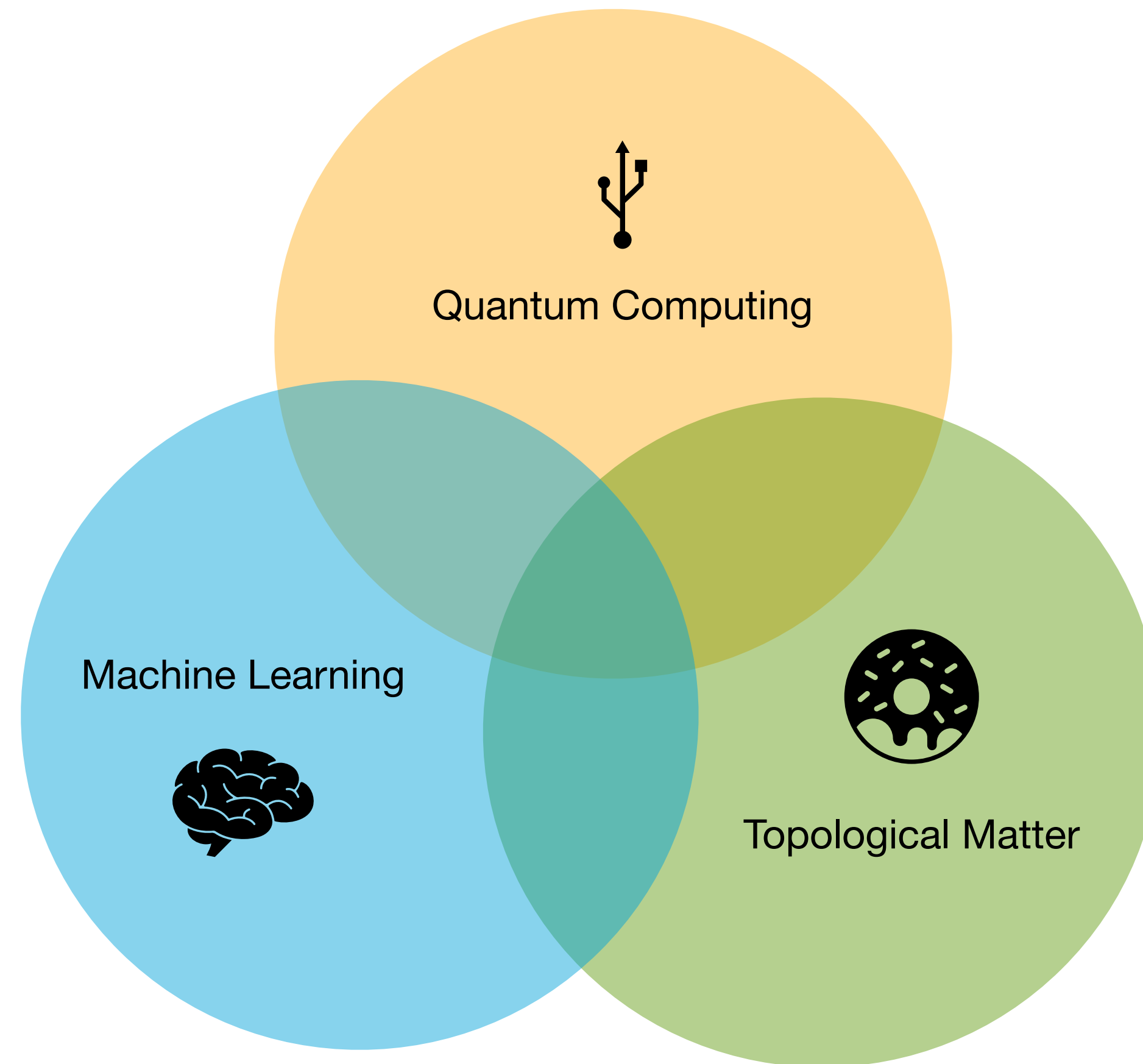


# Engineered Topological Matter and Machine Learning for Quantum Applications

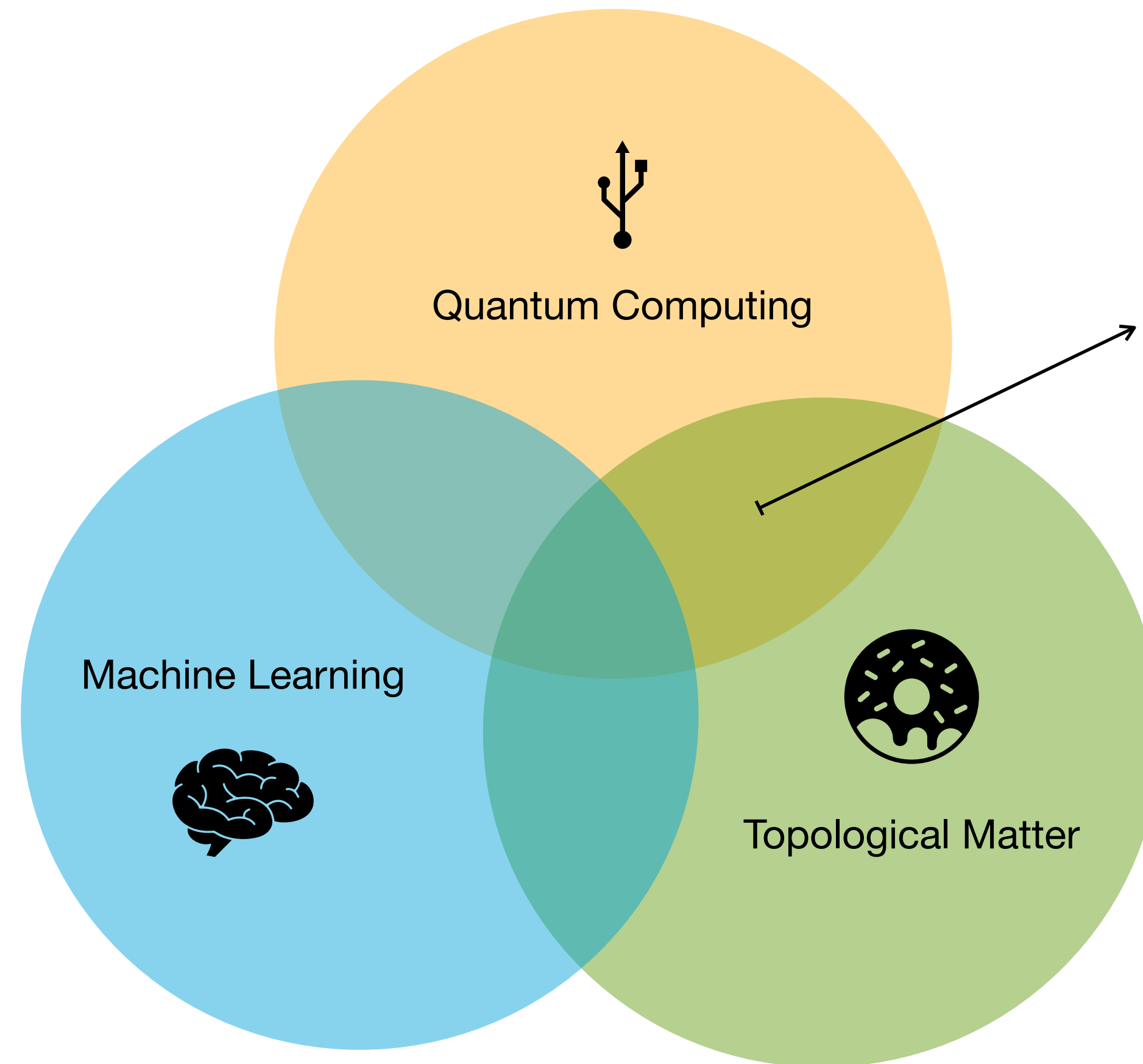
Eliška Greplová



# Topological Matter School '22



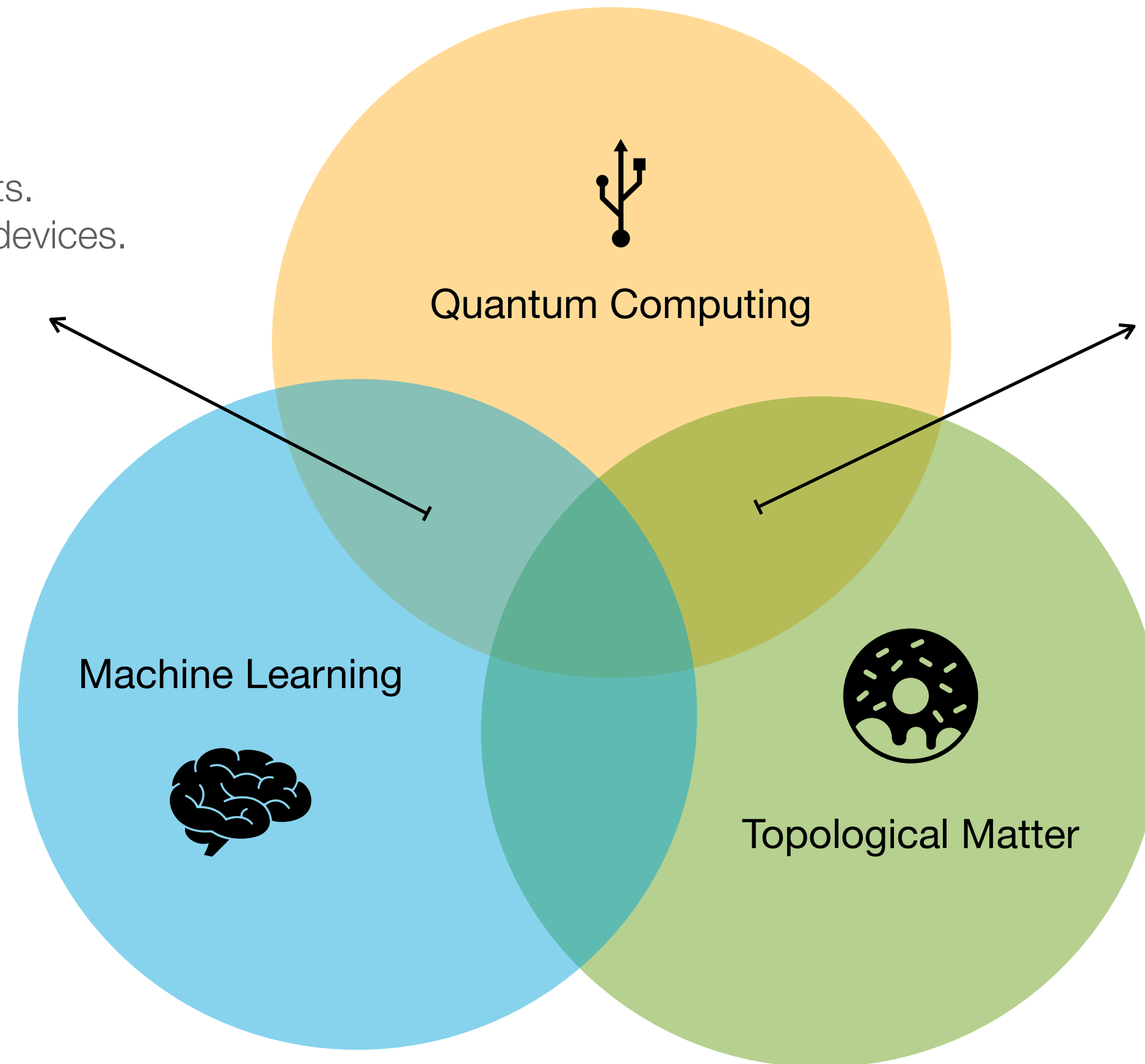
# Topological Matter School '22



Use topological excitations for quantum computing taking advantage of protection against errors.

# Topological Matter School '22

Model quantum circuits.  
Tune and control quantum devices.



Quantum Computing

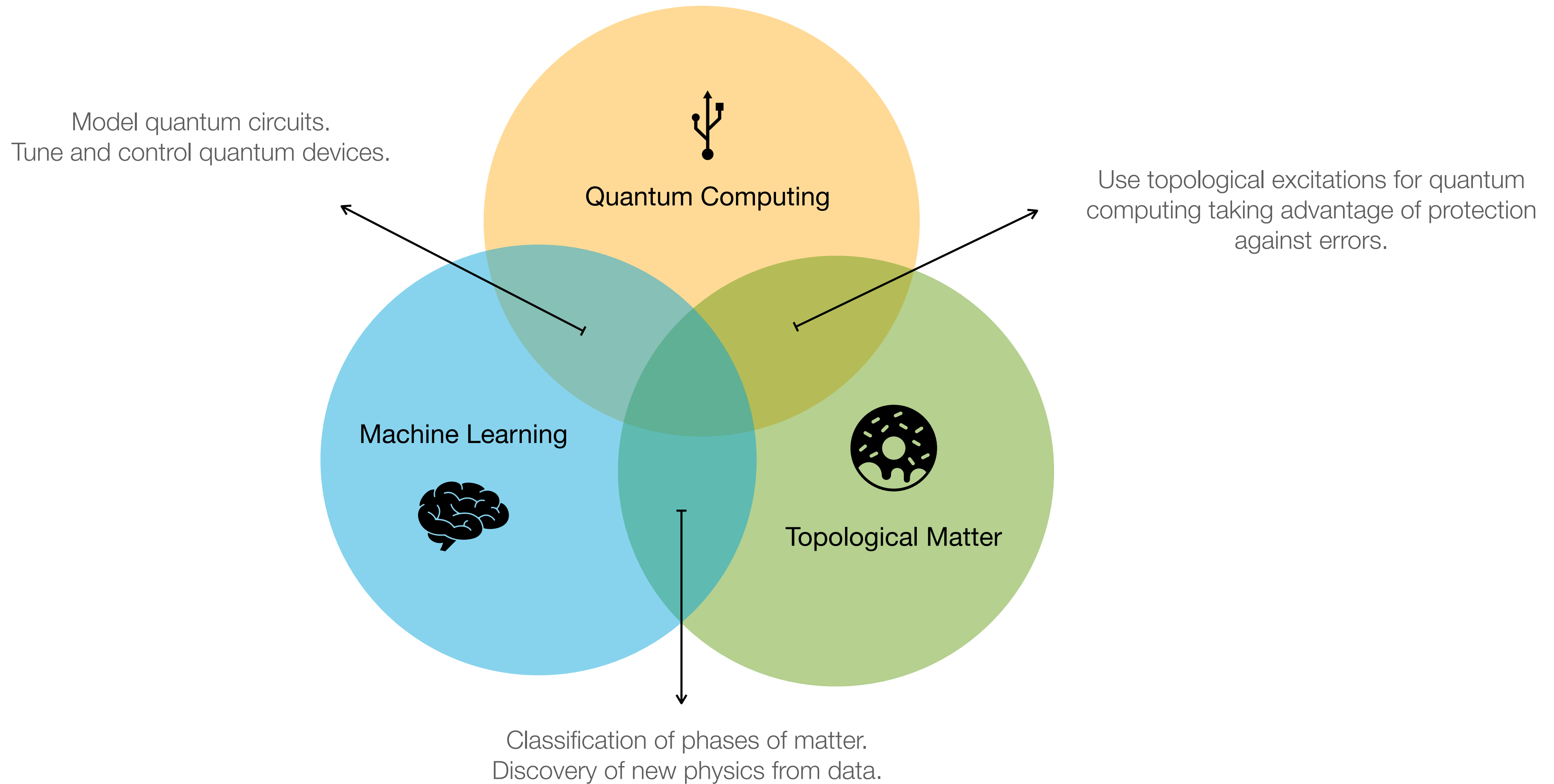
Machine Learning

Topological Matter

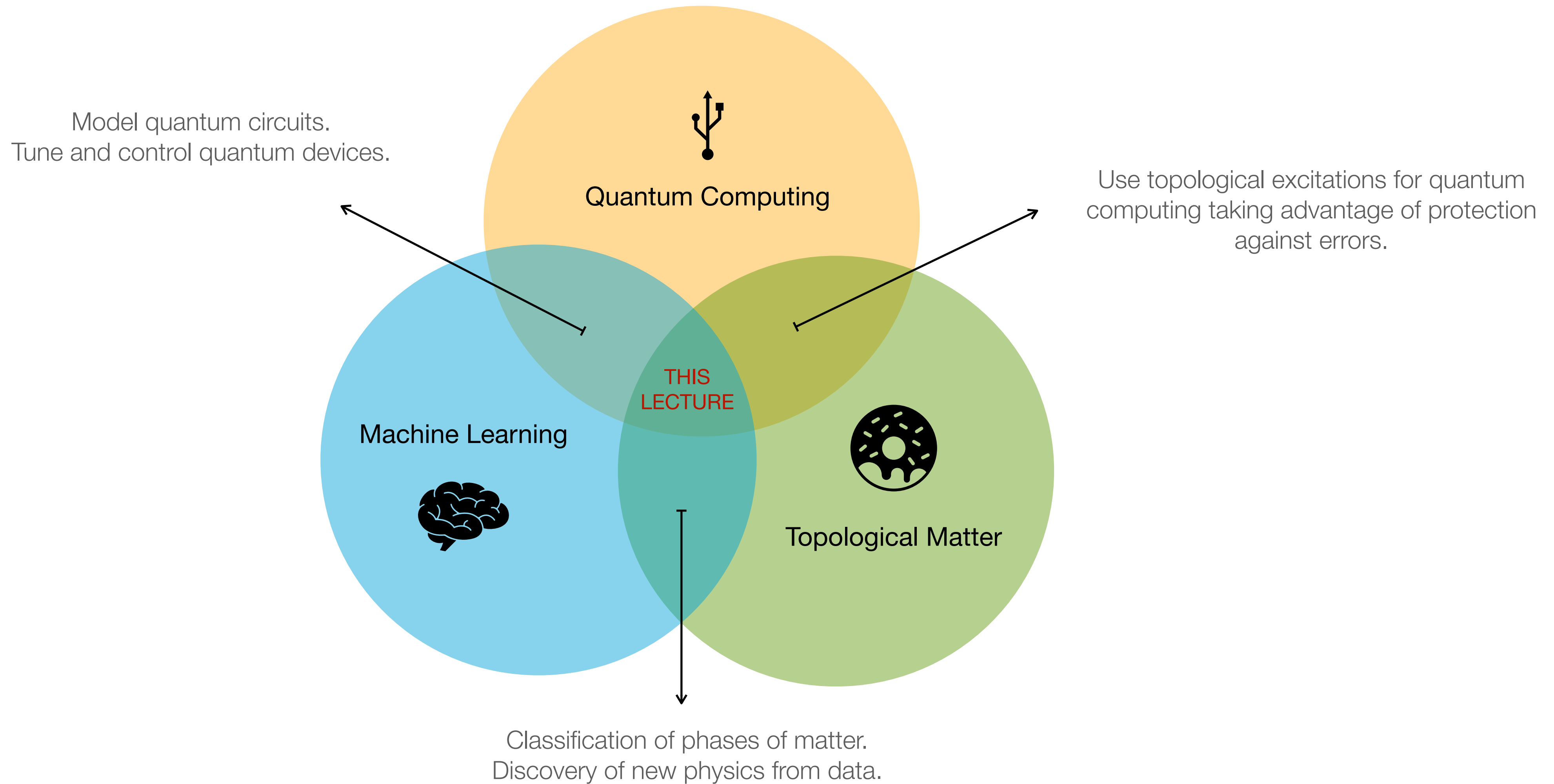
Use topological excitations for quantum computing taking advantage of protection against errors.



# Topological Matter School '22

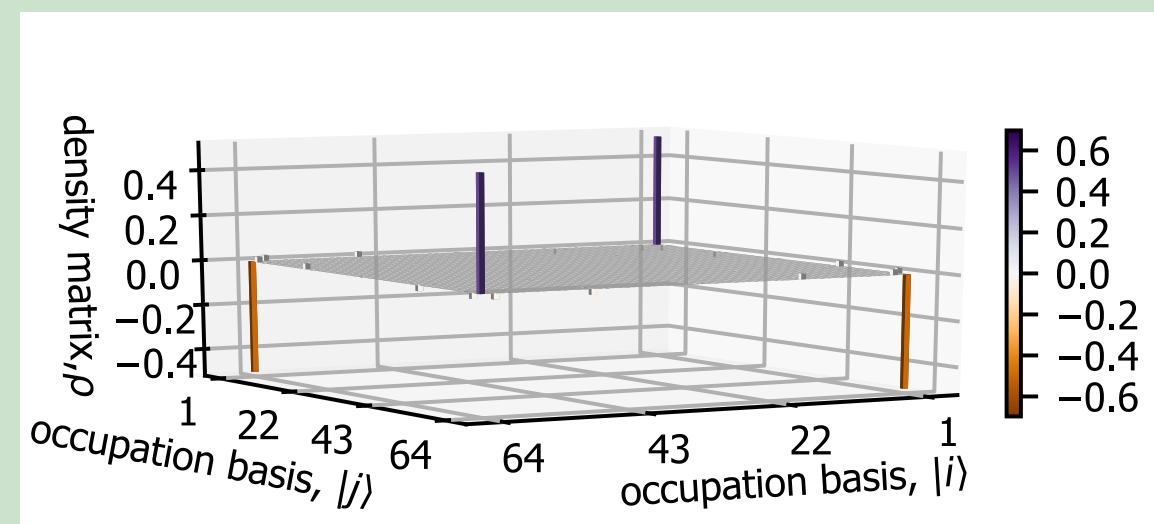


# Topological Matter School '22



## Motivation: Topological Metamaterials

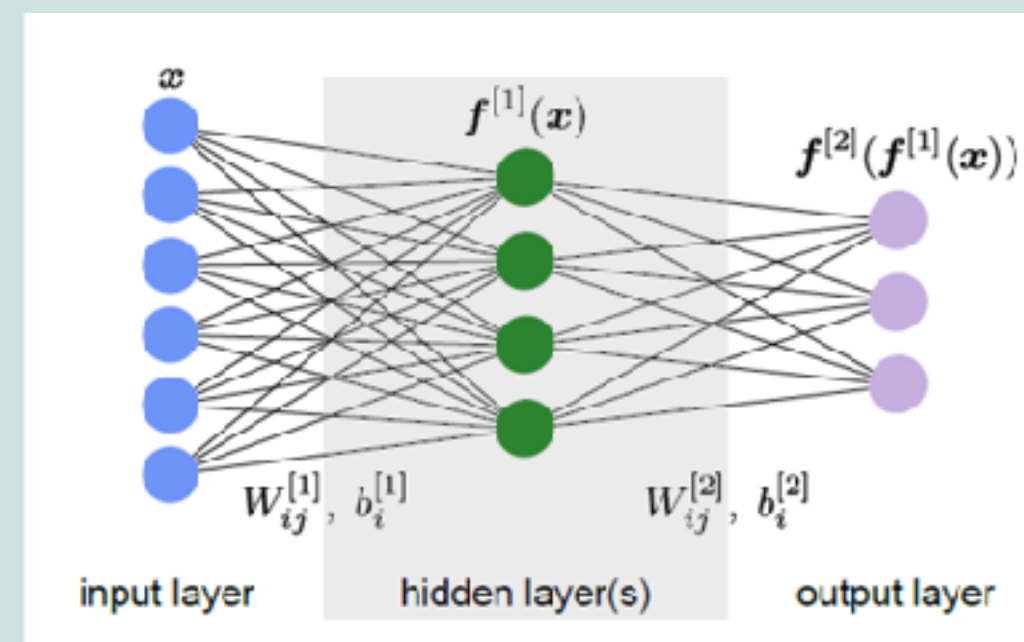
Stabilizing Entanglement in  
Superconducting Circuits Using  
Topology



arXiv:2205.09100

## ML Primer: Neural Networks Introduction

Learning Physics from Data: Why  
and How to Get Started



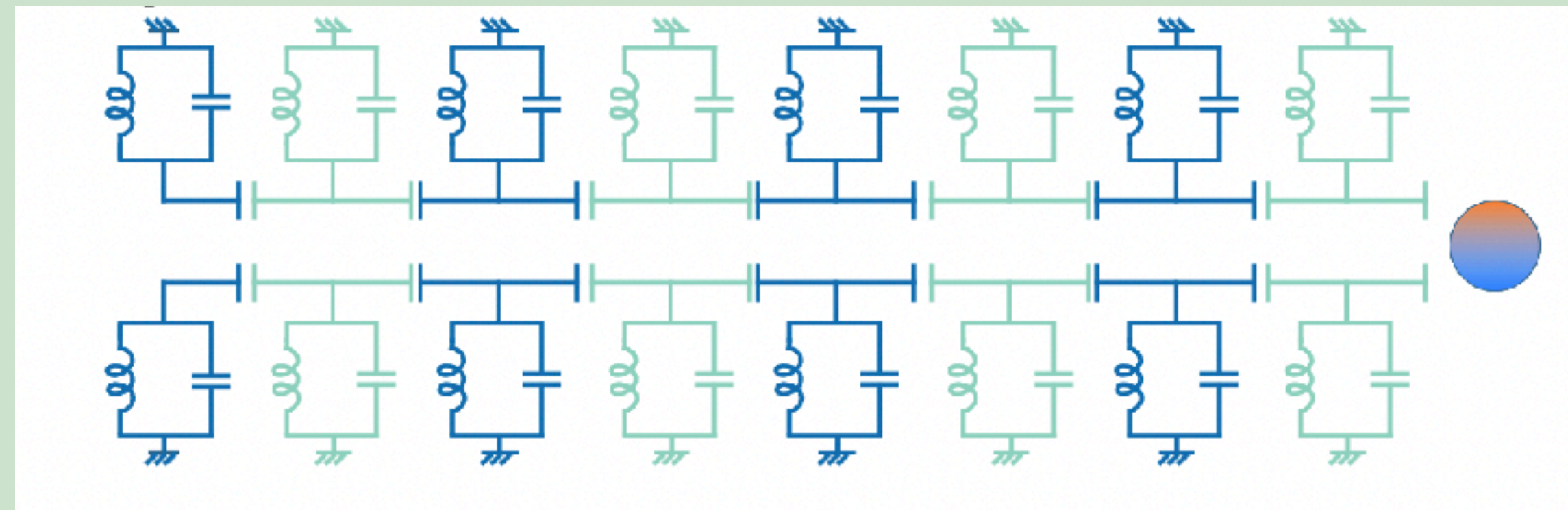
arXiv:2102.04883

## Hands-On: ML in Q-Computing Research

Writing Code to Classify Topological  
Phases in Superconducting Circuits

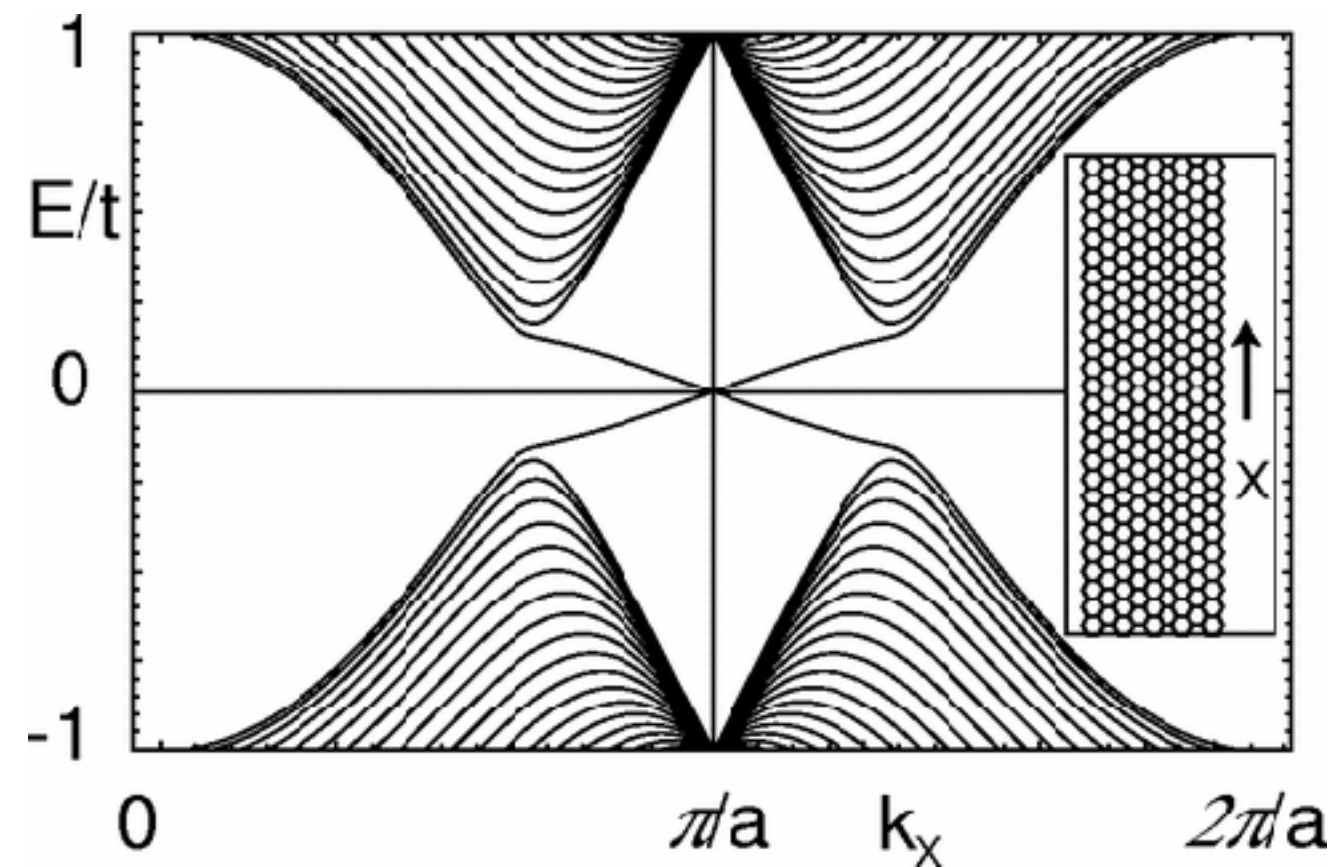
 PyTorch

Motivation:  
Quantum Topological Metamaterials with Superconducting Circuits

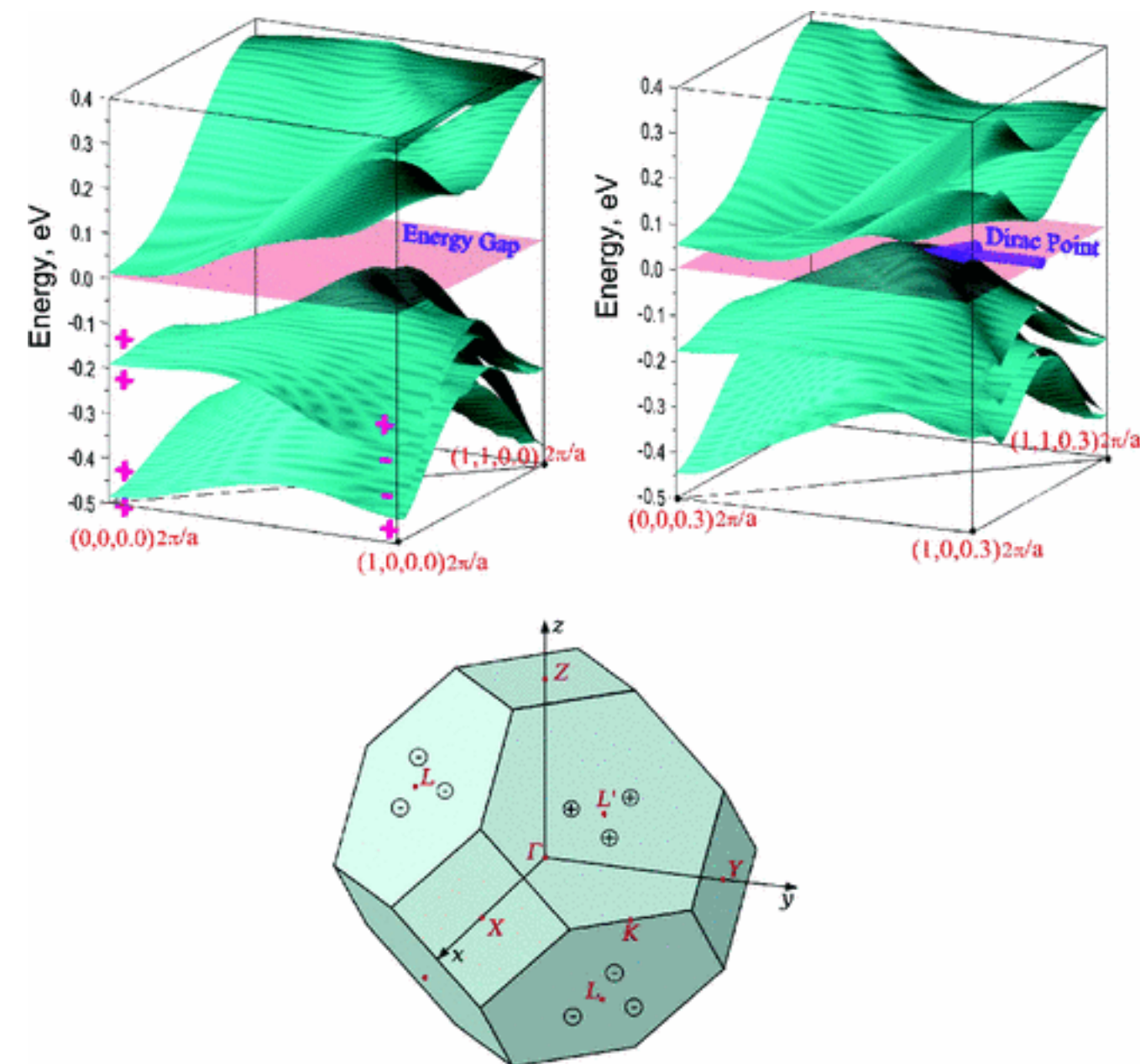




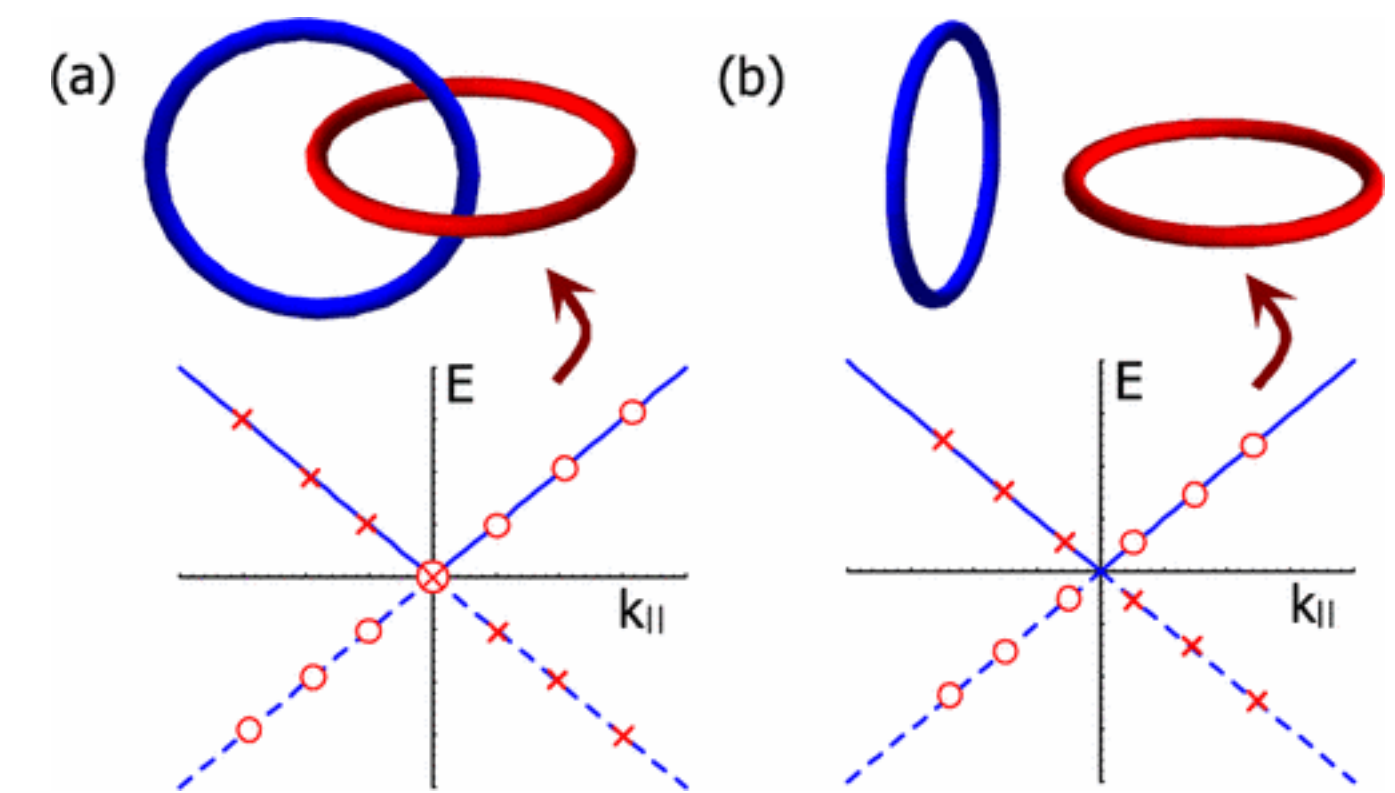
# Topology and Condensed Matter



C. L. Kane and E. J. Mele Phys. Rev. Lett. **95**, 226801



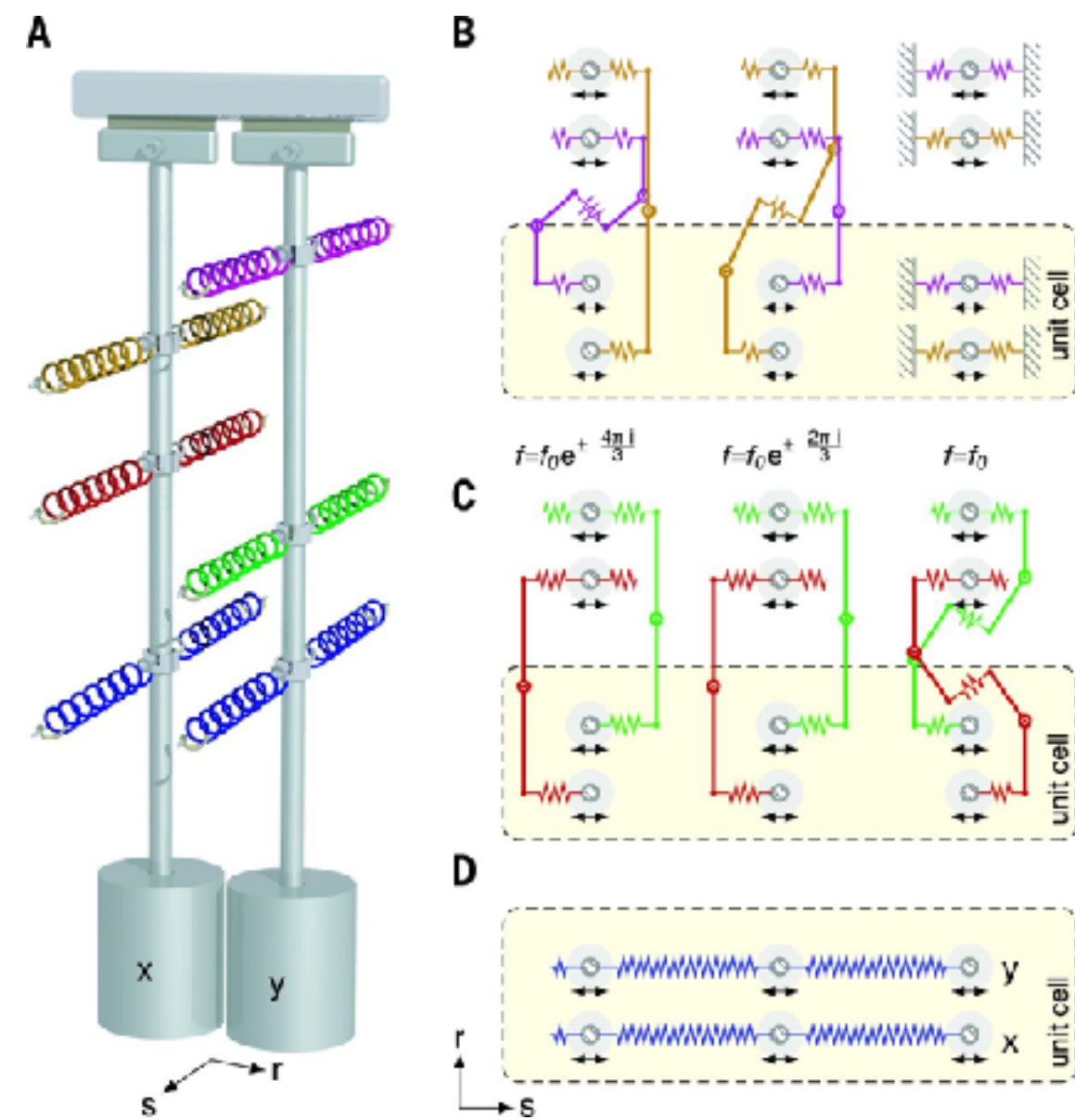
Xiangang Wan, Ari M. Turner, Ashvin Vishwanath, and Sergey Y. Savrasov Phys. Rev. B **83**, 205101



