Unit 9
Neural Networks

EE-UY 4563/EL-GY 9123: INTRODUCTION TO MACHINE LEARNING

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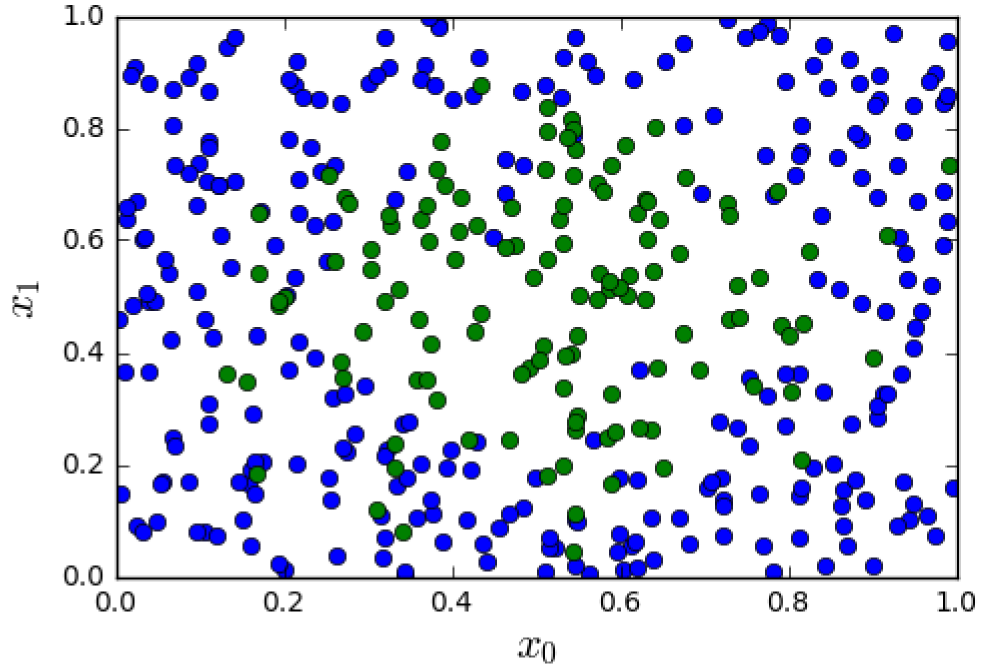
Learning Objectives

- ❑ Mathematically describe a neural network with a single hidden layer
  - Describe mappings for the hidden and output units
- ❑ Manually compute output regions for very simple networks
- ❑ Select the loss function based on the problem type
- ❑ Build and train a simple neural network in Keras
- ❑ Write the formulas for gradients using backpropagation
- ❑ Describe mini-batches in stochastic gradient descent

Outline

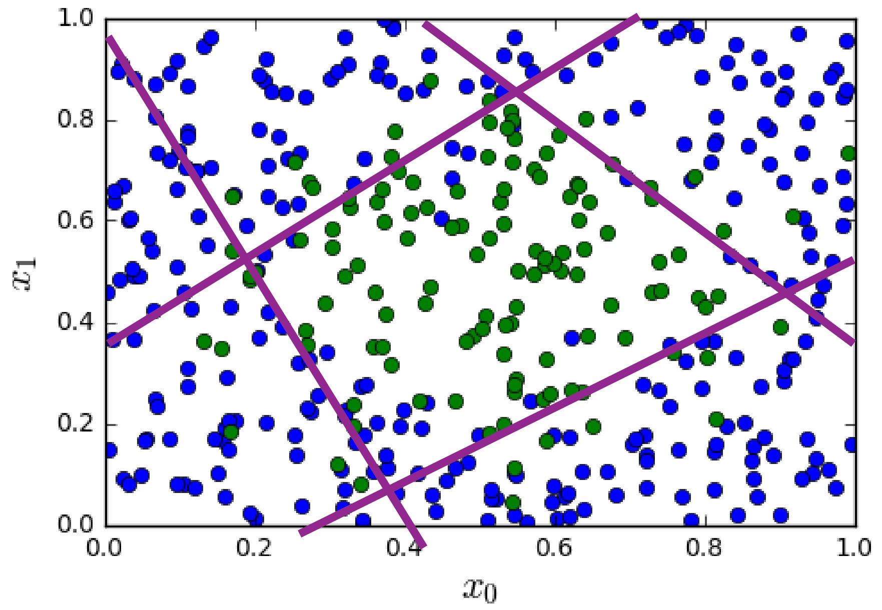
Most Datasets are not Linearly Separable



- Consider simple synthetic data
  - See figure to the left
  - 2D features
  - Binary class label
- Not separated linearly

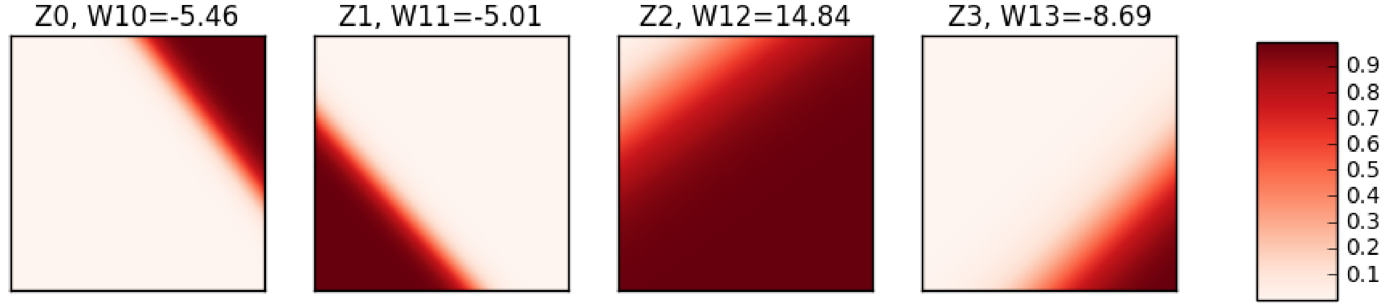
All code in https://github.com/sdrangan/introml/blob/master/neural/synthetic.ipynb

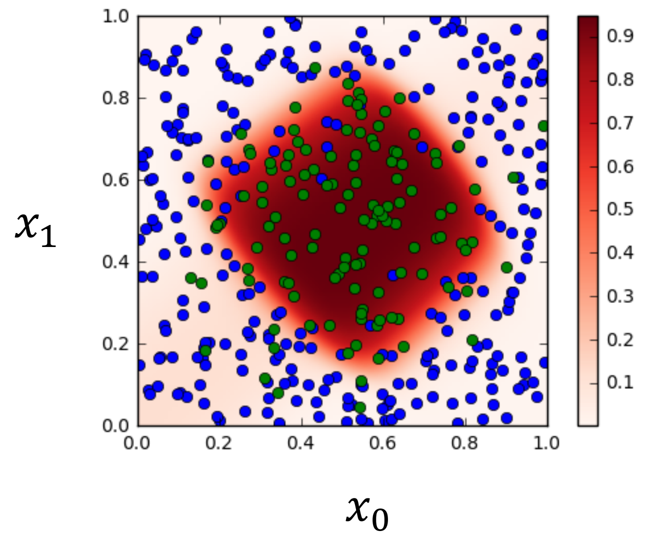
From Linear to Nonlinear



- Idea: Build nonlinear region from linear decisions
- Possible form for a classifier:
  - Step 1: Classify into small number of linear regions
  - Step 2: Predict class label from step 1 decisions

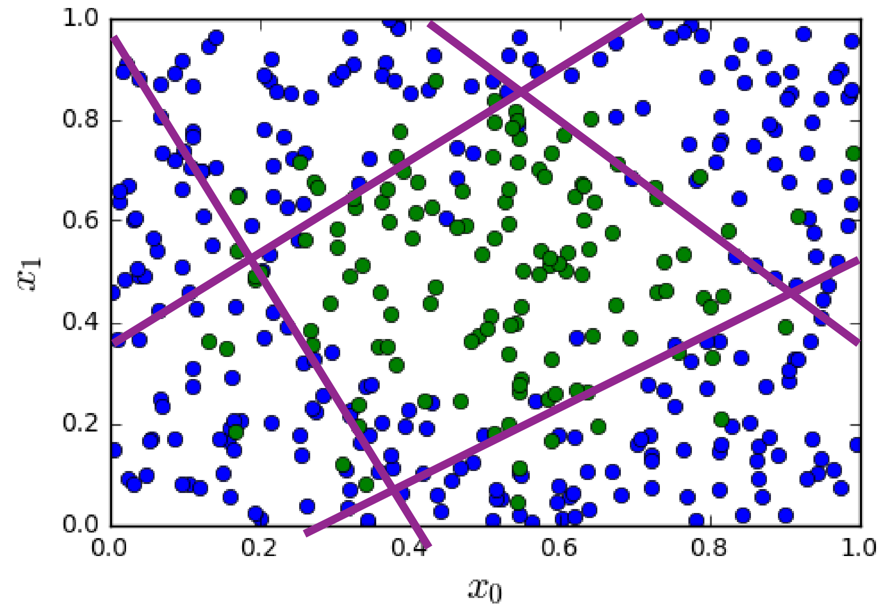
Step 1 Outputs and Step 2 Outputs





- Each output from step 1 is from a linear classifier with soft decision
  - Similar to logistic regression
- Final output is a weighted average of step 1 outputs using the weights
  - Weights are indicated on top of the figures

