3 - Activation, Loss and Optimization

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Introduction

Summary

- The vanishing gradients problem
- ReLU to the rescue
- Different activations: when and how
- Loss functions
- Optimizers
- Overfitting and model selection
- Regularization methods in ANN

Vanishing gradients

Vanishing gradients

Backpropagation in Activation and Loss

- Output neuron n of layer k receives input from m from layer i through weight j

$$\Delta w^j_{mkn} = -\eta \frac{\delta E^j_{kn}}{\delta s^j_{kn}} \frac{\delta s^j_{kn}}{\delta net^j_{kn}} \frac{\delta net^j_{kn}}{\delta w_{mkn}} = \eta(t^j - s^j_{kn})s^j_{kn}(1 - s^j_{kn})s^j_{im} = \eta \delta_{kn} s^j_{im}$$

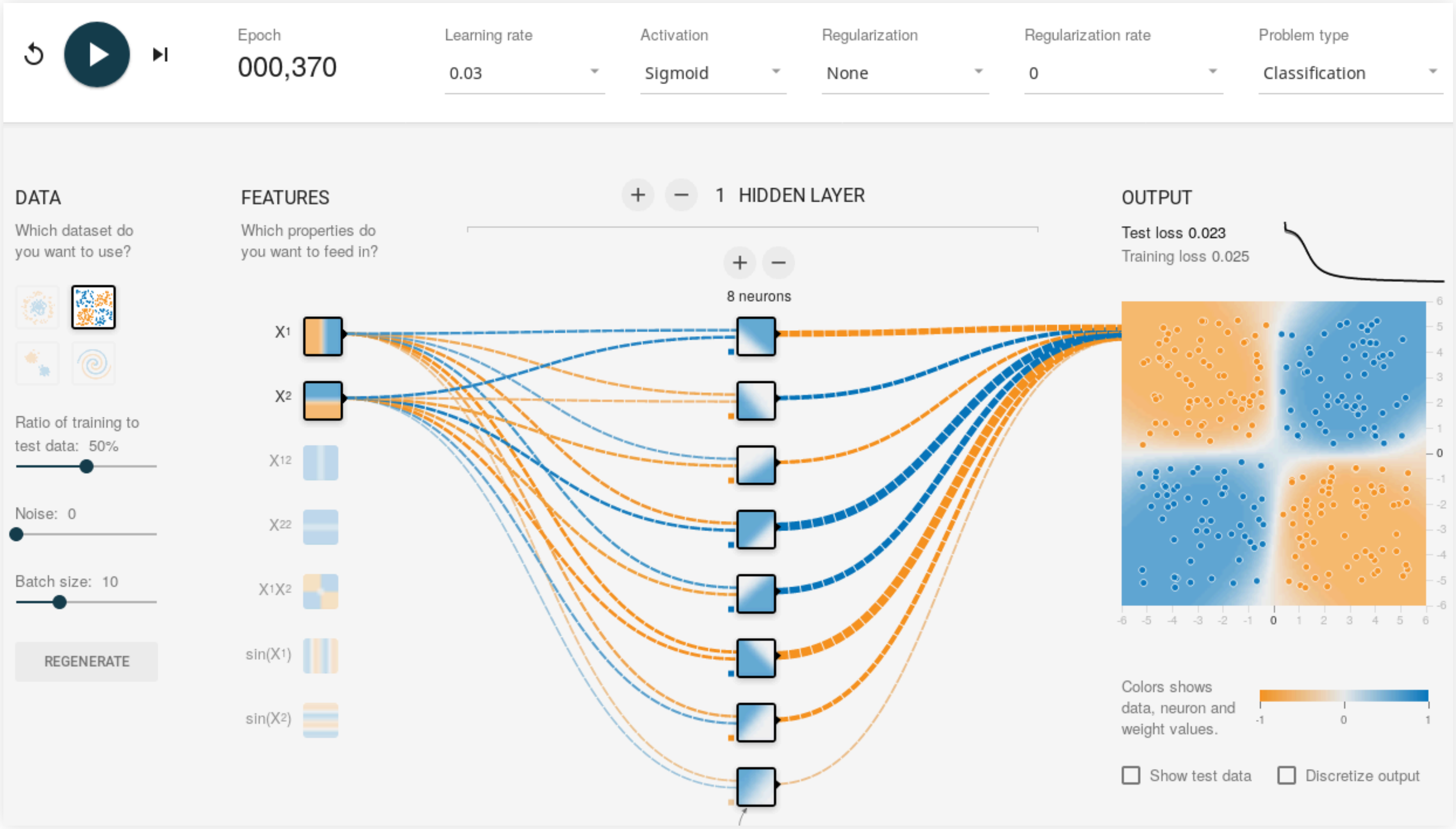
- For a weight m on hidden layer i, we must propagate the output error backwards from all neurons ahead

$$\Delta w^j_{min} = -\eta \left(\sum_p \frac{\delta E^j_{kp}}{\delta s^j_{kp}} \frac{\delta s^j_{kp}}{\delta net^j_{kp}} \frac{\delta net^j_{kp}}{\delta s^j_{in}} \right) \frac{\delta s^j_{in}}{\delta net^j_{in}} \frac{\delta net^j_{in}}{\delta w_{min}}$$

- If δs is small (vanishing gradient) backpropagation becomes ineffective as we increase depth
- This happens with sigmoid activation (or similar, such as TanH)

Vanishing gradients

- Single hidden layer, sigmoid, works fine here


Epoch 000,370
Learning rate 0.03
Activation Sigmoid
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

FEATURES
Which properties do you want to feed in?

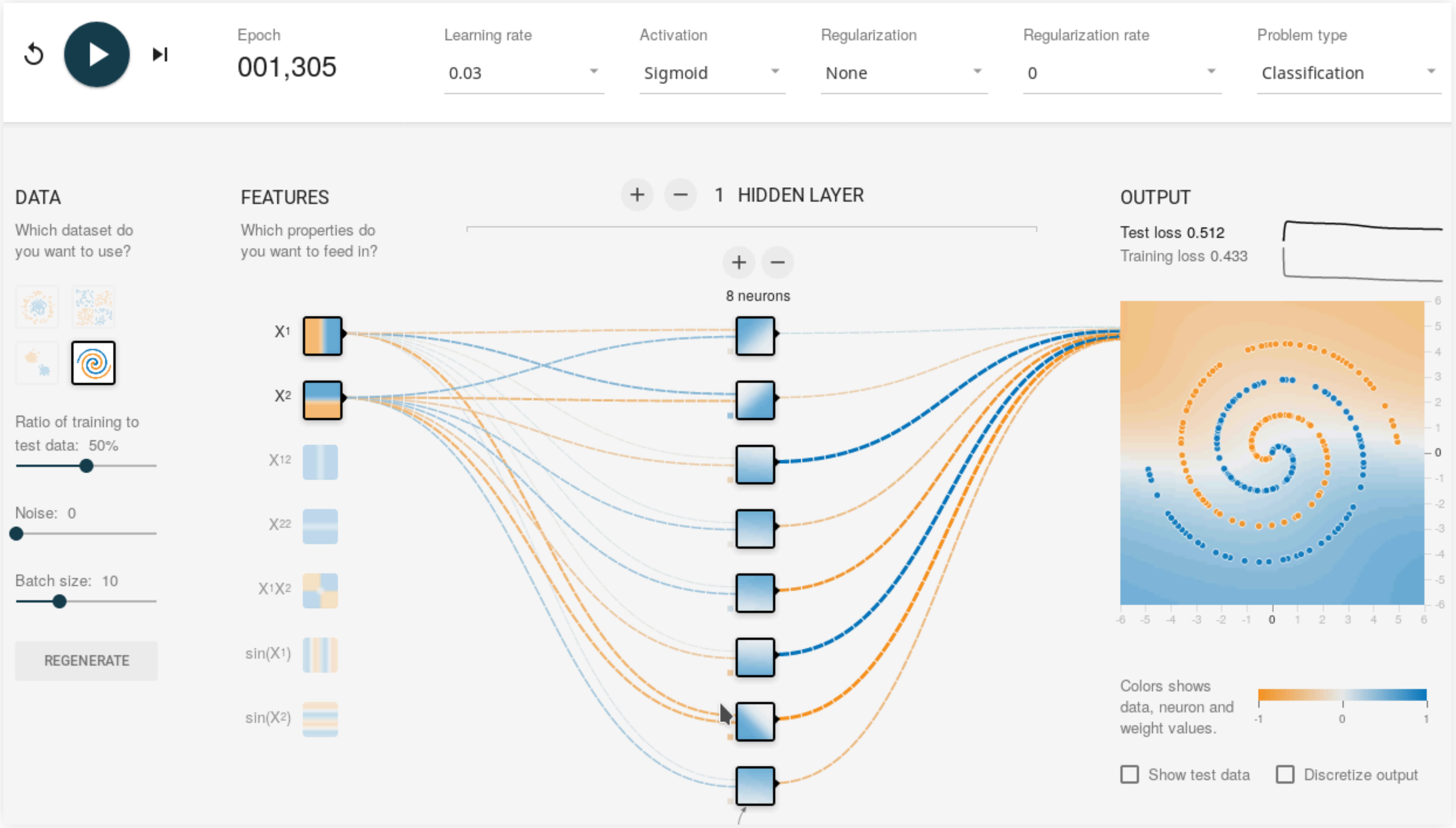
1 HIDDEN LAYER
8 neurons

OUTPUT
Test loss 0.023
Training loss 0.025

Colors shows data, neuron and weight values.

Vanishing gradients

- Single hidden layer, sigmoid, doesn't work here with 8 neurons


Epoch 001,305

Learning rate 0.03

Activation Sigmoid

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?

1 HIDDEN LAYER

8 neurons

OUTPUT

Test loss 0.512

Training loss 0.433

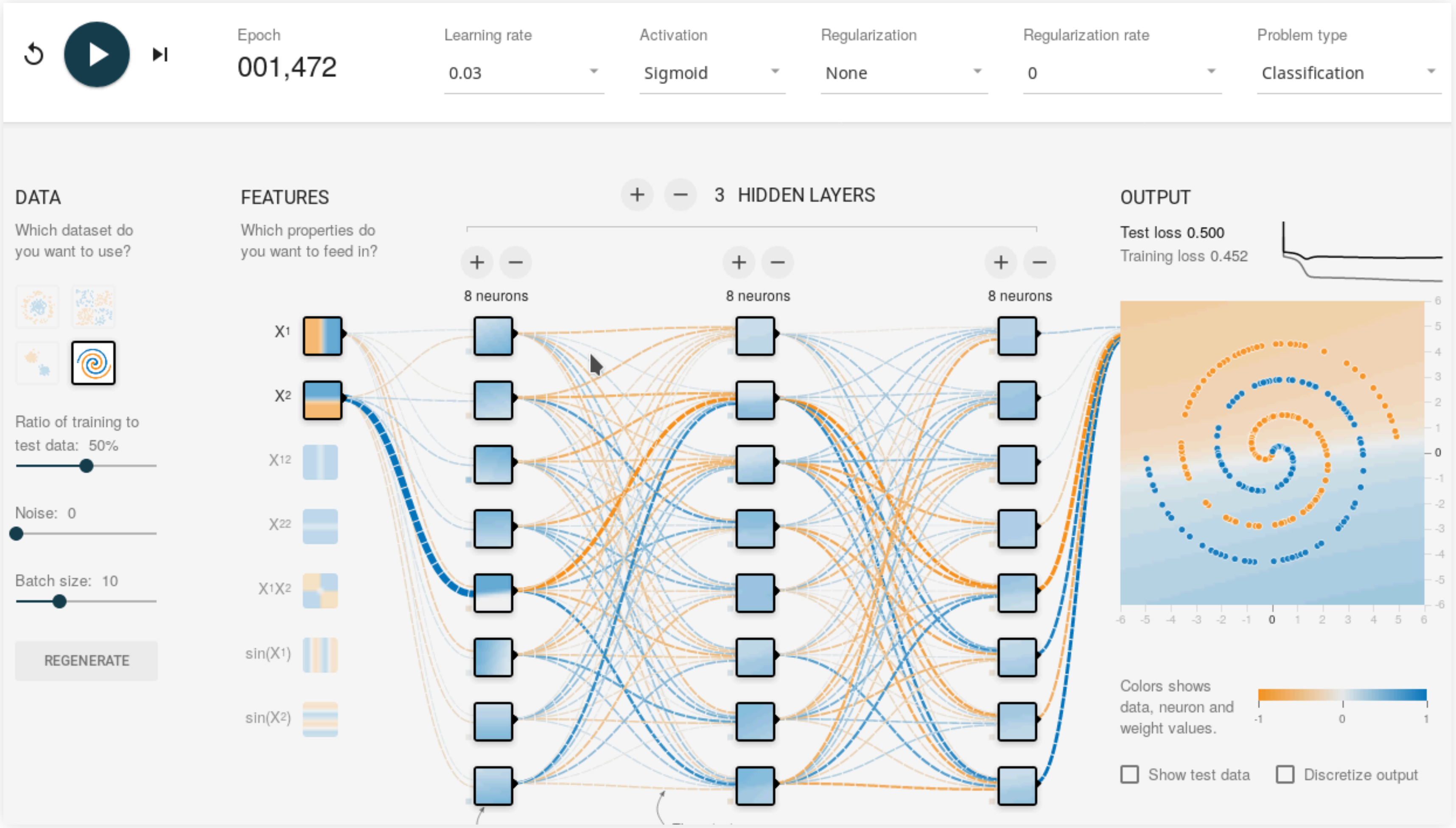
Colors shows data, neuron and weight values.

Show test data

Discretize output

Vanishing gradients

- Increasing depth does not seem to help



Epoch 001,472
Learning rate 0.03
Activation Sigmoid
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

FEATURES
Which properties do you want to feed in?

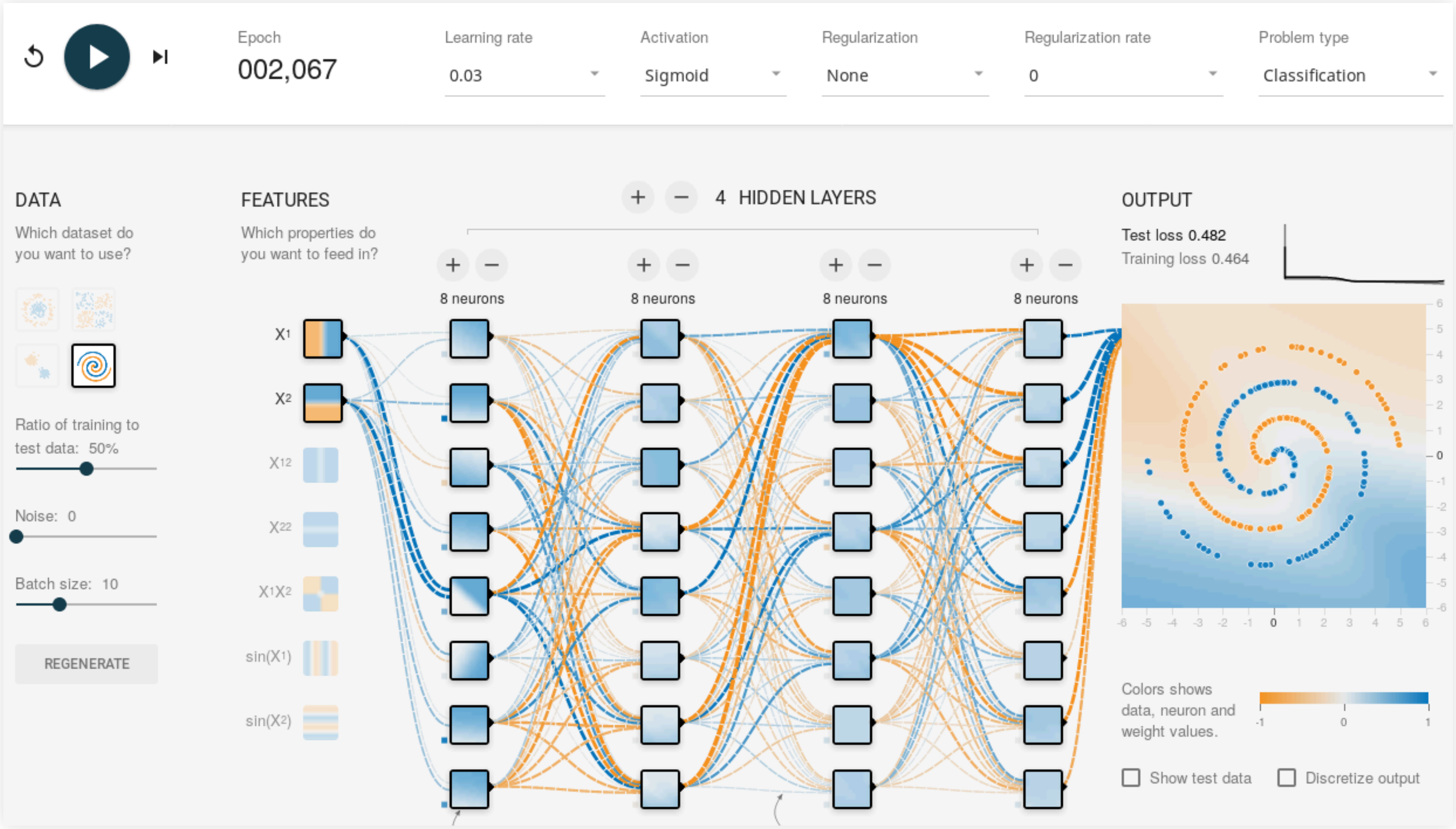
3 HIDDEN LAYERS
8 neurons
8 neurons
8 neurons

OUTPUT
Test loss 0.500
Training loss 0.452

Colors shows data, neuron and weight values.