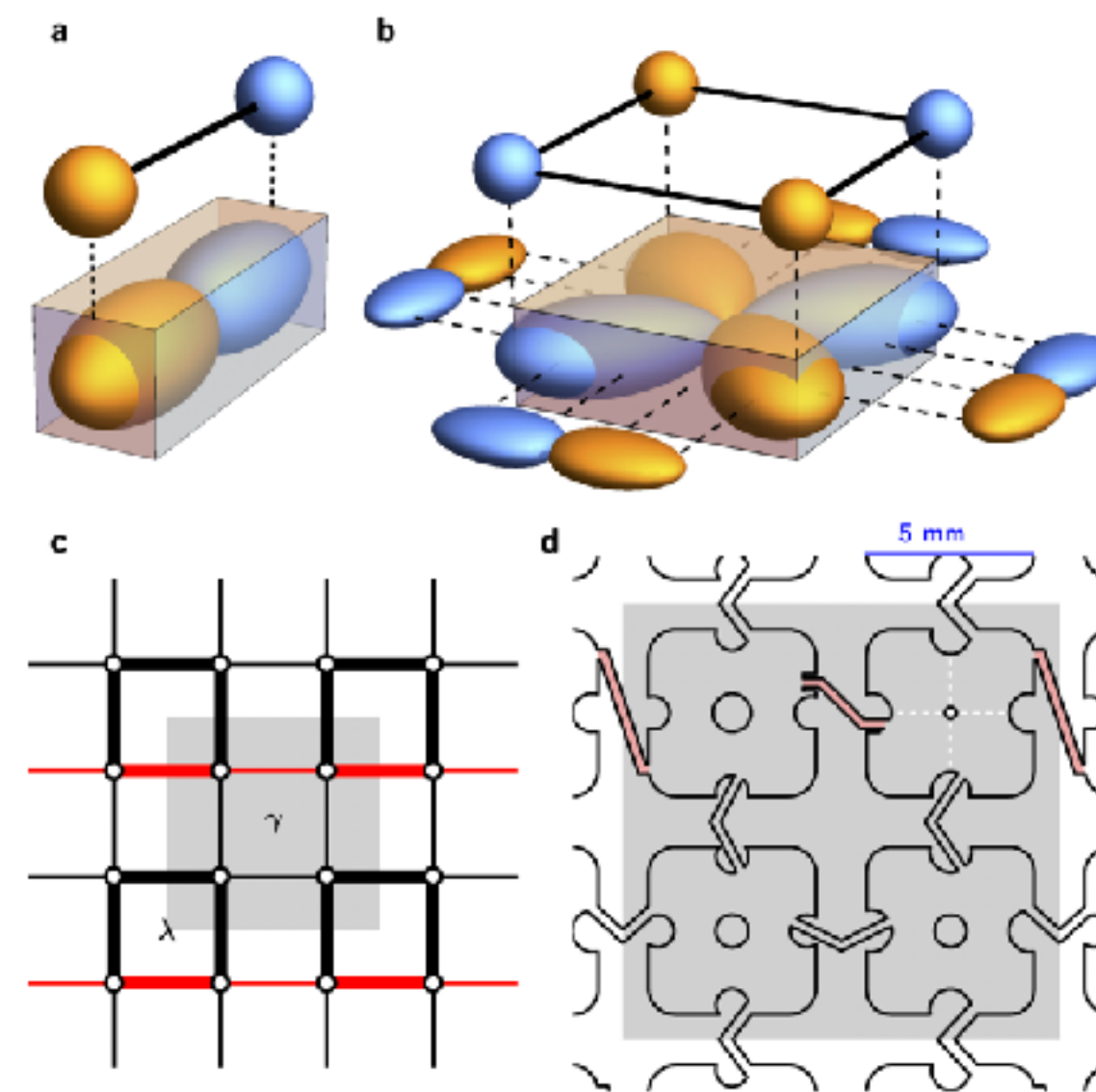
Xiao-Liang Qi, Taylor L. Hughes, S. Raghu, and Shou-Cheng Zhang Phys. Rev. Lett. **102**, 187001



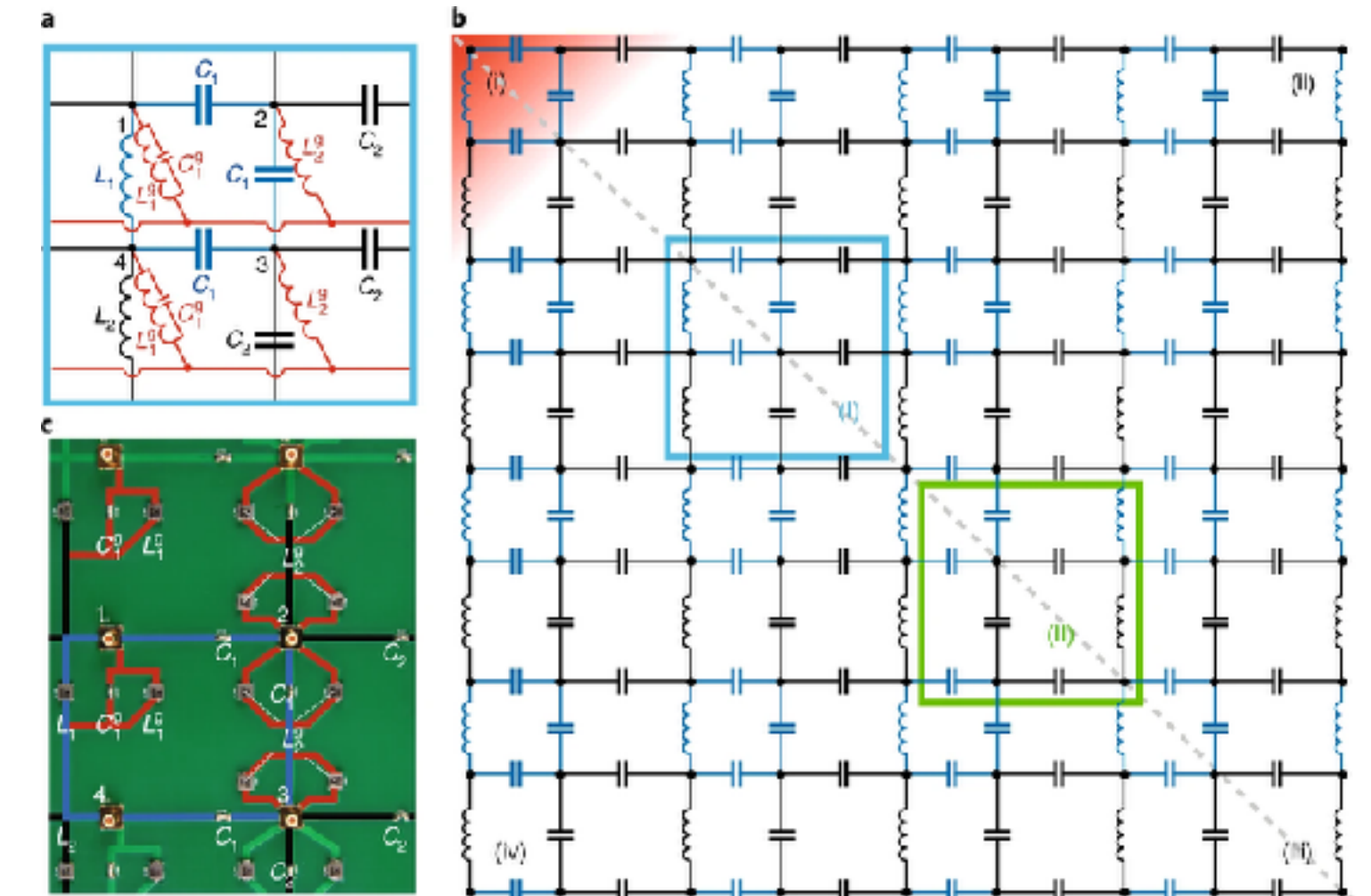
# Classical Topological Materials



Süsstrunk, Roman, and Sebastian D. Huber. "Observation of phononic helical edge states in a mechanical topological insulator." *Science* 349.6243 (2015): 47-50.

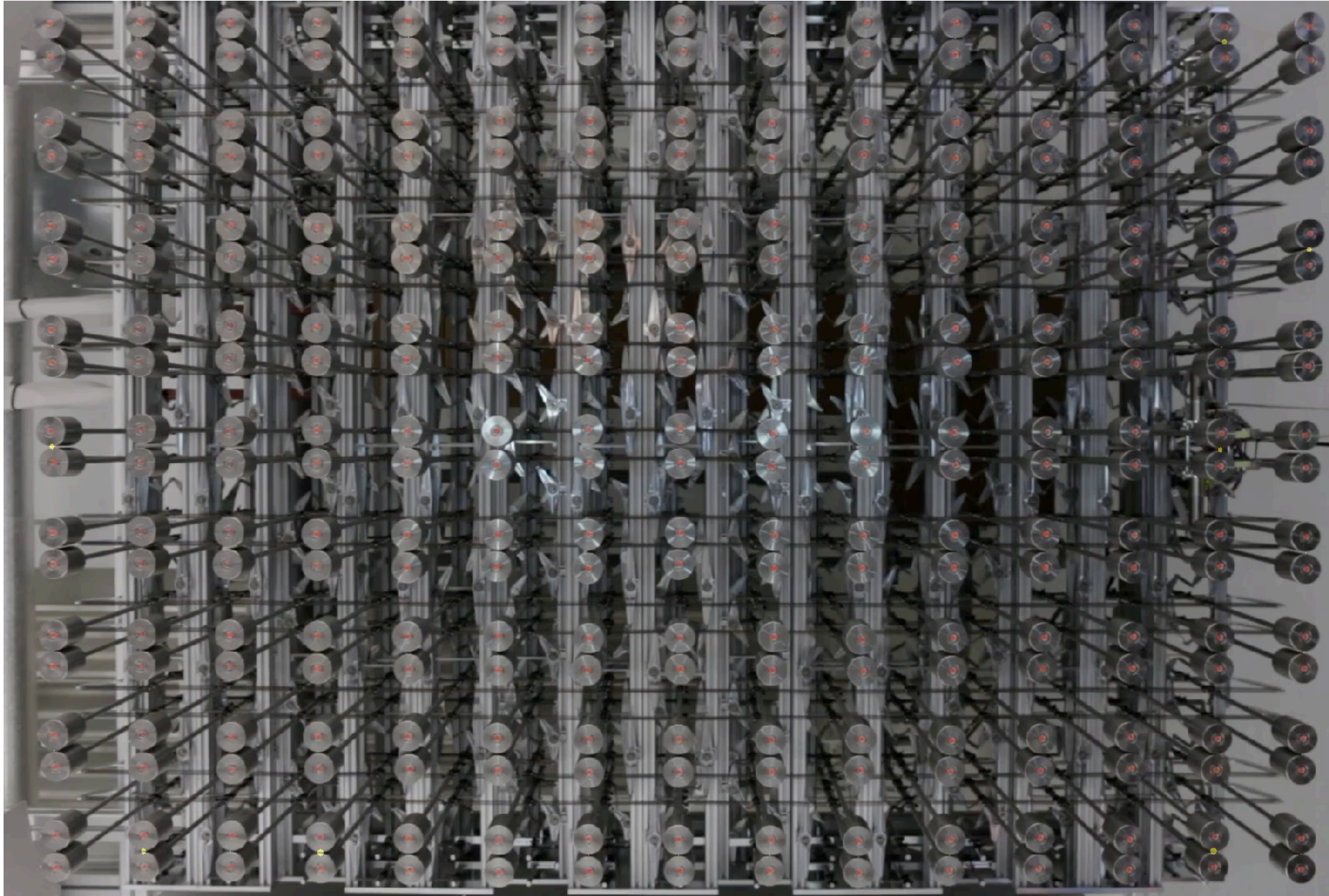


Serra-Garcia, Marc, et al. "Observation of a phononic quadrupole topological insulator." *Nature* 555.7696 (2018): 342-345.



Imhof, Stefan, et al. "Topoelectrical-circuit realization of topological corner modes." *Nature Physics* 14.9 (2018): 925-929.



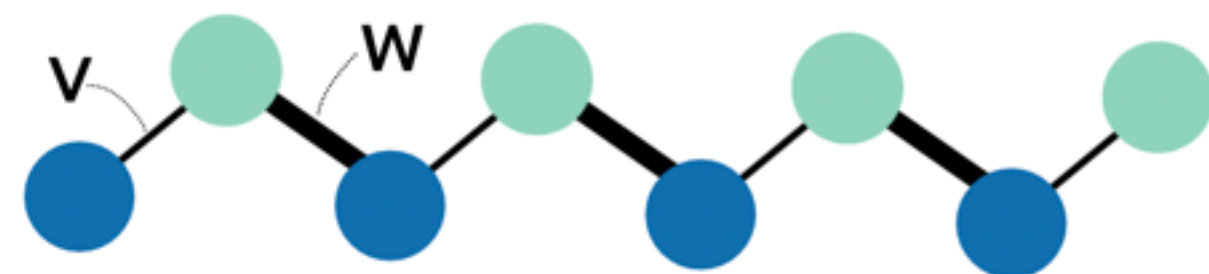


## Observation of phononic helical edge states in a mechanical topological insulator

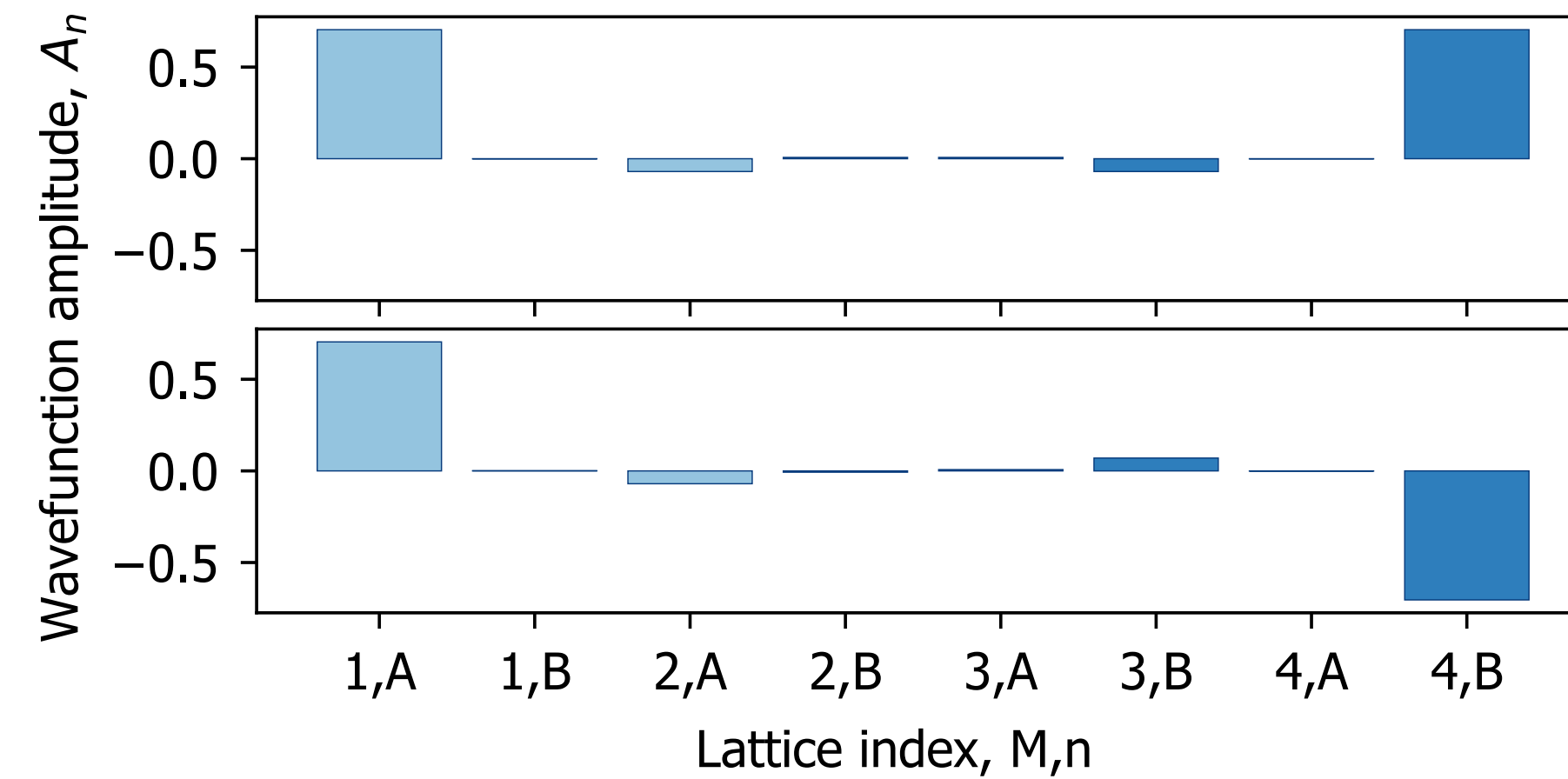
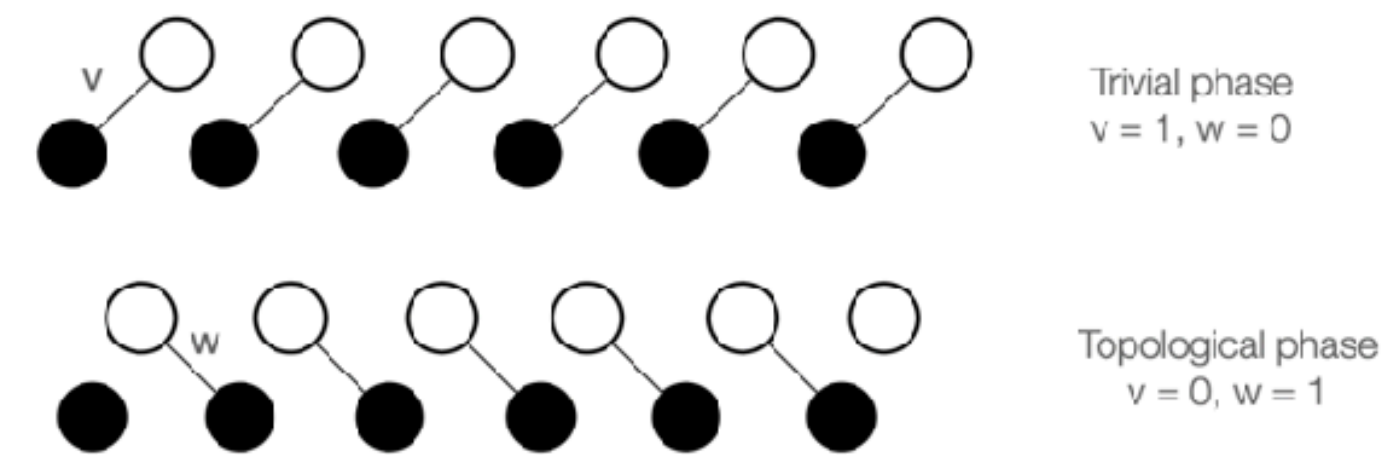
ROMAN SÜSSTRUNK AND SEBASTIAN D. HUBER  
*SCIENCE* • 3 Jul 2015 • Vol 349, Issue 6243



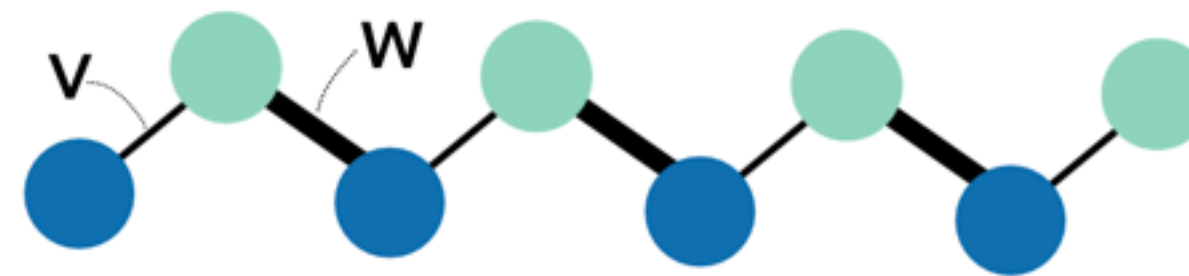
# Example: SSH model



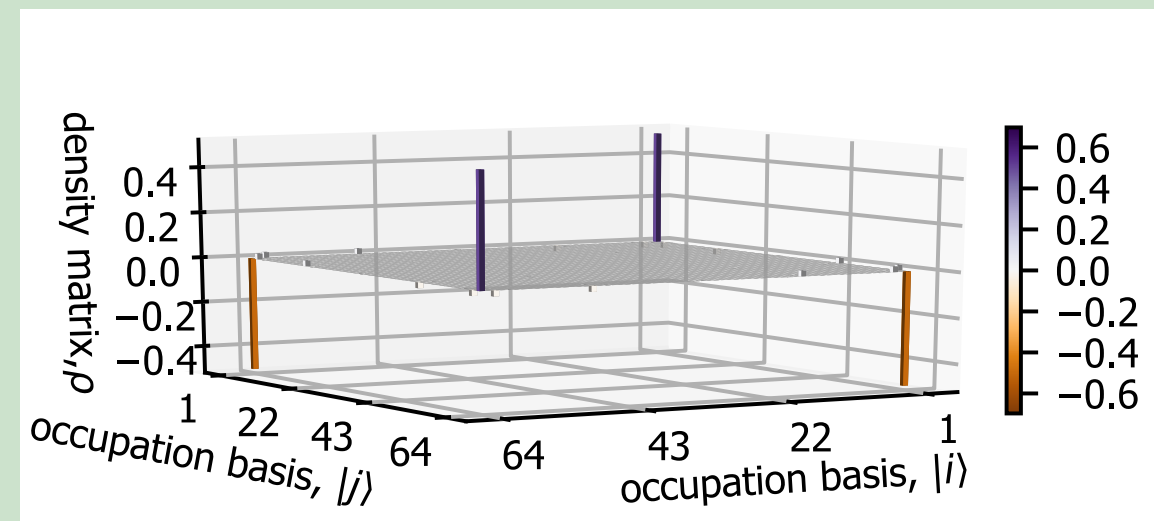
$$H_{SSH} = v \sum_{m=1}^N (|m, B\rangle \langle m, A| + h.c.) + w \sum_{m=1}^{N-1} (|m+1, A\rangle \langle m, B| + h.c.),$$



# SSH model in this lecture

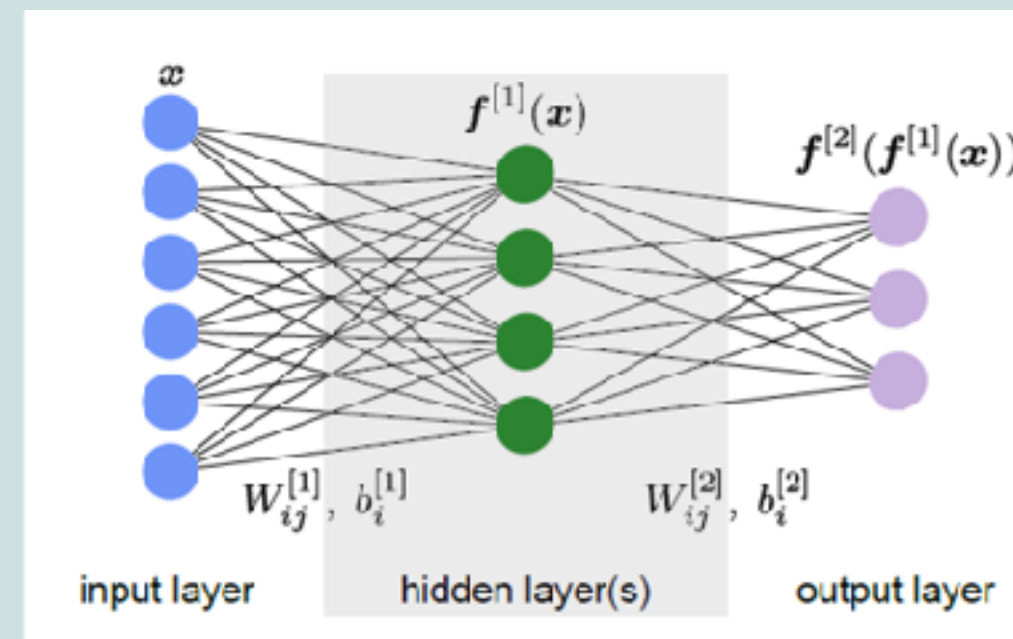


SSH in QMAI research



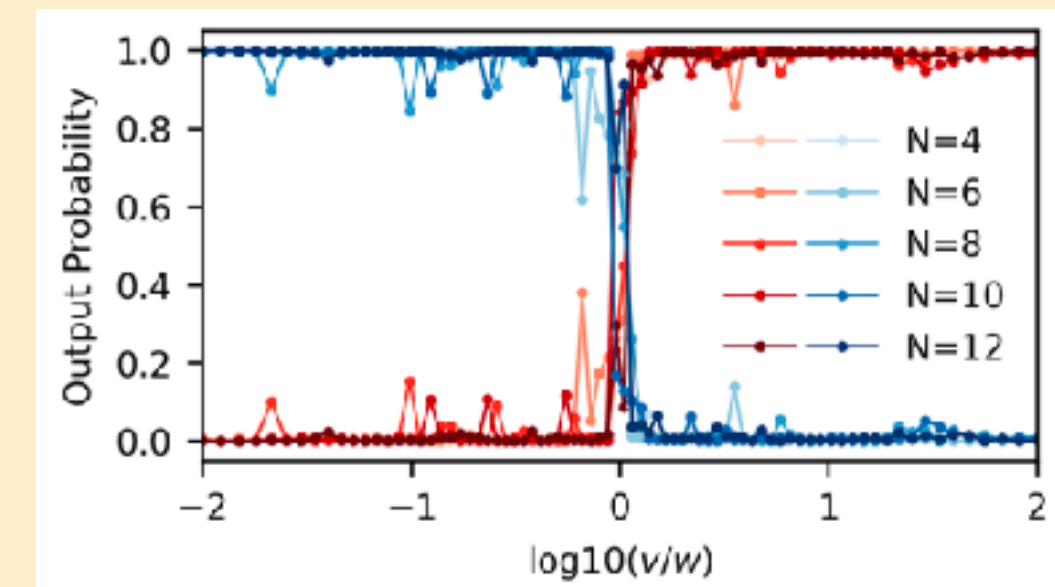
arXiv:2205.09100

ML generic intro

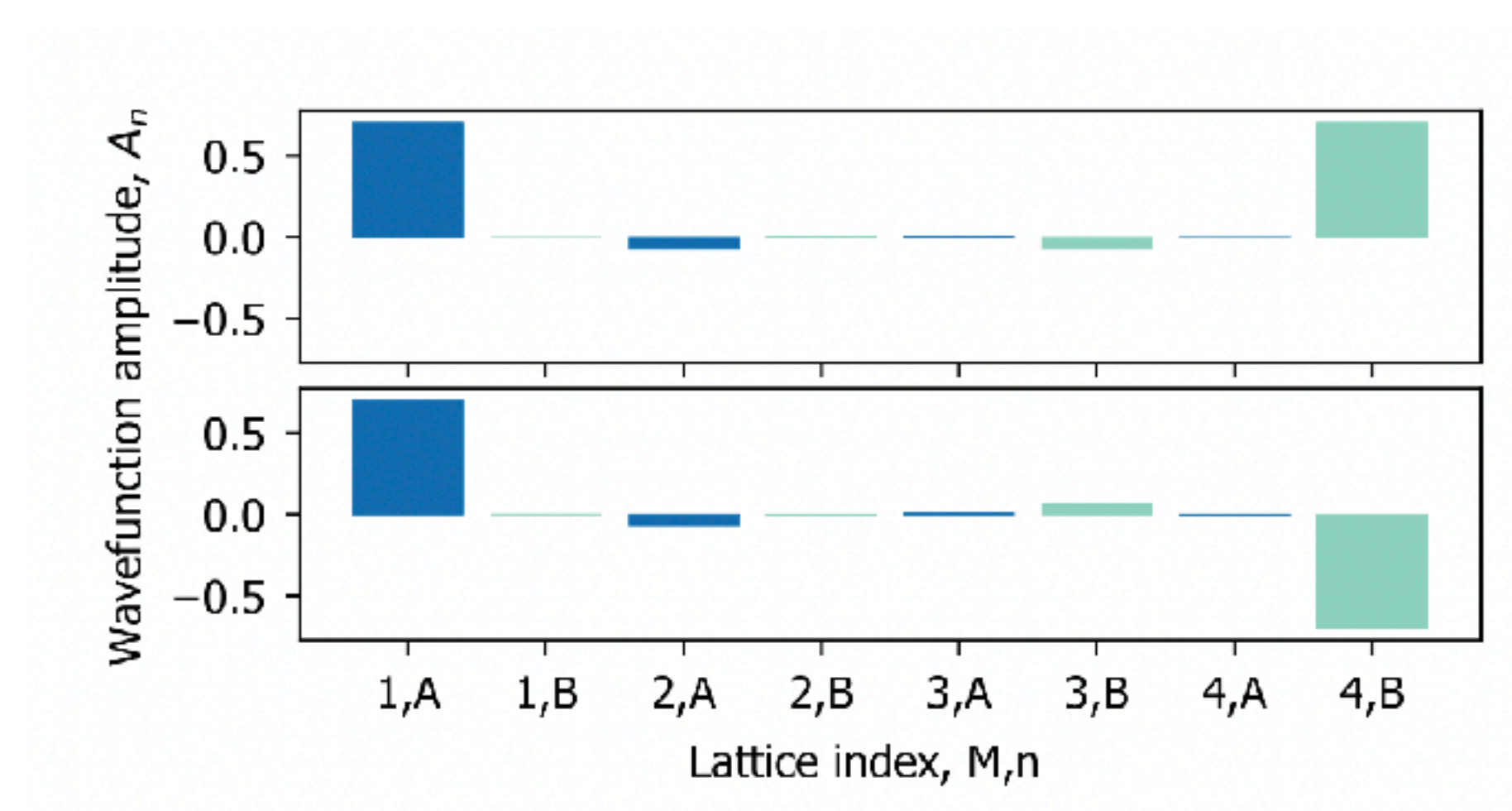
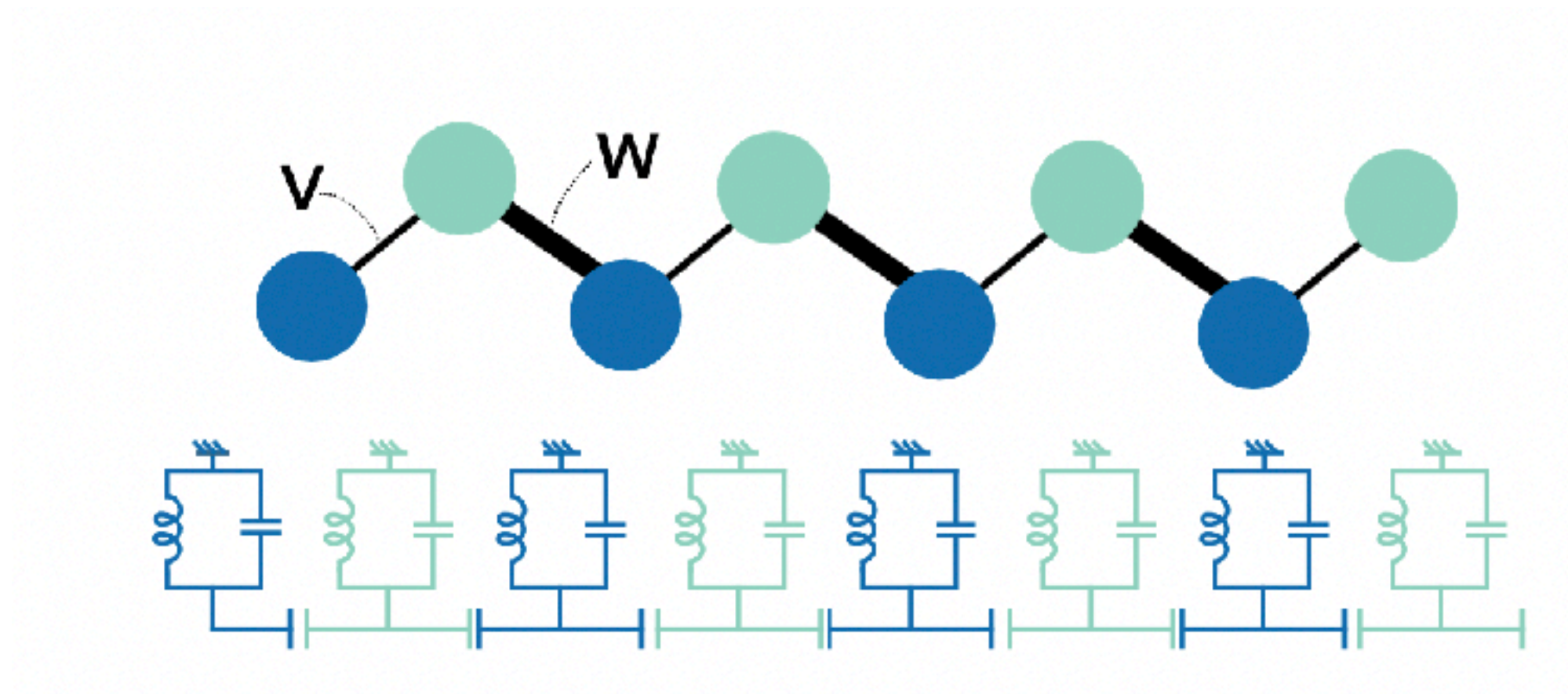


arXiv:2102.04883

ML applied on topological SSH states

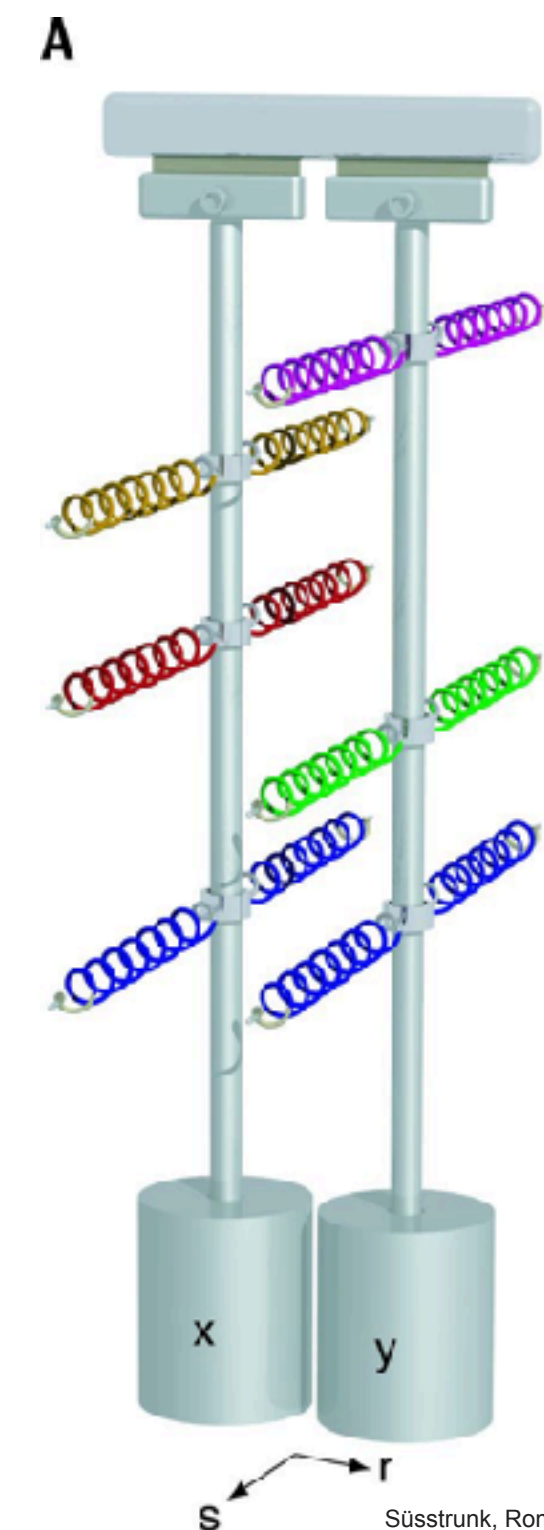
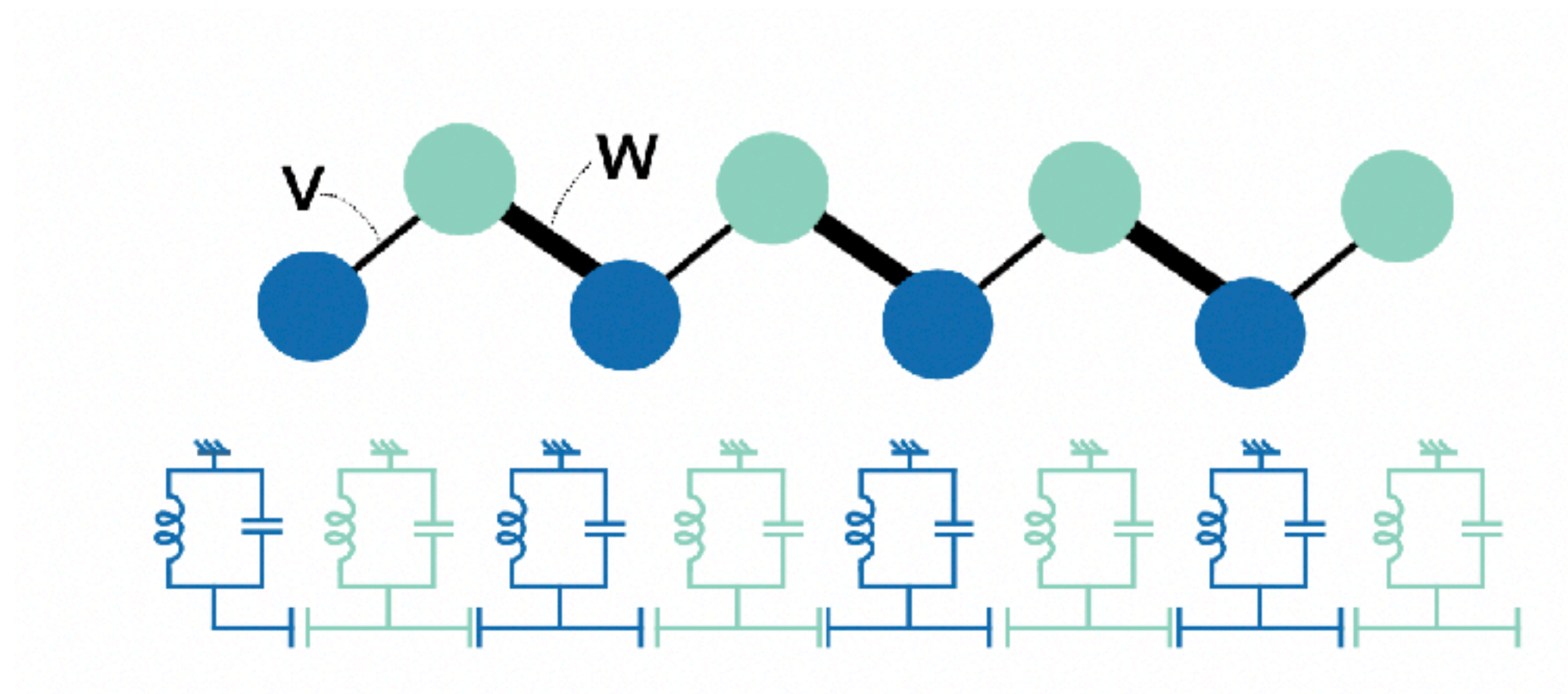


