The Physics of Neural Networks

Using physics to quantify “goodness”

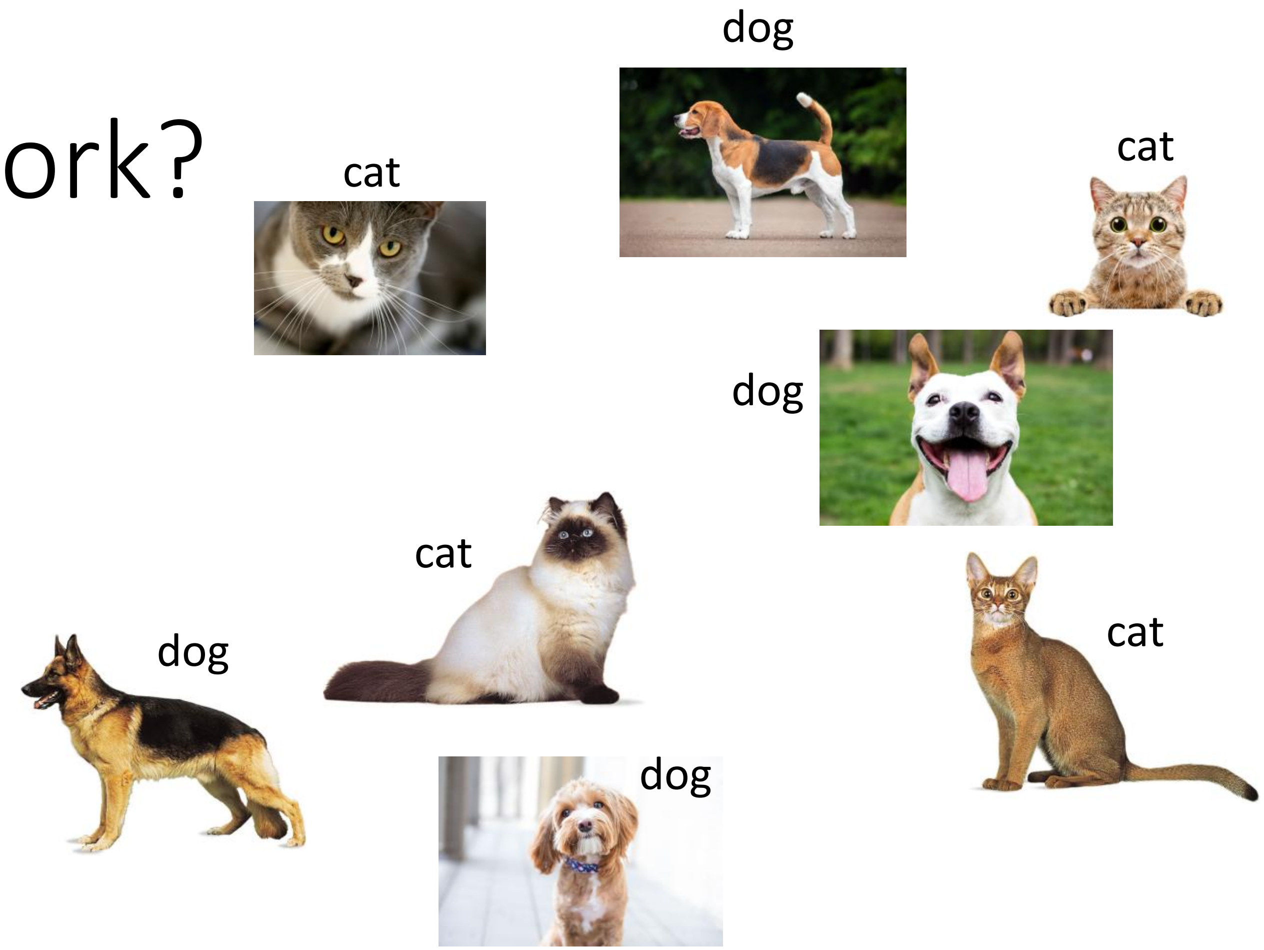
Hannah Day

In collaboration with: Yoni Kahn and Dan Roberts

What is a neural network?

(Spoiler alert: it’s just fancy regression!)

- Give it some labeled data



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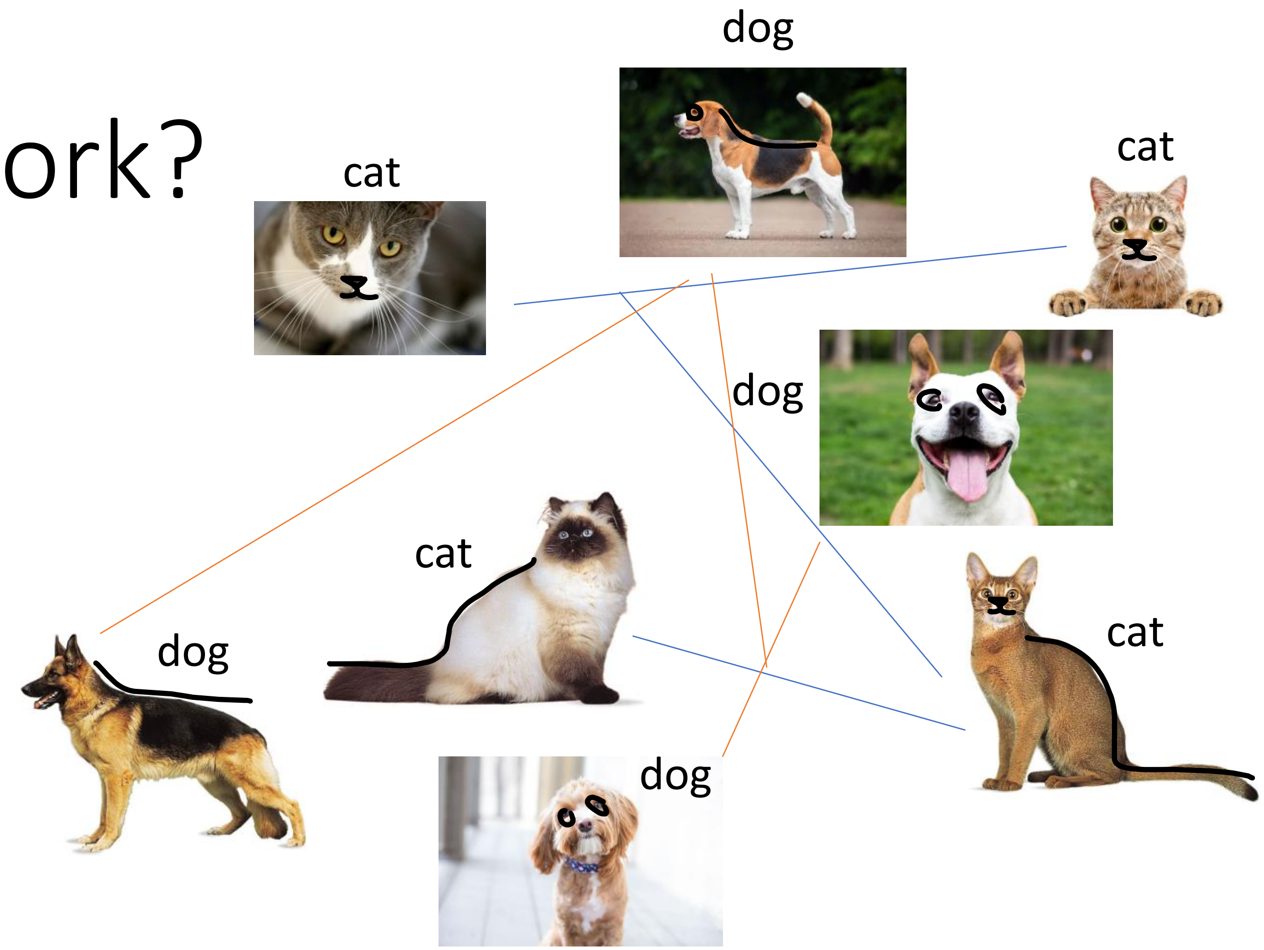
- Network learns patterns



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- Give it some unlabeled data

What is a neural network?

(Spoiler alert: it's just fancy regression!)

- Give it some labeled data

87% dog

90% cat

- Network learns patterns

72% dog

- Give it some unlabeled data

81% cat

- Network assigns labels with some percent confidence

What is a neural network?

(Spoiler alert: it’s just fancy regression!)

- Give it some labeled data
- Network learns patterns
- Give it some unlabeled data
- Network assigns labels with some percent confidence
- Adjust initial network parameters to improve accuracy

98% cat

95% dog

89% dog

93% cat

What is a neural network?

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- Give it some labeled data
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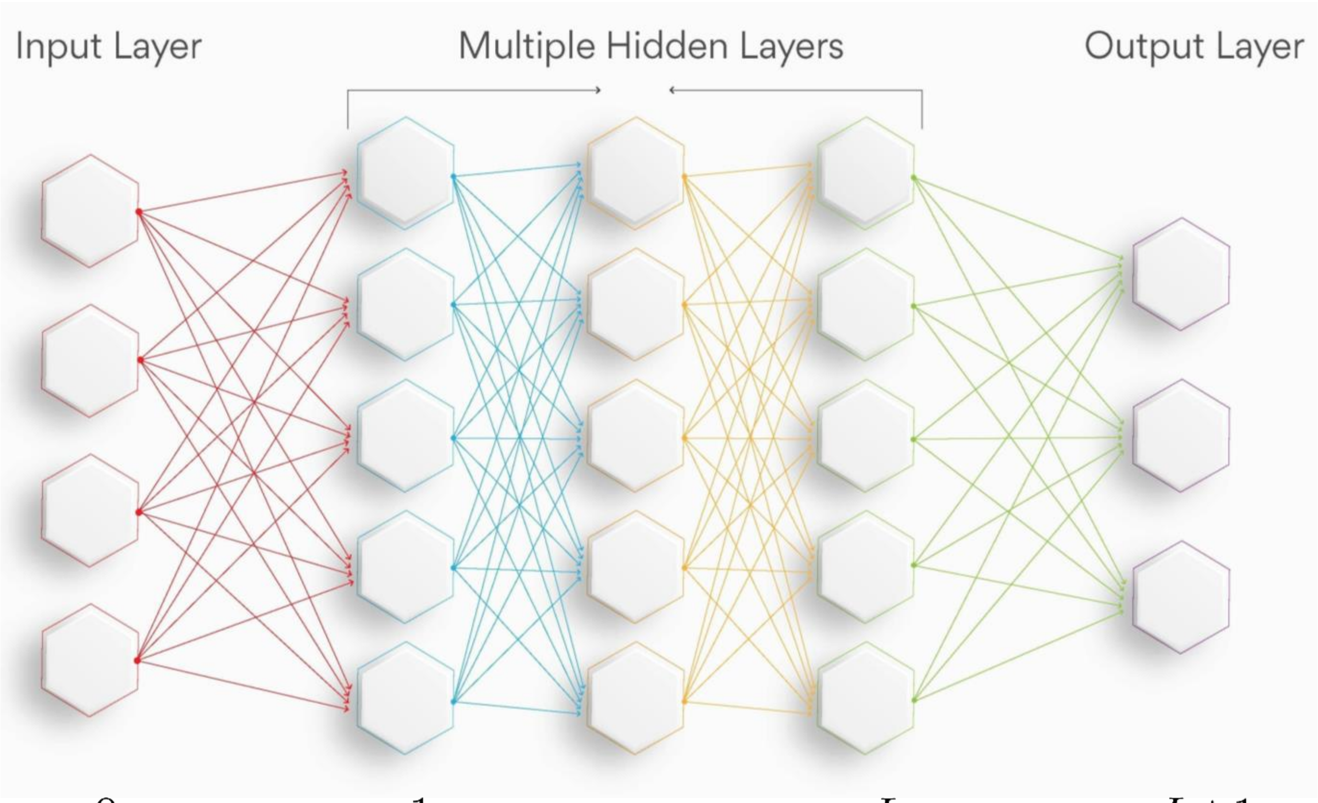
We want to avoid this step