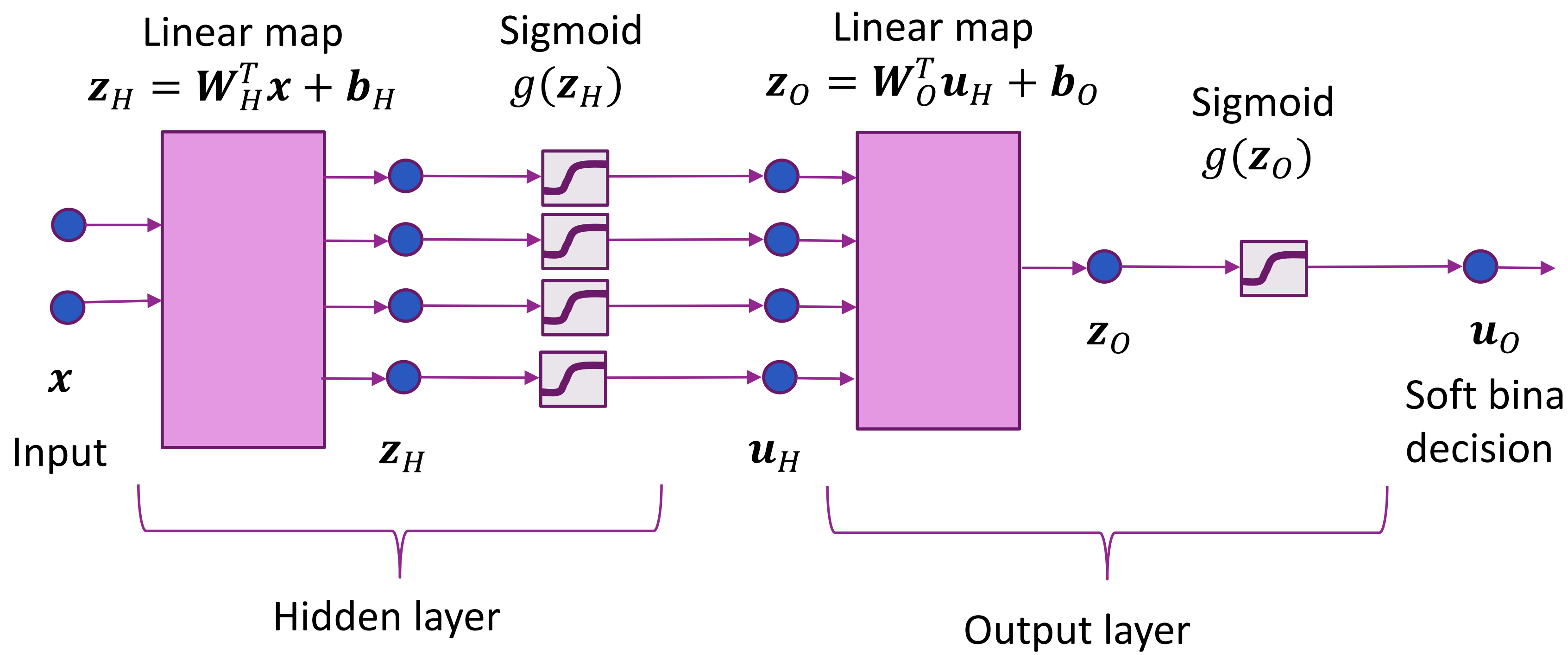
A Possible Two Stage Classifier



- Input sample: $\boldsymbol{x} = (x_1, x_2)^T$
- First step: Hidden layer
  - Take $N_H = 4$ linear discriminants
    $$z_{H,1} = \boldsymbol{w}_{H,1}^T x + b_{H,1}$$
    $$\vdots$$
    $$z_{H,N_H} = \boldsymbol{w}_{H,M}^T x + b_{H,M}$$
  - Make a soft decision on each linear region
    $$u_{H,m} = g\left(z_{H,m}\right) = 1/(1 + e^{-z_{H,m}})$$
- Second step: Output layer
  - Linear step $z_O = w_O^T u_H + b_O$
  - Soft decision: $u_O = g(z_O)$

Model Block Diagram

- Hidden layer: $\boldsymbol{z}_H = \boldsymbol{W}_H^T \boldsymbol{x} + \boldsymbol{b}_H, \quad \boldsymbol{u}_H = g(\boldsymbol{z}_H)$
- Output layer: $\boldsymbol{z}_O = \boldsymbol{W}_O^T \boldsymbol{u}_H + \boldsymbol{b}_O,\ u_O = g(\boldsymbol{z}_O)$



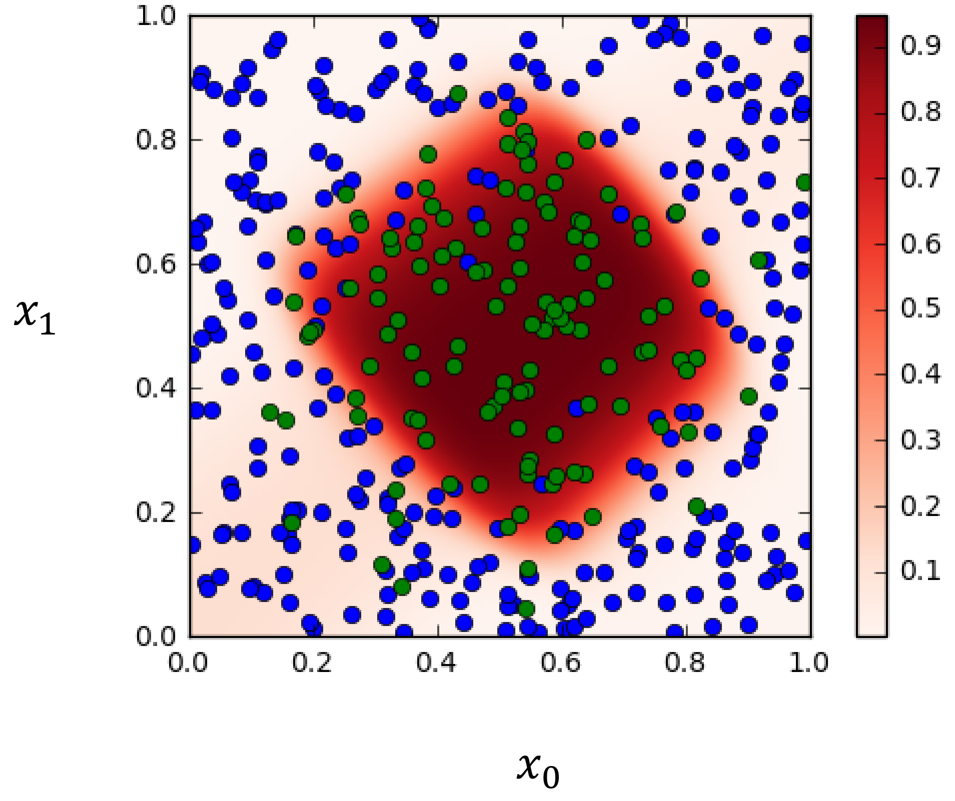
Training the Model

- Model in matrix form:
  - Hidden layer: $\boldsymbol{z}_H = \boldsymbol{W}_H^T \boldsymbol{x} + \boldsymbol{b}_H, \quad \boldsymbol{u}_H = g(\boldsymbol{z}_H)$
  - Output layer: $z_O = \boldsymbol{W}_O^T \boldsymbol{u}_H + \boldsymbol{b}_O, \ u_O = g(z_O)$
- $z_O = F(\boldsymbol{x}, \theta)$: Linear output from final stage
  - Parameters: $\theta = (\boldsymbol{W}_H, \boldsymbol{W}_O, b_H, b_O)$
- Get training data $(\boldsymbol{x}_i, y_i), i = 1, \ldots, N$
- Define loss function: $L(\theta) \coloneqq -\sum_{i=1}^{N} \ln P(y_i | x_i, \theta)$,
- Pick parameters to minimize loss:

$$\hat{\theta} = \arg\min_{\theta} L(\theta)$$

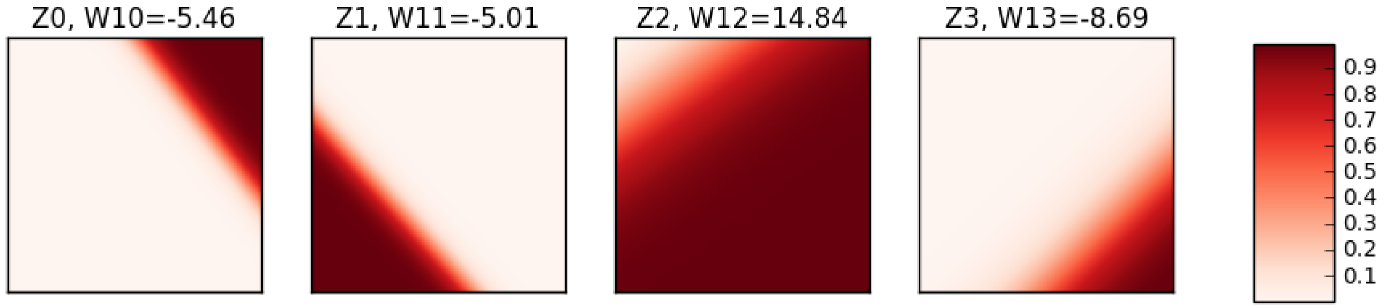
  - Will discuss how to do this minimization later

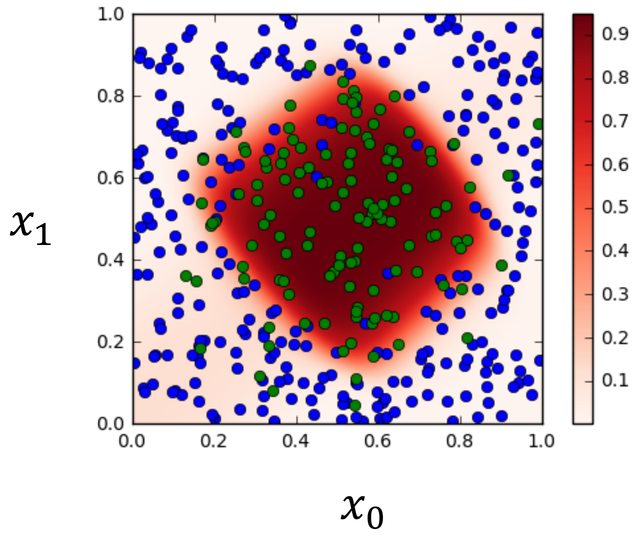
Results



- Neural network finds a nonlinear region
- Plot shows:
  - Blue circles: Negative samples
  - Greed circles: Positive samples
  - Red color: Classifier soft probability $g(z_O)$

Hidden Layer outputs and final outputs



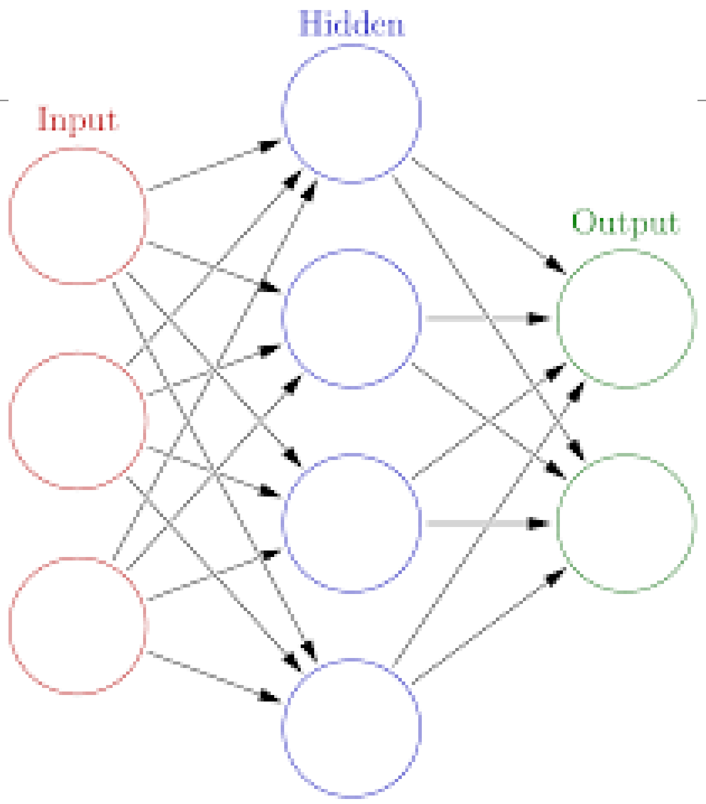


- ❑Each hidden node is a linear classifier with soft decision (Logistic regression)
- ❑Final output is a weighted average of step 1 outputs using the weights indicated on top of the figures