# SSH model with superconducting resonators



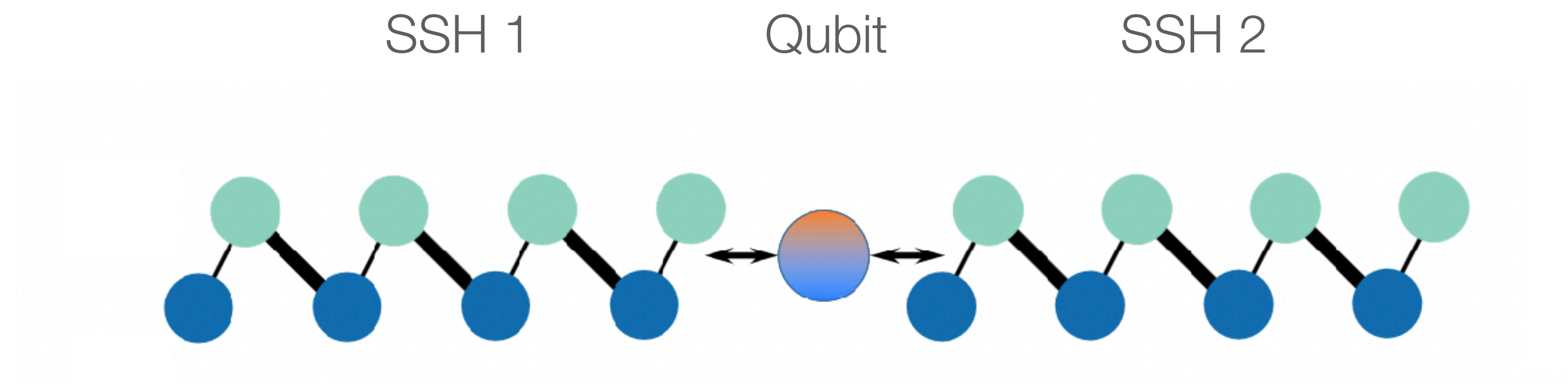


# Can we explore intrinsically quantum features?

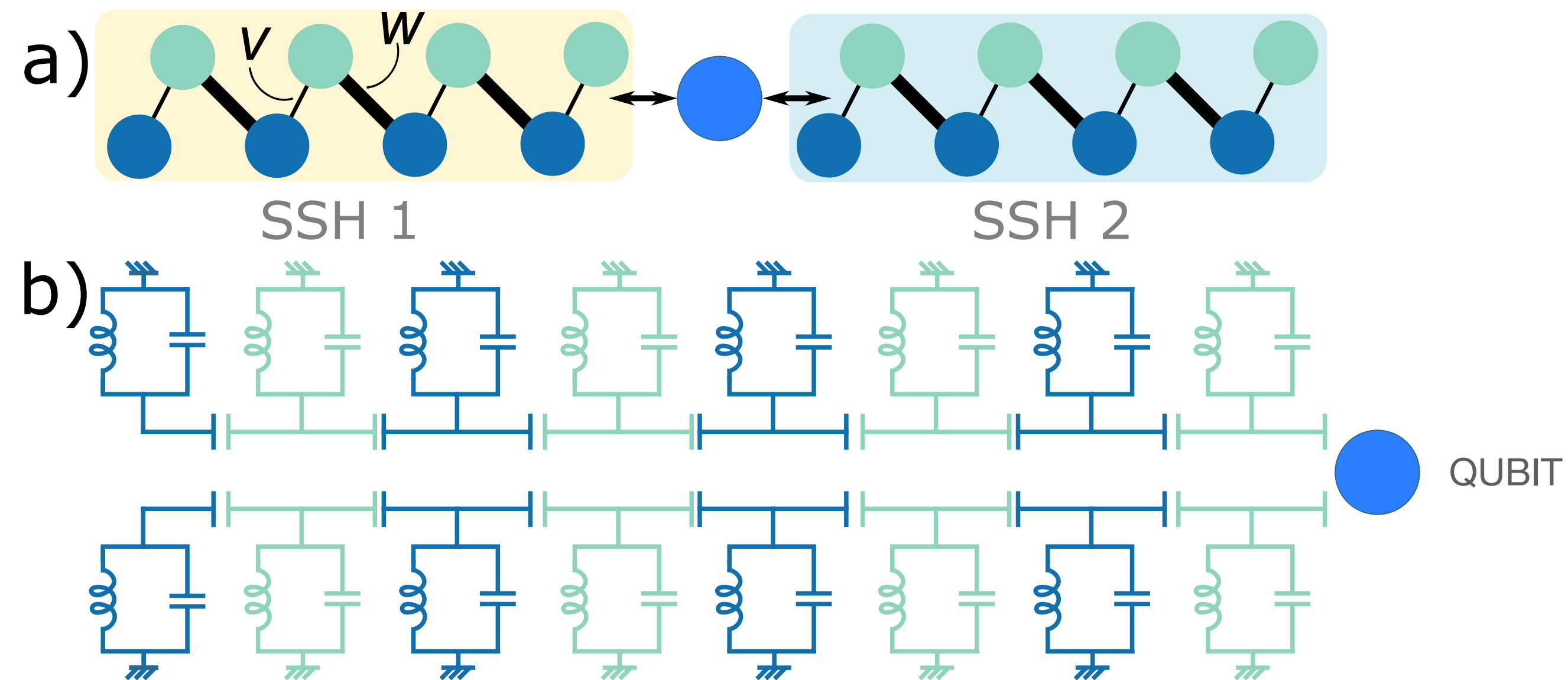


Süsstrunk, Roman, and Sebastian D. Huber. "Observation of phononic helical edge states in a mechanical topological insulator." *Science* 349.6243 (2015): 47-50.

# Generating entanglement of the topological modes



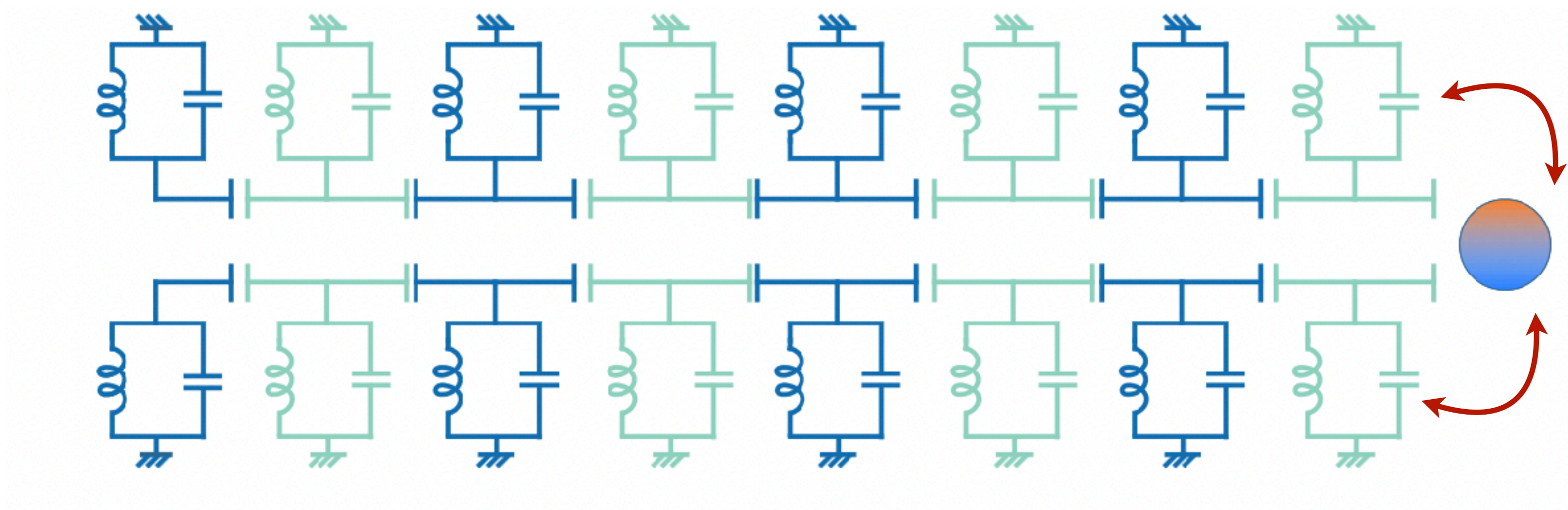
# Generating entanglement of the topological modes





# Entangling topo modes: Protocol

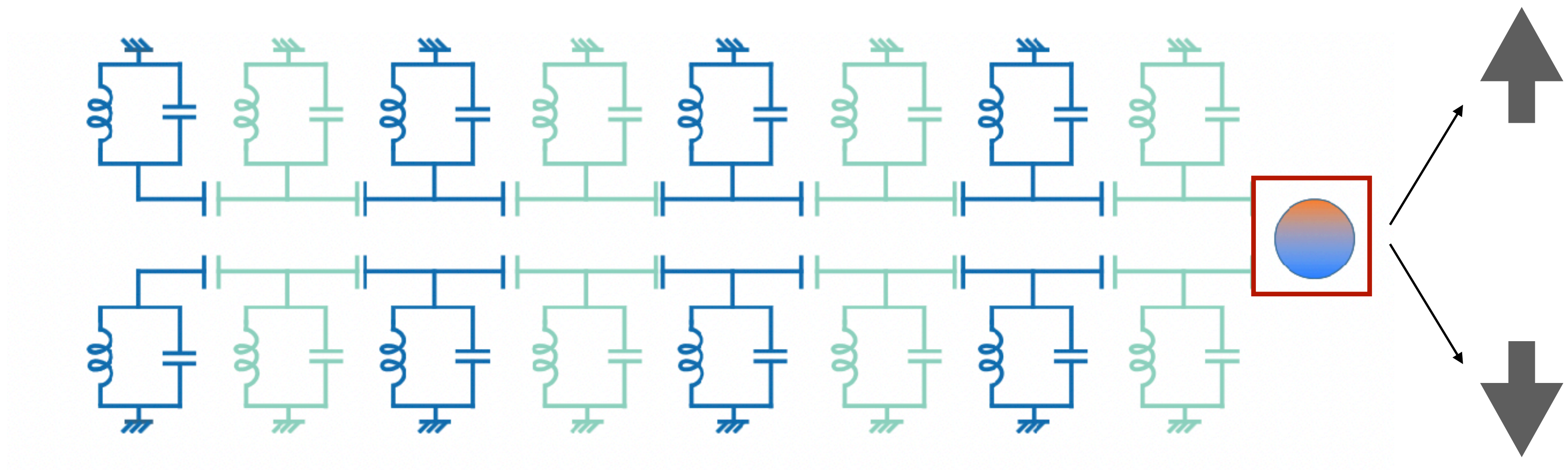
## Step 1: Couple





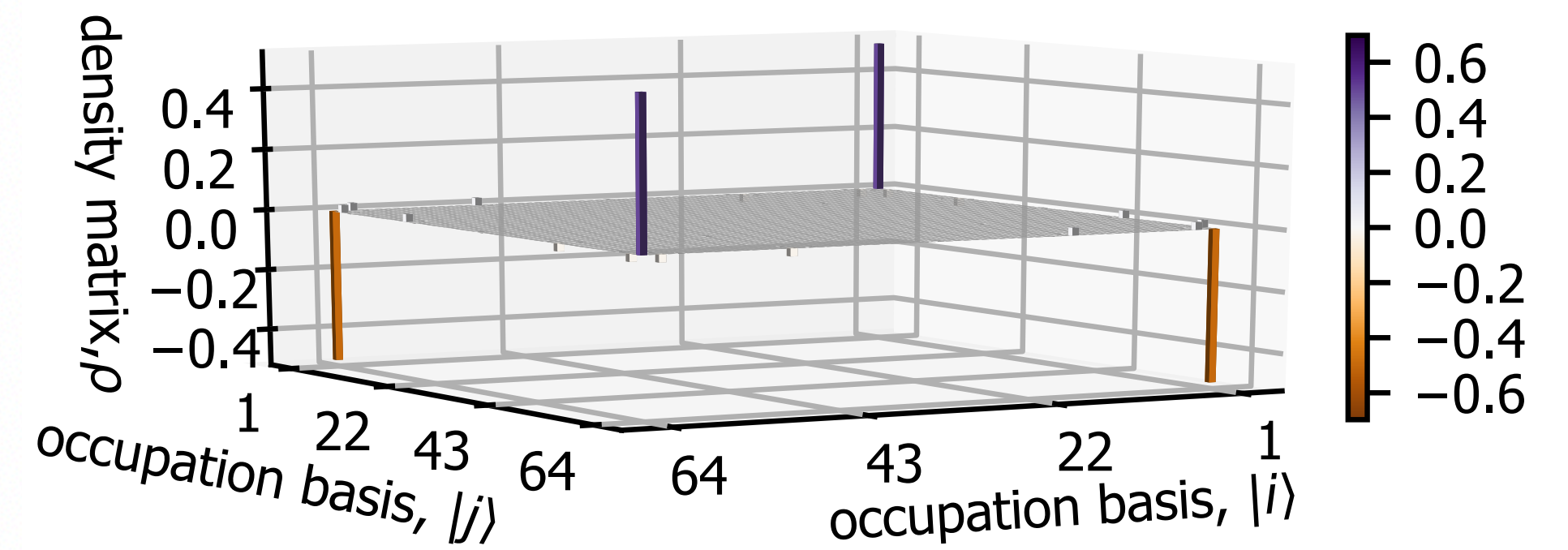
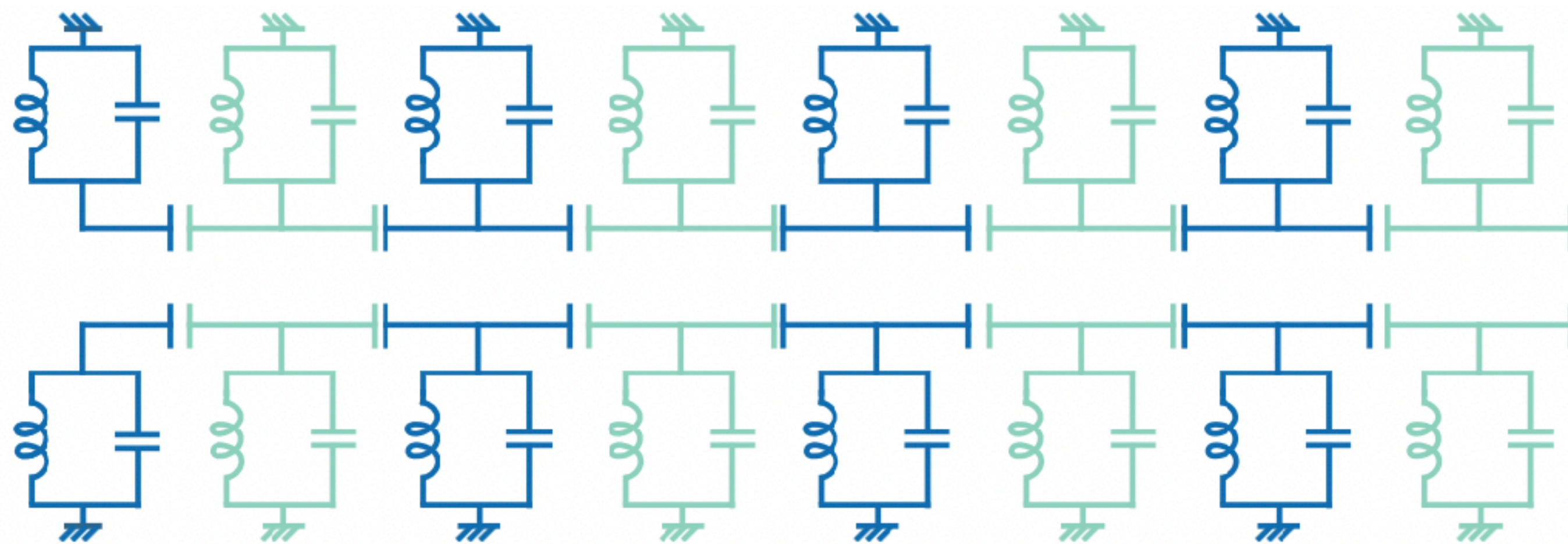
# Entangling topo modes: Protocol

## Step 2: Measure Qubit



# Entangling topo modes: Protocol

## Step 3: Maximally entangled state

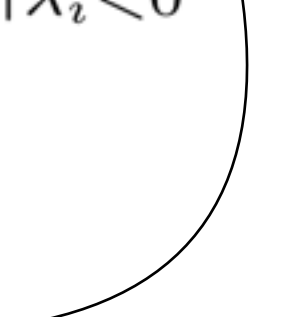


# Does topology help with the entanglement stability?

Entanglement Measure: Negativity

$$\mathcal{N}(\rho) = \left| \sum_{\lambda_i < 0} \lambda_i \right| = \sum_i \frac{|\lambda_i| - \lambda_i}{2},$$

Eigenvalues of the partially  
transposed density matrix



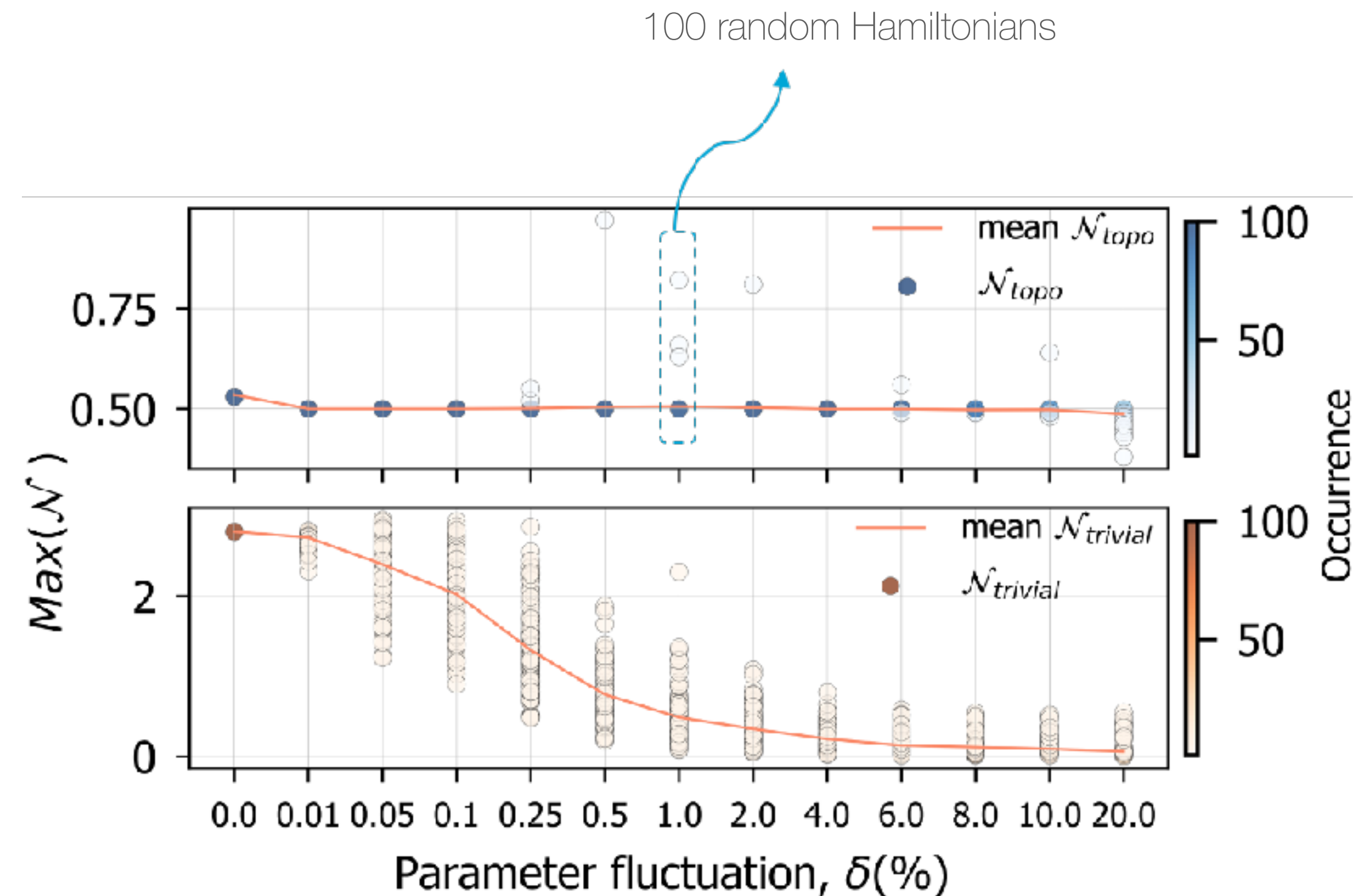


# Does topology help with the entanglement stability?

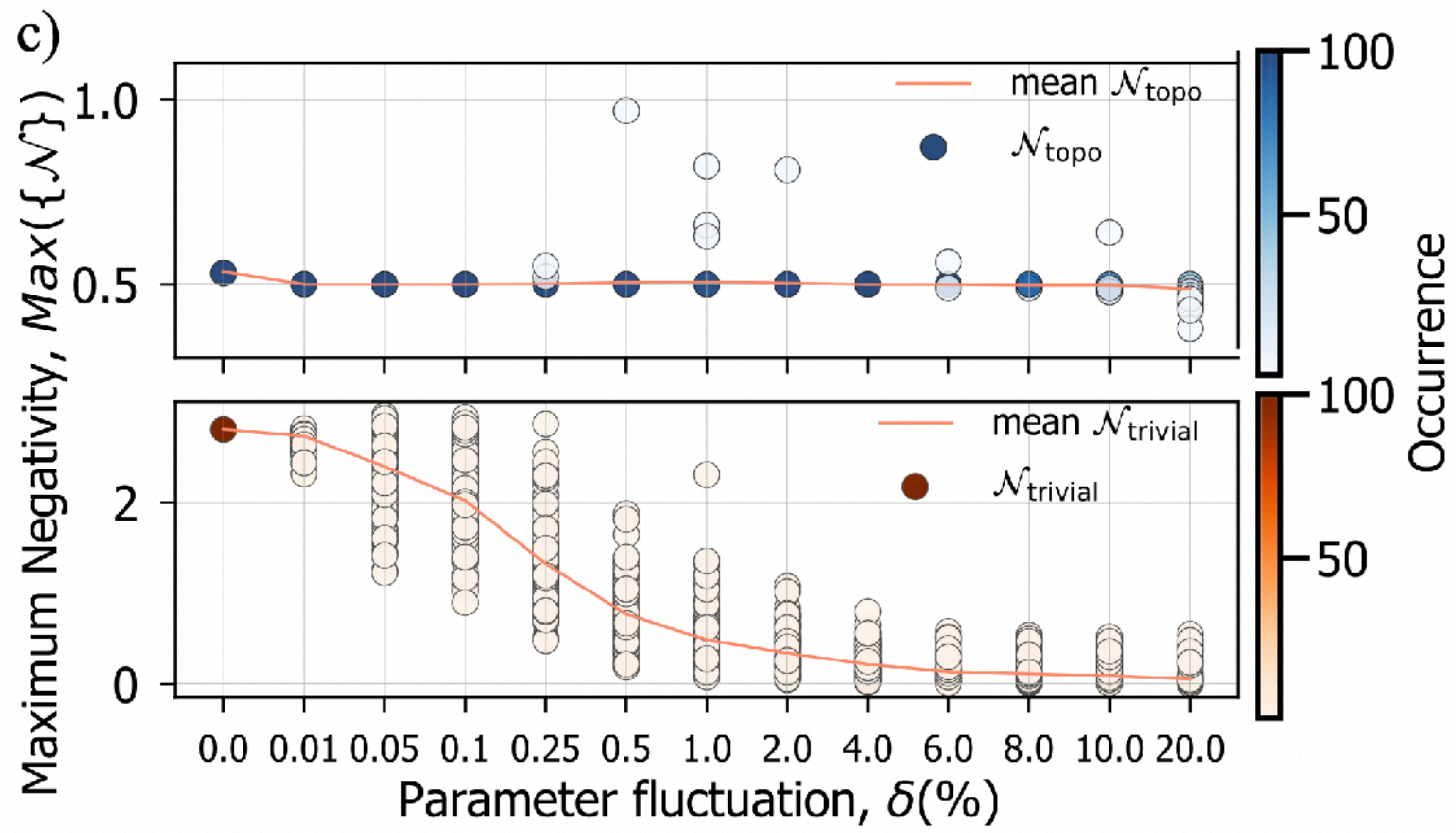
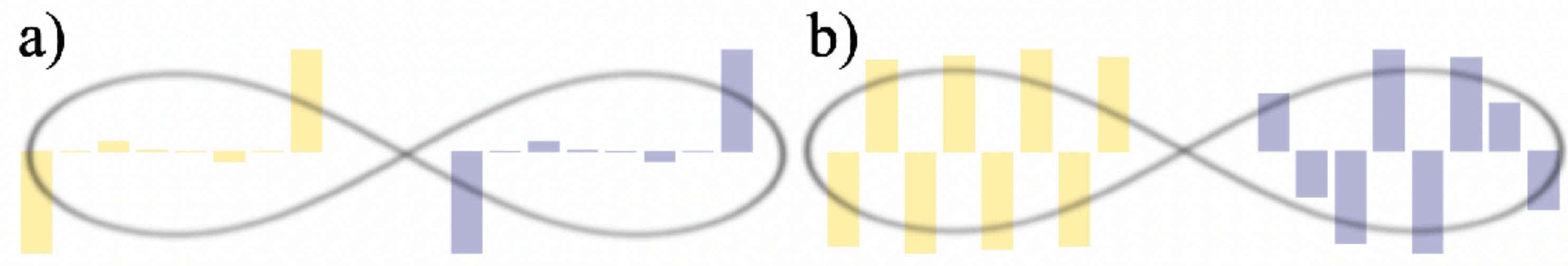
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Eigenvalues of the partially transposed density matrix

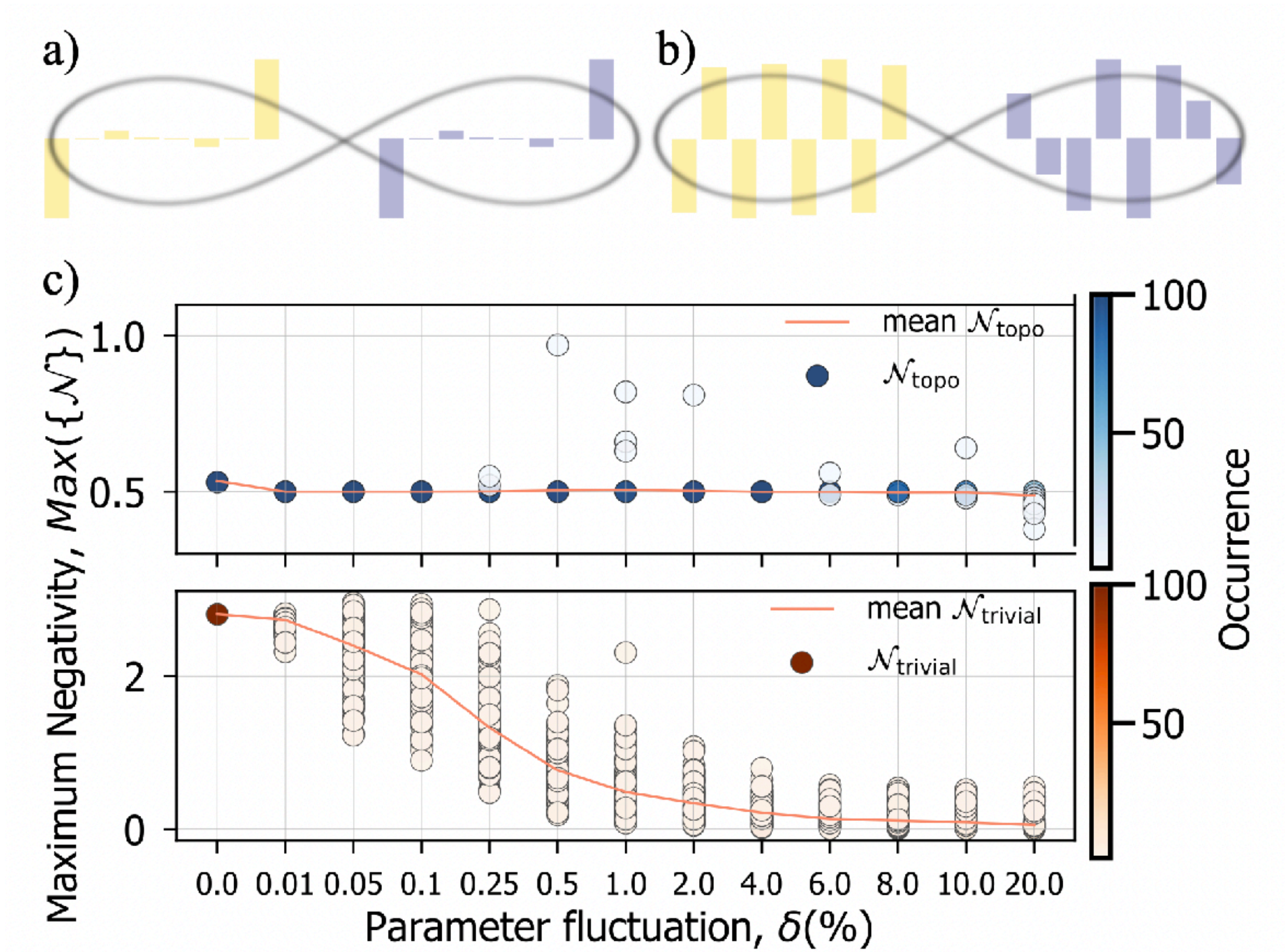
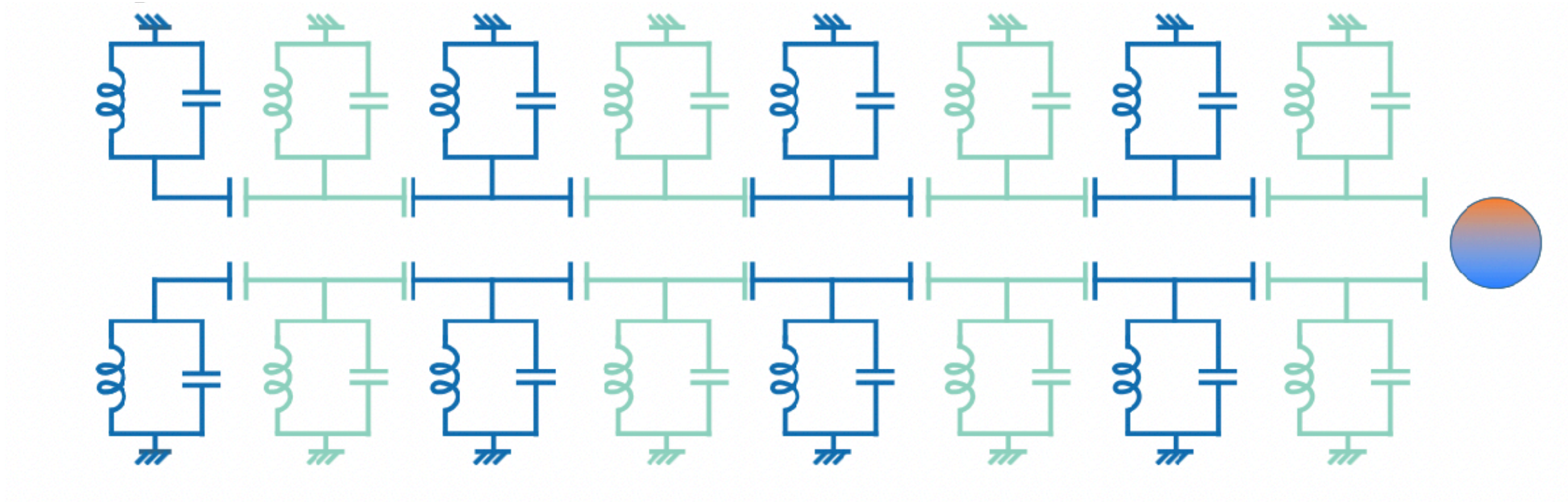


● topological  
● trivial





Simple topological model + on-chip engineering =  
practical entanglement stabilization