- ~~Adjust initial network parameters to improve accuracy~~

Basic neural network terminology



z^0 z^1 $\dots$ z^L z^{L+1}

$$\underbrace{\begin{pmatrix} z^{\ell+1} \end{pmatrix}}_{\text{layer vector}} = \underbrace{\begin{pmatrix} b^{\ell+1} \end{pmatrix}}_{\text{bias vector}} + \underbrace{\begin{pmatrix} W^{\ell+1} \end{pmatrix}}_{\text{weight matrix}} \begin{pmatrix} \sigma(z^{\ell}) \end{pmatrix}$$

activation function:
literally just some function applied to each element of the vector

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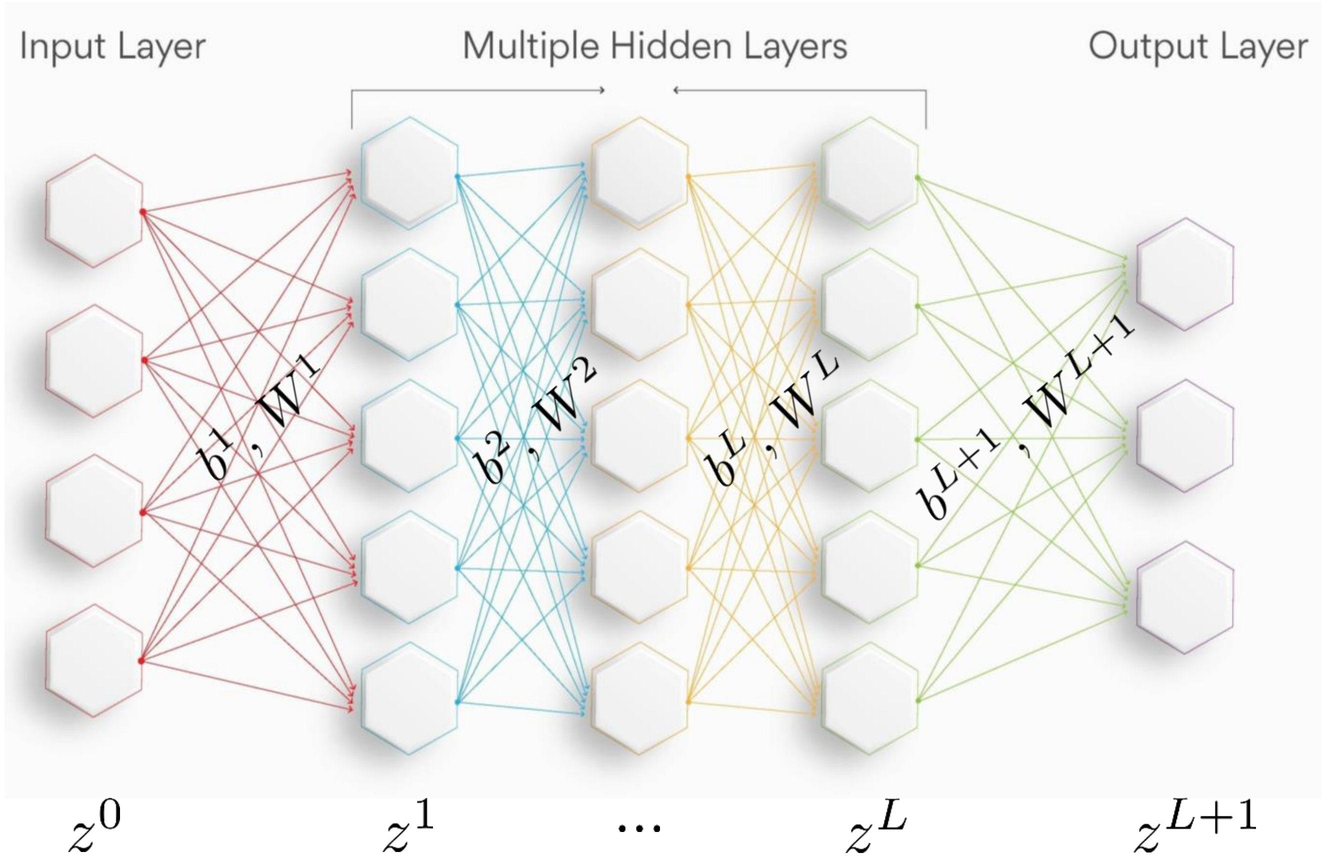

layer vector | bias vector | weight matrix

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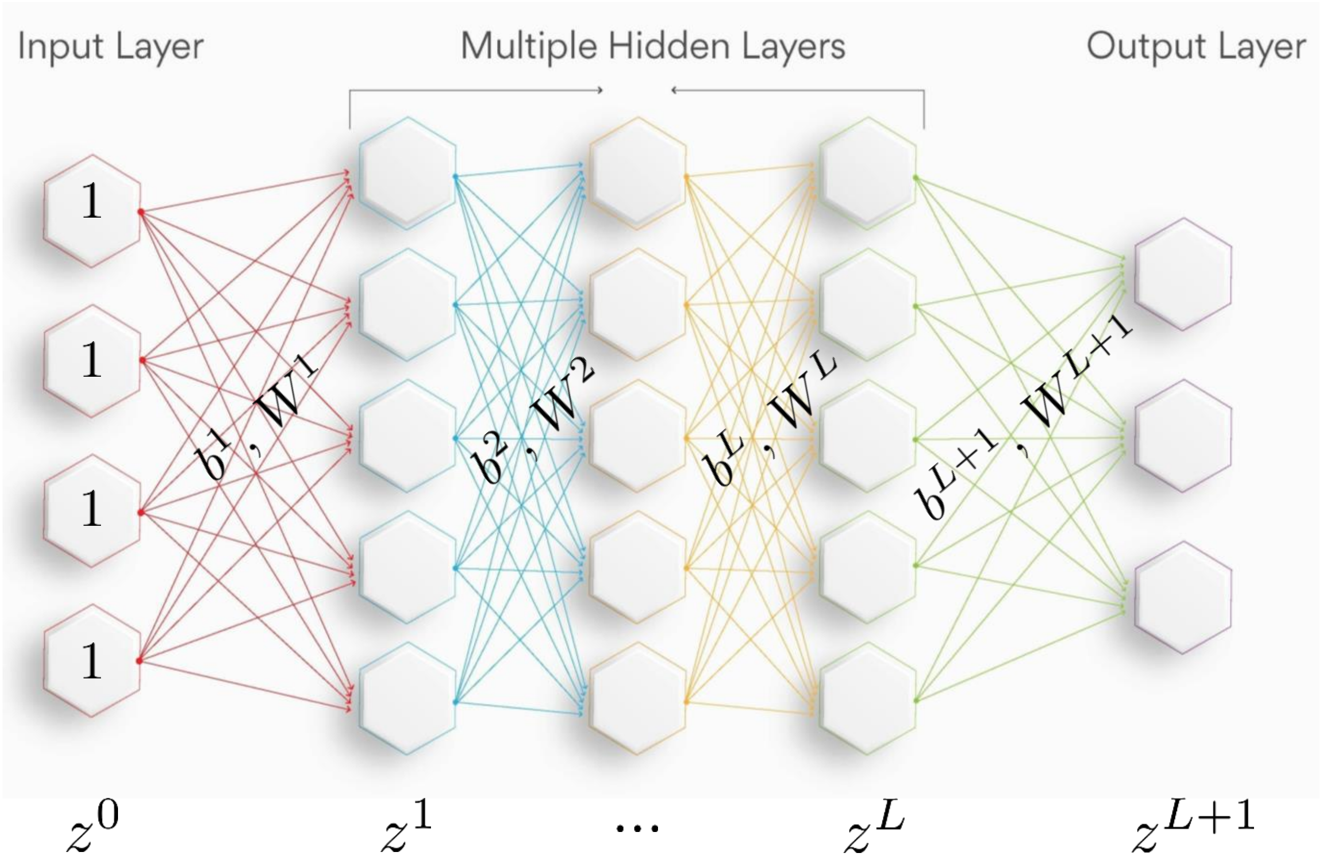

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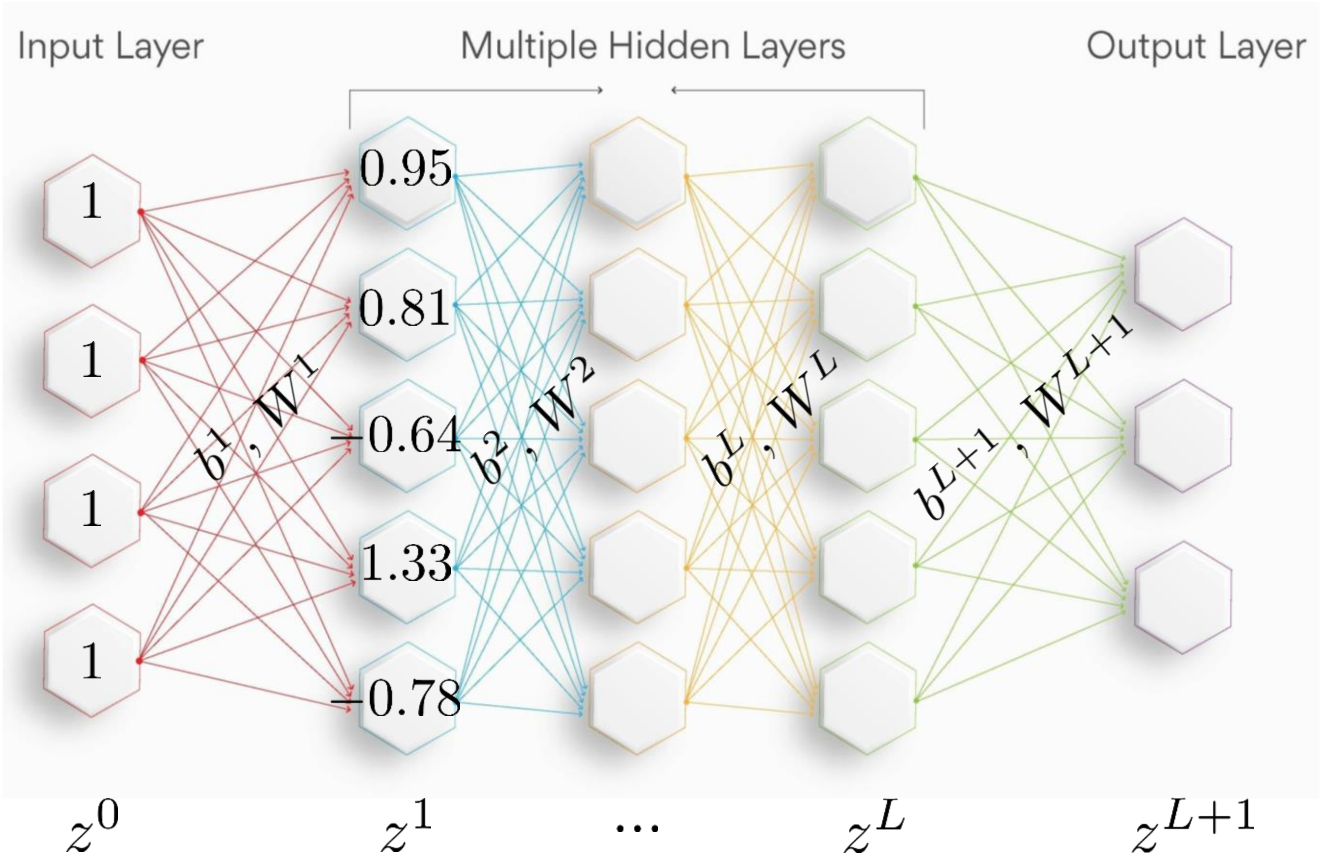