Vanishing gradients

- Increasing depth does not seem to help



Epoch 002,067

Learning rate: 0.03

Activation: Sigmoid

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?

4 HIDDEN LAYERS

8 neurons | 8 neurons | 8 neurons | 8 neurons

OUTPUT

Test loss 0.482

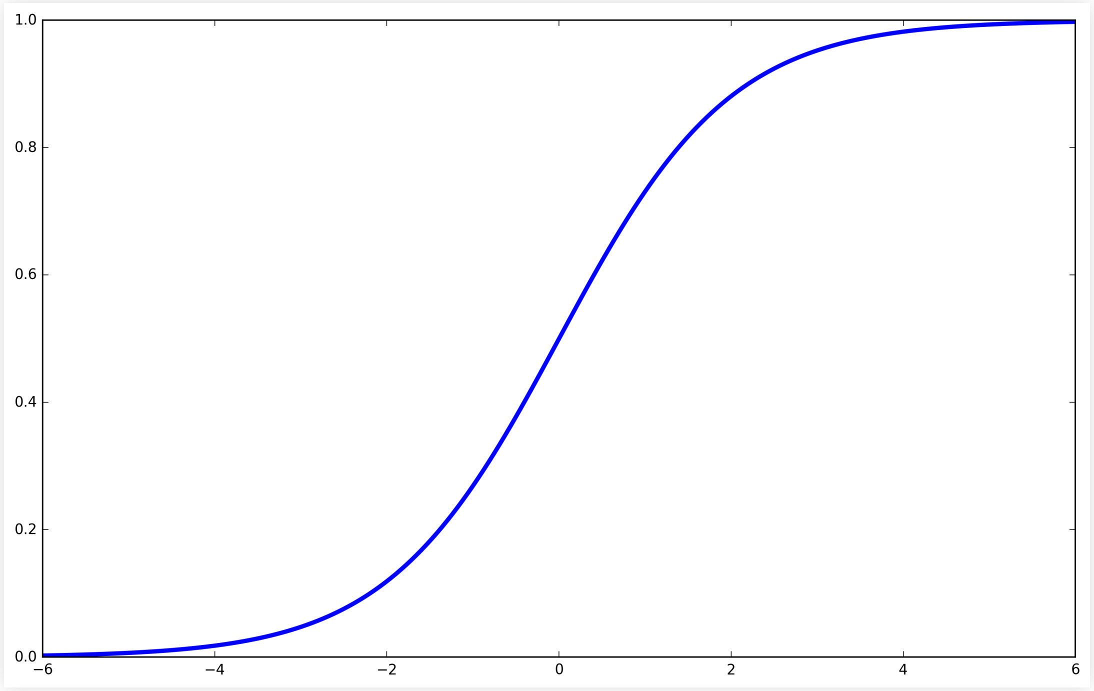
Training loss 0.464

Colors shows data, neuron and weight values.

☐ Show test data ☐ Discretize output

Vanishing gradients

- Increasing depth does not seem to help
- Sigmoid activation saturates and gradients vanish with large coefs.



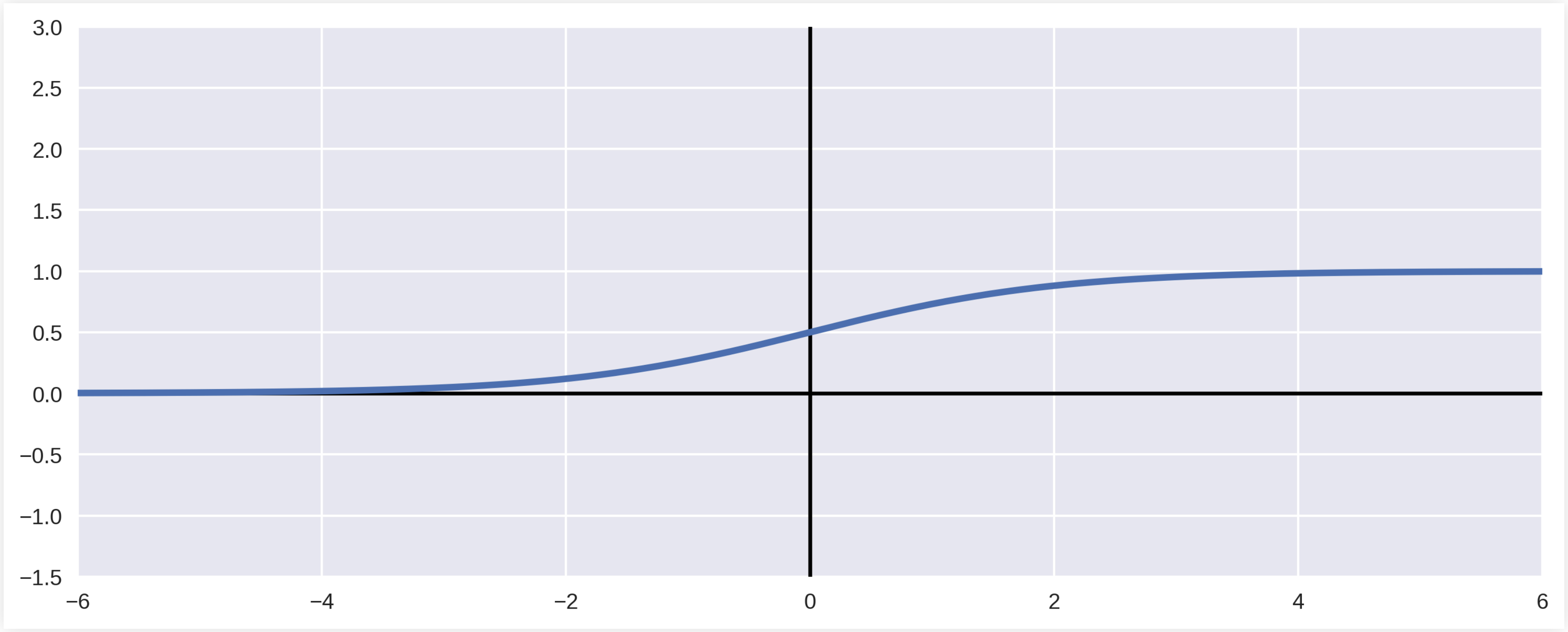
Rectified Linear Unit

ReLU

Rectified Linear Unit (ReLU)

- Sigmoid activation units saturate

$$y_i = \frac{1}{1 + e^{-x_i}}$$

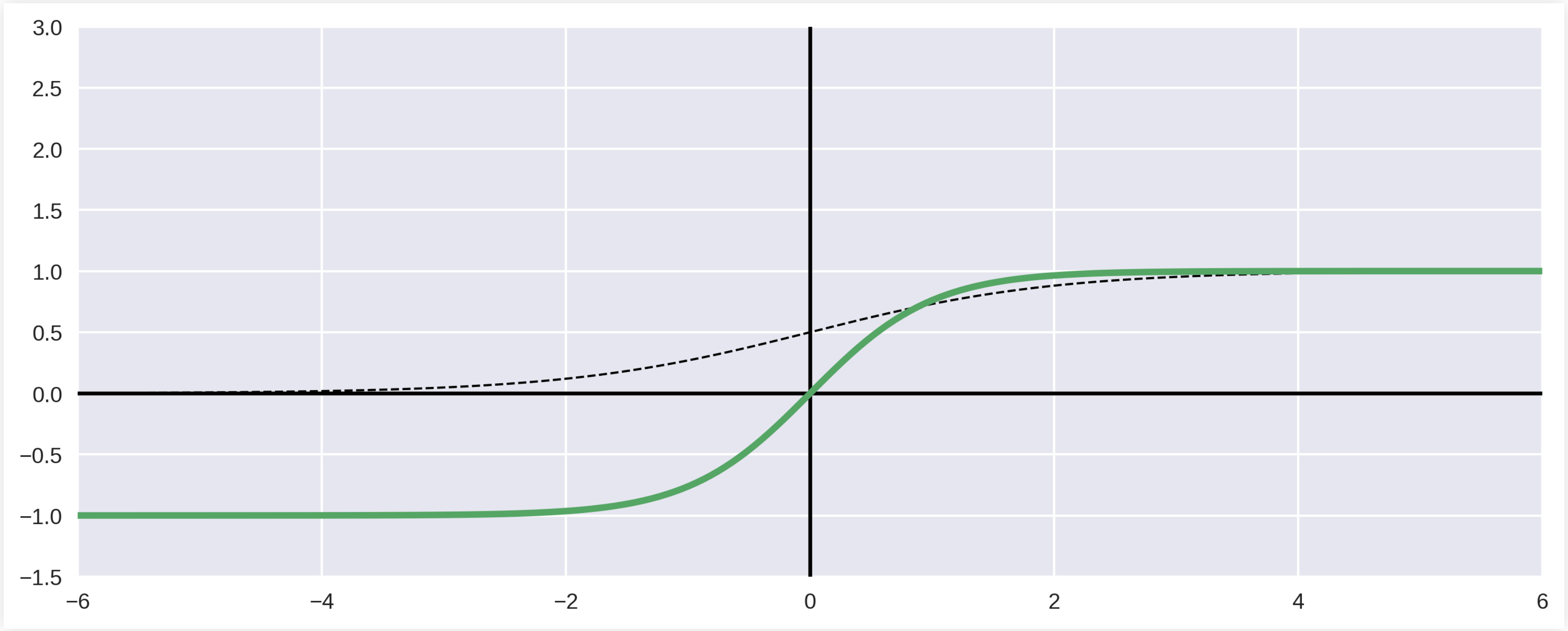


ReLU

Rectified Linear Unit (ReLU)

- The same happens with hyperbolic tangent

$$y_i = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

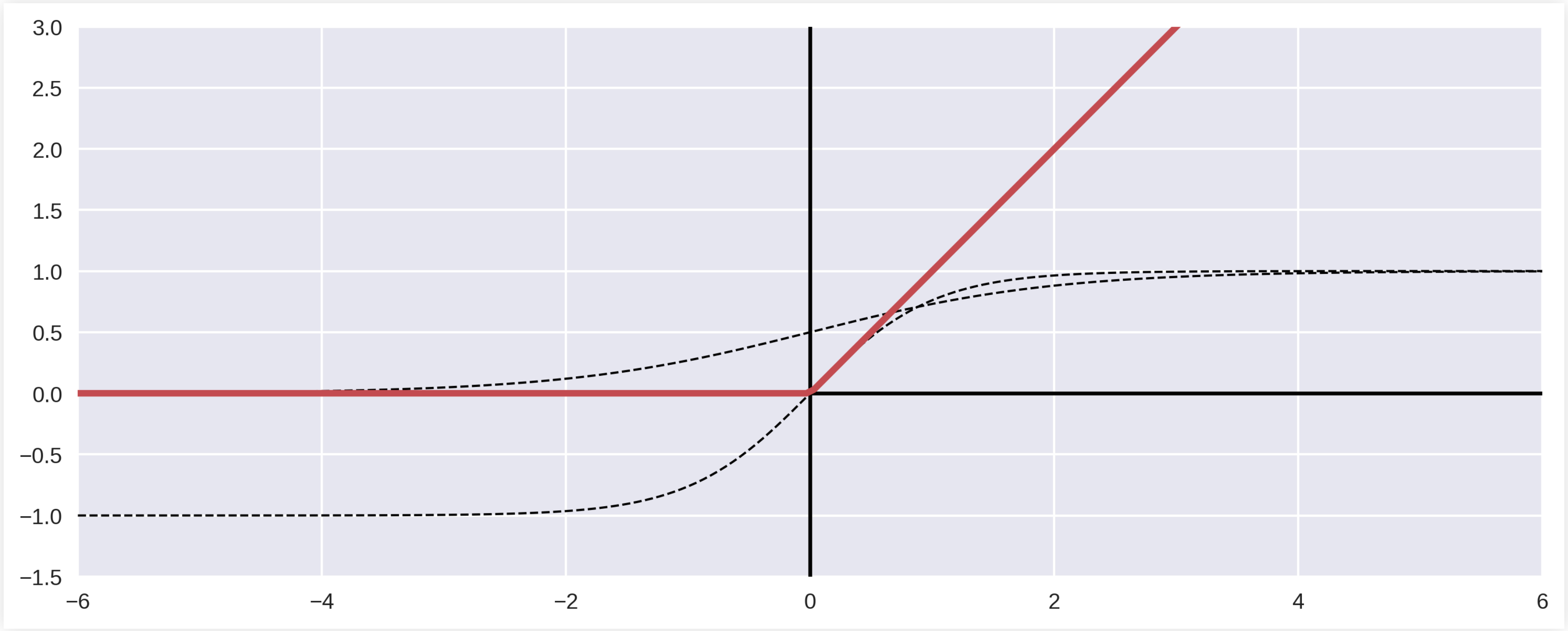


ReLU

Rectified Linear Unit (ReLU)

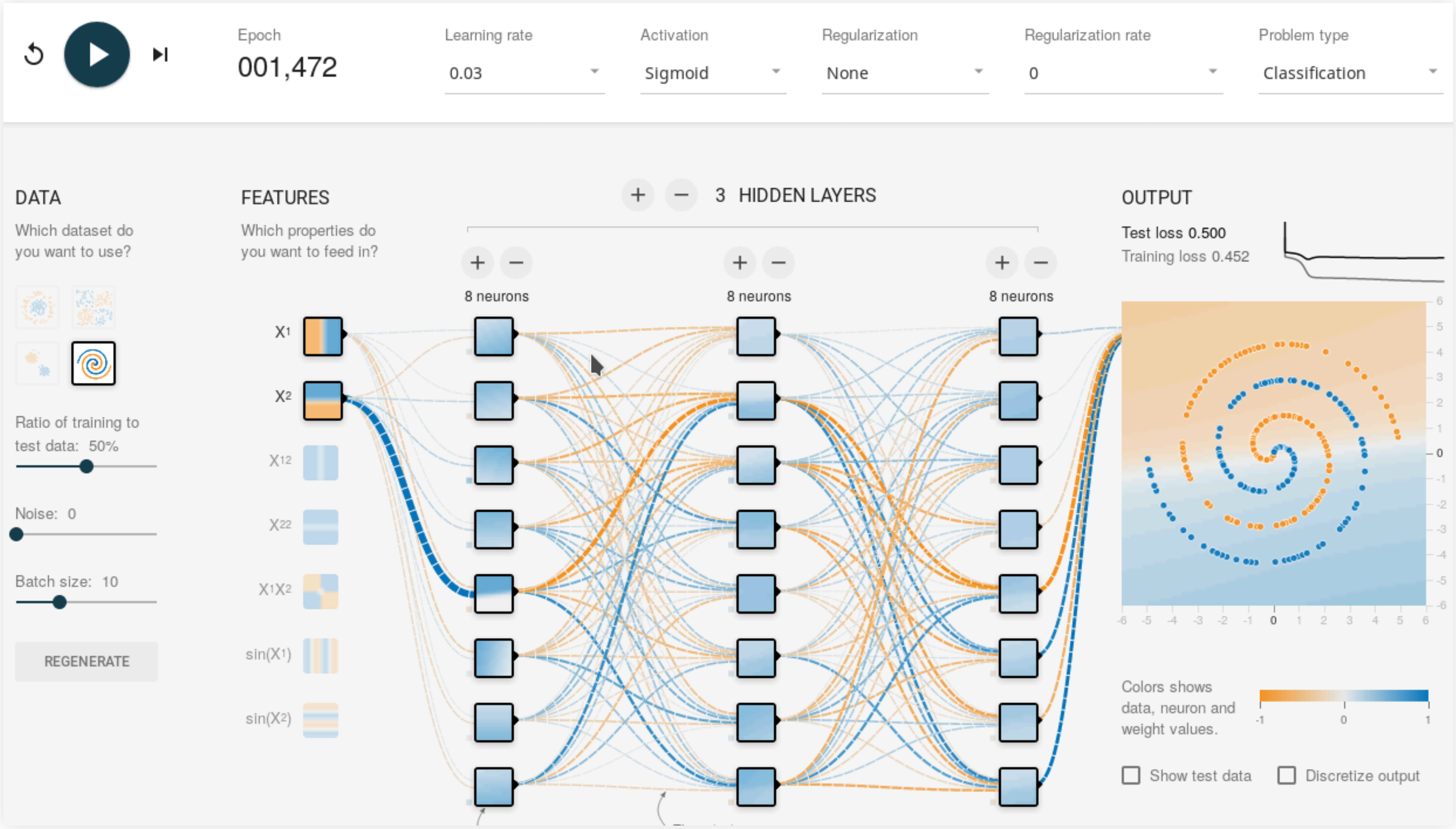
- Rectified linear units do not have this problem

$$y_i = \begin{cases} x_i & x_i > 0 \\ 0 & x_i \leq 0 \end{cases}$$



ReLU

- Sigmoid activation, 3 layers


Epoch 001,472

Learning rate 0.03

Activation Sigmoid

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

FEATURES

Which properties do you want to feed in?

