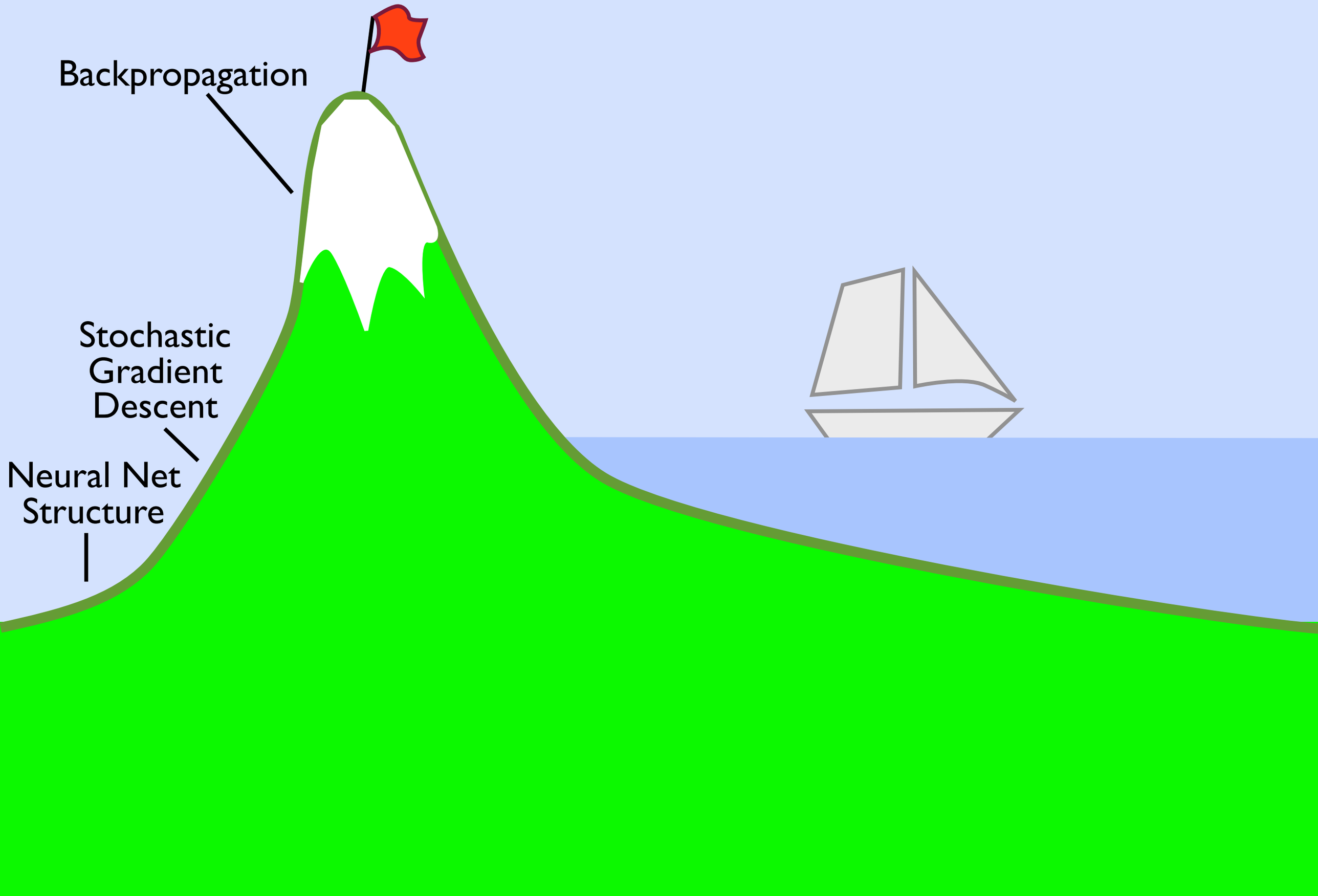
Machine Learning for Physicists

Lecture 4

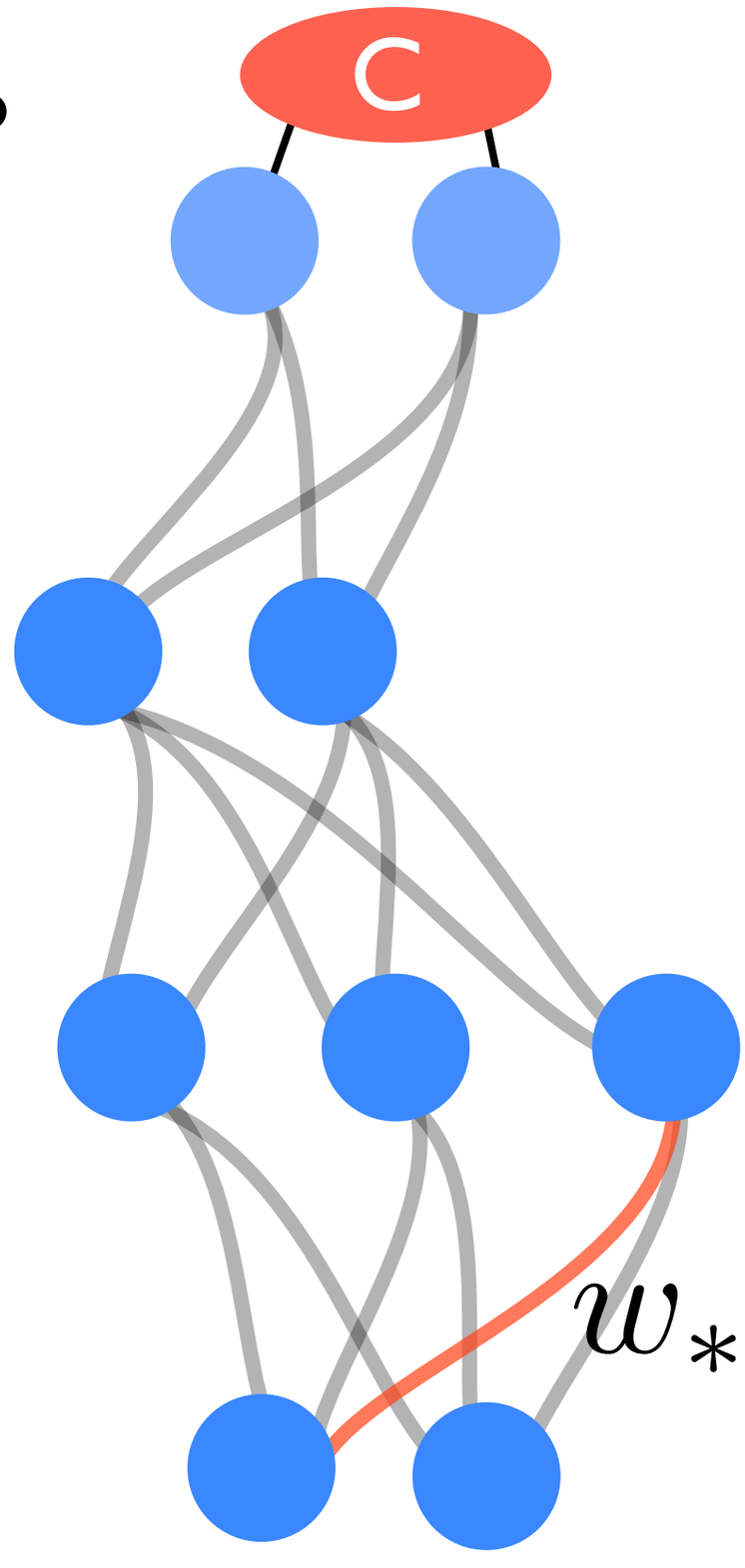
Summer 2017

University of Erlangen-Nuremberg
Florian Marquardt


Backpropagation
Stochastic Gradient Descent
Neural Net Structure

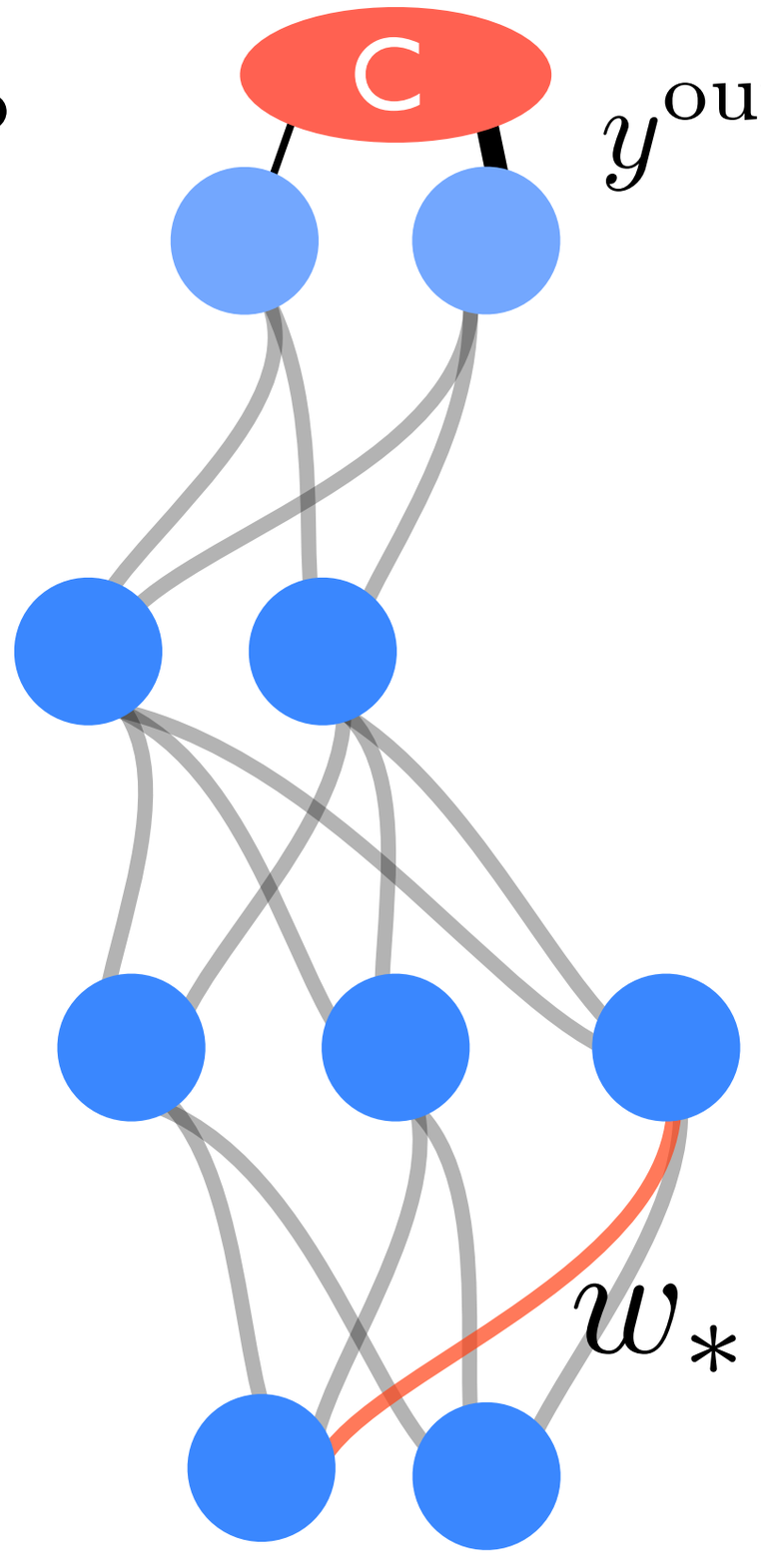
Backpropagation: the principle

$$\frac{\partial C}{\partial w_*} =?$$



Backpropagation: the principle

$$\frac{\partial C}{\partial w_*} =?$$

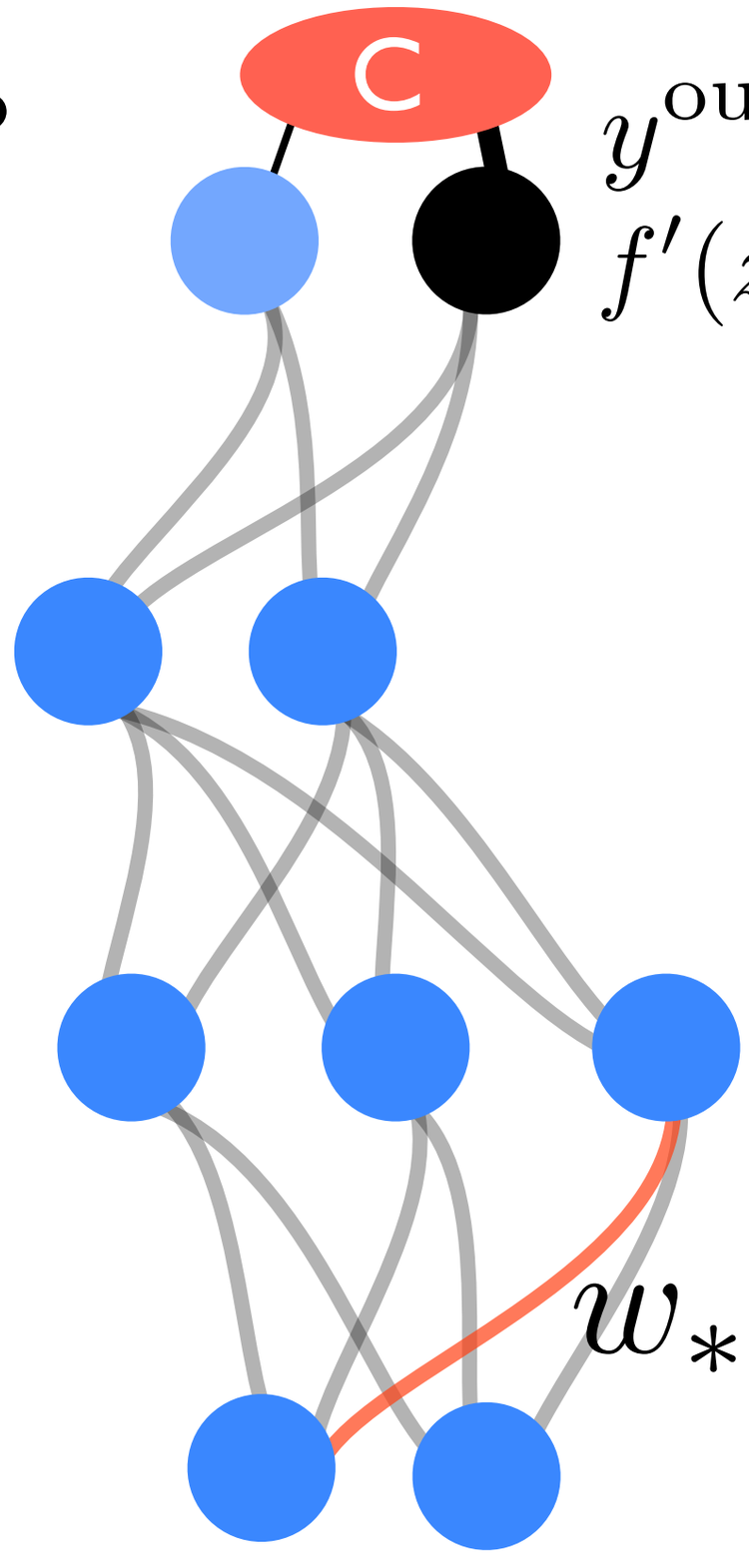


$$y^{\text{out}} - F(y^{\text{in}})$$

(omitting indices, should be clear from figure)