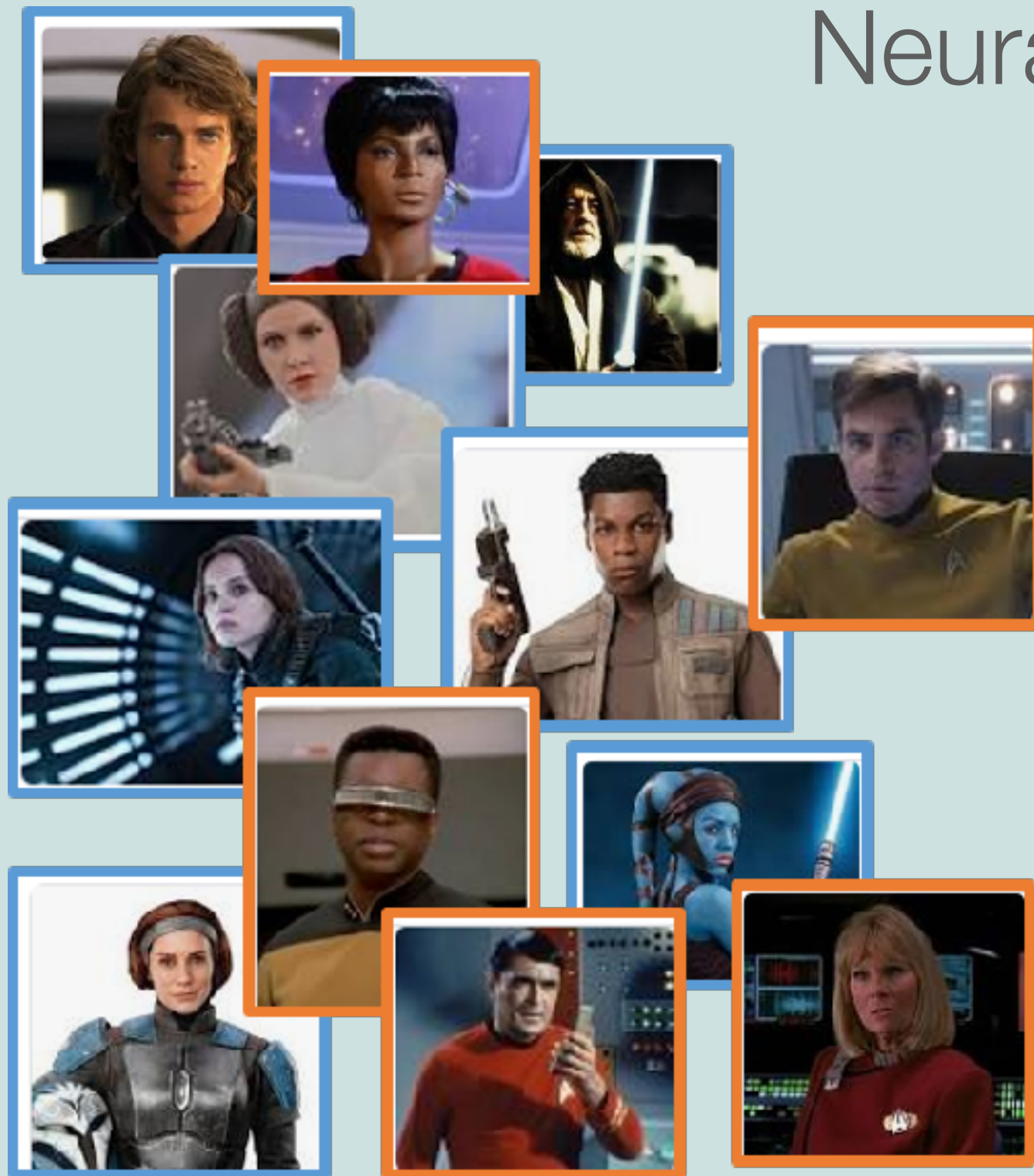


BREAK 10 mins



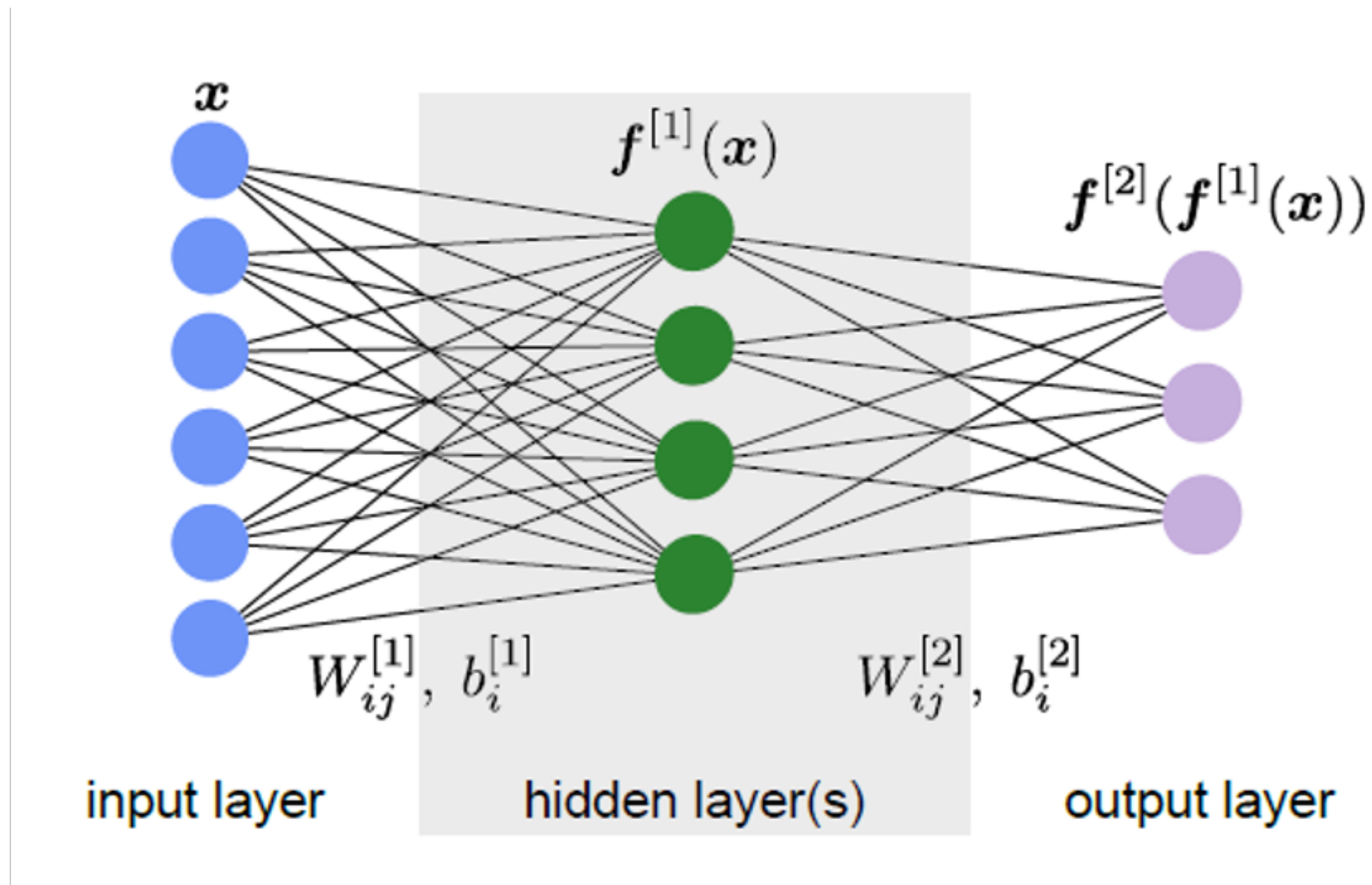


## Machine Learning Primer: Neural Network Introduction

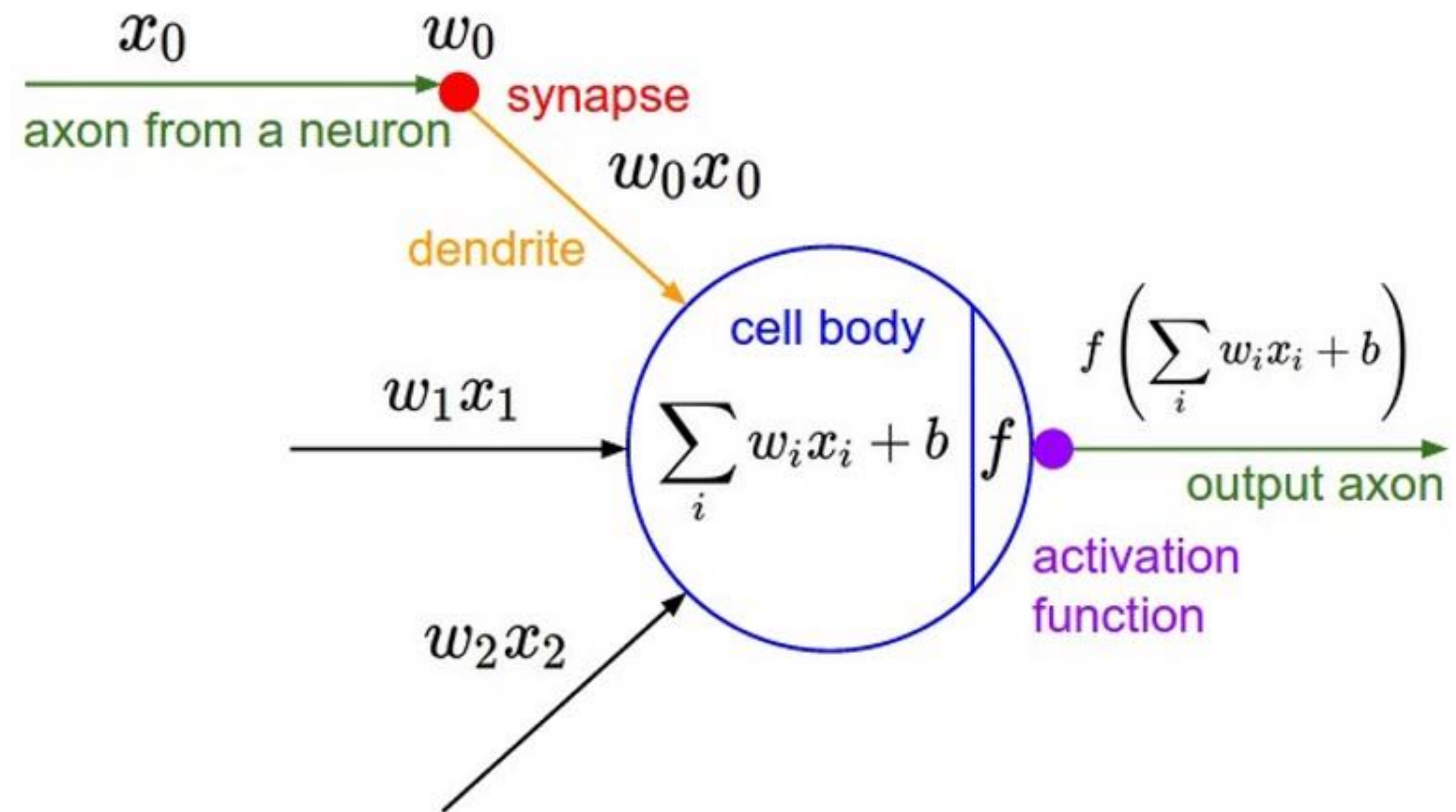


$$\frac{dL(f^{[2]})}{dW_{ij}^{[1]}} = \frac{dL}{df^{[2]}} \frac{df^{[2]}}{df^{[1]}} \frac{df^{[1]}}{dW^{[1]}}$$

# Neural Networks 101: Supervised learning

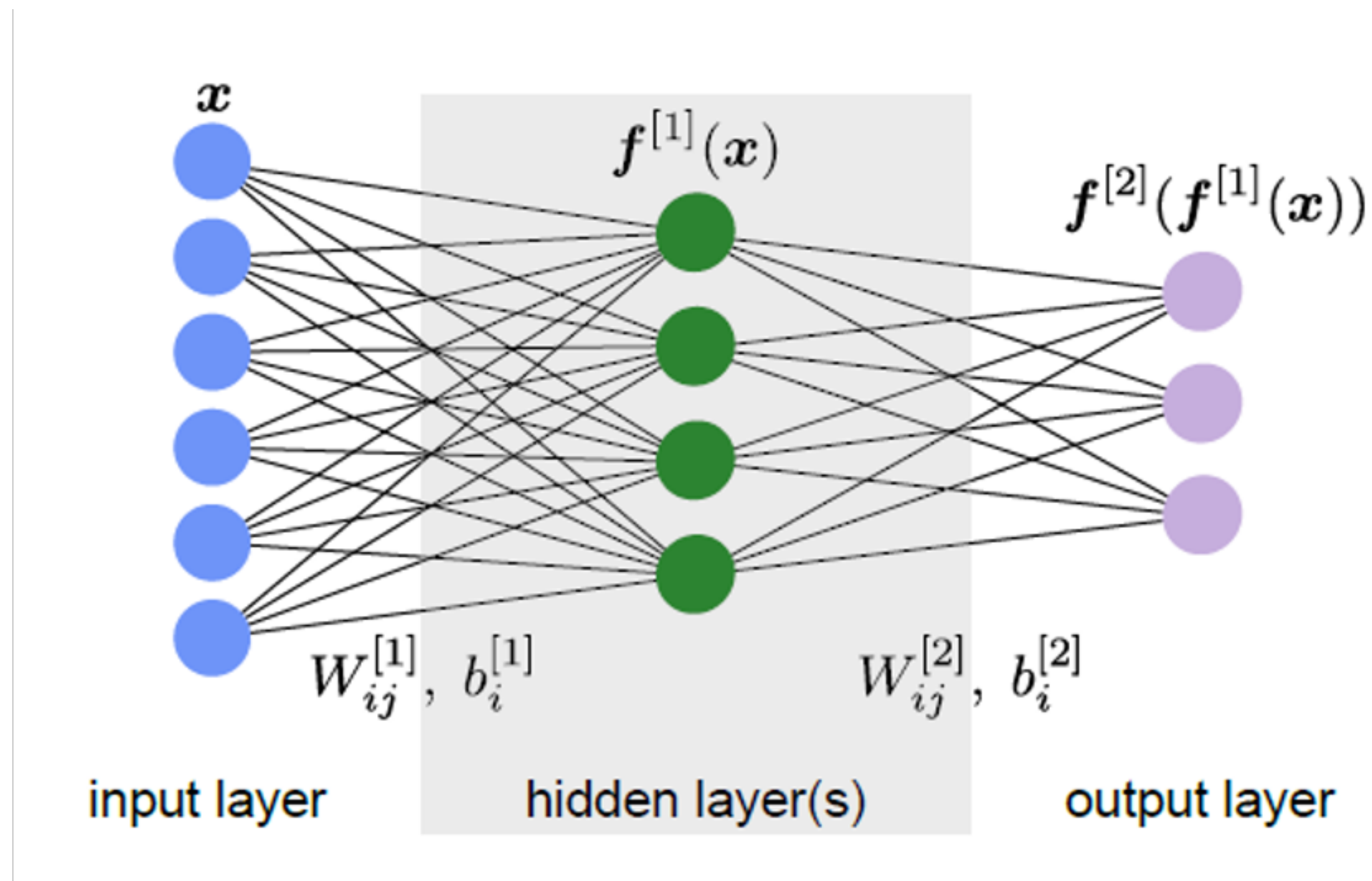


# What happens in a neuron?

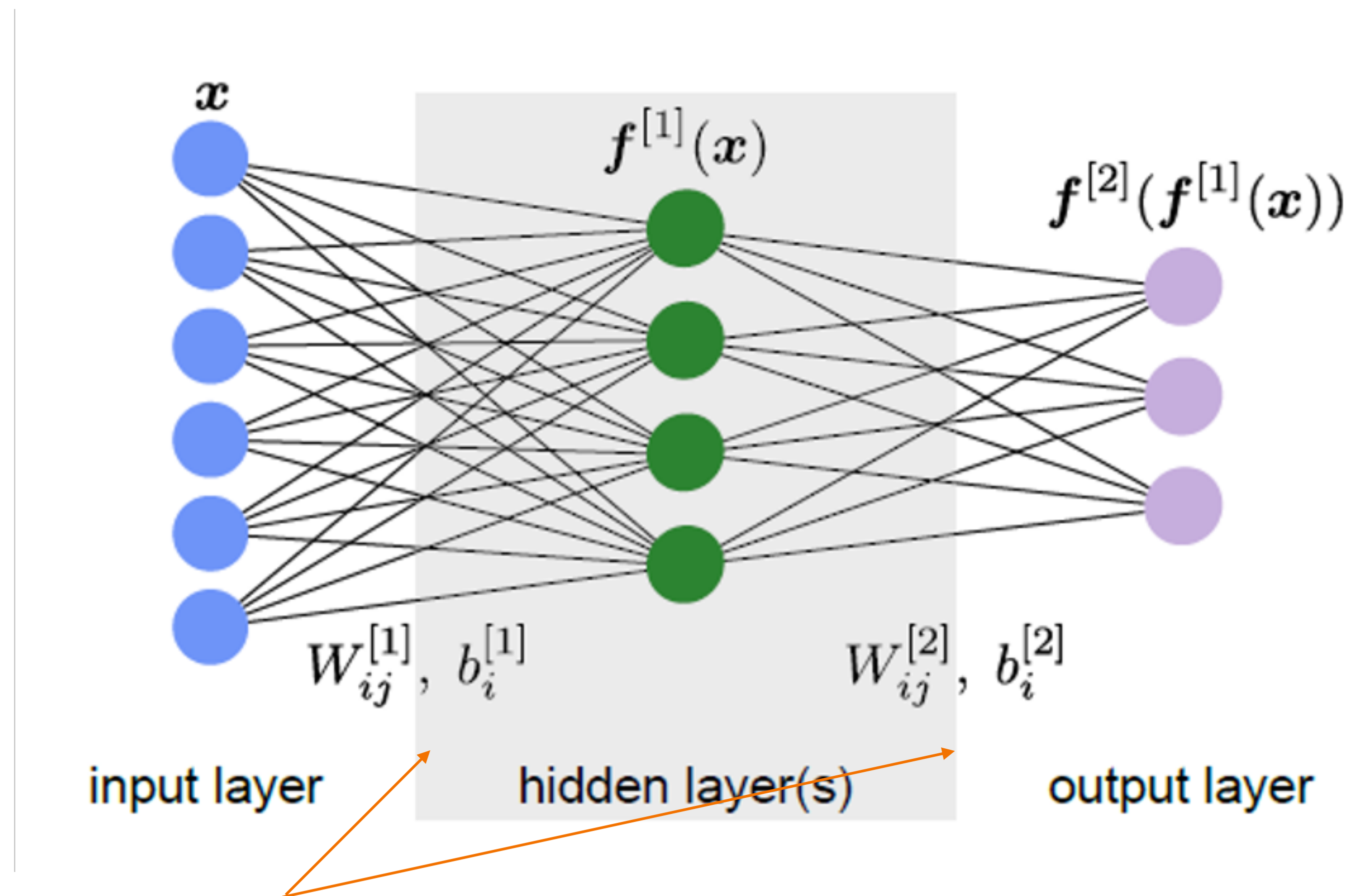




# Putting neurons in the networks

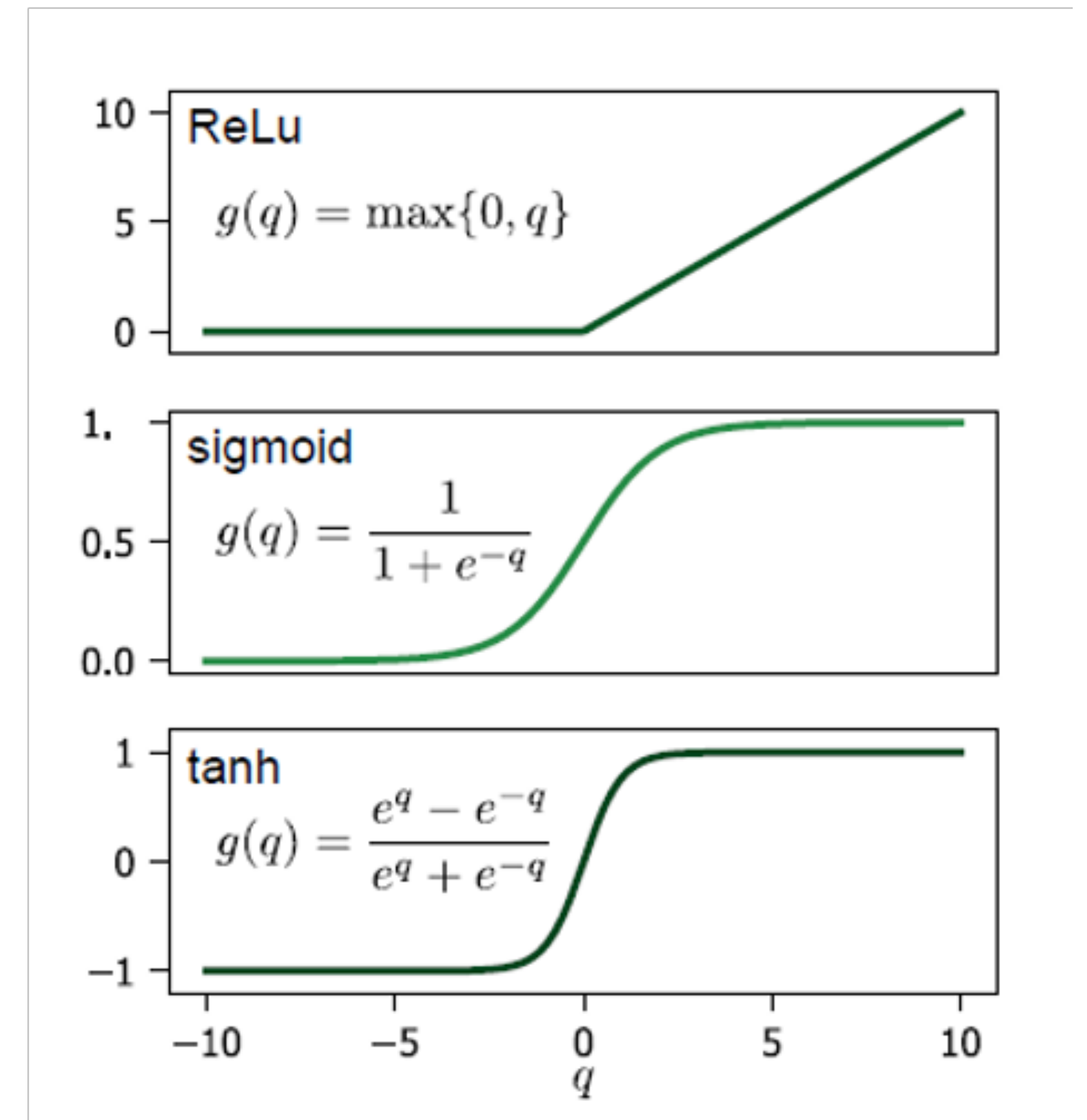
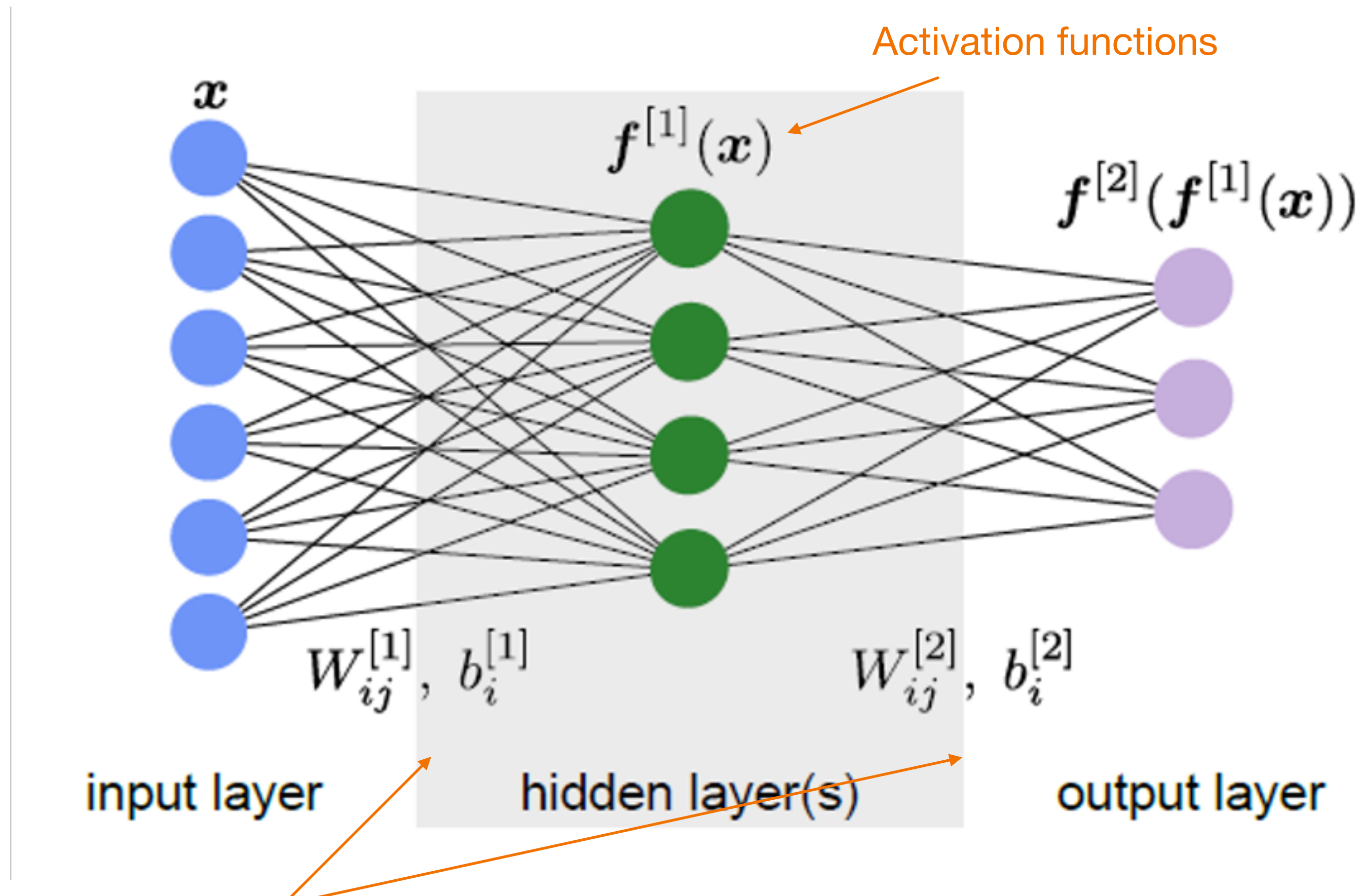


# Putting neurons in the networks



Weights (can be represented as matrices)

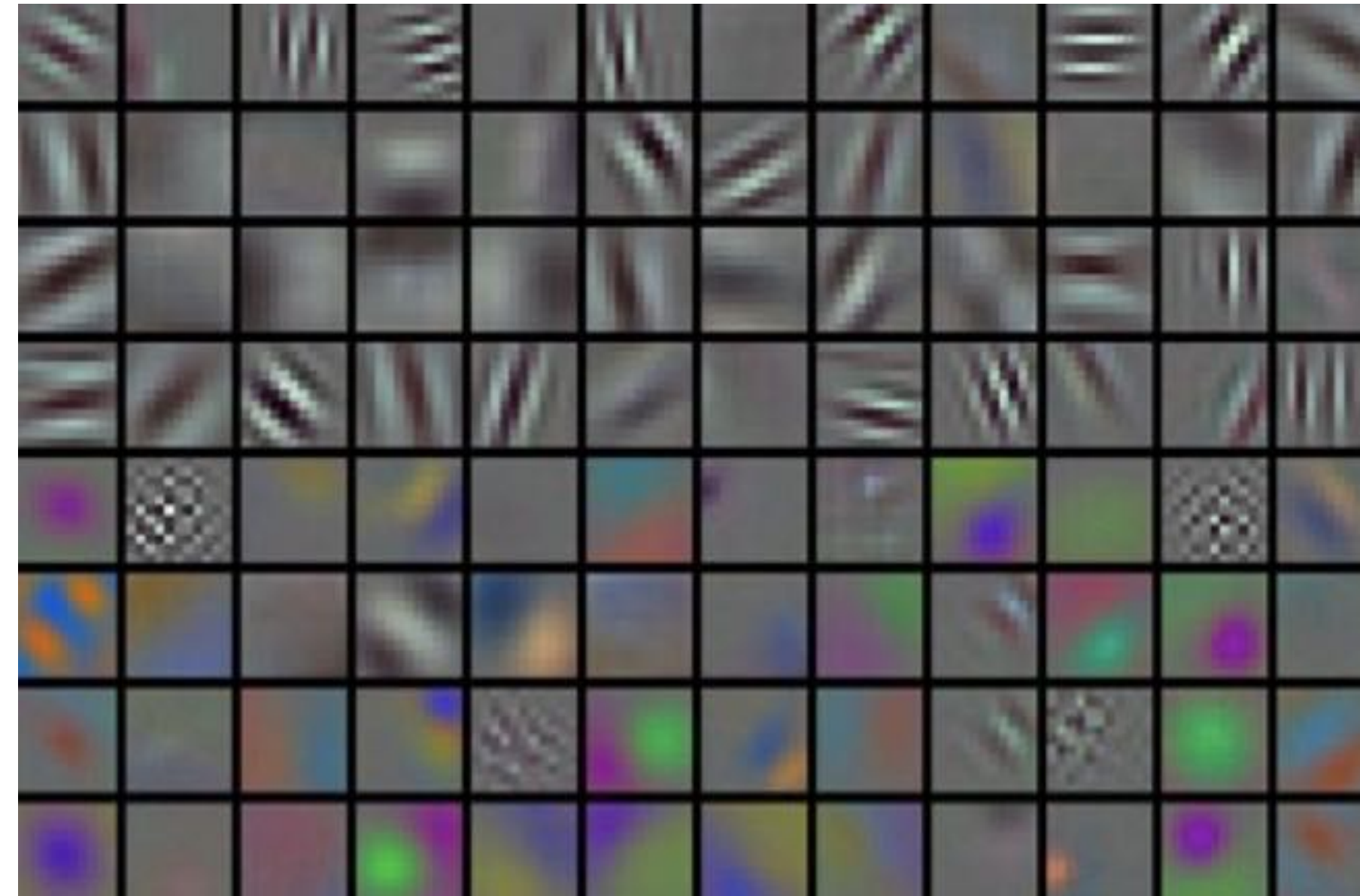
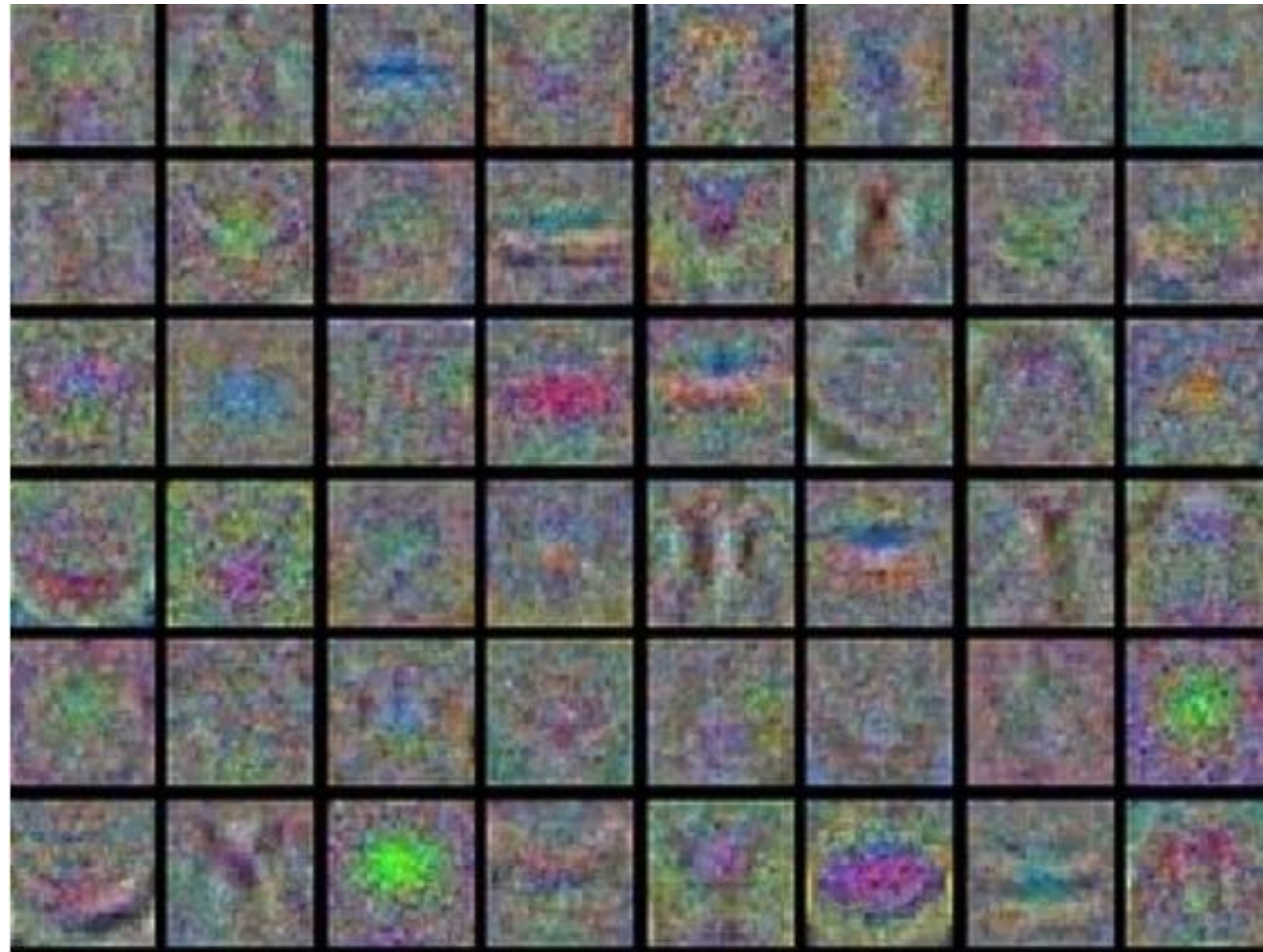
# Putting neurons in the networks



Weights (can be represented as matrices)



# How do the weights look like?



Weight matrices from a image recognition network:

- Left: badly trained network – the weights look noisy
- Right: well trained network – the weights clearly extract specific features in the data



# How do we train neural network?

- Define the loss function  $L(x)$  [ $x$  = our data] that we will minimise during training
- Calculate the derivative of  $L$  wrt weights and biases

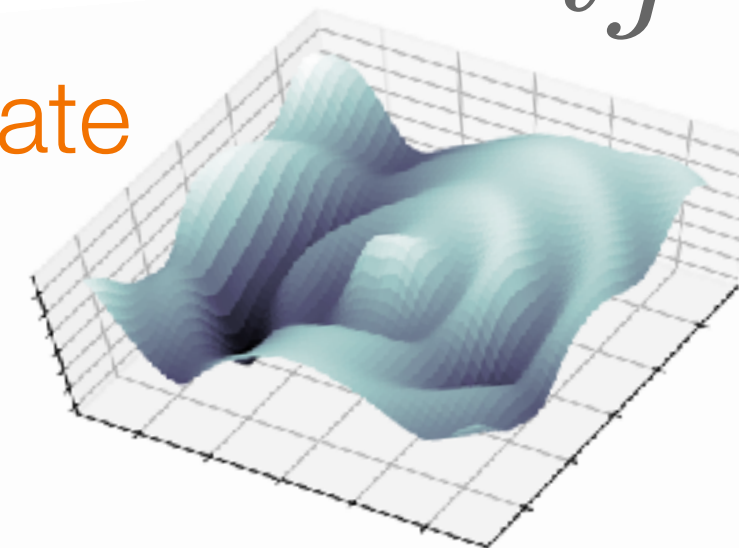
$$W_{ij} \rightarrow W_{ij} - \epsilon \frac{\partial L}{\partial W_{ij}}$$

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$$W_{ij} \rightarrow W_{ij} - \epsilon \frac{\partial L}{\partial W_{ij}}$$

learning rate





# How do we calculate the derivative?

- CHAIN RULE REMINDER:



# How do we calculate the derivative?



- CHAIN RULE REMINDER:

$$f(x) = g(h(x)) \Rightarrow \frac{df}{dx} = \frac{dg}{dh} * \frac{dh}{dx}$$



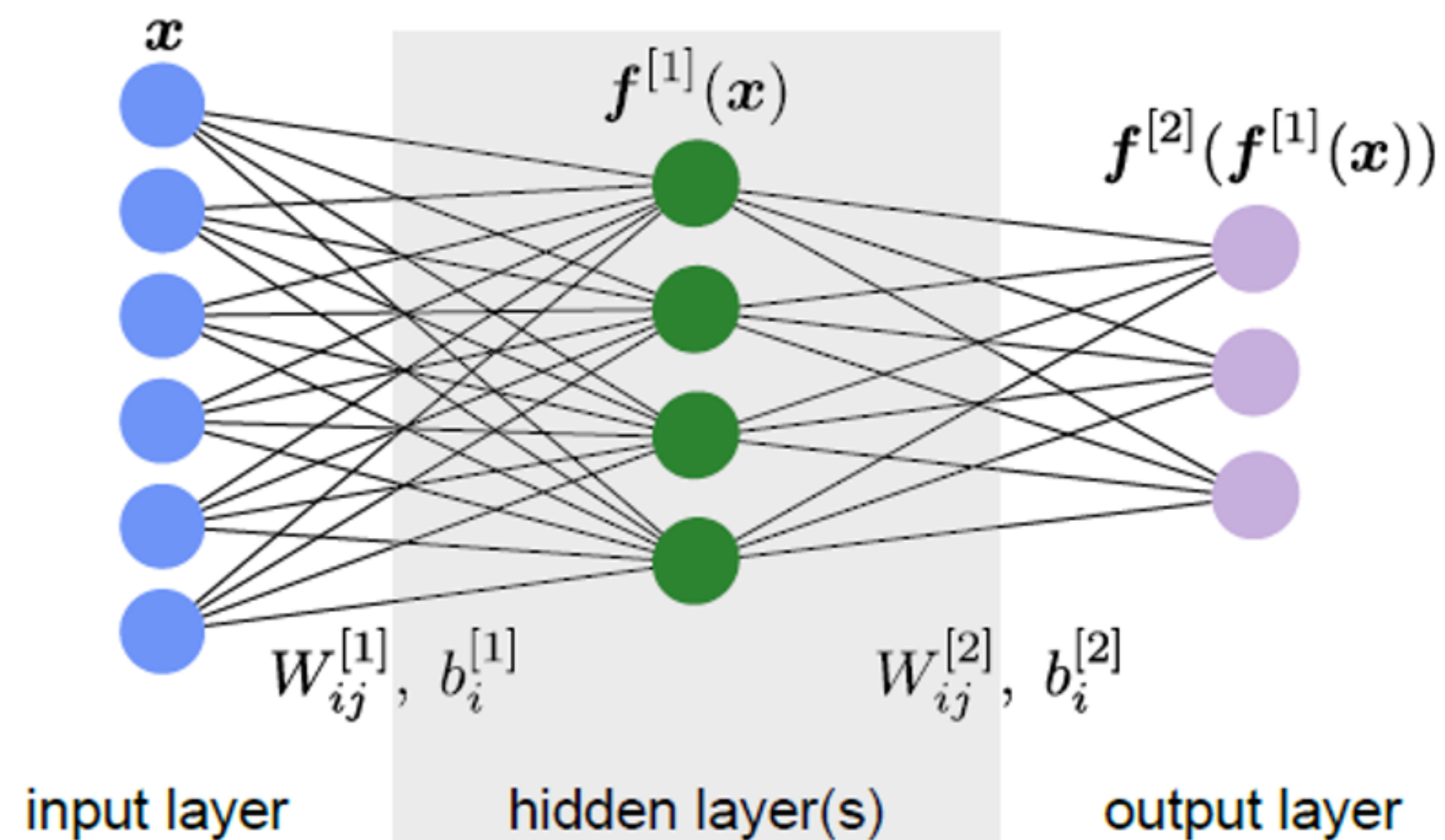
# How do we calculate the derivative?



