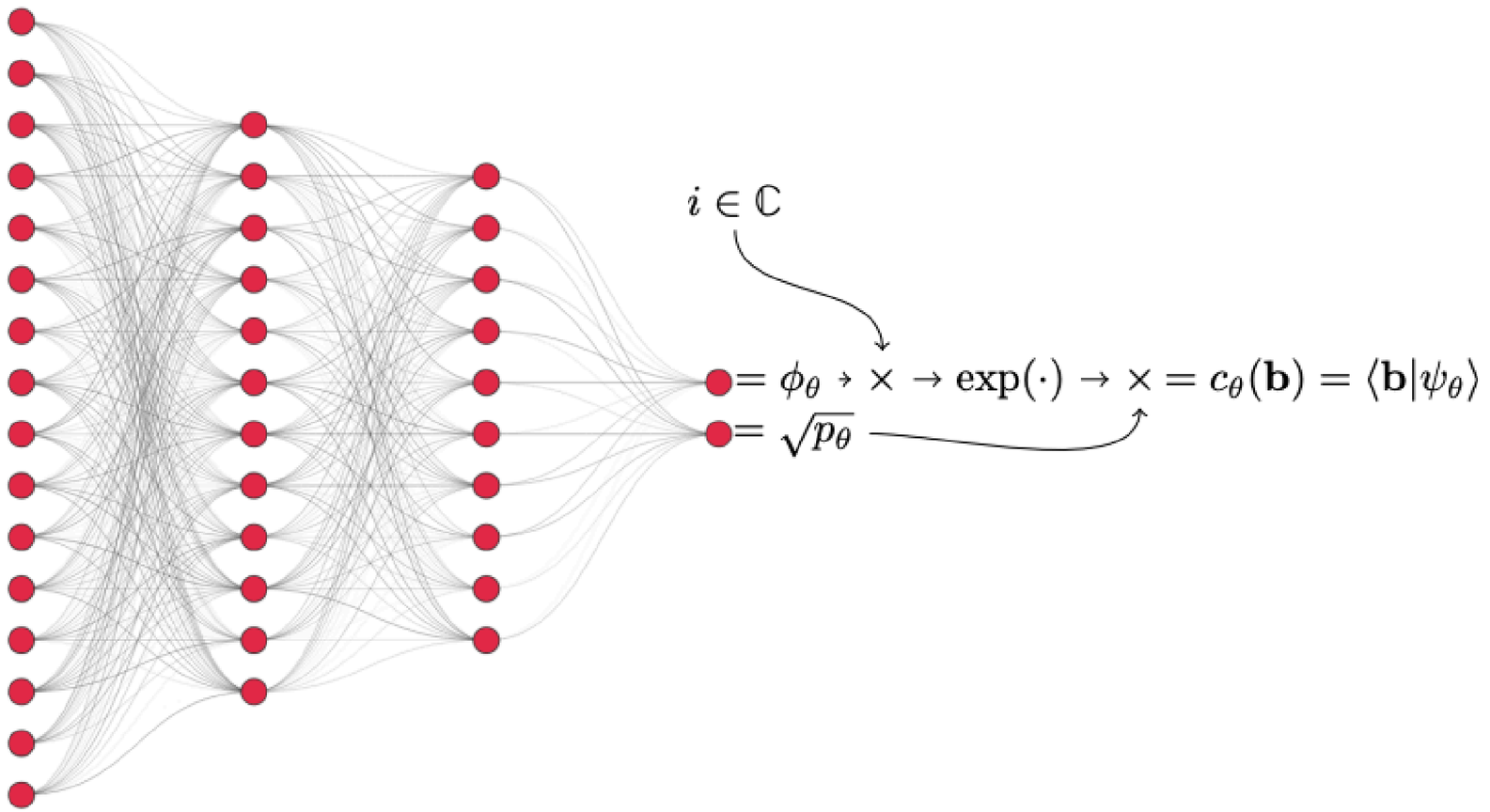
Variational parameters $\theta = \{J_1, J_2\}$