Outline

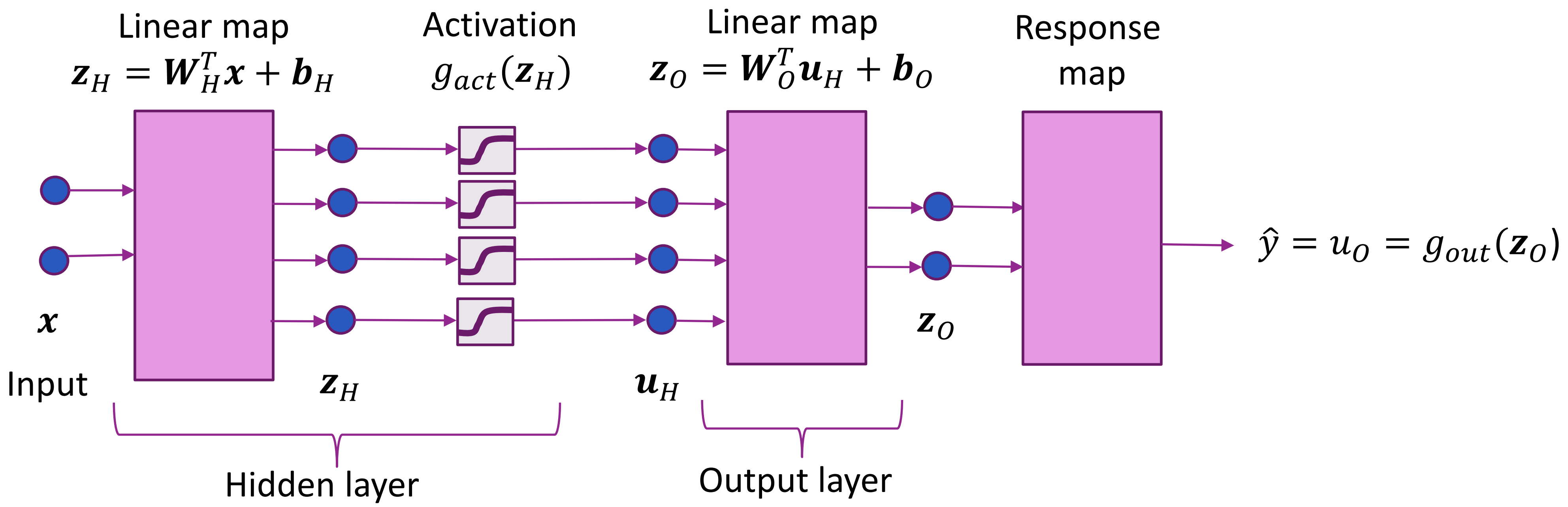
General Structure

- Input: $\boldsymbol{x} = (x_1, \cdots, x_d)$
  - N_I = number of features
- Hidden layer:
  - Linear transform: $\boldsymbol{z}_H = \boldsymbol{W}_H^T \boldsymbol{x} + \boldsymbol{b}_H$
  - Activation function: $\boldsymbol{u}_H = g_{act}(\boldsymbol{z}_H)$
  - Dimension: N_H hidden units
- Output layer:
  - Linear transform: $\boldsymbol{z}_O = \boldsymbol{W}_O^T \boldsymbol{u}_H + \boldsymbol{b}_O$
  - Output function: $\boldsymbol{u}_O = g_{out}(\boldsymbol{z}_O)$
  - Dimension: N_O = number of classes / outputs
- Can be used for classification or regression, with different decision functions



General Neural Net Block Diagram

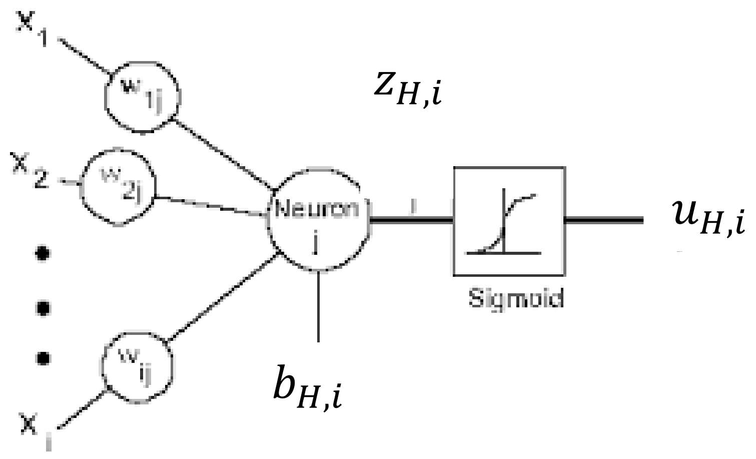
- Hidden layer: $\boldsymbol{z}_H = \boldsymbol{W}_H^T \boldsymbol{x} + \boldsymbol{b}_H, \quad \boldsymbol{u}_H = g_{act}(\boldsymbol{z}_H)$
- Output layer: $\boldsymbol{z}_O = \boldsymbol{W}_O^T \boldsymbol{u}_H + \boldsymbol{b}_O$
- Response map: $\hat{y} = u_O = g_{out}(\boldsymbol{z}_O)$ (for the case of binary classes)



Linear map
$\boldsymbol{z}_H = \boldsymbol{W}_H^T \boldsymbol{x} + \boldsymbol{b}_H$
Activation
$g_{act}(\boldsymbol{z}_H)$
Linear map
$\boldsymbol{z}_O = \boldsymbol{W}_O^T \boldsymbol{u}_H + \boldsymbol{b}_O$
Response map
$\boldsymbol{x}$
Input
$\boldsymbol{z}_H$
$\boldsymbol{u}_H$
$\boldsymbol{z}_O$
$\hat{y} = u_O = g_{out}(\boldsymbol{z}_O)$
Hidden layer
Output layer

Terminology

- ❑ Hidden variables: the variables $\boldsymbol{z}_H, \boldsymbol{u}_H$
  - These are not directly observed
- ❑ Hidden units: The functions that compute:
  - $z_{H,i} = \sum_j W_{H,ji} x_j + b_{H,i}, \quad u_{H,i} = g(z_{H,i})$
  - The function $g(z)$ called the activation function
- ❑ Output units: The functions that compute
  - $z_{O,i} = \sum_j W_{O,ji} u_{H,j} + b_{O,i}$

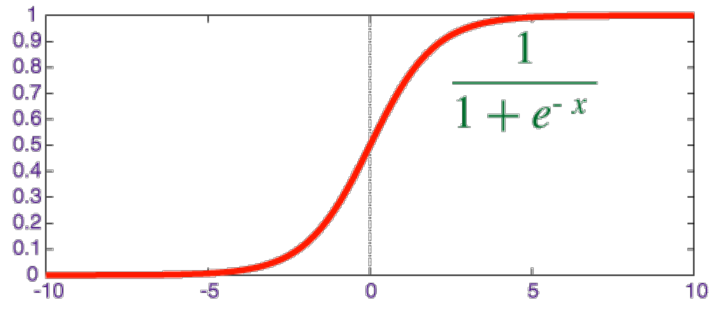


Response Map or Output Activation

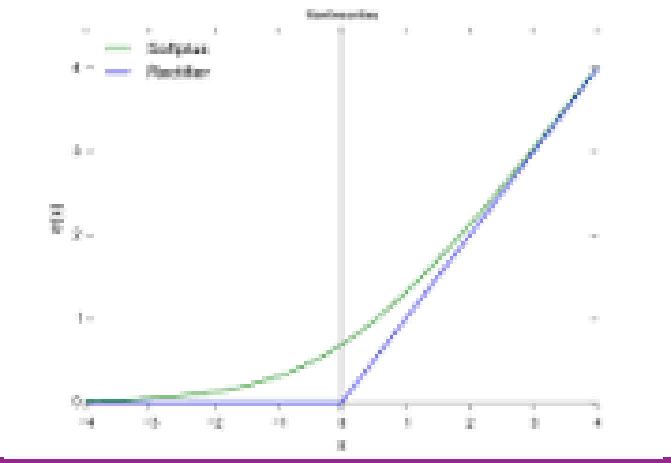
- Last layer depends on type of response
- Binary classification: $y = \pm 1$
  - z_O is a scalar
  - Hard decision: $\hat{y} = \text{sign}(z_O)$
  - Soft decision: $P(y = 1|x) = 1/(1 + e^{-z_O})$
- Multi-class classification: $y = 1, \dots, K$
  - $\boldsymbol{z}_O = \left[z_{O,1}, \cdots, z_{O,K}\right]^T$ is a vector
  - Hard decision: $\hat{y} = \arg\max_k z_{O,k}$
  - Soft decision: $P(y = k|x) = S_k(\boldsymbol{z}_O),\ \ S_k(\boldsymbol{z}_O) = \frac{e^{z_{O,k}}}{\sum_\ell e^{z_{O,\ell}}}$ (softmax)
- Regression: $\boldsymbol{y} \in R^K$
  - $\hat{\boldsymbol{y}} = \boldsymbol{z}_O$ (linear output layer)

Hidden Activation Function

- Two common activation functions
- Sigmoid:
  - $g_{act}(z) = 1/(1 + e^{-z})$
  - Benefits: Values are bounded
  - Often used for small networks



- Rectified linear unit (ReLU):
  - $g_{act}(z) = \max(0, z)$
  - Can add sparsity (more on this later)
  - Often used for larger networks
  - Esp. in combination with dropout

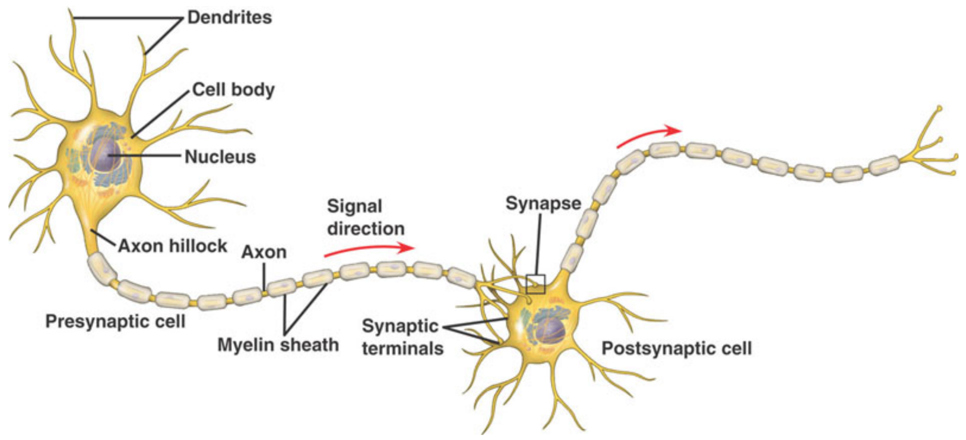


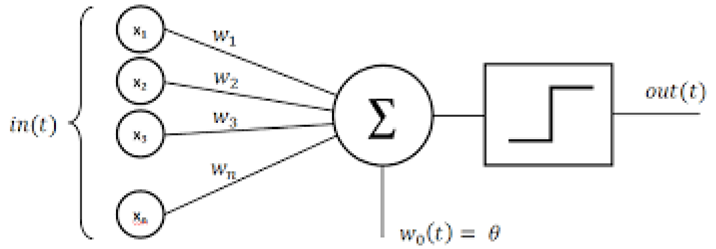
Number of Parameters

Layer	Parameter	Symbol	Number parameters
Hidden layer	Bias	b_H	N_H
	Weights	W_H	$N_H N_I$
Output layer	Bias	b_O	N_O
	Weights	W_O	$N_O N_H$
Total			$N_H(N_I + 1) + N_O(N_H + 1)$

- Sizes:
  - N_I = input dimension, N_H= number of hidden units, N_O=output dimension
- N_H= number of hidden units is a free parameter
- Discuss selection later

Inspiration from Biology





- Simple model of neurons
  - Dendrites: Input currents from other neurons
  - Soma: Cell body, accumulation of charge
  - Axon: Outputs to other neurons
  - Synapse: Junction between neurons
- Operation:
  - Take weighted sum of input current
  - Outputs when sum reaches a threshold
- Each neuron is like one unit in neural network