Backpropagation: the principle

$$\frac{\partial C}{\partial w_*} =?$$

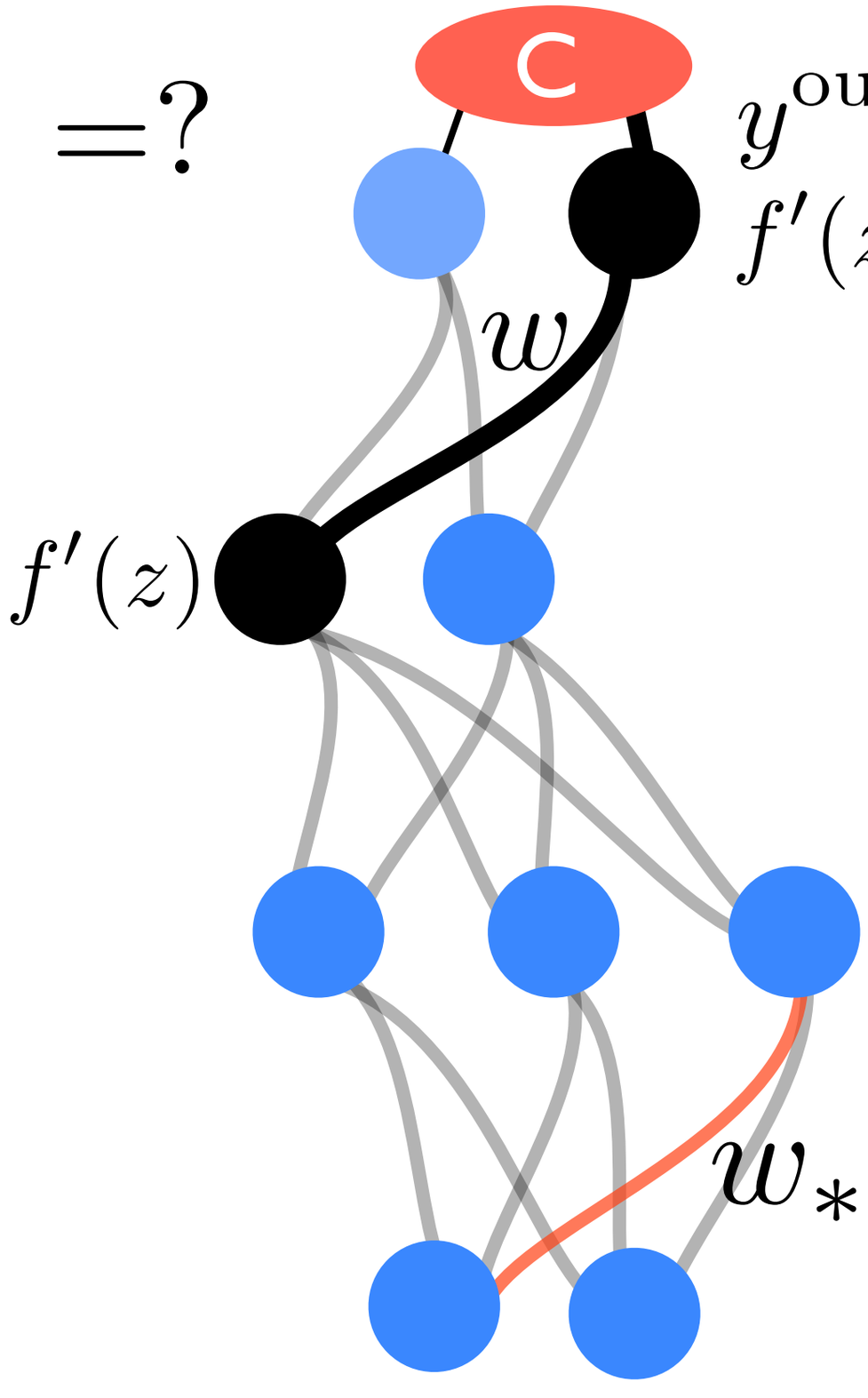


$$y^{\text{out}} - F(y^{\text{in}})$$
$$f'(z)$$

(omitting indices, should be clear from figure)

Backpropagation: the principle

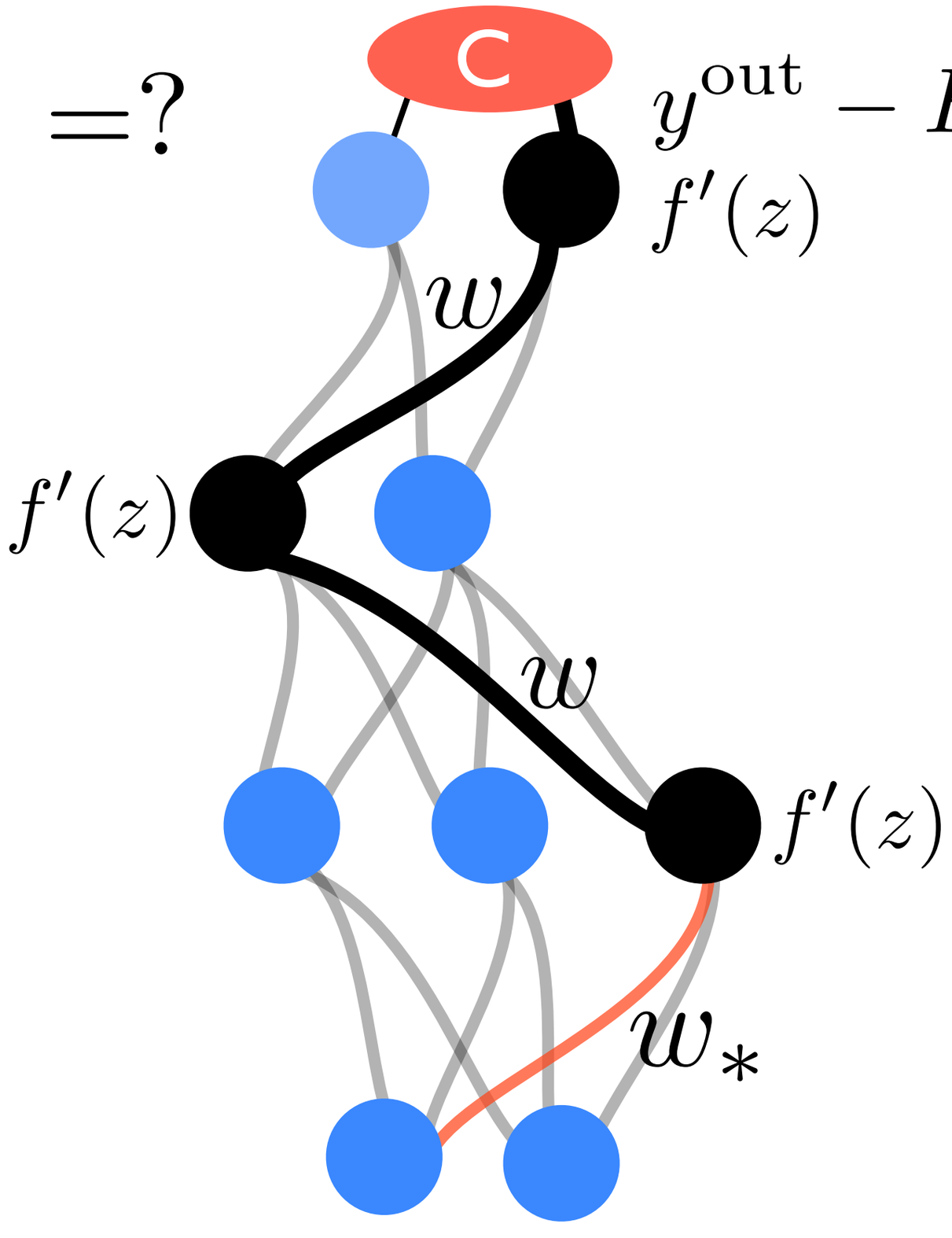
$$\frac{\partial C}{\partial w_*} =?$$



(omitting indices, should be clear from figure)

Backpropagation: the principle

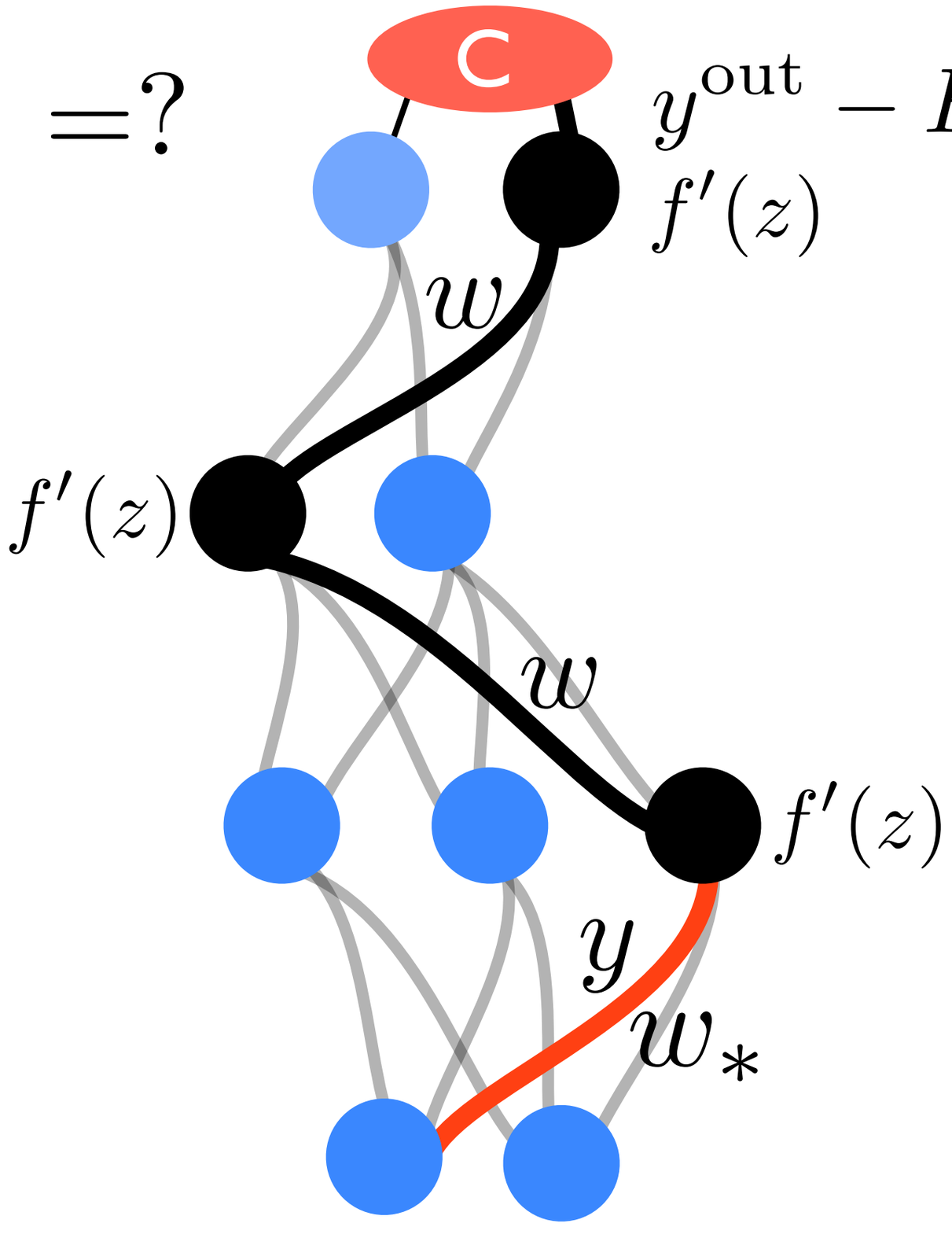
$$\frac{\partial C}{\partial w_*} =?$$



(omitting indices, should be clear from figure)

Backpropagation: the principle

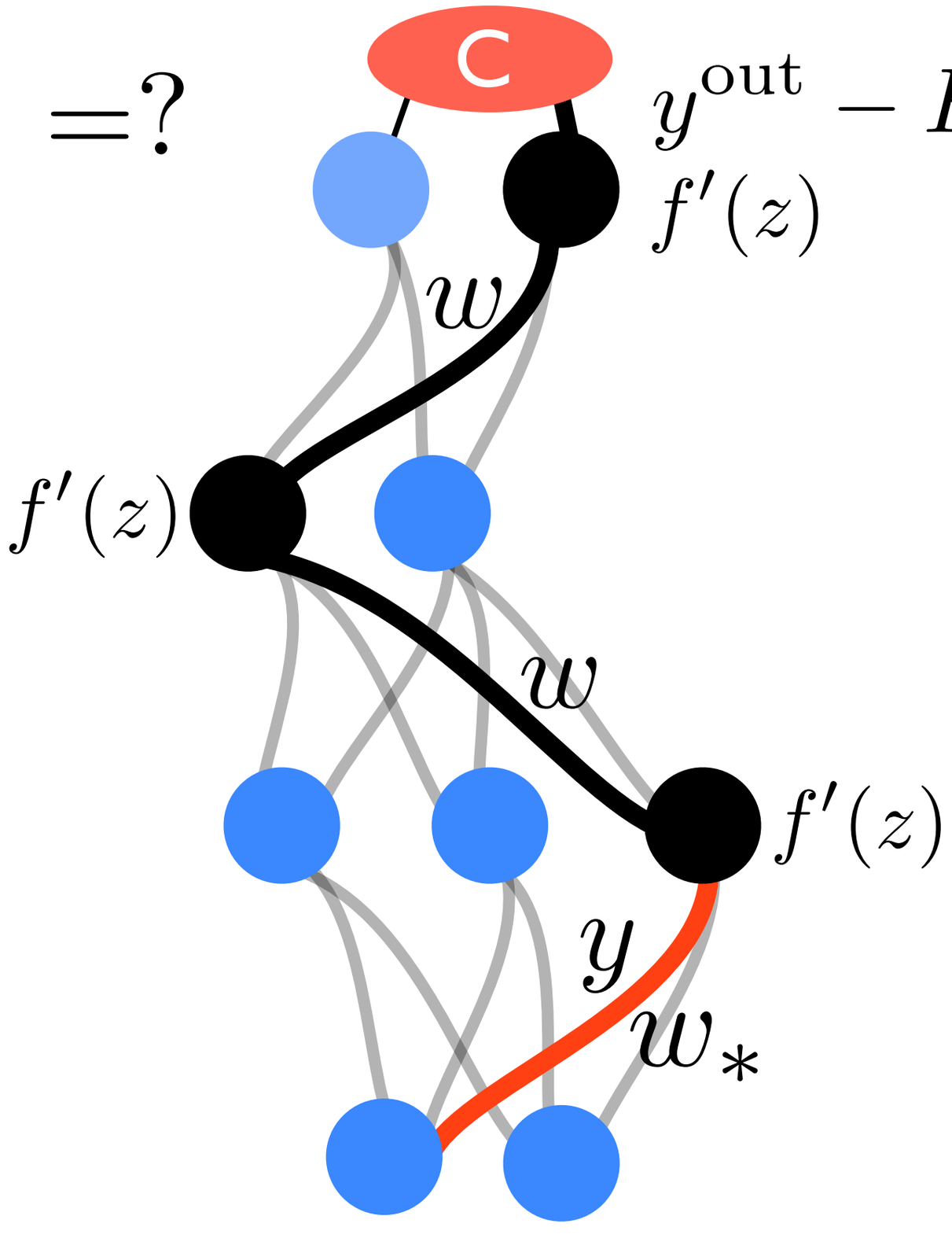
$$\frac{\partial C}{\partial w_*} =?$$



(omitting indices, should be clear from figure)