NQS Ground state search - Ising Model

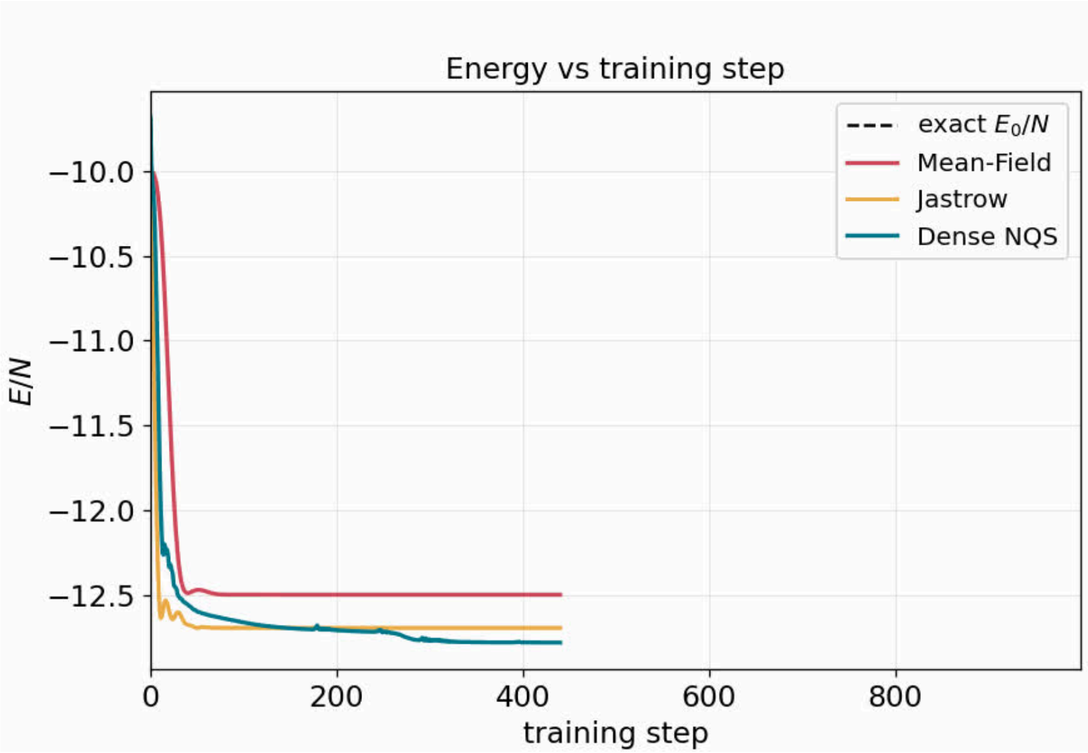
NQS Ansatz

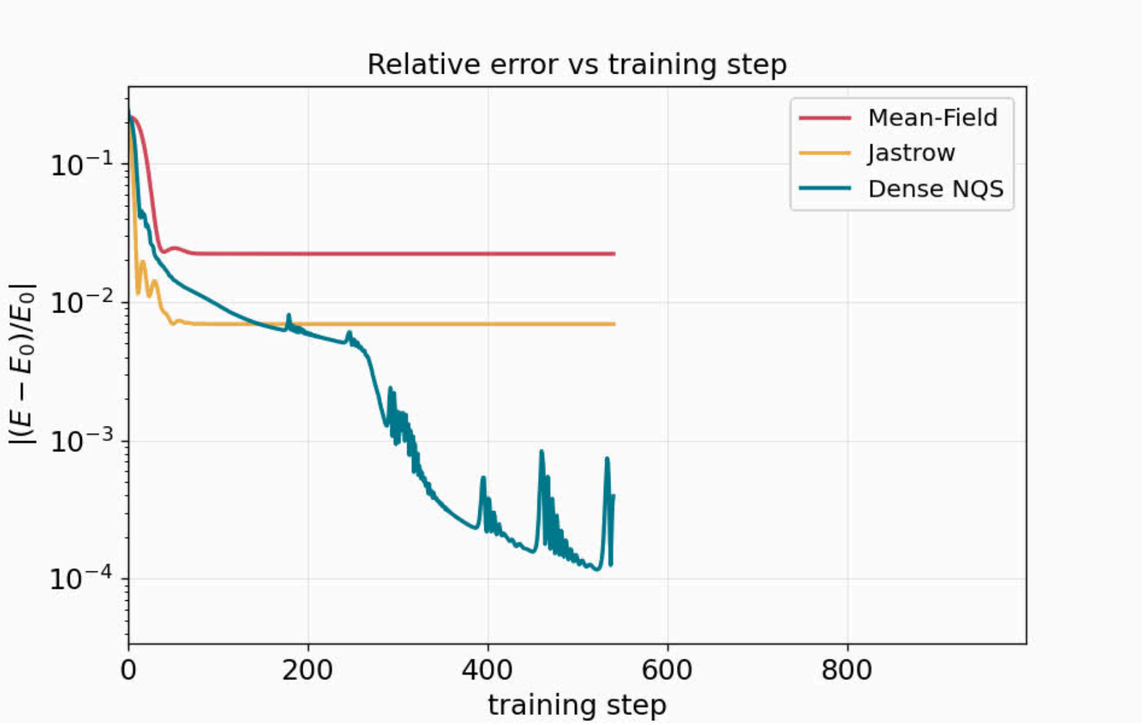


Dense Network

NQS Ground state search - Ising Model

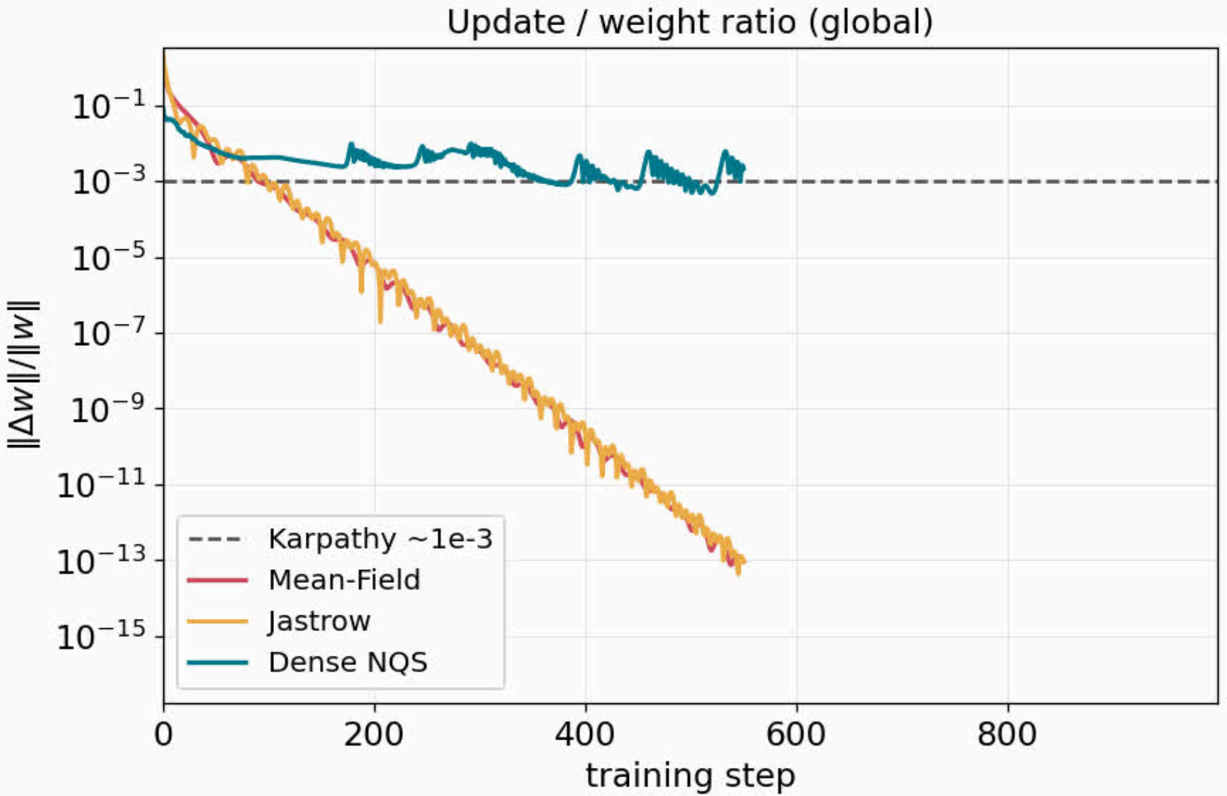
- NQS architecture outperforming Jastrow and mean-field ansatze?