History

- ❑Interest in understanding the brain for thousands of years
- ❑1940s: Donald Hebb. Hebbian learning for neural plasticity
  - Hypothesized rule for updating synaptic weights in biological neurons
- ❑1950s: Frank Rosenblatt: Coined the term perceptron
  - Essentially single layer classifier, similar to logistic classification
  - Early computer implementations
  - But, Limitations of linear classifiers and computer power
- ❑1960s: Backpropagation: Efficient way to train multi-layer networks
  - More on this later
- ❑1980s: Resurgence with greater computational power
- ❑2005+: Deep networks
  - Many more layers. Increased computational power and data
  - Enabled first breakthroughs in various image and text processing.
  - Next lecture

Outline

- ❑Motivating Idea: Nonlinear classifiers from linear features
- ❑Neural Networks
- ❑Neural Network Loss Function
- ❑Stochastic Gradient Descent
- ❑Building and Training a Network in Keras
  - Synthetic data
  - MNIST
- ❑Backpropagation Training

Training a Neural Network

- Given data: $(\boldsymbol{x}_i, y_i), i = 1, \ldots, N$
- Learn parameters: $\theta = (W_H, b_H, W_o, b_o)$
  - Weights and biases for hidden and output layers
- Will minimize a loss function: $L(\theta)$

$$\hat{\theta} = \arg\min_{\theta} L(\theta)$$

  - $L(\theta)$ = measures how well parameters θ fit training data $(\boldsymbol{x}_i, y_i)$

Note on Indexing

- Neural networks are often processed in batches
  - Set of training or test samples
- Need notation for single and batch input case
- For a single input $\boldsymbol{x}$
  - x_j = j-th feature of the input
  - $z_{H,j}, u_{H,j}, z_{O,j}$ = j-th component of hidden and output variables
  - H and O stand for Hidden and Output. Not an index
  - Write x, z_O, y if they are scalar (i.e. do not write index)
- For a batch of inputs $\boldsymbol{x}_1, \ldots.., \boldsymbol{x}_N$
  - x_{ij} = j-th feature of the input sample i
  - $z_{H,ij}, u_{H,ij}, z_{O,ij}$ = j-th component of hidden and output variables for sample i

Selecting the Right Loss Function

- Depends on the problem type
- Always compare final output z_{Oi} with target y_i

Problem	Target y_i	Output z_{Oi}	Loss function	Formula
Regression	y_i = Scalar real	z_{Oi} = Prediction of y_i Scalar output / sample	Squared / L2 loss	$\sum_i (y_i - z_{Oi})^2$
Regression with vector samples	$\boldsymbol{y}_i = (y_{i1}, \ldots, y_{iK})$	z_{Oik} = Prediction of y_{ik} K outputs / sample	Squared / L2 loss	$\sum_{ik} (y_{ik} - z_{Oik})^2$
Binary classification	$y_i = \{0,1\}$	z_{Oi} = "logit" score Scalar output / sample	Binary cross entropy	$\sum_i -y_i z_{Oi} + \ln(1 + e^{y_i z_i})$
Multi-class classification	$y_i = \{1, \ldots, K\}$	z_{Oik} = "logit" scores K outputs / sample	Categorical cross entropy	$\sum_i \ln\left(\sum_k e^{z_{Oik}}\right) - \sum_k r_{ik} z_{Oik}$

Loss Function: Regression

- Regression case:
  - y_i = scalar target variable for sample i
  - Typically continuous valued
- Output layer:
  - z_{Oi} = estimate of y_i
- Loss function: Use L2 loss

$$L(\theta) = \sum_{i=1}^{N} (y_i - z_{Oi})^2$$

- For vector $\boldsymbol{y}_i = (y_{i1}, \ldots, y_{iK}),$ use vector L2 loss

$$L(\theta) = \sum_{i=1}^{N} \sum_{j=1}^{K} (y_{ik} - z_{Oik})^2$$

Loss Function: Binary Classification

- Binary classification: $y_i = \{0,1\}$ = class label
- Loss function = negative log likelihood

$$L(\theta) = -\sum_{i=1}^{N} \ln P(y_i|x_i,\theta)\,, \qquad P(y_i = 1|x_i,\theta) = \frac{1}{1+e^{-z_{Oi}}}$$

  - Output z_{Oi} called the logit score
  - z_{Oi} scalar.
- From lecture on logistic regression:

$$\ln P(y_i|x_i,\theta) = y_i\, u_i + (1-y_i)\ln(1-u_i) \quad = y_i z_{oi} - \ln[1+e^{y_i z_{oi}}]$$

$$u_i = P(y_i = 1|x_i,\theta)$$

  - Called the binary cross-entropy

Loss Function: Multi-Class Classification 1

- $y_i = \{1, \ldots, K\}$ = class label
- Output: $\boldsymbol{z}_{Oi} = (z_{O,i1}, \ldots, z_{O,iK})$
  - K outputs. One per class
  - Also called the logit score
- Likelihood given by softmax:

$$P(y_i = k|\boldsymbol{x}_i, \theta) = g_k(z_{Oi}), \qquad g_k(z_{Oi}) = \frac{e^{z_{O,ik}}}{\sum_\ell e^{z_{O,i\ell}}}$$

  - Assigns class highest probability with highest logit score

Loss Function: Multi-Class Classification 2

- $y_i = \{1, \ldots, K\}$ = class label
- Define one-hot coded response

$$r_{ik} = \begin{cases} 1 & y_i = k \\ 0 & y_i \neq k \end{cases}$$

  - $\boldsymbol{r}_i = (r_{i1}, \ldots, r_{iK})$ is K-dimensional
- Negative log-likelihood given by:

$$\ln P(y_i = k|\boldsymbol{x}_i, \theta) = \sum_{k=1}^{K} r_{ik} \ln P(y_i = k|\boldsymbol{x}_i, \boldsymbol{\theta}), \qquad P(y_i = k|\boldsymbol{x}_i, \theta) = \frac{e^{z_{O,ik}}}{\sum_\ell e^{z_{O,il}}}$$

$$L(\theta) = -\sum_i r_{ik} P(y_i = k|\boldsymbol{x}_i, \theta) = \sum_i \ln\left(\sum_k e^{z_{Oik}}\right) - \sum_k r_{ik} z_{O,ik}$$

  - Called the categorical cross-entropy

Outline

- ❑ Motivating Idea: Nonlinear classifiers from linear features
- ❑ Neural Networks
- ❑ Neural Network Loss Function
- ❑ Stochastic Gradient Descent
- ❑ Building and Training a Network in Keras
  - Synthetic data
  - MNIST
- ❑ Backpropagation Training

Problems with Standard Gradient Descent

- Neural network training (like all training): Minimize loss function

$$\hat{\theta} = \arg\min_{\theta} L(\theta)\,, \qquad L(\theta) = \frac{1}{N}\sum_{i=1}^{N} L_i(\theta, \boldsymbol{x}_i, y_i)$$

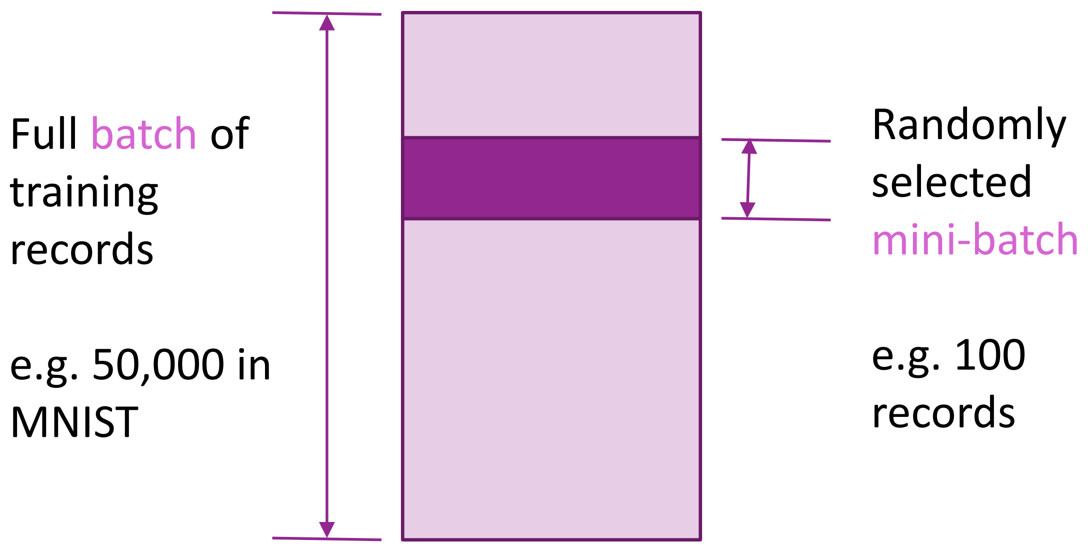
  - $L_i(\theta, \boldsymbol{x}_i, y_i)$ = loss on sample i for parameter θ

- Standard gradient descent:

$$\theta^{k+1} = \theta^k - \alpha \nabla L(\theta^k) = \theta^k - \frac{\alpha}{N}\sum_{i=1}^{N} \nabla L_i(\theta^k, \boldsymbol{x}_i, y_i)$$

  - Each iteration requires computing N loss functions and gradients
  - Will discuss how to compute later
  - But, gradient computation is expensive when data size N large

Stochastic Gradient Descent



- In each step:
  - Select random small “mini-batch”
  - Evaluate gradient on mini-batch

- For $t = 1$ to N_{steps}
  - Select random mini-batch $I \subset \{1, \ldots, N\}$
  - Compute gradient approximation:
    $$g^t = \frac{1}{|I|} \sum_{i \in I} \nabla L(x_i, y_i, \theta)$$
  - Update parameters:
    $$\theta^{t+1} = \theta^t - \alpha^t g^t$$

SGD Theory (Advanced)

- Mini-batch gradient = true gradient in expectation:

$$E(g^t) = \frac{1}{N}\sum_{i=1}^{N} \nabla L(x_i, y_i, \theta) = \nabla L(\theta^t)$$

- Hence can write $g^t = \nabla L(\theta^t) + \xi^t$,
  - ξ^t= random error in gradient calculation, $E(\xi^t) = 0$
  - SGD update: $\theta^{t+1} = \theta^t - \alpha^t g^t$, $\theta^{t+1} = \theta^t - \alpha^t \nabla L(\theta^t) - \alpha^t \xi^t$
- Robins-Munro: Suppose that $\alpha^t \to 0$ and $\sum_t \alpha^t = \infty$. Let $s_t = \sum_{k=0}^{t} \alpha^k$
  - Then $\theta^t \to \theta(s_t)$ where $\theta(s)$ is the continuous solution to the differential equation:

$$\frac{d\theta(s)}{ds} = -\nabla L(\theta)$$

- High-level take away:
  - If step size is decreased, random errors in sub-sampling are averaged out

SGD Practical Issues

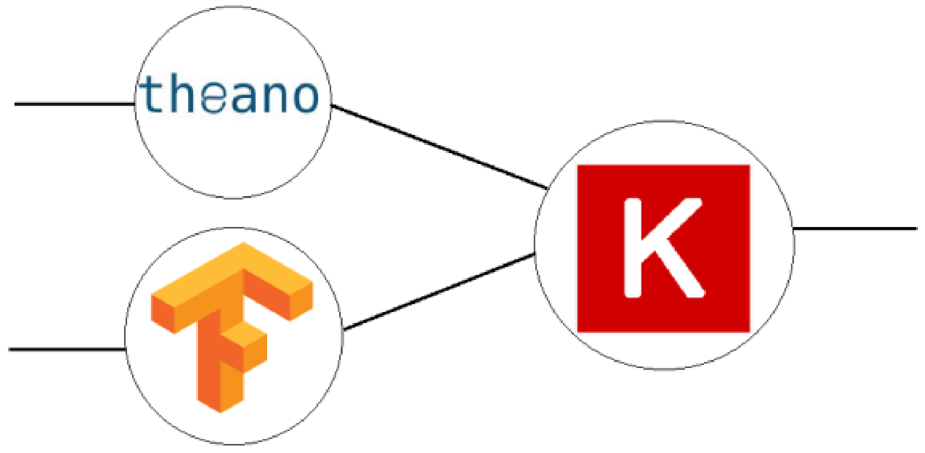
- Terminology:
  - Suppose minibatch size is B. Training size is N
  - Each training epoch includes updates going through all non-overlapping minibatches
  - There are $\frac{N}{B}$ steps per training epoch
- Data shuffling
  - Generally do not randomly pick a mini-batch
  - In each epoch, randomly shuffle training samples
  - Then, select mini-batches in order through the shuffled training samples.
  - It is critical to reshuffle in each epoch!