3 HIDDEN LAYERS

8 neurons

8 neurons

8 neurons

OUTPUT

Test loss 0.500

Training loss 0.452

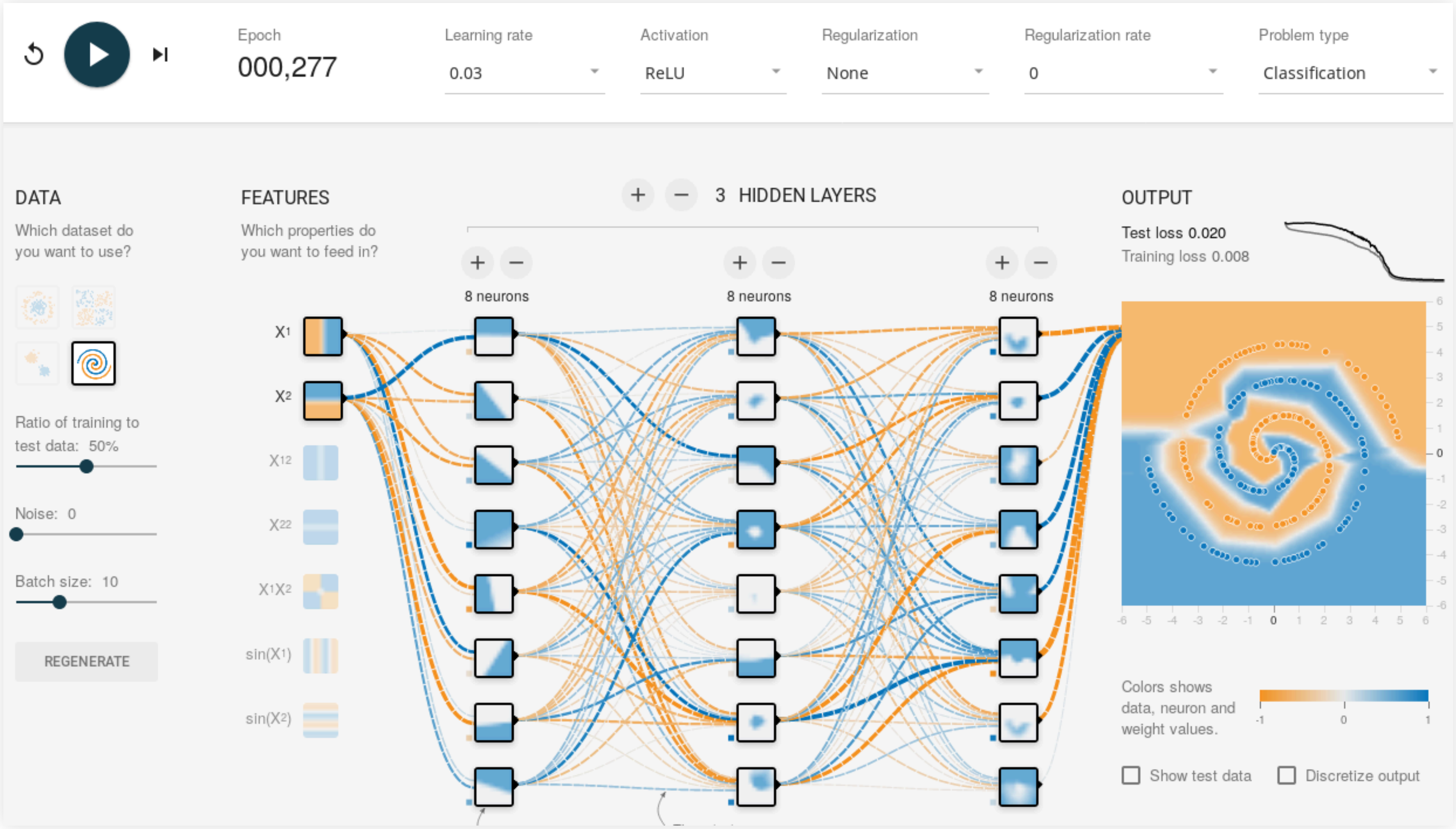
Colors shows data, neuron and weight values.

Show test data

Discretize output

ReLU

- ReLU activation, 3 layers



Epoch 000,277

Learning rate 0.03

Activation ReLU

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?

3 HIDDEN LAYERS

8 neurons

8 neurons

8 neurons

OUTPUT

Test loss 0.020

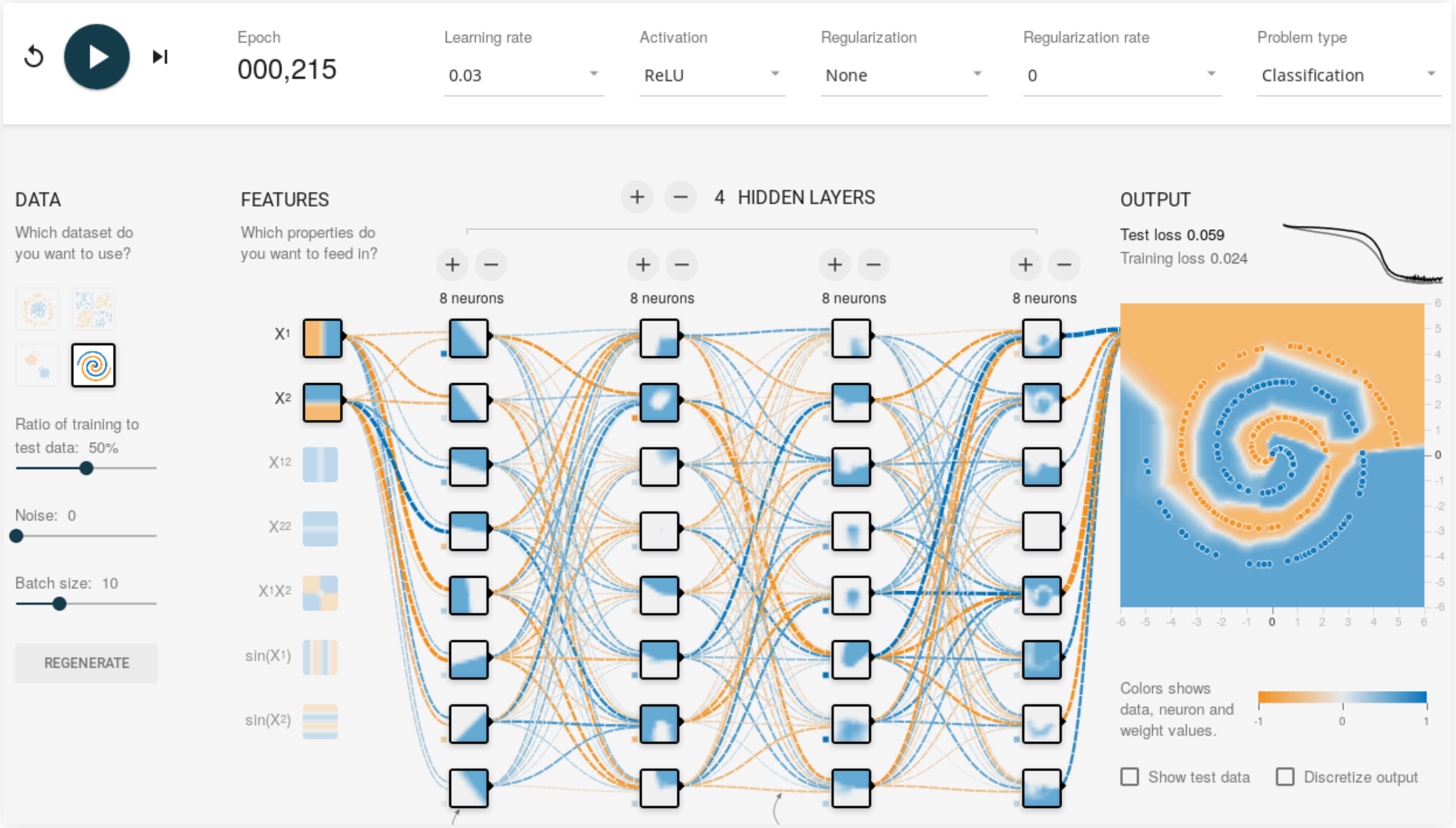
Training loss 0.008

Colors shows data, neuron and weight values.

☐ Show test data ☐ Discretize output

ReLU

- ReLU activation, 4 layers



Epoch 000,215

Learning rate 0.03

Activation ReLU

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?

4 HIDDEN LAYERS

8 neurons

8 neurons

8 neurons

8 neurons

OUTPUT

Test loss 0.059

Training loss 0.024

Colors shows data, neuron and weight values.

Show test data

Discretize output

ReLU

Rectified Linear Unit (ReLU)

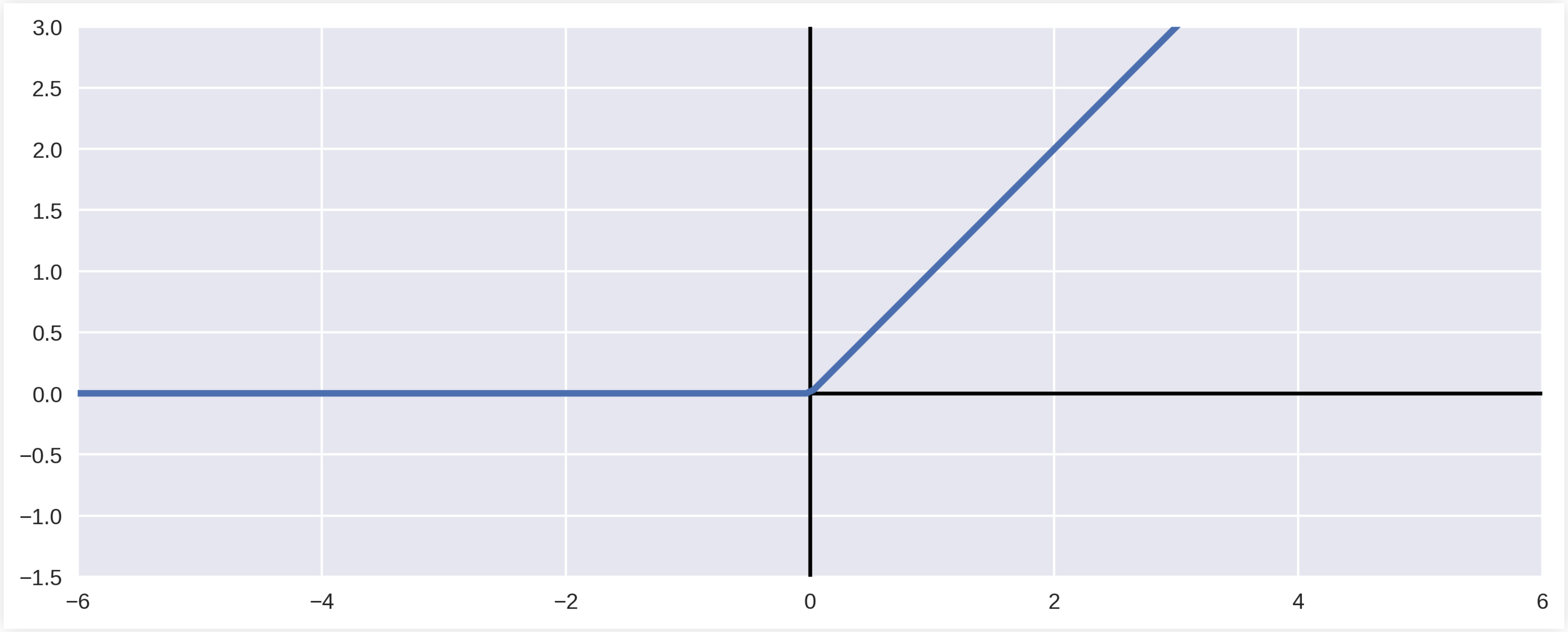
- Advantages of ReLU activation:
  - Fast to compute
  - Does not saturate for positive values, and gradient is always 1
- Disadvantage:
  - ReLU units can "die" if training makes their weights very negative
  - The unit will output 0 and the gradient will become 0, so it will not "revive"
- There are variants that try to fix this problem