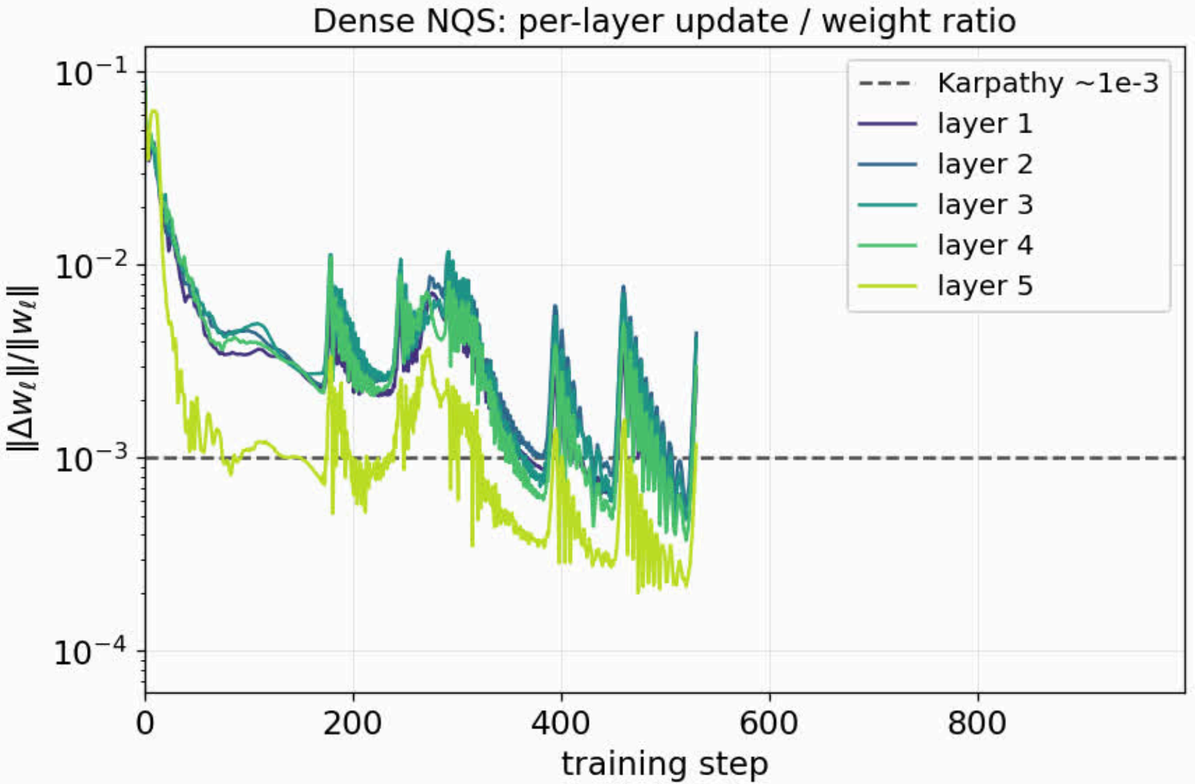




NQS Ground state search - Ising Model

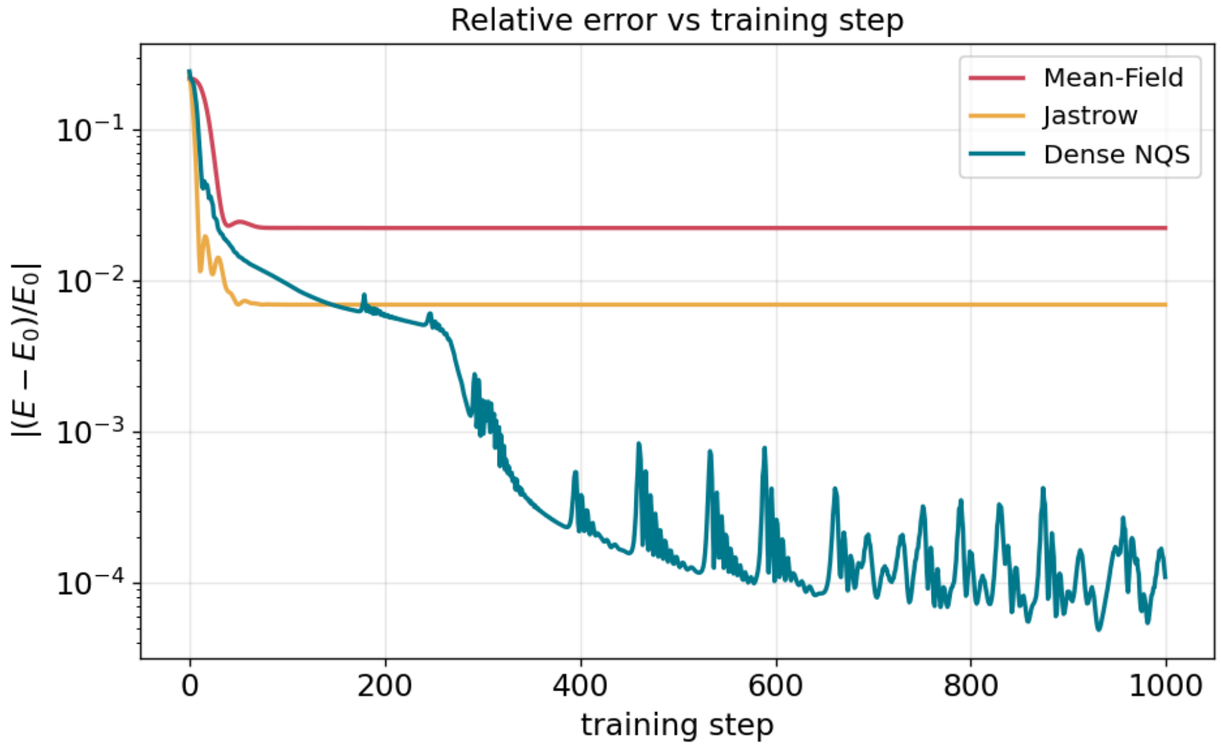
- Yes - our metrics (update ratio) and layer-norms look relatively healthy

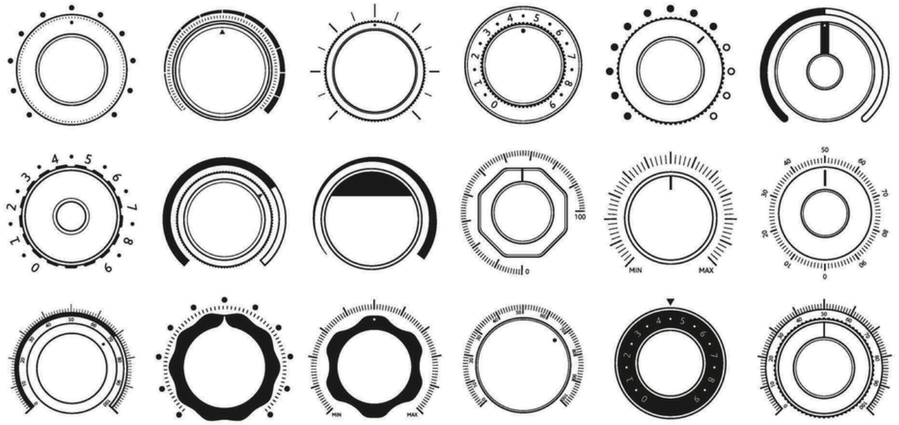




NQS Ground state search - Ising Model

- Is this the best we can do though?