Outline

Deep Learning Zoo

- Torch
- Caffe
- Theano (Keras, Lasagne)
- CuDNN
- Tensorflow
- Mxnet
- Etc.

Keras Package
Python Deep Learning Library



Keras
High-level language

Low-level backend
(e.g. Tensorflow, Theano, CNTK, …)

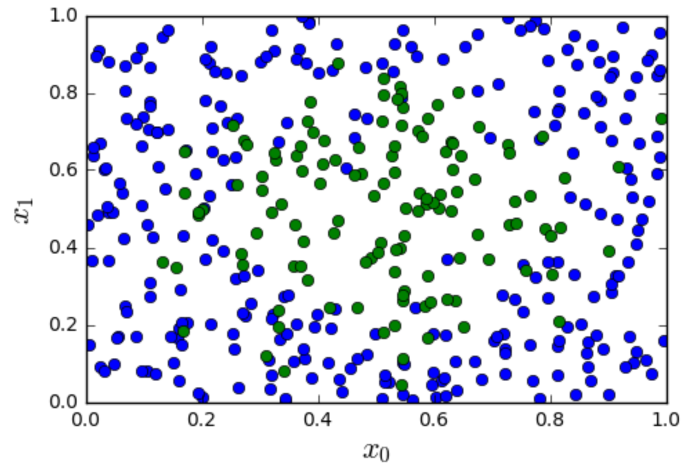
- ❑ High-level neural network language in Python
- ❑ Runs on top of a backend
  - Much simpler than raw backend language
  - Very fast coding
  - Uniform language for all backend
- ❑ Keras has been incorporated into TF
- ❑ But…
  - Slightly less flexible
  - Not as fast sometimes
- ❑ In this class, we use Keras

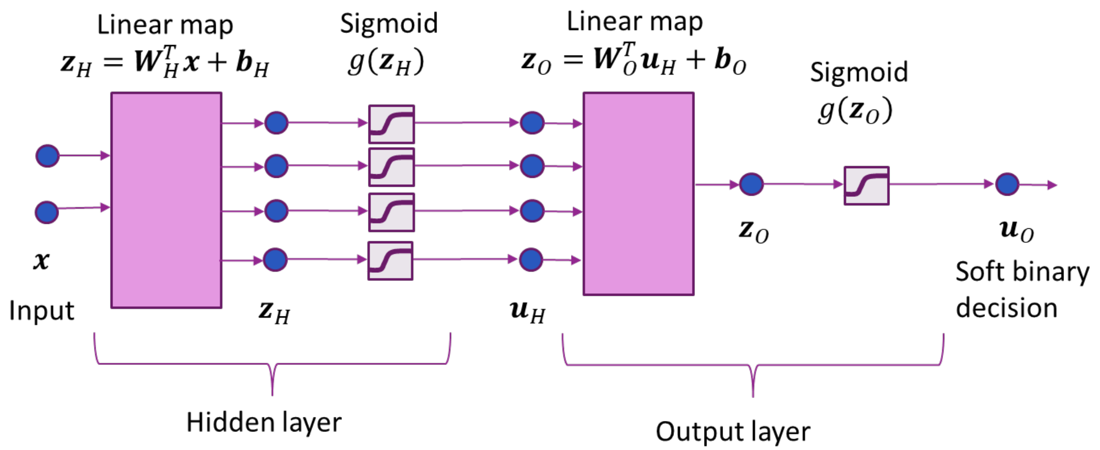
Keras Recipe

- ❑Step 1. Describe model architecture
  - Number of hidden units, output units, activations, …
- ❑Step 2. Select an optimizer
- ❑Step 3. Select a loss function and compile the model
- ❑Step 4. Fit the model
- ❑Step 5. Test / use the model

Synthetic Data Example

- Try a simpler two-layer NN
  - Input x = 2 dim
  - 4 hidden units
  - 1 output unit (binary classification)



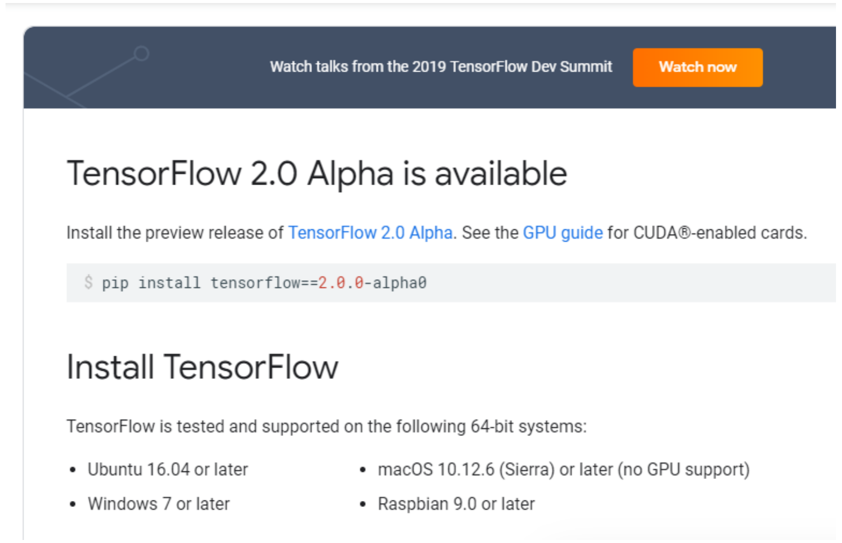


Step 0: Import the Packages

- ❑Install Tensorflow
- ❑For this lab, you can use the CPU version
- ❑If you are using Google Collaboratory, TF is pre-installed

```
import tensorflow as tf
```

https://www.tensorflow.org/install



TensorFlow 2.0 Alpha is available

Install the preview release of TensorFlow 2.0 Alpha. See the GPU guide for CUDA®-enabled cards.

```
$ pip install tensorflow==2.0.0-alpha0
```

Install TensorFlow

TensorFlow is tested and supported on the following 64-bit systems:

- Ubuntu 16.04 or later
- Windows 7 or later
- macOS 10.12.6 (Sierra) or later (no GPU support)
- Raspbian 9.0 or later

Step 1: Define Model

```
from tensorflow.keras.models import Model, Sequential
from tensorflow.keras.layers import Dense, Activation
```

```
import tensorflow.keras.backend as K
K.clear_session()
```

```
nin = nx   # dimension of input data
nh = 4     # number of hidden units
nout = 1   # number of outputs = 1 since this is binary
model = Sequential()
model.add(Dense(units=nh, input_shape=(nx,), activation='sigmoid', name='hidden'))
model.add(Dense(units=nout, activation='sigmoid', name='output'))
```

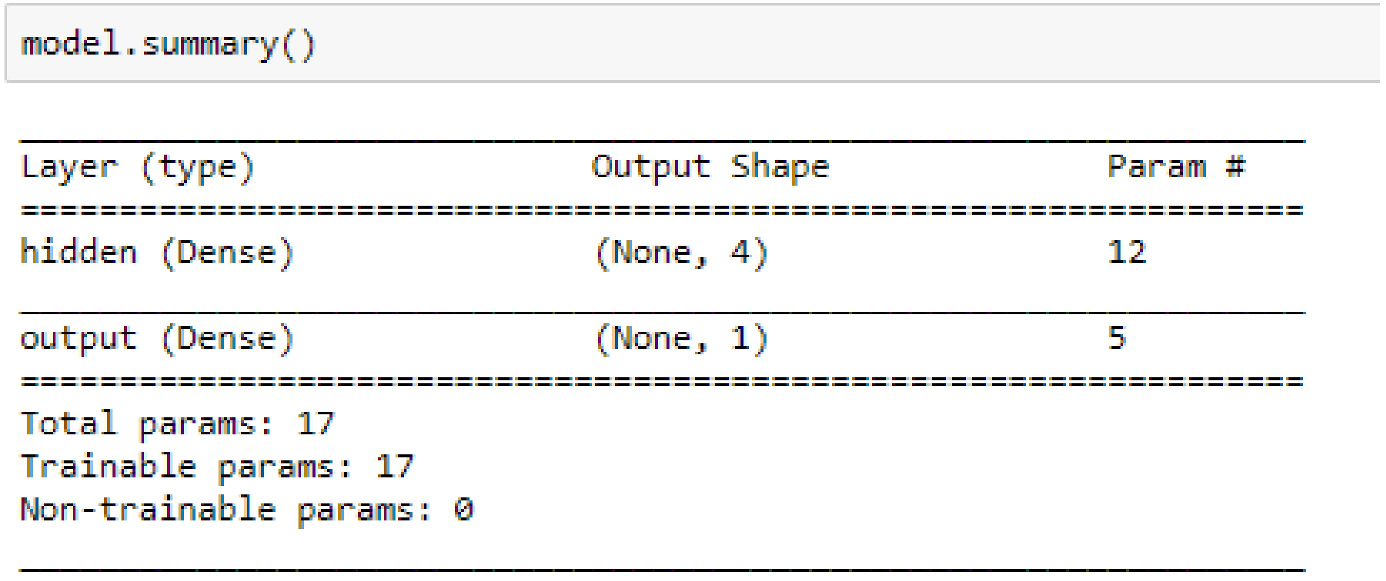
- ❑Load modules for layers
- ❑Clear graph (extremely important!)
- ❑Build model
  - This example: dense layers
  - Give each layer a dimension, name & activation

Step 1: Continued

- Print the model summary
- For each layers
  - Shows dimensions and shape
- Note shapes:
  - (None, 4)