ReLU

(Some) ReLU variants

- Simple ReLU can die if coefficients are negative

$$y_i = \begin{cases} x_i & x_i > 0 \\ 0 & x_i \leq 0 \end{cases}$$

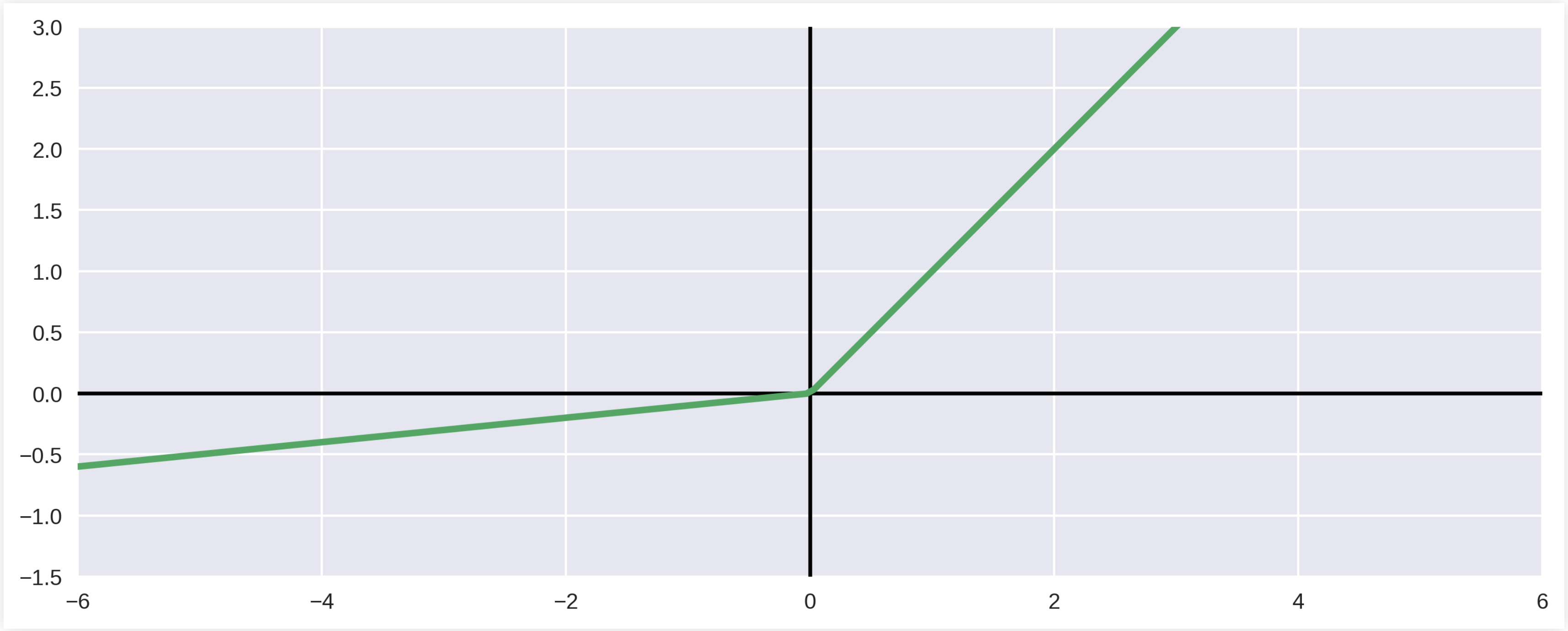


ReLU

ReLU variant: Leaky ReLU

- Leaky ReLU gradient is never 0

$$y_i = \begin{cases} x_i & x > 0 \\ \frac{x_i}{a_i} & x_i \le 0 \end{cases}$$

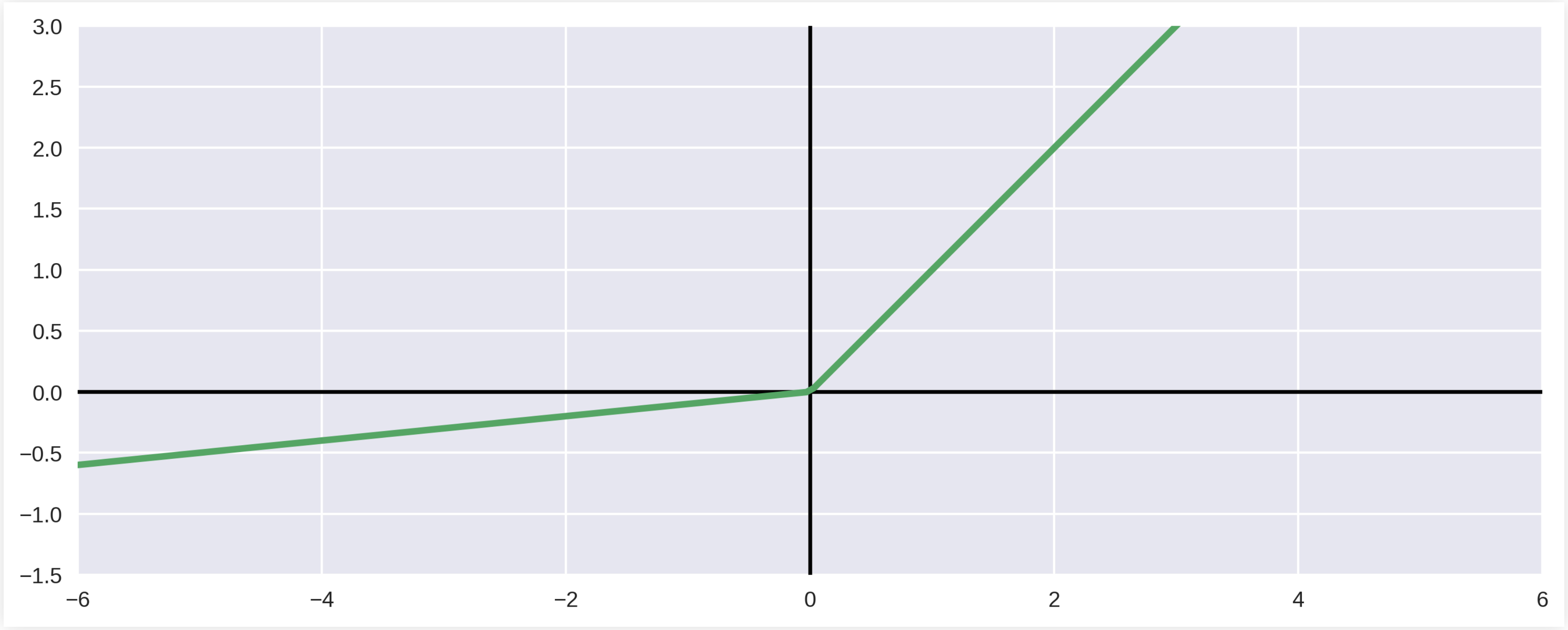


ReLU

ReLU variant: Leaky ReLU

- Note: in Tensorflow

$$y_i = \begin{cases} x_i & x > 0 \\ a_i x_i & x_i \leq 0 \end{cases}$$

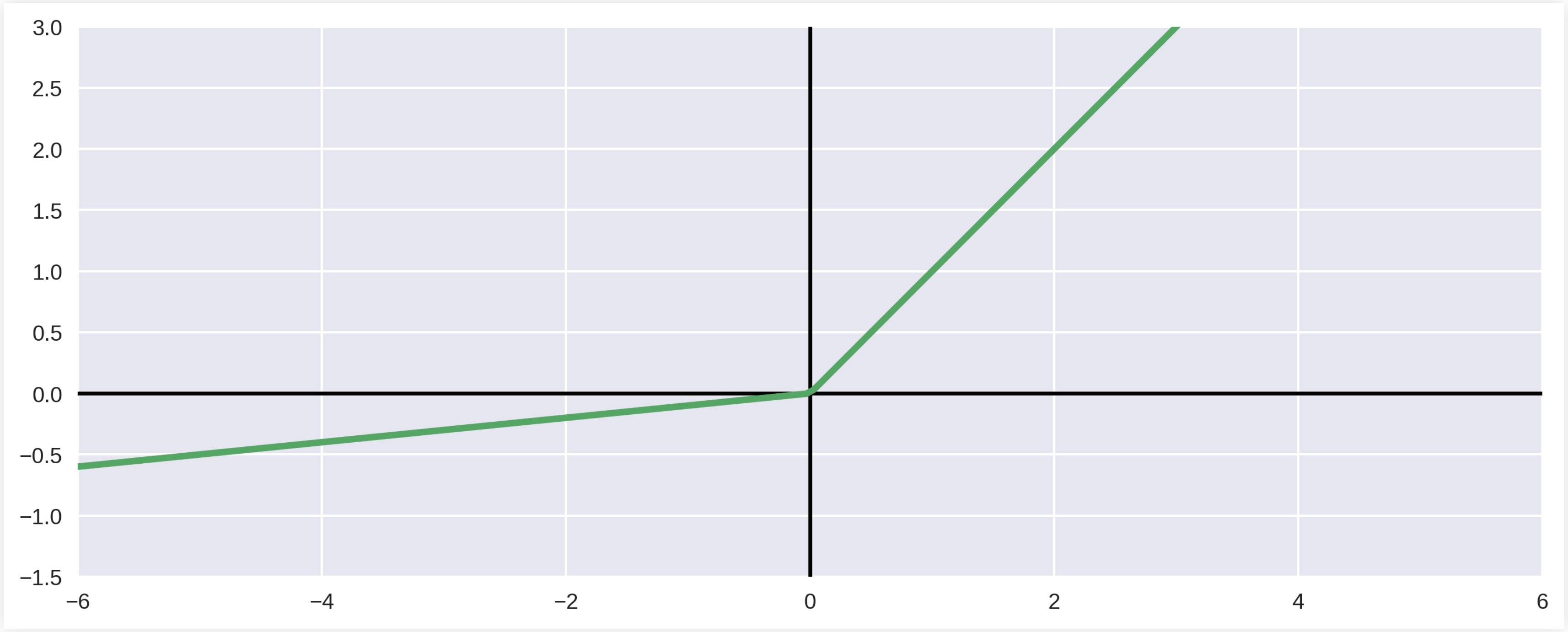


ReLU

ReLU variant: Parametric ReLU

- Same as leaky, but a_i is also learned

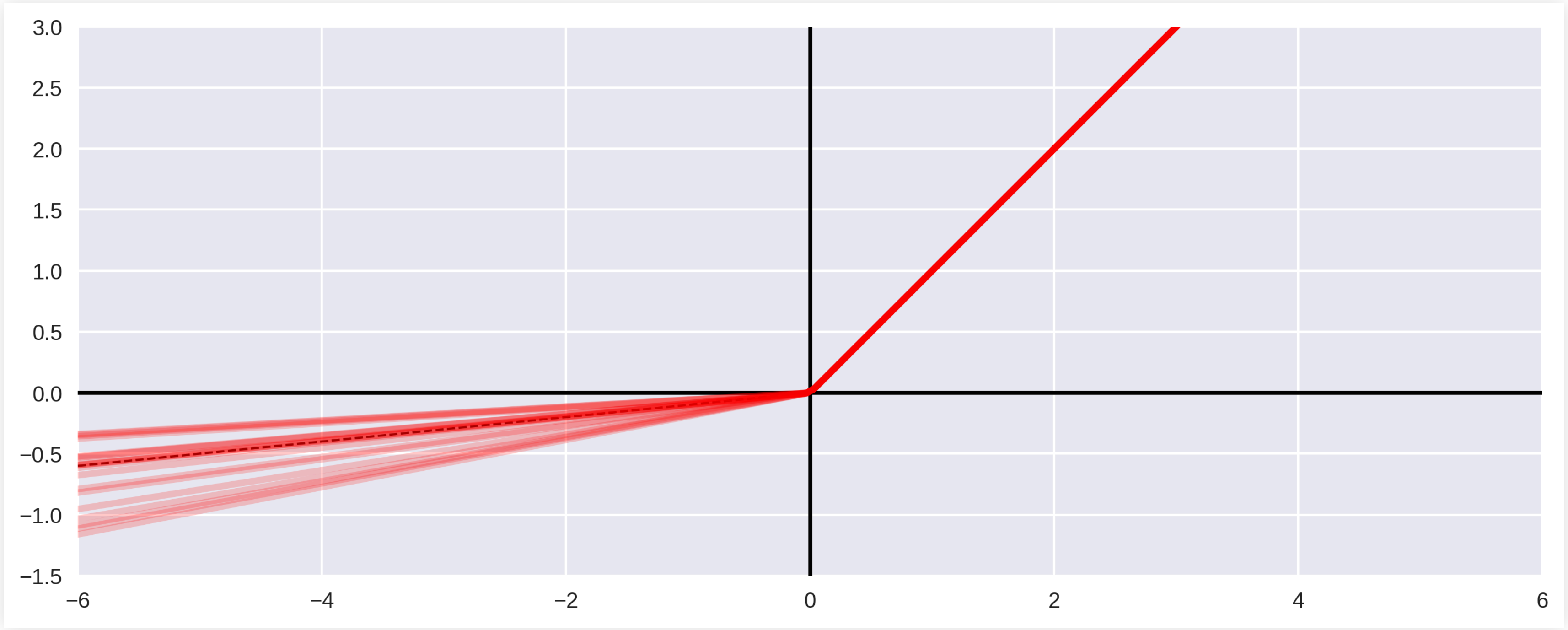
$$y_i = \begin{cases} x_i & x > 0 \\ \frac{x_i}{a_i} & x_i \leq 0 \end{cases}$$



ReLU variant: Randomized Leaky ReLU

- Similar, but $a_i \sim U(l, u)$ (average of l, u in test)

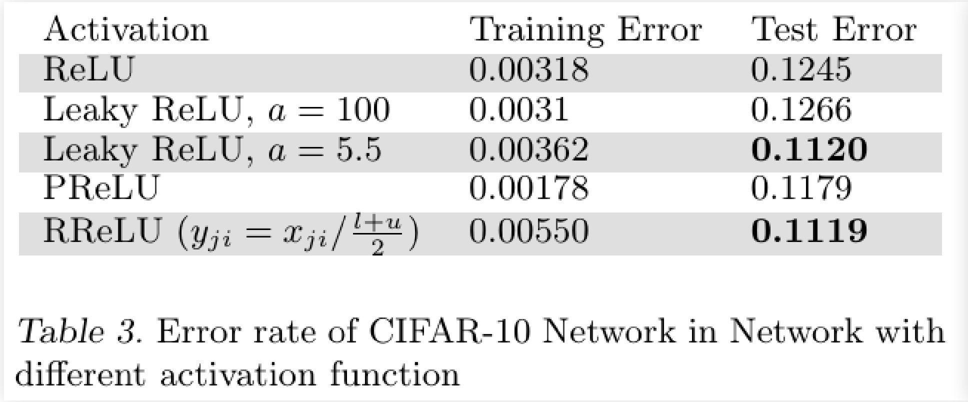
$$y_i = \begin{cases} x_i & x > 0 \\ a_i x_i & x_i \leq 0 \end{cases}$$



Comparing ReLU variants

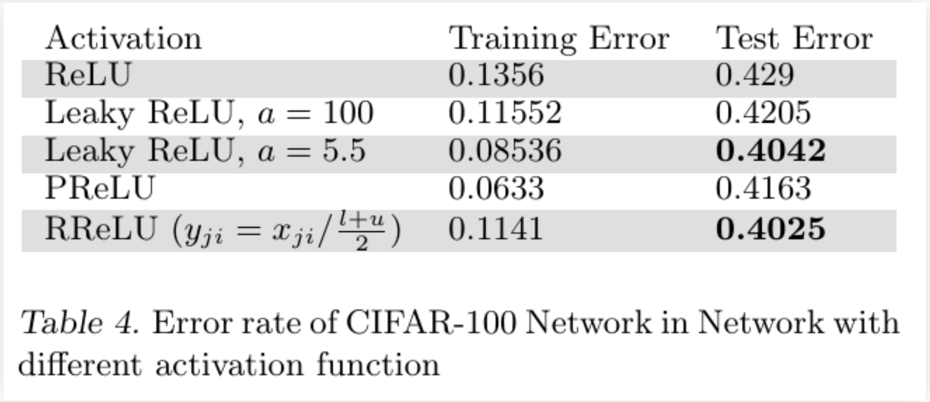
Empirical Evaluation of Rectified Activations in Convolution Network (Xu et. al. 2015)

- Compared on 2 data sets
  - CIFAR-10: 60000 32x32 color images in 10 classes of 6000 each
  - CIFAR-100: 60000 32x32 color images in 100 classes of 600 each



Activation	Training Error	Test Error
ReLU	0.00318	0.1245
Leaky ReLU, $a = 100$	0.0031	0.1266
Leaky ReLU, $a = 5.5$	0.00362	**0.1120**
PReLU	0.00178	0.1179
RReLU ($y_{ji} = x_{ji}/\frac{l+u}{2}$)	0.00550	**0.1119**

Table 3. Error rate of CIFAR-10 Network in Network with different activation function



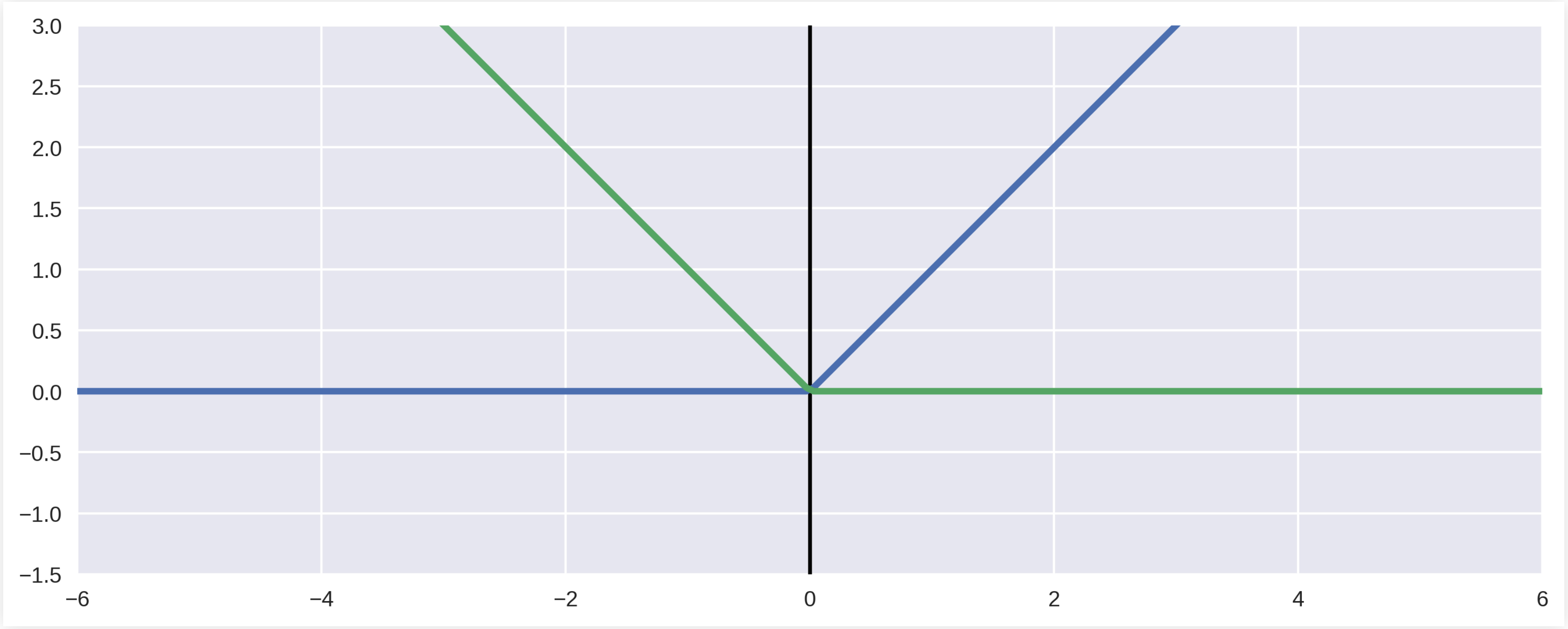
Activation	Training Error	Test Error
ReLU	0.1356	0.429
Leaky ReLU, $a = 100$	0.11552	0.4205
Leaky ReLU, $a = 5.5$	0.08536	**0.4042**
PReLU	0.0633	0.4163
RReLU ($y_{ji} = x_{ji}/\frac{l+u}{2}$)	0.1141	**0.4025**