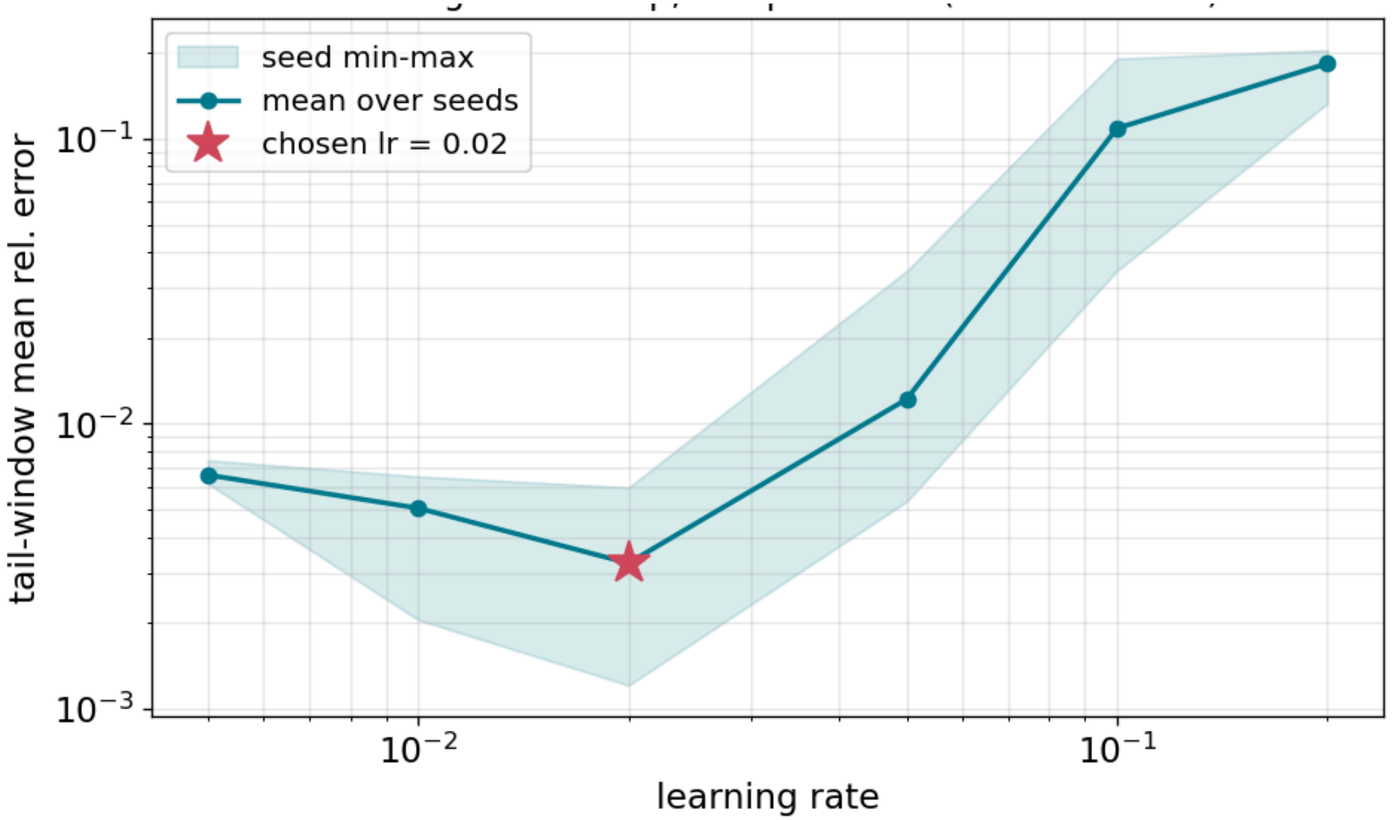




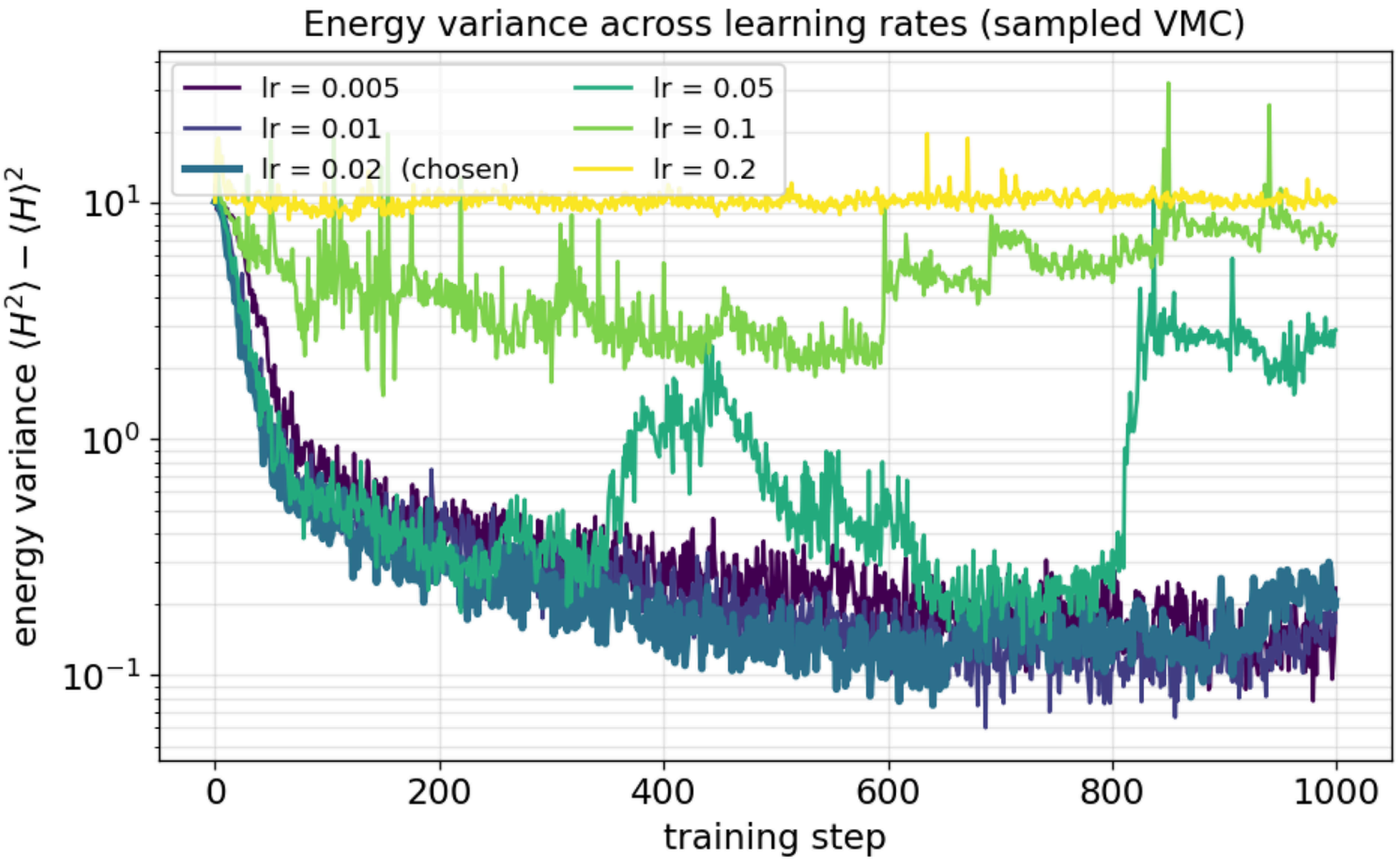
Let’s do some hyperparameter tuning (!)