- CHAIN RULE REMINDER:

$$f(x) = g(h(x)) \Rightarrow \frac{df}{dx} = \frac{dg}{dh} * \frac{dh}{dx}$$

- APPLY TO NEURAL NET:

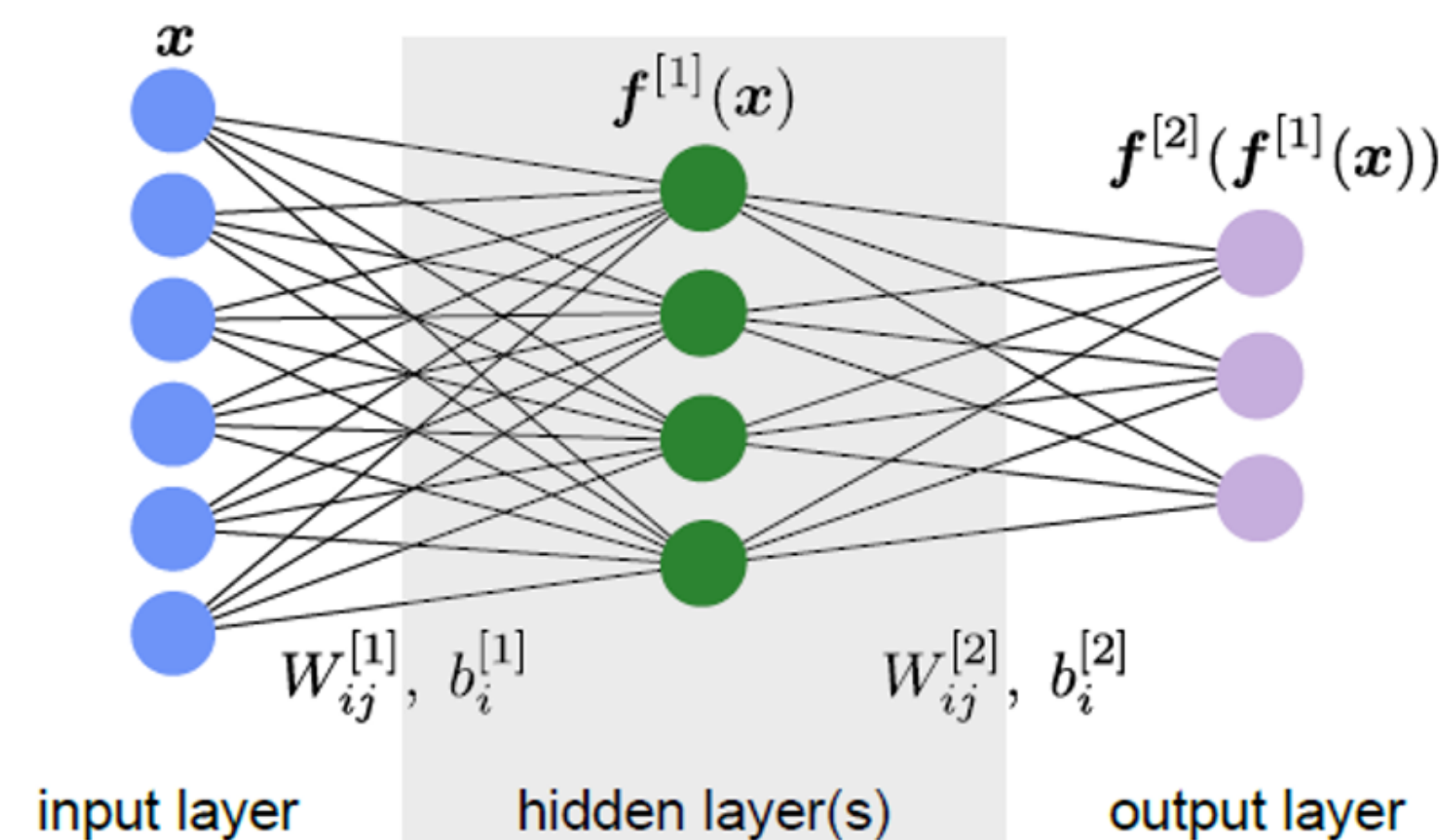


# How do we calculate the derivative?



$$\frac{dL(f^{[2]})}{dW_{ij}^{[1]}} = \frac{dL}{df^{[2]}} \frac{df^{[2]}}{df^{[1]}} \frac{df^{[1]}}{dW^{[1]}}$$

- APPLY TO NEURAL NET:





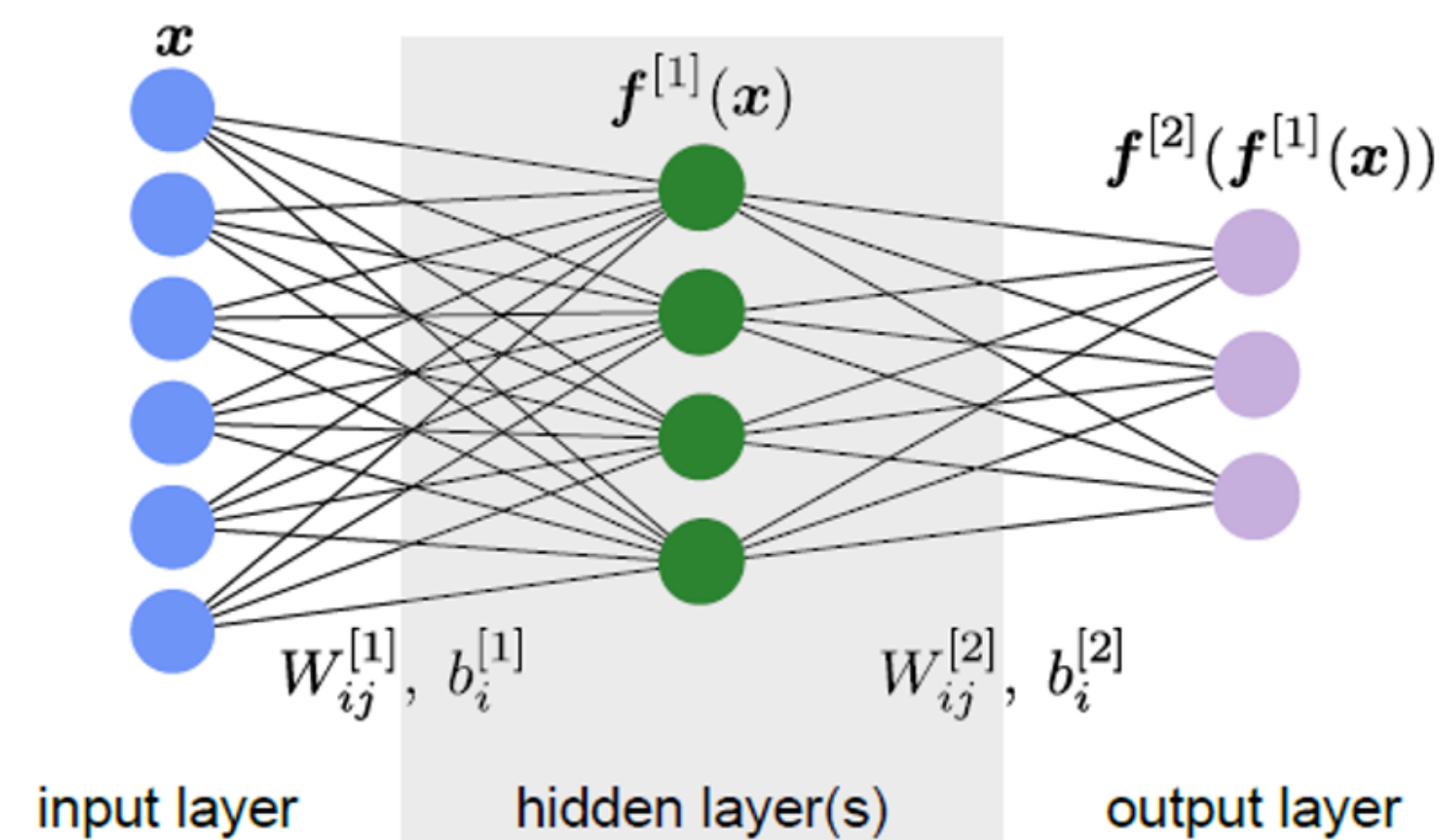
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$$\frac{dL(f^{[2]})}{dW_{ij}^{[1]}} = \frac{dL}{df^{[2]}} \frac{df^{[2]}}{df^{[1]}} \frac{df^{[1]}}{dW^{[1]}}$$

First calculate this using  
the network's output

- APPLY TO NEURAL NET:



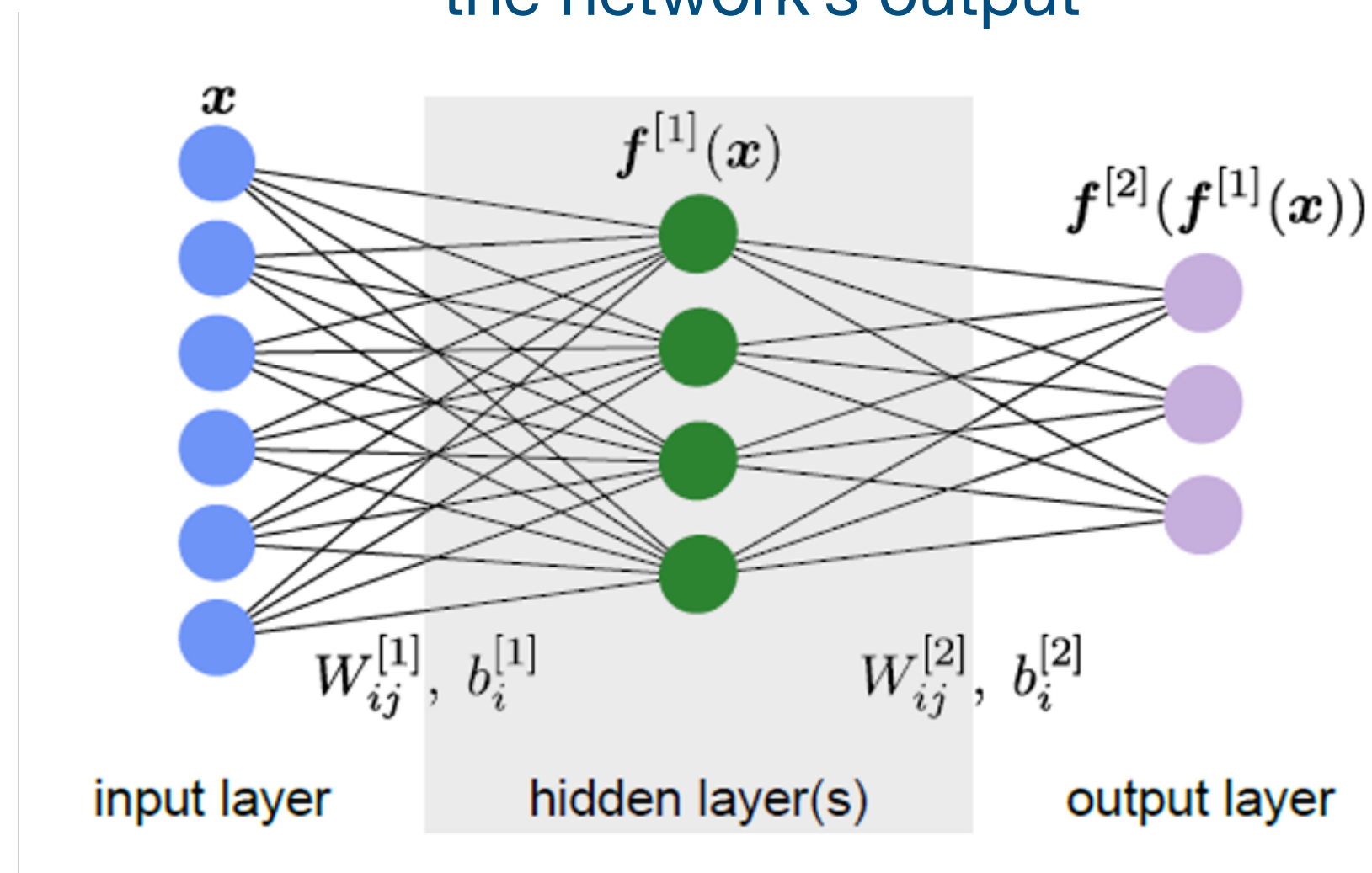
# How do we calculate the derivative?

$$\frac{dL(f^{[2]})}{dW_{ij}^{[1]}} = \frac{dL}{df^{[2]}} \frac{df^{[2]}}{df^{[1]}} \frac{df^{[1]}}{dW^{[1]}}$$

Calculate this using estimate of  $f^{[2]}$  from previous step

First calculate this using the network's output

- APPLY TO NEURAL NET:





# How do we calculate the derivative?

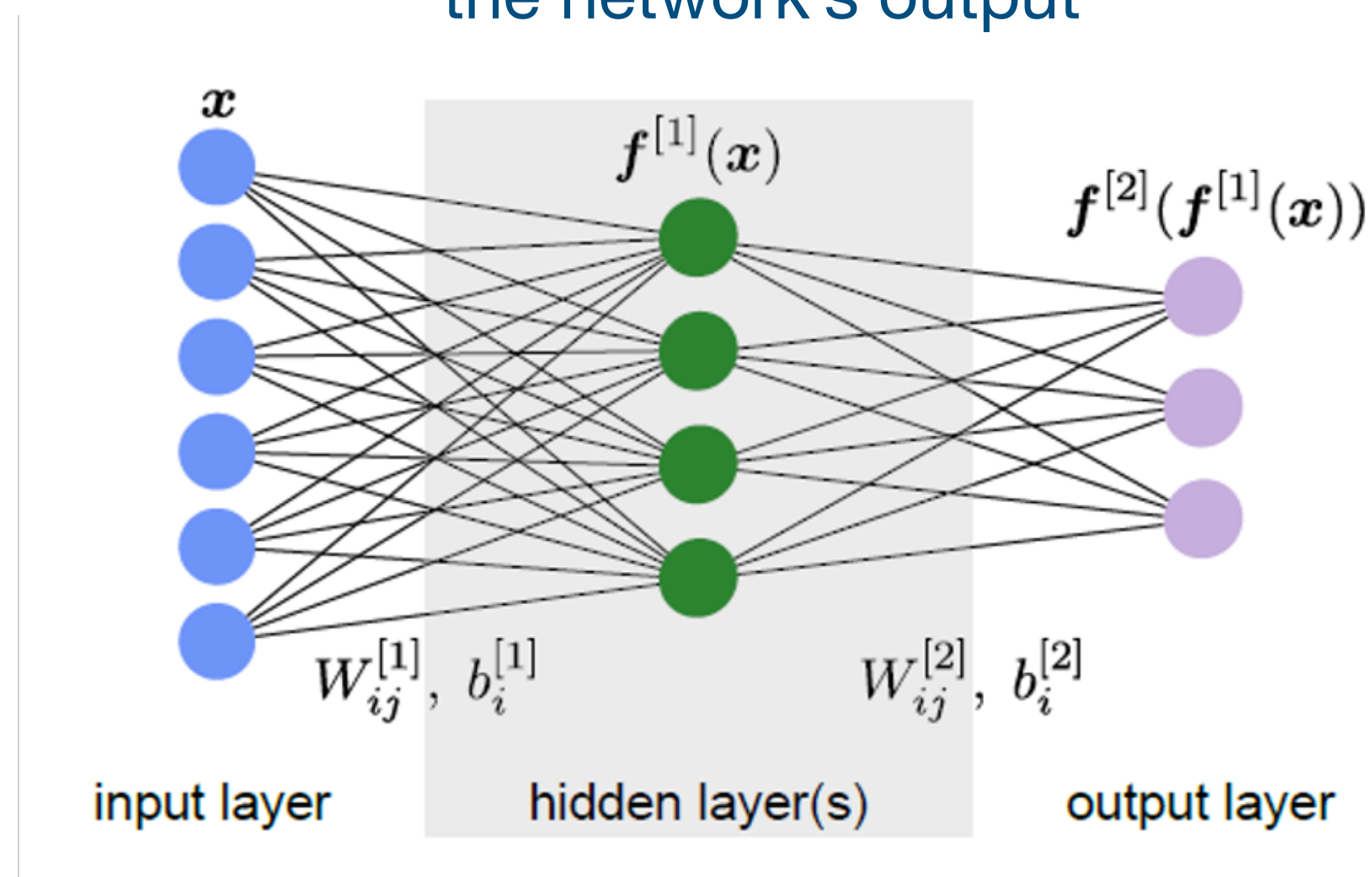
$$\frac{dL(f^{[2]})}{dW_{ij}^{[1]}} = \frac{dL}{df^{[2]}} \frac{df^{[2]}}{df^{[1]}} \frac{df^{[1]}}{dW^{[1]}}$$

Calculate this using estimate of  $f^{[2]}$  from previous step

First calculate this using the network's output

..and so on: we calculate each derivative from the back

- APPLY TO NEURAL NET:



# Backpropagation algorithm



**WHEN EXACTLY DO YOU USE THE CHAIN RULE AGAIN?**



**WHEN THERE'S A FUNCTION WITHIN A FUNCTION, IT'S A TYPE OF ...**

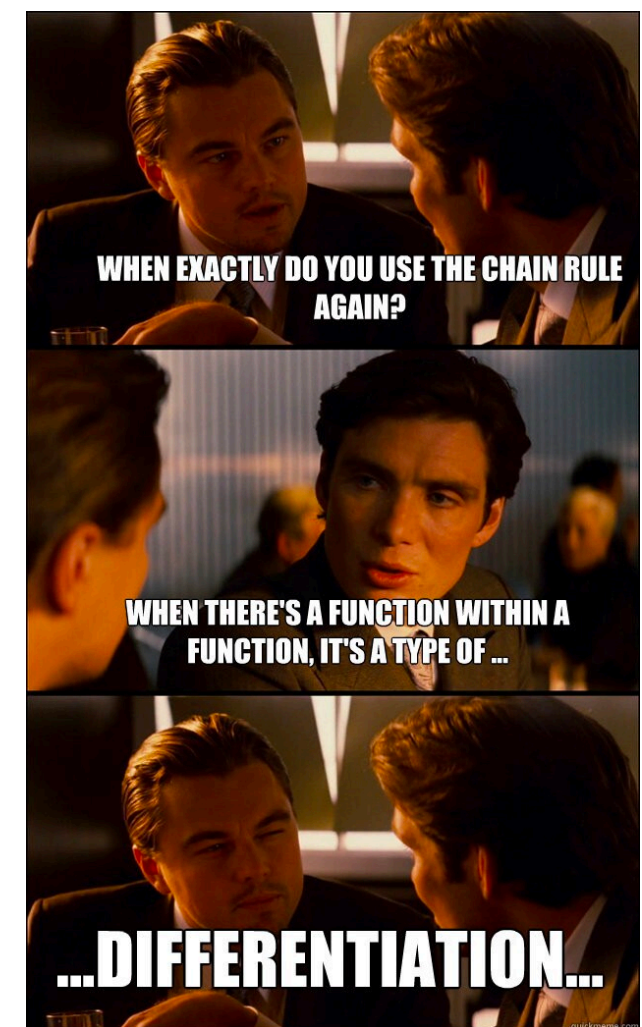
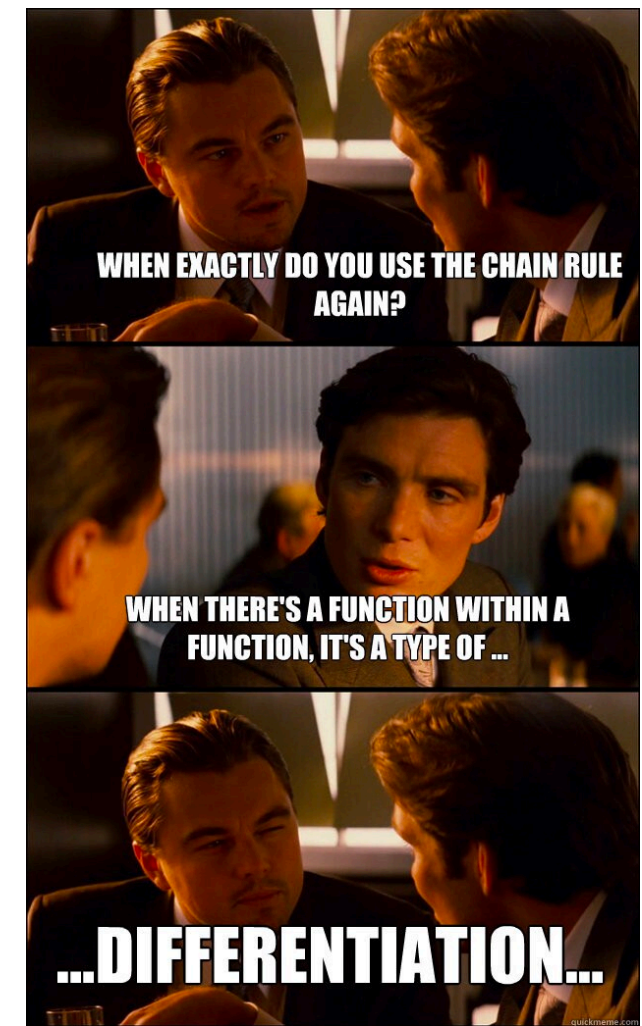
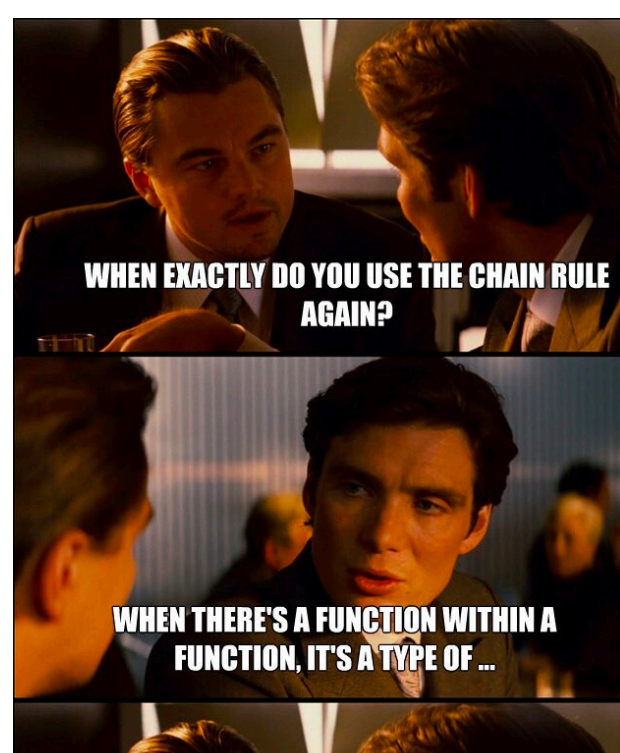
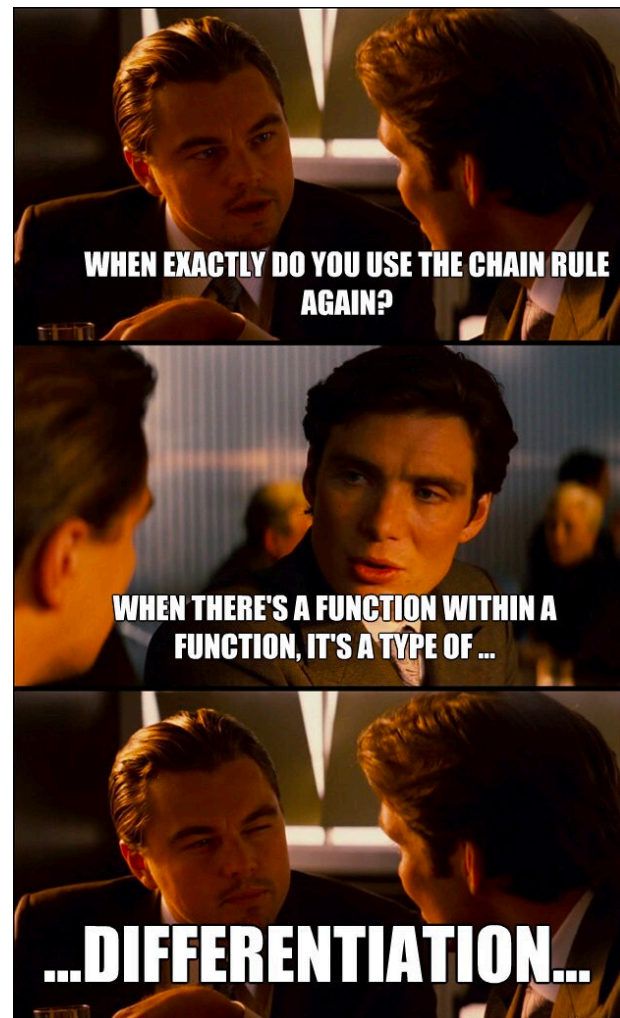
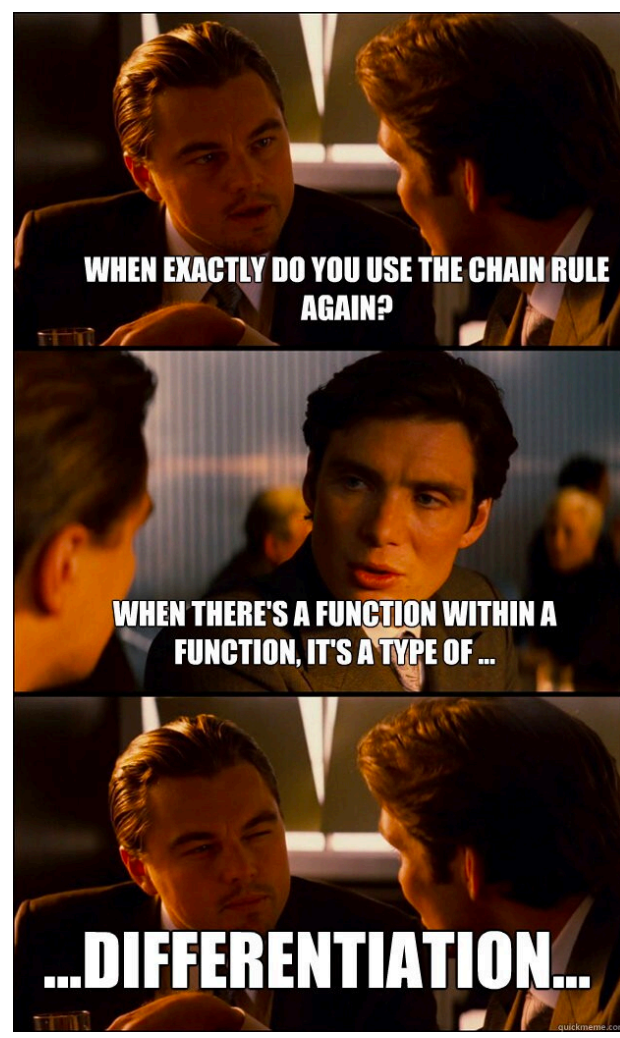


**...DIFFERENTIATION...**



# Backpropagation algorithm

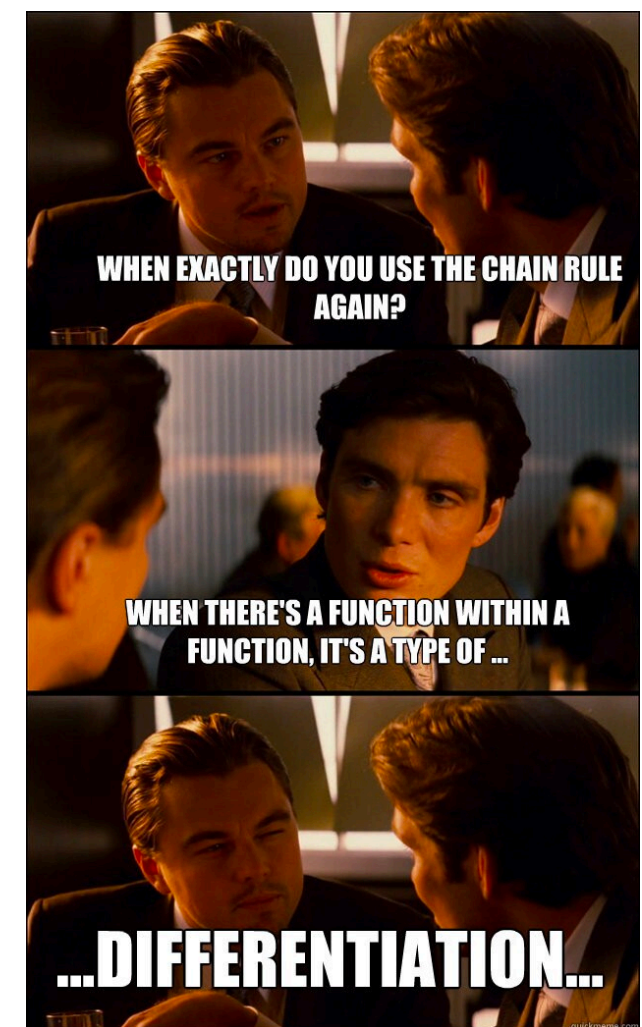
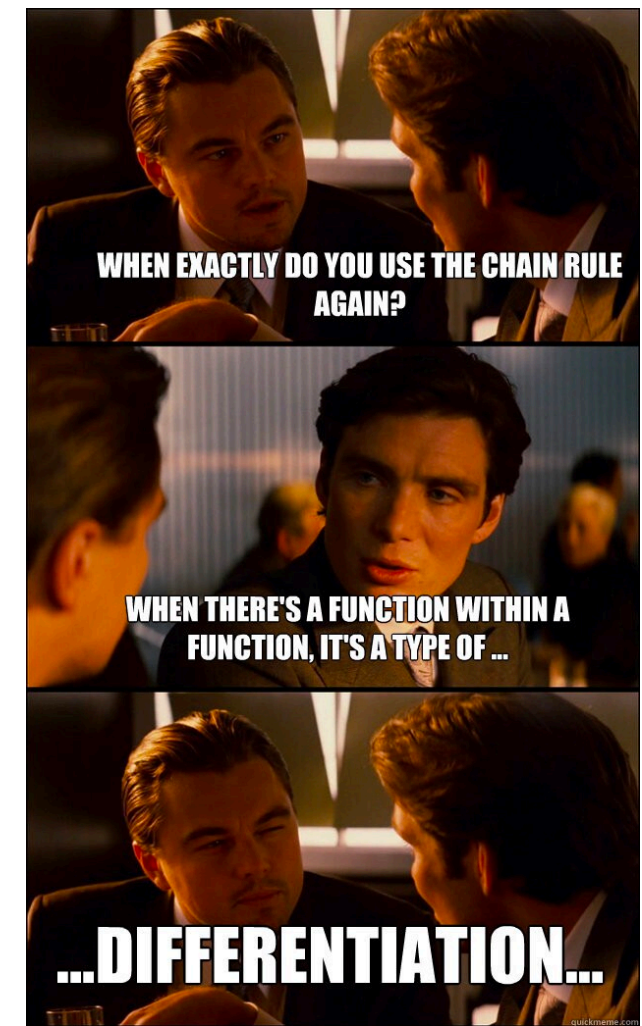
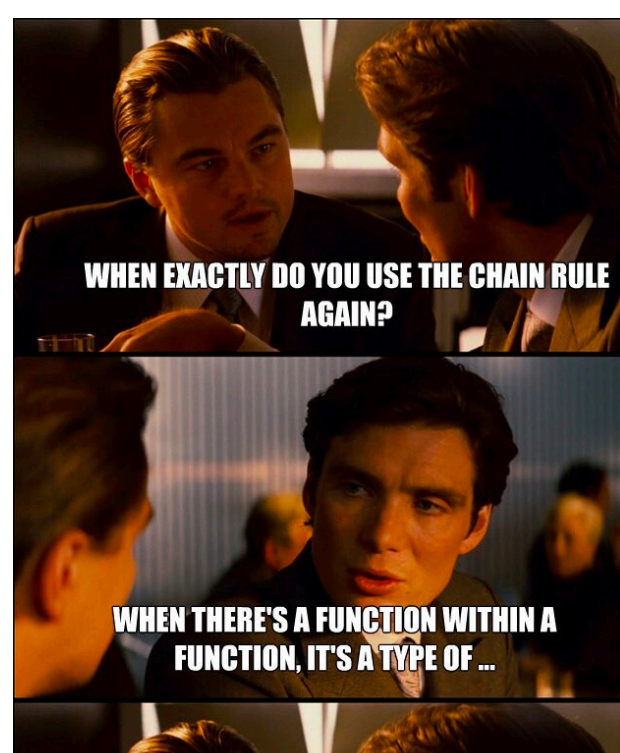
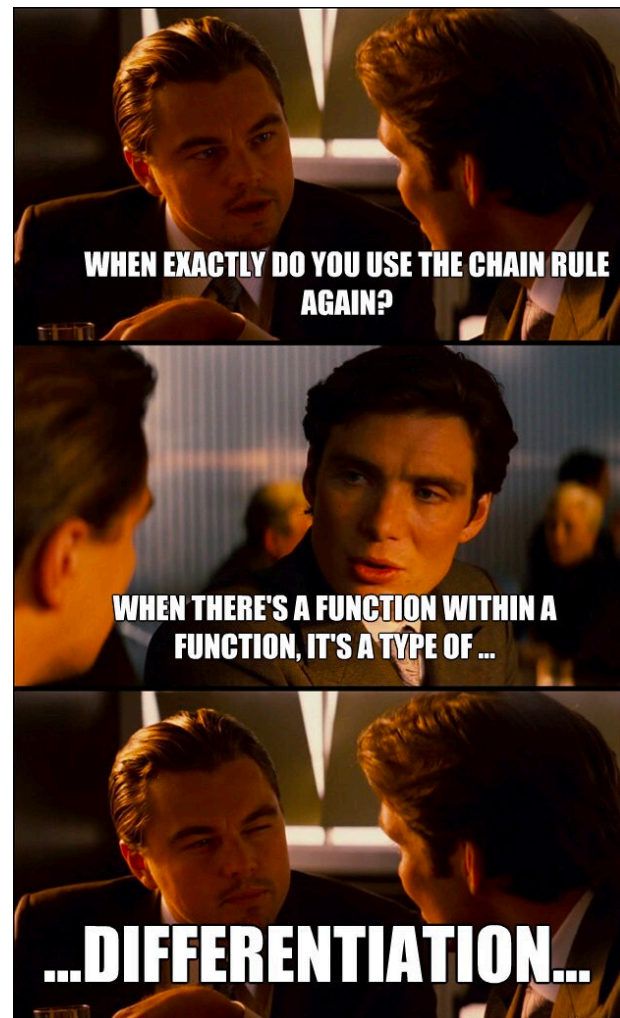
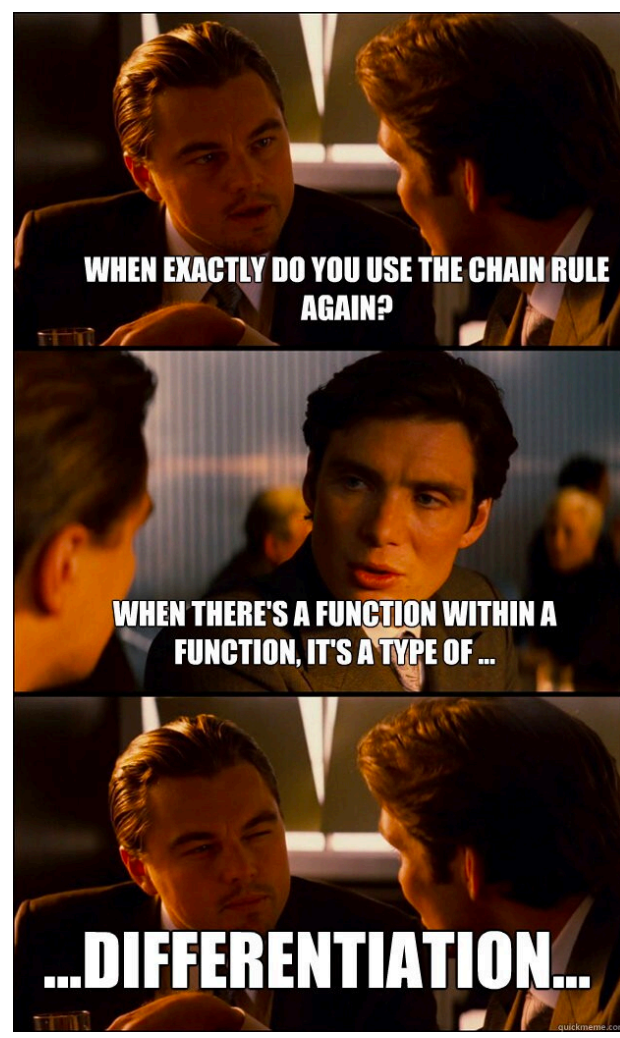
1. Calculate forward propagation of the network
2. Calculate the backward phase
  - a: Estimate the error in the final layer
  - b: Propagate that error into the previous layer
  - c: Evaluate the derivative of each parameter in the network
3. Combine all partial gradients into the final gradient
4. Update the weights using the calculated gradients to minimise the loss





# Backpropagation algorithm

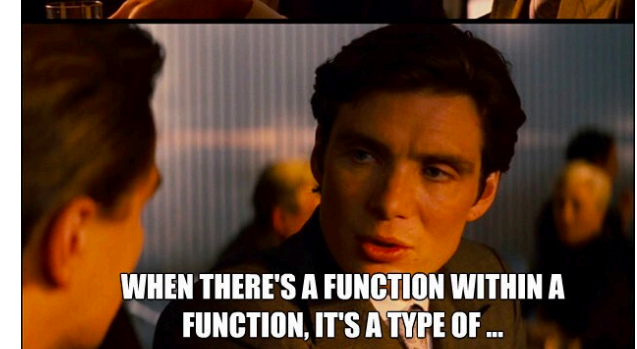
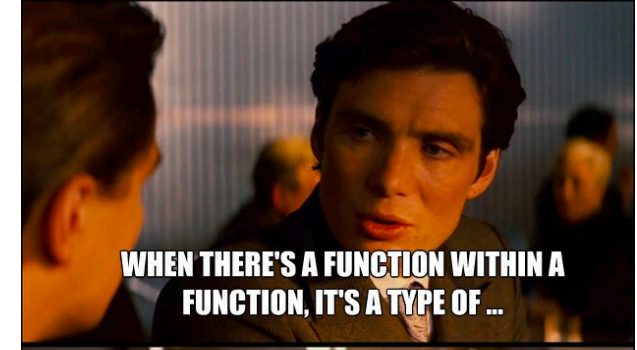
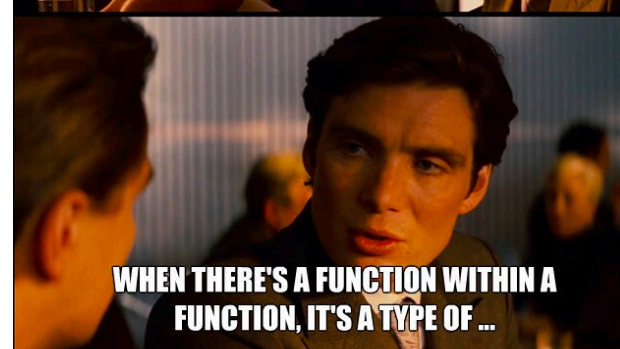
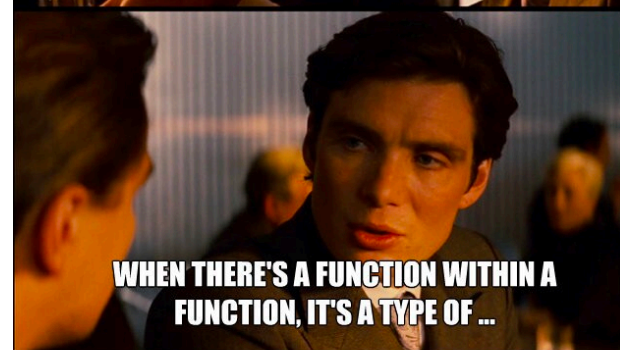
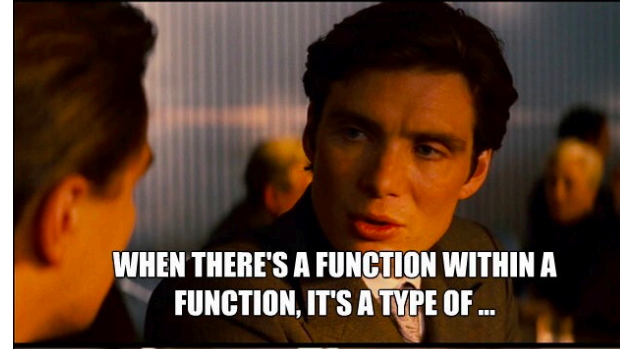
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# Backpropagation algorithm