Batch size
This is not fixed

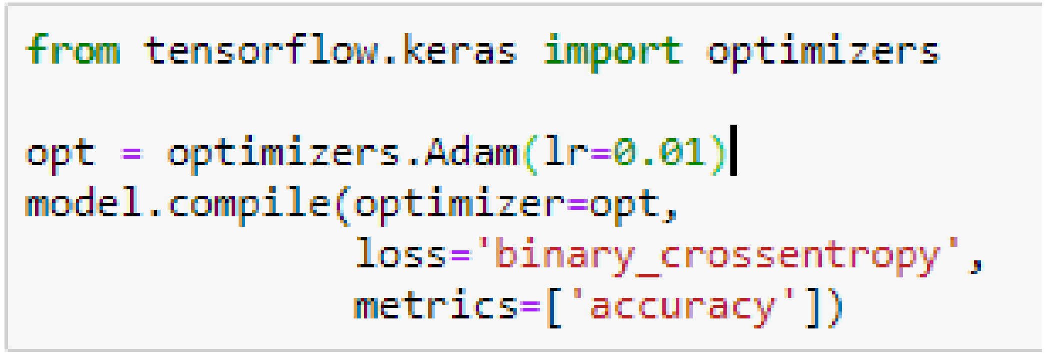
Dim per sample in batch



```
model.summary()
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #   
=================================================================
hidden (Dense)               (None, 4)                 12        
_________________________________________________________________
output (Dense)               (None, 1)                 5         
=================================================================
Total params: 17
Trainable params: 17
Non-trainable params: 0
_________________________________________________________________
```

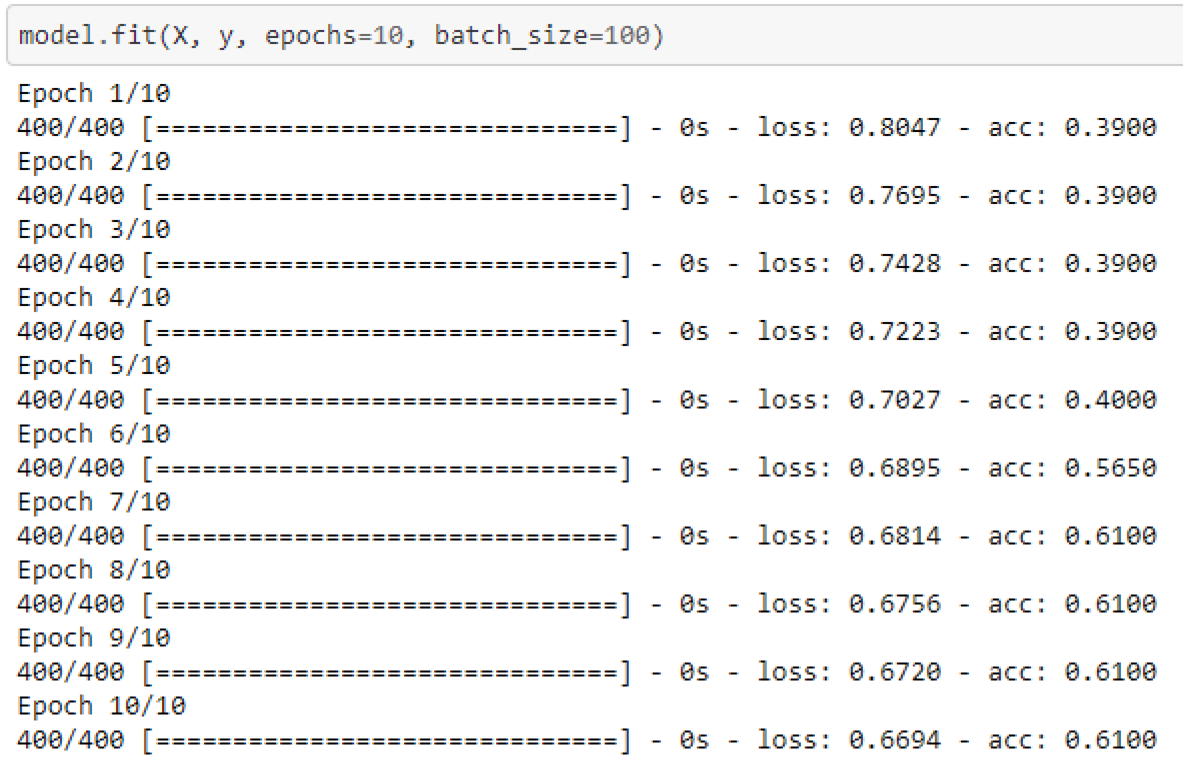
Step 2, 3: Select an Optimizer & Compile



```
from tensorflow.keras import optimizers

opt = optimizers.Adam(lr=0.01)
model.compile(optimizer=opt,
              loss='binary_crossentropy',
              metrics=['accuracy'])
```

- Adam optimizer generally works well for most problems
  - In this case, had to manually set learning rate
  - You often need to play with this.
- Use binary cross-entropy loss
- Metrics indicate what will be printed in each epoch

Step 4: Fit the Model



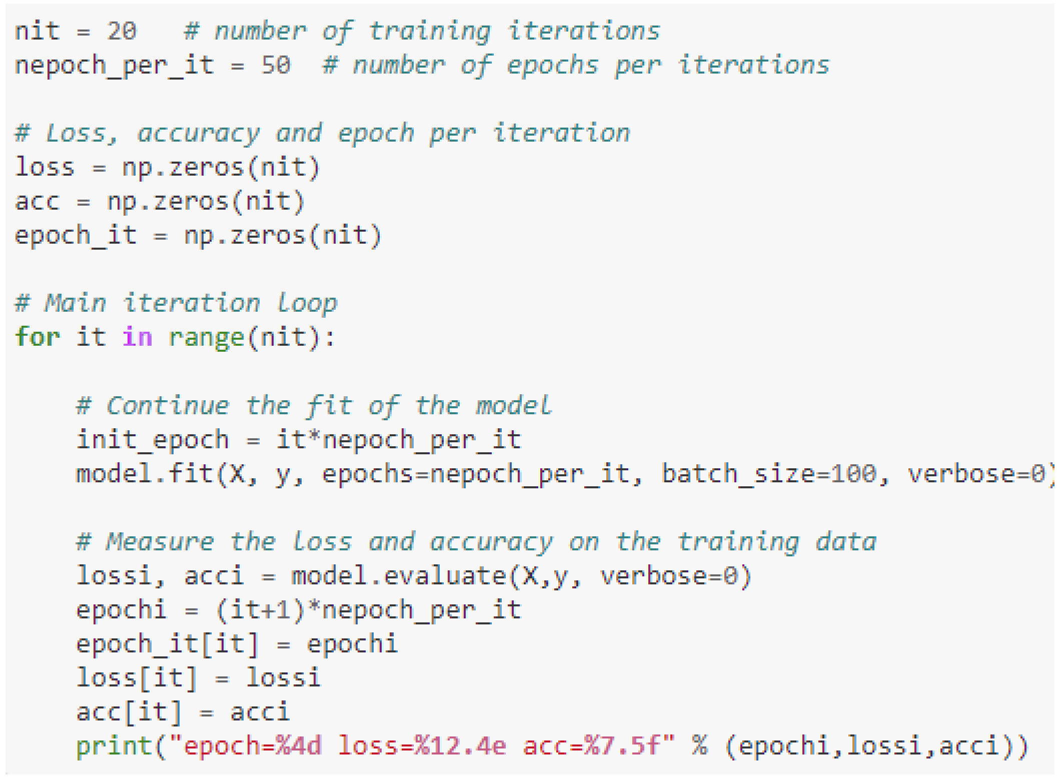
```
model.fit(X, y, epochs=10, batch_size=100)
```

```
Epoch 1/10
400/400 [==============================] - 0s - loss: 0.8047 - acc: 0.3900
Epoch 2/10
400/400 [==============================] - 0s - loss: 0.7695 - acc: 0.3900
Epoch 3/10
400/400 [==============================] - 0s - loss: 0.7428 - acc: 0.3900
Epoch 4/10
400/400 [==============================] - 0s - loss: 0.7223 - acc: 0.3900
Epoch 5/10
400/400 [==============================] - 0s - loss: 0.7027 - acc: 0.4000
Epoch 6/10
400/400 [==============================] - 0s - loss: 0.6895 - acc: 0.5650
Epoch 7/10
400/400 [==============================] - 0s - loss: 0.6814 - acc: 0.6100
Epoch 8/10
400/400 [==============================] - 0s - loss: 0.6756 - acc: 0.6100
Epoch 9/10
400/400 [==============================] - 0s - loss: 0.6720 - acc: 0.6100
Epoch 10/10
400/400 [==============================] - 0s - loss: 0.6694 - acc: 0.6100
```

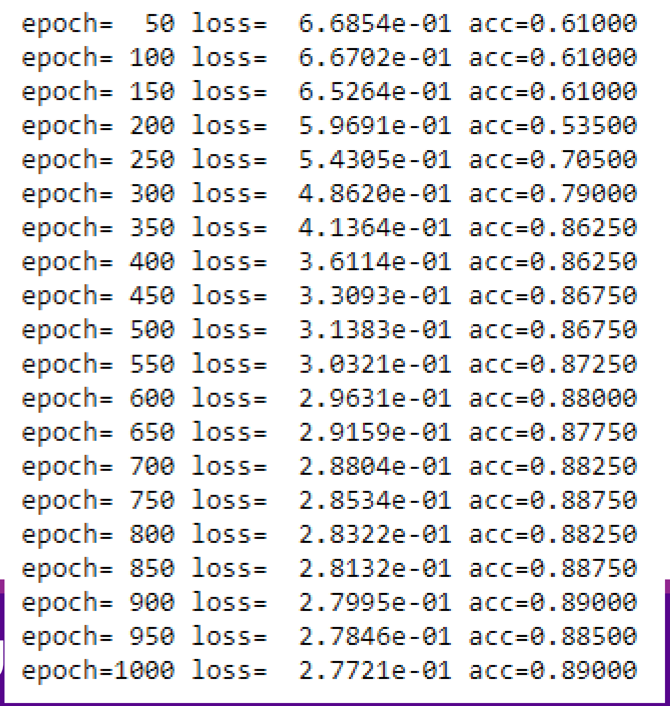
- Use keras fit function
  - Specify number of epoch & batch size
- Prints progress after each epoch
  - Loss = loss on training data
  - Acc = accuracy on training data

Fitting the Model with Many Epochs

- This example requires large number of epochs (~1000)
- Do not want to print progress on each epoch
- Rewrite code to manually print progress
- Can also use a callback function



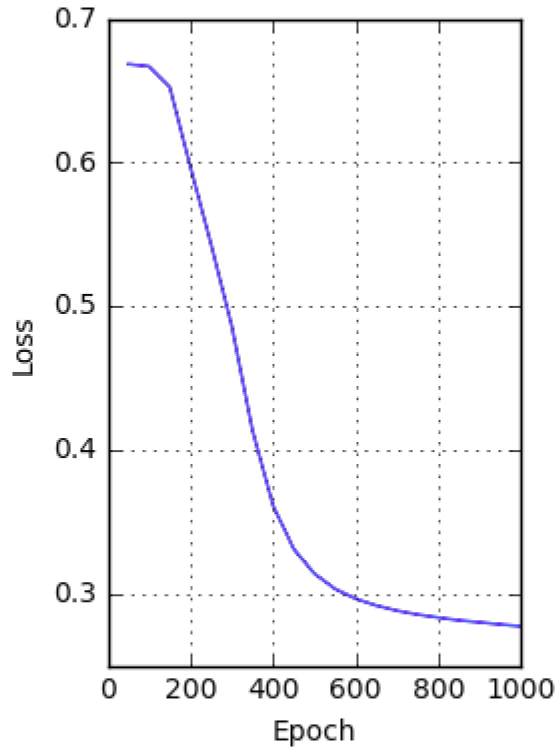
```python
nit = 20   # number of training iterations
nepoch_per_it = 50  # number of epochs per iterations

# Loss, accuracy and epoch per iteration
loss = np.zeros(nit)
acc = np.zeros(nit)
epoch_it = np.zeros(nit)

# Main iteration loop
for it in range(nit):

    # Continue the fit of the model
    init_epoch = it*nepoch_per_it
    model.fit(X, y, epochs=nepoch_per_it, batch_size=100, verbose=0)

    # Measure the loss and accuracy on the training data
    lossi, acci = model.evaluate(X,y, verbose=0)
    epochi = (it+1)*nepoch_per_it
    epoch_it[it] = epochi
    loss[it] = lossi
    acc[it] = acci
    print("epoch=%4d loss=%12.4e acc=%7.5f" % (epochi,lossi,acci))
```