Table 4. Error rate of CIFAR-100 Network in Network with different activation function

CReLU

- Concatenated ReLU combine two ReLU for x and $-x$

$$y_i = \begin{cases} x_i & x_i > 0 \\ 0 & x_i \leq 0 \end{cases} \qquad z_i = \begin{cases} 0 & x_i > 0 \\ -x_i & x_i \leq 0 \end{cases}$$



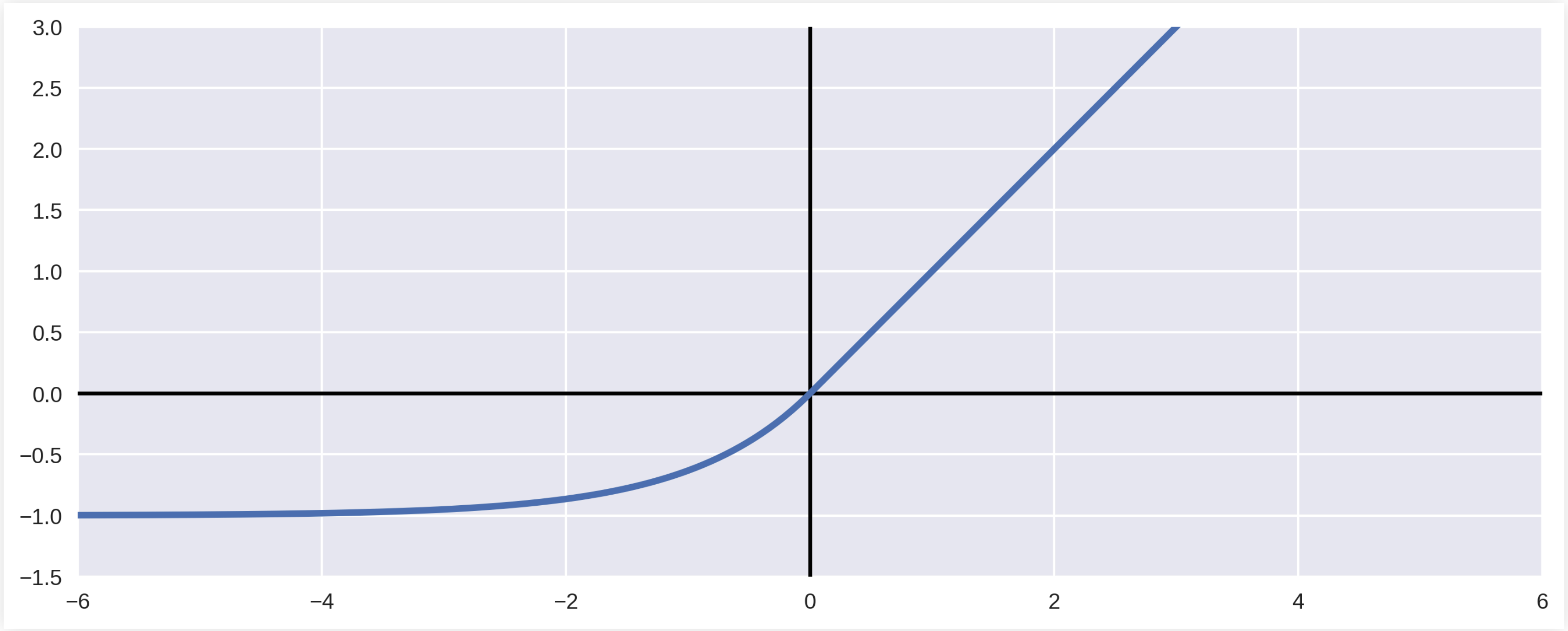
Shang et. al., Understanding and Improving CNN via CReLUs, 2016

ELU

Exponential Linear Unit

- Exponential in negative part

$$y_i = \begin{cases} x_i & x_i > 0 \\ a(e^{x_i} - 1) & x_i \leq 0 \end{cases}$$



Clevert et. al. Fast and Accurate Deep Network Learning by ELUs, 2015

Activations: which, when, why?

Choosing activations

Hidden layer activations

- Hidden layers perform nonlinear transformations
  - Without nonlinear activation functions, all layers would just amount to a single linear transformation
- Activation functions should be fast to compute
- Activation functions should avoid vanishing gradients
- This is why ReLU (esp. leaky variants) are the recommended choice for hidden layers
  - Except for specific applications.
  - E.g. LSTM, Long short-term memory recurrent networks

Choosing activations

Output layer activations

- Output layers are a different case.
  - Choice depends on what we want the model to do
- For regression, output should generally be linear
  - We do not want bounded values and there is little need for nonlinearity in the last layer
- For binary classification, sigmoid is a good choice
  - The output value $[0, 1]$ is useful as a representation of the probability of C_1, like in logistic regression
- Sigmoid is also good for multilabel classification
  - One example may fit with several labels at the same time
  - Use one sigmoid output per label

Choosing activations

Output layer activations

- For multiclass classification, use softmax:
  - Note: multiclass means each example fits only one of several classes

$$\sigma : \mathbb{R}^K \to [0,1]^K \qquad \sigma(\vec{x})_j = \frac{e^{x_j}}{\sum_{k=1}^{K} e^{x_k}}$$

- Softmax returns a vector where $\sigma_j \in [0,1]$ and $\sum_{k=1}^{K} \sigma_k = 1$
- This can fit a probability of example belonging to each class C_j
- Softmax is a generalization of the logistic function
  - It combines the activations of several neurons

Activation, Loss and Optimization

Loss and likelihood

Likelihood

Basic concepts

- We have a set of labelled data

$$\{(\vec{x}^1, y^1), \ldots, (\vec{x}^n, y^n)\}$$

- We want to approximate some function $F(X) : X \rightarrow Y$ by fitting our parameters
- Given some training set, what are the best parameter values?

Simple example, linear regression

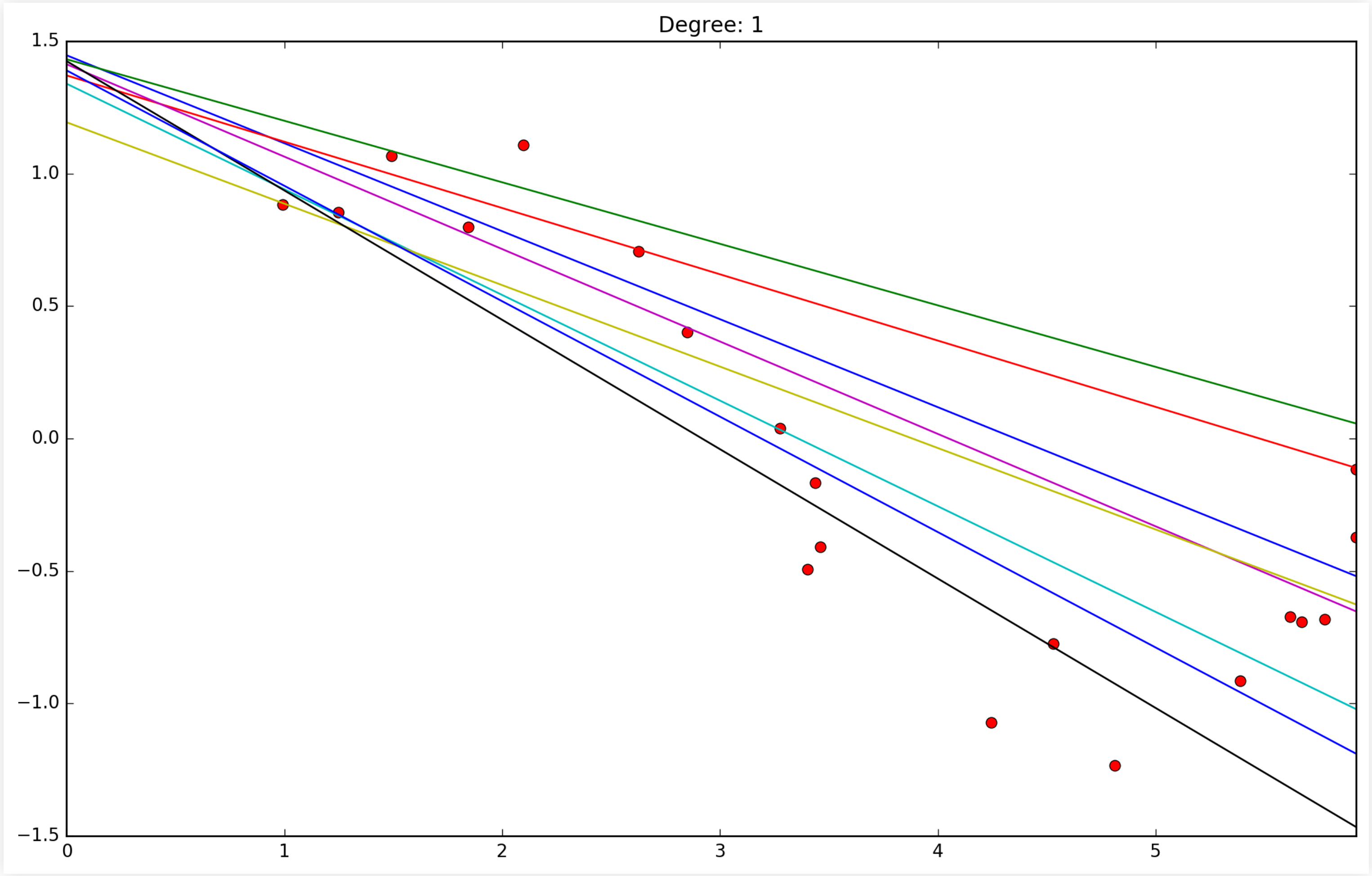
$$y = \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_{n+1}$$

- We have a set of (x, y) examples and want to fit the best line:

$$y = \theta_1 x + \theta_2$$

Likelihood

What to optimize?



Likelihood

What to optimize?

- Assume y is a function of x plus some error:

$$y = F(x) + \epsilon$$

- We want to approximate $F(x)$ with some $g(x, \theta)$
- Assuming $\epsilon \sim N(0, \sigma^2)$ and $g(x, \theta) \sim F(x)$, then:

$$p(y|x) \sim \mathcal{N}(g(x, \theta), \sigma^2)$$

- Given $\mathcal{X} = \{x^t, y^t\}_{t=1}^{N}$ and knowing that $p(x, y) = p(y|x)p(x)$

$$p(X, Y) = \prod_{t=1}^{n} p(x^t, y^t) = \prod_{t=1}^{n} p(y^t|x^t) \times \prod_{t=1}^{n} p(x^t)$$

Likelihood

What to optimize?

- The probability of (X, Y) given $g(x, \theta)$ is the $\boxed{\text{likelihood}}$ of θ:

$$l(\theta|\mathcal{X}) = \prod_{t=1}^{n} p(\vec{x}^t, y^t) = \prod_{t=1}^{n} p(y^t|x^t) \times \prod_{t=1}^{n} p(x^t)$$

Likelihood

- The examples $(\vec{x}, y)$ are randomly sampled from all possible values
- But θ is not a random variable
- Find the θ for which the data is most probable

- In other words, find the θ of maximum likelihood

Likelihood

Maximum likelihood for linear regression

$$l(\theta|\mathcal{X}) = \prod_{t=1}^{n} p(x^t, y^t) = \prod_{t=1}^{n} p(y^t|x^t) \times \prod_{t=1}^{n} p(x^t)$$

- First, take the logarithm (same maximum)

$$L(\theta|\mathcal{X}) = log\left(\prod_{t=1}^{n} p(y^t|x^t) \times \prod_{t=1}^{n} p(x^t)\right)$$

- We ignore $p(X)$, since it's independent of θ

$$L(\theta|\mathcal{X}) \propto log\left(\prod_{t=1}^{n} p(y^t|x^t)\right)$$

- Replace the expression for the normal distribution:

$$\mathcal{L}(\theta|\mathcal{X}) \propto log \prod_{t=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-[y^t - g(x^t|\theta)]^2/2\sigma^2}$$

Likelihood

Maximum likelihood for linear regression

$$\mathcal{L}(\theta|\mathcal{X}) \propto log \prod_{t=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-[y^t - g(x^t|\theta)]^2/2\sigma^2}$$

- Simplify:

$$\mathcal{L}(\theta|\mathcal{X}) \propto log \prod_{t=1}^{n} e^{-[y^t - g(x^t|\theta)]^2}$$

$$\mathcal{L}(\theta|\mathcal{X}) \propto -\sum_{t=1}^{n} [y^t - g(x^t|\theta)]^2$$

Likelihood

Maximum likelihood for linear regression

$$\mathcal{L}(\theta|\mathcal{X}) \propto -\sum_{t=1}^{n}[y^t - g(x^t|\theta)]^2$$

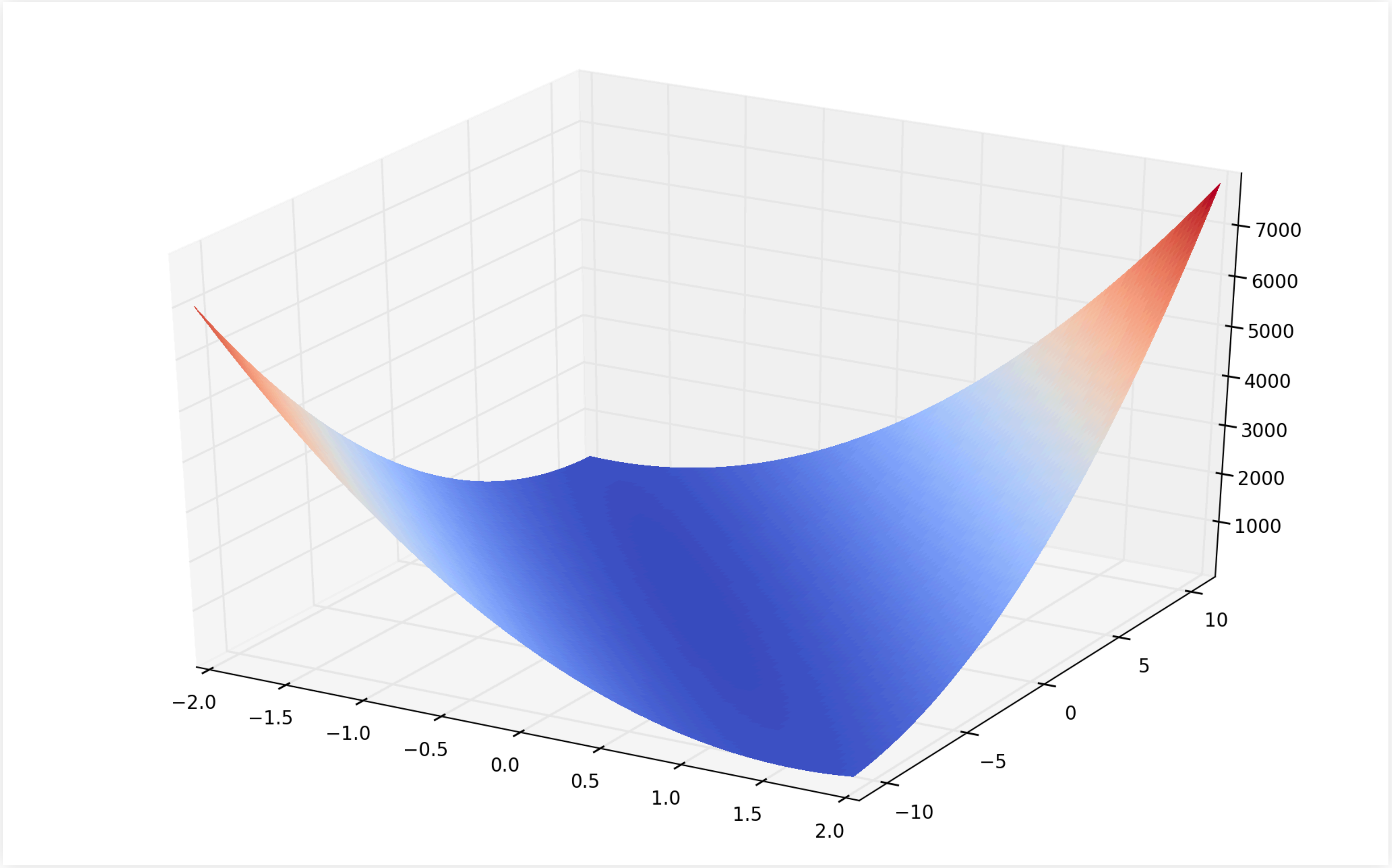
- Max(likelihood) = Min(squared error)