Backpropagation: the principle

$$\frac{\partial C}{\partial w_*} =?$$



$$y^{\text{out}} - F(y^{\text{in}})$$

$$f'(z)$$

and now:
sum over ALL possible paths!

similar to Feynman sum over paths (path integral)

efficient implementation: repeated matrix/vector multiplication

(omitting indices, should be clear from figure)

Backpropagation: the code

```
def net_f_df(z): # calculate f(z) and f'(z)
    val=1/(1+exp(-z))
    return(val,exp(-z)*(val**2)) # return both f and f'
```

```
def forward_step(y,w,b): # calculate values in next layer
z=dot(y,w)+b # w=weights, b=bias vector for next layer
    return(net_f_df(z)) # apply nonlinearity
```

```
def apply_net(y_in): # one forward pass through the network
    global Weights, Biases, NumLayers
    global y_layer, df_layer # store y-values and df/dz
    y=y_in # start with input values
    y_layer[0]=y
    for j in range(NumLayers): # loop through all layers
        # j=0 corresponds to the first layer above input
        y,df=forward_step(y,Weights[j],Biases[j])
        df_layer[j]=df # store f'(z)
        y_layer[j+1]=y # store f(z)
    return(y)
```

only 30 lines of code!

```
def backward_step(delta,w,df):
    # delta at layer N, of batchsize x layersize(N))
    # w [layersize(N-1) x layersize(N) matrix]
    # df = df/dz at layer N-1, of batchsize x layersize(N-1)
    return( dot(delta,transpose(w))*df )
```

```
def backprop(y_target): # one backward pass
    global y_layer, df_layer, Weights, Biases, NumLayers
    global dw_layer, db_layer # dCost/dw and dCost/db
  #(w,b=weights,biases)
    global batchsize

    delta=(y_layer[-1]-y_target)*df_layer[-1]
    dw_layer[-1]=dot(transpose(y_layer[-2]),delta)/batchsize
    db_layer[-1]=delta.sum(0)/batchsize
    for j in range(NumLayers-1):
        delta=backward_step(delta,Weights[-1-j],df_layer[-2-j])
        dw_layer[-2-j]=dot(transpose(y_layer[-3-j]),delta)/batchsize
        db_layer[-2-j]=delta.sum(0)/batchsize
```

Neural networks: the ingredients

General purpose algorithm: feedforward & backpropagation (implement once, use often)

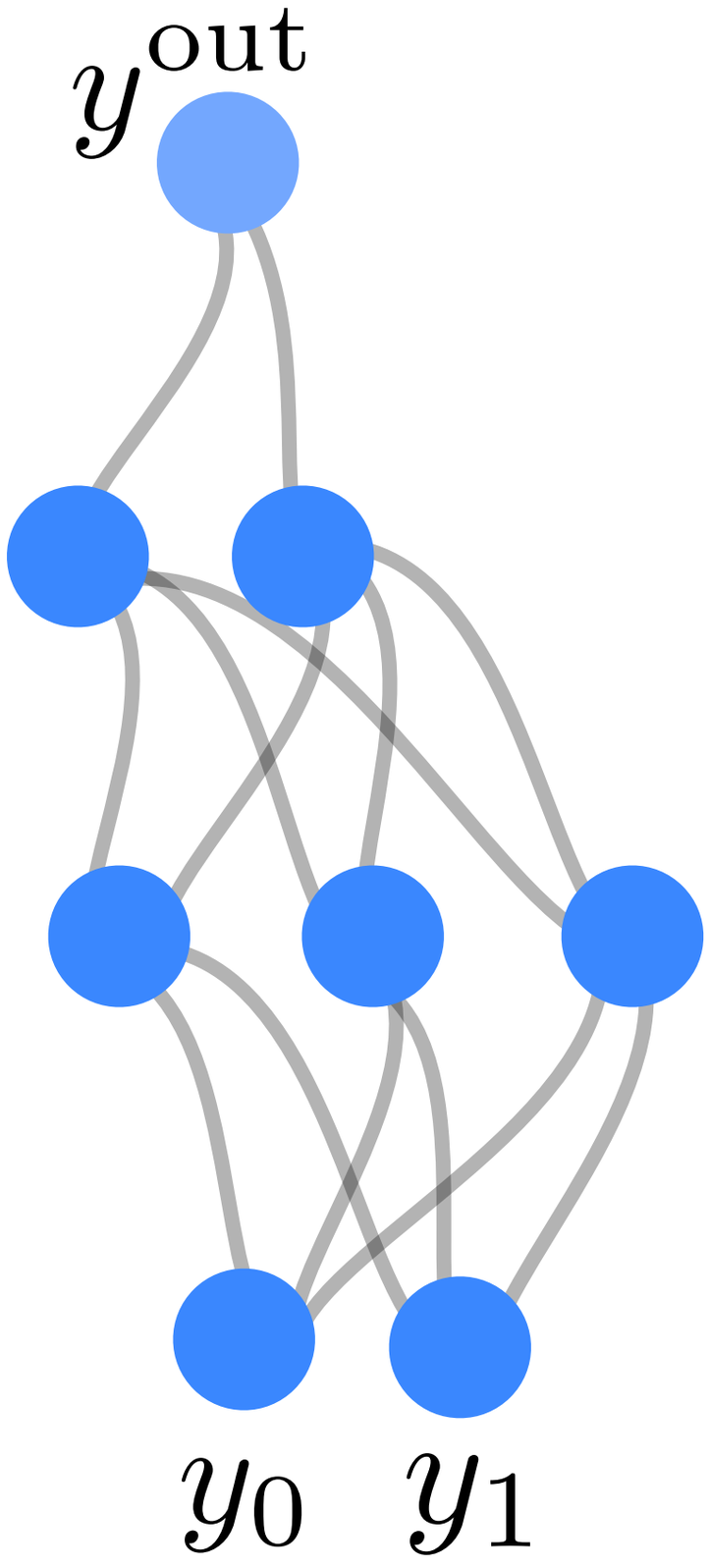
Problem-specific:
Choose network layout (number of layers, number of neurons in each layer, type of nonlinear functions, maybe specialized structures of the weights) **"Hyperparameters"**

Generate training (& validation & test) samples: load from big databases (that have to be compiled from the internet or by hand!) or produce by software

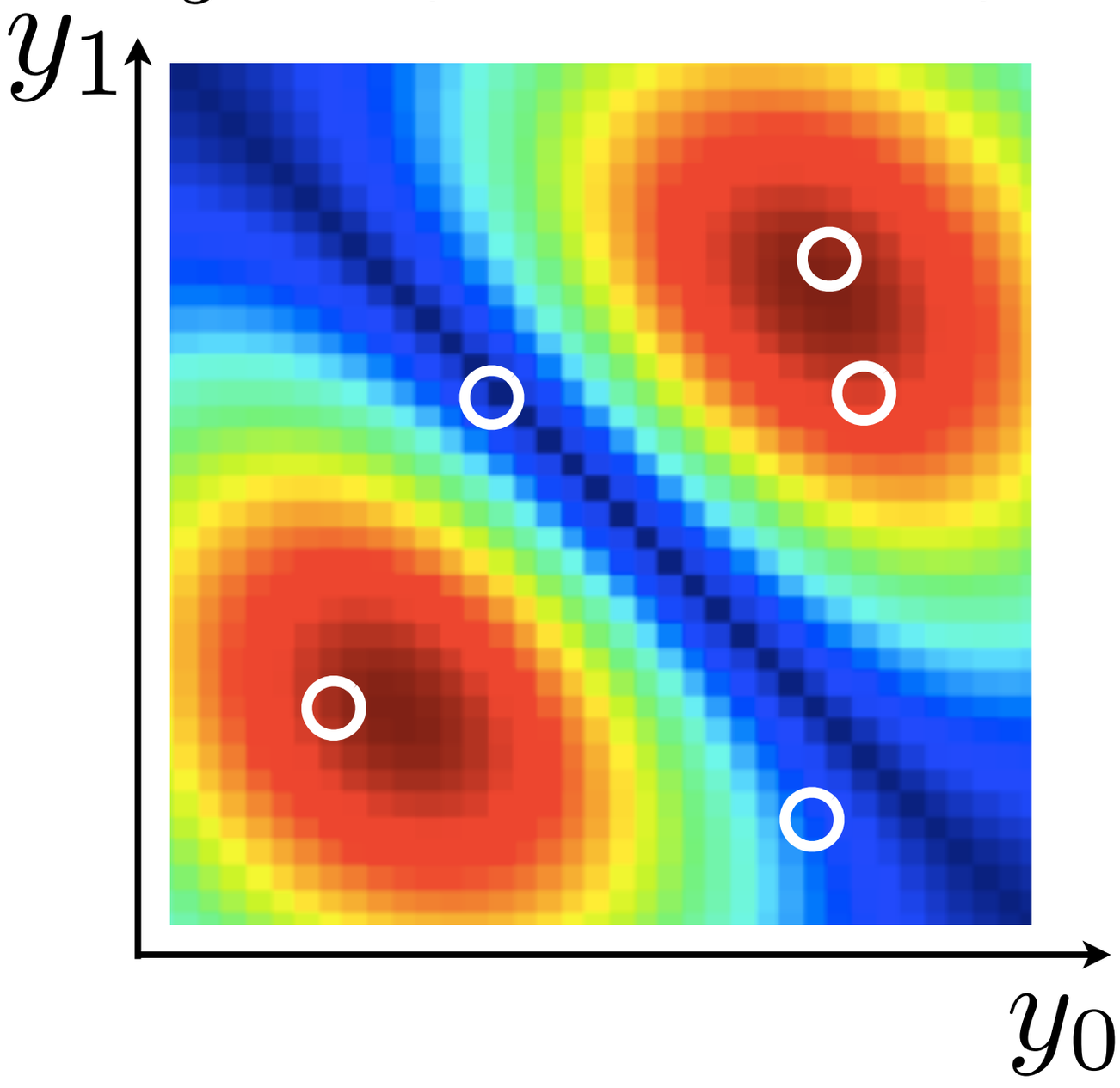
Monitor/optimize training progress (possibly choose learning rate and batch size or other parameters, maybe try out many combinations) **"Hyperparameters"**

Example: Learning a 2D function

see notebook (on website): **MultiLayerBackProp**



y^{out} (values as color)



Evaluate at sample points

Example: Learning a 2D function

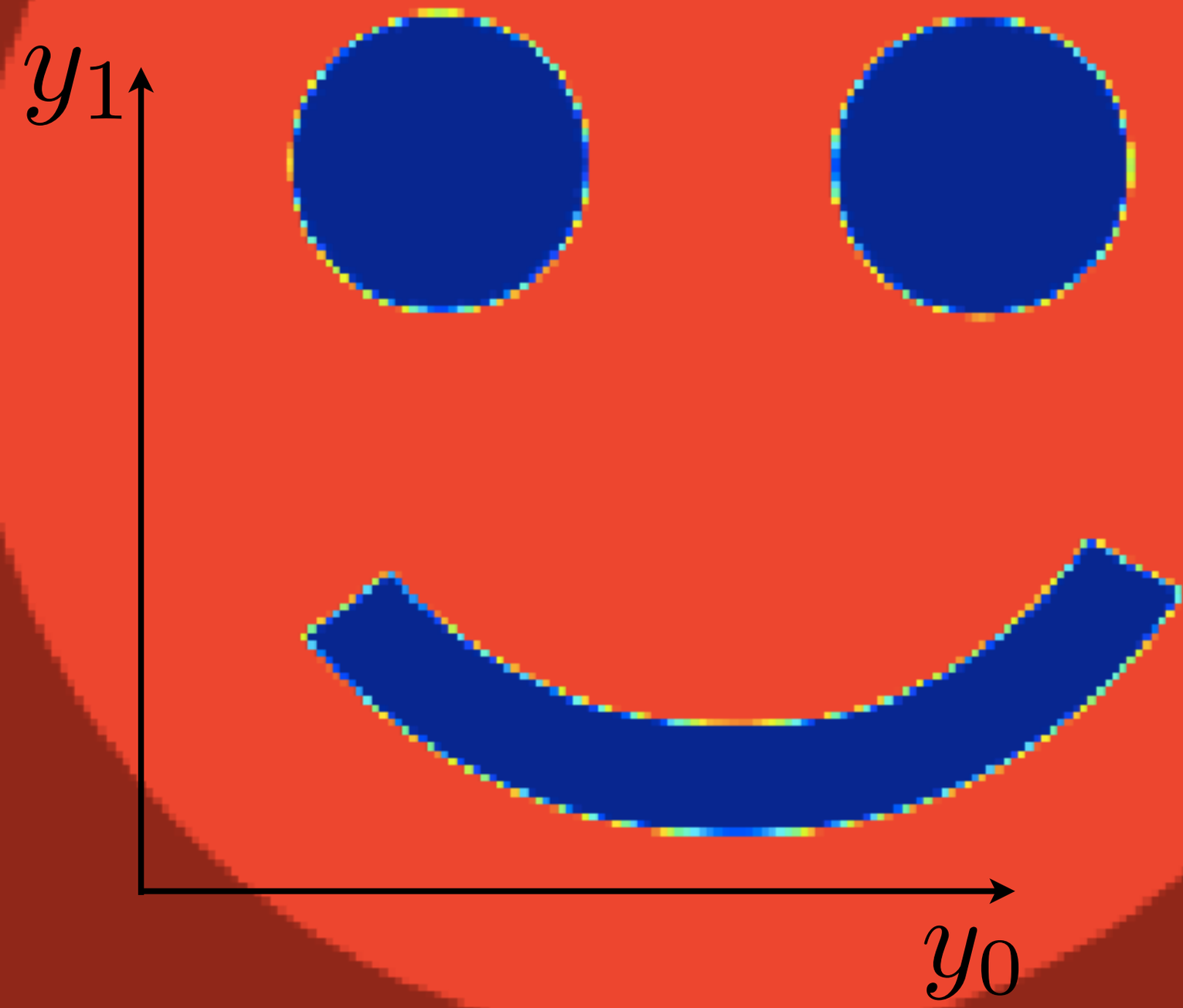
see notebook (on website): **MultiLayerBackProp**