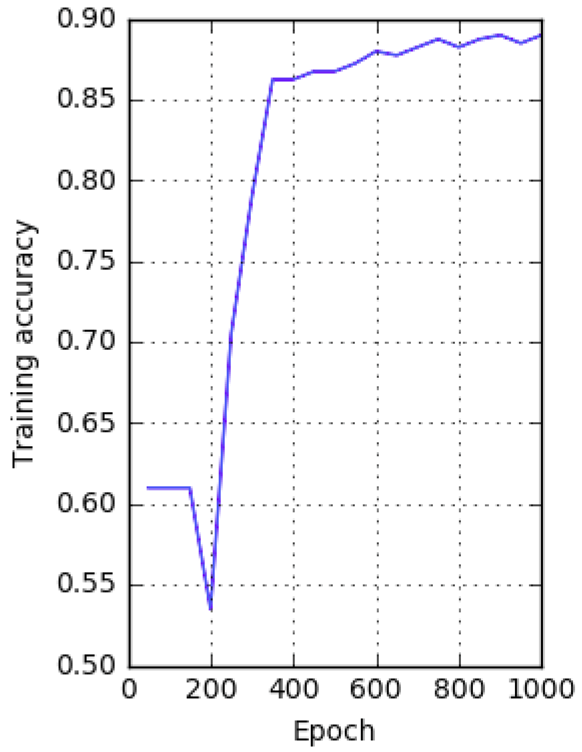


```
epoch=  50 loss=  6.6854e-01 acc=0.61000
epoch= 100 loss=  6.6702e-01 acc=0.61000
epoch= 150 loss=  6.5264e-01 acc=0.61000
epoch= 200 loss=  5.9691e-01 acc=0.53500
epoch= 250 loss=  5.4305e-01 acc=0.70500
epoch= 300 loss=  4.8620e-01 acc=0.79000
epoch= 350 loss=  4.1364e-01 acc=0.86250
epoch= 400 loss=  3.6114e-01 acc=0.86250
epoch= 450 loss=  3.3093e-01 acc=0.86750
epoch= 500 loss=  3.1383e-01 acc=0.86750
epoch= 550 loss=  3.0321e-01 acc=0.87250
epoch= 600 loss=  2.9631e-01 acc=0.88000
epoch= 650 loss=  2.9159e-01 acc=0.87750
epoch= 700 loss=  2.8804e-01 acc=0.88250
epoch= 750 loss=  2.8534e-01 acc=0.88750
epoch= 800 loss=  2.8322e-01 acc=0.88250
epoch= 850 loss=  2.8132e-01 acc=0.88750
epoch= 900 loss=  2.7995e-01 acc=0.89000
epoch= 950 loss=  2.7846e-01 acc=0.88500
epoch=1000 loss=  2.7721e-01 acc=0.89000
```

Performance vs Epoch

- Can observe loss function slowly converging

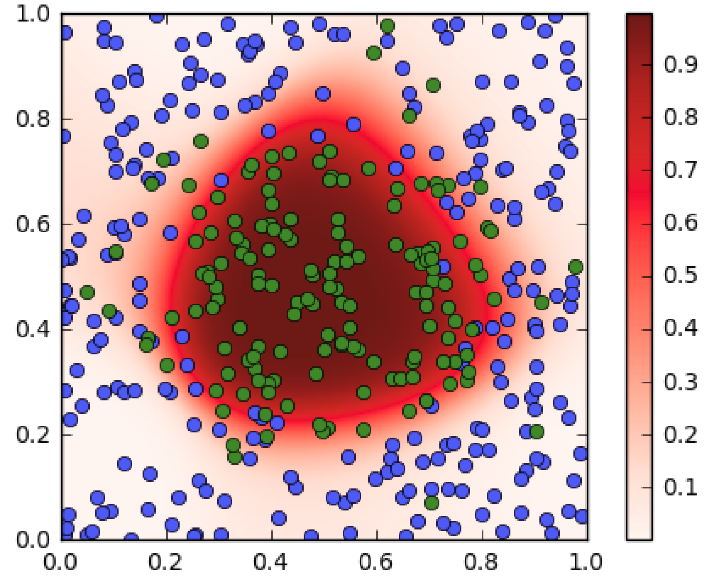




Step 5. Visualizing the Decision Regions

- Feed in data $x = (x_1, x_2)$ over grid of points in $[0,1] \times [0,1]$
- Use predict to observe output for each input point
- Plot outputs $u_O = sigmoid(z_O)$

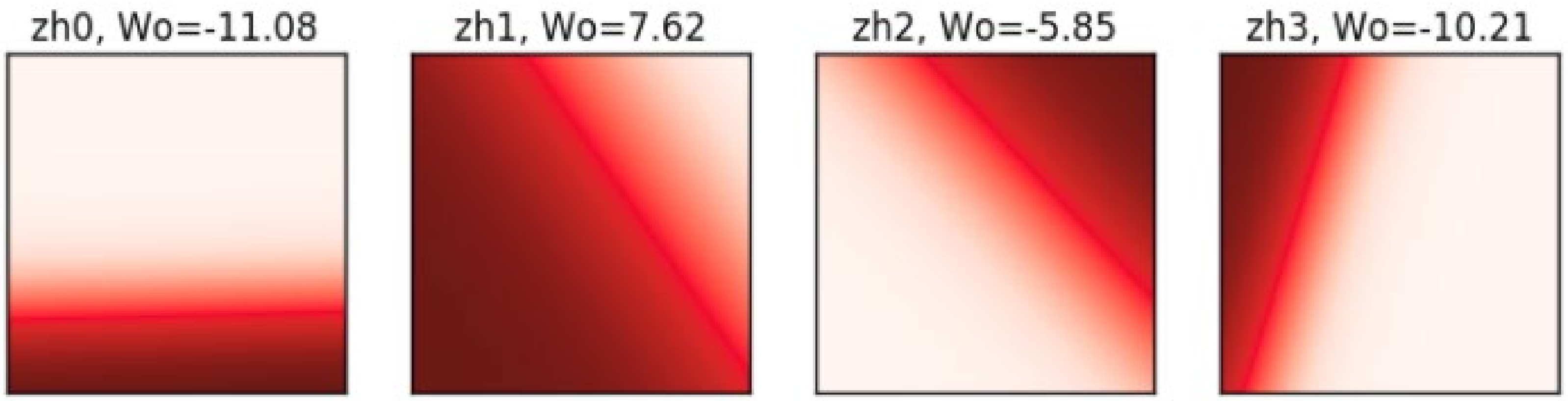
```
# Limits to plot the response.
xmin = [0,0]
xmax = [1,1]

# Use meshgrid to create the 2D input
nplot = 100
x0plot = np.linspace(xmin[0],xmax[1],nplot)
x1plot = np.linspace(xmin[0],xmax[1],nplot)
x0mat, x1mat = np.meshgrid(x0plot,x1plot)
Xplot = np.column_stack([x0mat.ravel(), x1mat.ravel()])

# Compute the output
yplot = model.predict(Xplot)
yplot_mat = yplot[:,0].reshape((nplot, nplot))

# Plot the recovered region
plt.imshow(np.flipud(yplot_mat), extent=[xmin[0],xmax[0],xmin[0],xmax[1]], cmap=plt.cm.Reds)
plt.colorbar()
```



Visualizing the Hidden Layers

```
# Get the response in the hidden units
layer_hid = model.get_layer('hidden')
model1 = Model(inputs=model.input,
               outputs=layer_hid.output)
zhid_plot = model1.predict(Xplot)
zhid_plot = zhid_plot.reshape((nplot,nplot,nh))
```

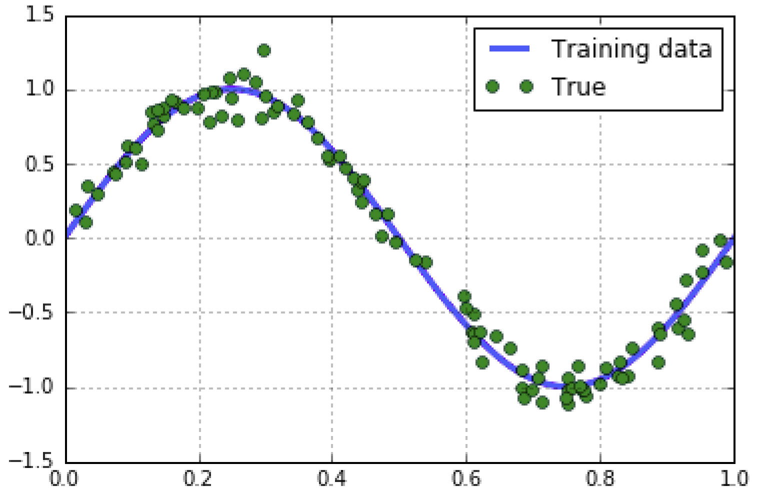
- ❑Create a new model with hidden layer output
- ❑Feed in data $x = (x_1, x_2)$ over $[0,1] \times [0,1]$
- ❑Predict outputs from hidden outputs



Each hidden layer is a logistic regression layer with a different separating line!

In-Class Exercise

- Go to in class exercise in github



Now try to have a neural network *learn* the relation `y=f(x)`.

