CME 213, ME 339—Spring 2021

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“Physics is the universe's operating system.” (Steven R Garman)

Final project

Goal

Implementing a neural network in order to recognize hand-written digits

Logistics

Turn in	Date	Grade
Preliminary report + code	Friday May 28th	20%
Final report (4 pages) + code	Sunday June 6th	80%

Preliminary report

Focus is on correctness

Final report

Profiling and analysis, performance, quality of report

What are the performance bottlenecks in your code?

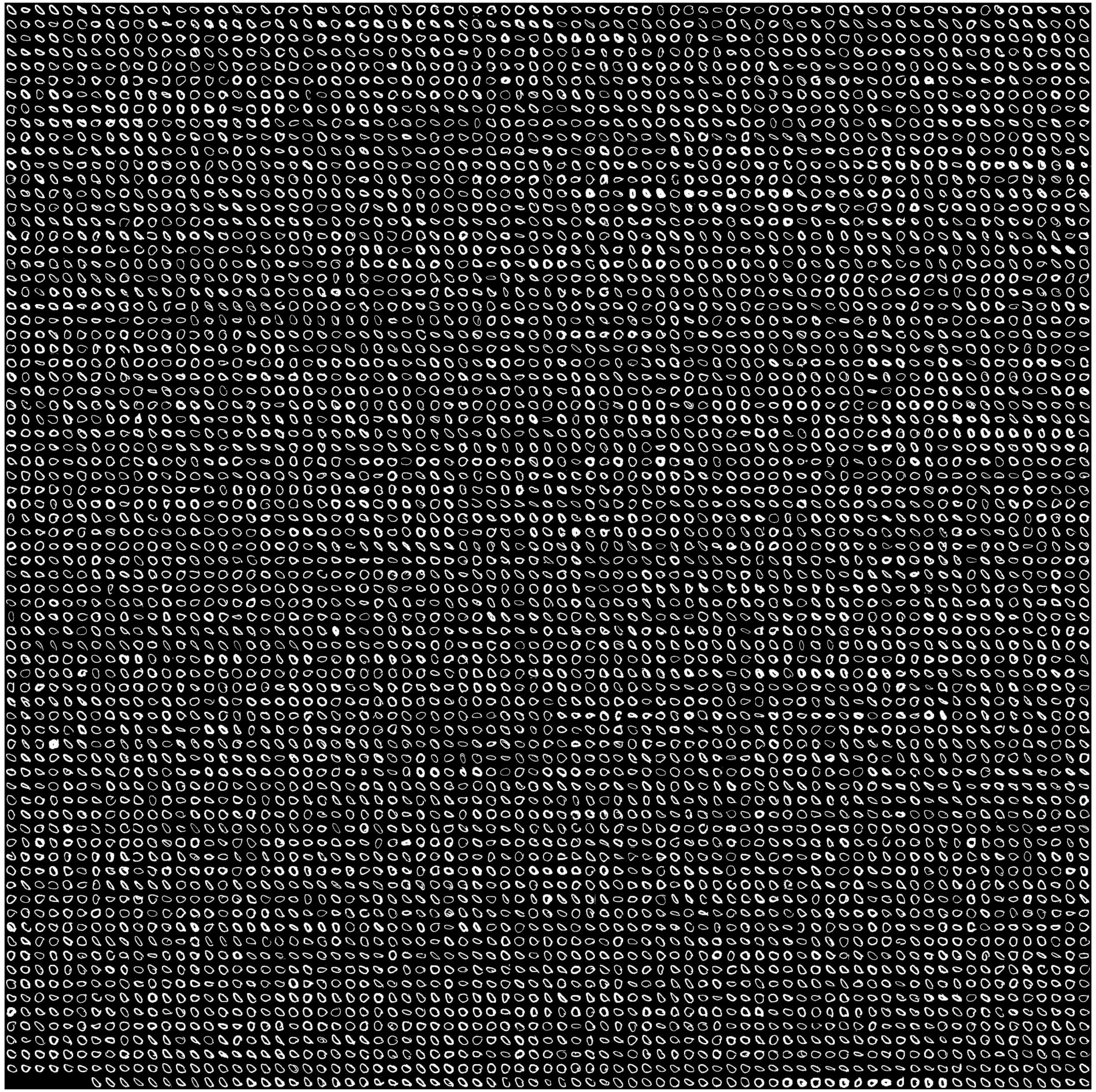
How can they be addressed?