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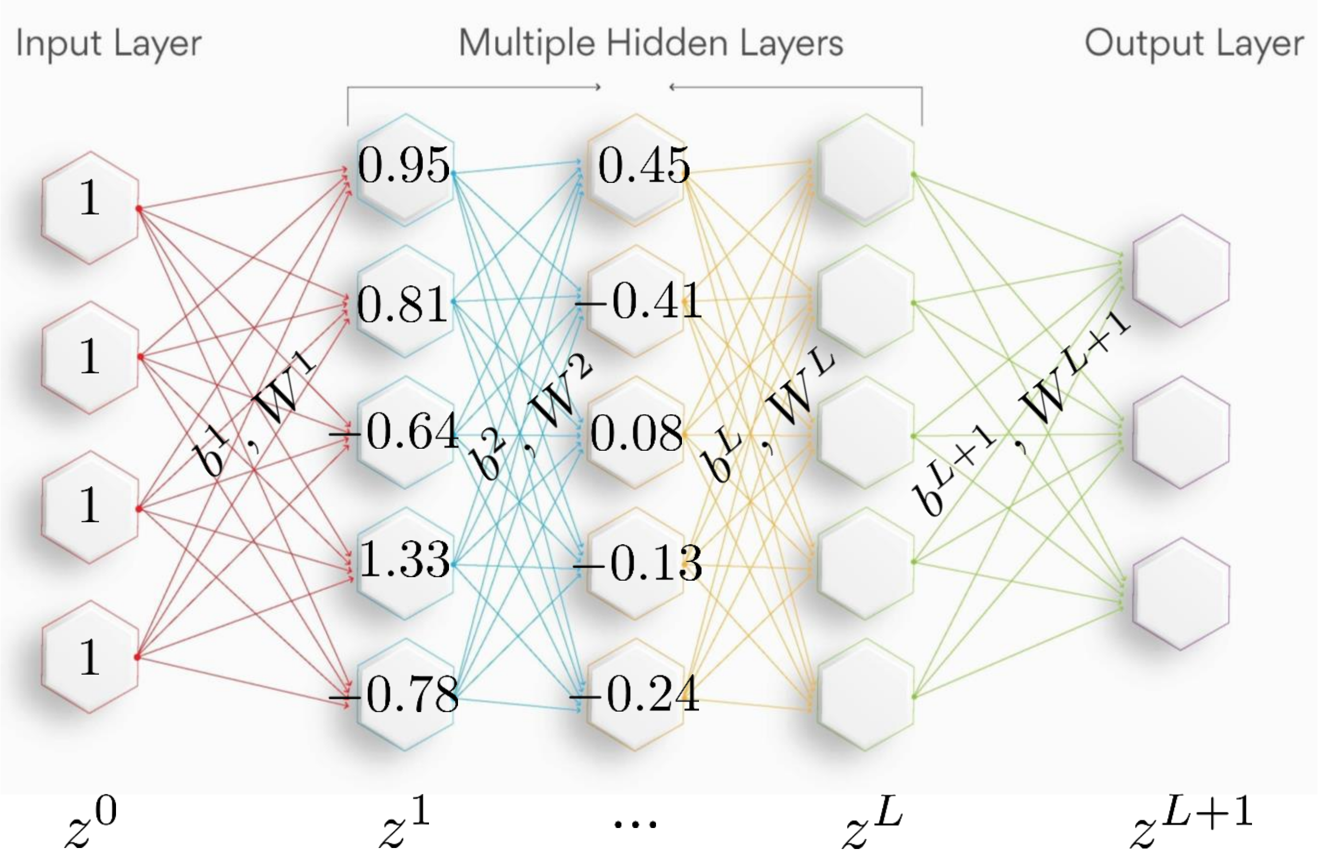

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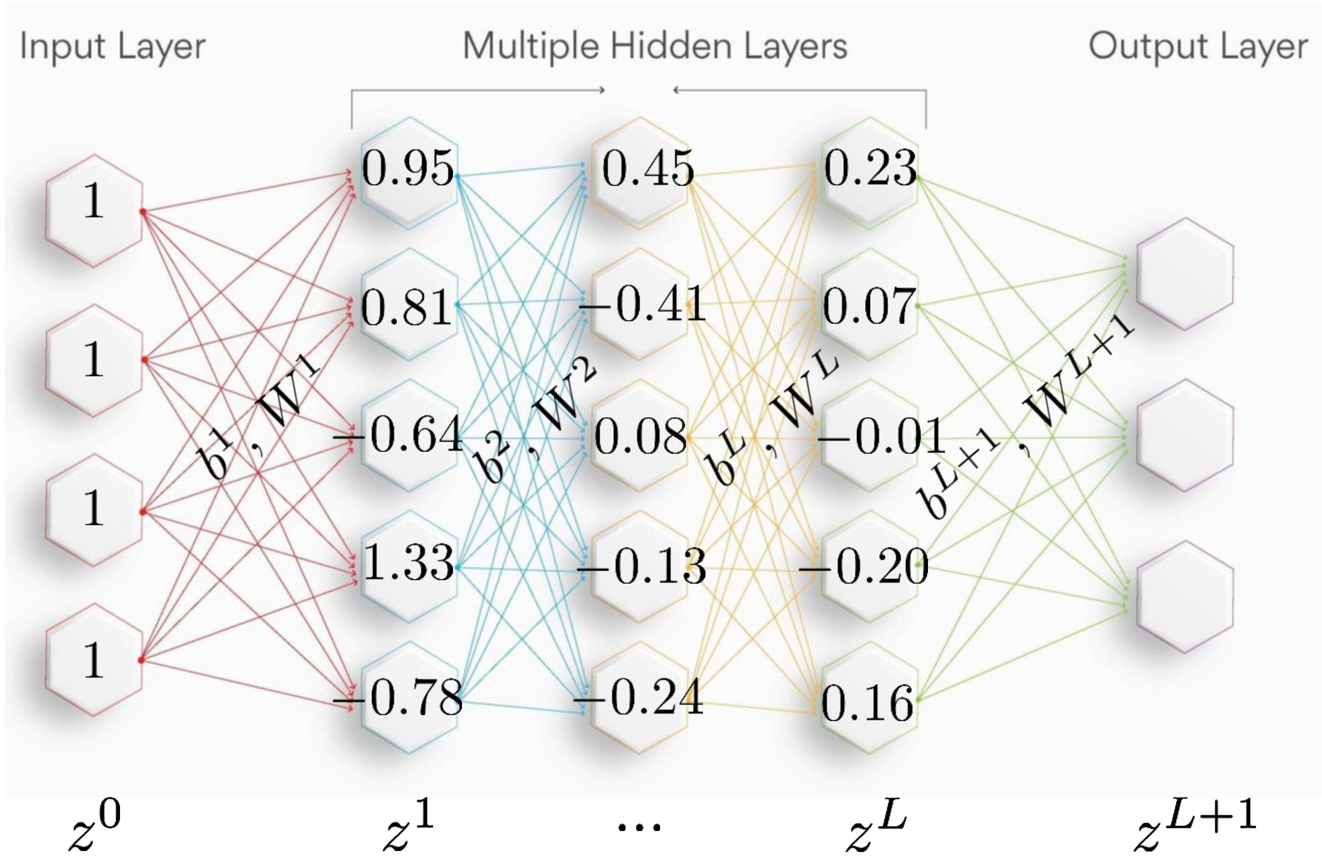

layer vector, bias vector, weight matrix

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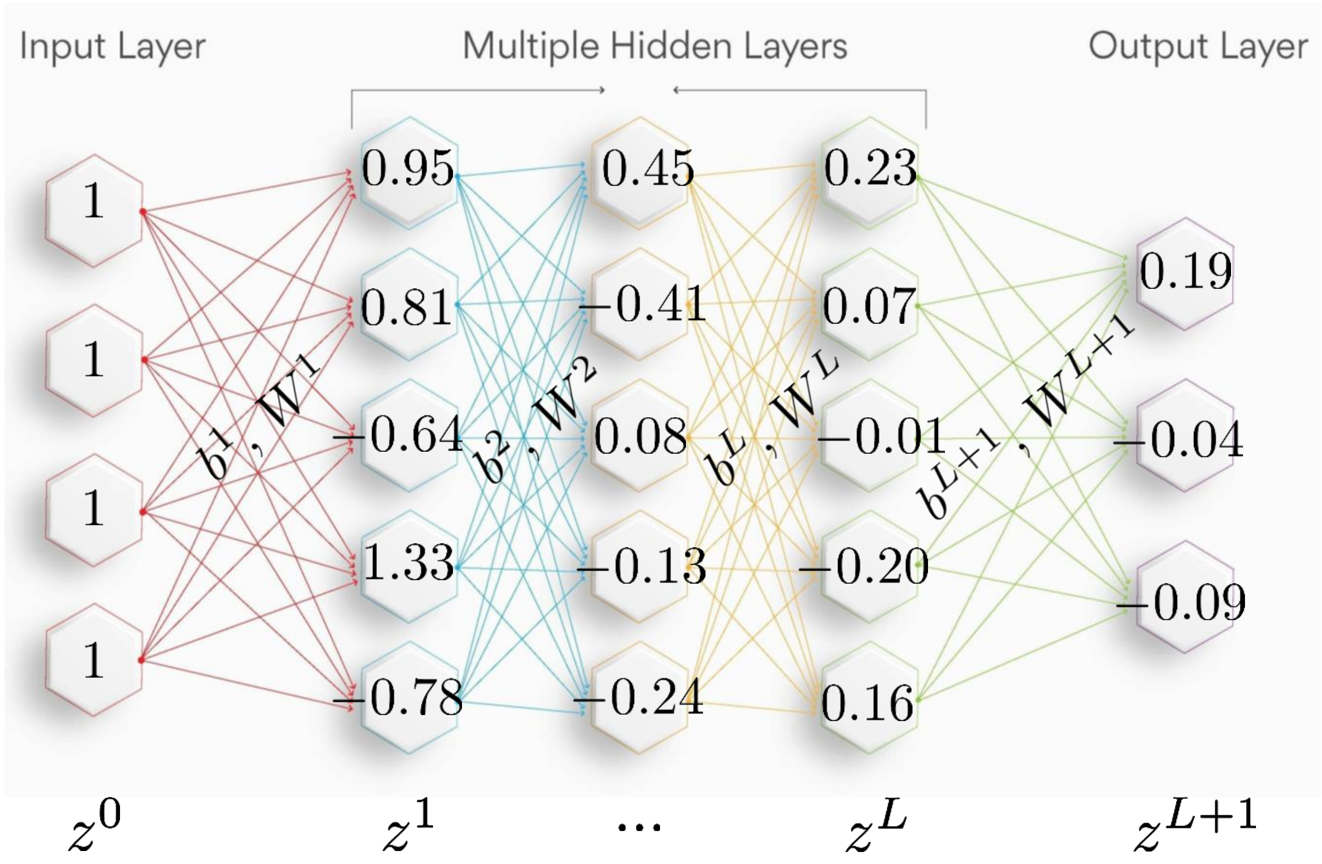