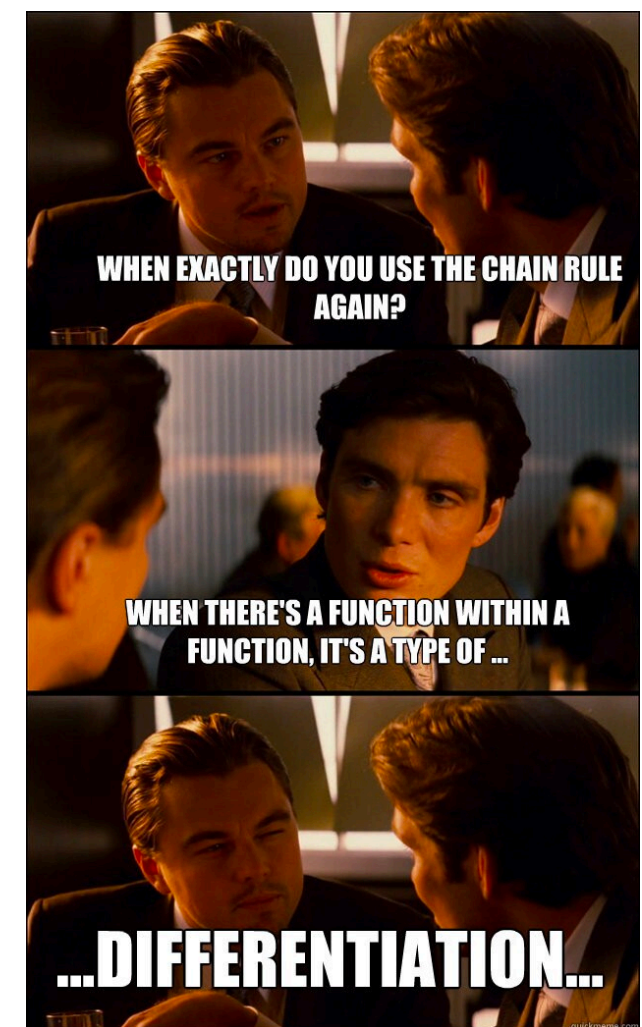
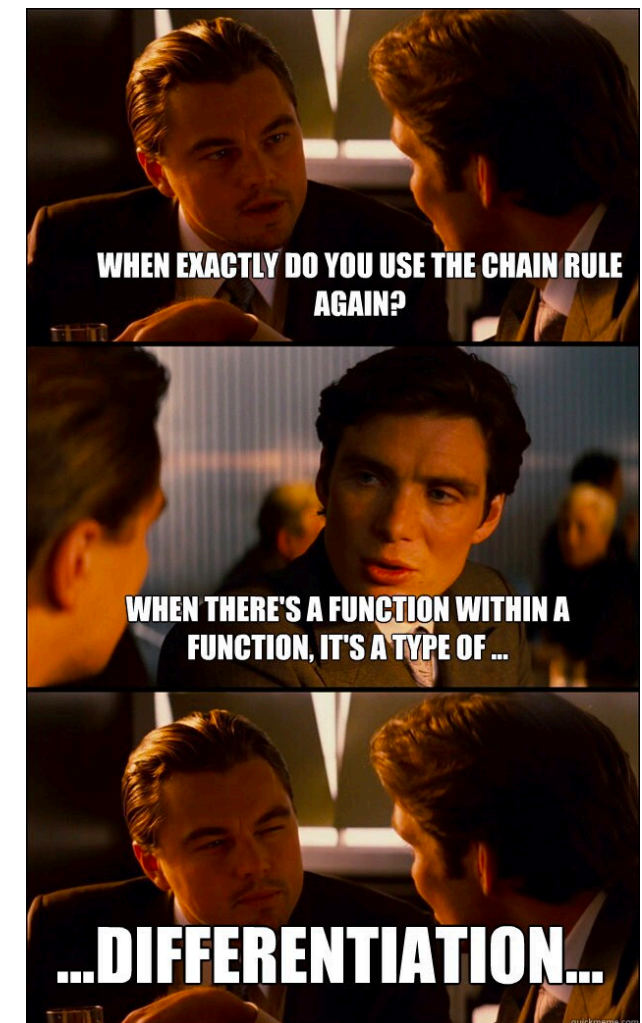
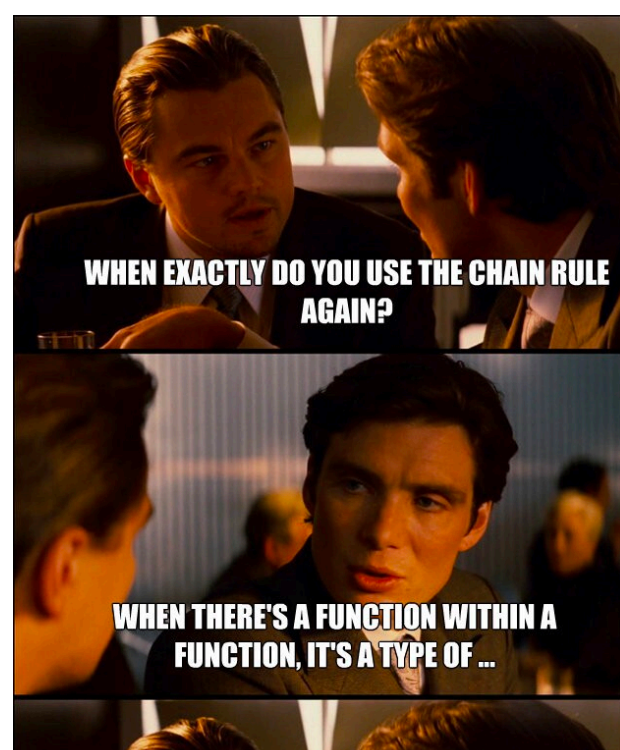
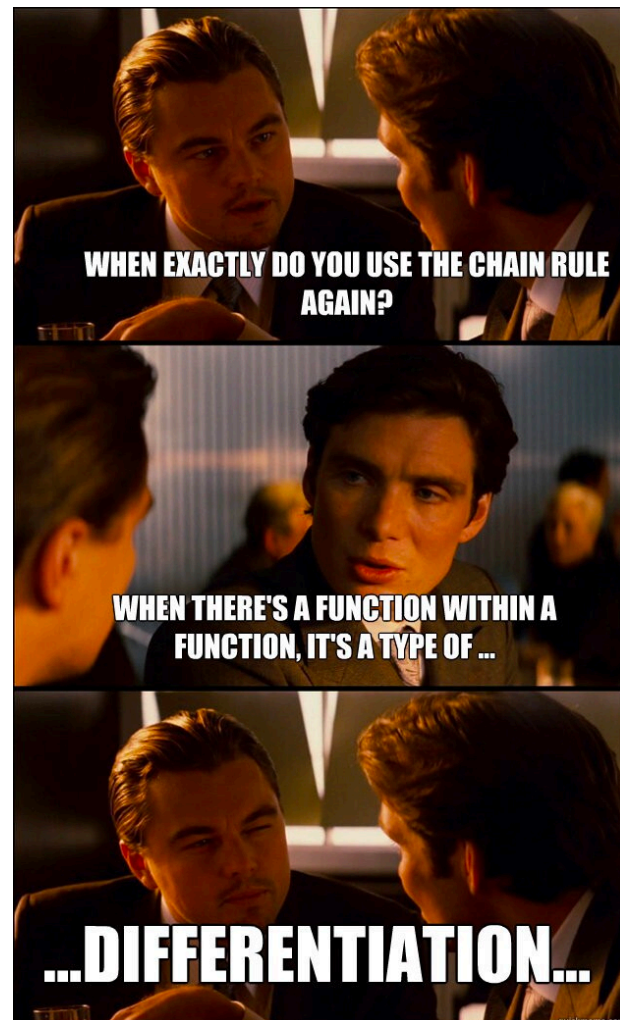
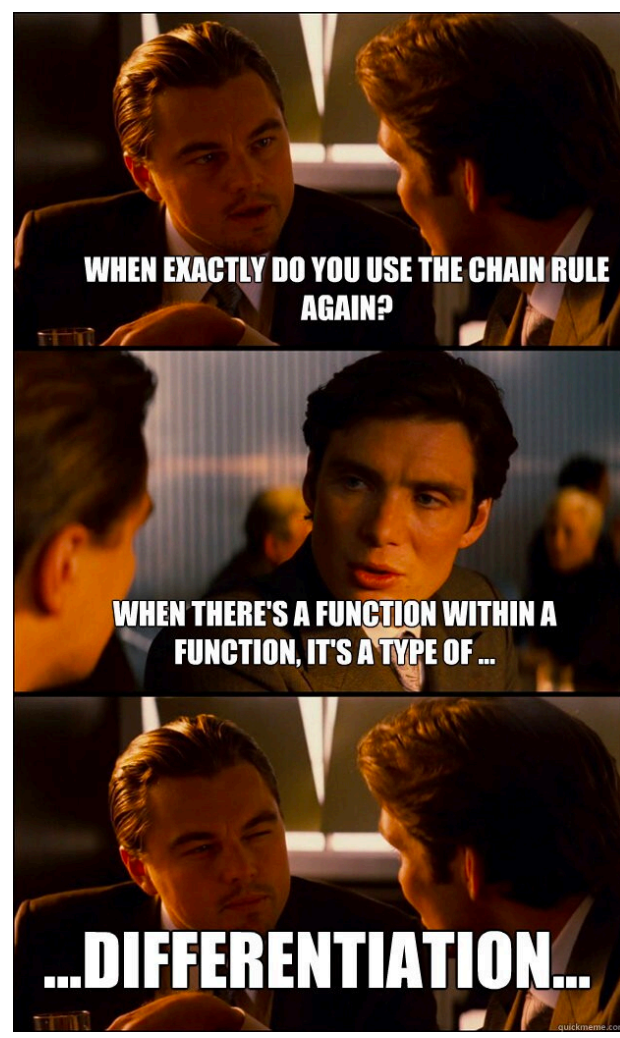
1. Calculate forward propagation of the network
2. Calculate the backward phase
  - a: Estimate the error in the final layer
  - b: Propagate that error into the previous layer
  - c: Evaluate the derivative of each parameter in the network
3. Combine all partial gradients into the final gradient
4. Update the weights using the calculated gradients to minimise the loss





# Backpropagation algorithm

1. Calculate forward propagation of the network
2. Calculate the backward phase
  - a: Estimate the error in the final layer
  - b: Propagate that error into the previous layer
  - c: Evaluate the derivative of each parameter in the network
3. Combine all partial gradients into the final gradient
4. Update the weights using the calculated gradients to minimise the loss





# Setting up the neural network

Classification: Does a picture belong into the class "A" or class "B"?

Build a network with two outputs that tell you the probability from which movie franchise your character is from.



# Output and loss function

- LAST LAYER ACTIVATION FUNCTION:

(normalises the output and maps it on the probability distribution)

$$f(z)_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

- LOSS FUNCTION:

(calculate the difference between predicted and correct outcome during training)

$$L = - \sum_x p(x) \log q(x)$$



# Classification: a mini example



Label:  $p(x)$

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Network output:  $q(x)$

$$\begin{bmatrix} q(\text{class A}) \\ q(\text{class B}) \end{bmatrix}$$

Loss:

$$-1 \log(q(\text{class A})) - 0 \log(q(\text{class B}))$$

$$-0 \log(q(\text{class A})) - 1 \log(q(\text{class B}))$$

# Classification: a mini example



Label:  $p(x)$

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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$$\begin{bmatrix} q(\text{class A}) \\ q(\text{class B}) \end{bmatrix}$$

Loss:

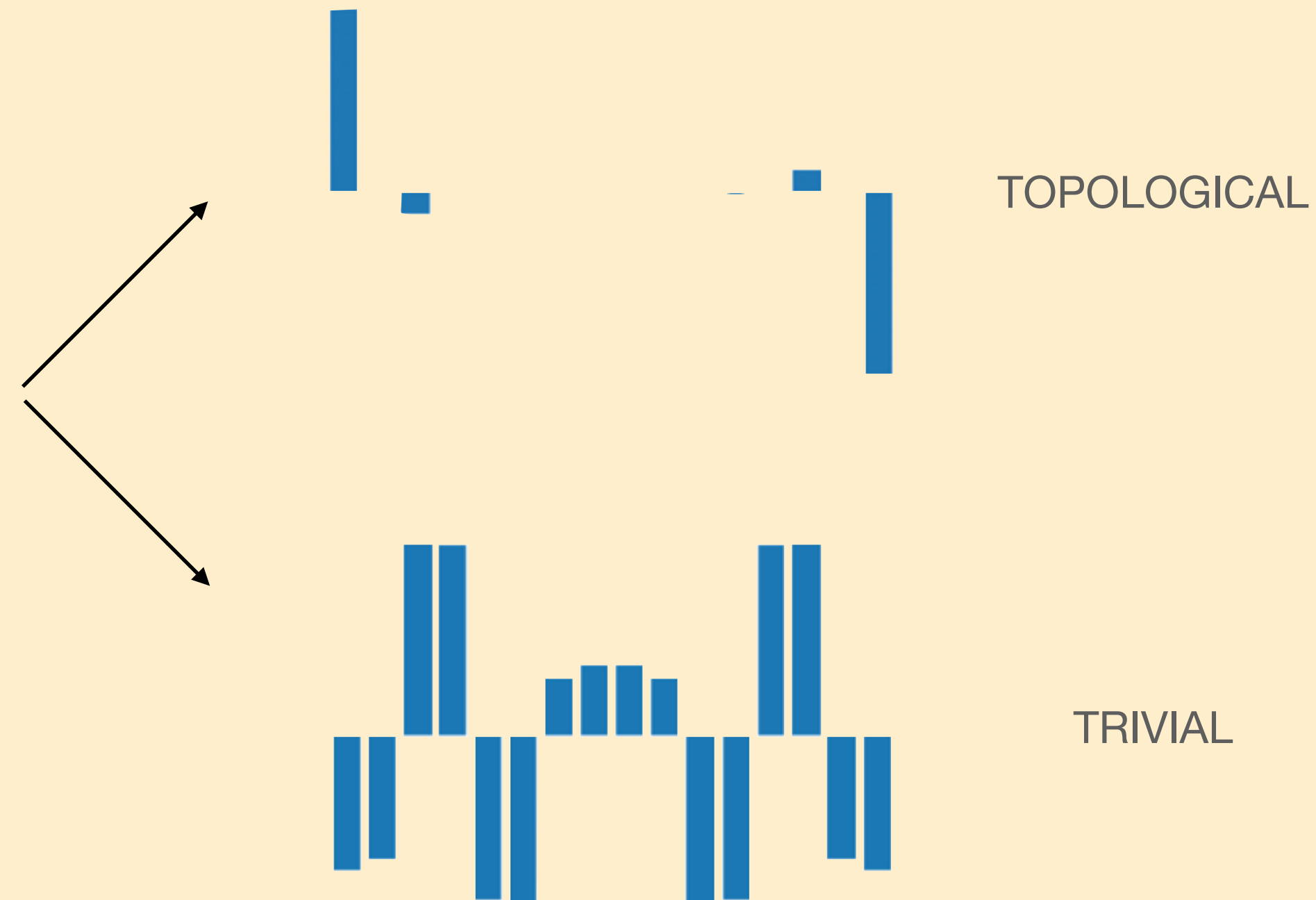
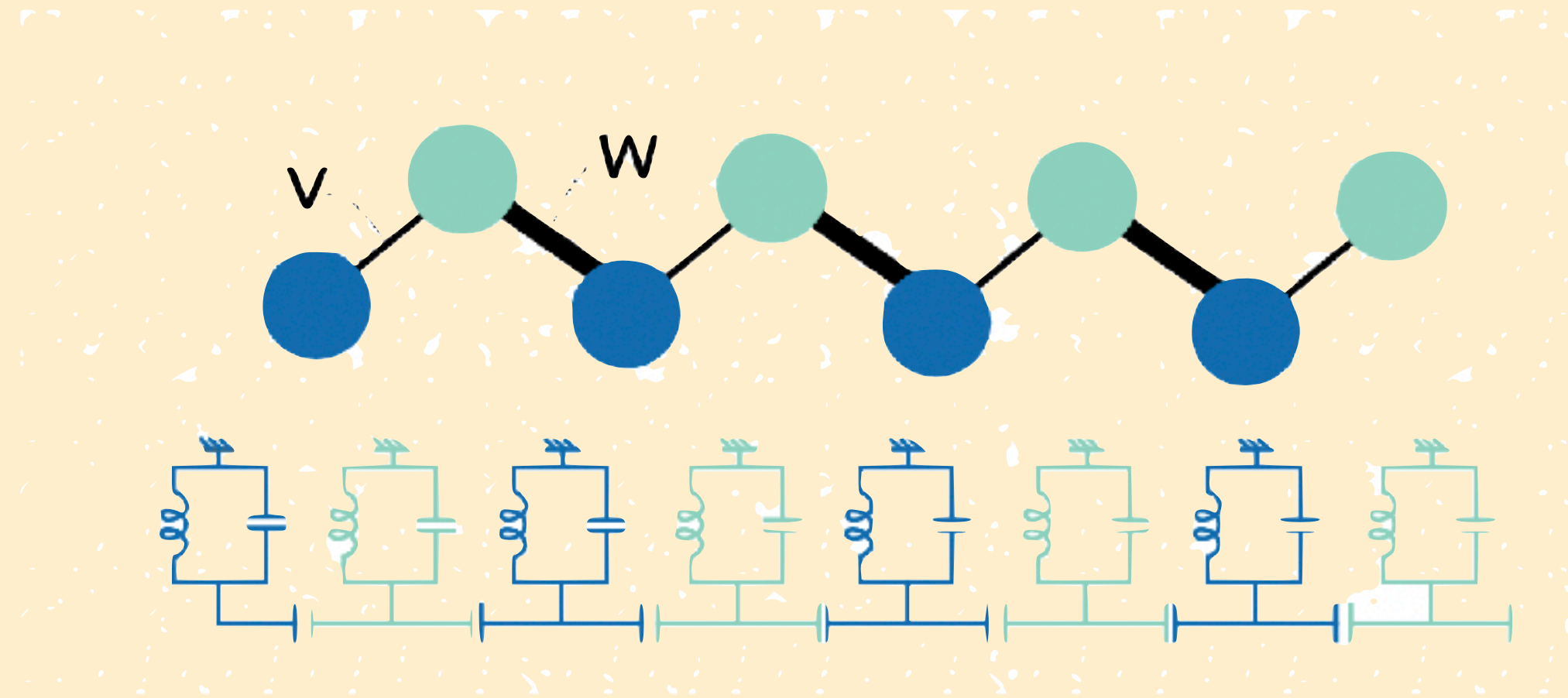
$$-1 \log(q(\text{class A})) - 0 \log(q(\text{class B}))$$

$$-0 \log(q(\text{class A})) - 1 \log(q(\text{class B}))$$

!the loss is minimal if  $q(x)$  matches the labels!

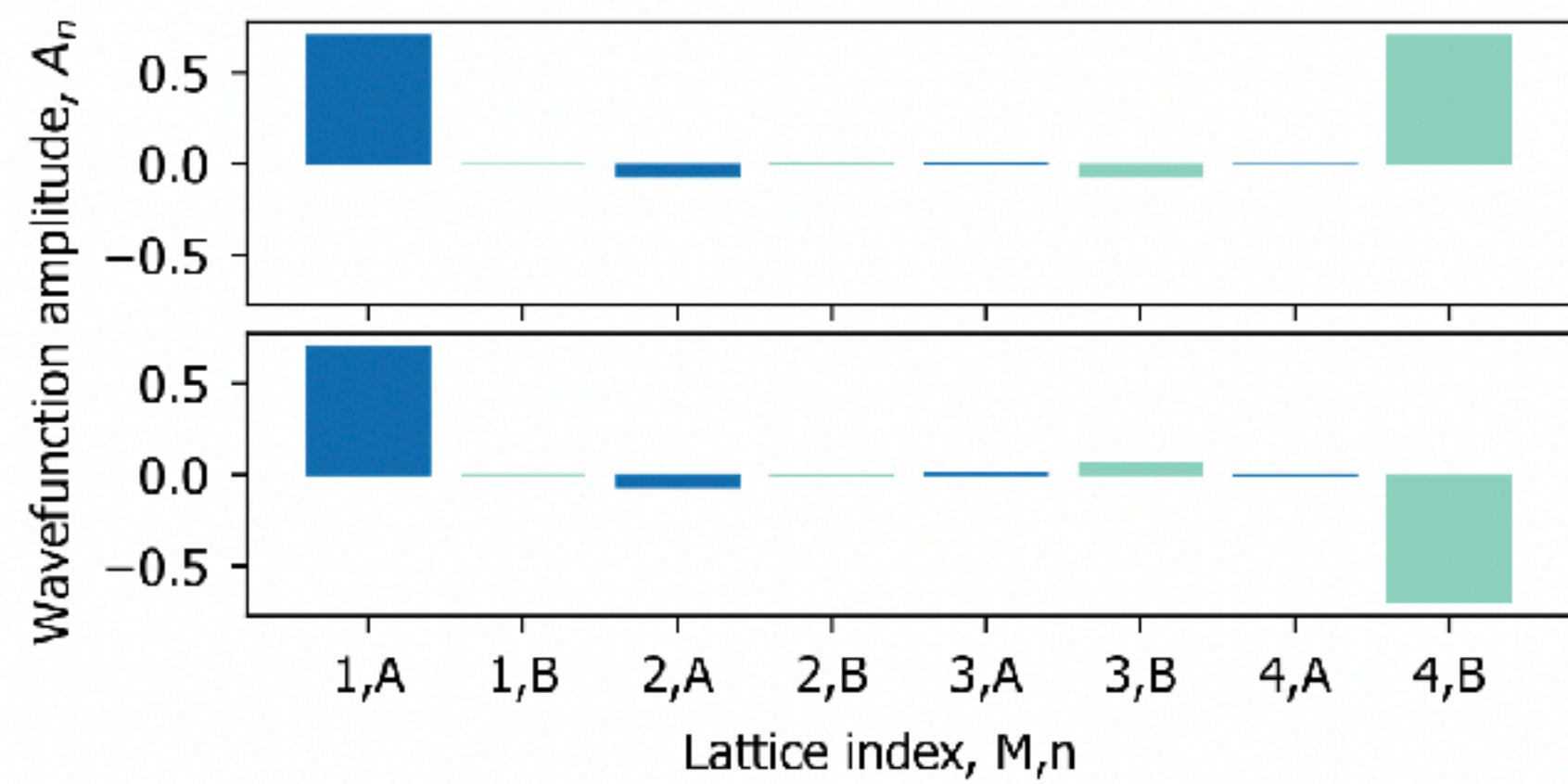


# Hands-On: Machine Learning in (Topological) Superconducting Circuits

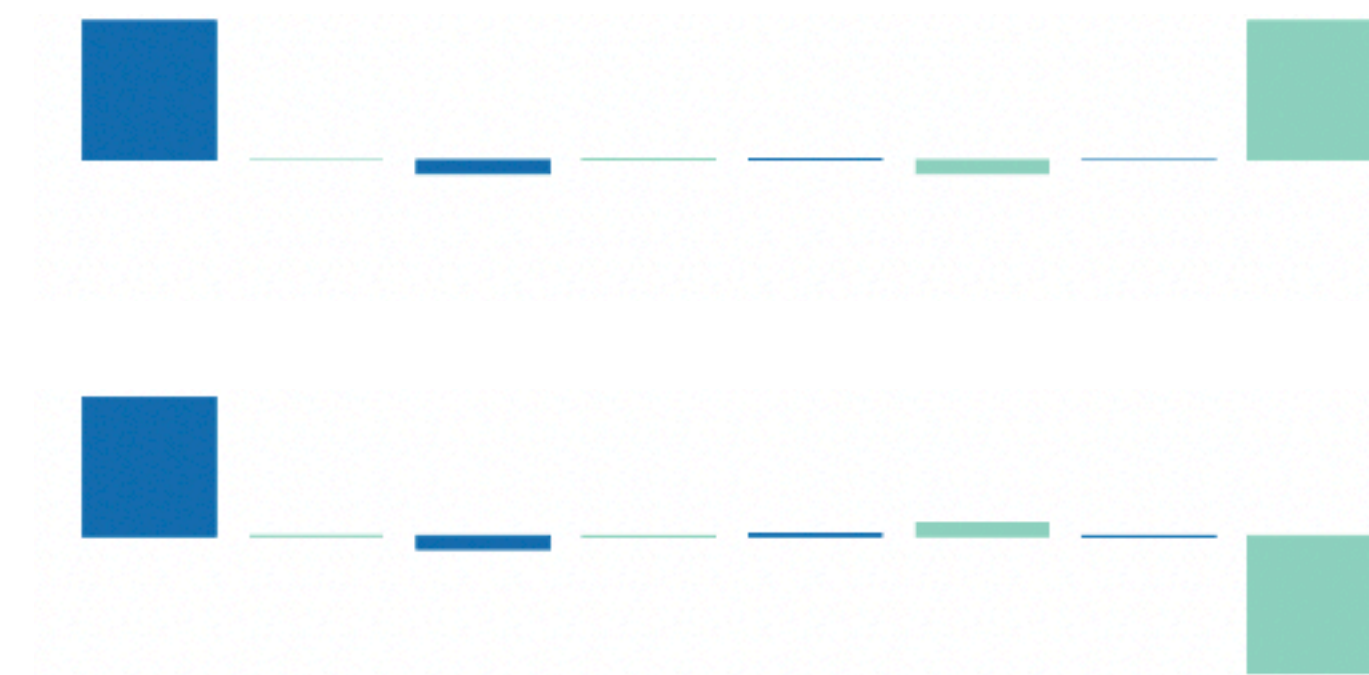


# Classification: a mini example

Wave-function amplitude at spatial position



Visual representation





# Classification: a mini example



Label:  $p(x)$

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Network output:  $q(x)$

$$\begin{bmatrix} q(\text{class A}) \\ q(\text{class B}) \end{bmatrix}$$

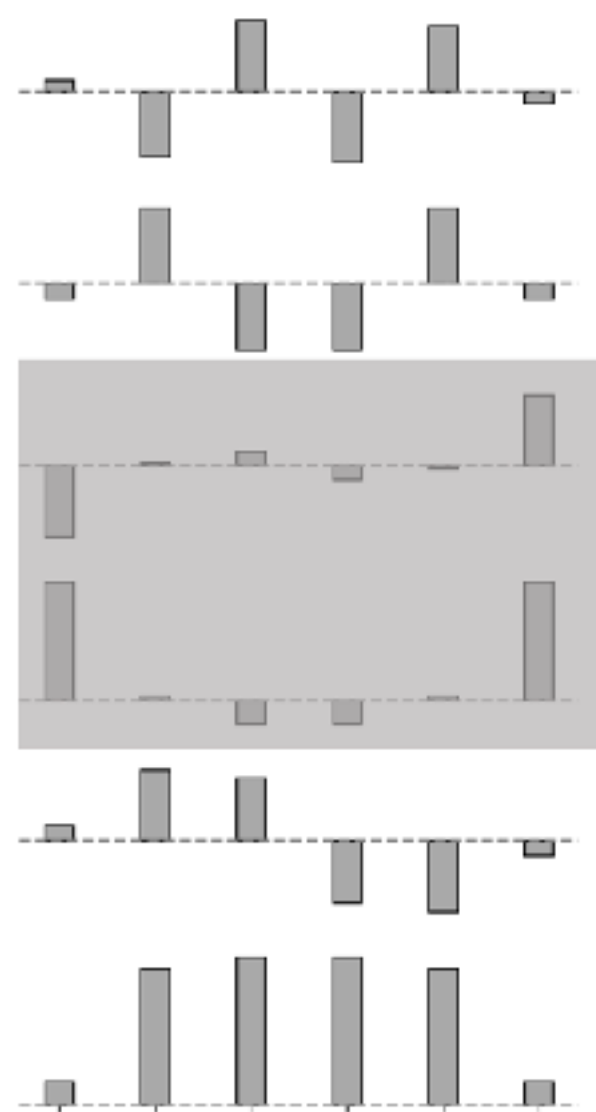
Loss:

$$-1 \log(q(\text{class A})) - 0 \log(q(\text{class B}))$$

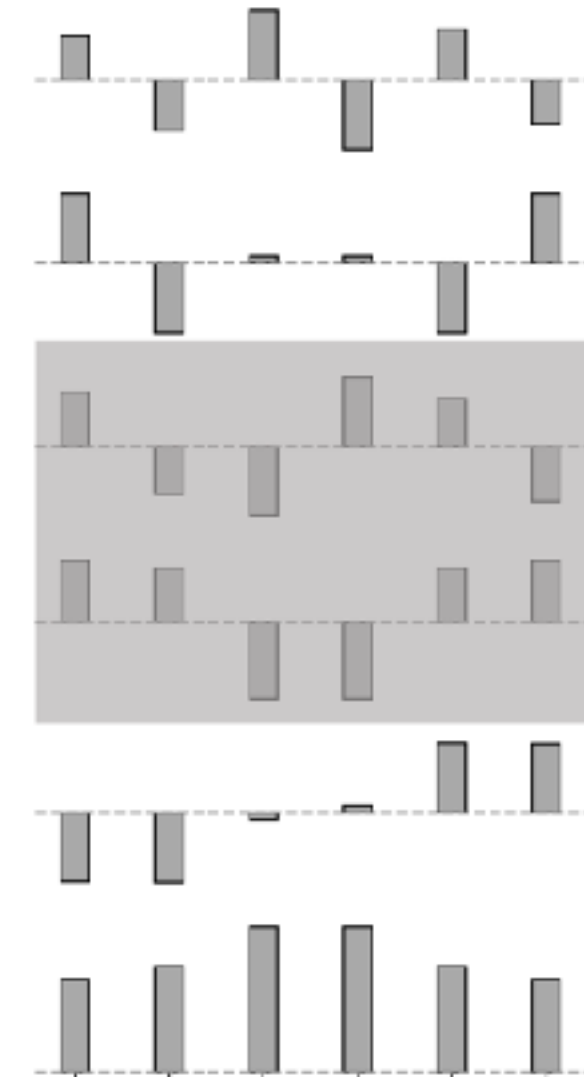
$$-0 \log(q(\text{class A})) - 1 \log(q(\text{class B}))$$

!the loss is minimal if  $q(x)$  matches the labels!

# Back to physics



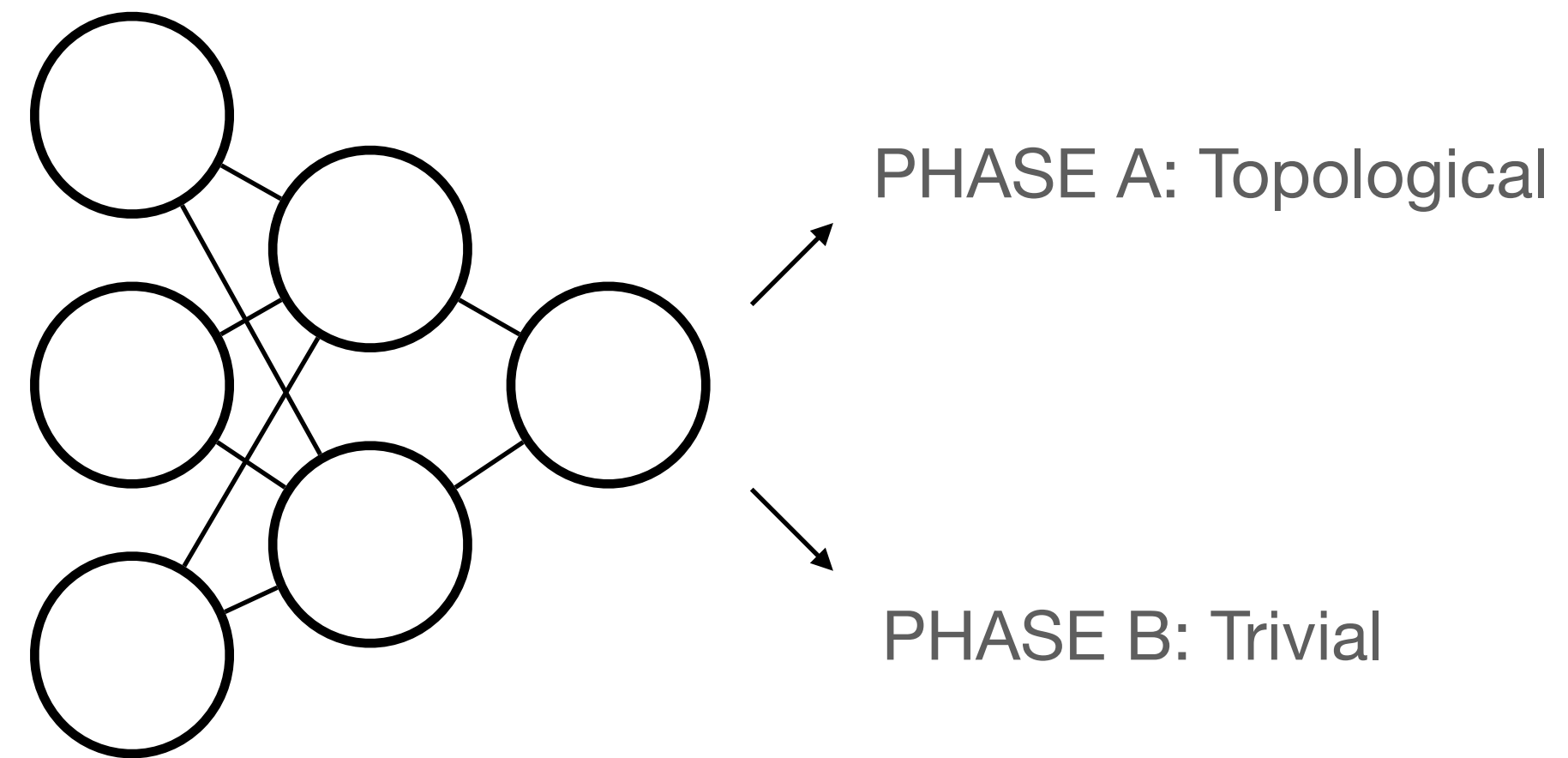
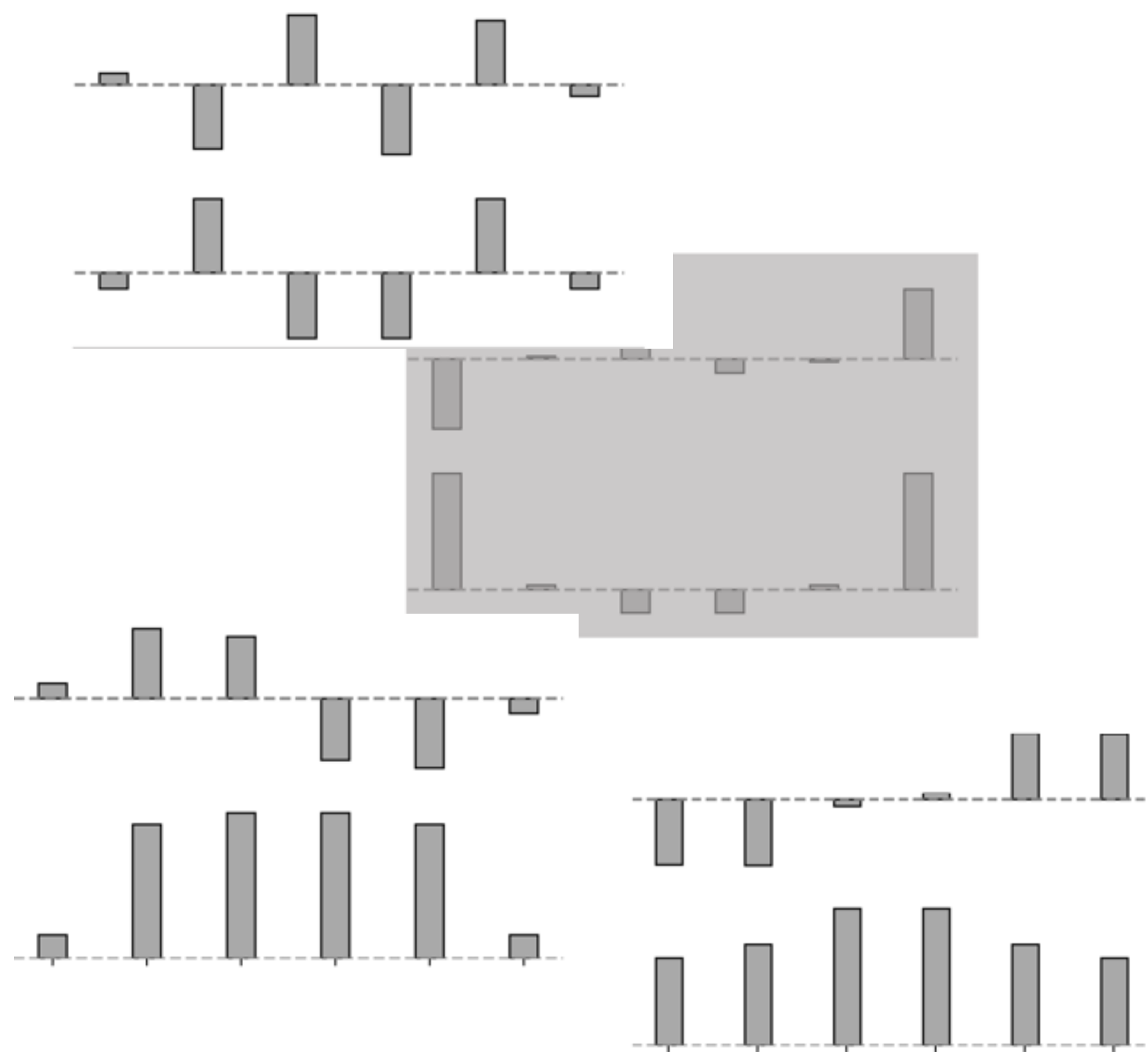
← Topological