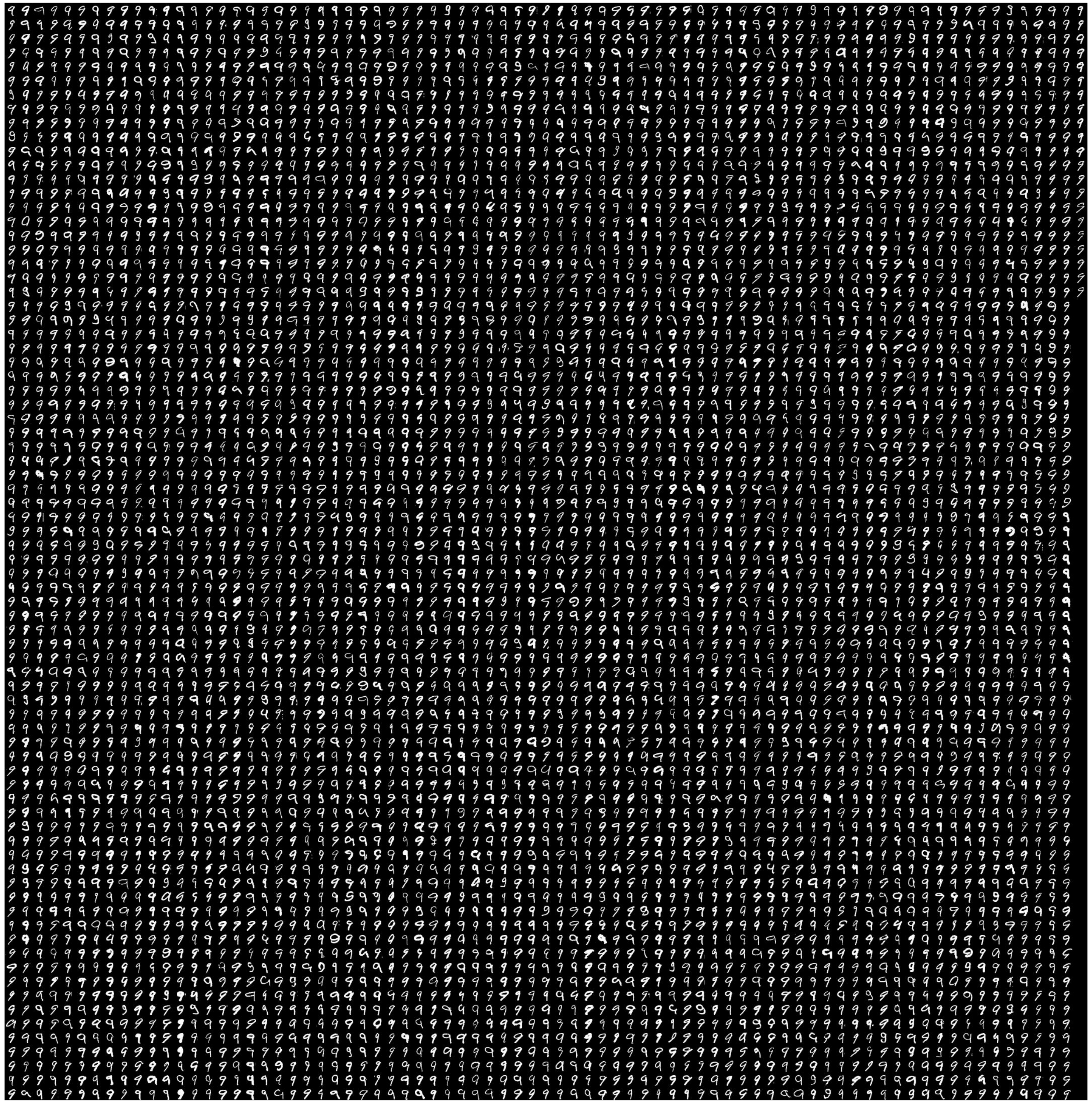
Correctness

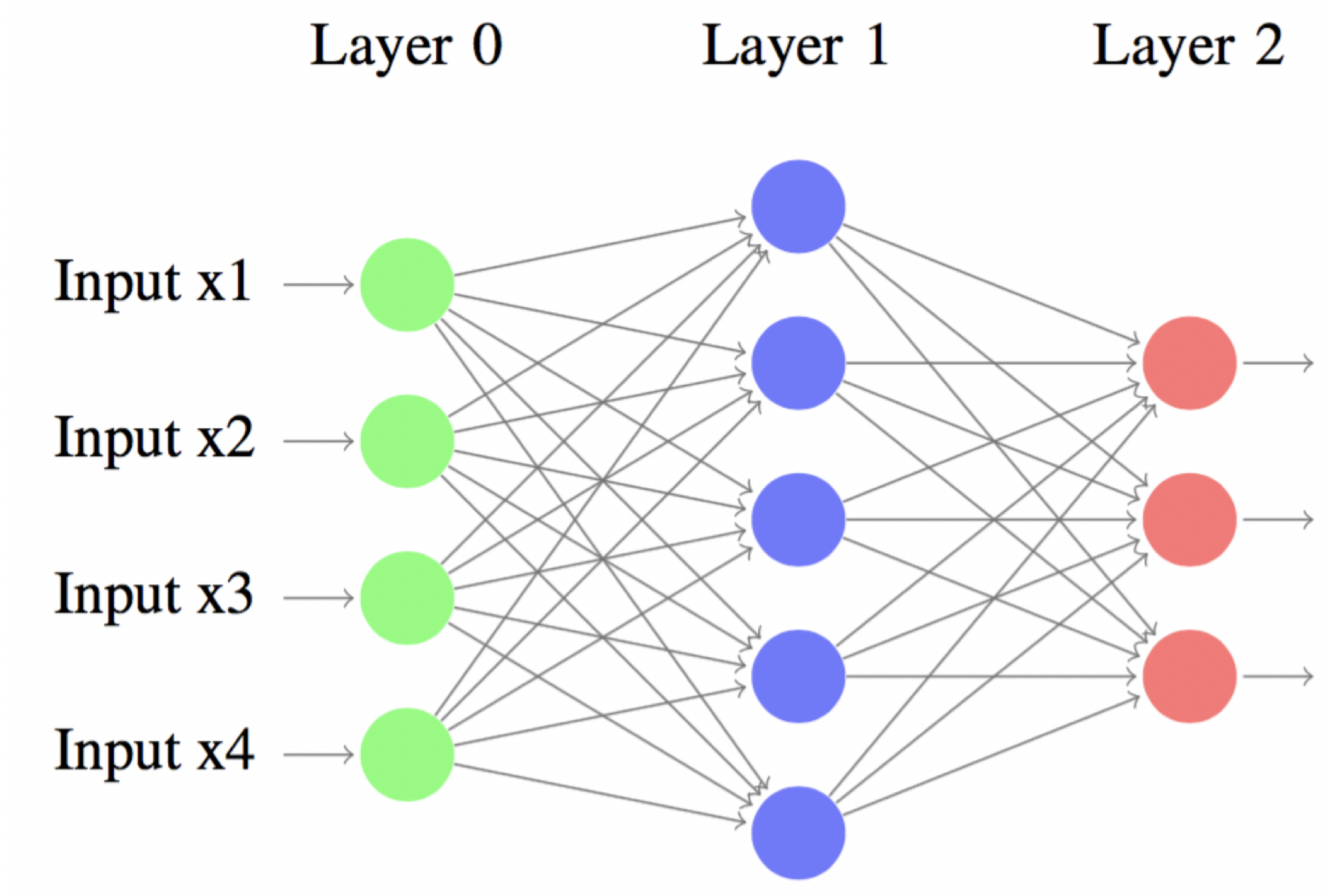
Discuss your strategy to test your code

Test outputs for valid inputs

Make sure you distinguish roundoff errors from genuine bugs






Layer 0
Layer 1
Layer 2
Input x1
Input x2
Input x3
Input x4

Input layer: image

Hidden layer: `-n num`; variable size

Output layer: `softmax` vector with 10 digits

Softmax

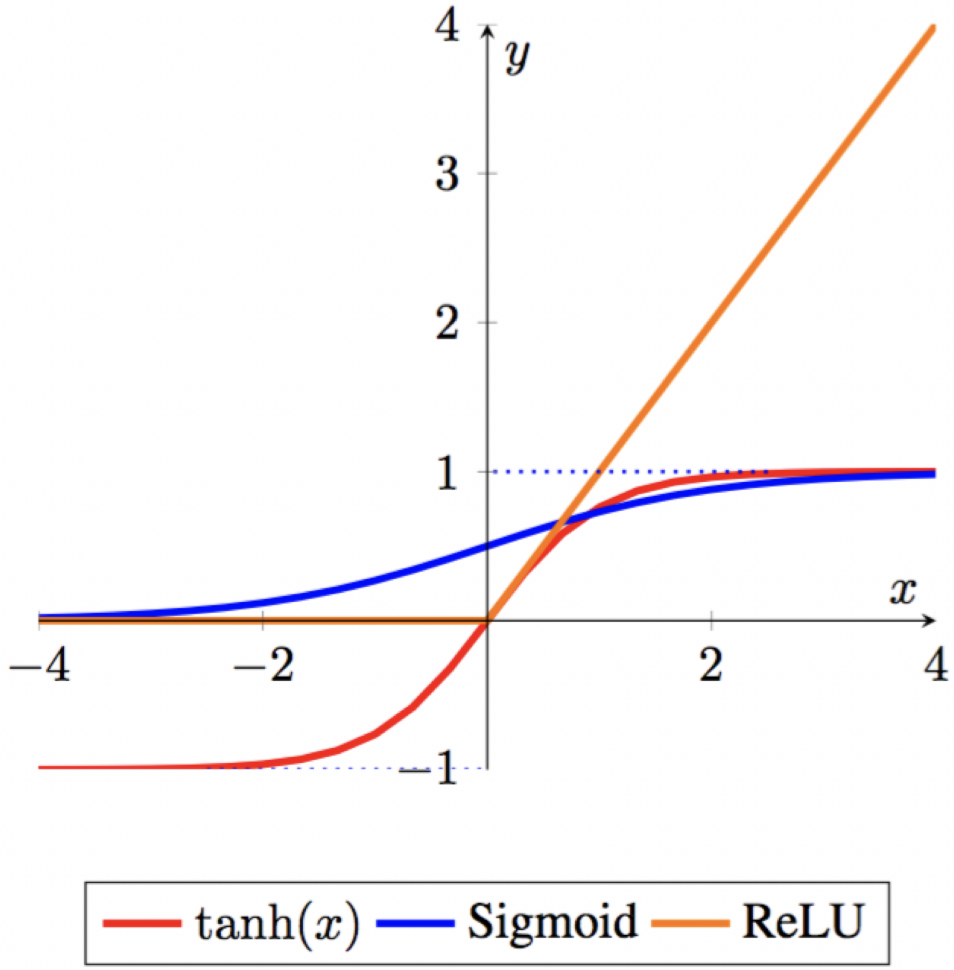
$$\mathrm{softmax}(z)_j = \frac{\exp(z_j)}{\sum_{i=0}^{9} \exp(z_i)}$$

Interpreted as a probability

Each layer is a matrix multiplication and a non-linear function

$$z = Wx + b$$

$$a = \sigma(z)$$



We will use sigmoid

How do you train a network?

Many methods but most are based on gradient descent

Error function

$$J(p) = \frac{1}{N} \sum_{i=1}^{N} \mathrm{error}^{(i)}(y_i, \hat{y}_i)$$

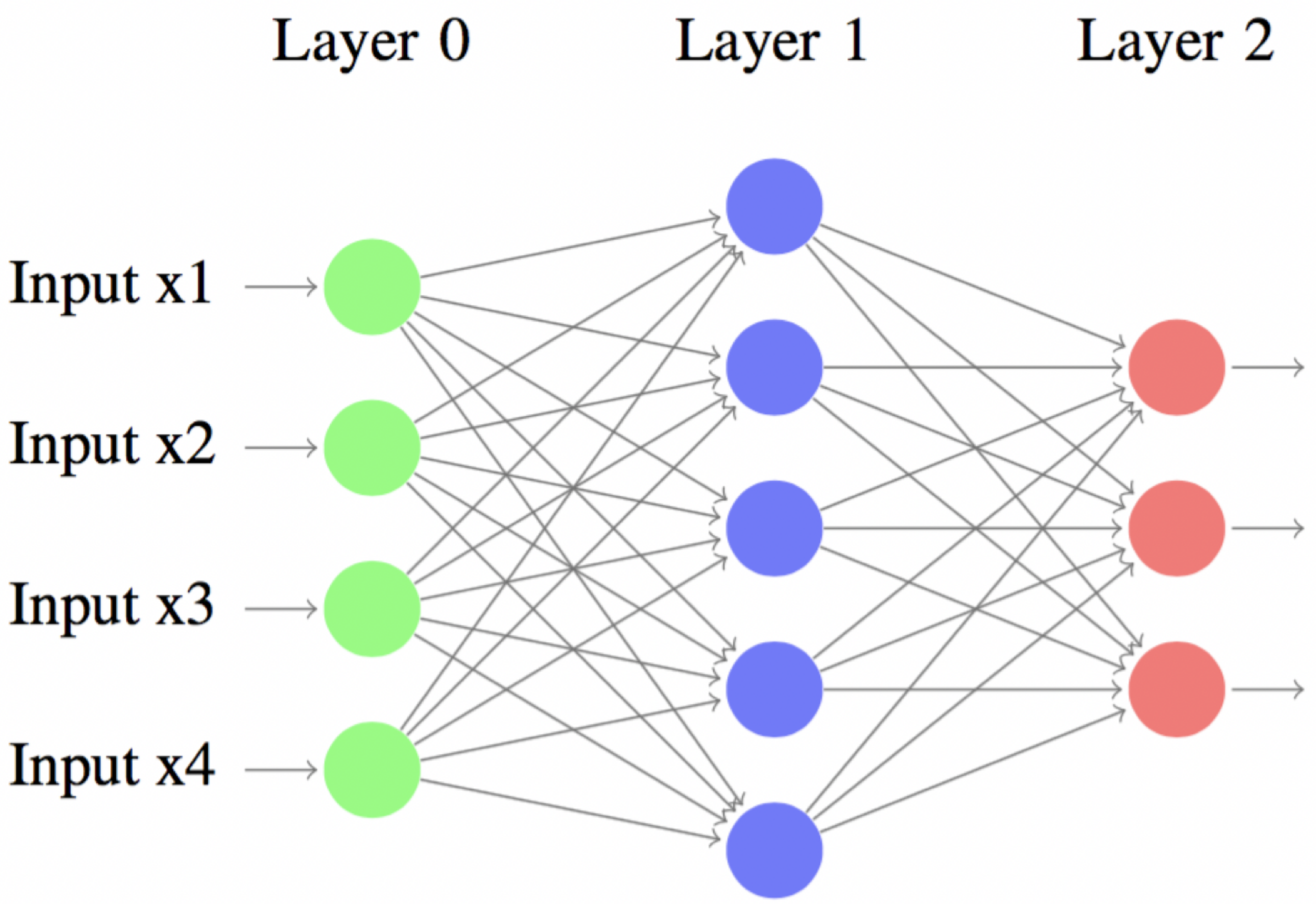
p: weights and biases of network = all parameters