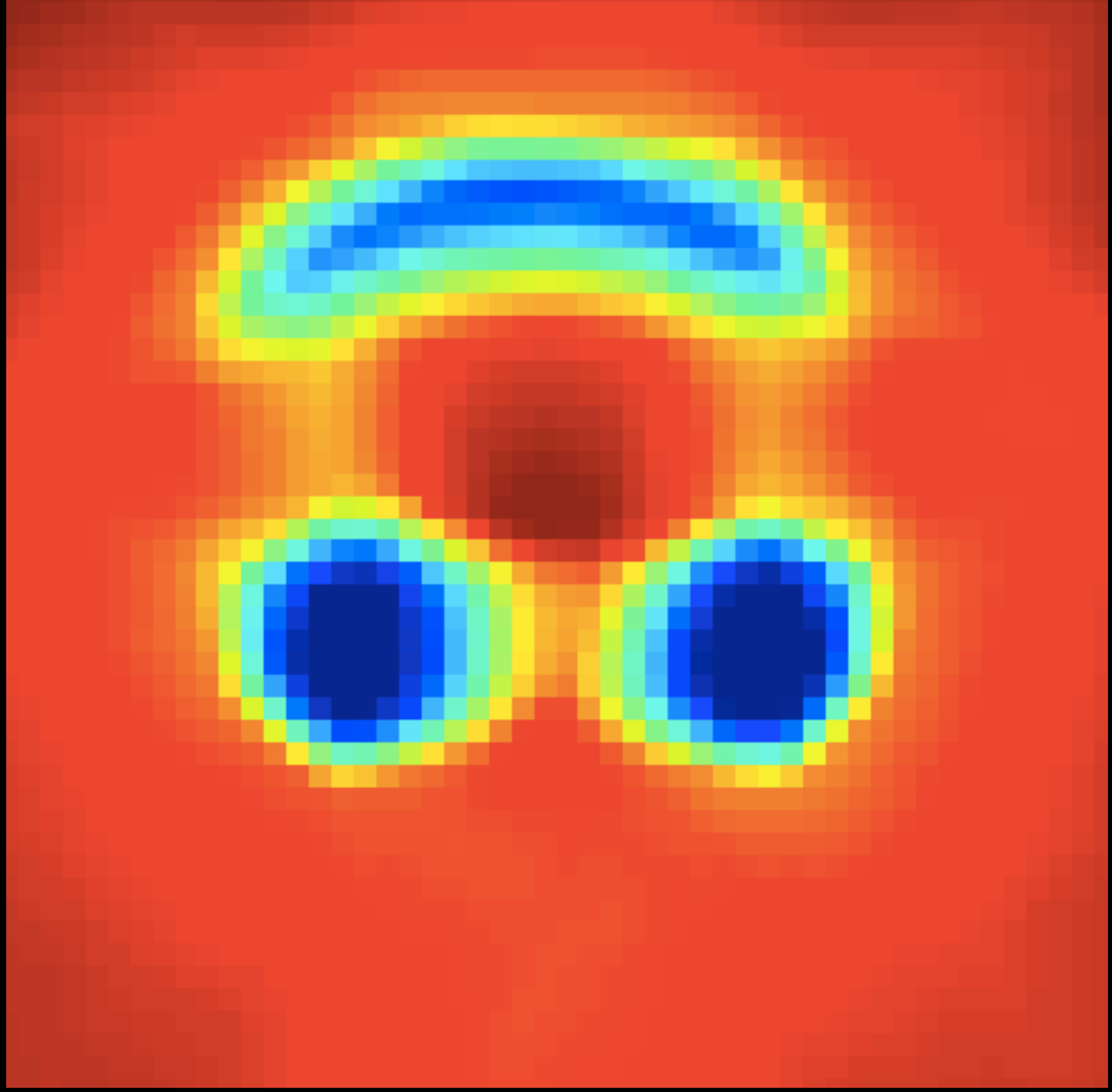
```
# pick batchsize random positions in the 2D square
def make_batch():
    global batchsize

    inputs=random.uniform(low=-0.5,high=+0.5,size=[batchsize,2])
    targets=zeros([batchsize,1]) # must have right dimensions
    targets[:,0]=myFunc(inputs[:,0],inputs[:,1])
    return(inputs,targets)
```

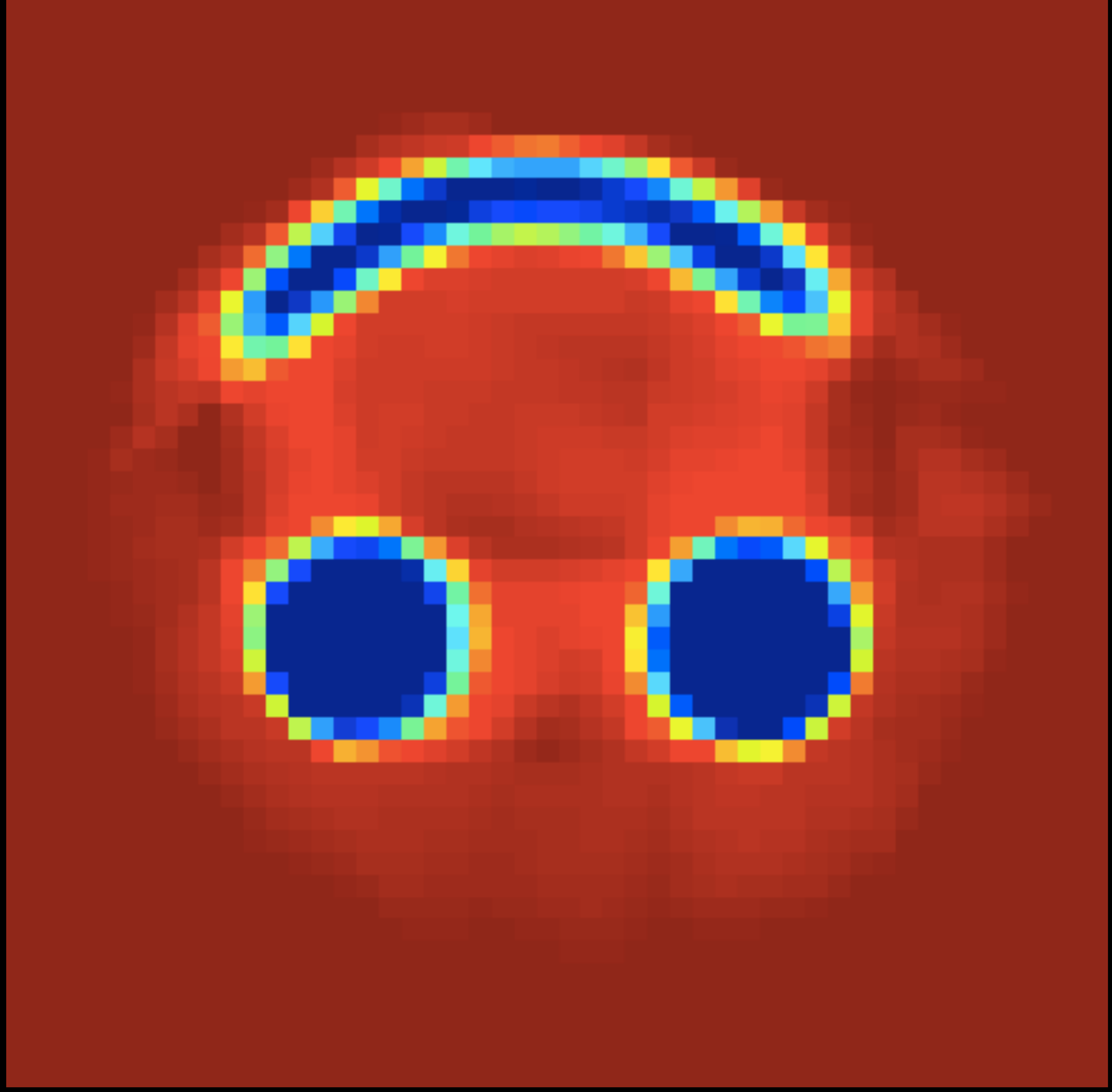
```
eta=.1
batchsize=1000
batches=2000
costs=zeros(batches)

for k in range(batches):
    y_in,y_target=make_batch()
    costs[k]=train_net(y_in,y_target,eta)
```

Example: Learning a 2D image

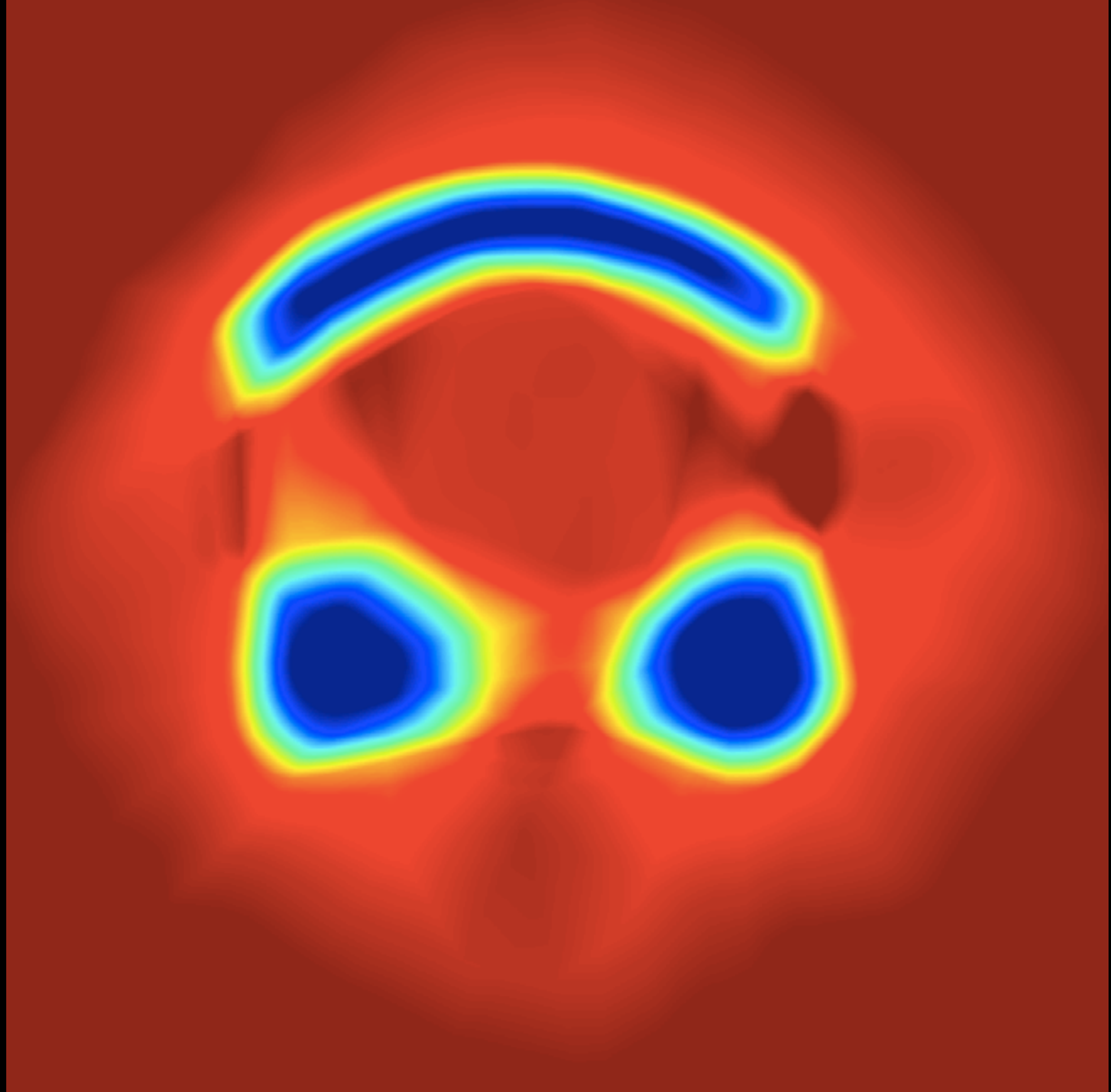
see notebook (on website): **MultiLayer_ImageCompression**







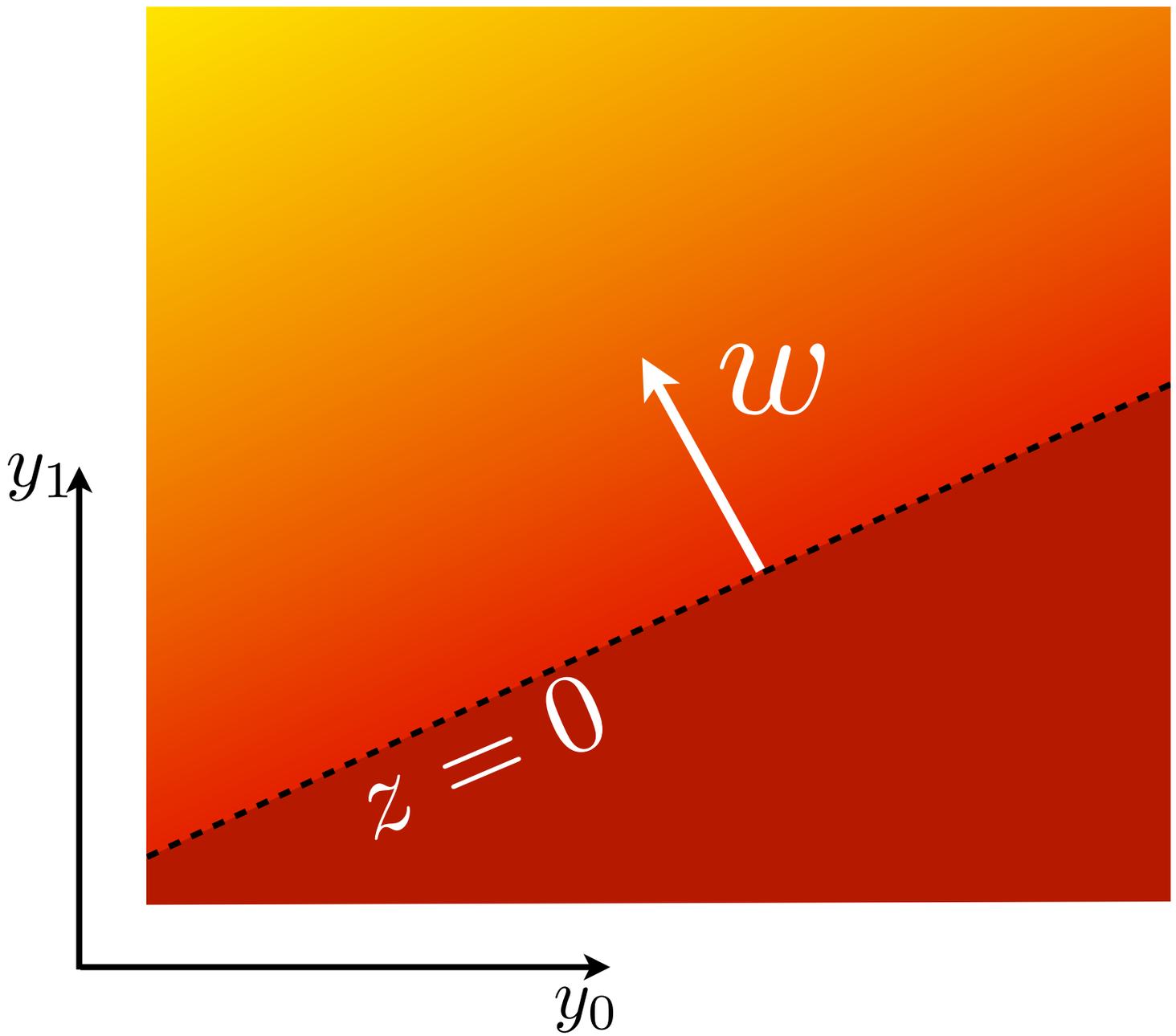
Network layers: 2,150,150,100,1 neurons
(after about 2min of training, ~4 Mio. samples)