- Note: the squared error is often written like this for convenience:

$$E(\theta|\mathcal{X}) = \frac{1}{2}\sum_{t=1}^{n}[y^t - g(x^t|\theta)]^2$$

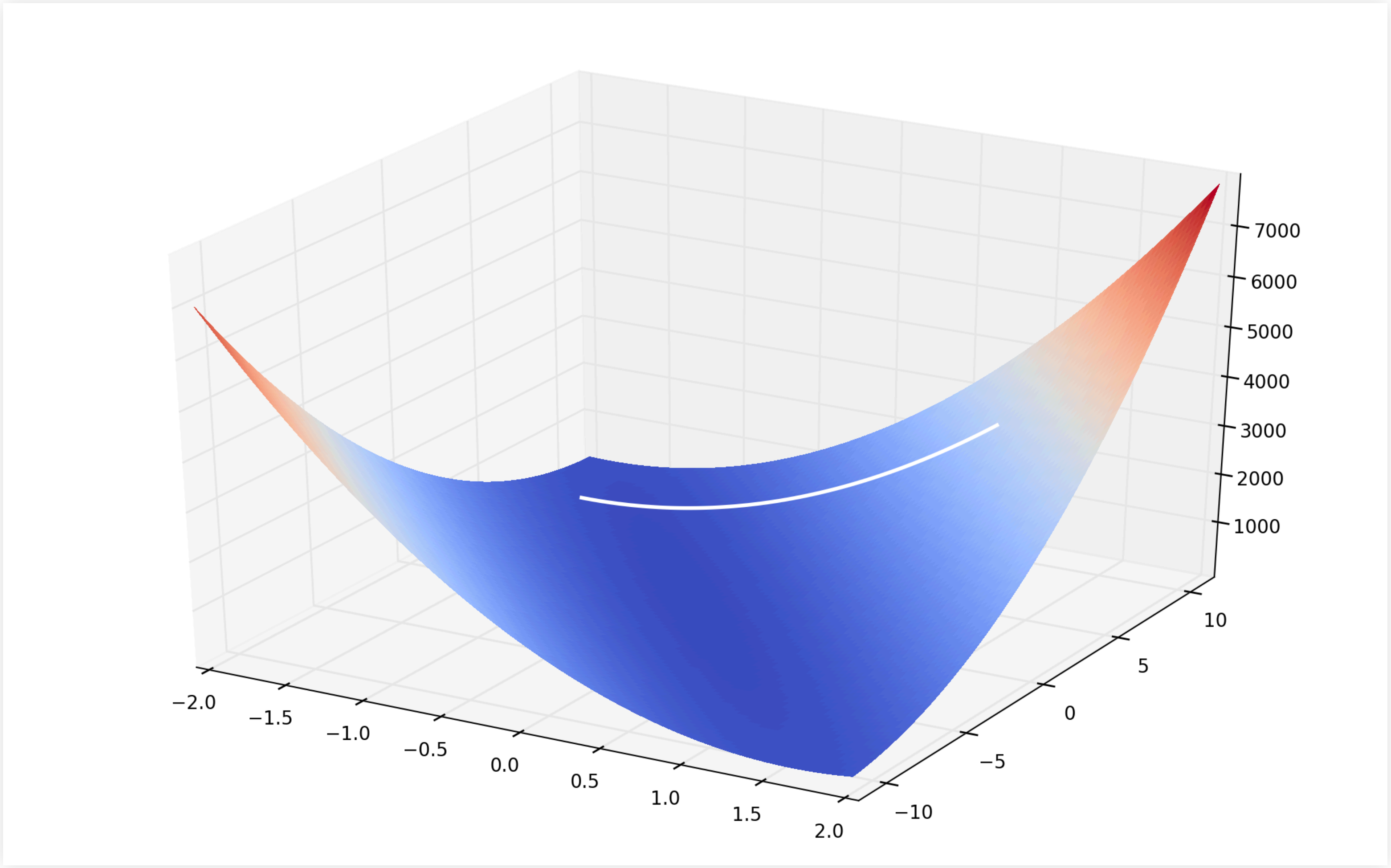
Likelihood

- Having the Loss function, we do gradient descent



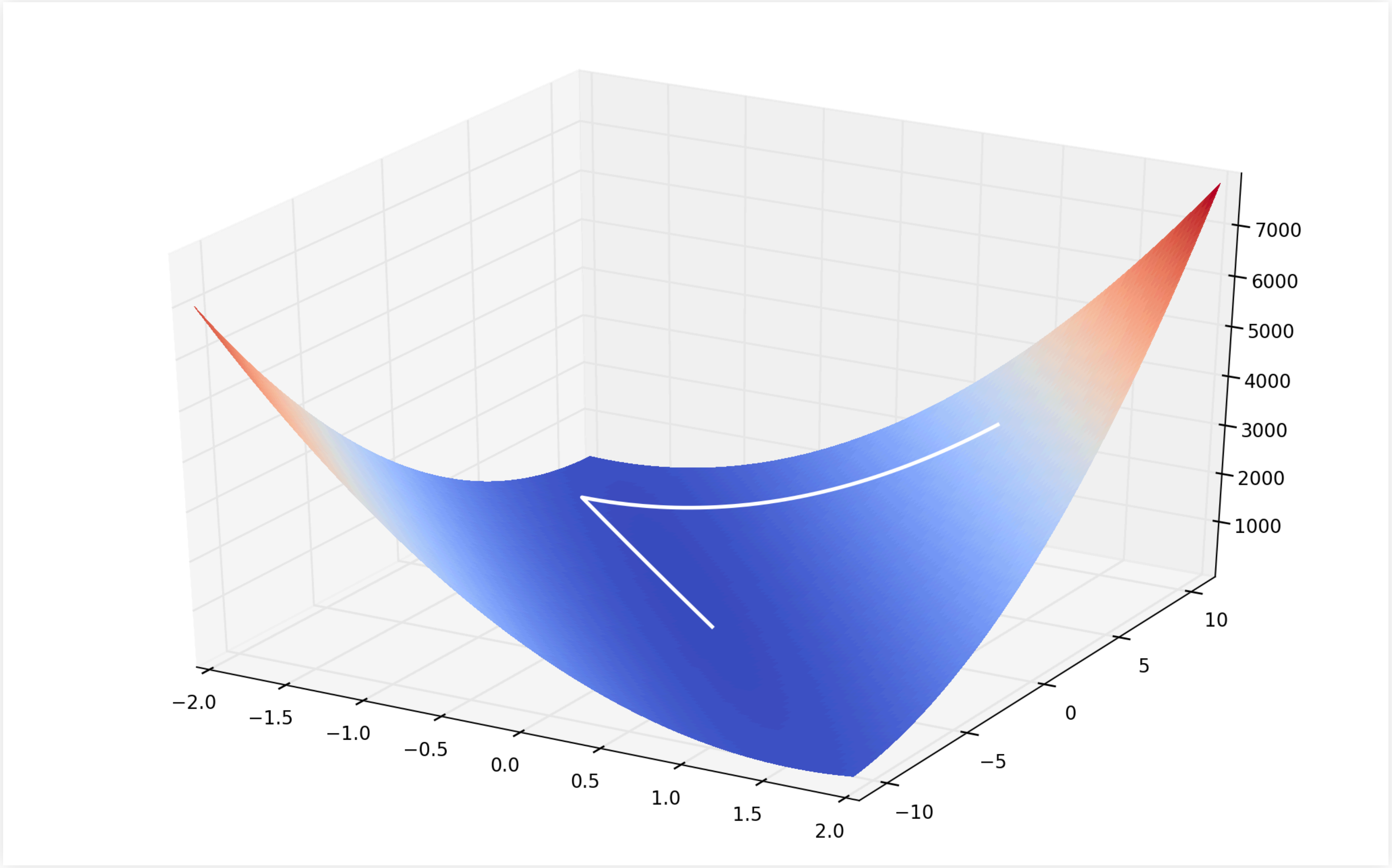
Likelihood

- Having the Loss function, we do gradient descent



Likelihood

- Having the Loss function, we do gradient descent



Maximum Likelihood

Finding a loss function by ML

$$\theta_{ML} = \arg\max_{\theta} P(Y|X;\theta) = \arg\max_{\theta} \sum_{i=1}^{m} \log P(y^i|\vec{x}^i;\theta)$$

- We want to maximize likelihood
- This means minimizing cross entropy between model and data
- Loss function depends on the model output:

- Regression: linear output, mean squared error
- Binary classification: class probability, sigmoid output, logistic loss
- (Also for multilabel classification, with probability for each label)
- N-ary classification, use softmax and the softmax cross entropy:

$$-\sum_{c=1}^{C} y_c \log \frac{e^{a_c}}{\sum_{k=1}^{C} e^{a_k}}$$

Optimizers

Optimizers

Minimizing the loss function

- We want to minimize the loss function (e.g. cross-entropy for ML) to obtain θ from some data
- Numerical optimization is outside the scope of this course

- But it's useful to have some knowledge of the optimizers

Optimizers

Minimizing the loss function

- So far we saw `tf.optimizers.SGD`
  - Basic gradient descent algorithm, single learning rate.
  - Stochastic gradient descent: use gradient computed at each example, selected at random
  - Mini-batch gradient descent: updates after computing the total gradient from a batch of randomly selected examples.
  - Can include momentum (and you should use momentum, in general)
- This is just an alias for the `tf.keras.optimizers.SGD` class
  - We'll be using Keras explicitely from now on

Optimizers

Minimizing the loss function:

- Different parameters may best be changed at different rates

- `tf.keras.optimizers.Adagrad`
- Keeps sum of past (squared) gradients for all parameters
- Divides learning rate of each parameter by this sum
- Parameters with small gradients will have larger learning rates, and vice-versa
- Since Adagrad sums previous gradients, learning rates will shrink
- (good for convex problems)

Optimizers

Minimizing the loss function:

- Some parameters may be left with too large or too small gradients

- `tf.keras.optimizers.RMSProp`
- Keeps moving root of the mean of the squared gradients (RMS)
- Divides gradient by this moving RMS
- Updates will tend to be similar for all parameters.
- Since it uses a moving average, learning rates don't shrink
- Good for non-convex problems, and often used in recurrent neural networks
- Most famous unpublished optimizer

Optimizers

Minimizing the loss function

- `tf.keras.optimizers.Adam`
  - Adaptive Moment Estimation (Adam)
  - Momentum and different learning rates using an exponentially decaying average over the previous gradients
- `tf.keras.optimizers.AdamW`
  - Adaptive Moment Estimation (Adam)
  - Similar to Adam but with Weight Decay, generalizes better than Adam
  - Fast to learn but may have convergence problems

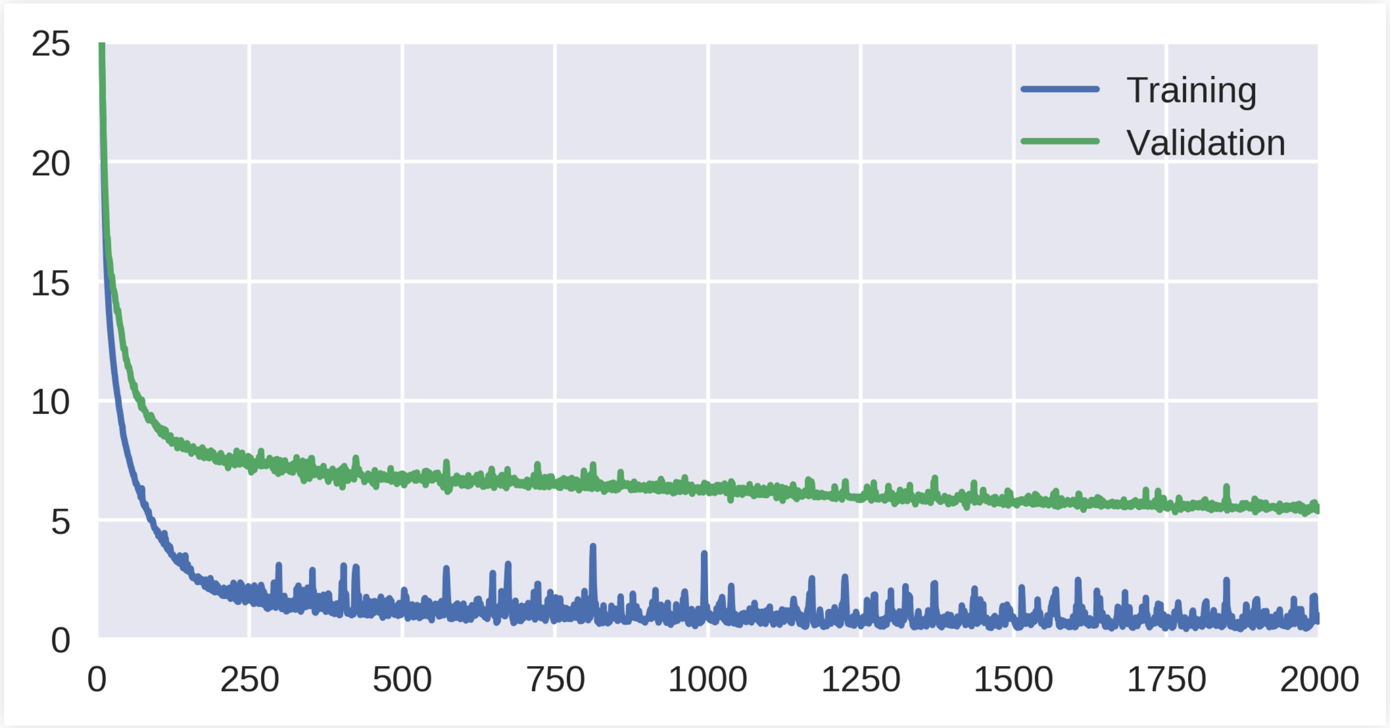
How to choose?

- There is no solid theoretical foundation for this
- So you must choose empirically
  - Which is just a fancy way of saying try and see what works...

Learning Rate

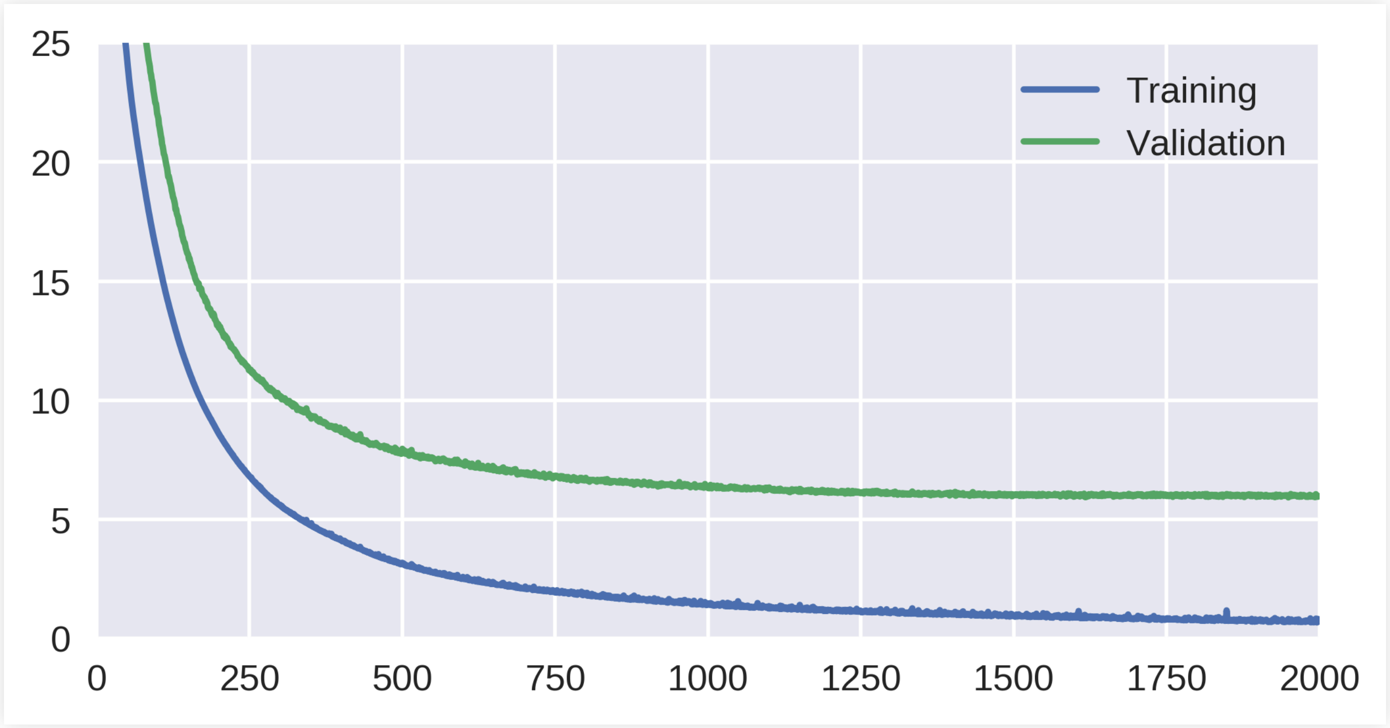
Choosing the best learning rate

- Optimizers can have other parameters, but all have a learning rate
- Too high a learning rate can lead to convergence problems