Gradient update

$$p \leftarrow p - \alpha \nabla_p J$$

Gradient is computed by repeated application of the chain rule

Backpropagation


Layer 0
Layer 1
Layer 2
Input x1
Input x2
Input x3
Input x4

Stochastic gradient descent

$$J_r(p) = \frac{1}{N} \sum_{i \in \text{random subset}} \text{error}^{(i)}(y_i, \hat{y}_i)$$

$$p \leftarrow p - \alpha \nabla_p J_r$$

If we use a small subset, this allows more updates to the DNN coefficients

$\Rightarrow$ more accurate

Randomness of subset selection allows avoiding local minima and escaping saddle points

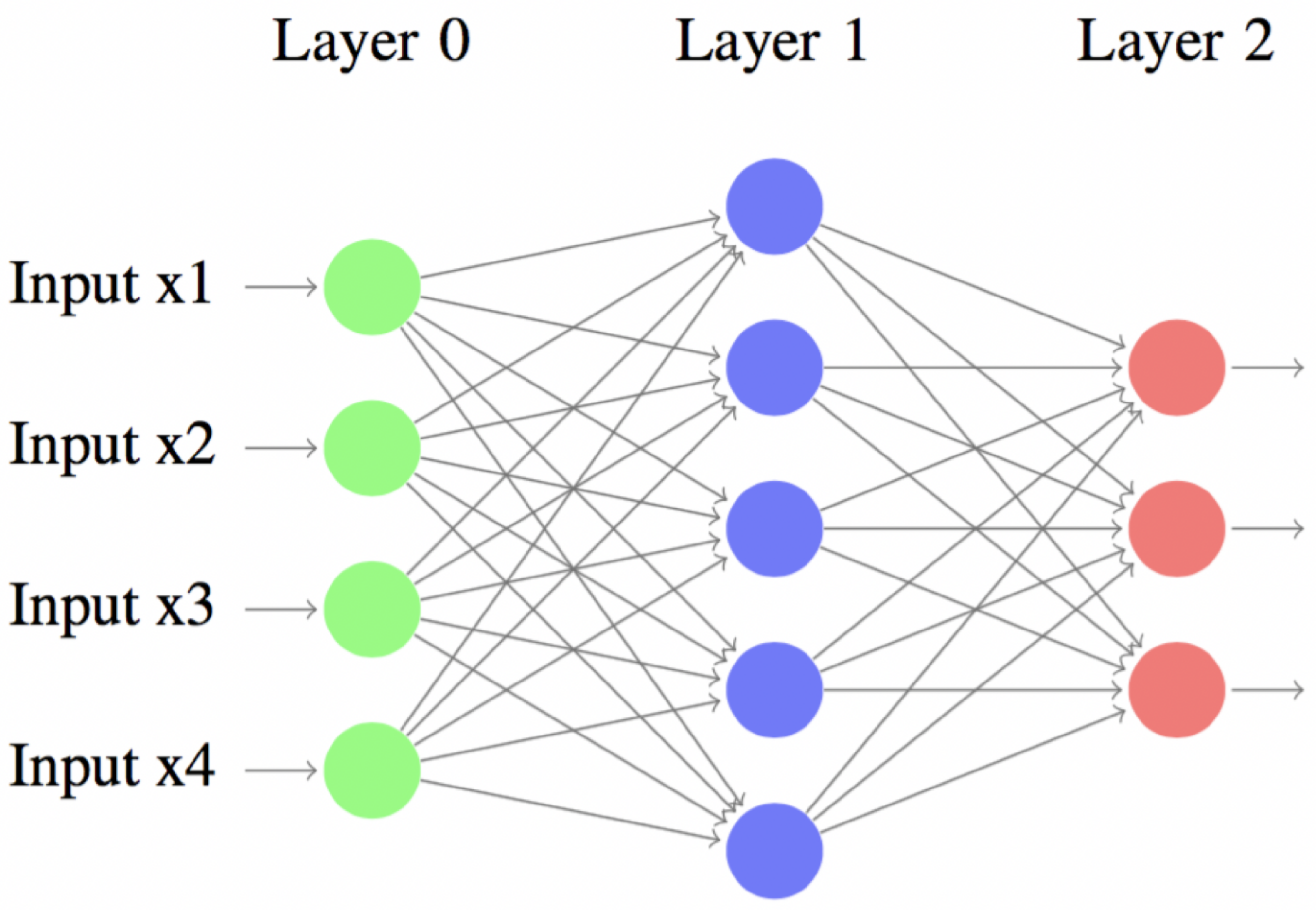
$\Rightarrow$ better convergence

Sequence of operations

Forward pass = left to right; DNN prediction; compare with label

Backward propagation = right to left; chain rule; compute gradient and update DNN