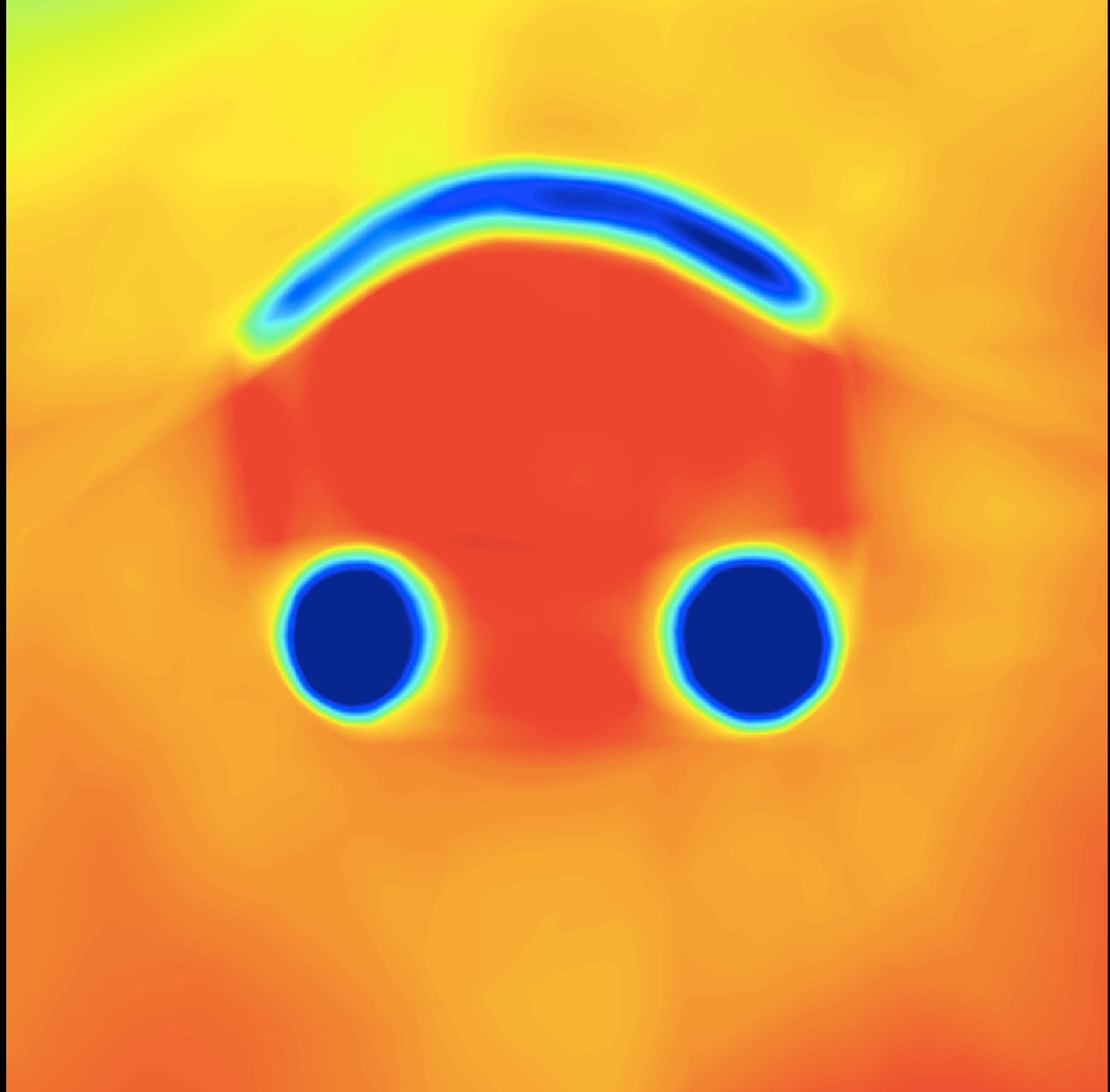


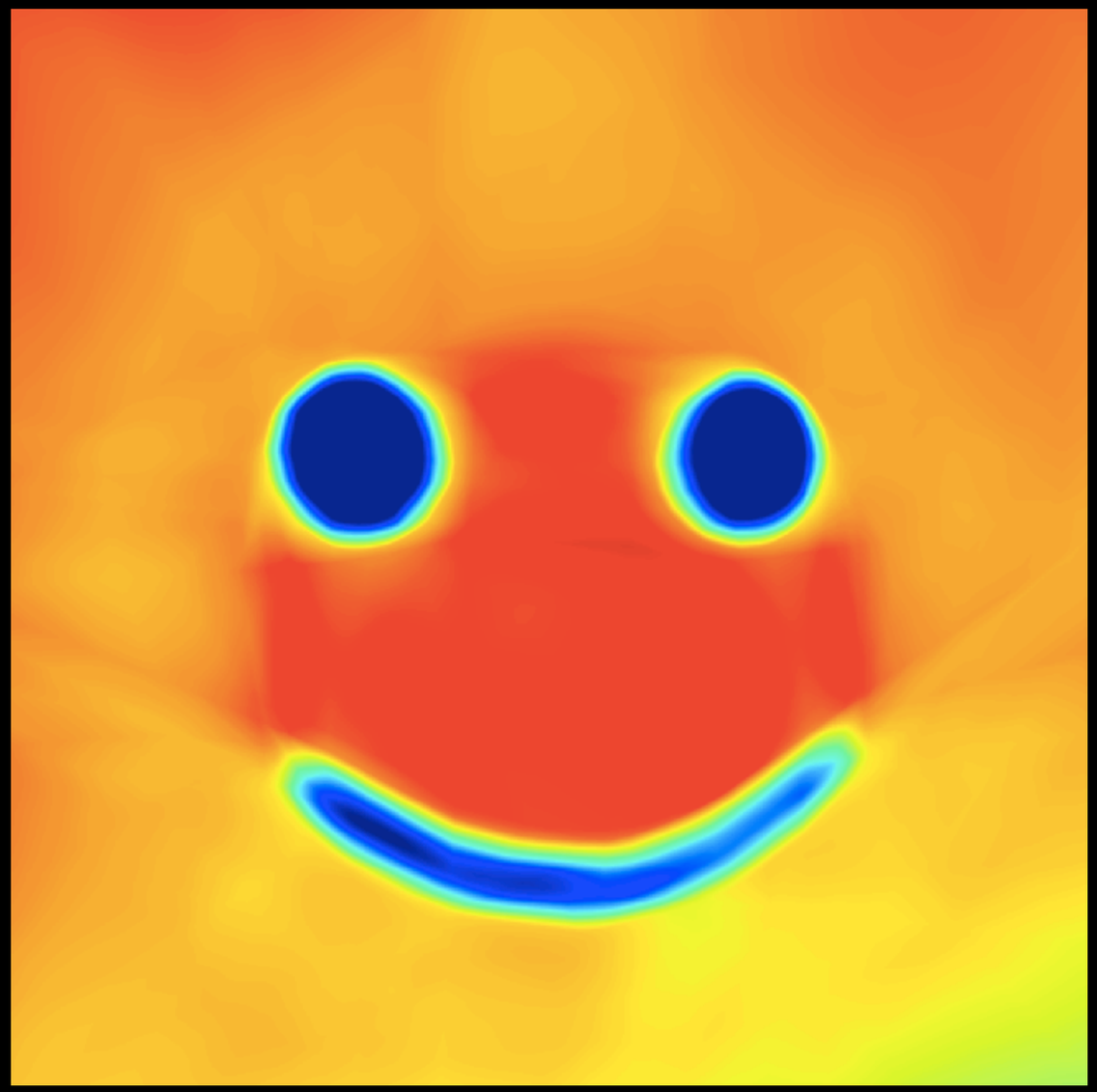
Reminder: ReLU (rectified linear unit)

$$f(z) = \begin{matrix} z \text{ for } z > 0 \\ 0 \text{ for } z \leq 0 \end{matrix}$$

$$z = wy + b$$







à la Franz Marc?

Try to understand how the network operates!

Switching on only a single neuron of the last hidden layer

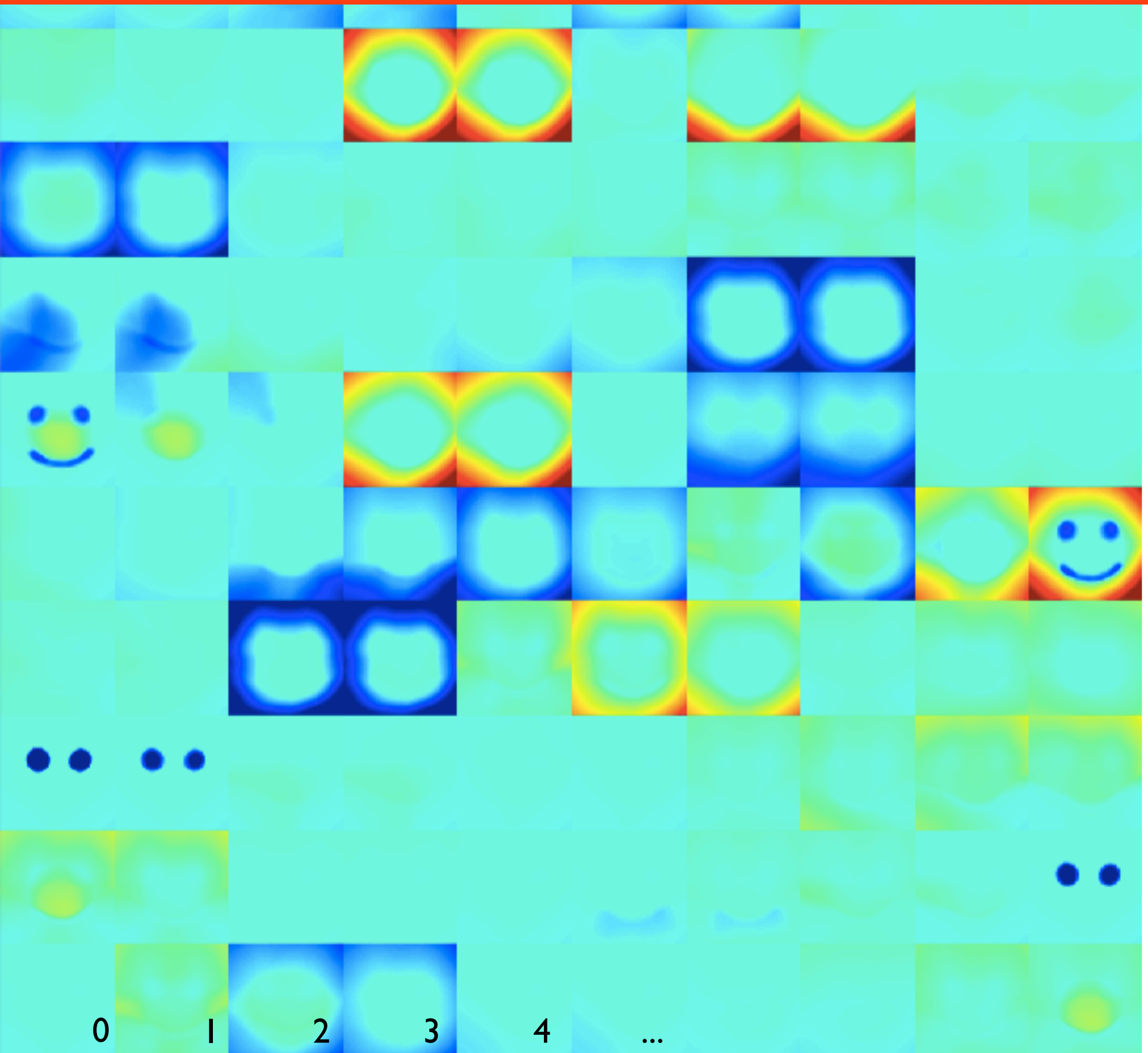
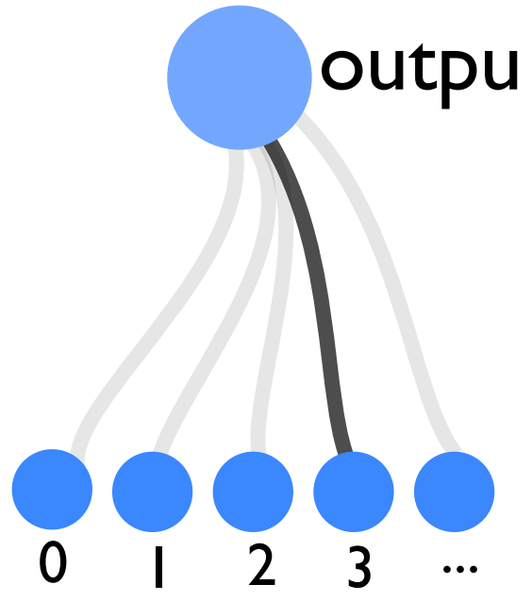
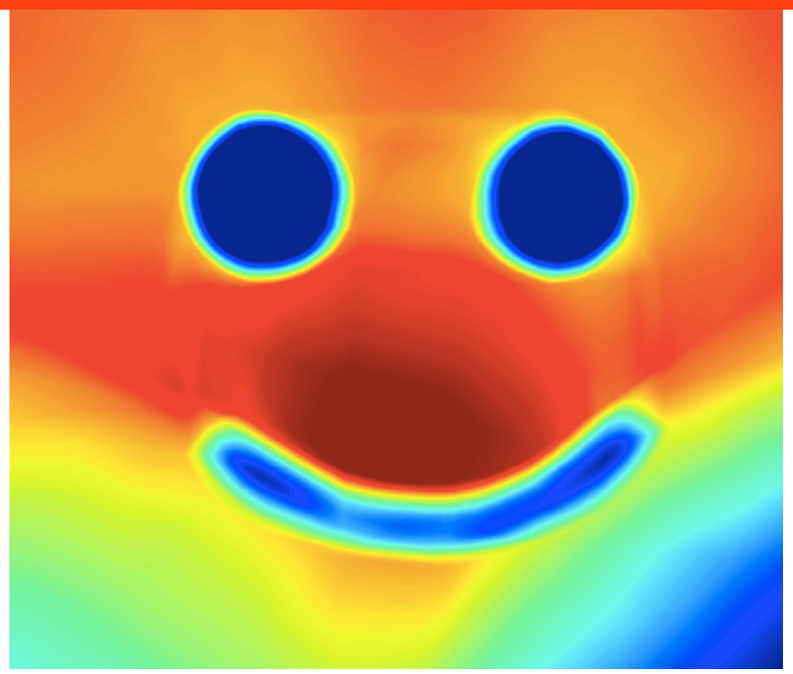