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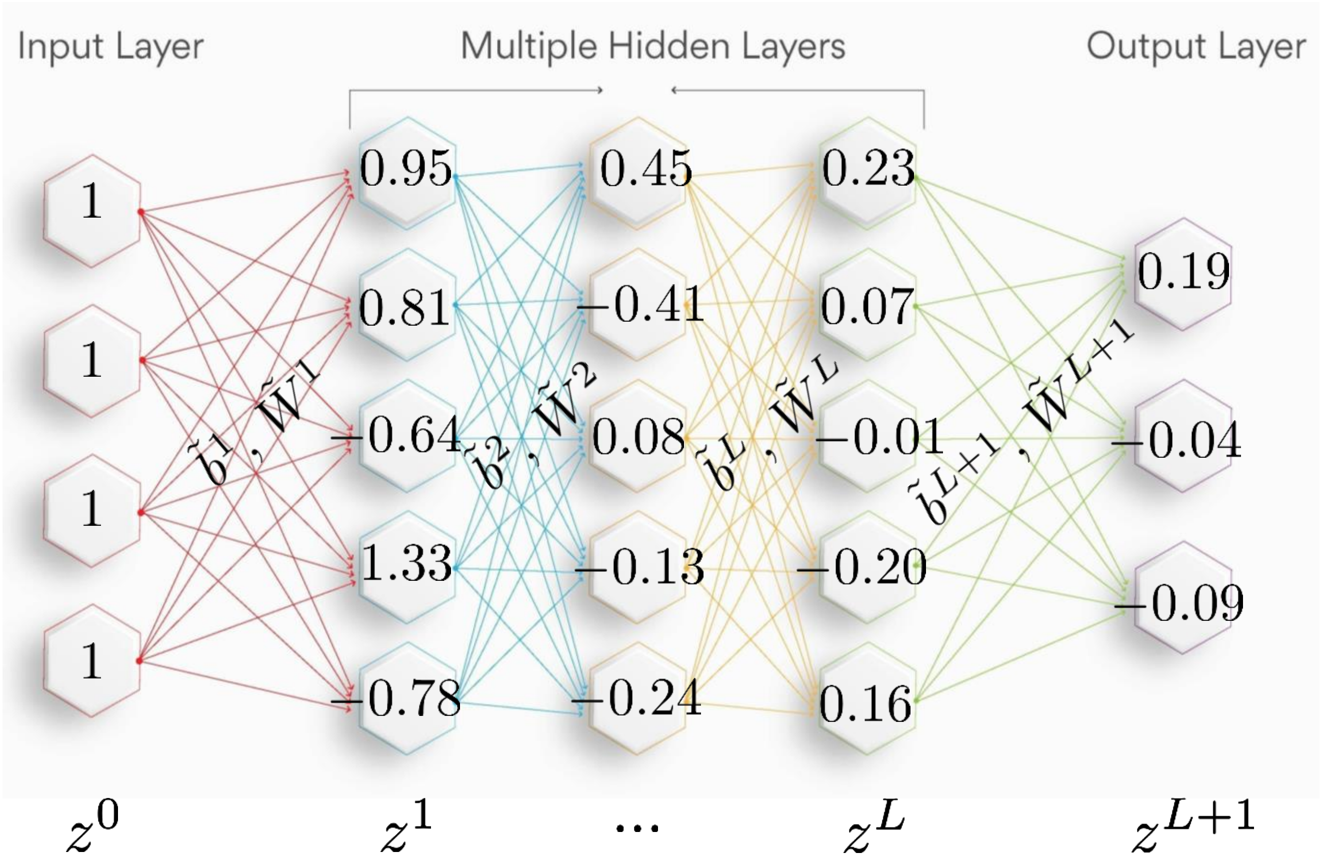

layer vector bias vector weight matrix

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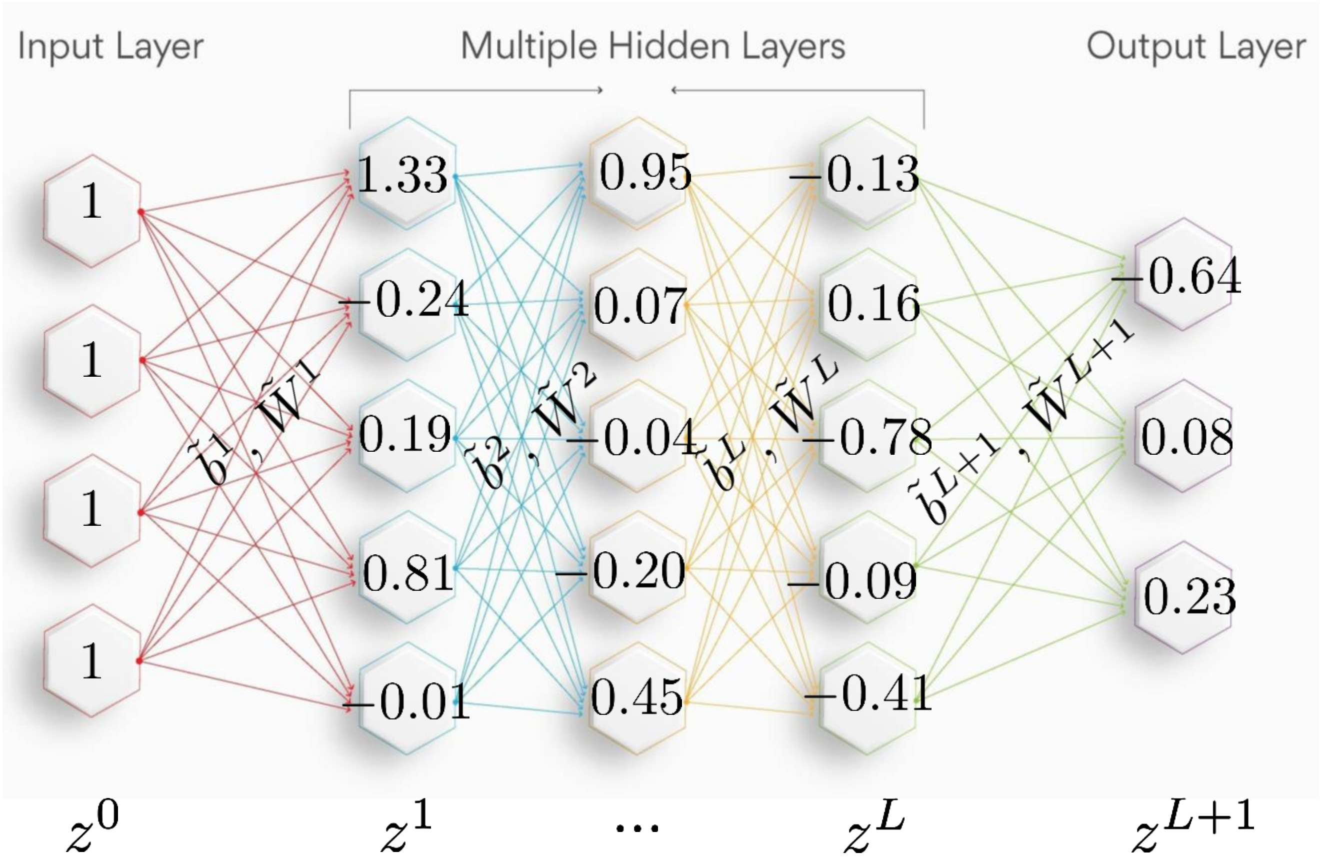

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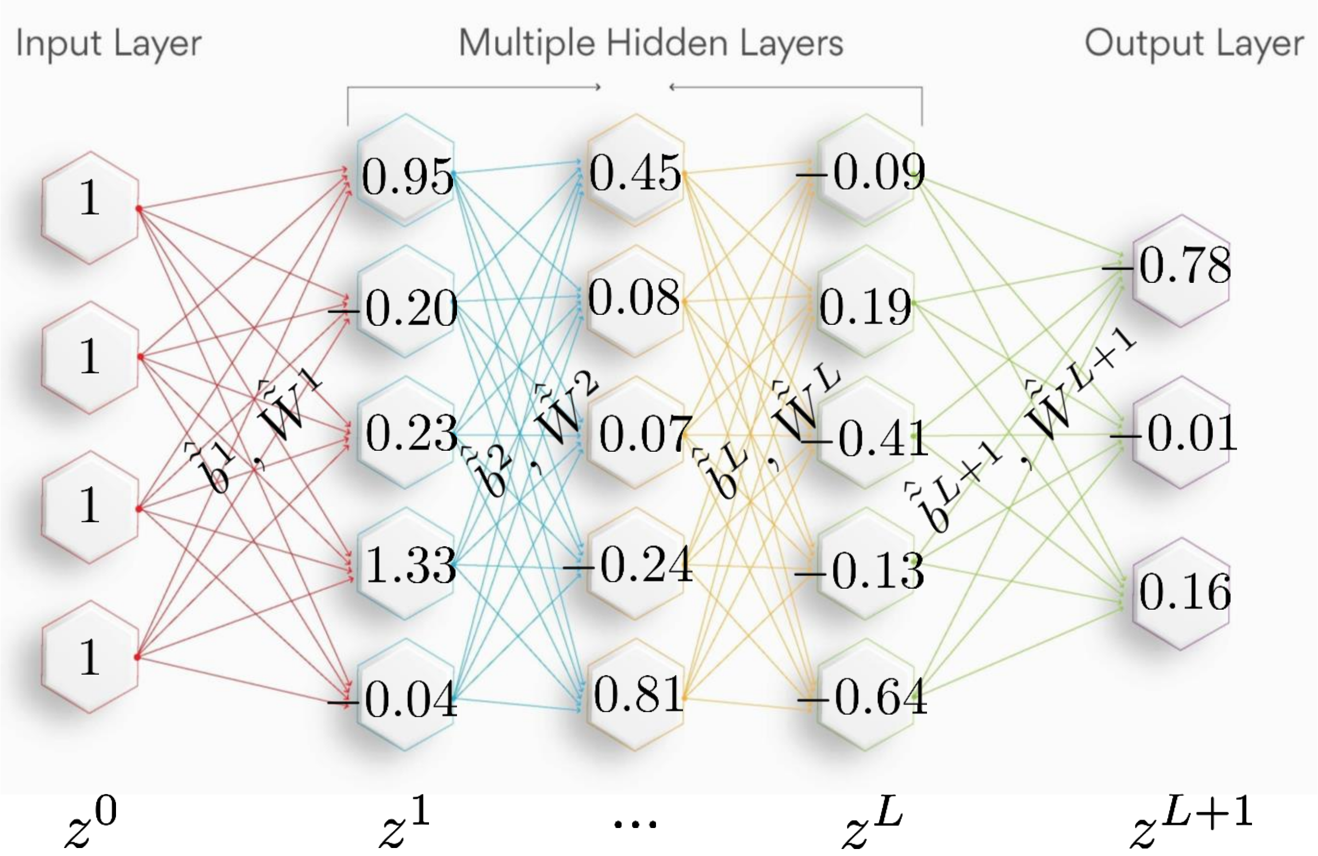

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$$\left(z^{\ell+1} \right) = \left(b^{\ell+1} \right) + \left(\quad W^{\ell+1} \quad \right) \left(\sigma(z^\ell) \right)$$

activation function:
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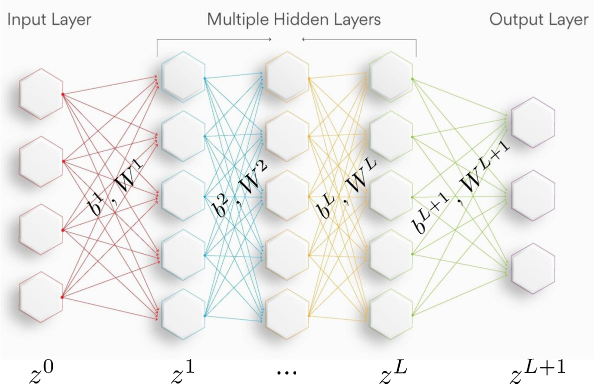
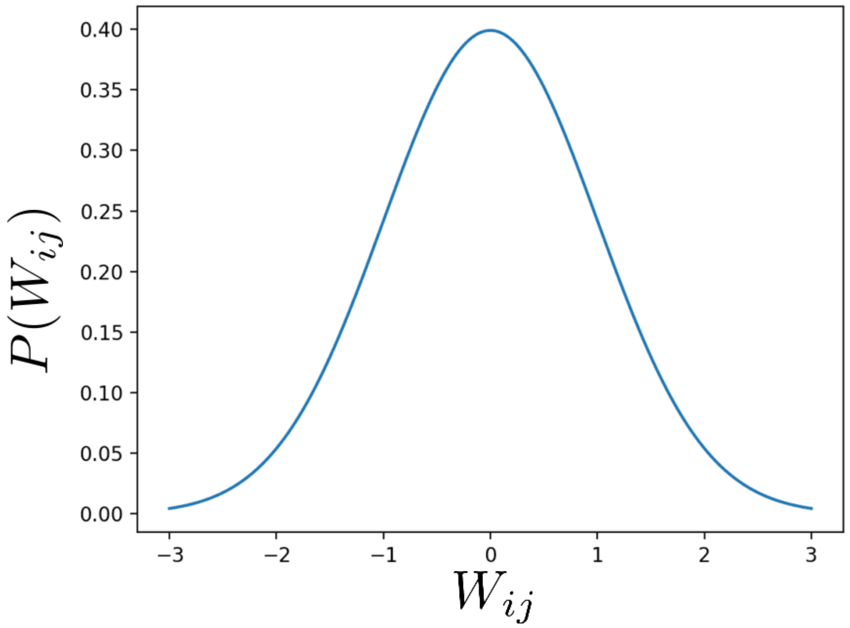
- *Initializing the network* means picking <u>starting</u> values for biases and weights
- Data *propagates* through the network
- Biases and weights *evolve* during training
- A *trained network* has "learned" the best biases and weights for optimal performance



Where's the physics?