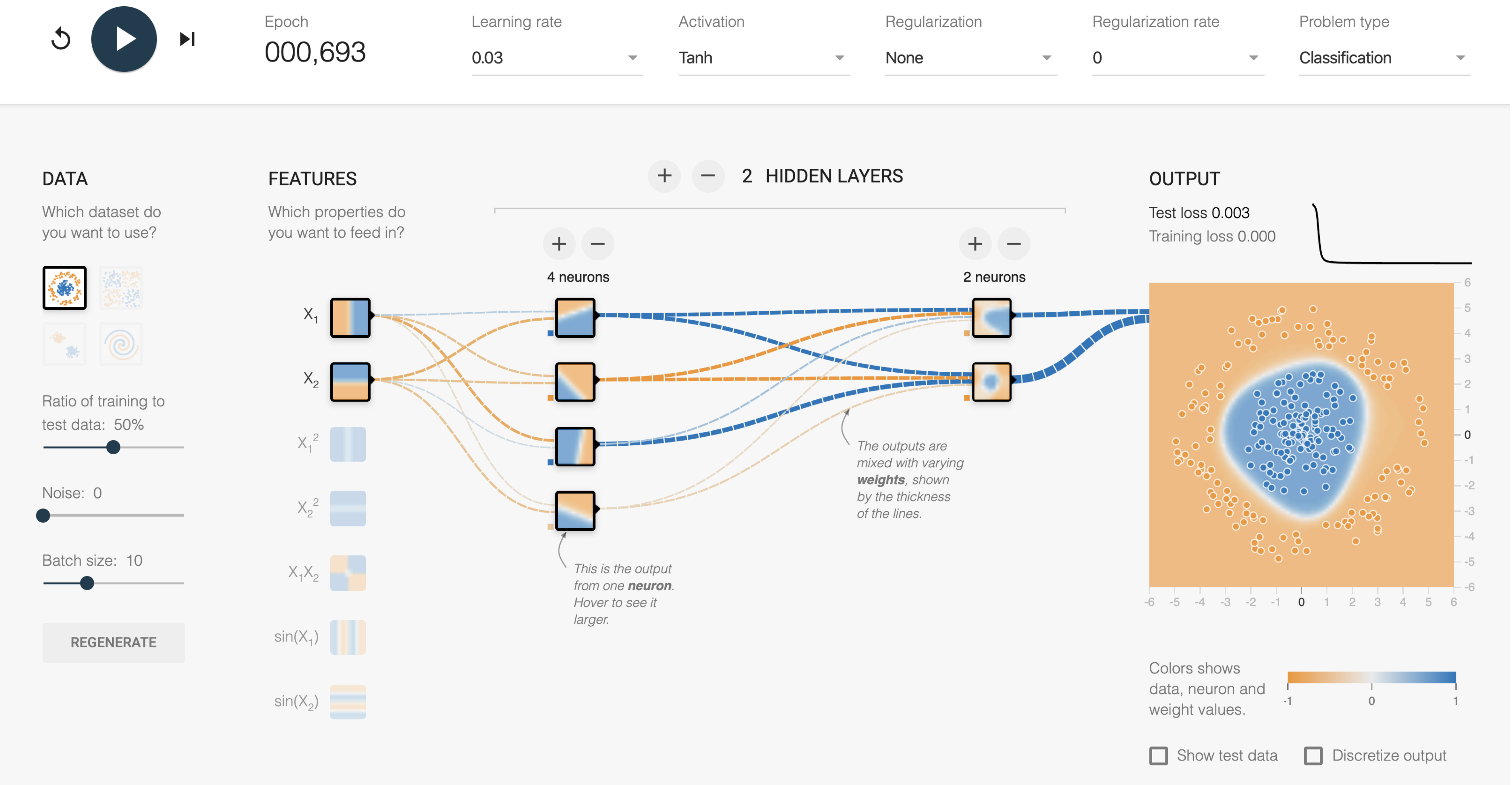
Iterate until convergence

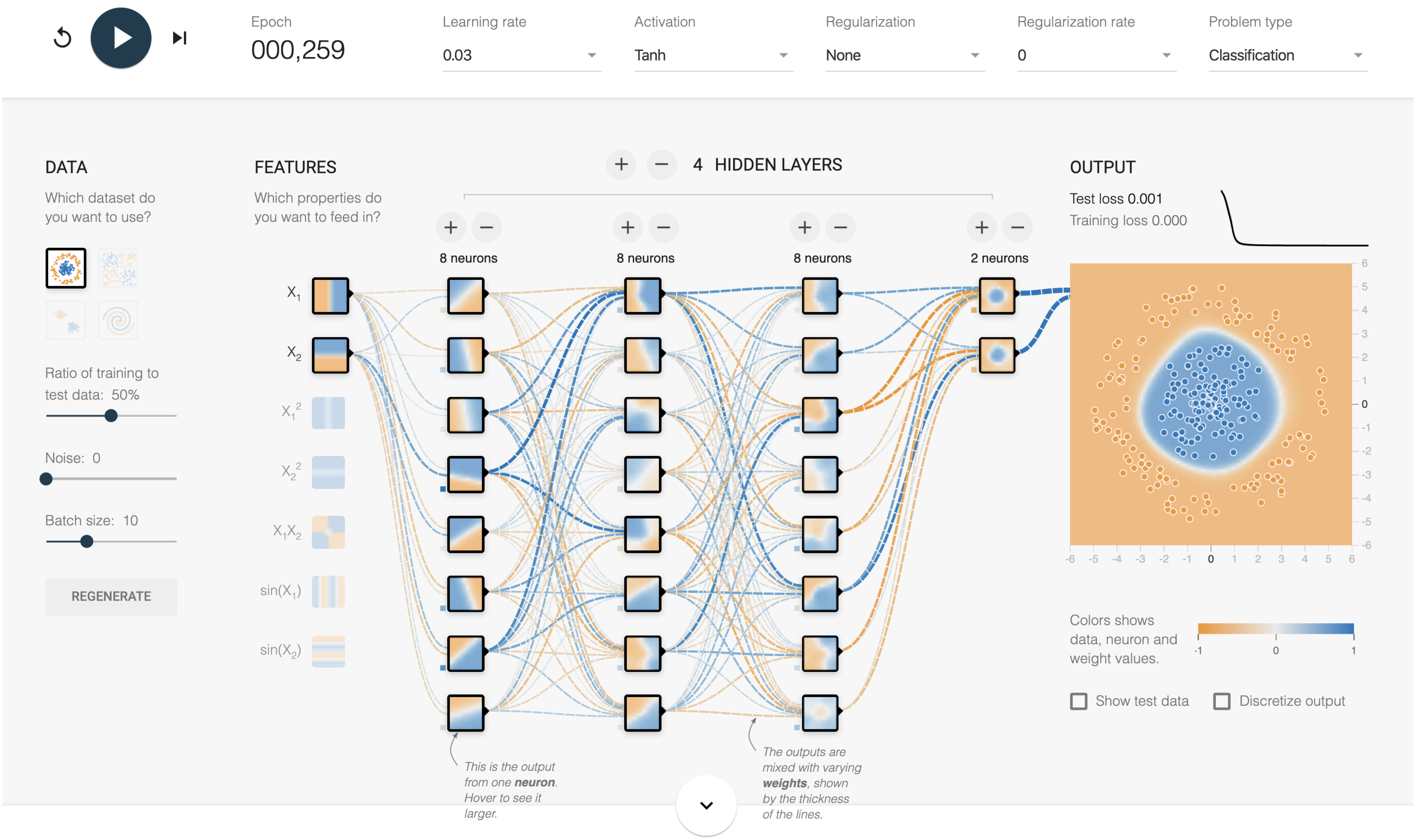

Layer 0
Layer 1
Layer 2
Input x1
Input x2
Input x3
Input x4

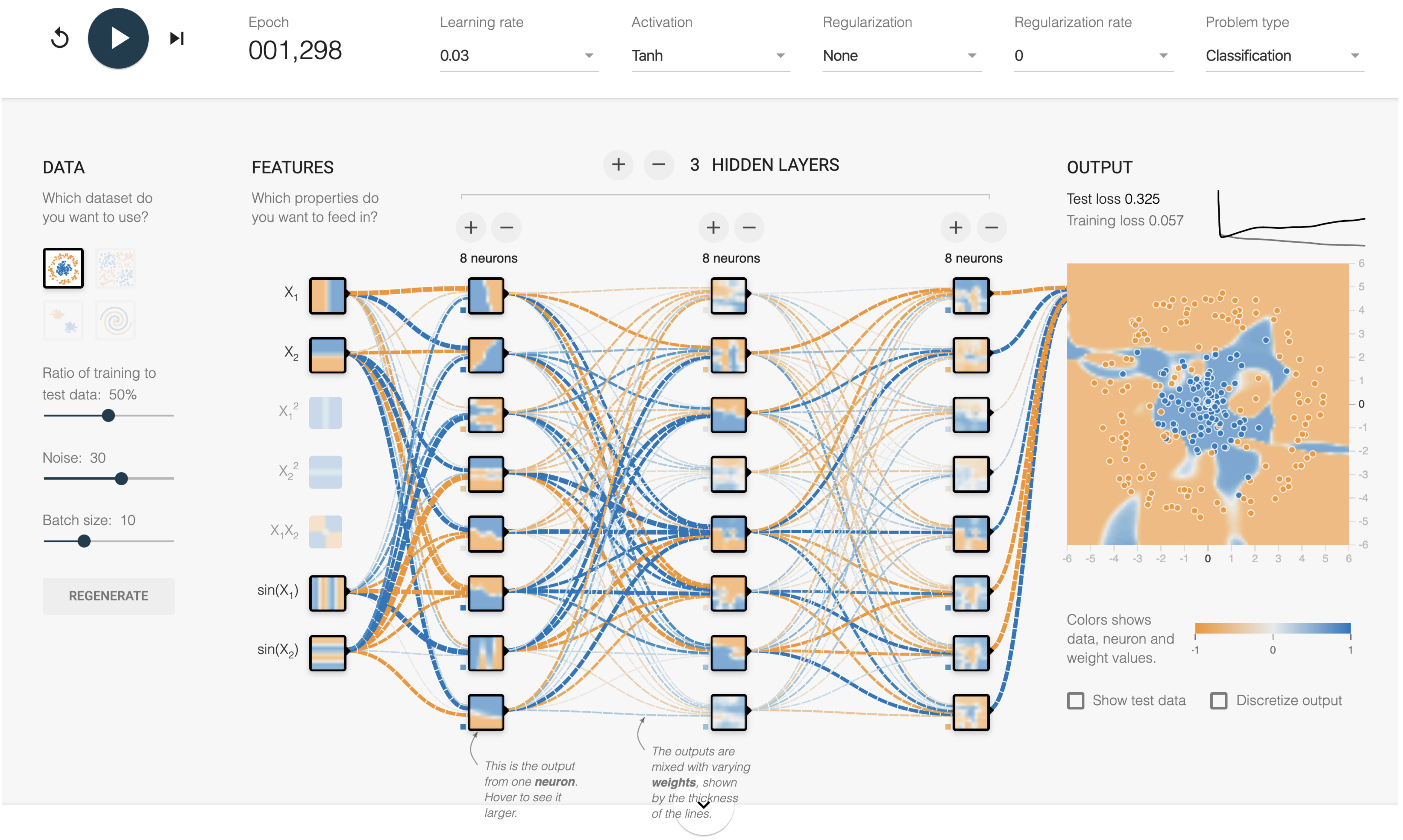
Core building blocks to implement

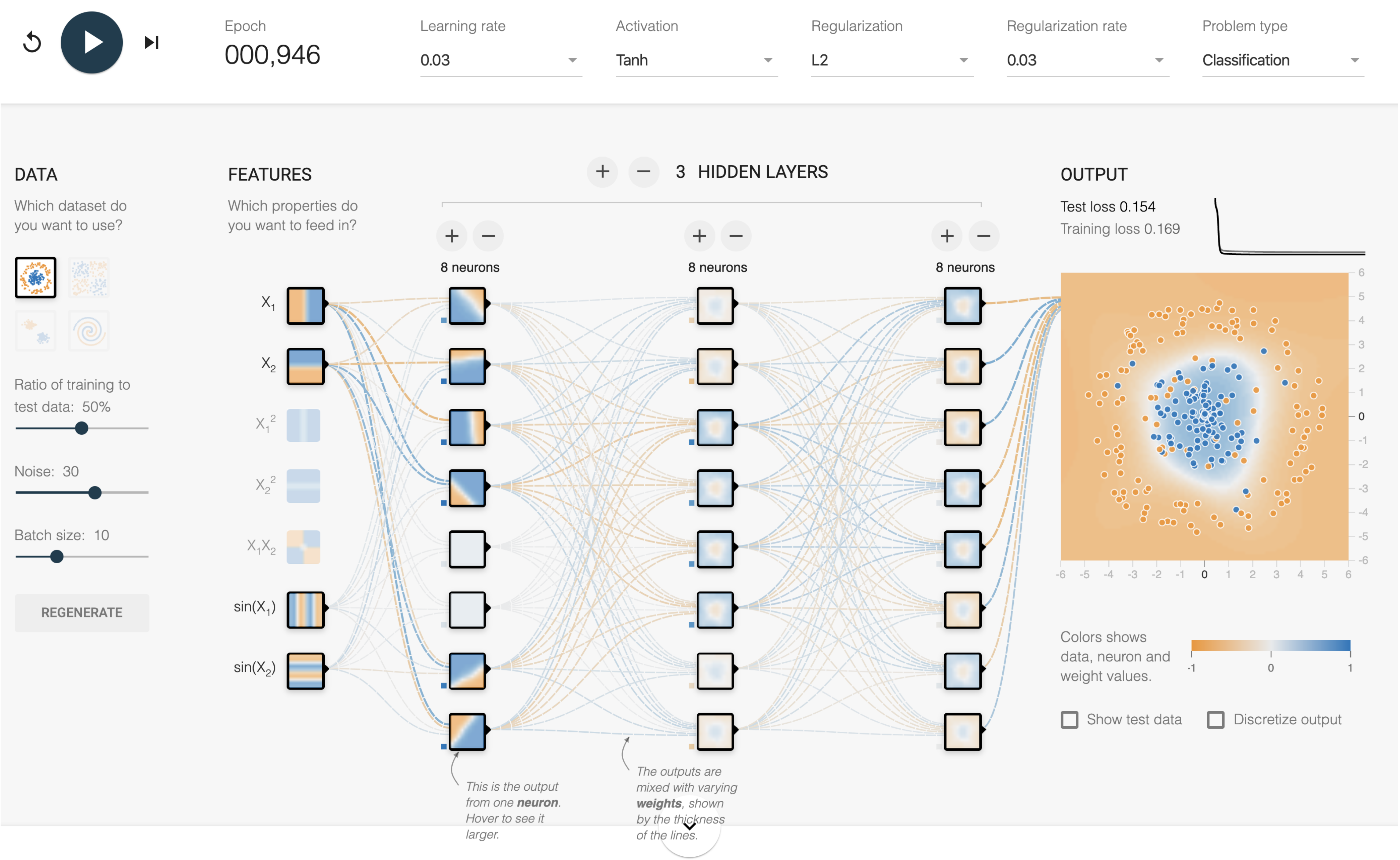
- Matrix-matrix products
- Non-linear activation functions

https://playground.tensorflow.org


Epoch
000,693
Learning rate
0.03
Activation
Tanh
Regularization
None
Regularization rate
0
Problem type
Classification
DATA
Which dataset do you want to use?
Ratio of training to test data: 50%
Noise: 0
Batch size: 10
REGENERATE
FEATURES
Which properties do you want to feed in?
X1
X2
X1^2
X2^2
X1X2
sin(X1)
sin(X2)
2 HIDDEN LAYERS
4 neurons
2 neurons
This is the output from one neuron. Hover to see it larger.
The outputs are mixed with varying weights, shown by the thickness of the lines.
OUTPUT
Test loss 0.003
Training loss 0.000
Colors shows data, neuron and weight values.
Show test data
Discretize output