Trivial →

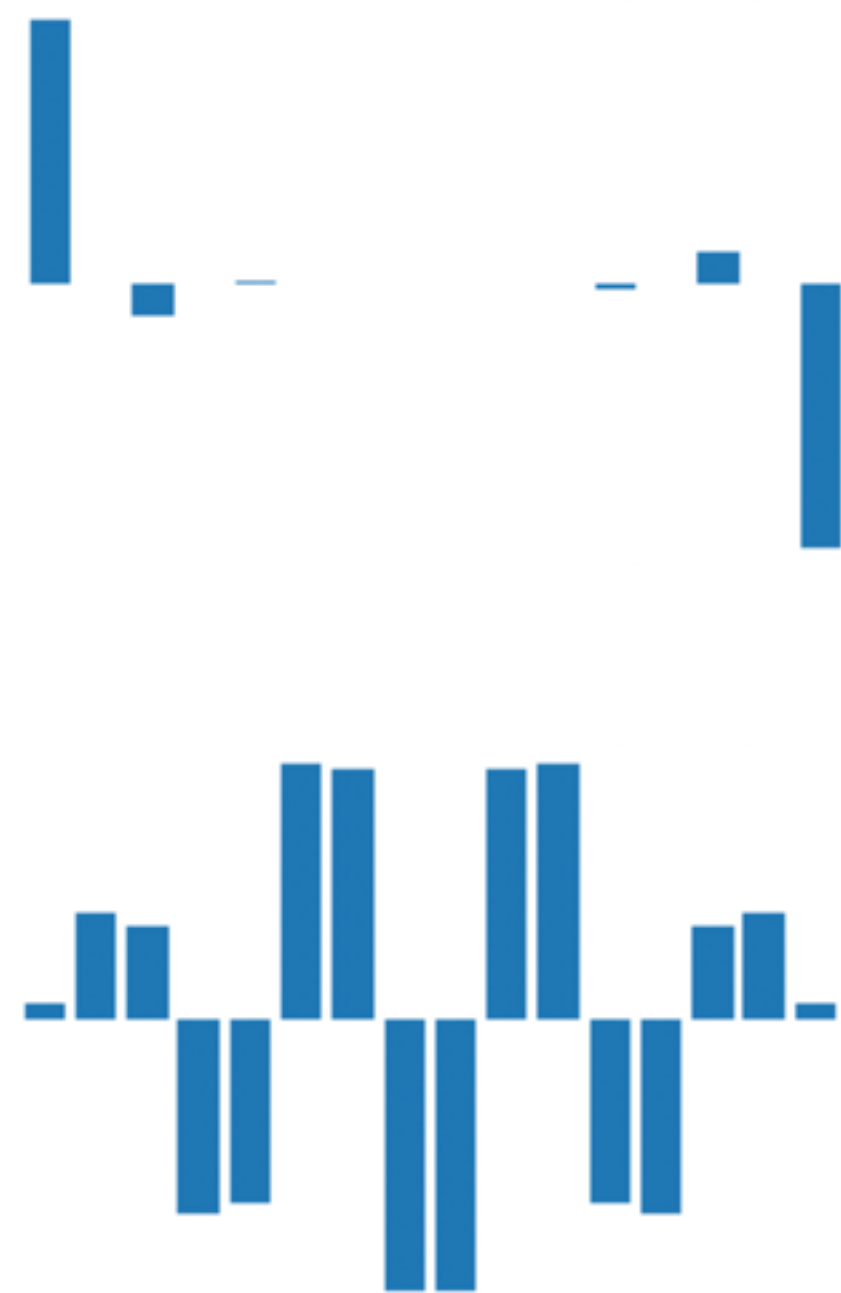


# Notebook 1: Supervised learning



# Quiz: SSH Human Classification

A



B





# Quiz: SSH Human Classification

A



PHASE A: Topological

B



PHASE B: Trivial

# Notebook 1: Supervised learning

```
Using cpu device
NeuralNetwork(
  (flatten): Flatten()
  (linear_relu_stack): Sequential(
    (0): Linear(in_features=256, out_features=32, bias=True)
    (1): ReLU()
    (2): Linear(in_features=32, out_features=16, bias=True)
    (3): ReLU()
    (4): Linear(in_features=16, out_features=2, bias=True)
  )
)
```

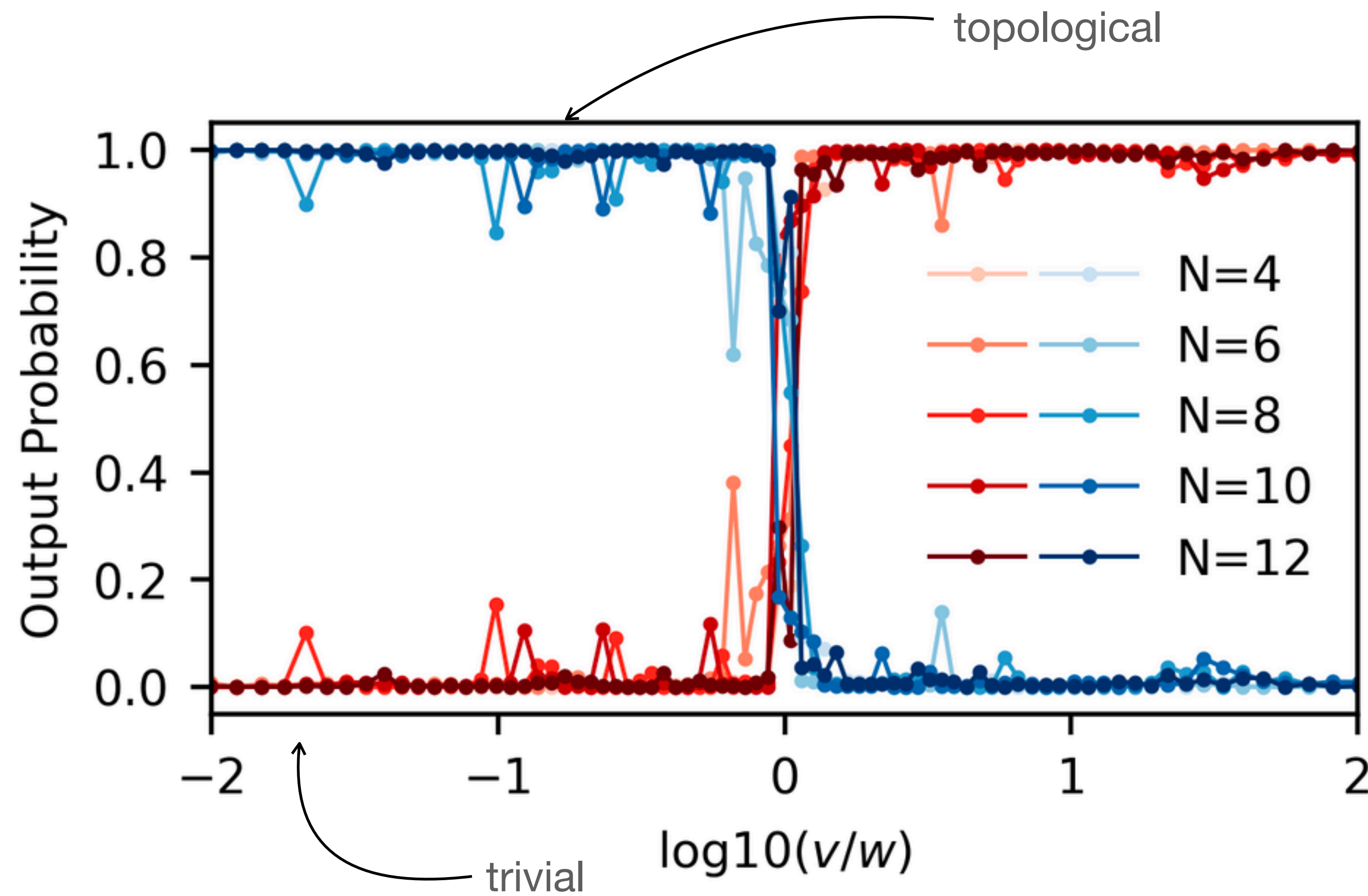
INPUT: 16 sites x 16 eigenstates = 256

2 HIDDEN LAYERS

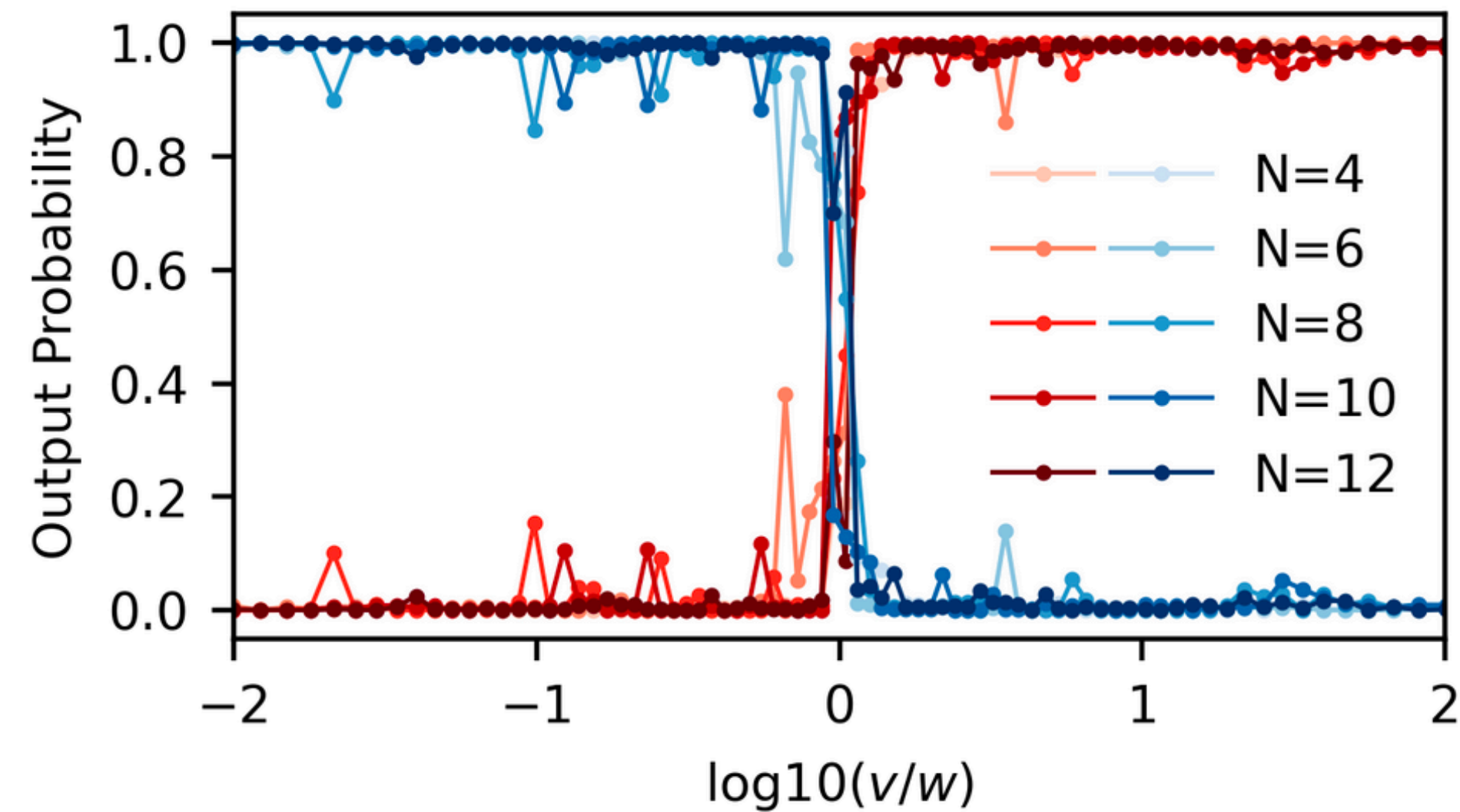
2 OUTPUTS: topo and trivial



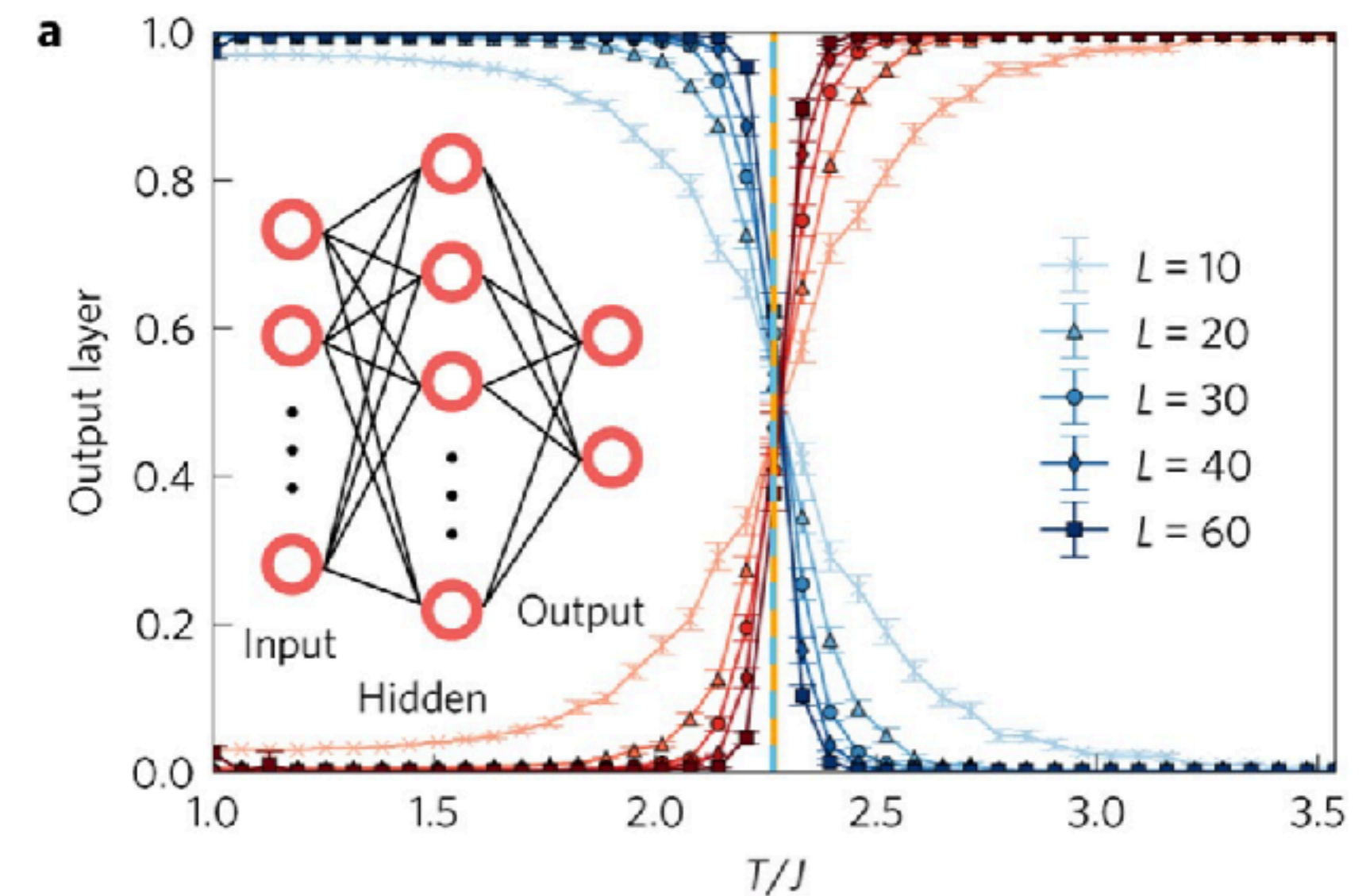
# How does NN learn the phase transition?



# How does NN learn the phase transition?



From your exercise notebook

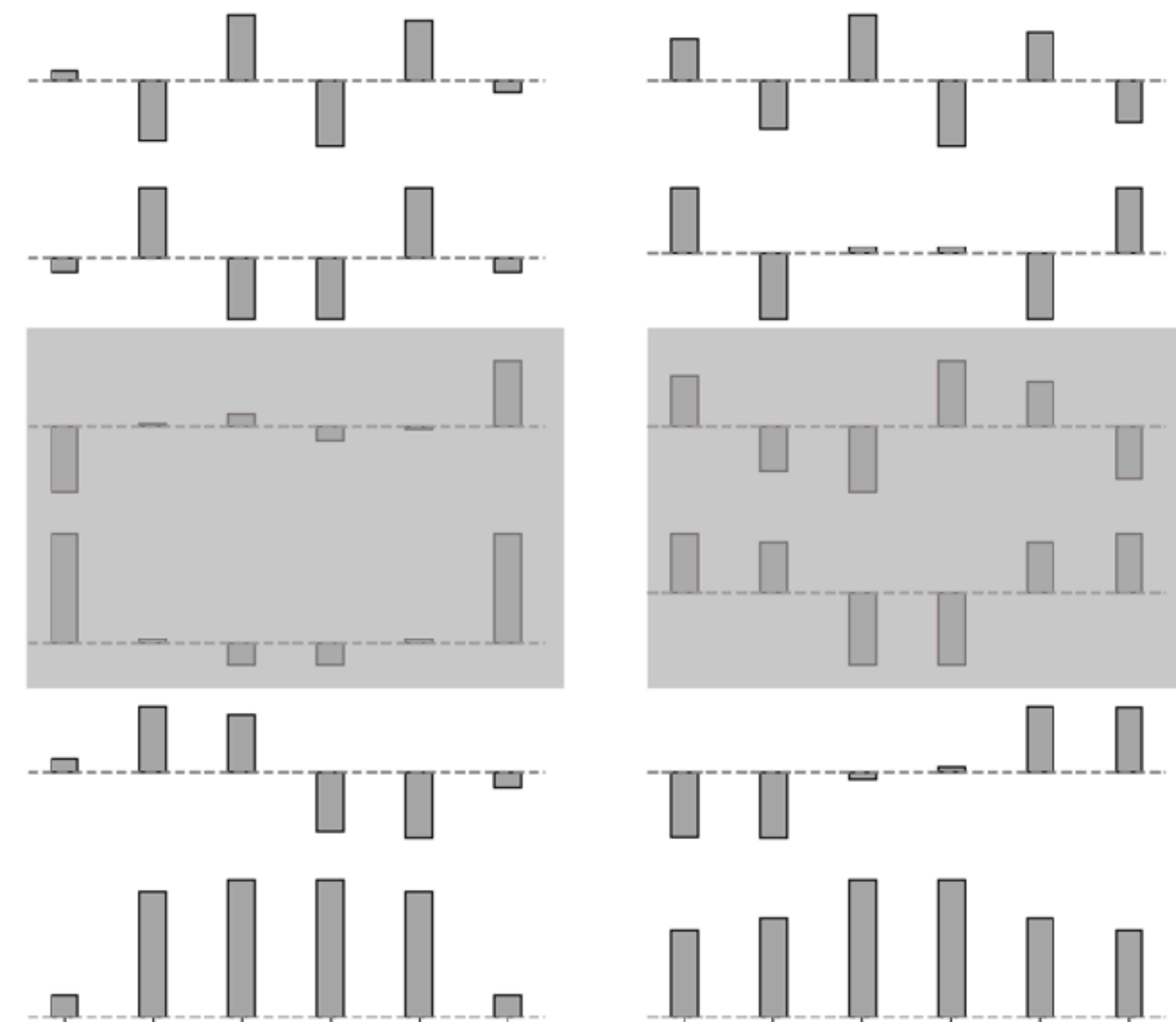


Carrasquilla&Melko, Nature Physics **13**, 431–434(2017)



# Let's make the classification more challenging

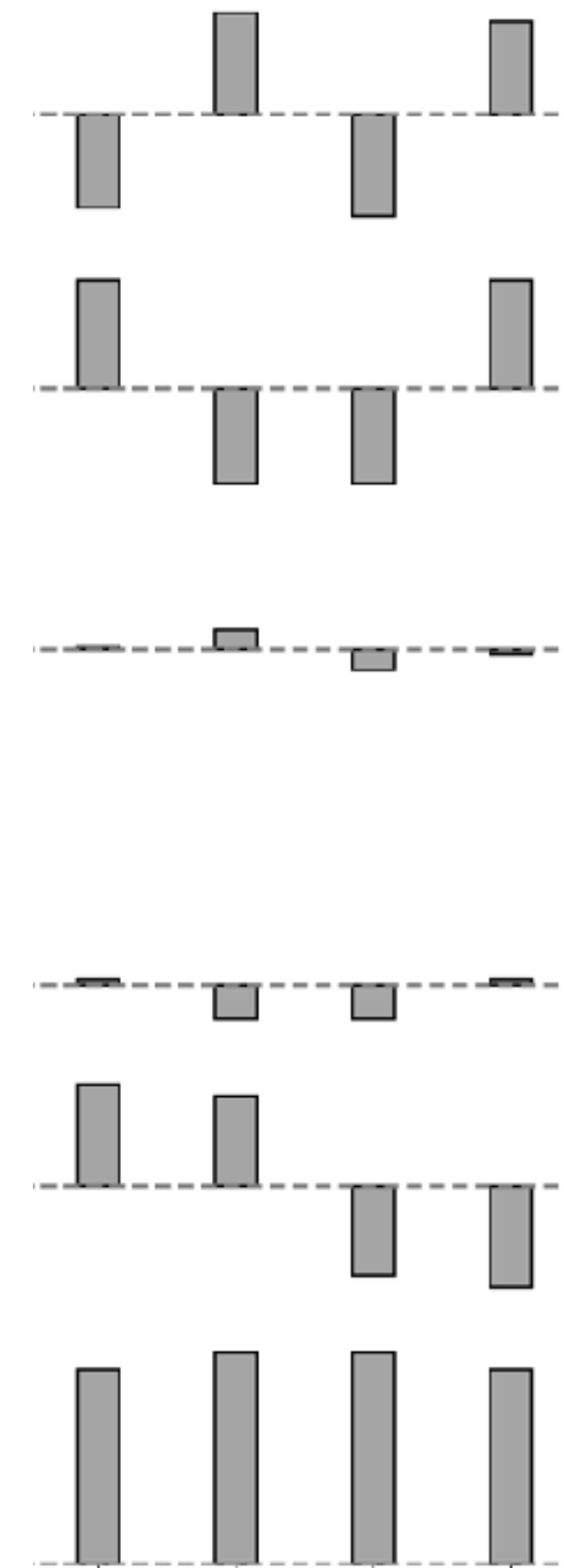
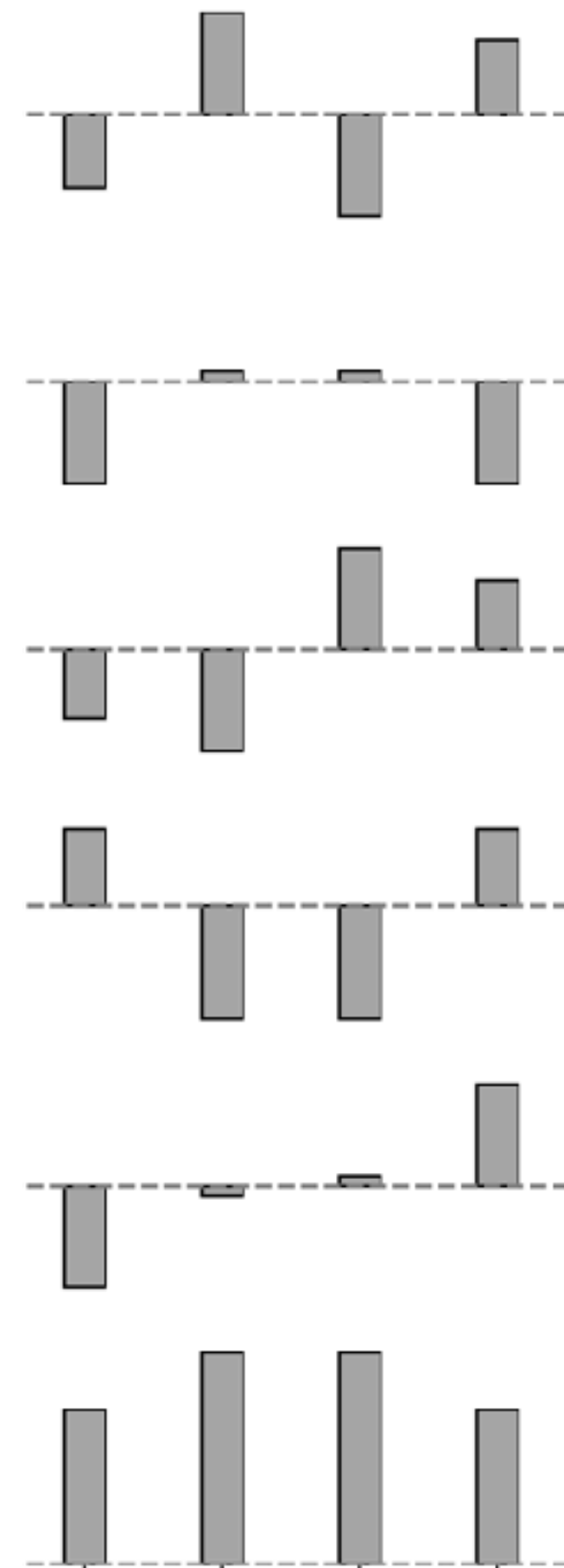
What about the wave function allows you to immediately determine the topology?