Learning Rate

- However, if learning rate is too small training can take too long
- Try to make it as high as you can while still converging to low error
- (you can experiment with a subset of your training set, even if overfitting)



Batch Normalization

Normalizing (standardizing) activations

- Compute running averages and standard deviations during training
  - And standardize the inputs to each layer
- Just like we do for the inputs to the network, do for hidden layers too
  - Makes learning easier by preventing extreme values
  - Eliminates shifts in mean and variance during training
  - Reduces the need for each layer to adapt to the changes in the previous one
- This can be done easily in Keras
  - The mean, standard deviation and rescaling can all be part of backpropagation
  - AutoDiff takes care of the derivatives
  - So we can add batch normalization as an additional layer

Overfitting and Validation

Overfitting and Validation

The goal of (supervised) learning is prediction

- And we want to predict outside of what we know

Overfitting

- The problem of adjusting too much to training data
  - and losing generalization
- Two ways of solving this:
  - Select the right model: model selection
  - Adjust training: regularization

Overfitting and Validation

How to check for overfitting

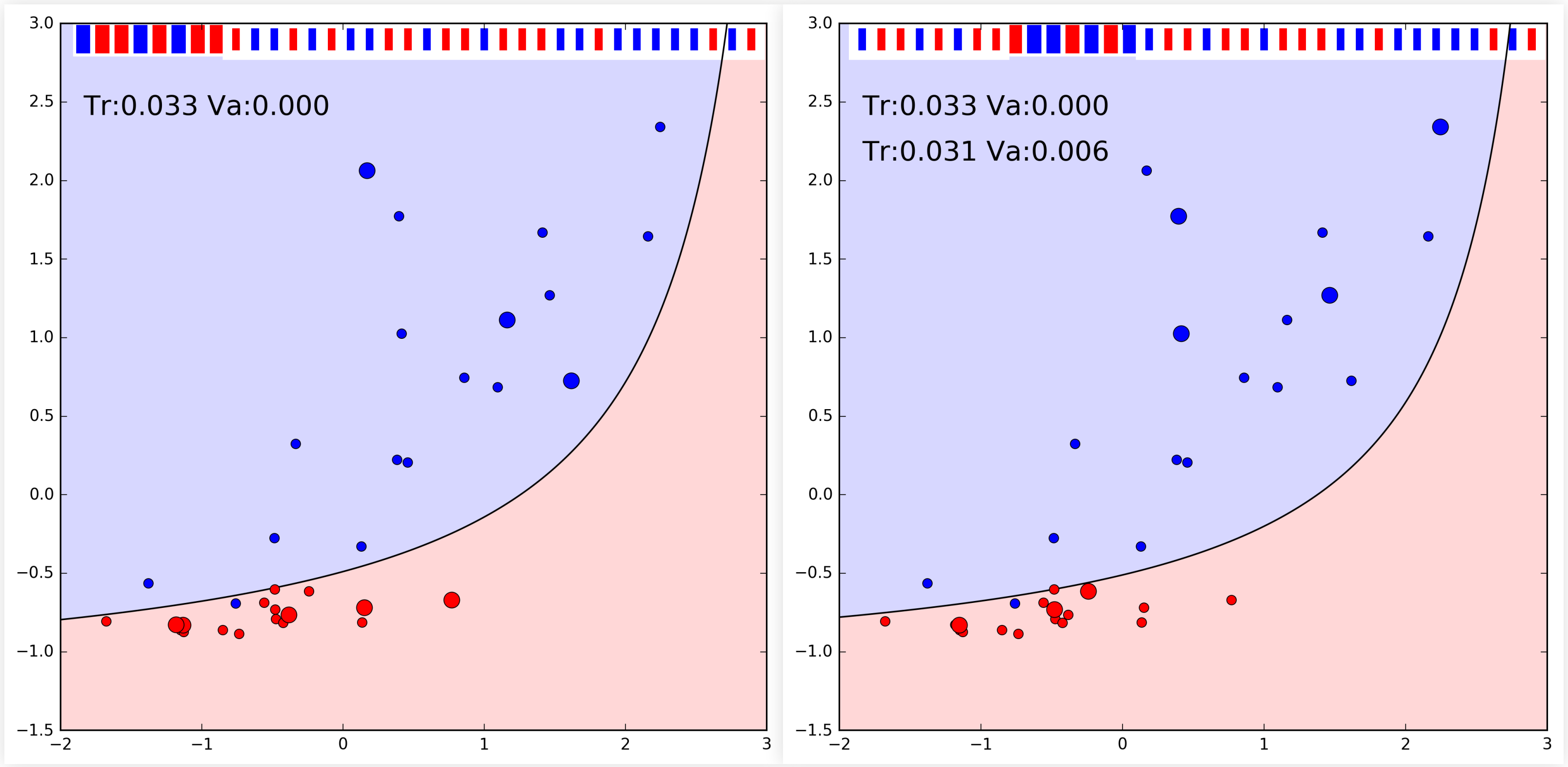
- We need to evaluate performance outside the training set
  - Test set: we need to keep this for final evaluation of error rate
- We can use a validation set
- Or we can use cross-validation

Overfitting and Validation

How to check for overfitting

- Cross-Validation:

- Split training set into K folds, average validations training on the k-1



Overfitting and Validation

How to check for overfitting

- Cross-Validation:

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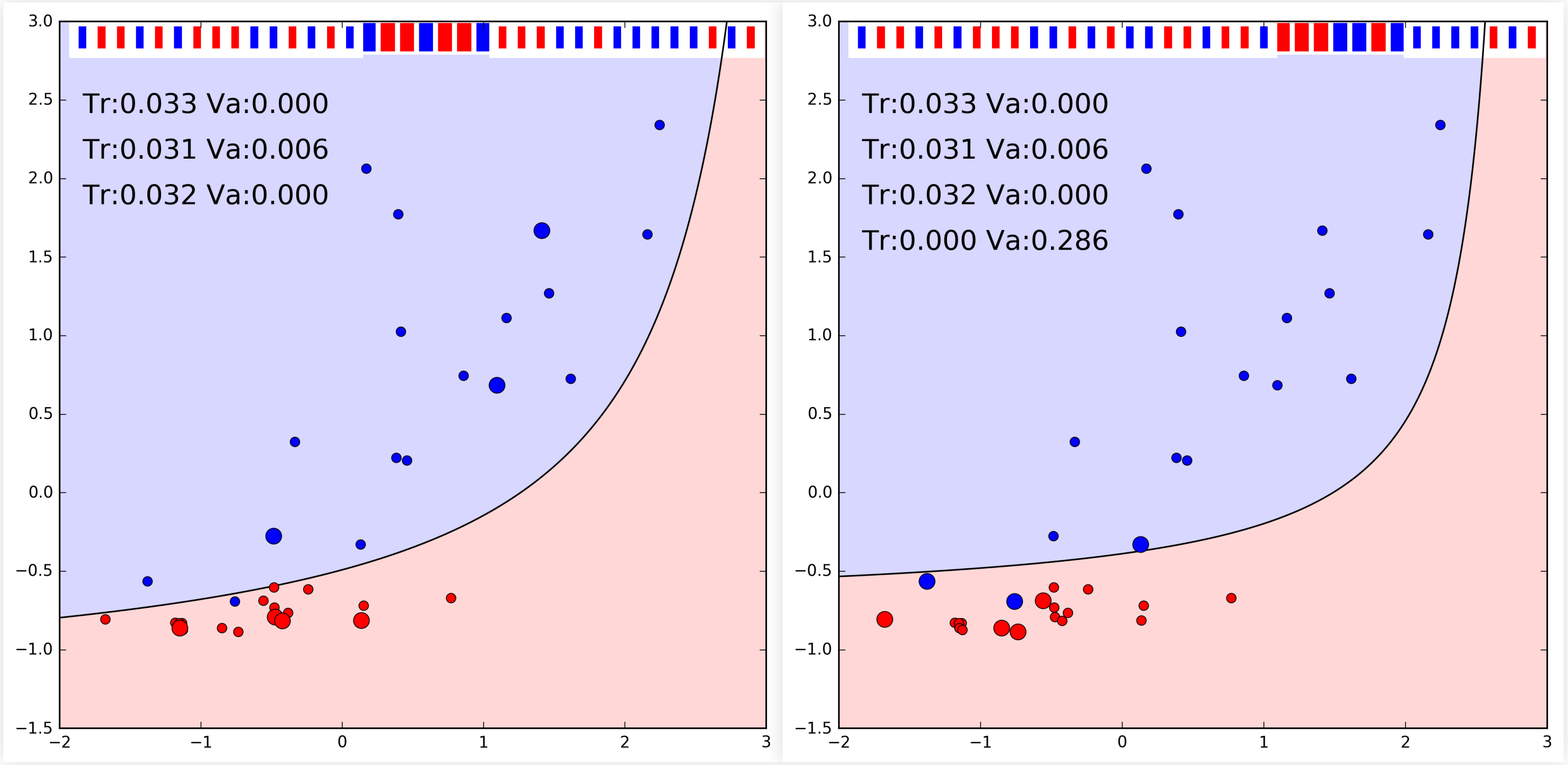


Overfitting and Validation

How to check for overfitting

- Option 1: Cross-validation on training set, test
  - Good when data is scarcer
  - Better estimate of true error
  - More computationally demanding
- Option 2: train, validation for preventing overfitting, test
  - Good when we have lots of data (which is generally the case for DL)
- Cross-validation is widely used outside deep learning
- With deep learning training and validation is more common
  - Deep networks take some time to train

Overfitting and Validation

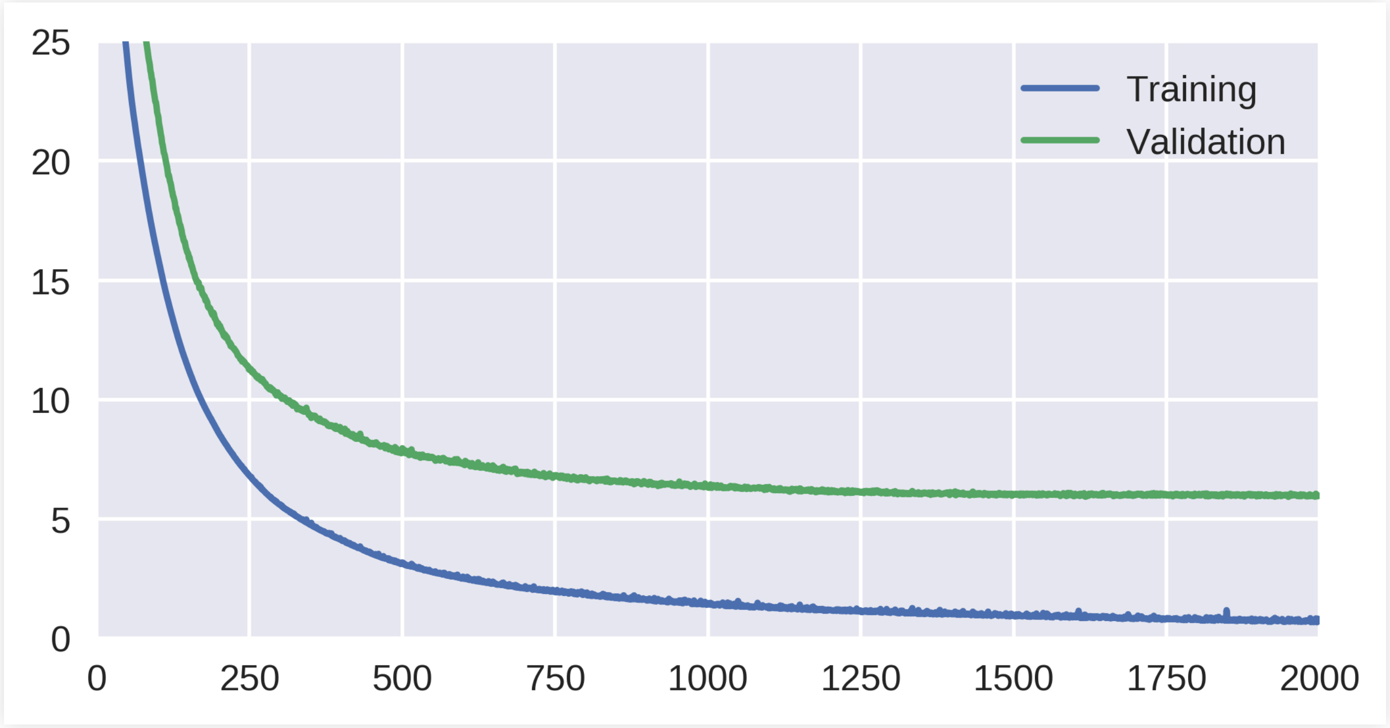
Estimating the true error

- True error: the expected error over all possible data
  - We cannot measure this, since we would need all possible data
- Must be estimated with a test set, outside the training set
- This cannot be the validation set if the validation set was used to optimize hyperparameters
  - We choose the combination with the smallest validation error, this makes the estimate biased.
- Solution: reserve a test set for final estimate of true error
  - This set should not be used for any choice or optimization

Model Selection

- If the model adapts too much to the data, the training error may be low but the true error high

- Example: Auto MPG problem, 100-50-10-1 network.

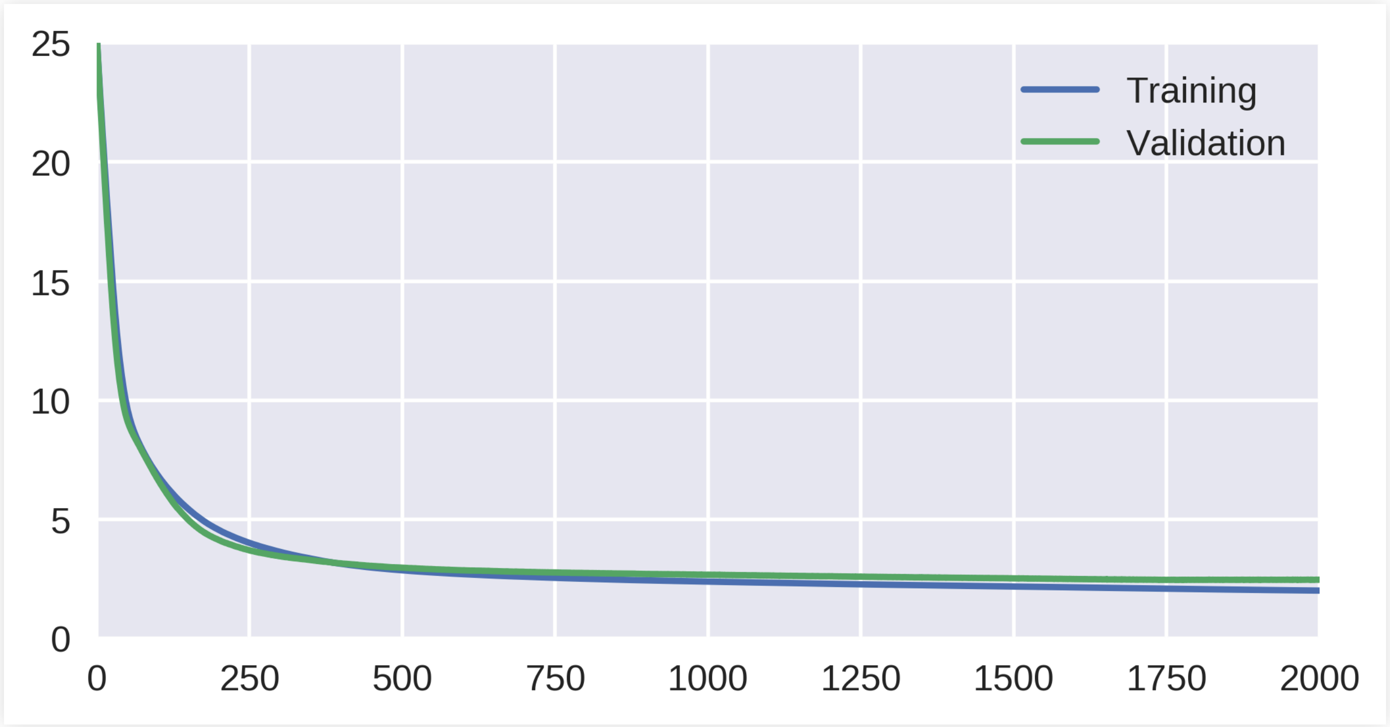


Overfitting

Model Selection

- One way of solving this problem is to use a simpler model (assuming it can fit the data)

- Example: Auto MPG problem, 30-10-1 network.