- Initial weights and biases are randomly selected from a *distribution*

For example, sampling from a standard Gaussian distribution means the initial weight matrices could look like this:

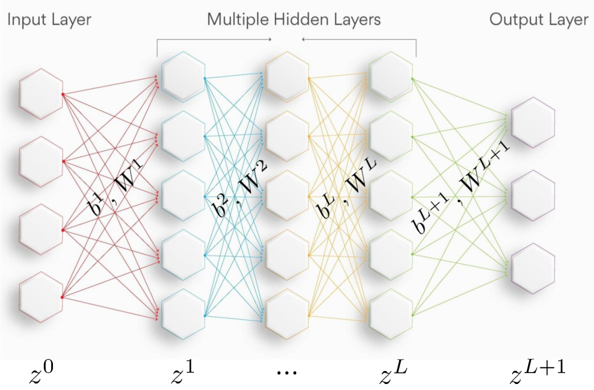


$$W^1 = \begin{pmatrix} -0.34 & -0.09 & -0.05 & 0.03 \\ 0.76 & 0.98 & -0.53 & -1.13 \\ 0.50 & -0.97 & 0.51 & 0.61 \\ 0.59 & -0.14 & 0.76 & 0.69 \end{pmatrix}$$

$$W^2 = \begin{pmatrix} 0.11 & 0.54 & -0.30 & 0.42 \\ 0.01 & 0.06 & -0.10 & -0.47 \\ 0.58 & -0.08 & -0.27 & 0.76 \\ 0.53 & -0.37 & 0.28 & 0.92 \end{pmatrix}$$

$$W^3 = \begin{pmatrix} -0.02 & -0.06 & -0.50 & -0.73 \\ 0.54 & 0.49 & -0.35 & 0.67 \\ -0.99 & -0.02 & -0.56 & 0.01 \\ -0.68 & 0.29 & -0.03 & -0.40 \end{pmatrix}$$

Where's the physics?

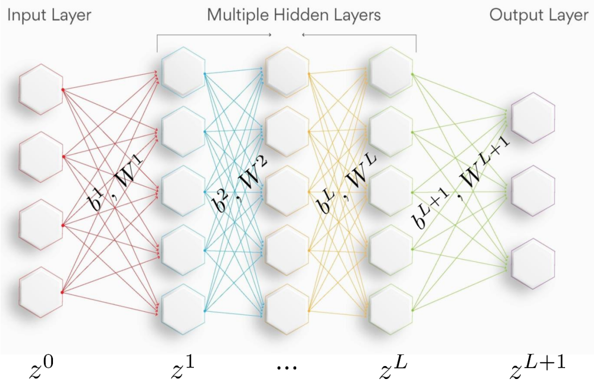


- Initial weights and biases are randomly selected from a *distribution*
- Deep networks must be tuned to *criticality*

$$z^0 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \xrightarrow{b^1,\, W^1} z^1 = \begin{pmatrix} 0.95 \\ 0.81 \\ -0.64 \\ 1.33 \end{pmatrix} \xrightarrow{b^2,\, W^2} z^2 = \begin{pmatrix} 0.45 \\ -0.41 \\ 0.08 \\ -0.13 \end{pmatrix} \xrightarrow{b^3,\, W^3} z^3 = \begin{pmatrix} 0.23 \\ 0.07 \\ -0.01 \\ -0.20 \end{pmatrix}$$

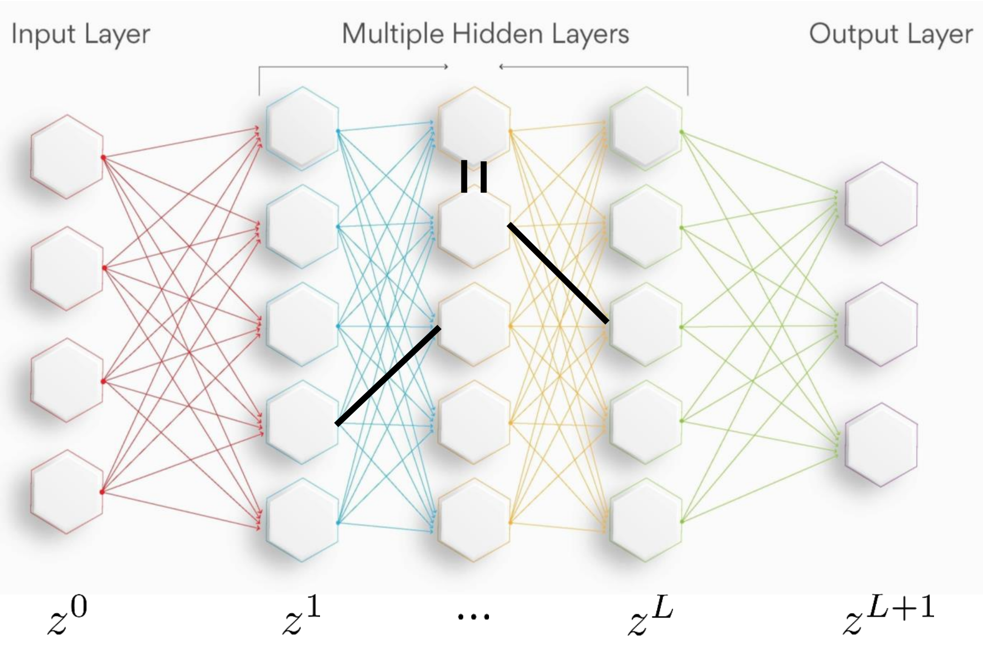
versus

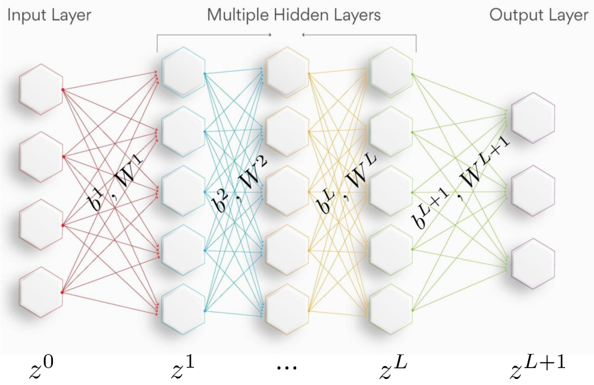
$$z^0 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \xrightarrow{b^1,\, W^1} z^1 = \begin{pmatrix} -1.59 \\ 0.70 \\ 1.66 \\ -0.23 \end{pmatrix} \xrightarrow{b^2,\, W^2} z^2 = \begin{pmatrix} 0.22 \\ 0.75 \\ -2.04 \\ 1.39 \end{pmatrix} \xrightarrow{b^3,\, W^3} z^3 = \begin{pmatrix} 1.03 \\ -1.34 \\ -0.77 \\ 1.12 \end{pmatrix}$$



Where's the physics?

- Initial weights and biases are randomly selected from a *distribution*
- Deep networks must be tuned to *criticality*
- Interactions between network nodes can be quantified with *couplings*





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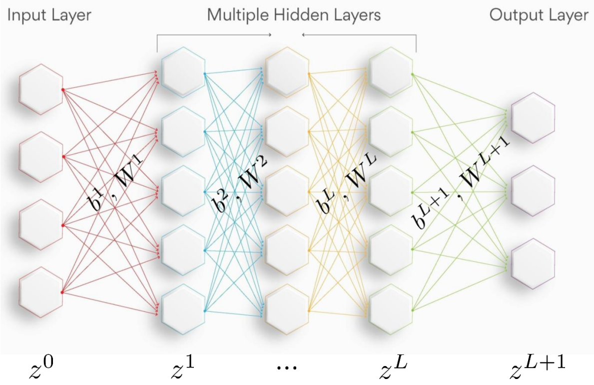
Sounds suspiciously like stat mech!

- Infinite-width neural network = free field theory
- Finite width $\Longrightarrow$ interactions
- Signals propagation = renormalization group flow
- Critically tuned weights and biases = marginal couplings / critical point

Where's the physics?



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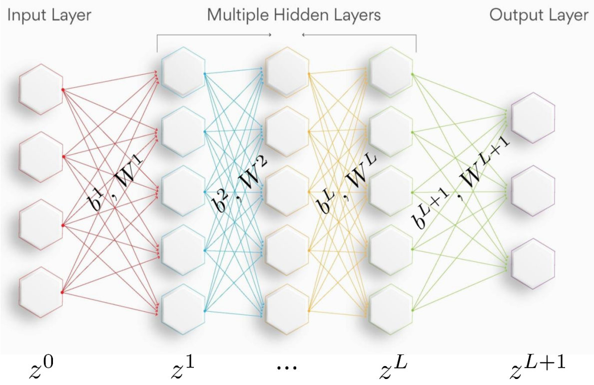
Given our initial network conditions,
can we predict how the network will evolve?



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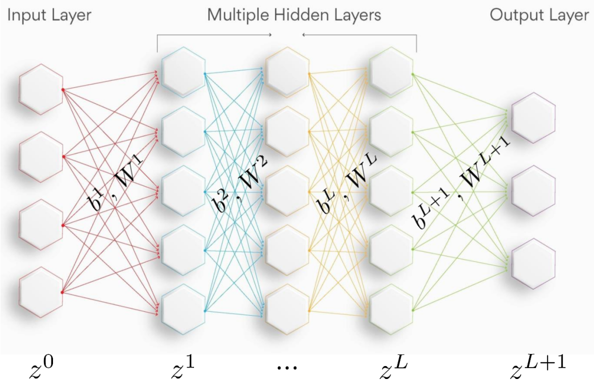
Given how we want the network to evolve,
can we determine the necessary initial conditions?



What makes a network "good"?