Image shows results of switching on individually each of 100 neurons

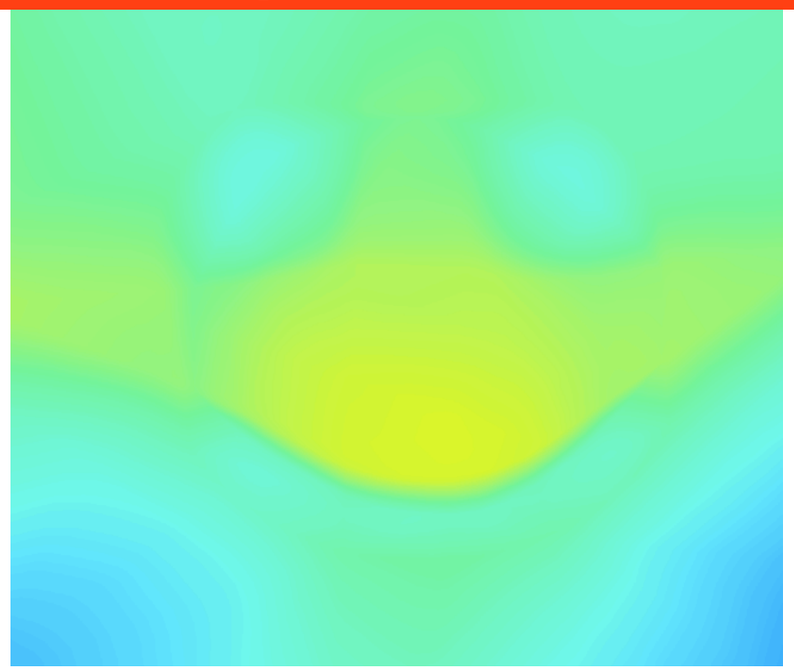


Weights from last hidden layer to output

deleted first 50 weights



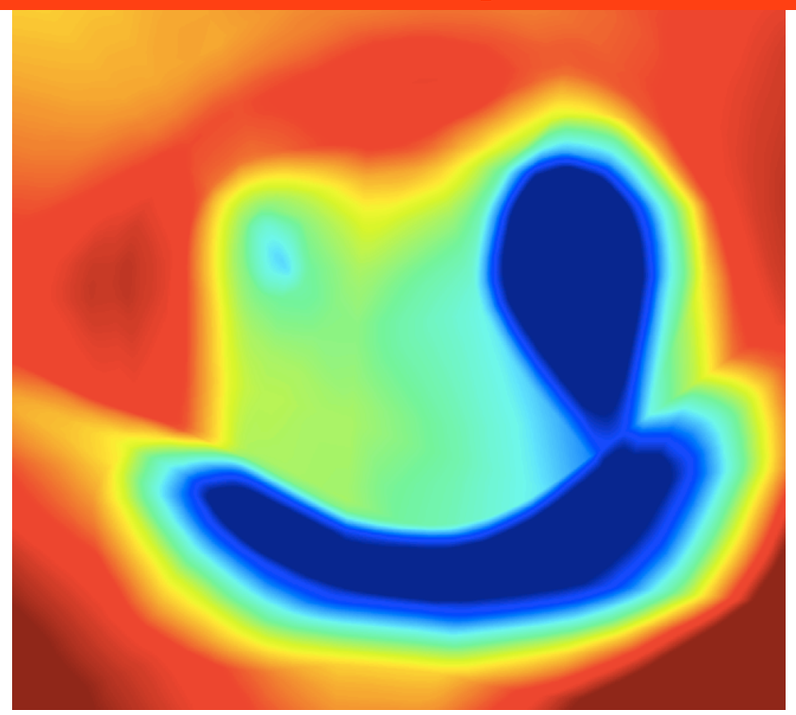
deleted last 50 weights



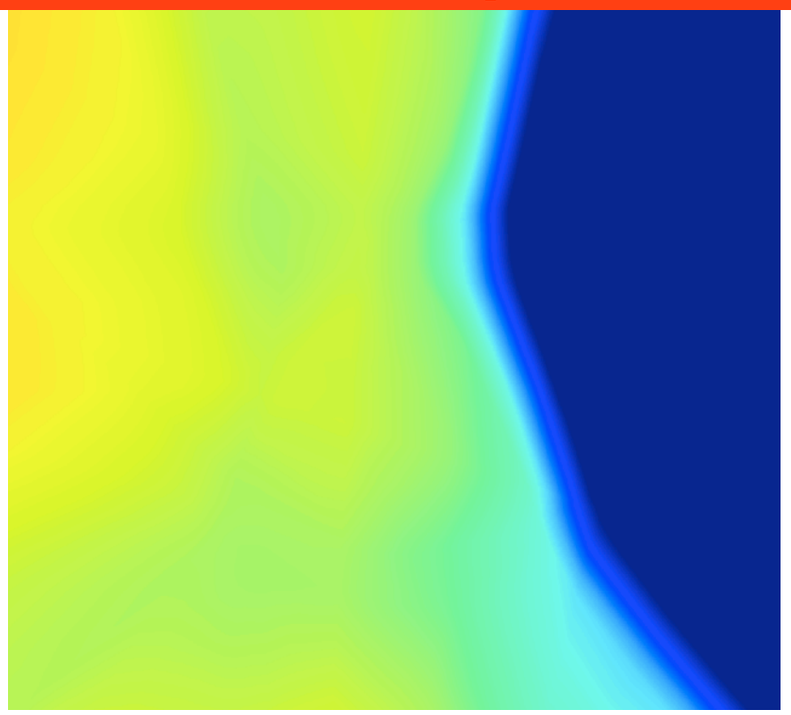
kept only 10 out of 100

Weights from 2nd hidden layer to last hidden layer

deleted first 75

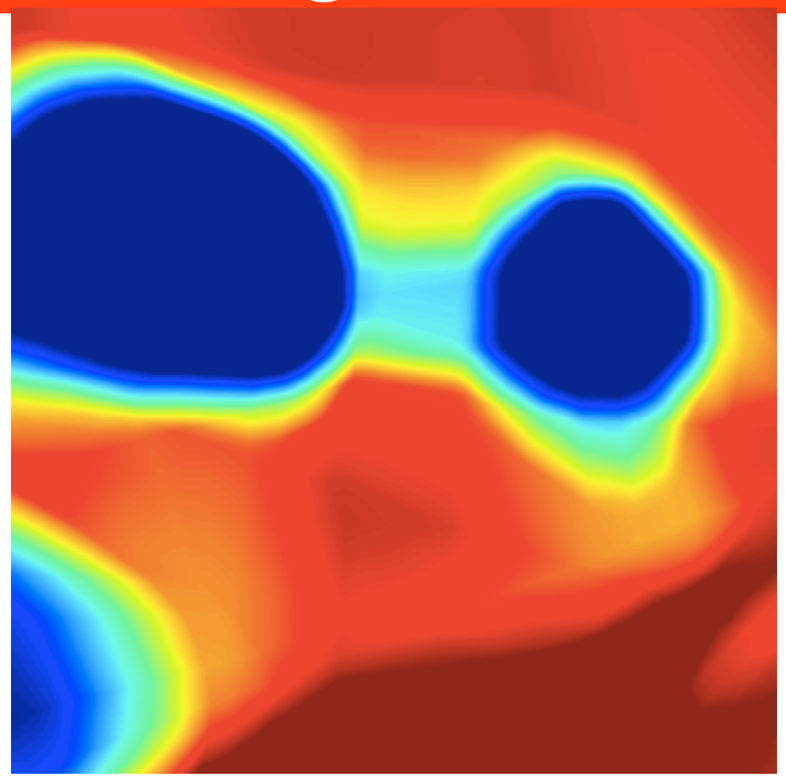


deleted last 75

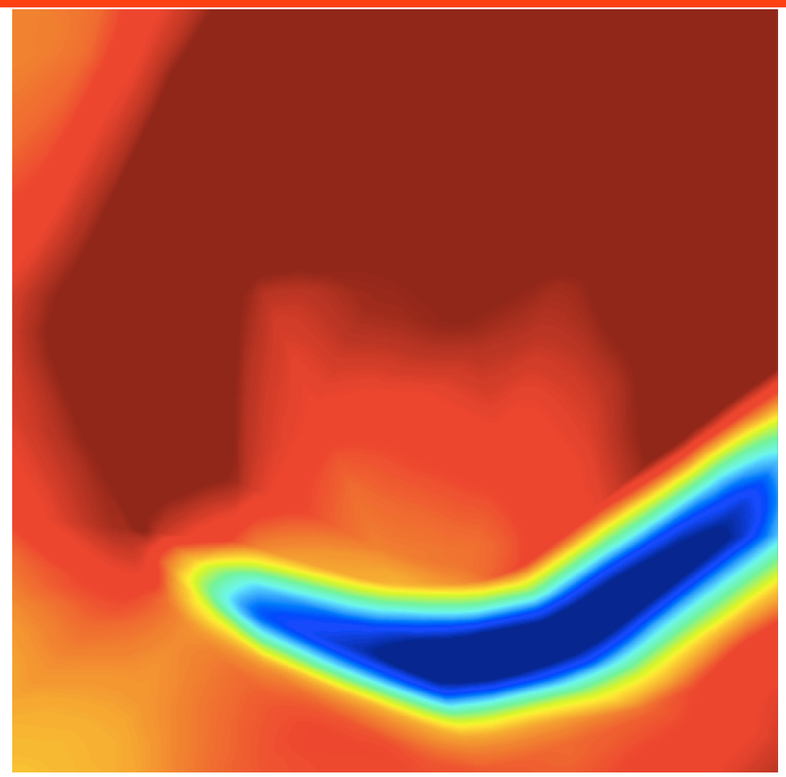


kept only 10 out of 150