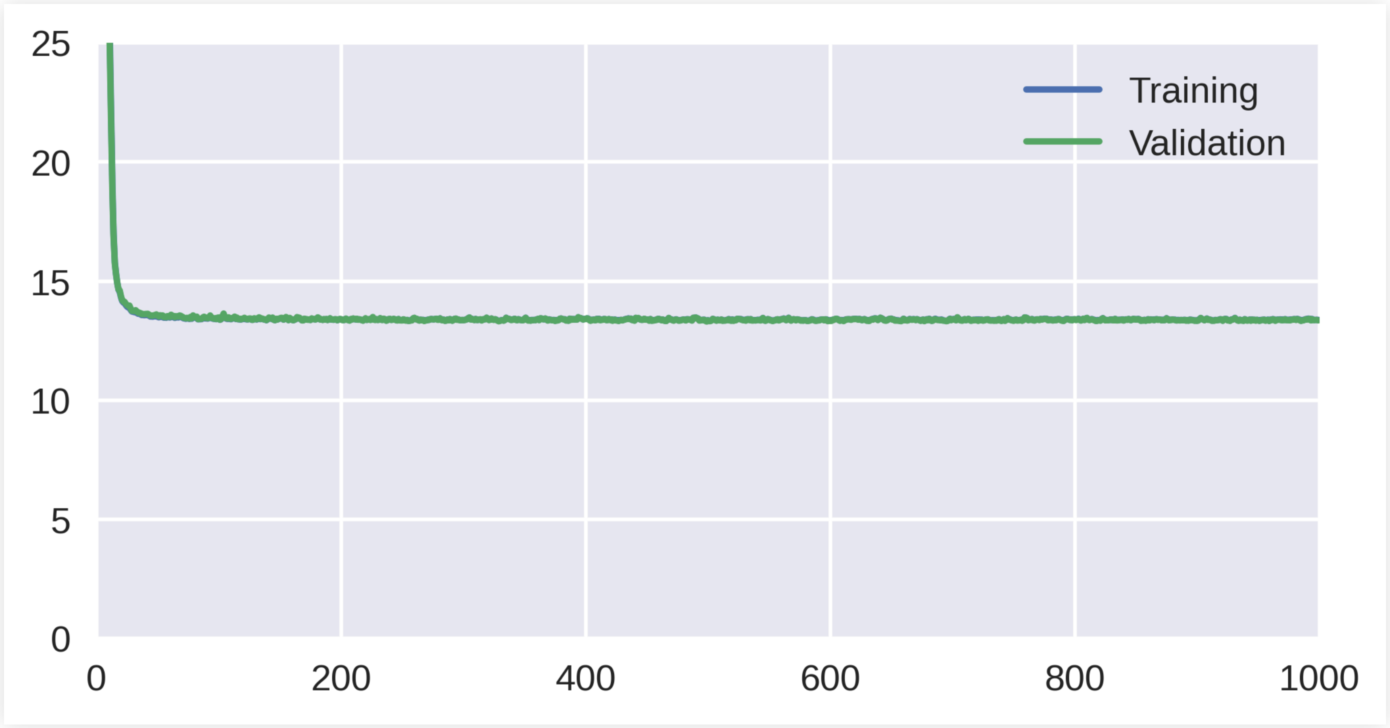


Overfitting

Model Selection

- If the model is too simple, then error may become high

- (Underfitting)
- Example: Auto MPG problem, 3-2-1 network.



Regularization in ANN

Regularization

Penalizing parameter size

- To reduce variance, we can force parameters to remain small by adding a penalty to the objective (cost) function:

$$\tilde{J}(\theta; X, y) = J(\theta; X, y) + \alpha\Omega(\theta)$$

- Where α is the weight of the regularization

- Note: in ANN, generally only the input weights at each neuron are penalized and not the bias weights.

- The norm function $\Omega(\theta)$ usually takes these forms:

- L^2 Regularization (ridge regression): penalize $||\theta||^2$
- L^1 Regularization: penalize $\sum_i |\theta_i|$

Regularization

L^2 Regularization is weight decay

- If we penalize w^2, the gradient becomes:

$$\nabla \tilde{J}(\theta; X, y) = \nabla J(\theta; X, y) + 2\alpha w$$

- This means the update rule for the weight becomes

$$w \leftarrow w - \epsilon 2\alpha w - \epsilon \nabla J(\theta; X, y)$$

- We decrease the magnitude of w to $(1 - \epsilon 2\alpha)$ per update
- This causes weights that do not contribute to reducing the cost function to shrink

Regularization

L^1 Regularization

- If we penalize $|w|$, the gradient becomes:

$$\nabla \tilde{J}(\theta; X, y) = \nabla J(\theta; X, y) + \alpha \, sign(w)$$

- This penalizes parameters by a constant value, leading to a sparse solution

- Some weights will have an optimal value of 0

L^1 vs L^2 Regularization

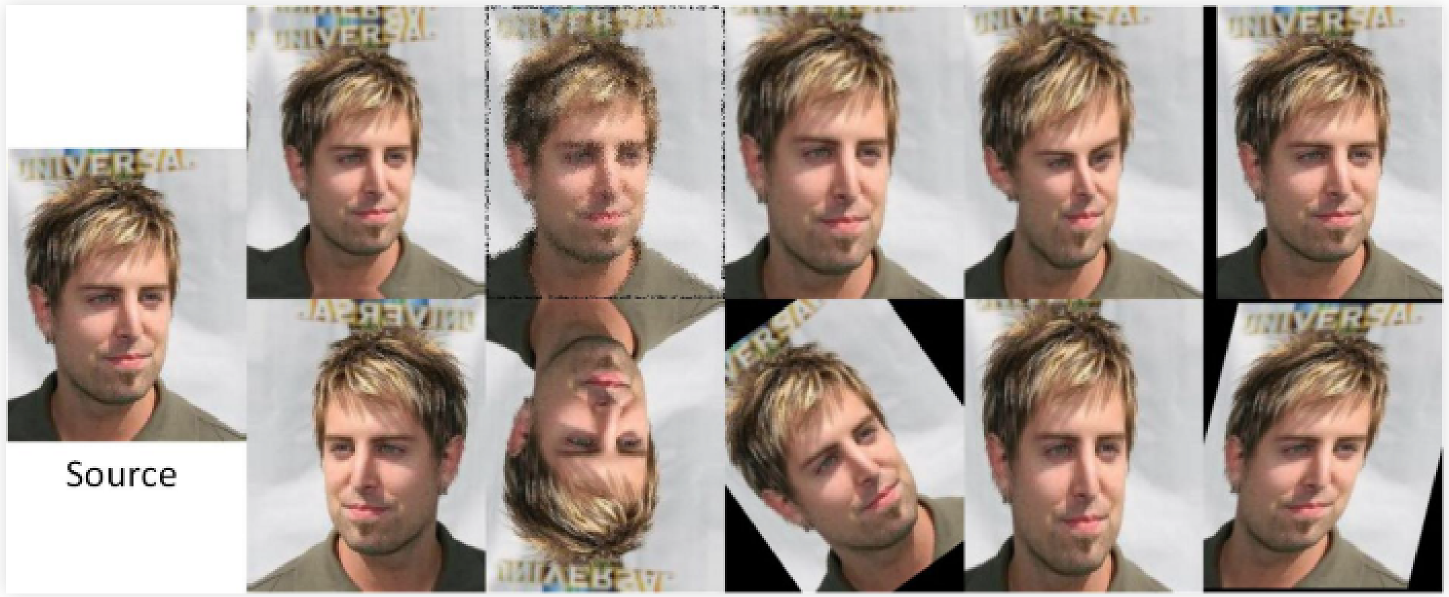
- L^1 minimizes number of non-zero weights
- L^2 minimizes overall weight magnitude

Regularization

Dataset augmentation

- More data is generally better, although not always readily available
- But sometimes we can make more data
- E.g. Image classification:

• Translate images. Rotate or flip, if appropriate (not for character recognition)



Wang et al, 2019, "A survey of face data augmentation".

Regularization

Dataset augmentation by noise injection

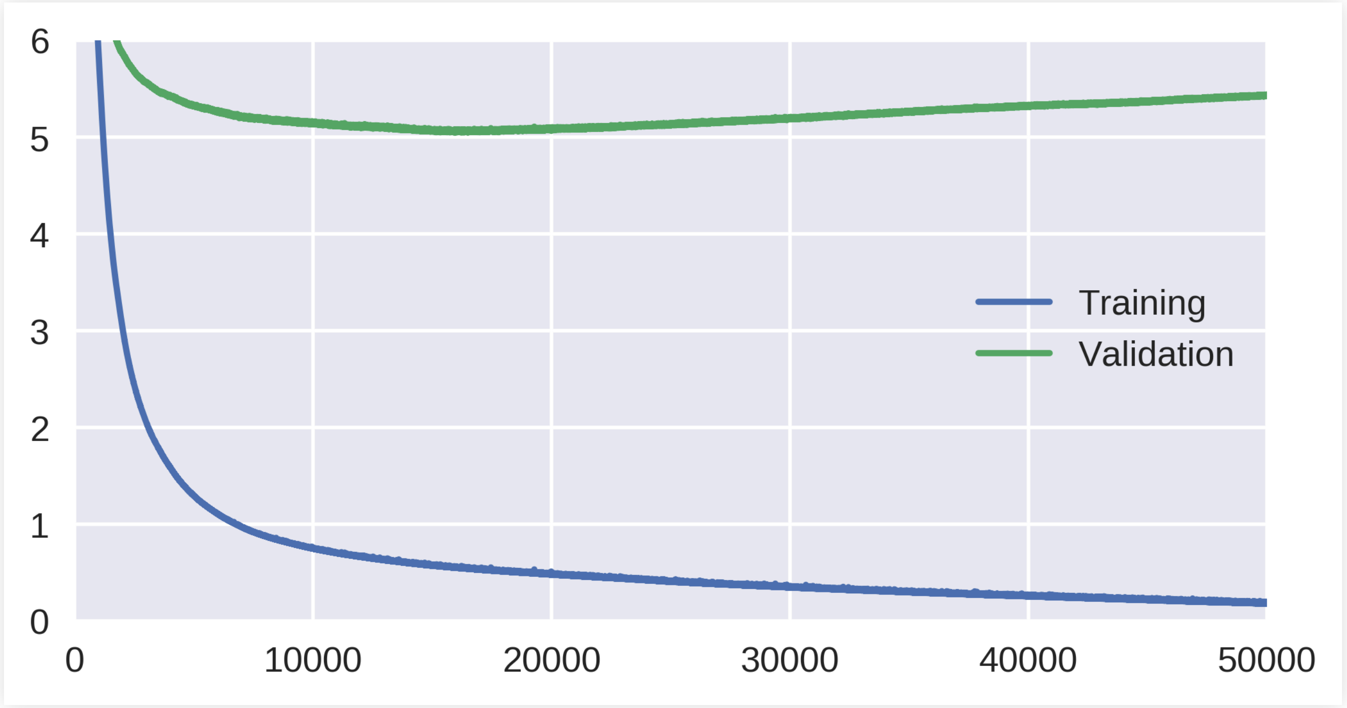
- Noise injection is an (implicit) form of dataset augmentation
- Add (carefully) noise to inputs, or even to some hidden layers
- Noise can also be applied to the weights
- Or even the output
- There may be errors in labelling
- Or for label smoothing: use $\frac{\epsilon}{(k-1)}$ and $1-\epsilon$ instead of 0 and 1 for target
- This prevents pushing softmax or sigmoid to infinity

Regularization

Early stopping

- Use validation to stop at best point

- Constrains weights to be closer to starting distribution



Regularization

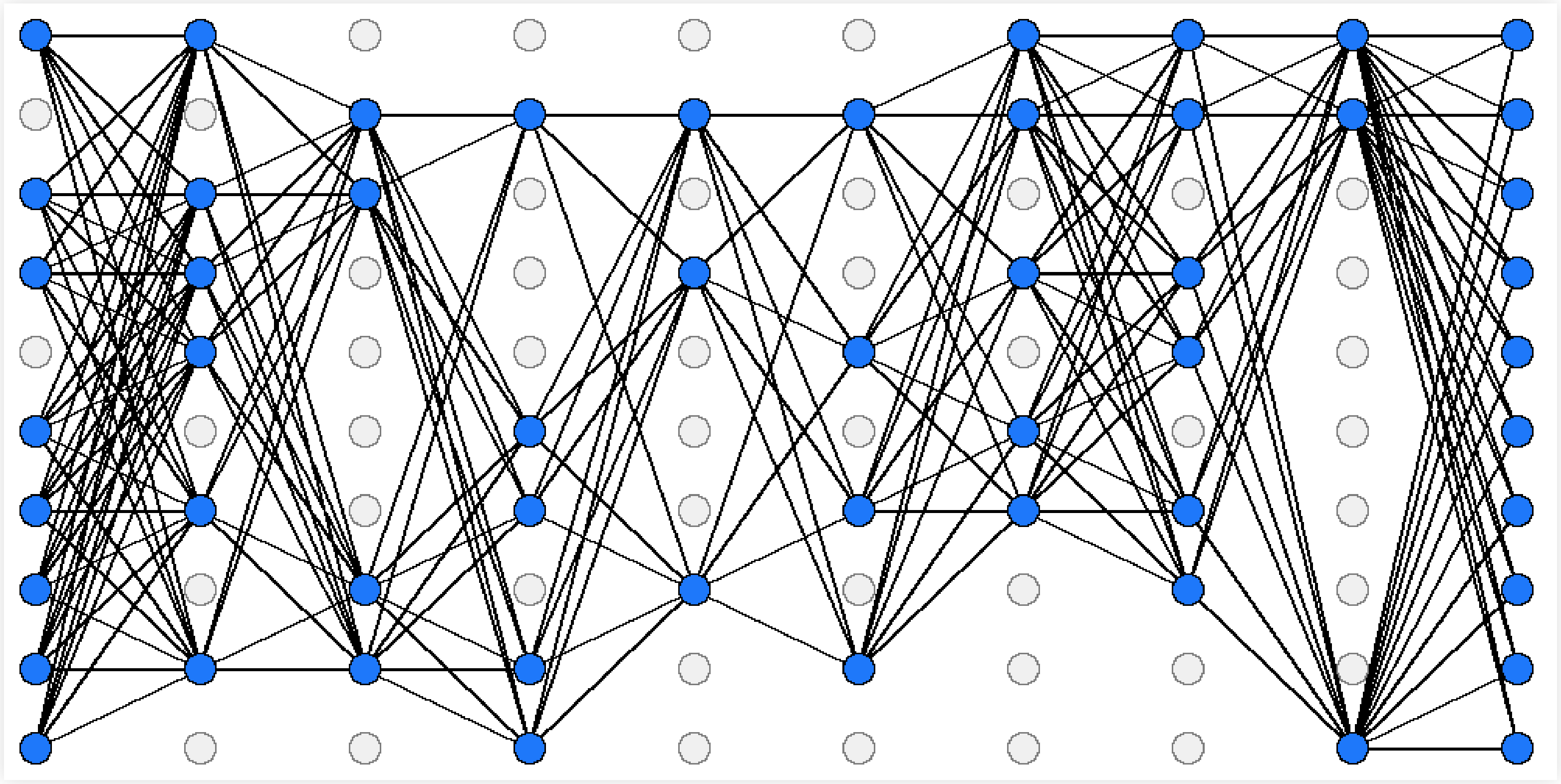
Bagging

- Training a set of models on different subsets of the data
- use the average response (or majority vote)
- Improves performance, as it reduces variance without affecting bias, and ANN can have high variance
- However, it can be costly to train and use many deep models.

Regularization

Dropout

- "Turns off" random input and hidden neurons in each minibatch



Regularization

Dropout

- Dropout does model averaging implicitely
- Turning off neurons at random trains an ensemble of many different networks
- After training, weights are scaled by the probability of being "on"
  - (same expected activation value)
- Keras automatically adjust for this when we use a Dropout layer

Activation, Loss and Optimization

Summary

Activation and Loss

Summary

- The vanishing gradients problem, ReLU
- Activations for hidden and output layers
- Loss functions
- Optimizers, learning rate, batch normalization
- Model selection and Regularization

Further reading:

- Goodfellow et.al, Deep learning, Chaps 5-7 and 11, Sects 8.4; 8.7.1
- Tensorflow, activation functions:

• https://www.tensorflow.org/api_guides/python/nn#Activation_Functions