Epoch
000,259
Learning rate
0.03
Activation
Tanh
Regularization
None
Regularization rate
0
Problem type
Classification
DATA
Which dataset do you want to use?
Ratio of training to test data: 50%
Noise: 0
Batch size: 10
REGENERATE
FEATURES
Which properties do you want to feed in?
X1
X2
X1 2
X2 2
X1X2
sin(X1)
sin(X2)
4 HIDDEN LAYERS
8 neurons
8 neurons
8 neurons
2 neurons
This is the output from one neuron. Hover to see it larger.
The outputs are mixed with varying weights, shown by the thickness of the lines.
OUTPUT
Test loss 0.001
Training loss 0.000
Colors shows data, neuron and weight values.
-1
0
1
Show test data
Discretize output


Epoch
001,298
Learning rate
0.03
Activation
Tanh
Regularization
None
Regularization rate
0
Problem type
Classification
DATA
Which dataset do you want to use?
Ratio of training to test data: 50%
Noise: 30
Batch size: 10
REGENERATE
FEATURES
Which properties do you want to feed in?
X_1
X_2
X_1^2
X_2^2
X_1X_2
$\sin(X_1)$
$\sin(X_2)$
3 HIDDEN LAYERS
8 neurons
8 neurons
8 neurons
This is the output from one **neuron**. Hover to see it larger.
The outputs are mixed with varying **weights**, shown by the thickness of the lines.
OUTPUT
Test loss 0.325
Training loss 0.057
Colors shows data, neuron and weight values.
-1
0
1
Show test data
Discretize output


Epoch
000,946
Learning rate
0.03
Activation
Tanh
Regularization
L2
Regularization rate
0.03
Problem type
Classification
DATA
Which dataset do you want to use?
Ratio of training to test data: 50%
Noise: 30
Batch size: 10
REGENERATE
FEATURES
Which properties do you want to feed in?
3 HIDDEN LAYERS
8 neurons
8 neurons
8 neurons
This is the output from one neuron. Hover to see it larger.
The outputs are mixed with varying weights, shown by the thickness of the lines.
OUTPUT
Test loss 0.154
Training loss 0.169
Colors shows data, neuron and weight values.
Show test data
Discretize output

Regularization

$$J(p) = \frac{1}{N} \sum_{i=1}^{N} \mathrm{error}^{(i)}(y_i, \hat{y}_i) + \frac{1}{2}\,\lambda\,||p||_2^2$$

p: weights and biases of the network

$$z = Wx + b$$

$$a = \sigma(z)$$

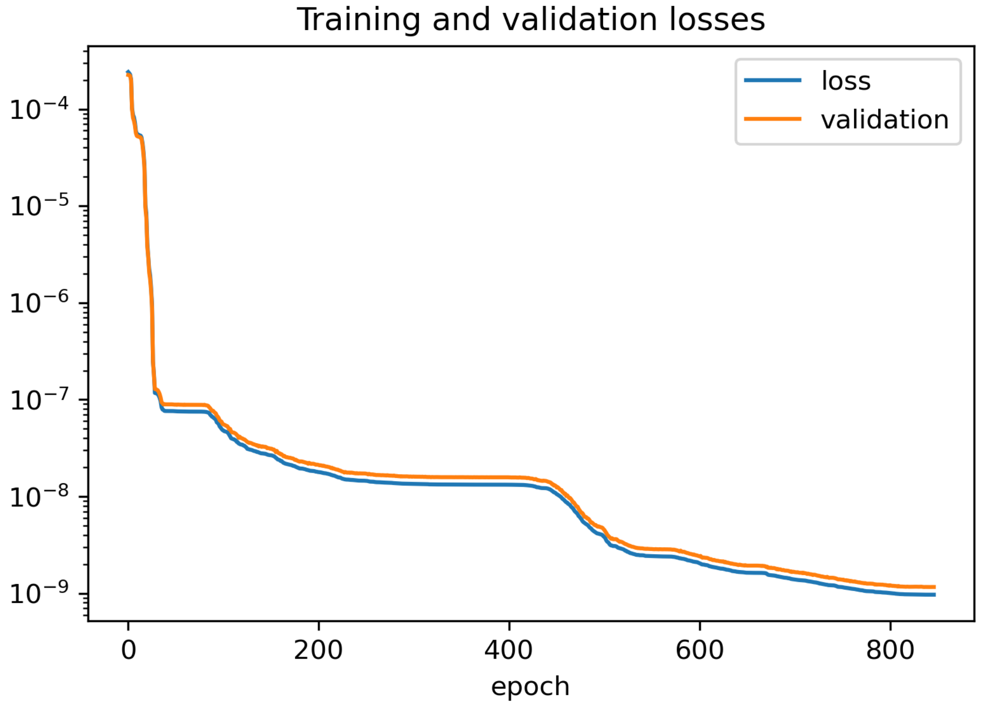
Regularization makes the DNN more linear

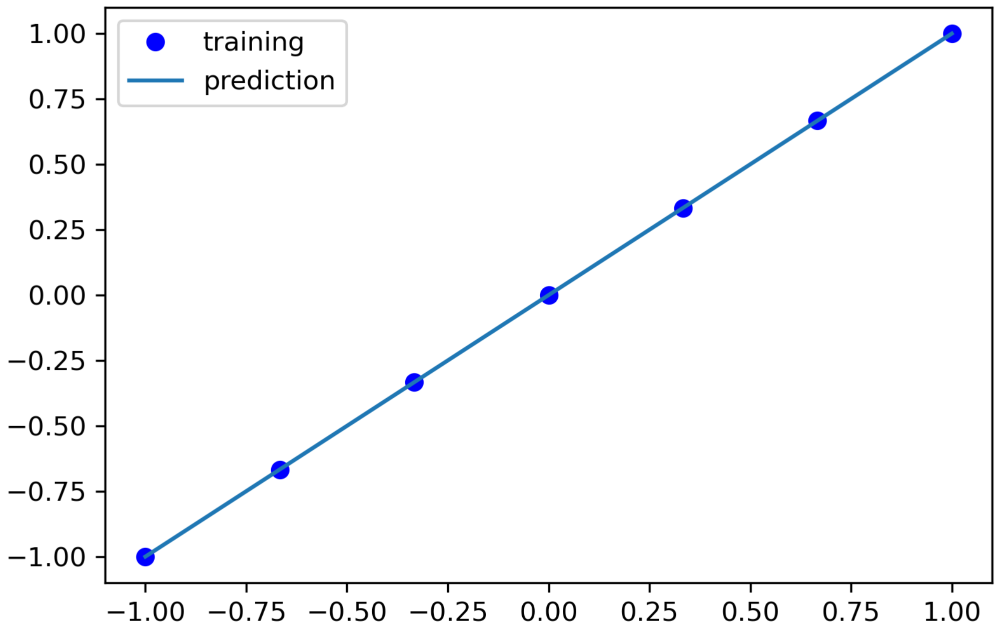
How can we figure out how much regularization is needed?

Training set: used to minimize loss; involved in defining the gradient

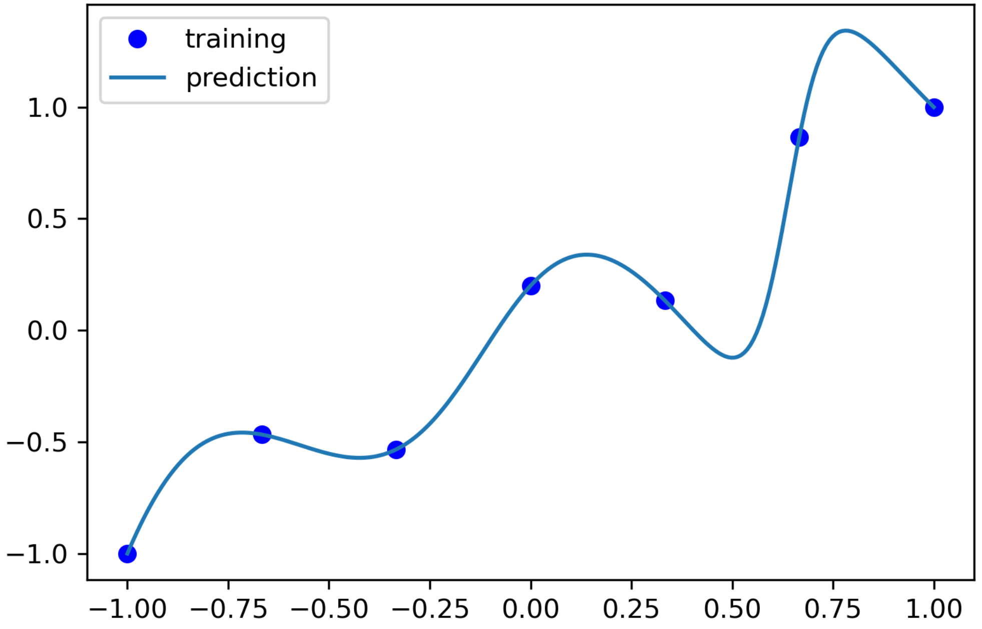
Validation set: used to evaluate model; how accurate is it? Avoids overfitting