- High percentage of correct prediction
- Similar inputs should go to similar outputs
- Expect similar results every time you use the network

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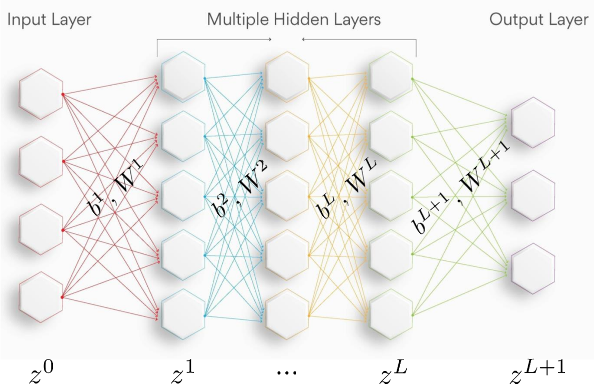

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Especially important for physics applications

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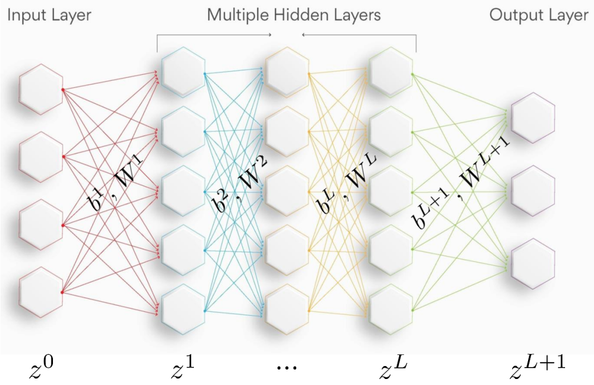

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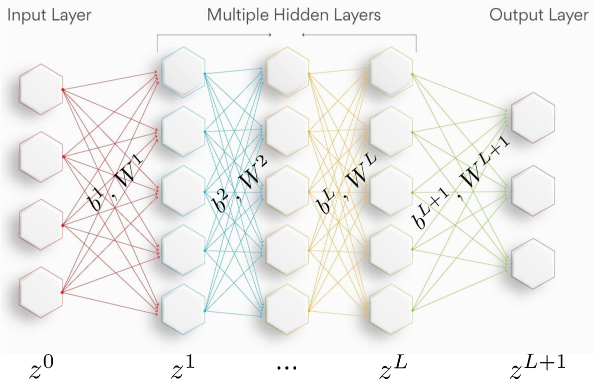
Especially important for physics applications:

E.g.
- 2 top quark jet images should receive similar classification
- That classification should be the same every time

What makes a network "good"?



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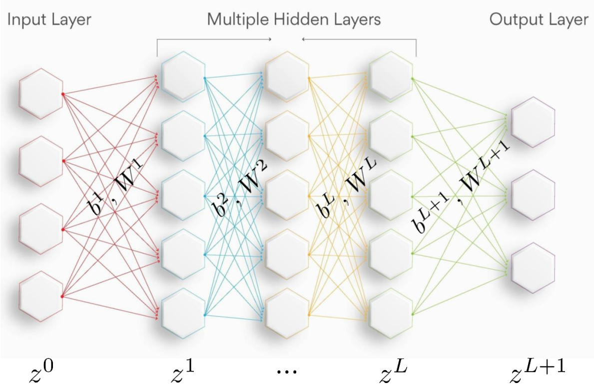
Especially important for physics applications

? Perhaps introducing physically motivated interactions will improve "goodness" of network

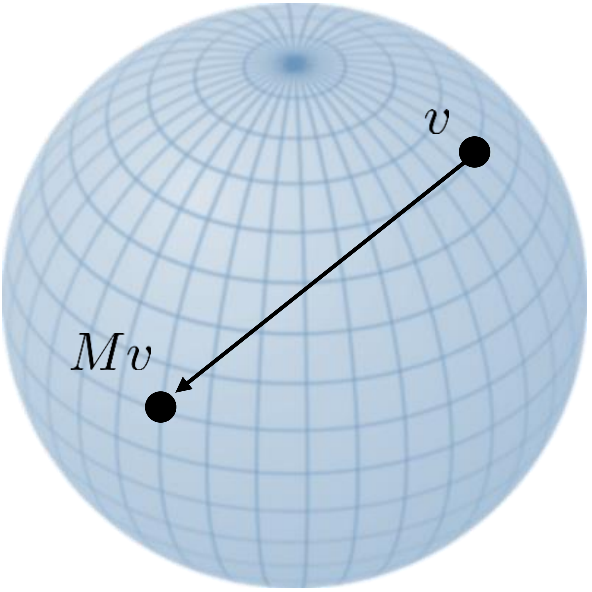
? Perhaps we can quantify the "goodness" of a network based on initial network parameters



The orthogonal distribution

(Physically motivated interactions)

- An orthogonal matrix rotates points on a sphere
  $\Rightarrow$ automatically preserves vector norms
- Naturally limits explosions and decays



layer vector | bias vector | weight matrix

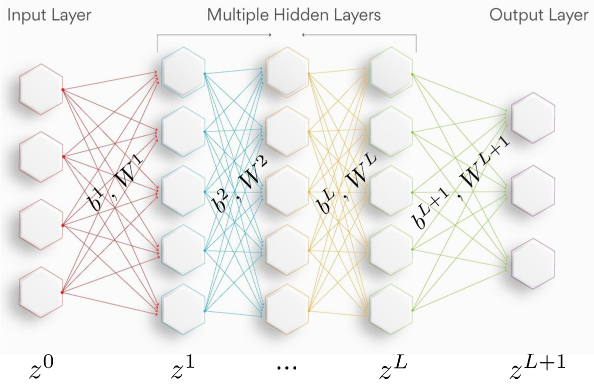
$$\begin{pmatrix} z^{\ell+1} \end{pmatrix} = \begin{pmatrix} b^{\ell+1} \end{pmatrix} + \begin{pmatrix} W^{\ell+1} \end{pmatrix} \begin{pmatrix} \sigma(z^{\ell}) \end{pmatrix}$$

bias initialization can always be set to zero

An orthogonal weight matrix will not change the magnitude of a vector

activation function: literally just some function applied to each element of the vector

What to measure?



- Stat mech relies on probabilities which require randomness
  - Initialize network 100 times to get 100 sets of parameters
  - Take averages over initializations to get expectation values
- Measure properties of initialization that inform network performance

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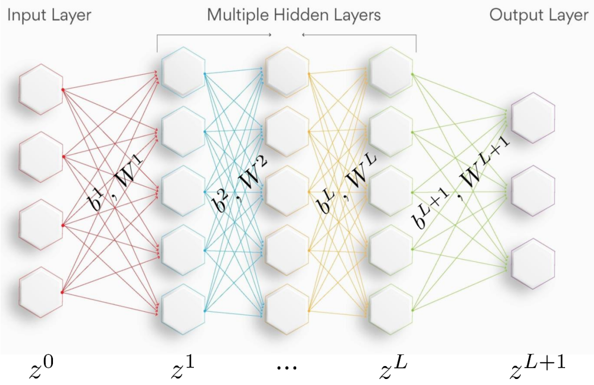

- Stat mech relies on probabilities which require randomness
  - Initialize network 100 times to get 100 sets of parameters
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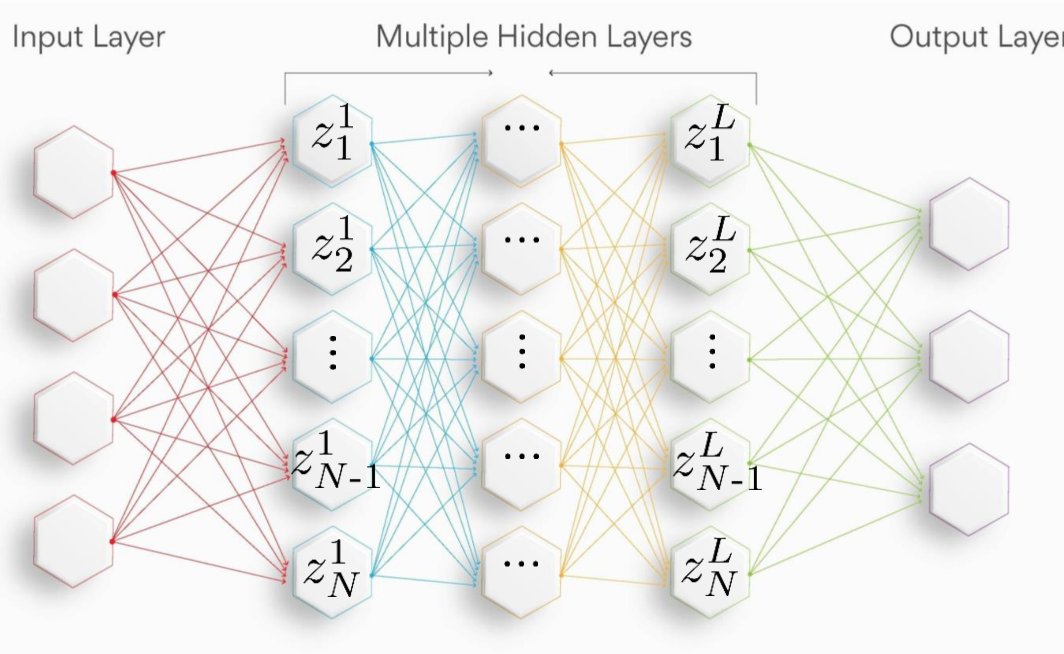
- Measure properties of initialization that inform network performance
  - Similar inputs should go to similar outputs ⇒ n-point functions
  - Expect similar results every time you use the network ⇒ NTK

$$\underset{\text{layer vector}}{\left(z^{\ell+1}\right)} = \underset{\text{bias vector}}{\left(b^{\ell+1}\right)} + \underset{\text{weight matrix}}{\left(\quad W^{\ell+1} \quad\right)}\left(\sigma(z^{\ell})\right)$$

N-point functions

- Average of products of different combinations of neurons in each layer
- Similar inputs → similar outputs
  ⇒ want minimal layer-dependence
  (limit explosions and decays)