Weights from 1st hidden layer to 2nd hidden layer



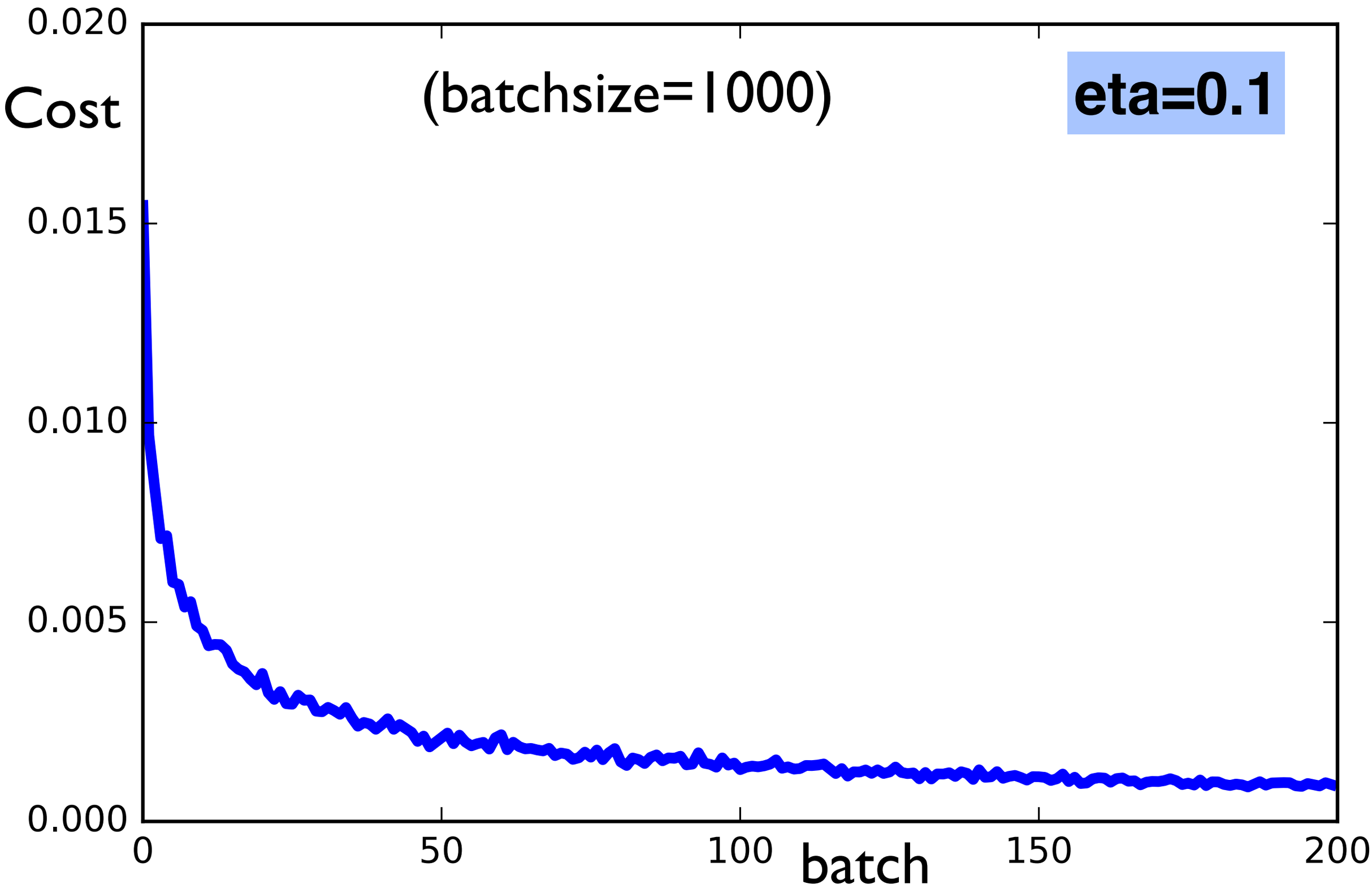
deleted first 75



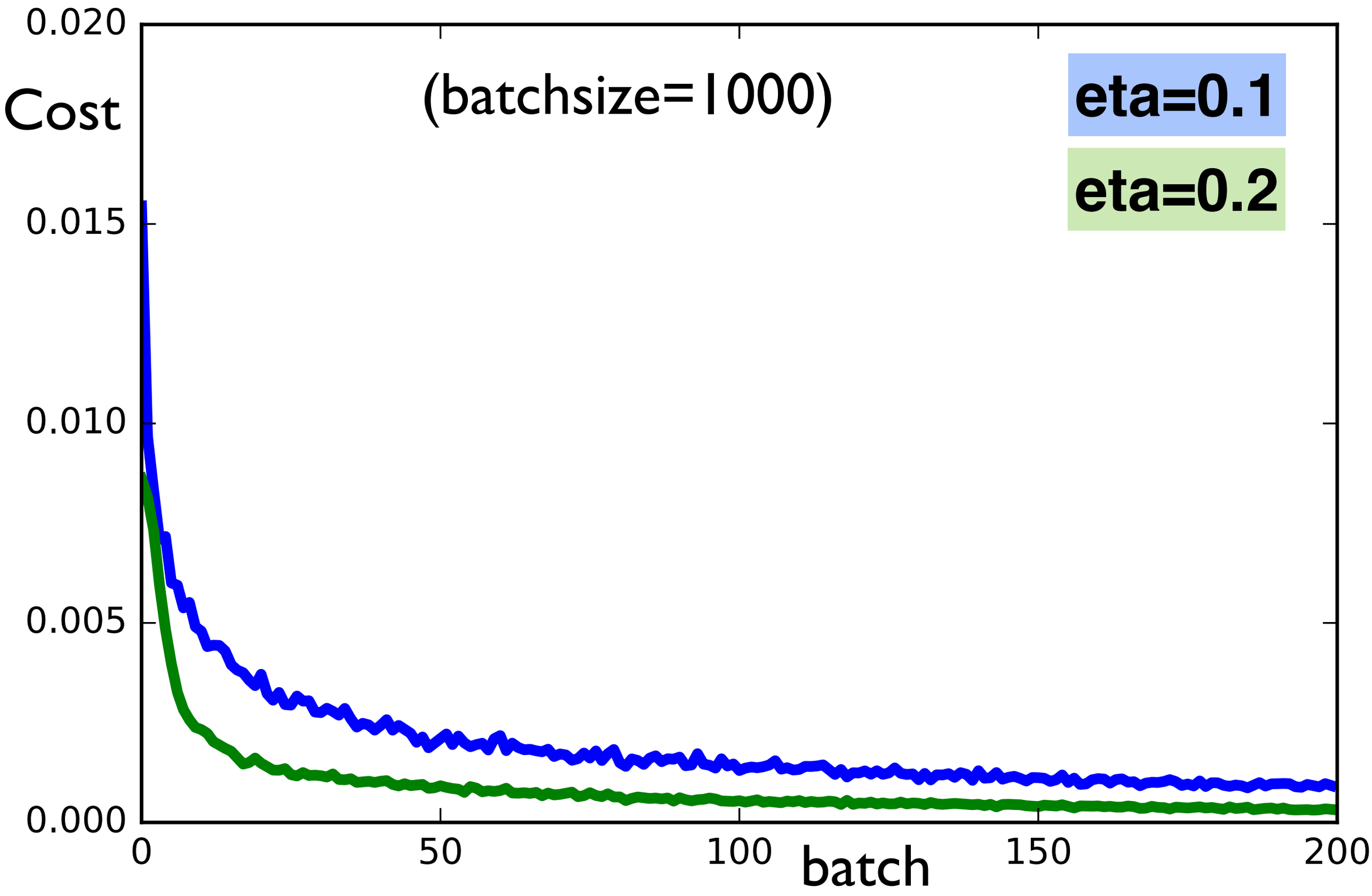
deleted last 75

kept only 10 out of 150

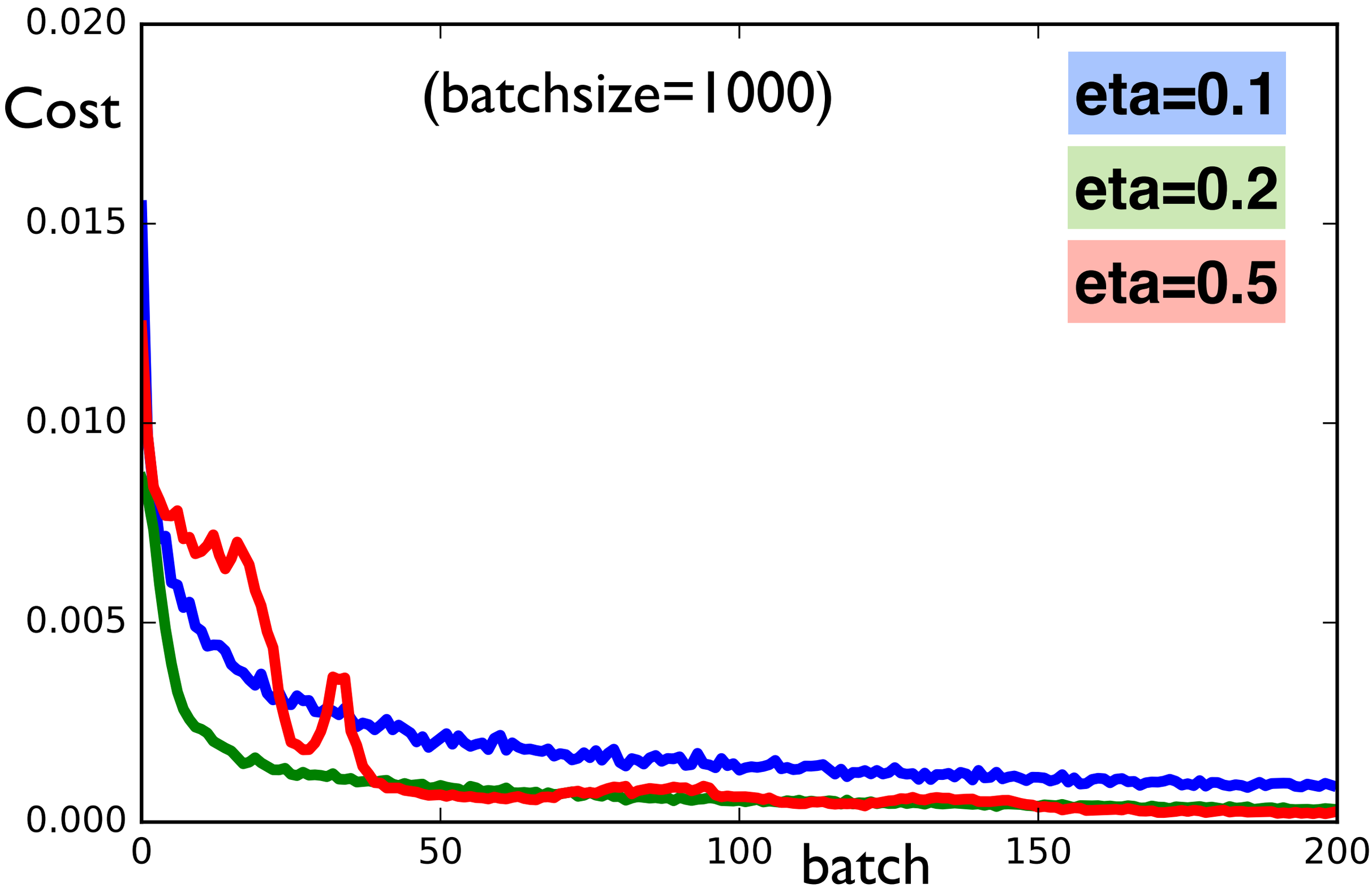
Influence of learning rate (stepsize)



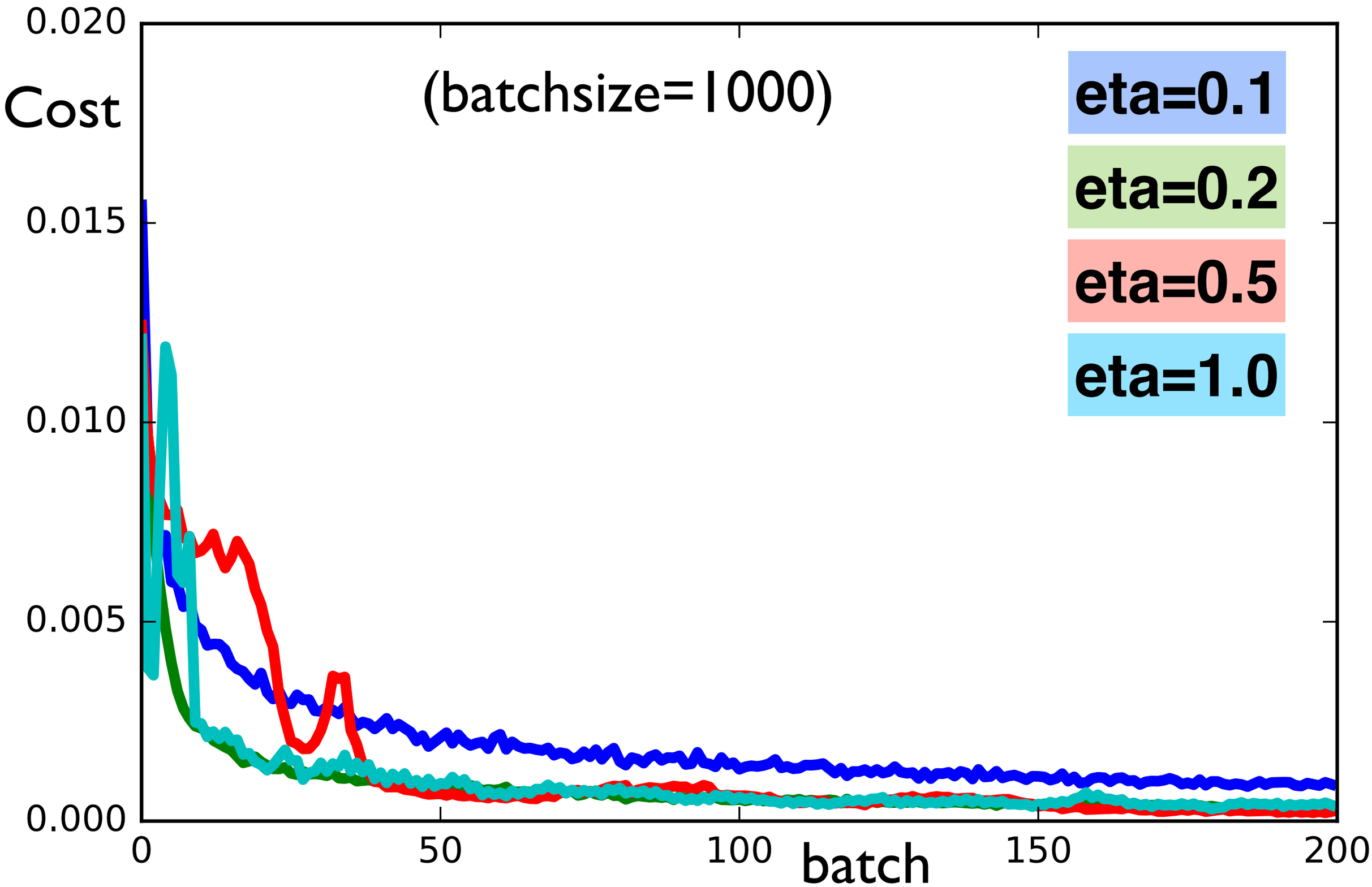
Influence of learning rate (stepsize)



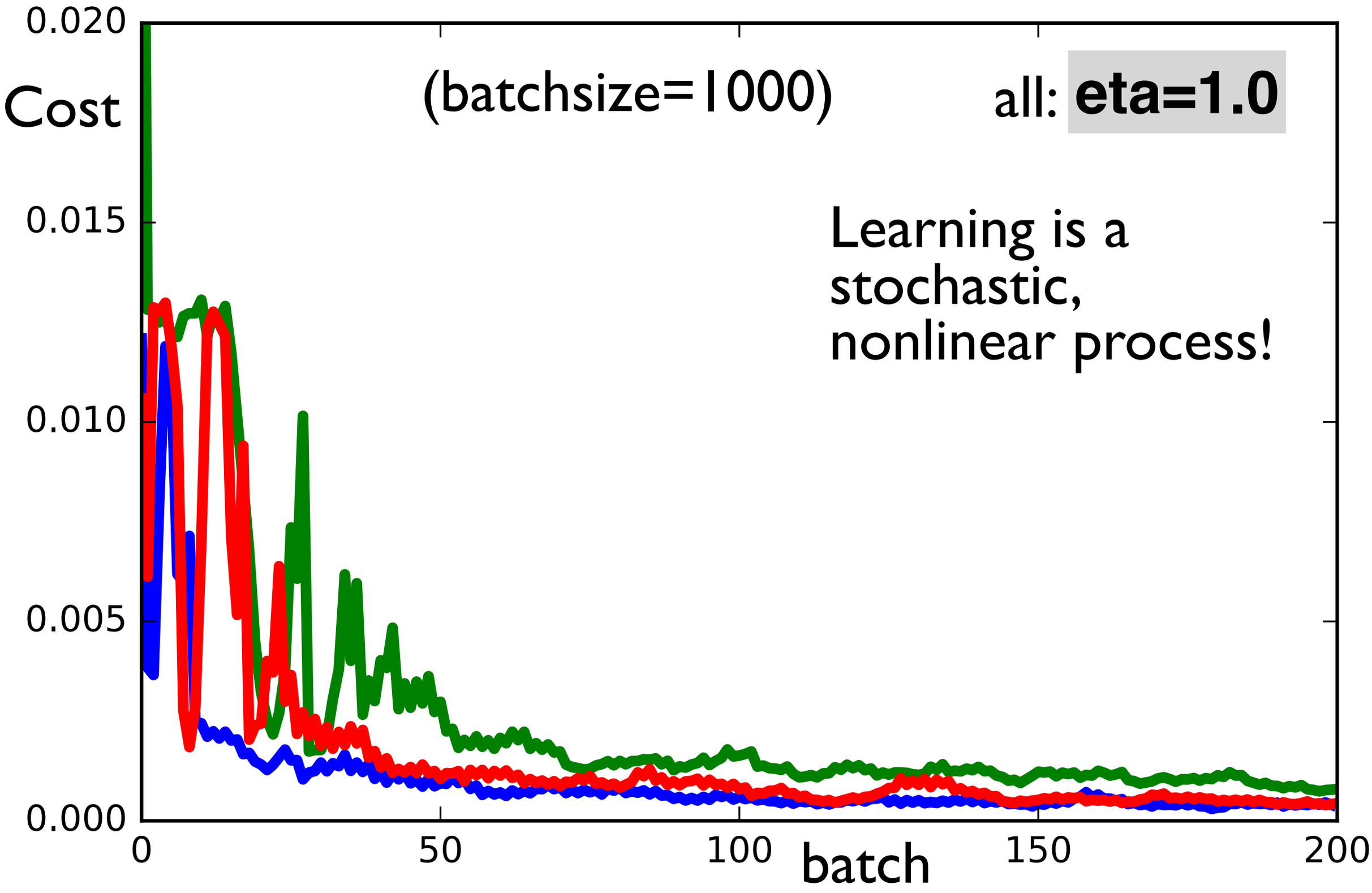
Influence of learning rate (stepsize)



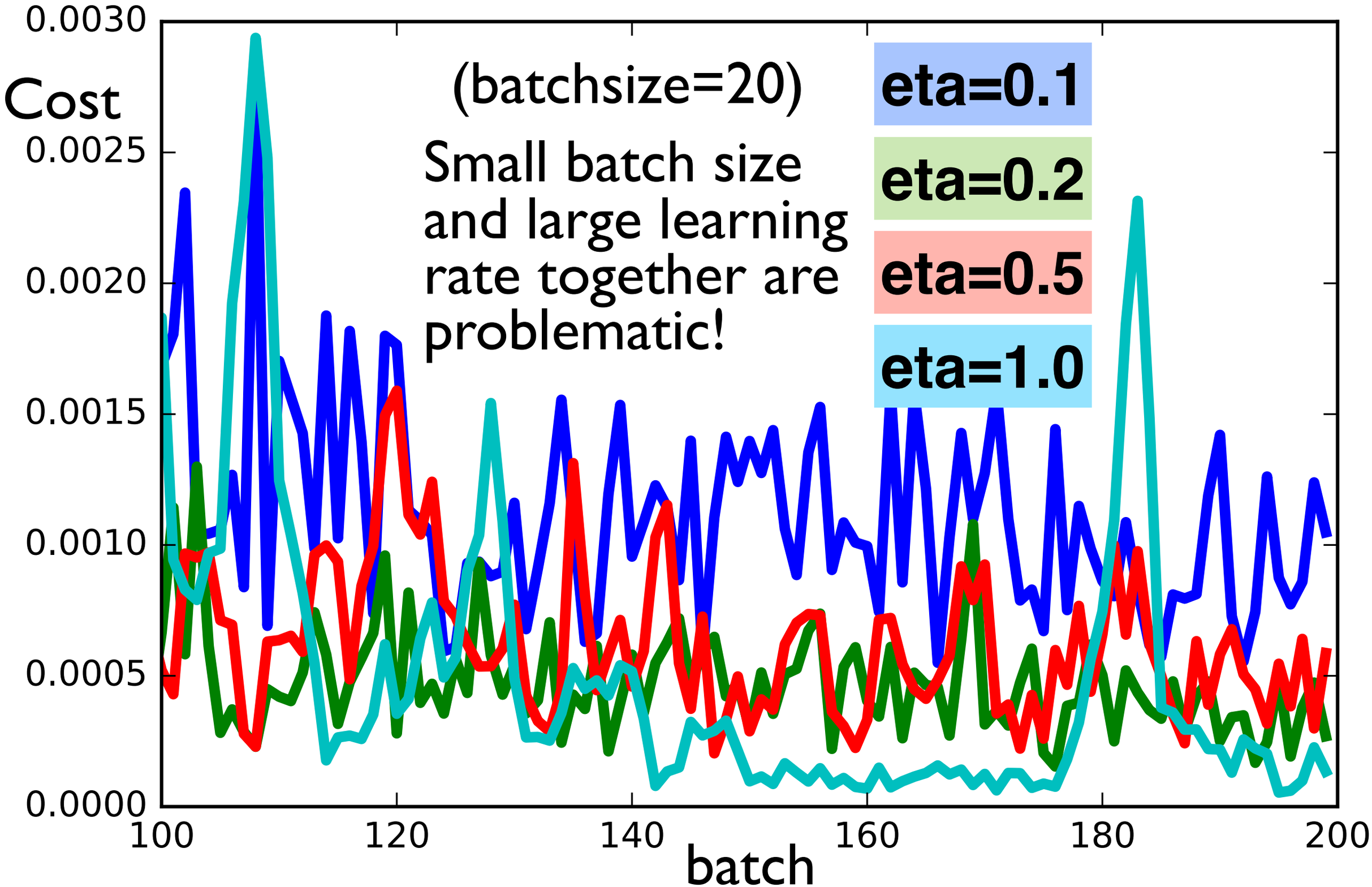
Influence of learning rate (stepsize)