Example: small 2-layer DNN with width 8

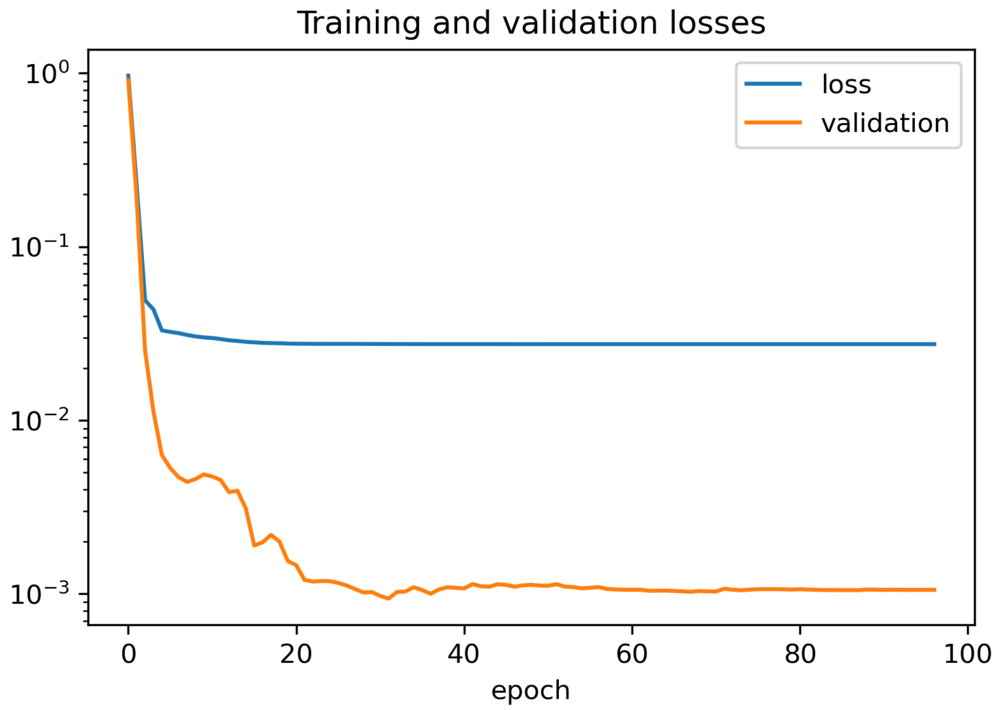


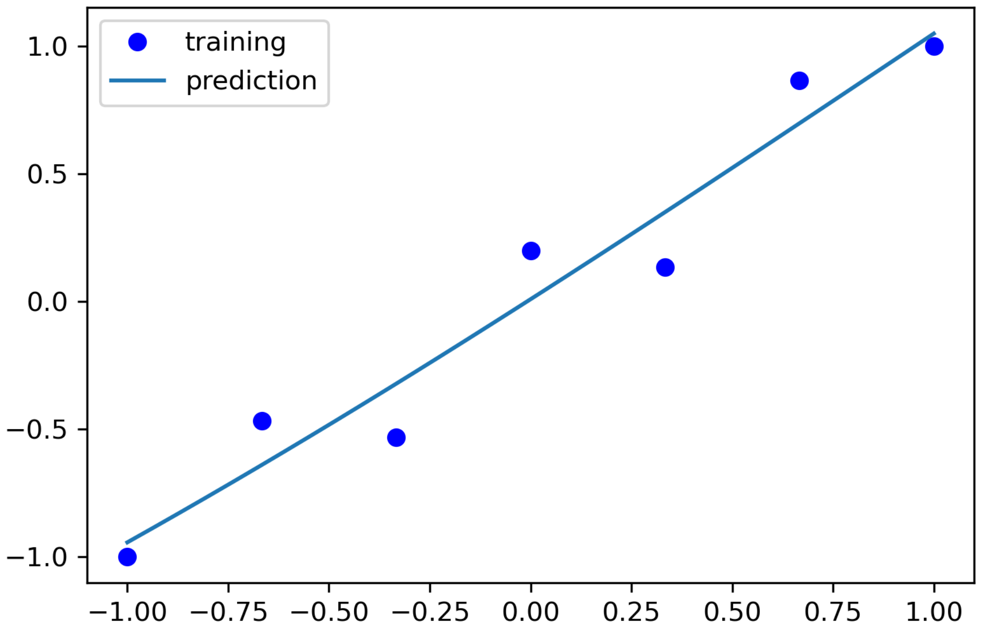


With noise added to data

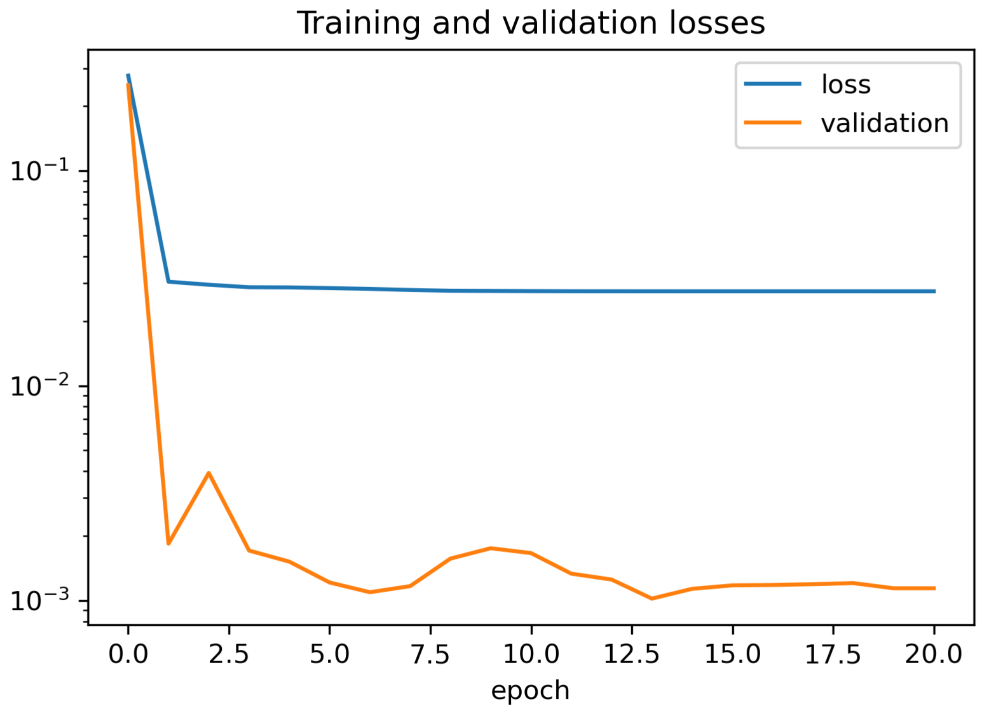


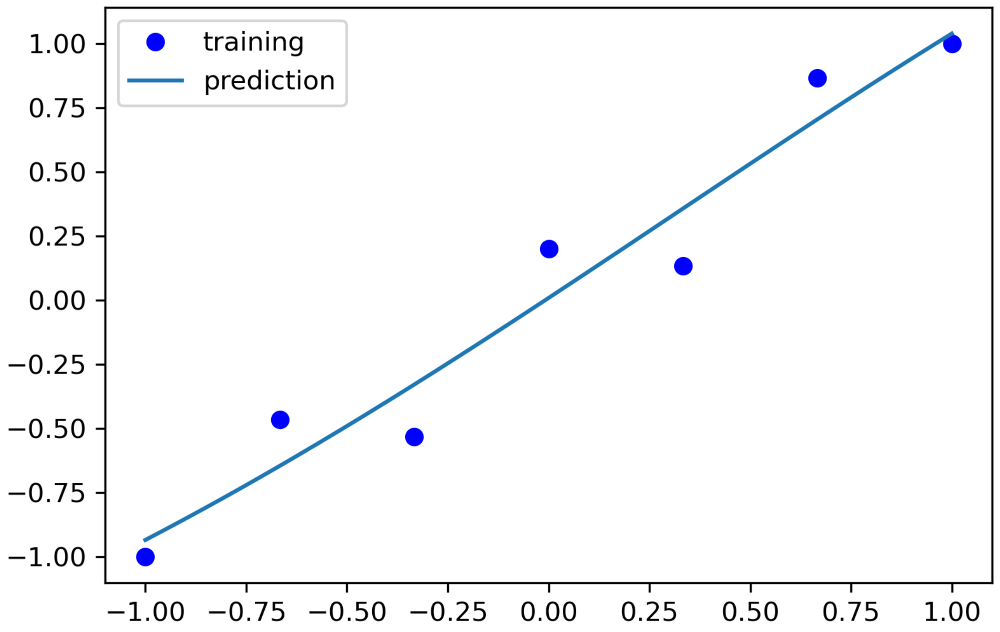
Fix 1: reduce the size of the DNN; for example with width 1

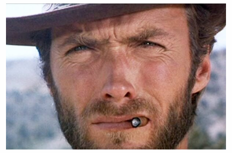
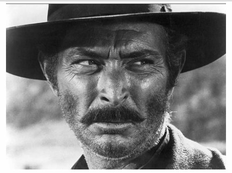
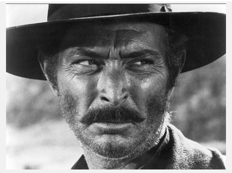
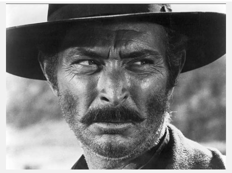
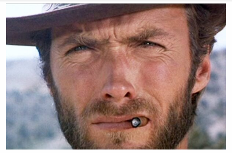
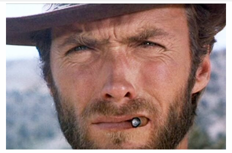