NQS Ground state search - Ising Model

1. Finding a good learning rate:

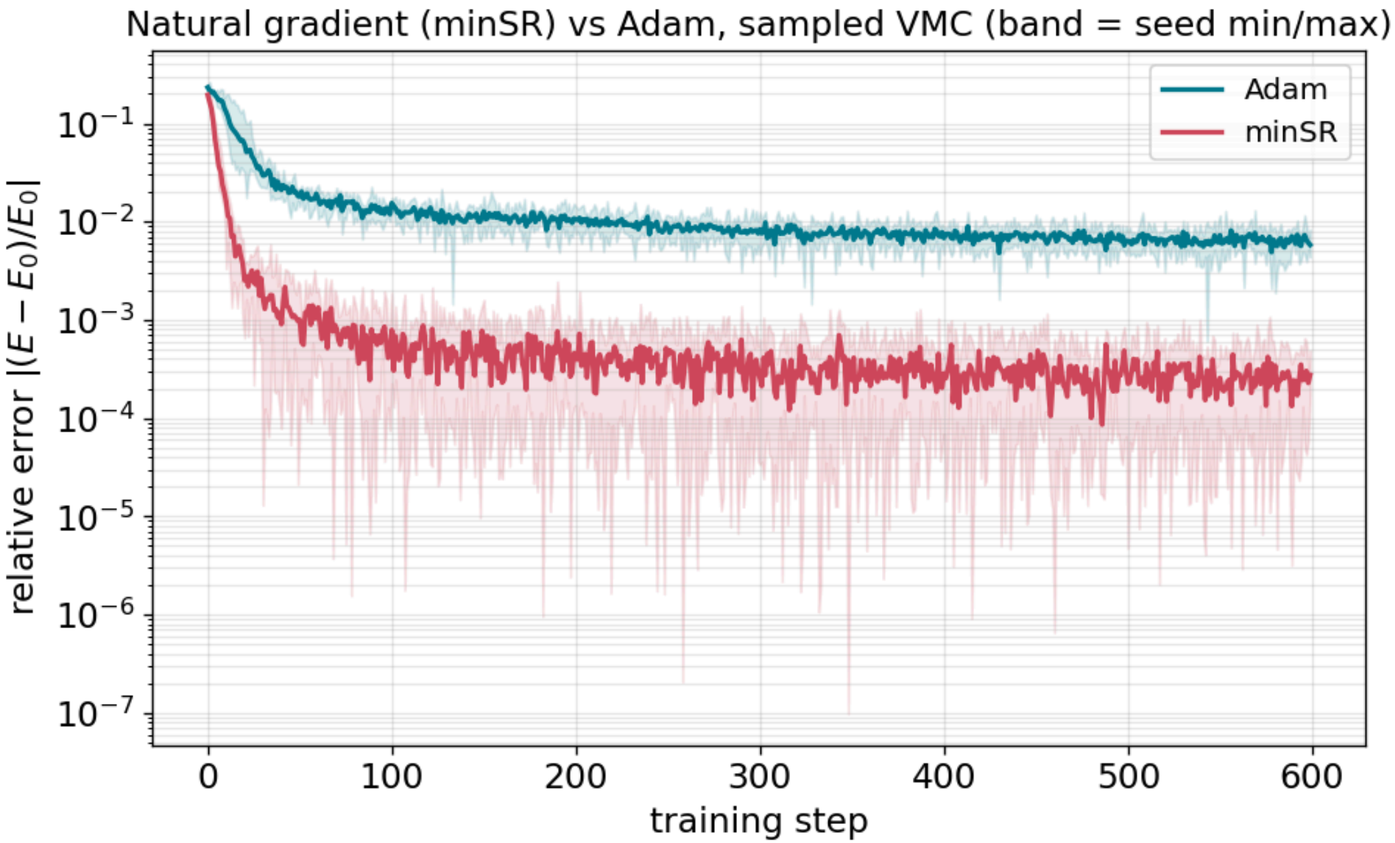


Zero-variance principle in practise:



NQS Ground state search - Ising Model

2. Optimiser - ADAM vs minSR (Heyl 2023)



NQS Ground state search - Ising Model

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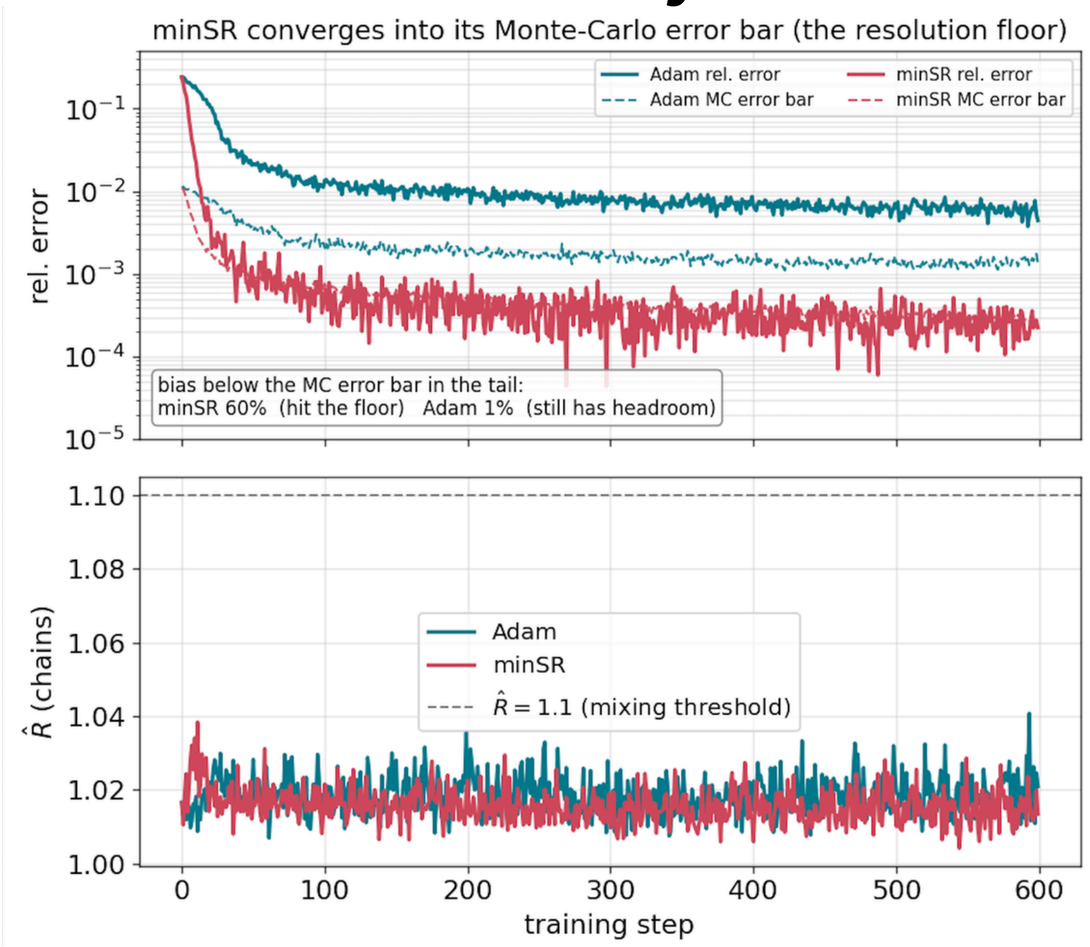