PHASE A: Topological

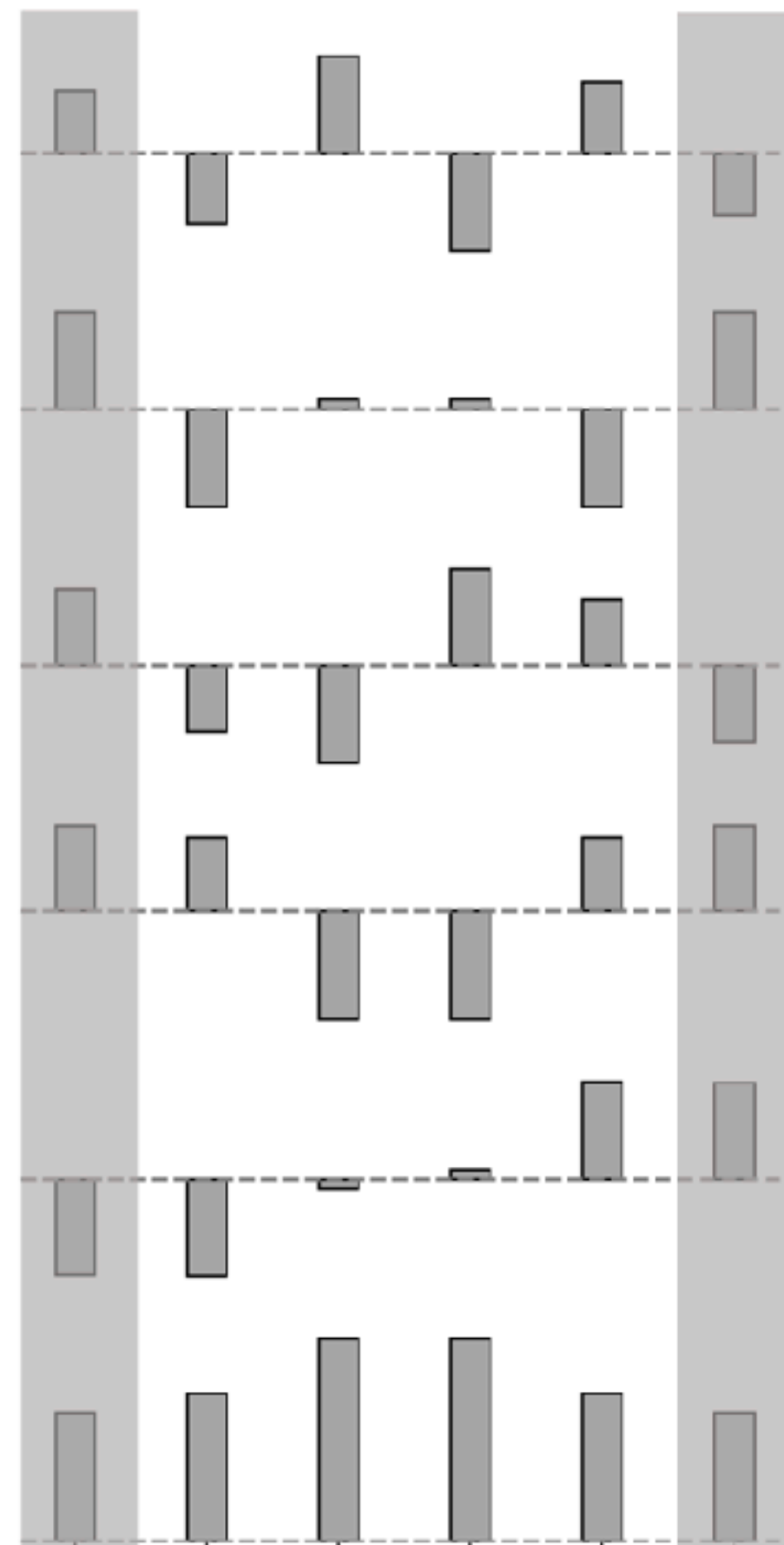
PHASE B: Trivial

# Quiz 2:SSH Human Classification

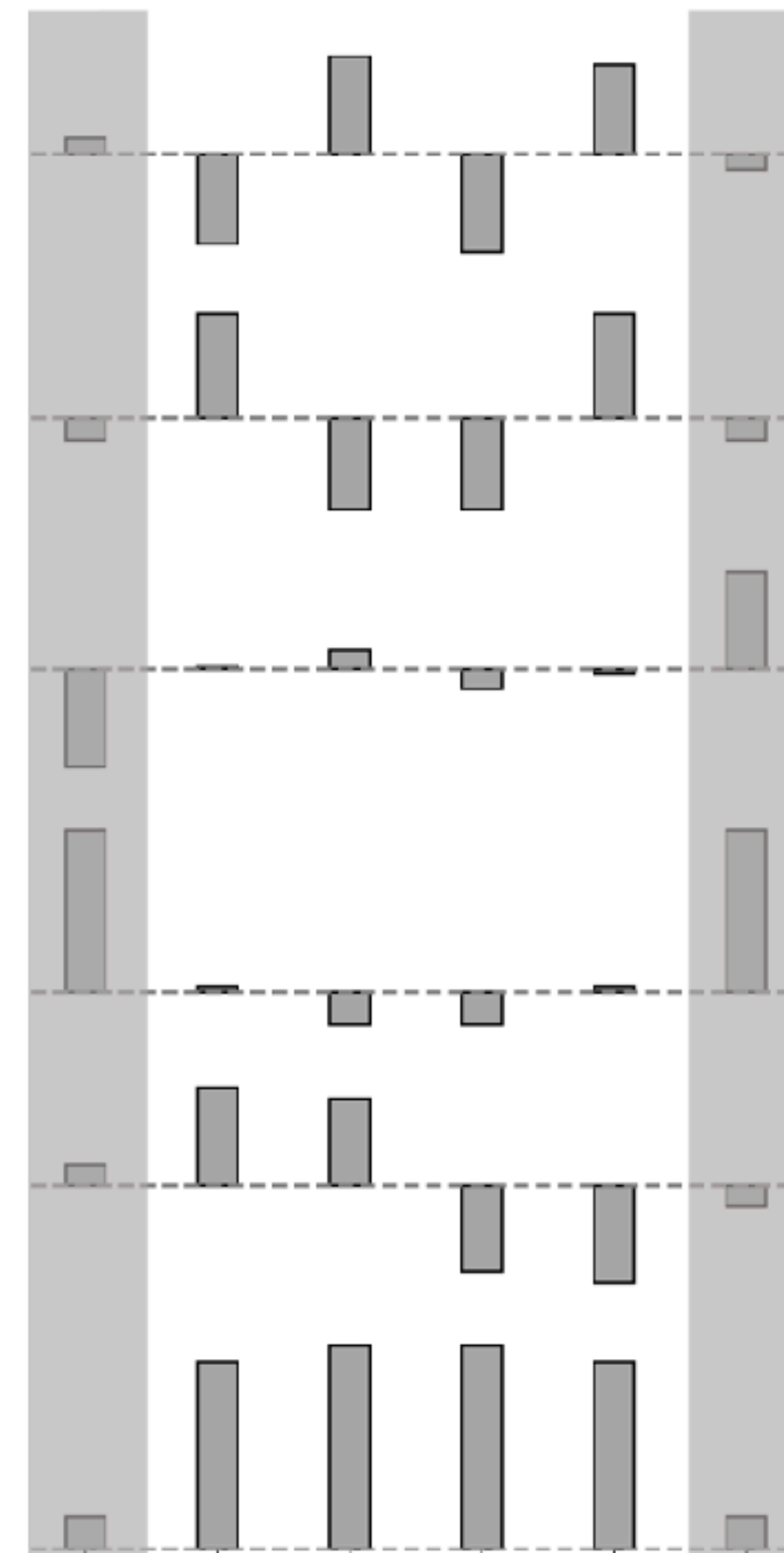




# Quiz 2:SSH Human Classification

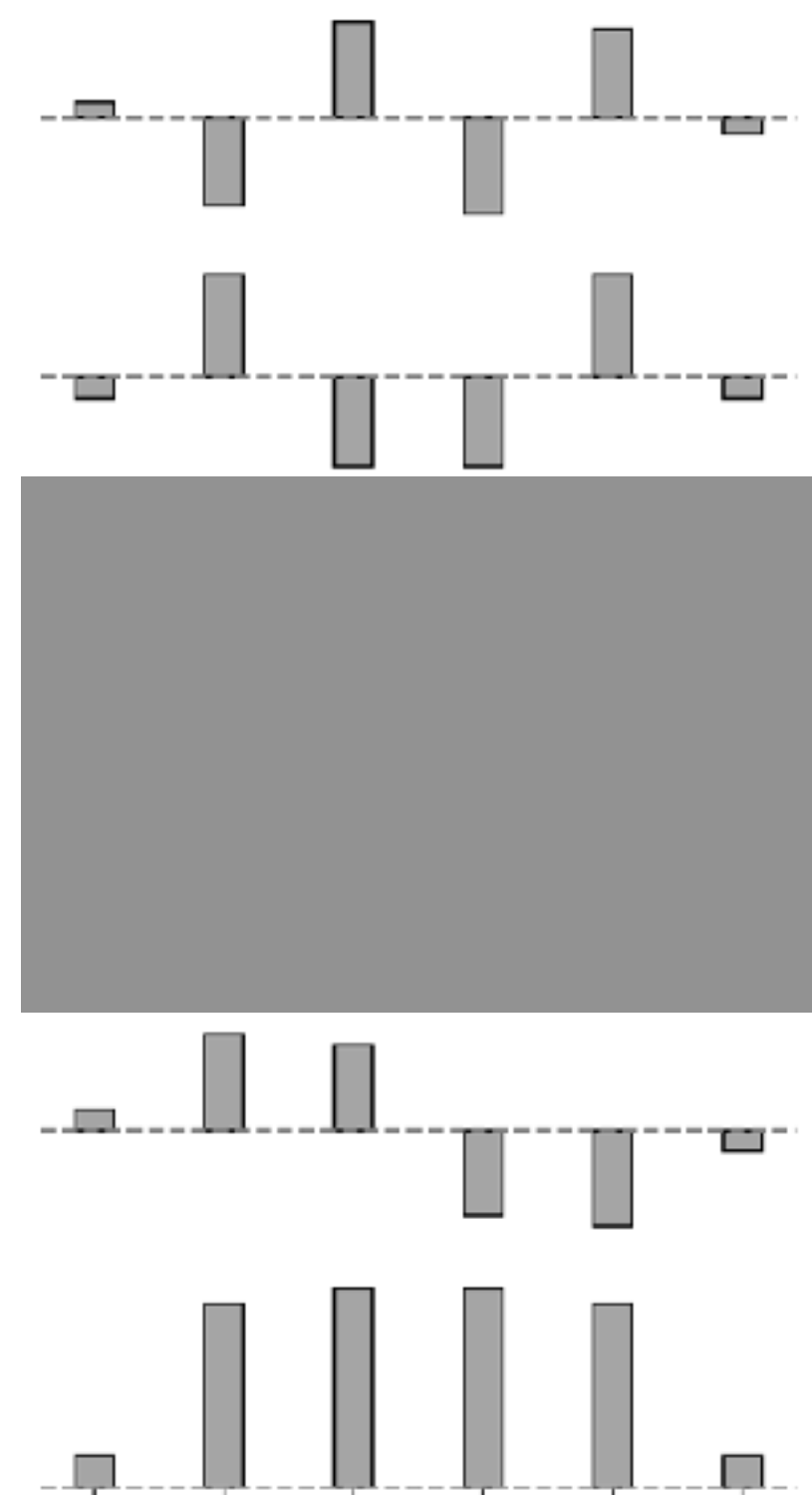


PHASE B: Trivial



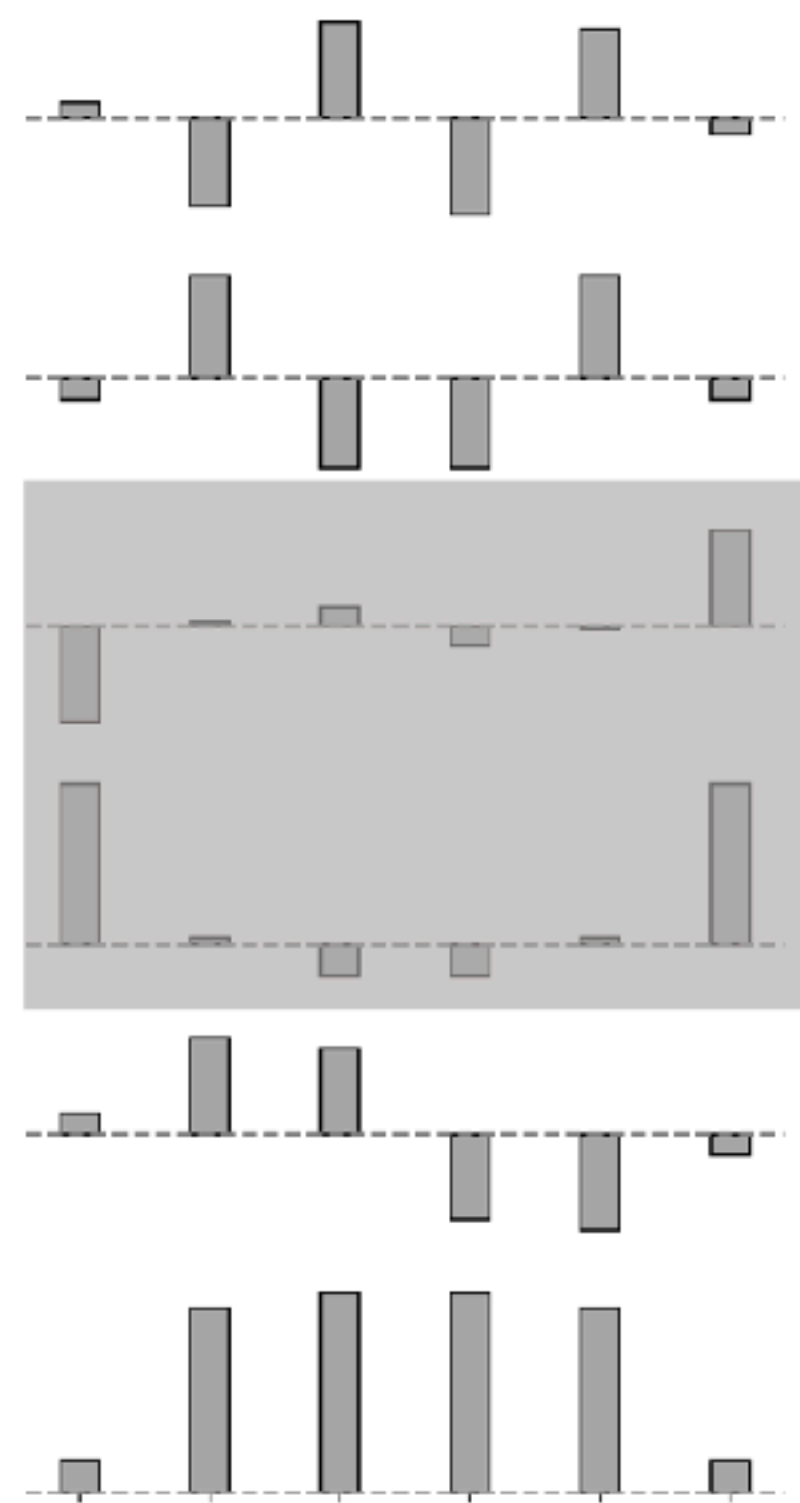
PHASE A: Topological

# Quiz 3: SSH Human Classification

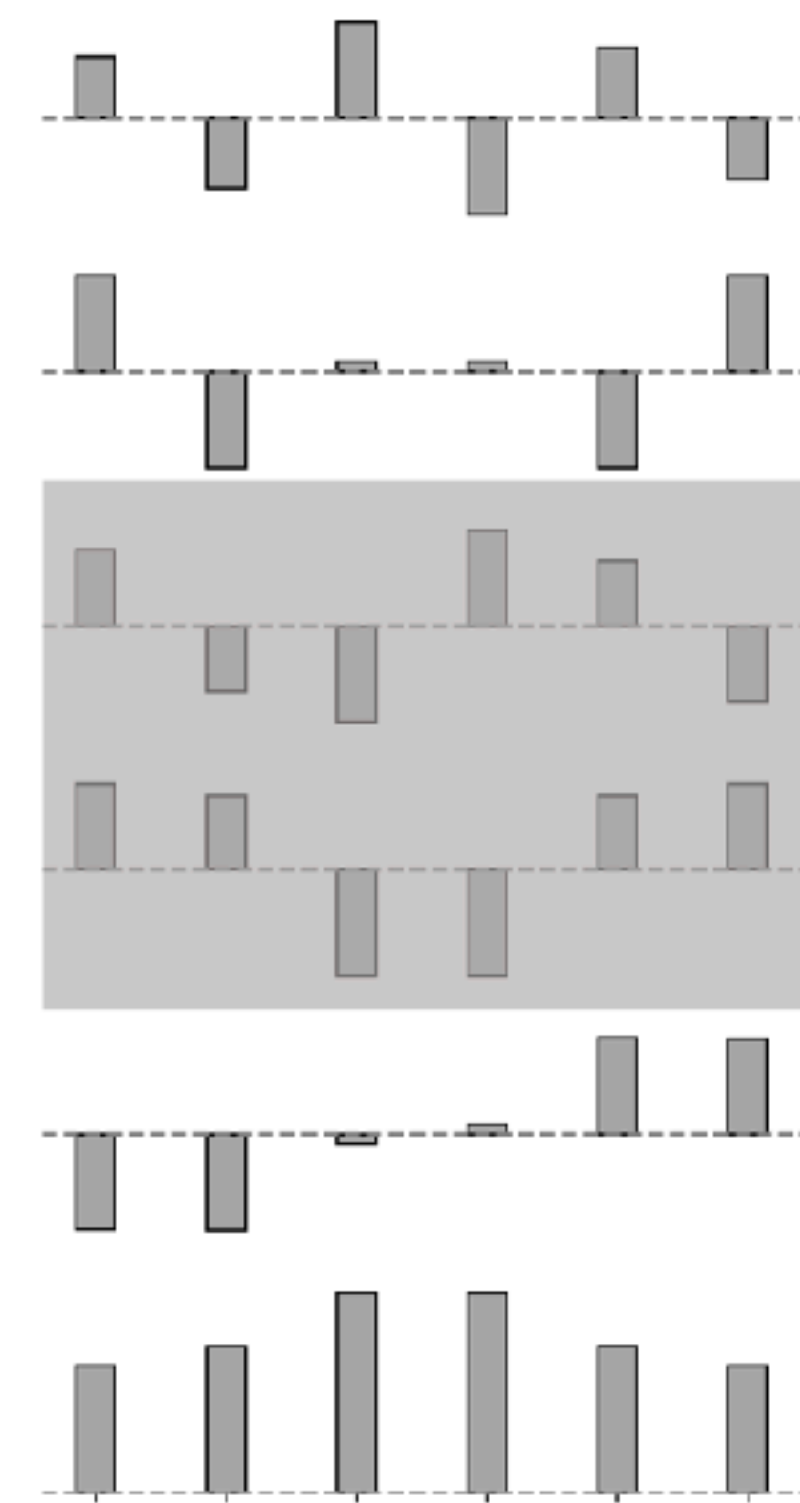




# Quiz 3:SSH Human Classification



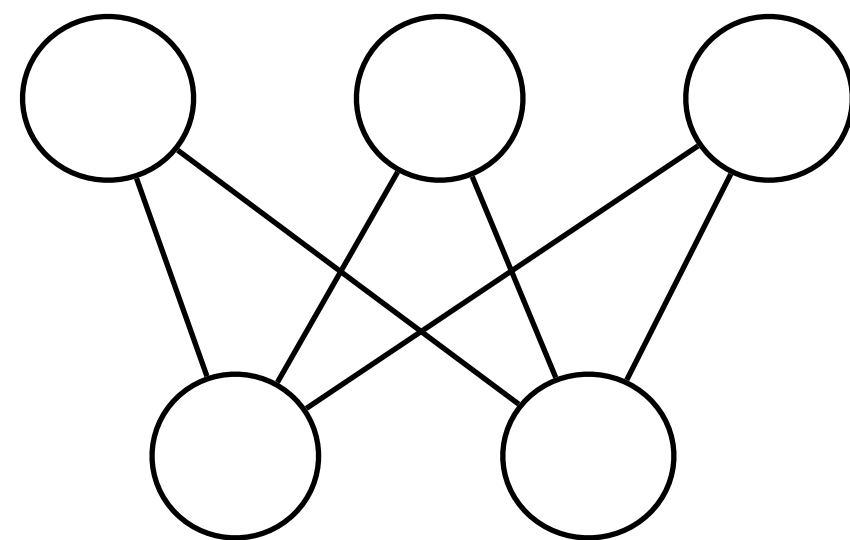
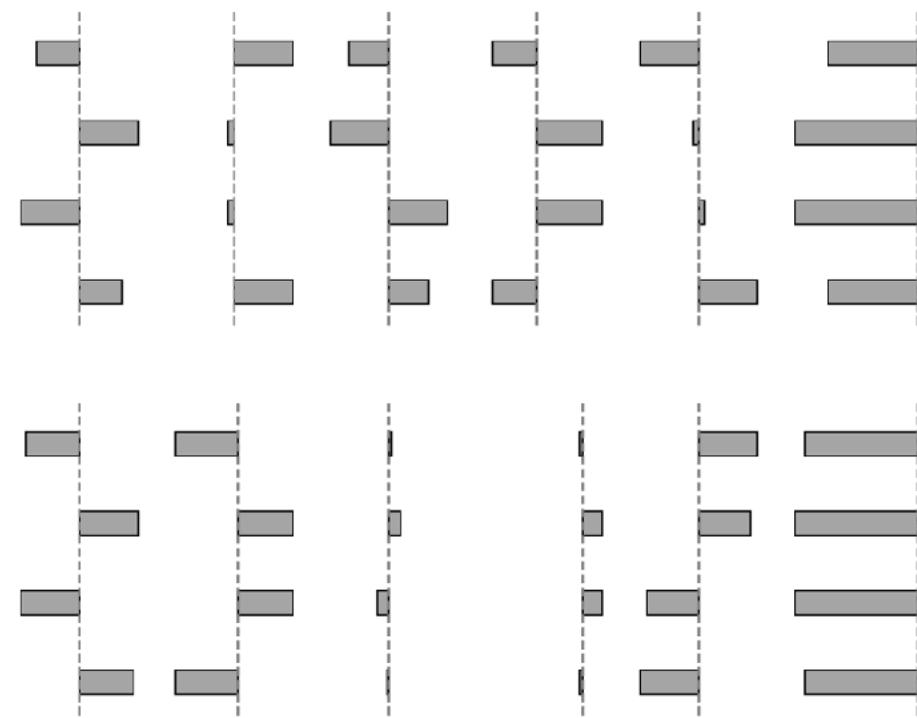
PHASE A: **Topological**



PHASE B: **Trivial**

# Notebook 2: Classification with limited data

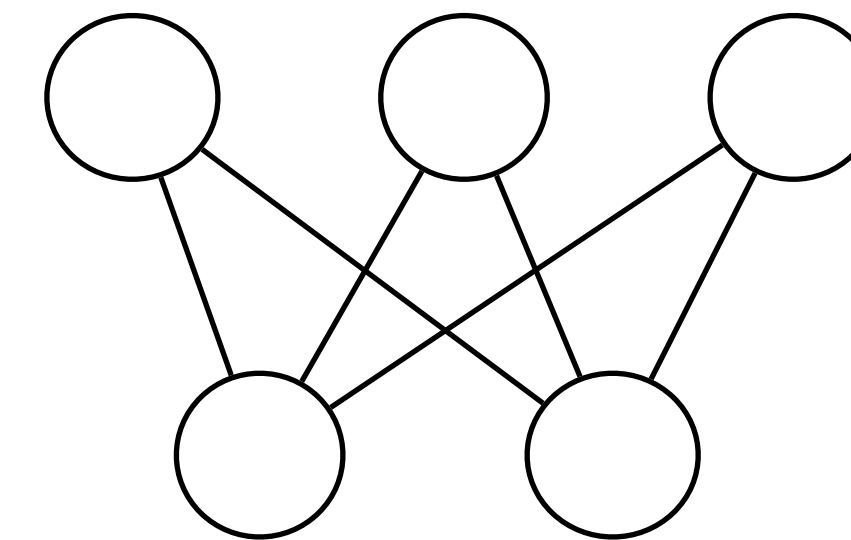
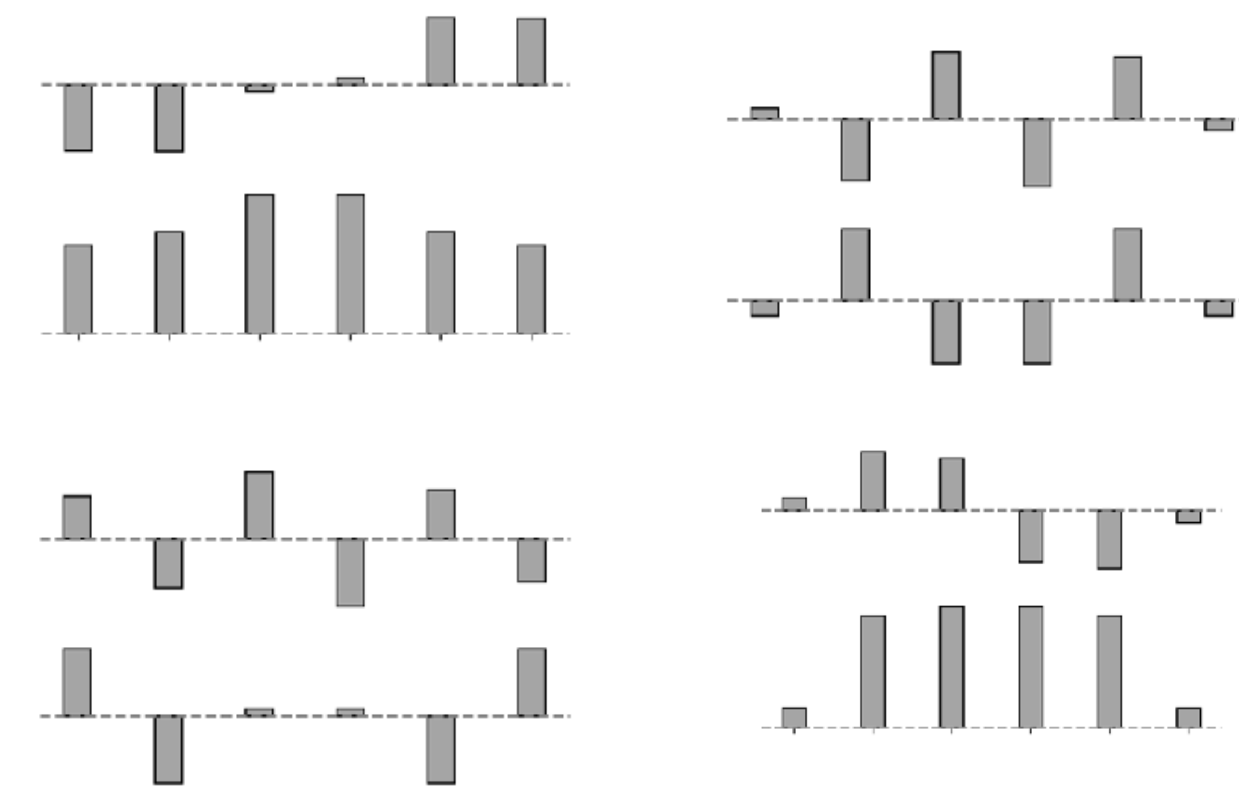
Data without edge sites



TOPO

TRIVIAL

Data without edge modes



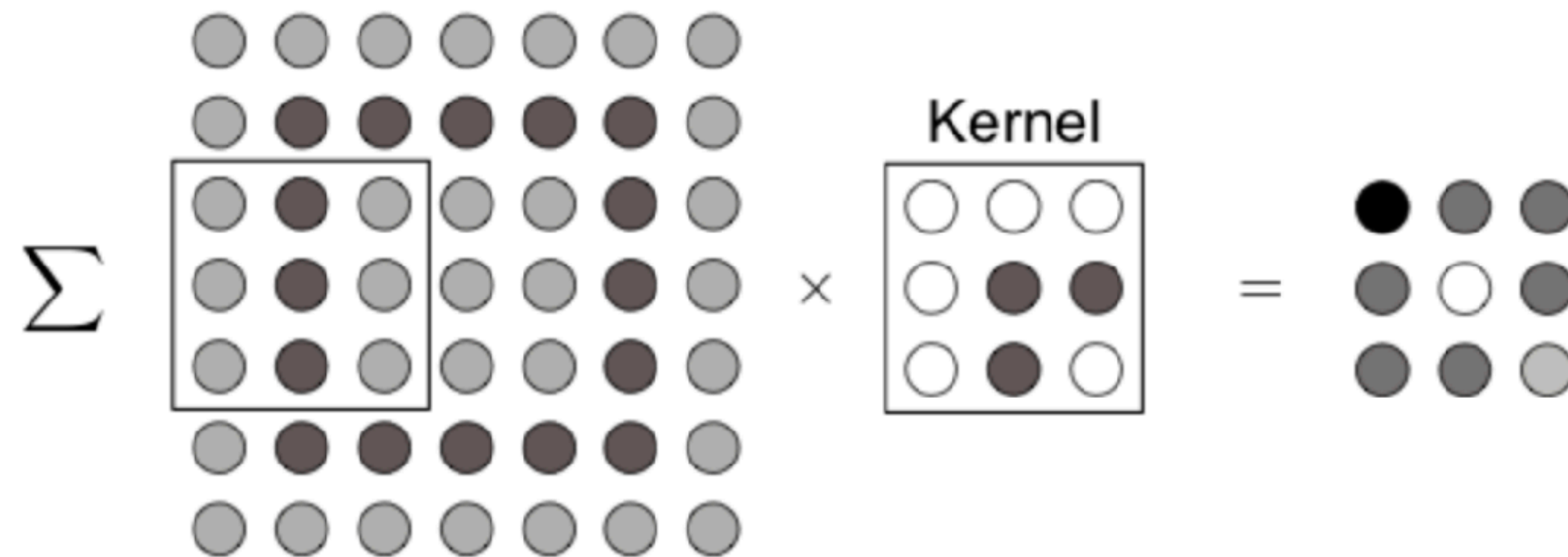
TOPO

TRIVIAL

# Fine-tuning your network

- Add different types of layers

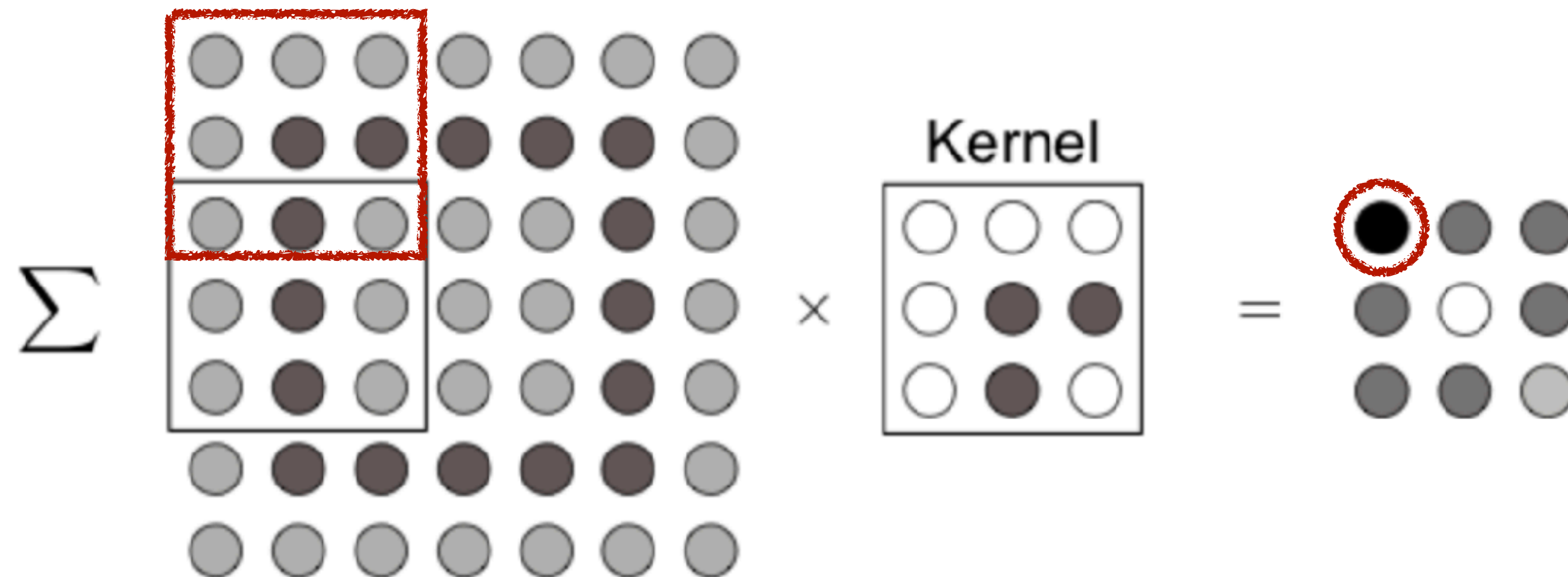
CONVOLUTIONS:





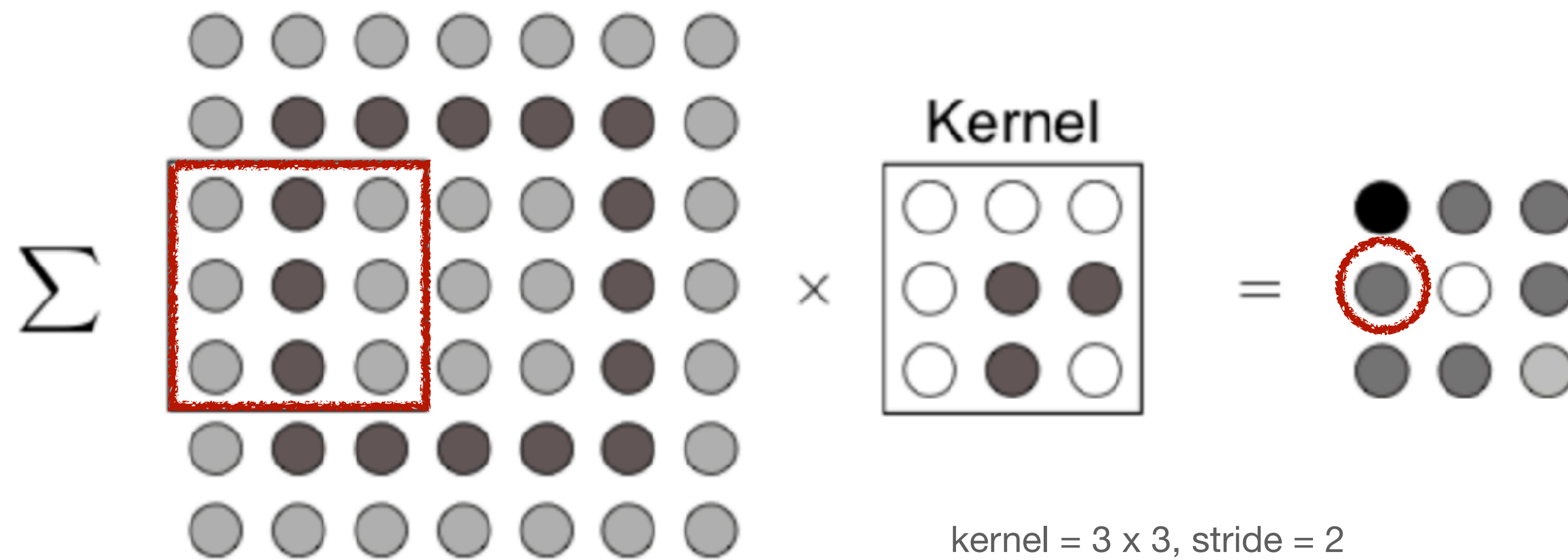
# Fine-tuning your network

- Add different types of layers



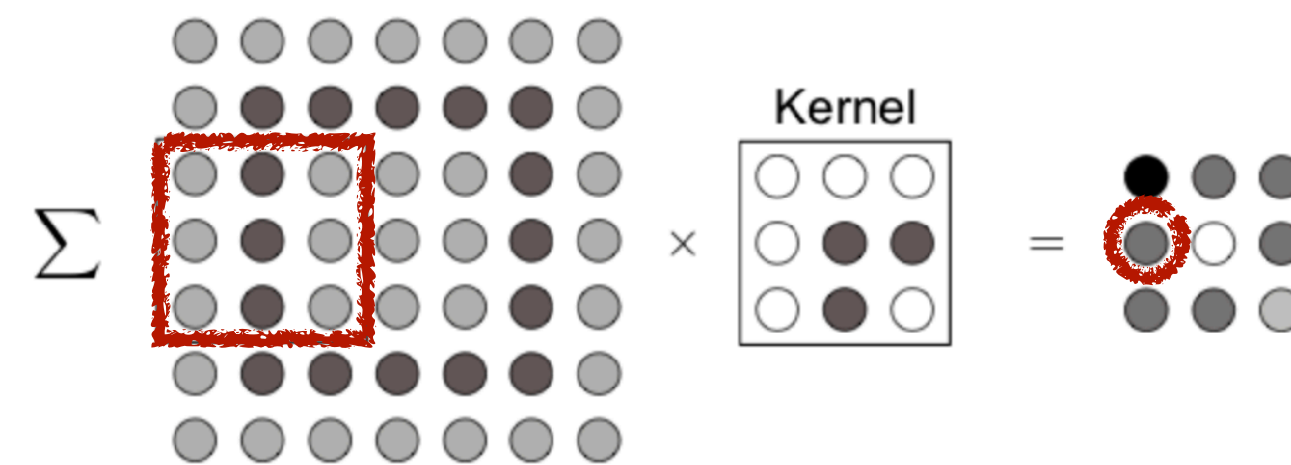
# Fine-tuning your network

- Add different types of layers

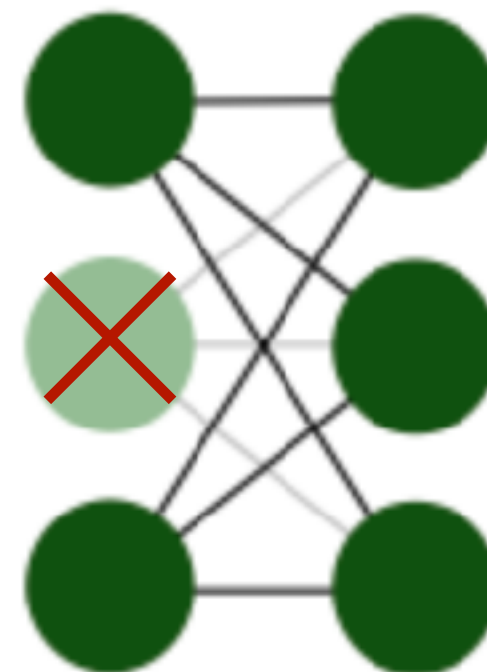


# Fine-tuning your network

- Add different types of layers



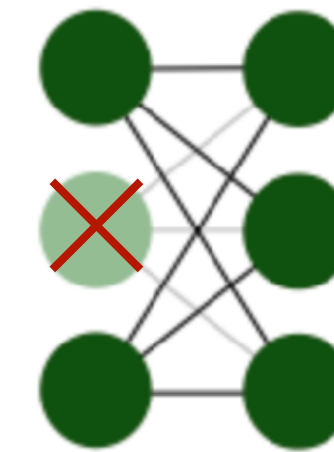
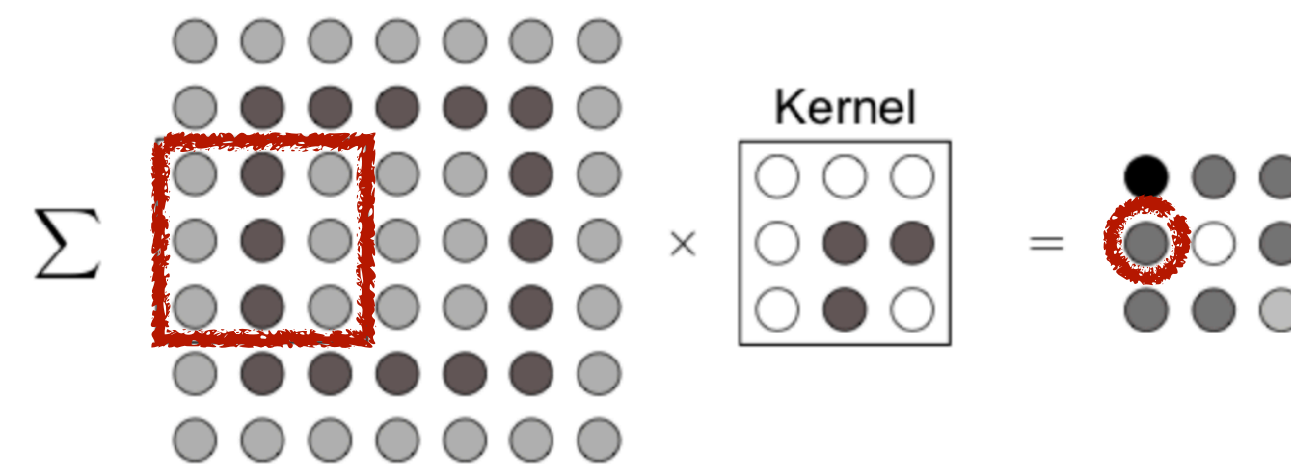
DROPOUT:



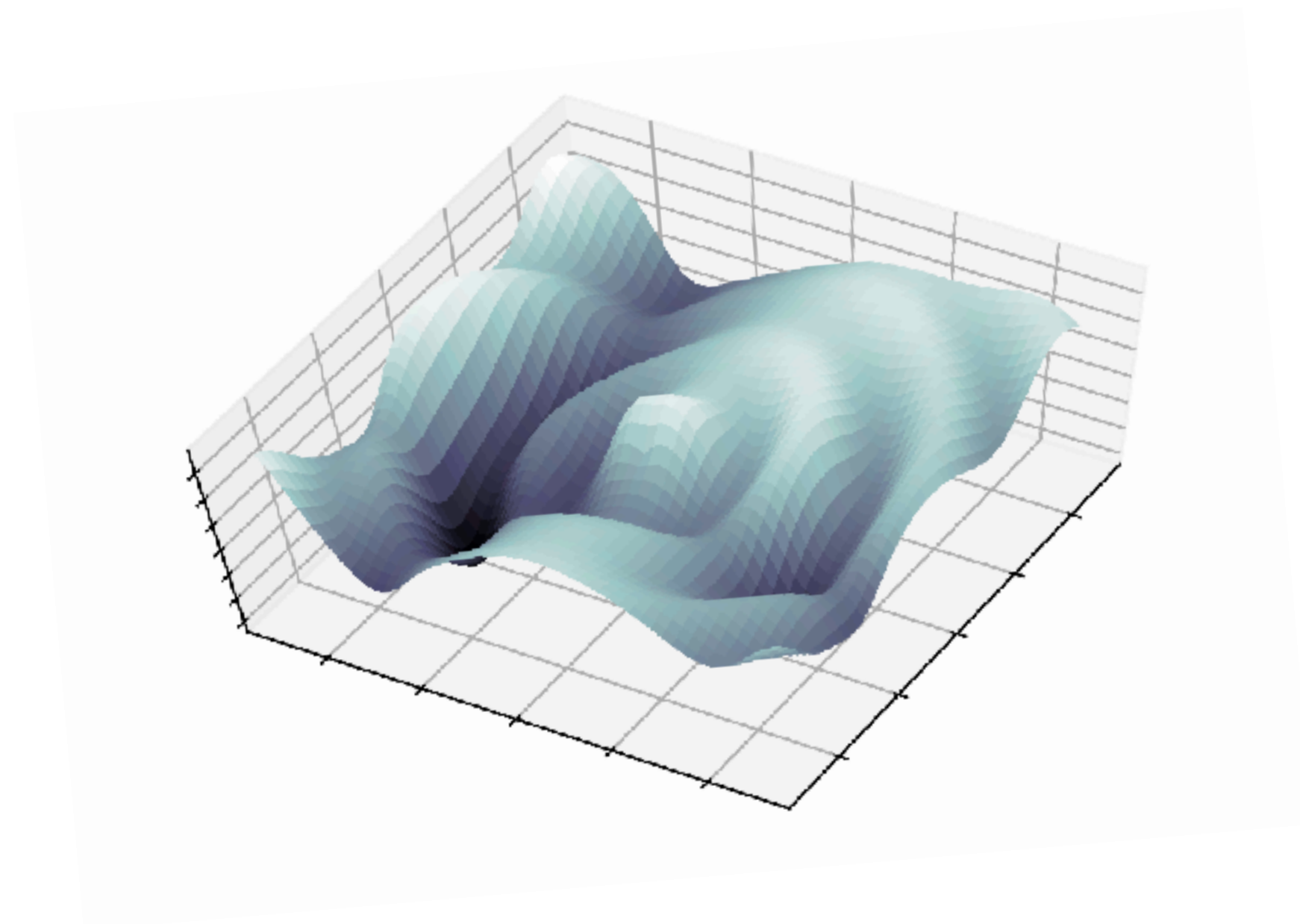


# Fine-tuning your network

- Add different types of layers

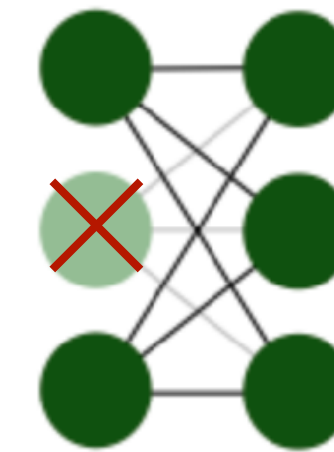
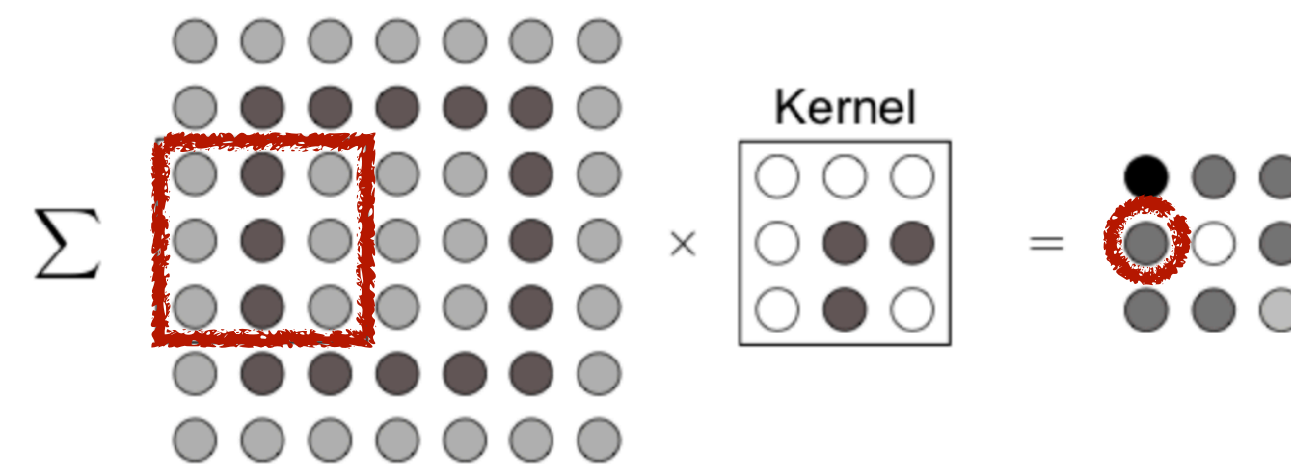


- Vary learning rate

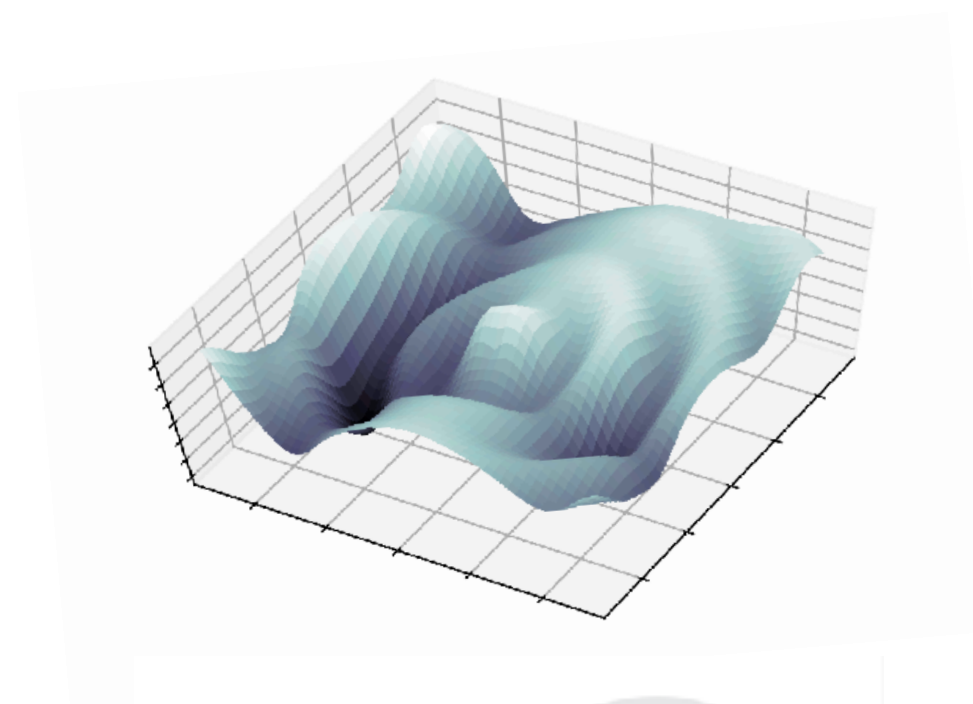


# Fine-tuning your network

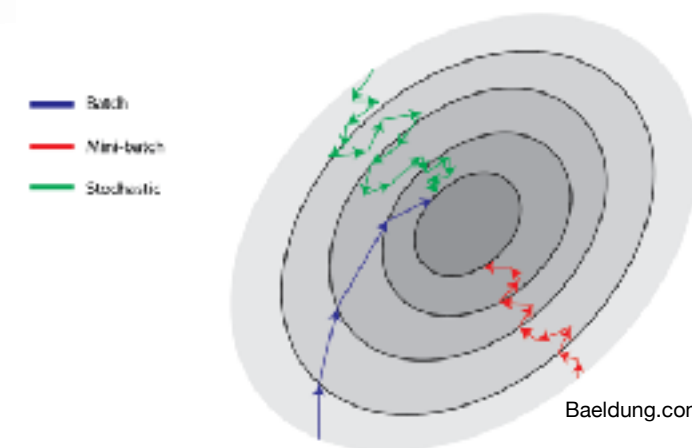
- Add different types of layers



- Vary learning rate



- Vary batch size



More tips and links at the end of Notebook 1!

# Fine-tuning your network

<https://tms-dipc.org/hands-on-information/>

## Topological Matter School DIPC 2022: Notebook 1

In the lecture we learned how topology can be used to stabilize entanglement in the quantum computing context. In this notebook we will get hands-on experience diagonalizing Su-Schrieffer-Heeger model and learn to classify its phases: topological and trivial one.

Authors: Eliska Greplova, Guliuxin Jin, Naoual El Yazidi

Structurally based on [this](#) PyTorch tutorial

```
[ ] # First we load the libraries
import numpy as np
import scipy as sp
import matplotlib.pyplot as plt
import matplotlib
from sklearn.utils import shuffle

## Machine learning related libraries:
import torch
import torch.nn as nn # base class used to develop all neural network models
from torch.utils.data import DataLoader # easy and organized data loading to the ML model
from torch.utils.data import Dataset #for nice loadable dataset creation
```



BREAK 20 mins

**Paper: "We used 8 2080Ti GPUs  
to train our..."**



# Exercise Notebooks

<https://tms-dipc.org/hands-on-information/>

## Notebook 1

- supervised learning topological and trivial SSH
- data preparation and loading
- build your own neural network and train it!!

## Notebook 2

- supervised learning topological and trivial SSH  
with limited data
- data slicing info

**You will work in team: MAKE GROUPS OF THREE PLEASE!**