Fix 2: add regularization, e.g., $\lambda = 10^{-3}$





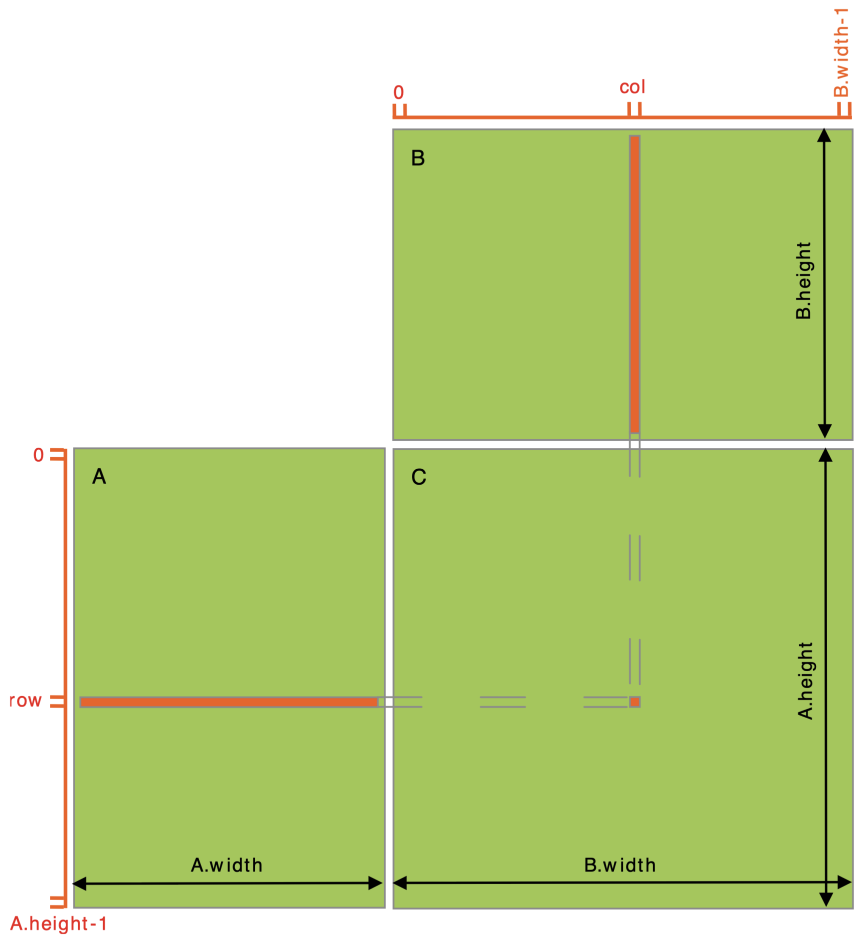
Training	Validation	Diagnostic
		Overfitting; ↑ λ
		Too much regularization; ↓ λ
		Regularization is good

- Training set: optimize DNN parameters
- Validation set: optimize regularization

Two main tasks in the project

1. Implement a matrix-matrix product (GEMM) algorithm
2. Implement the MPI algorithm for distributed memory

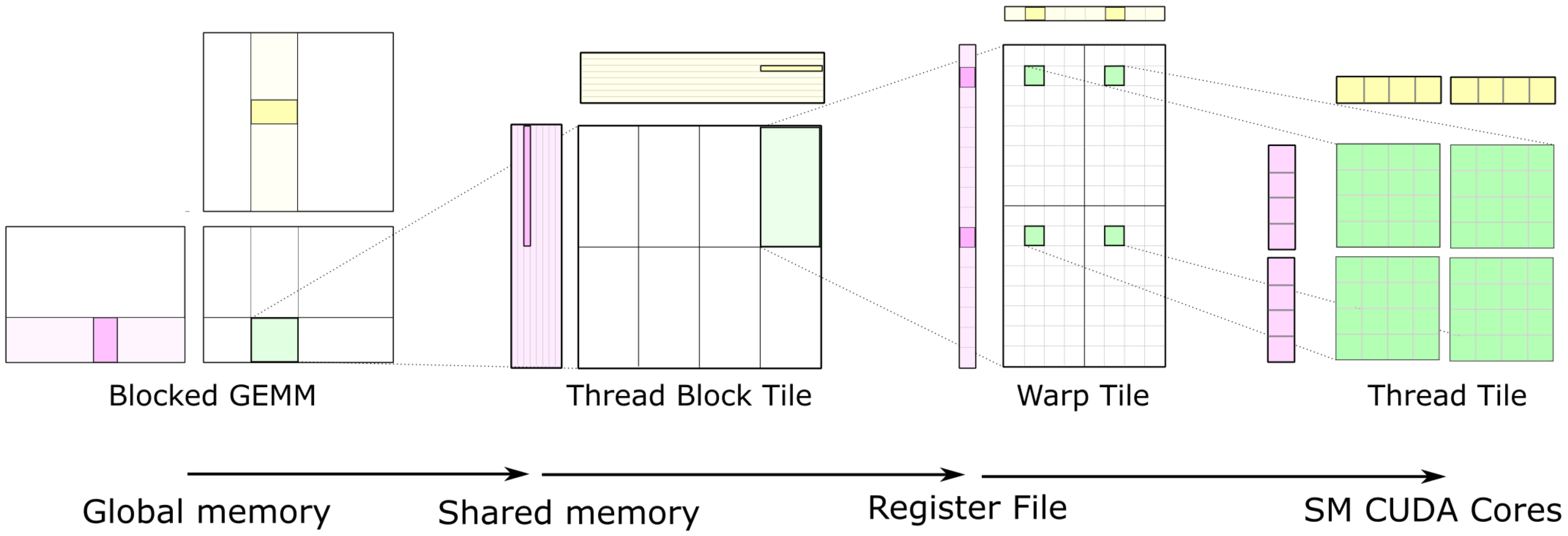
Naive implementation; shared memory is not used



GEMM performance

The key is to increase the arithmetic intensity.

This requires reducing the memory traffic.


Blocked GEMM
Thread Block Tile
Warp Tile
Thread Tile
Global memory
Shared memory
Register File
SM CUDA Cores

$$c_{ij} = \sum_k a_{ik} b_{kj}$$

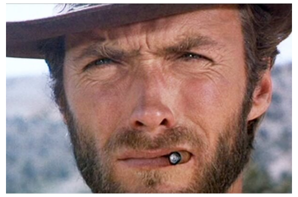
$$c_{ij} \leftarrow c_{ij} + a_{ik} b_{kj}$$

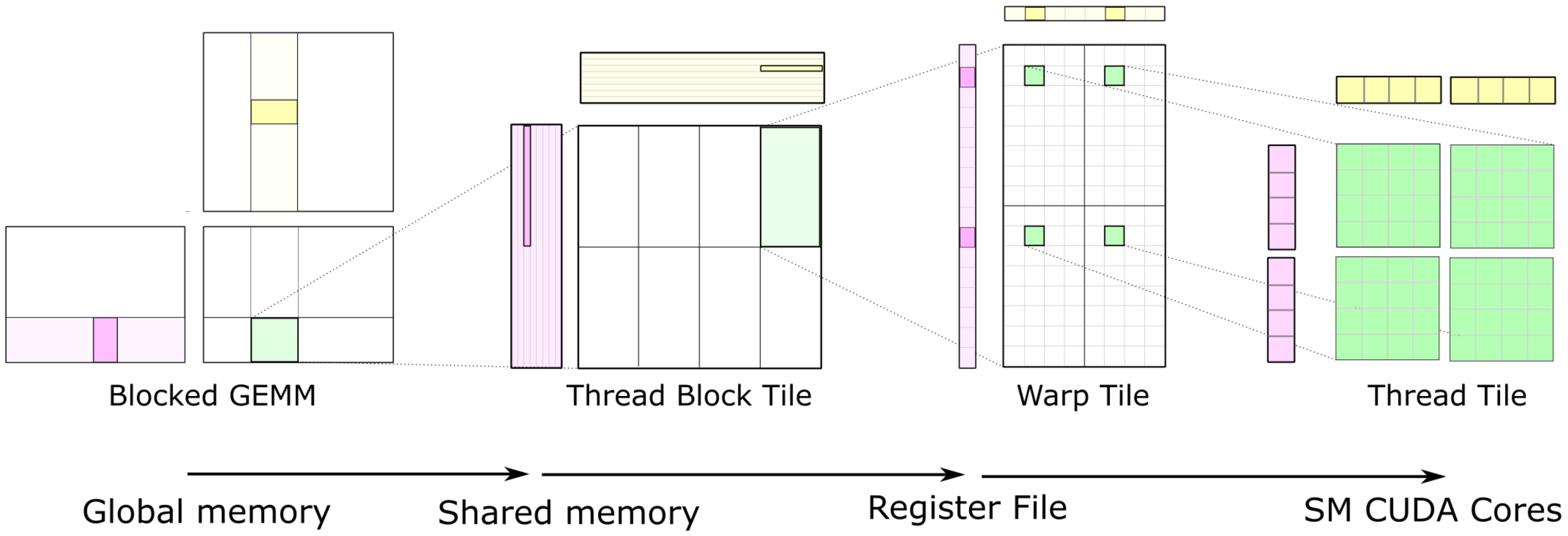
$$c_{ij} \leftarrow c_{ij} + a_{ik} b_{kj}$$

Block size: b

Memory traffic: $2b$

Flops: b^2

High arithmetic intensity 


Blocked GEMM
Thread Block Tile
Warp Tile
Thread Tile
Global memory
Shared memory
Register File
SM CUDA Cores