NQS Ground state search - Ising Model

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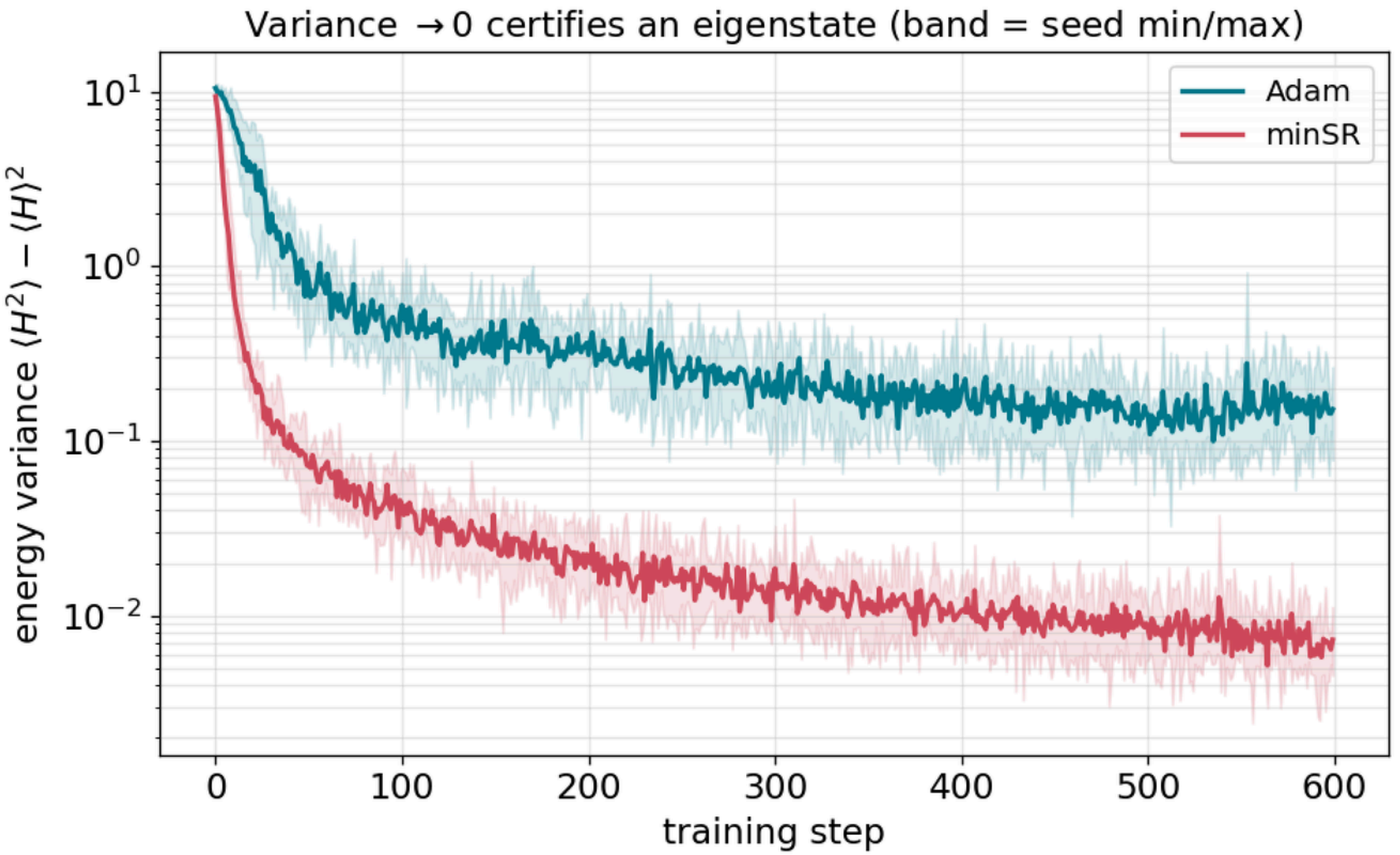
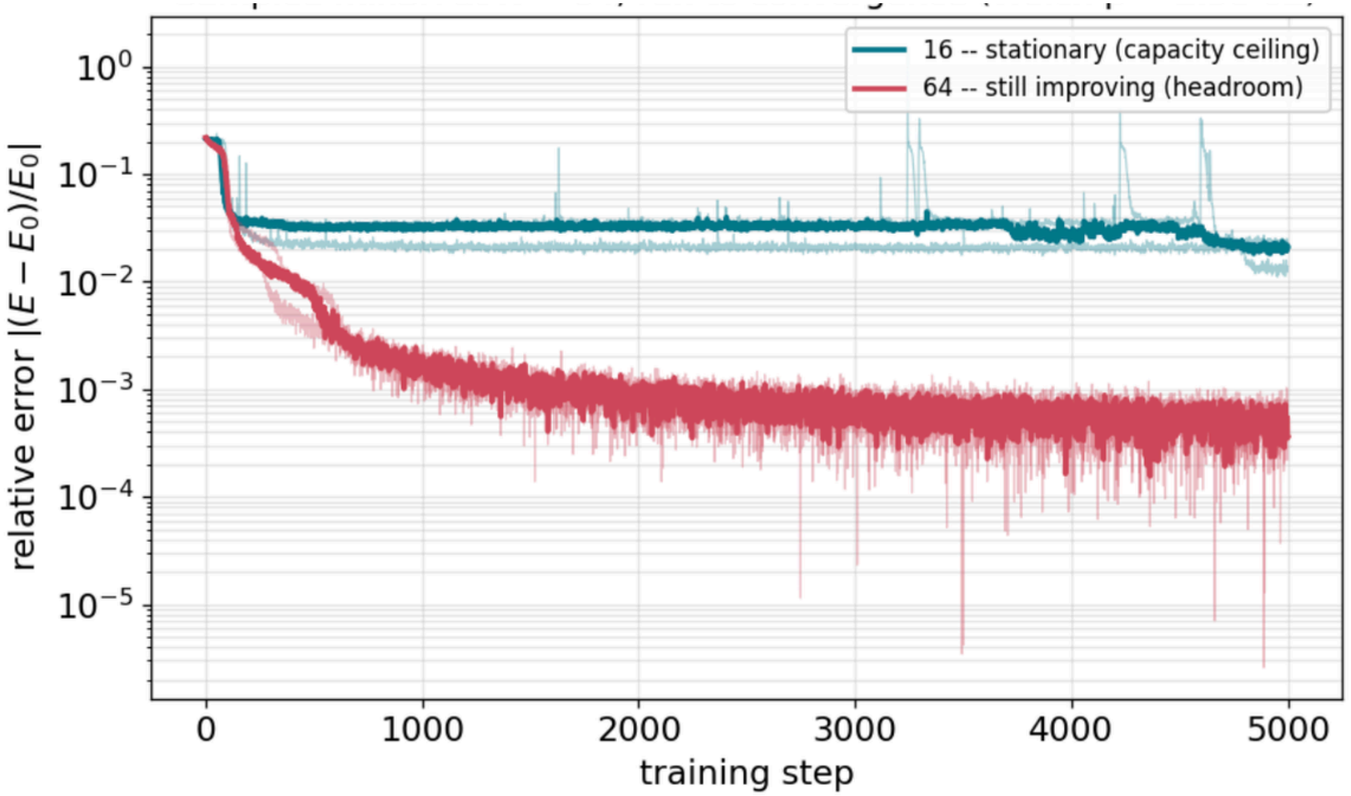
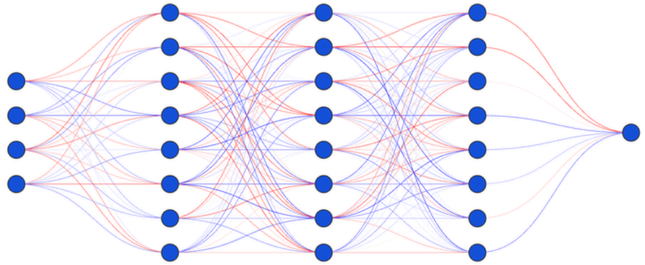