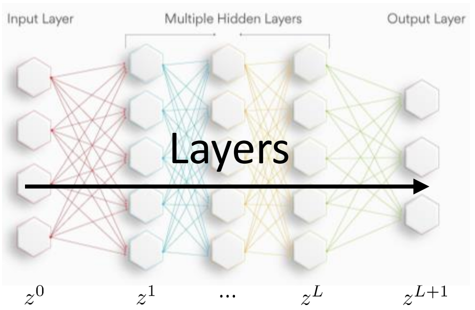


$$\mathbb{E}[z^{\ell}_{i_1} z^{\ell}_{i_2}]$$

$$\mathbb{E}[z^{\ell}_{i_1} z^{\ell}_{i_2} z^{\ell}_{i_3} z^{\ell}_{i_4}]$$

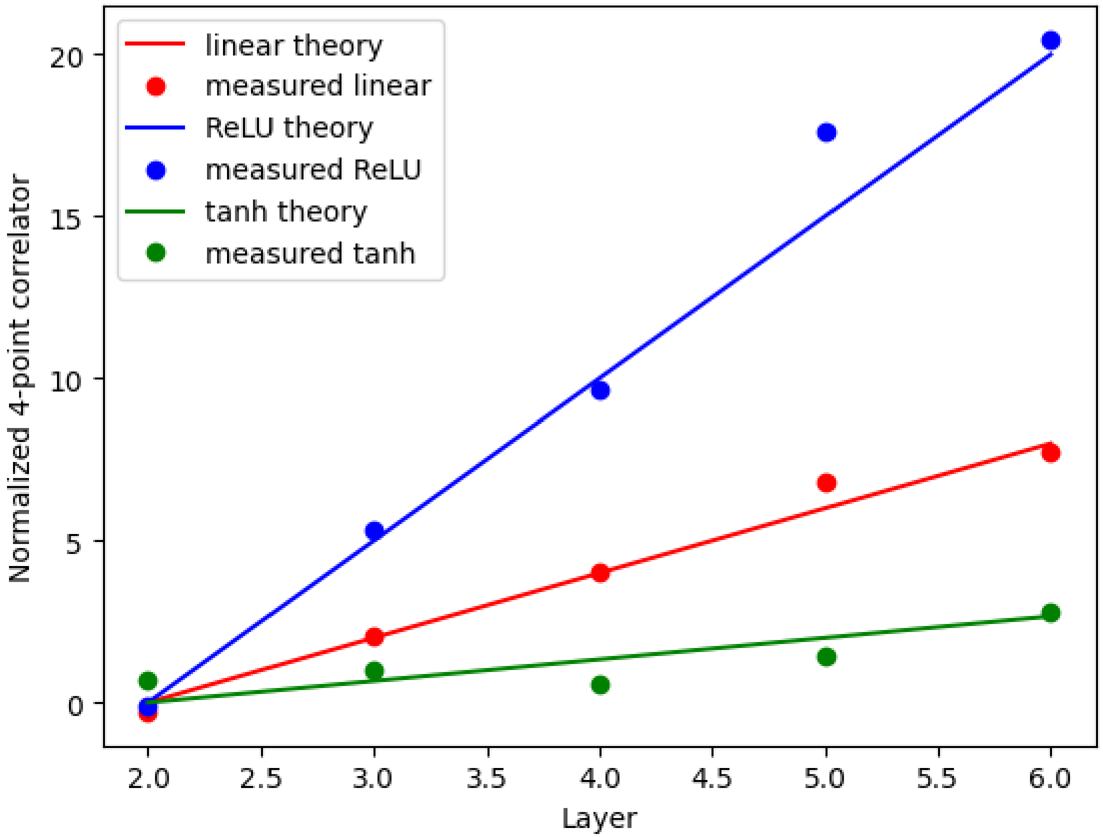
$$\mathbb{E}[z^{\ell}_{i_1} z^{\ell}_{i_2} z^{\ell}_{i_3} z^{\ell}_{i_4}]|_{\text{conn.}} = \mathbb{E}[z^{\ell}_{i_1} z^{\ell}_{i_2} z^{\ell}_{i_3} z^{\ell}_{i_4}] - \mathbb{E}[z^{\ell}_{i_1} z^{\ell}_{i_2}]\mathbb{E}[z^{\ell}_{i_3} z^{\ell}_{i_4}] - \mathbb{E}[z^{\ell}_{i_1} z^{\ell}_{i_3}]\mathbb{E}[z^{\ell}_{i_2} z^{\ell}_{i_4}] - \mathbb{E}[z^{\ell}_{i_1} z^{\ell}_{i_4}]\mathbb{E}[z^{\ell}_{i_2} z^{\ell}_{i_3}]$$

$$\vdots$$

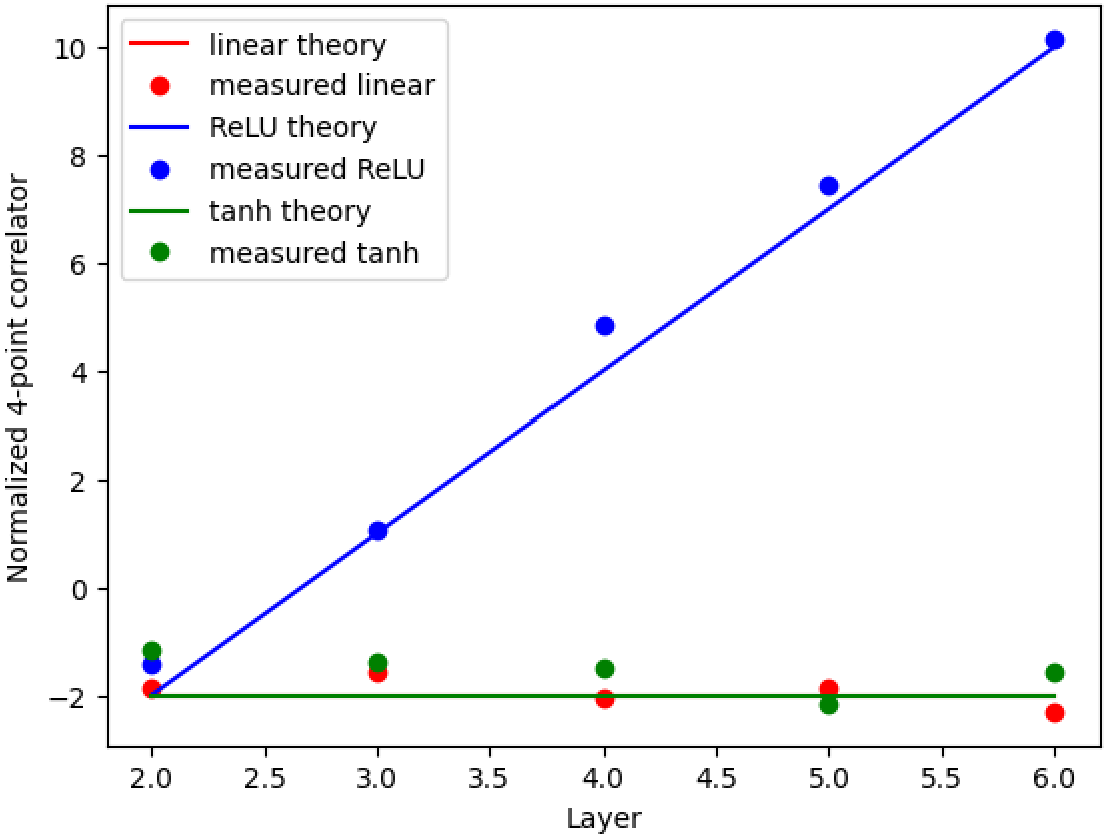


N-point functions

Gaussian weight initialization

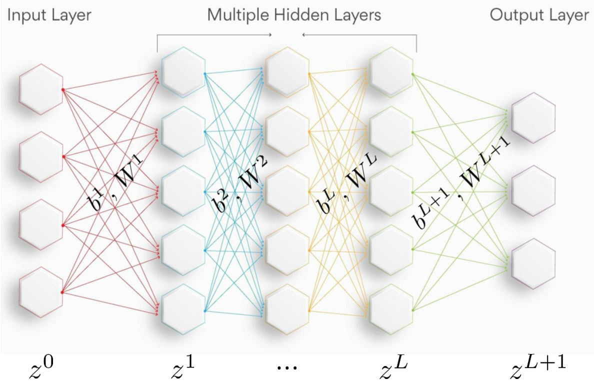


orthogonal weight initialization



Orthogonal initialization removes layer dependance!

HD, Y. Kahn, D. Roberts [arXiv:23XX.XXXX]



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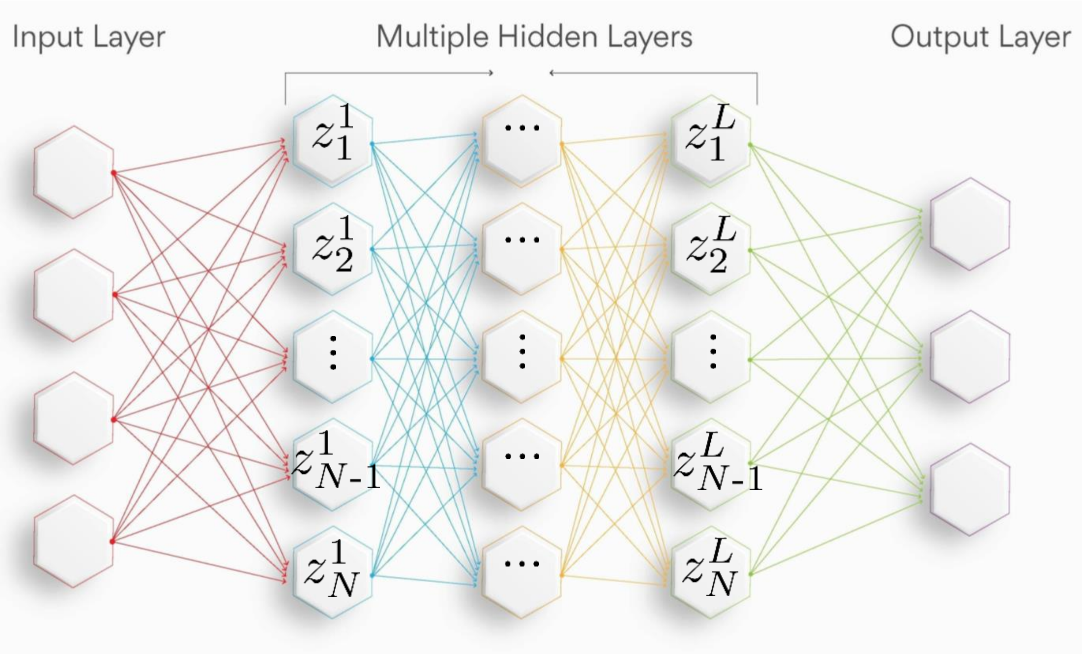
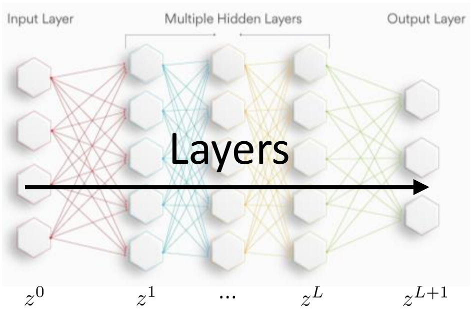
The neural tangent kernel (NTK)

- Change in layer outputs as biases and weights are updated during training
- Governs *feature learning*, i.e. whether something useful happens during training
- Consistent results

  ⇒ want minimal layer-dependance
- But beware of tradeoff with learning, which requires layer-dependence



$$\widehat{H}^{(\ell)} \propto \frac{dz^{(\ell)}}{d\theta}\frac{dz^{(\ell)}}{d\theta} \ , \quad \theta \in \{b, W\}$$



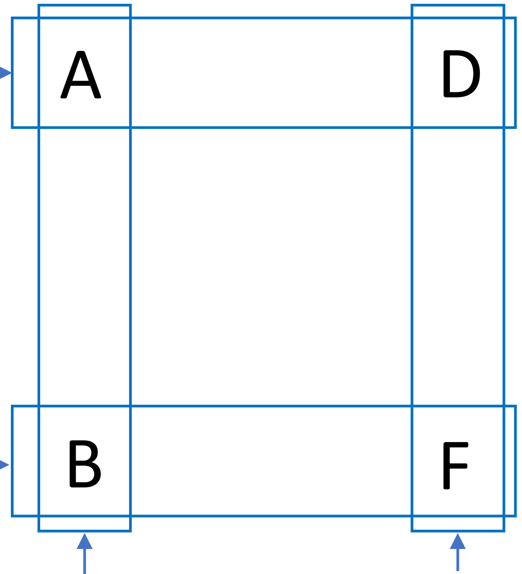
NTK: Gaussian vs. orthogonal

do not affect NTK evolution
(only induce noise)

$$\widehat{H}^{\ell+1} \neq f(A^\ell, D^\ell)$$

update NTK during training
(allow feature learning)