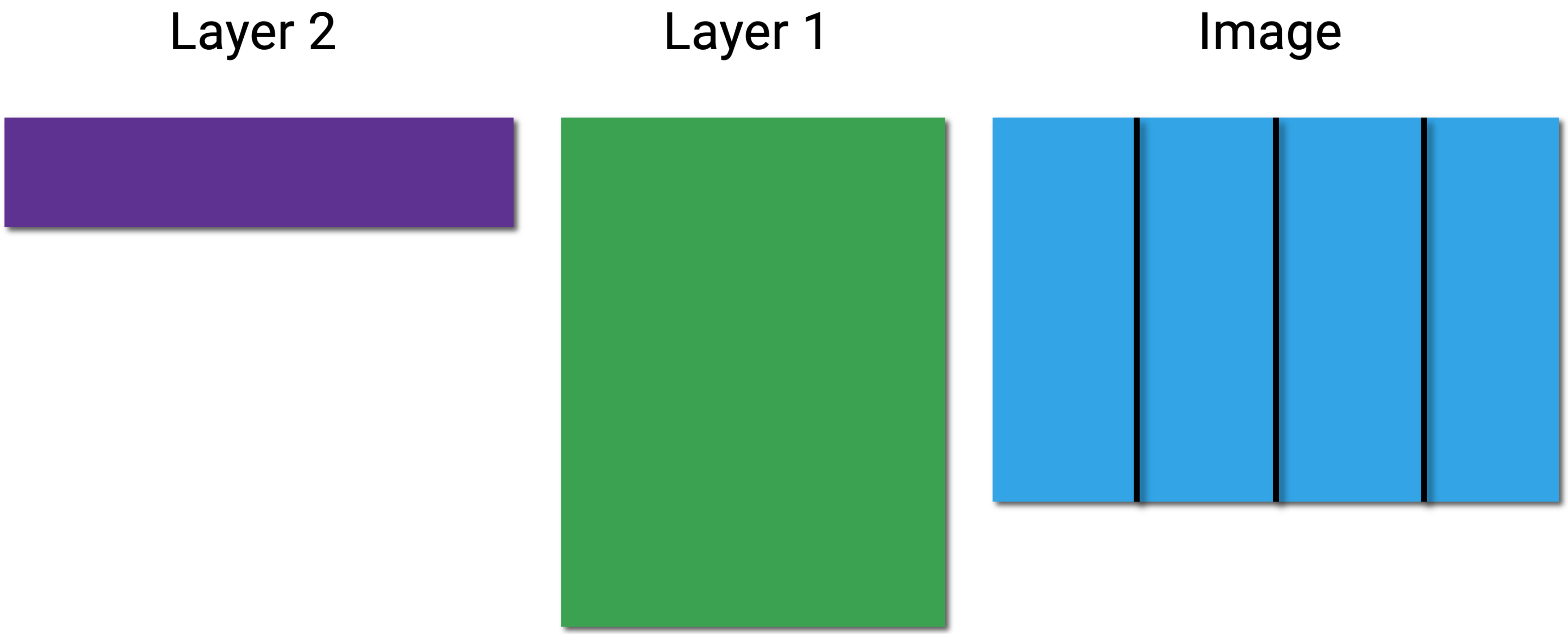
MPI, distributed memory algorithm

Topic of upcoming lectures

High-level discussion of approaches

Layer 2 Layer 1 Image

Data parallelism



Communication

$$J(p) = \frac{1}{N} \sum_{i=1}^{N} \mathrm{error}^{(i)}(y_i, \hat{y}_i)$$

Sum is required over all input images to compute gradient

Parallel reduction to get $\nabla_p J$

= Reduction for all DNN coefficients across all nodes

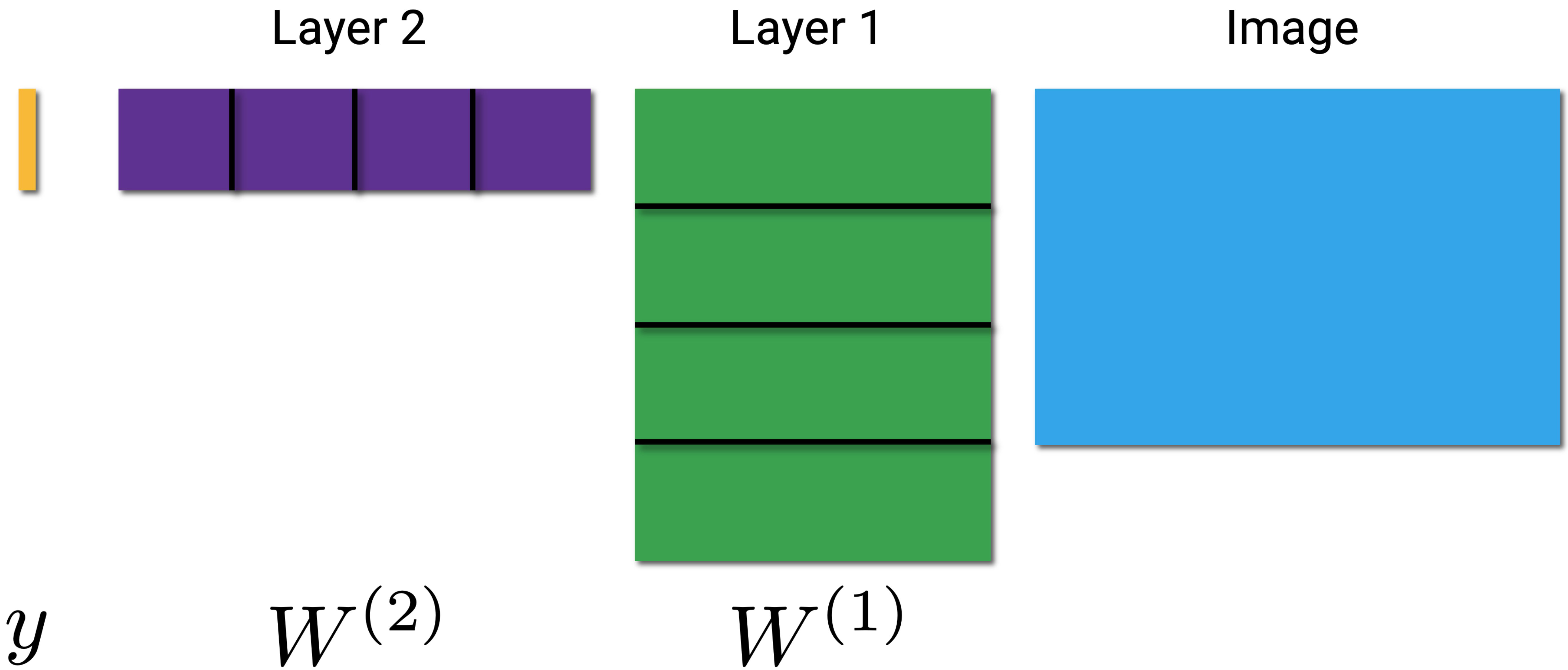
Layer 2 | Layer 1 | Image

Time for MPI communication is fairly significant.

A better implementation exists!

Model parallelism

Much more complicated to understand but implementation is not more difficult than previous approach

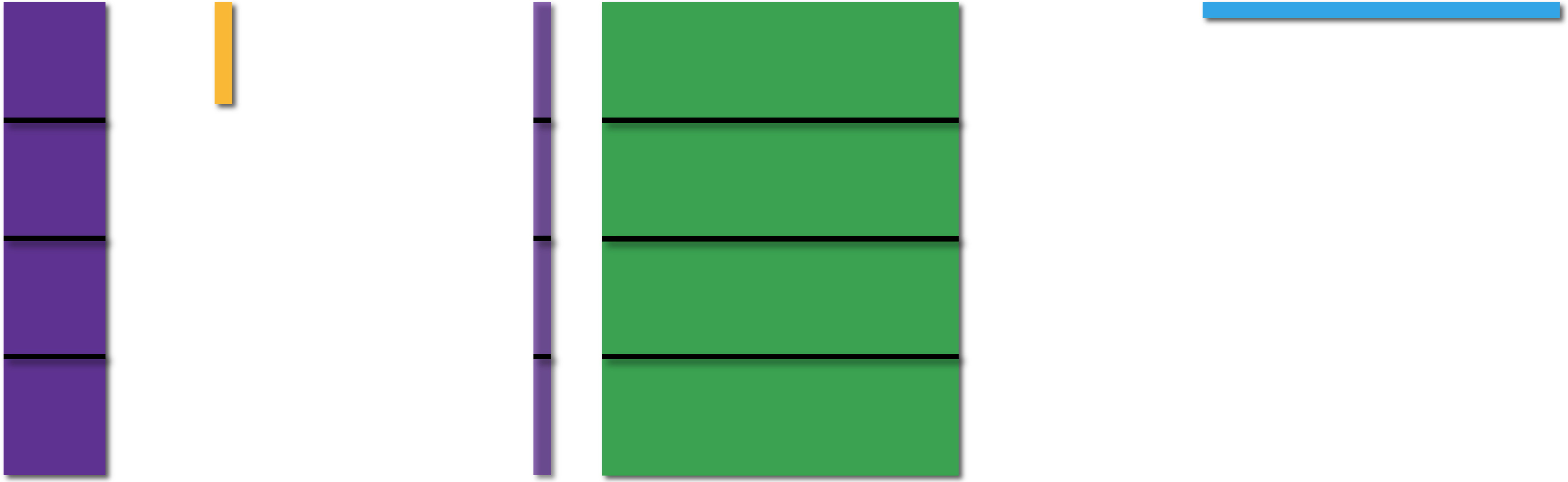

Layer 2
Layer 1
Image
y
$W^{(2)}$
$W^{(1)}$

Reduction is required at the end to get the output labels y

Backpropagation

You have not seen the details yet. So, it will be hard to follow.

The take-home message is that no MPI communication is required between nodes.



$$[W^{(2)}]^T \; y \qquad W^{(1)} \leftarrow W^{(1)} - \alpha[(W^{(2)})^T y]x^T \qquad x^T$$

Warning!

Equations in previous slide were simplified for clarity

See `Part1` write-up for details

No communication is required during the backpropagation

This implementation is much more efficient


good
luck!