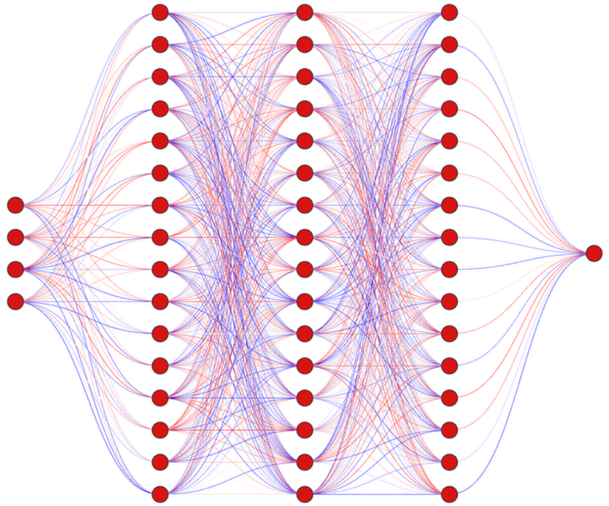
NQS Ground state search - Ising Model

3. **Changing architectures' width**



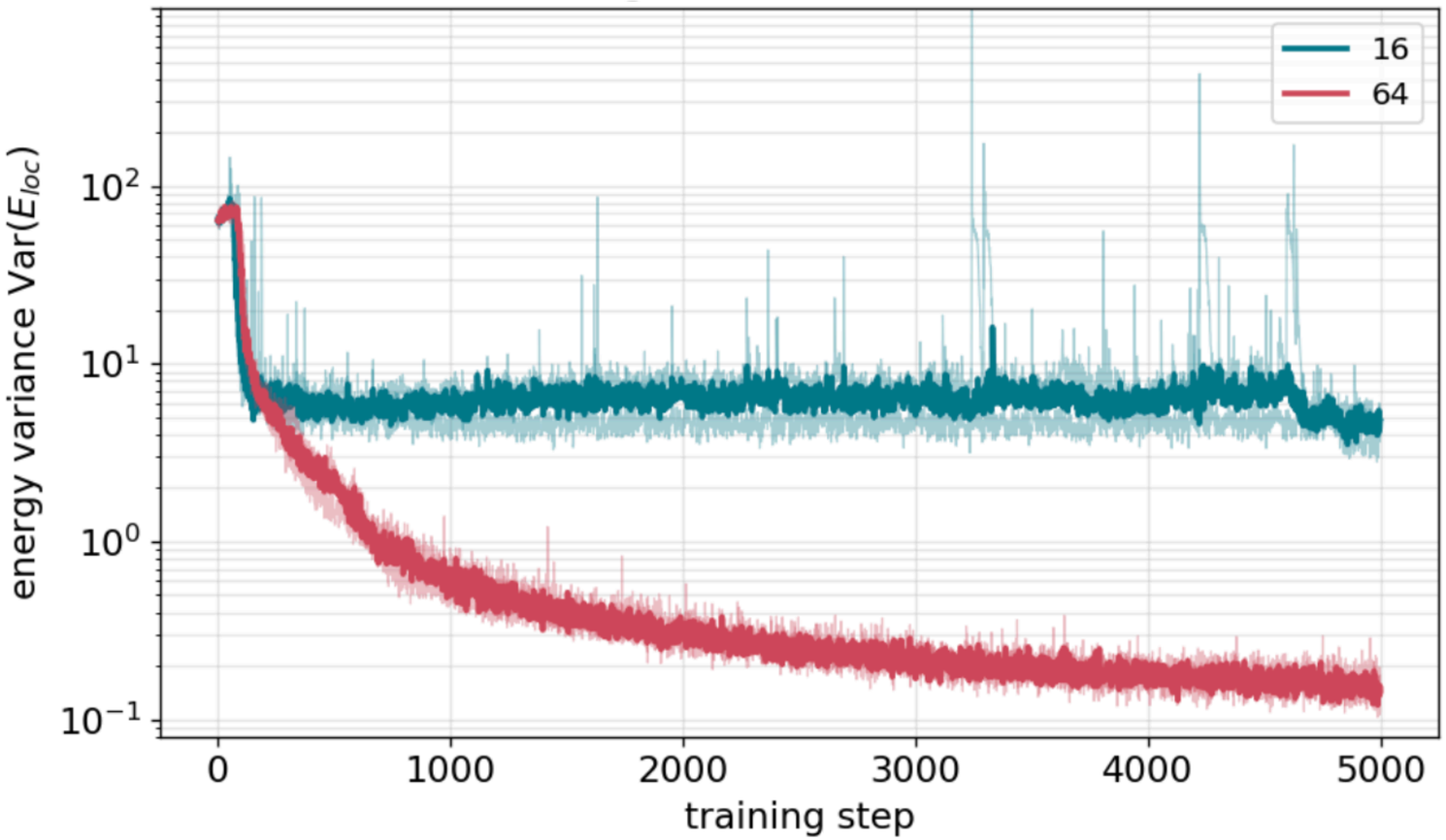


VS



NQS Ground state search - Ising Model

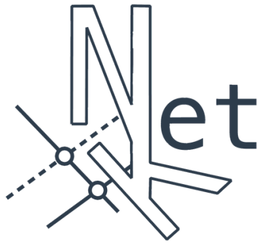
3. **Changing architectures' width - zero variance principle**