$$\widehat{H}^{\ell+1} = f(B^\ell, F^\ell)$$

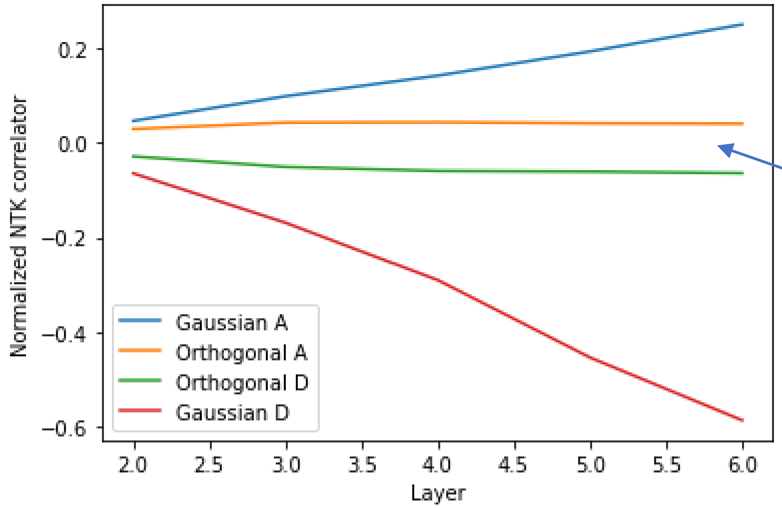


NTK fluctuations

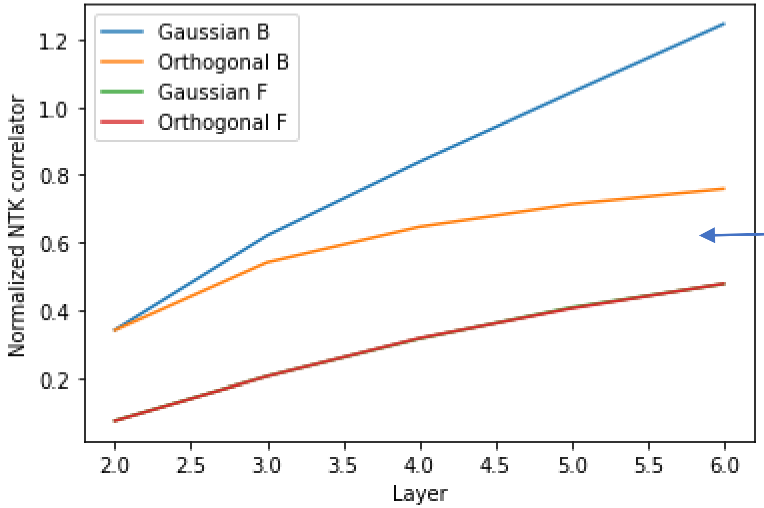
$$\mathbb{E}[\widehat{\Delta H}^2]$$

interactions between
NTK and layer output

$$\mathbb{E}[z^2 \widehat{\Delta H}]$$

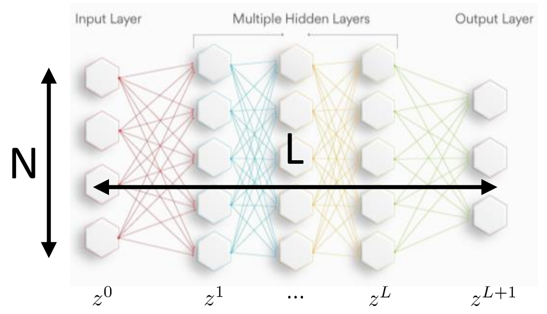


“bad” correlators become depth-independent



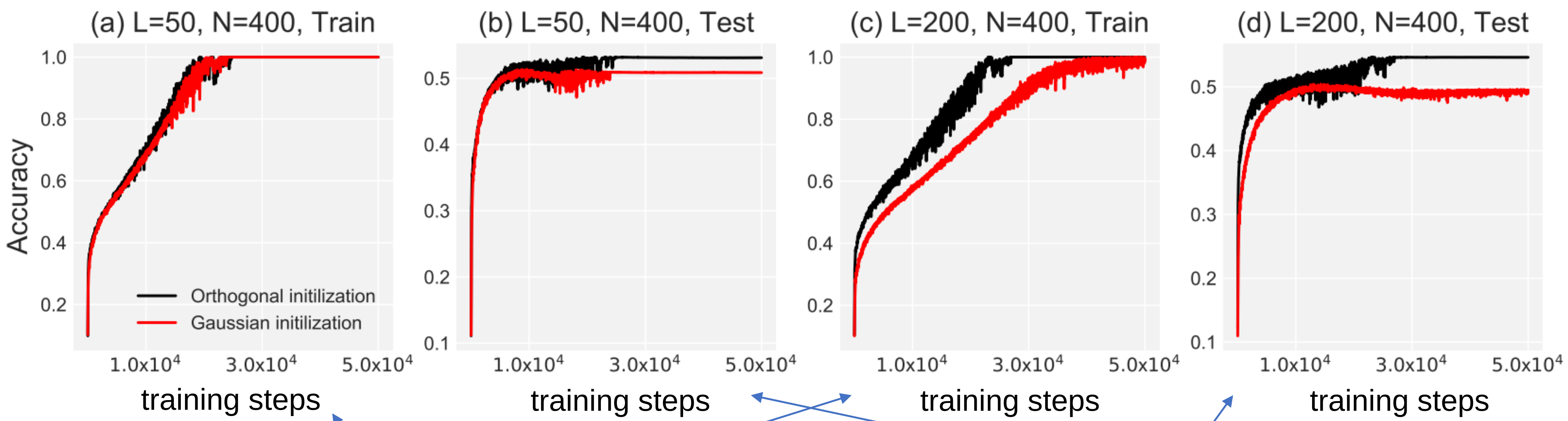
“good” correlators maintain depth-dependence

HD, Y. Kahn, D. Roberts [arXiv:23XX.XXXX]



Are the predictors right?

(Does reducing “bad” depth dependance improve network learning?)



Gaussian takes longer to train when depth increases
Orthogonal trains at approximately the same rate

Gaussian test accuracy plateaus sooner and lower than orthogonal as training steps increase

W. Huang, W. Du, R. Xu [arXiv:2004.05867]

Are the predictors right?

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Future work:

- Does variance in accuracy also decrease with orthogonal initialization?
- What happens with other types of networks (e.g. convolutional)?
- Can we generically determine the best initialization distribution?
- How does the type of data or dataset affect results?
- How far does the analogy go? (Feynman diagrams?)

Conclusion

- Neural networks can be described using statistical mechanics
- Network outputs can be both stochastic (governed by statistics) and deterministic (predictable) – just like in stat mech!
- Techniques from stat mech can be used for network optimization
- Measurements at initialization can predict training success

Daniel A. Roberts and Sho Yaida. *The Principles of Deep Learning Theory*. [arXiv:2106.10165]

Wei Huang, Weitao Du, and Richard Yi Da Xu. *On the NTK of Deep Networks with Orthogonal Initialization.* [arXiv:2004.05867]

Jared Kaplan. *Notes on Contemporary Machine Learning for Physicists*. (Great introductory text)

Explosions and disappearances

(What does criticality mean?)

- Large weight initialization ⇒ large network output

$$|W^i| = \mathcal{O}(100) \implies |z^L| \to \infty$$

- Small weight initialization ⇒ small network output

$$|W^i| = \mathcal{O}(0.01) \implies |z^L| \to 0$$

- Network cannot learn in either case

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~~Similar inputs should go to similar outputs~~

~~Expect similar results every time you use the network~~

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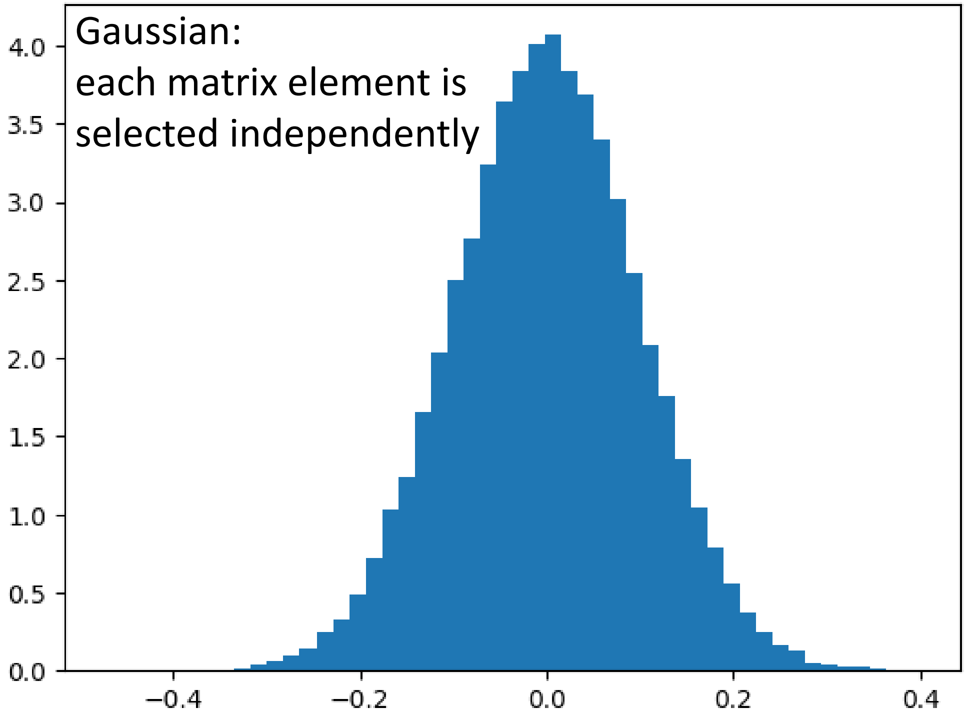
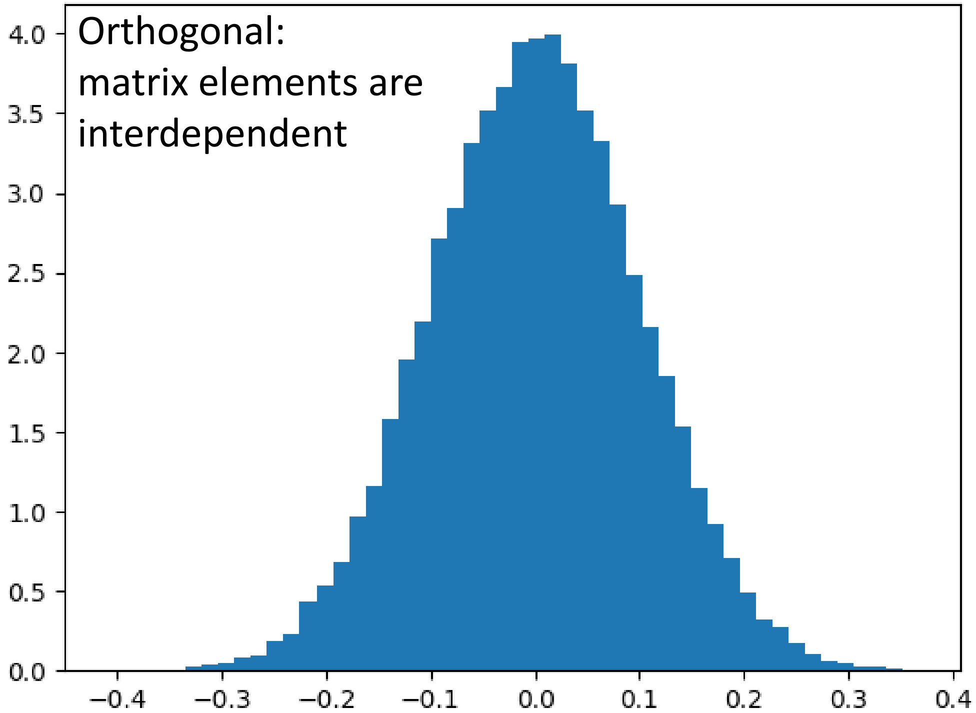
*This reduces signal growth and decay, but does not eliminate it
(that would be bad too)

Gaussian vs orthogonal weights

- Gaussian distribution is the limiting distribution – all distributions become Gaussian at infinite width
- Orthogonal distribution corresponds to points on a sphere





Comparing weight initialization distributions

Recall

- Initial weights and biases are randomly selected from a distribution
- Infinite-width neural network = free (Gaussian) field theory

- Finite width $\Longrightarrow$ interactions

$$\underbrace{\begin{pmatrix} z^{\ell+1} \end{pmatrix}}^{\text{layer vector}} = \overbrace{\begin{pmatrix} b^{\ell+1} \end{pmatrix}}^{\text{bias vector}} + \overbrace{\begin{pmatrix} \quad W^{\ell+1} \quad \end{pmatrix}}^{\text{weight matrix}} \begin{pmatrix} \sigma(z^{\ell}) \end{pmatrix}$$

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➡ Non-Gaussian initializations are perturbations away from (infinite-width) Gaussian limit

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*even Gaussian initializations become non-Gaussian at finite-width!

Perhaps introducing physically-motivated interactions to our network will improve learning