Randomness (initial weights, learning samples)



Influence of batch size / learning rate



Influence of batch size / learning rate

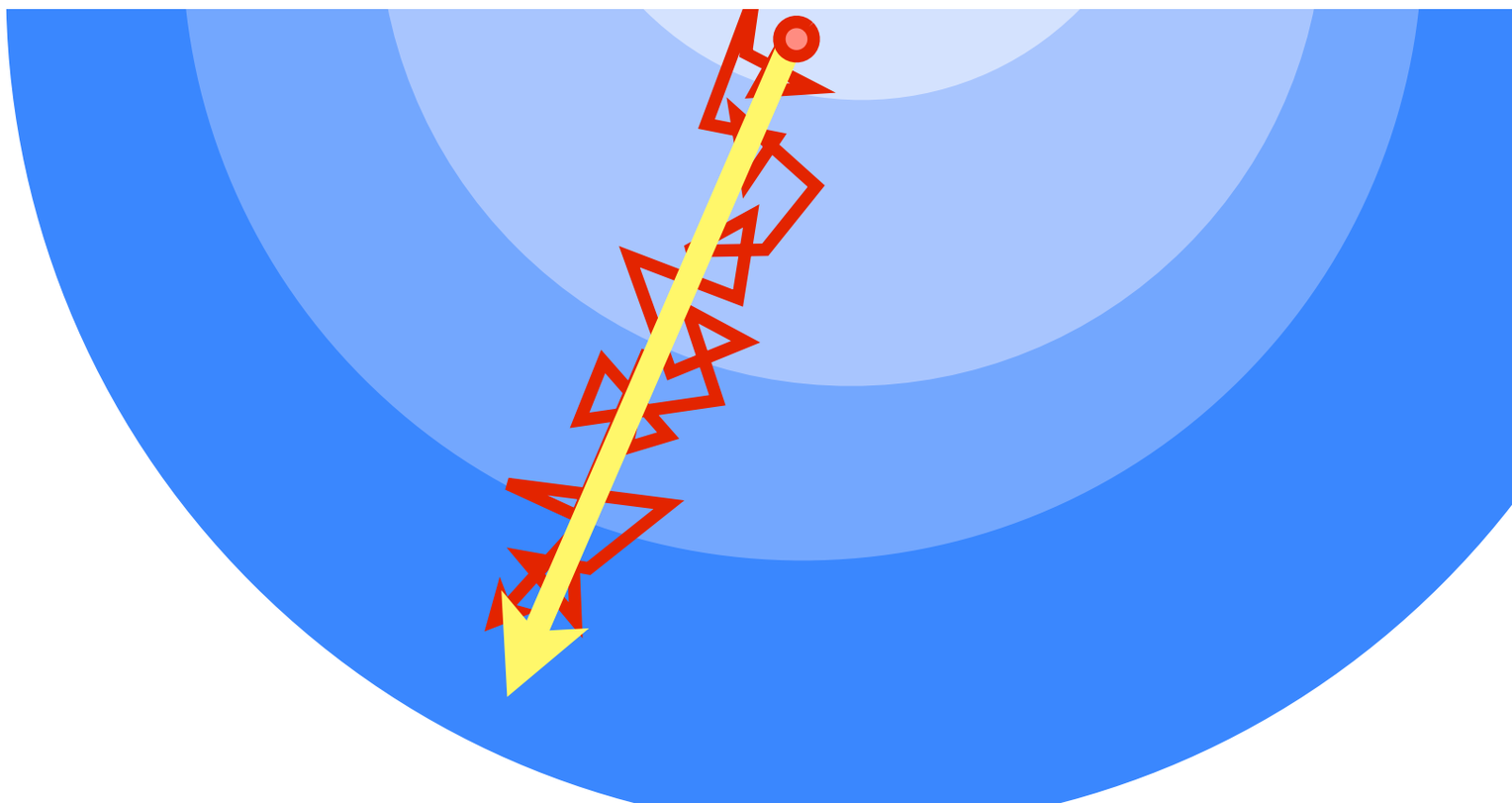
$$C(w - \eta \nabla_w C) \approx C(w) - \eta (\nabla_w C)(\nabla_w C) + \dots$$

new weights

always >0

decrease in C!

higher order in η



Influence of batch size / learning rate

$$C(w - \eta \nabla_w C) \approx C(w) - \eta (\nabla_w C)(\nabla_w C) + \ldots$$

always >0

new weights

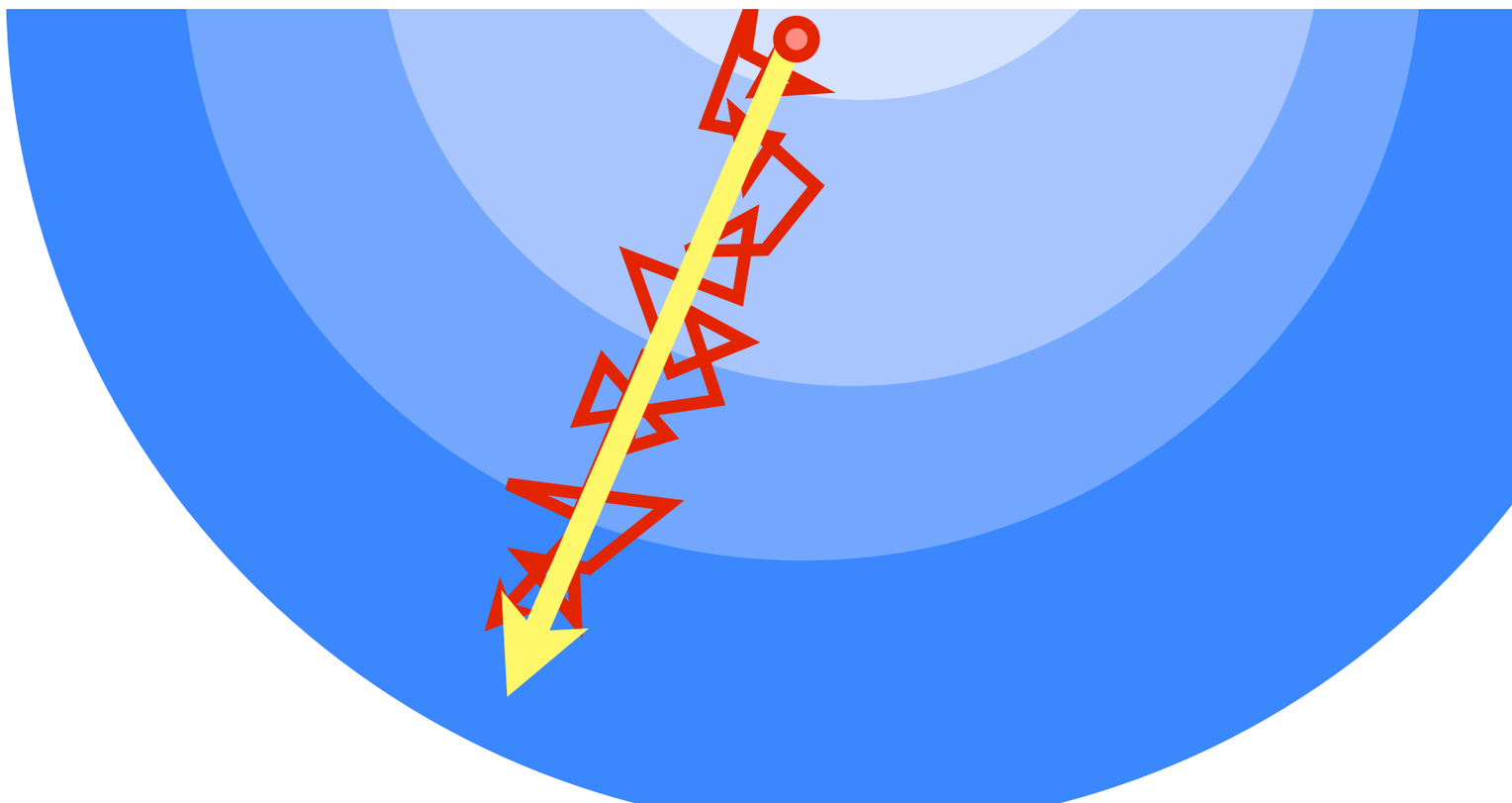
decrease in C!

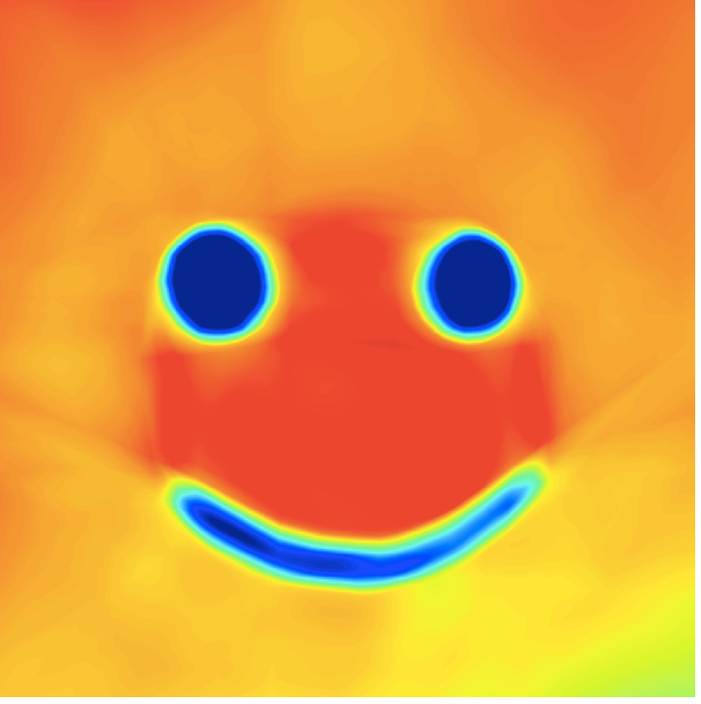
higher order in η

Potential problems:

- step too large: need higher-order terms
  [will not be a problem near minimum of C]
- approx. of C bad [small batch size: approx. C fluctuates]

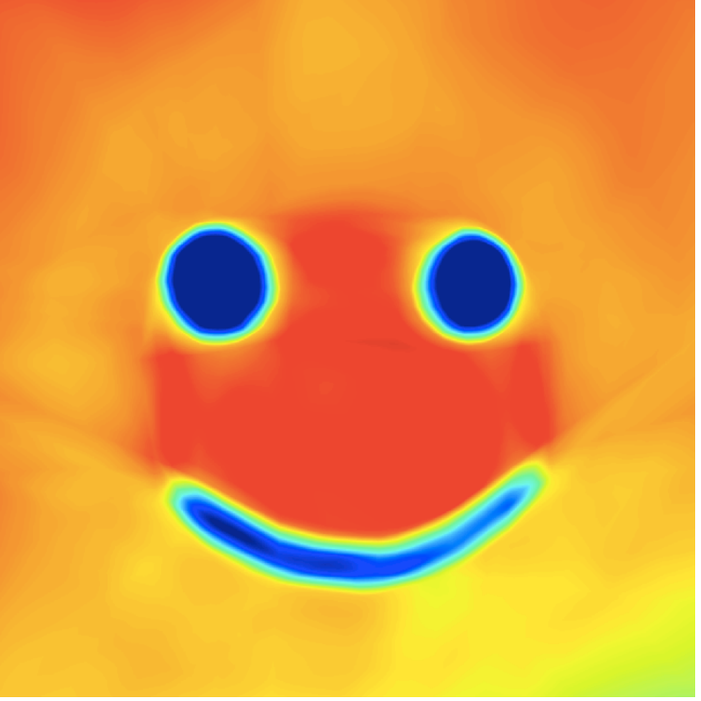
Sufficiently small learning rate: multiple training steps (batches) add up, and their average is like a larger batch





Programming a general multilayer neural network & backpropagation was not so hard (once you know it!)

Could now go on to image recognition etc. with the same program!



Programming a general multilayer neural network & backpropagation was not so hard (once you know it!)

Could now go on to image recognition etc. with the same program!

But: want more flexibility and added features!

For example:

- Arbitrary nonlinear functions for each layer
- Adaptive learning rate
- More advanced layer structures (such as convolutional networks)
- etc.

Keras

- Convenient neural network package for python
- Set up and training of a network in a few lines
- Based on underlying neural network / symbolic differentiation package [which also provides run-time compilation to CPU and GPU]: either ‘theano’ or ‘tensorflow’ [User does not care]

Keras

From the website **keras.io**

“Keras is a high-level neural networks API, written in Python and capable of running on top of either TensorFlow or Theano. It was developed with a focus on enabling fast experimentation. Being able to go from idea to result with the least possible delay is key to doing good research.”

```
from keras import *
from keras.models import Sequential
from keras.layers import Dense
```

Defining a network

layers with 2,150,150,100,1 neurons

```
net=Sequential()
net.add(Dense(150, input_shape=(2,), activation='relu'))
net.add(Dense(150, activation='relu'))
net.add(Dense(100, activation='relu'))
net.add(Dense(1, activation='relu'))
```

‘Compiling’ the network

```
net.compile(loss='mean_squared_error',
                optimizer=optimizers.SGD(lr=0.1),
                metrics=['accuracy'])
```

```
from keras import *
from keras.models import Sequential
from keras.layers import Dense
```

Defining a network

"Sequential": the usual neural network, with several layers

```
net=Sequential()
net.add(Dense(150, input_shape=(2,), activation='relu'))
net
net
```

"Dense": "fully connected layer" (all weights there)

input_shape: number of input neurons

'relu': rectified linear unit

'Compiling' the network

SGD=stoch. gradient descent

'loss'=cost

```
net.compile(loss='mean_squared_error',
            optimizer=optimizers.SGD(lr=0.1),
            curacy'])
```

lr=learning rate=stepsize

Training the network

```
batchsize=20
batches=200
costs=zeros(batches)

for k in range(batches):
    y_in,y_target=make_batch()
    costs[k]=net.train_on_batch(y_in,y_target)[0]
```

y_in array dimensions ‘batchsize’ x 2

y_target array dimensions ‘batchsize’ x 1

(just like before, for our own python code)

Predicting with the network

```
y_out=net.predict_on_batch(y_in)
```

y_in array dimensions ‘batchsize’ x 2

y_out array dimensions ‘batchsize’ x 1

(just like before, for our own python code)

Homework

Explore how well the network can reproduce various features of target images, and how that depends on the network layout!

Aspects to consider (& I do not claim to know all the answers!):

How good are other nonlinear functions? [e.g. sigmoids or your own favorite f(z)]

Given a fixed total number of weights, is it better to go deep (many layers) or shallow?

Bonus: After training, try to 'prune' the network, i.e. delete neurons whose deletion does not increase the cost function too much!