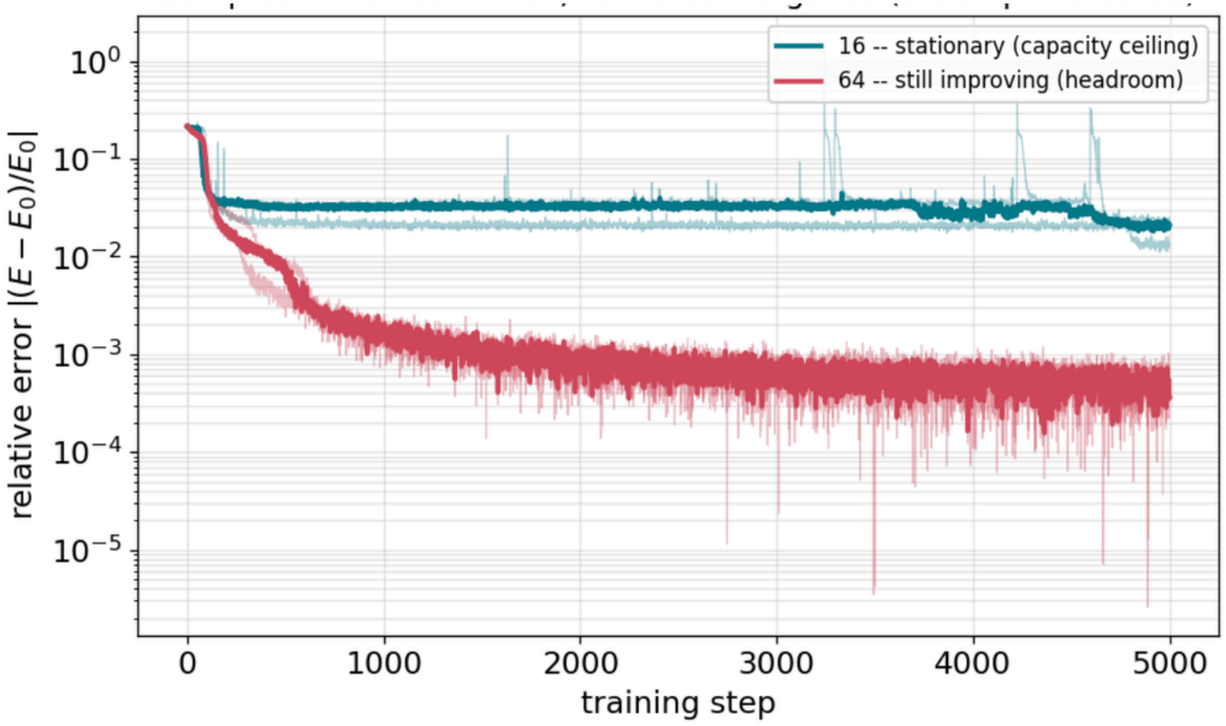
CONTENT

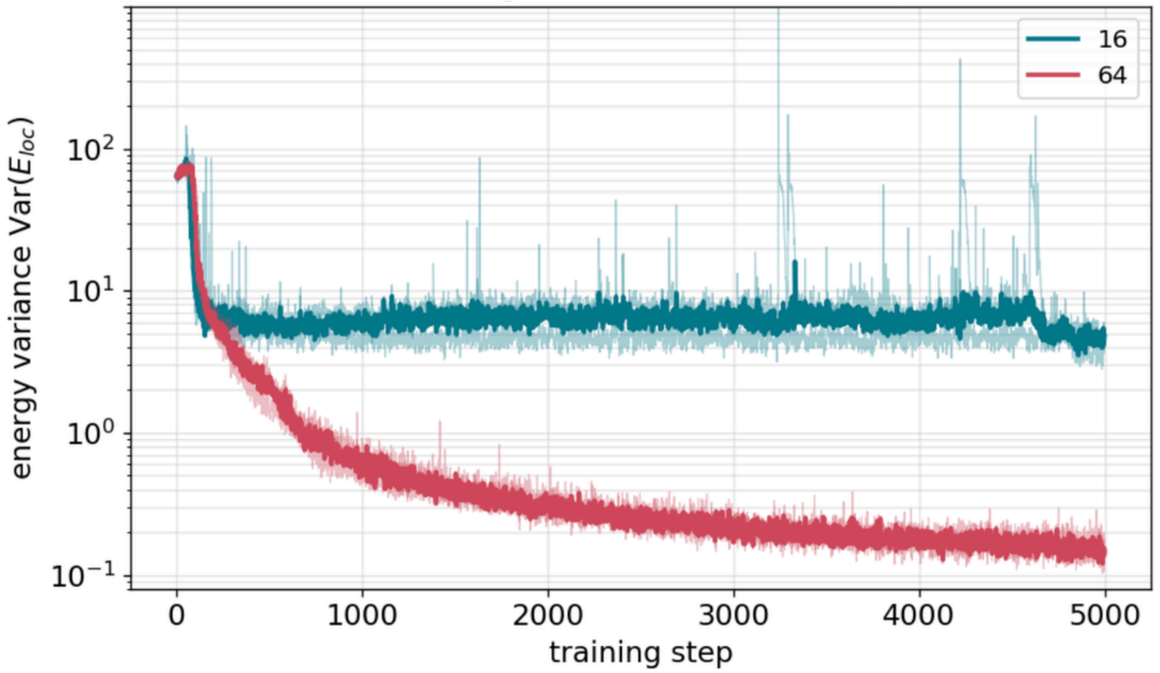
CONTENT

Practical



- **Beat the current neural net for the Ising model….**





Practical

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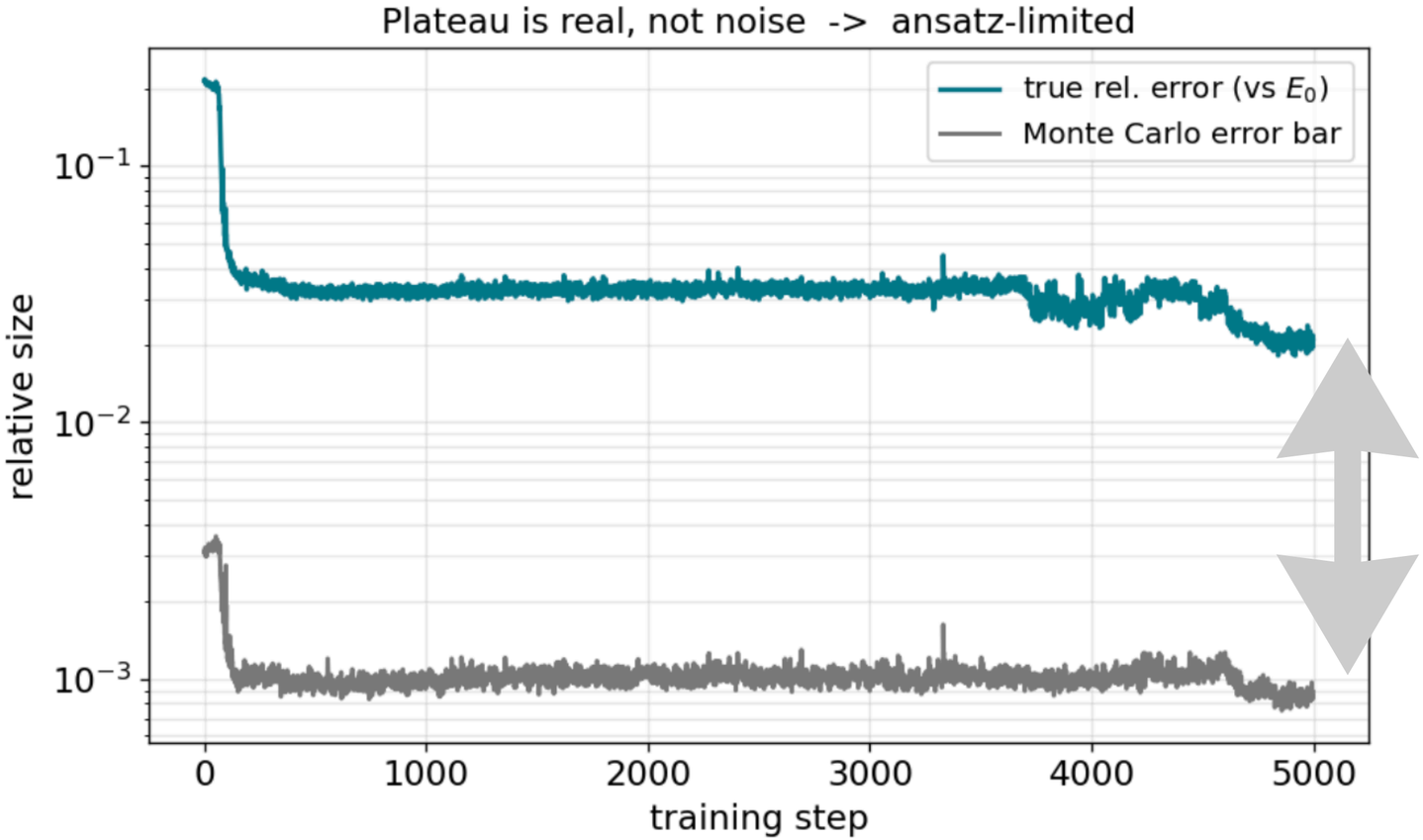
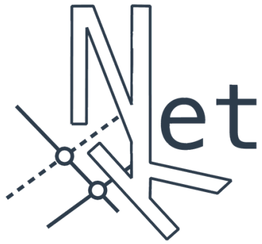


- If we plot the shot noise, we can see there is still room for improvement (!)

Practical

- **Two notebooks**
  a. Install packages (jax, flax, optax, netket)
  b. Notebook 1 - Current best
  c. Notebook 2 - Your model (!)