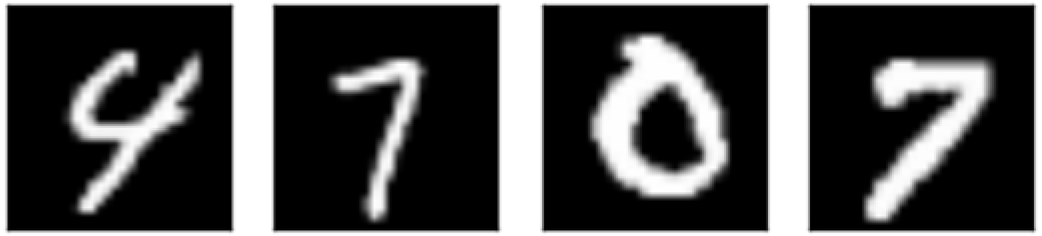
- Clear the keras session
- Create a neural network with 4 hidden units, 1 output unit
- Use a sigmoid activation for the hidden units and no output activation
- Compile with `mean_squared_error` for the `loss` and `metrics`
- Fit the model
- Plot the predicted and true function

Outline

- ❑ Motivating Idea: Nonlinear classifiers from linear features
- ❑ Neural Networks
- ❑ Neural Network Loss Function
- ❑ Stochastic Gradient Descent
- ❑ Building and Training a Network in Keras
  - Synthetic data
  - MNIST
- ❑ Backpropagation Training

Recap: MNIST data

- Classic MNIST problem:
  - Detect hand-written digits
  - Each image is 28 x 28 = 784 pixels
- Dataset size:
  - 50,000 training digits
  - 10,000 test
  - 10,000 validation (not used here)
- Can be loaded with sklearn and many other packages



Simple MNIST Neural Network

- 784 inputs, 100 hidden units, 10 outputs

```
nin = Xtr.shape[1]  # dimension of input data
nh = 100     # number of hidden units
nout = int(np.max(ytr)+1)    # number of outputs = 10 since there are 10 classes
model = Sequential()
model.add(Dense(units=nh, input_shape=(nin,), activation='sigmoid', name='hidden'))
model.add(Dense(units=nout, activation='softmax', name='output'))
```

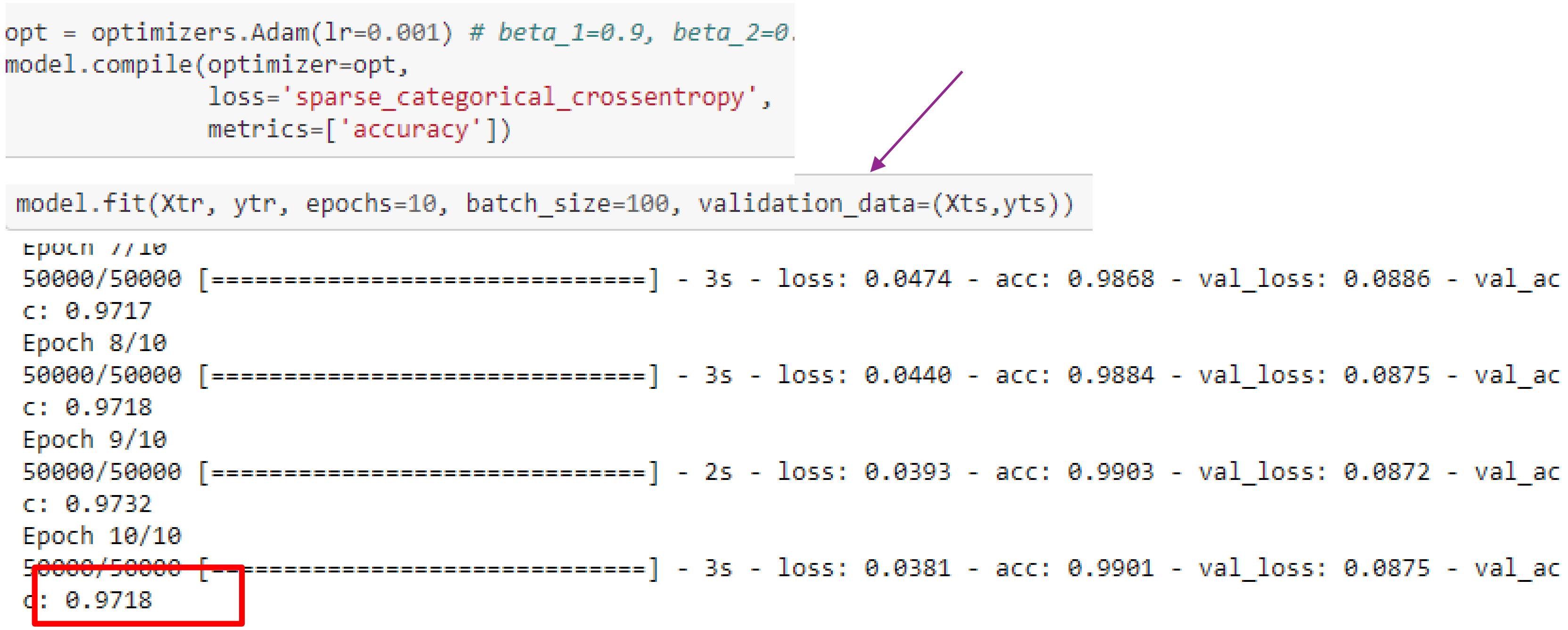
```
model.summary()
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #   
=================================================================
hidden (Dense)               (None, 100)               78500     
_________________________________________________________________
output (Dense)               (None, 10)                1010      
=================================================================
Total params: 79,510
Trainable params: 79,510
Non-trainable params: 0
```

Why 78500 parameters in hidden layer?

Fitting the Model

- ❑Run for 20 epochs, ADAM optimizer, batch size = 100
- ❑Final accuracy = 0.972
- ❑Not great, but much faster than SVM. Also CNNs we study later do even better.

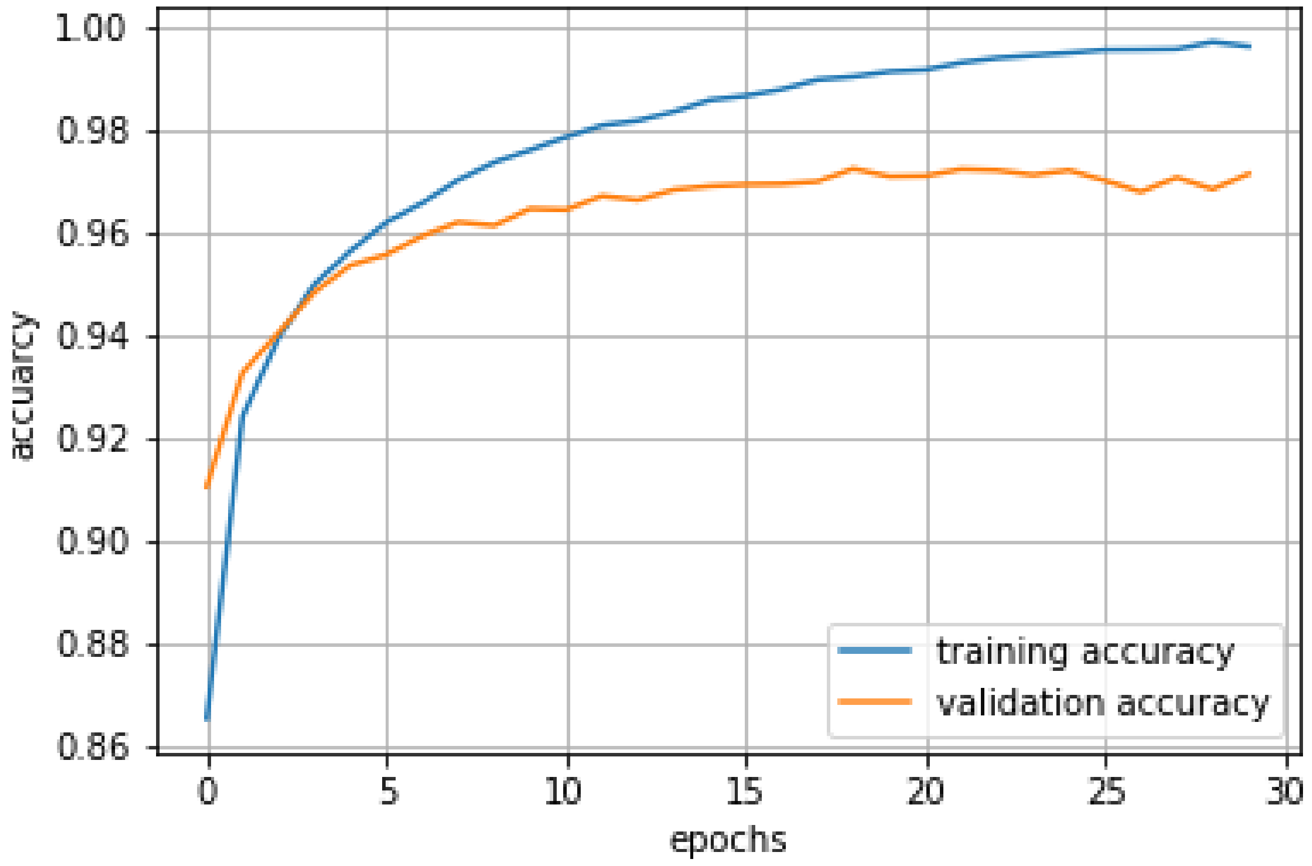


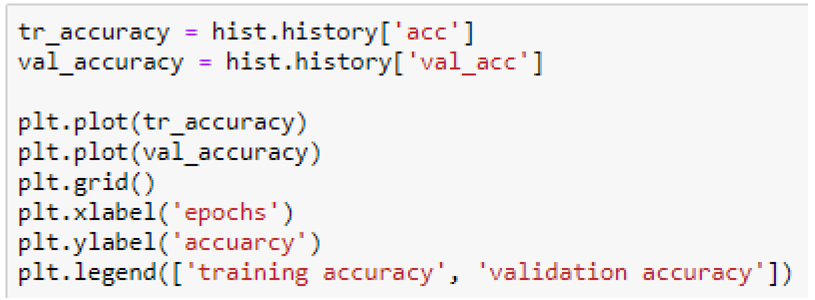
```
opt = optimizers.Adam(lr=0.001) # beta_1=0.9, beta_2=0.
model.compile(optimizer=opt,
              loss='sparse_categorical_crossentropy',
              metrics=['accuracy'])
```

```
model.fit(Xtr, ytr, epochs=10, batch_size=100, validation_data=(Xts,yts))
```

```
Epoch 7/10
50000/50000 [==============================] - 3s - loss: 0.0474 - acc: 0.9868 - val_loss: 0.0886 - val_ac
c: 0.9717
Epoch 8/10
50000/50000 [==============================] - 3s - loss: 0.0440 - acc: 0.9884 - val_loss: 0.0875 - val_ac
c: 0.9718
Epoch 9/10
50000/50000 [==============================] - 2s - loss: 0.0393 - acc: 0.9903 - val_loss: 0.0872 - val_ac
c: 0.9732
Epoch 10/10
50000/50000 [==============================] - 3s - loss: 0.0381 - acc: 0.9901 - val_loss: 0.0875 - val_ac
c: 0.9718
```

Training and Validation Accuracy





```
tr_accuracy = hist.history['acc']
val_accuracy = hist.history['val_acc']

plt.plot(tr_accuracy)
plt.plot(val_accuracy)
plt.grid()
plt.xlabel('epochs')
plt.ylabel('accuarcy')
plt.legend(['training accuracy', 'validation accuracy'])
```

- Training accuracy continues to increase
- Validation accuracy eventually flattens and sometimes starts to decrease.
- Should stop when the validation accuracy starts to decrease.
- This indicates overfitting.

Outline

- ❑Motivating Idea: Nonlinear classifiers from linear features
- ❑Neural Networks
- ❑Neural Network Loss Function
- ❑Stochastic Gradient Descent
- ❑Building and Training a Network in Keras
  - Synthetic data
  - MNIST
- ❑Backpropagation Training

Stochastic Gradient Descent

- ❑Training uses SGD
- ❑In each step:
  - Select a subset of sample for minibatch $I \subset \{1, \ldots, N\}$
  - Evaluate mini-batch loss $L(\theta^t) = \sum_{i \in I} L_i(\theta^t, \boldsymbol{x}_i, y_i)$
  - Evaluate mini-batch gradient $\boldsymbol{g}^t = \sum_{i \in I} \nabla L_i(\theta^t, \boldsymbol{x}_i, y_i)$
  - Take SGD step: $\theta^{t+1} = \theta^t - \alpha \boldsymbol{g}^t$
- ❑Question: How do we compute gradient?

Gradients with Multiple Parameters

- For neural net problem: $\theta = (W_H, b_H, W_o, b_o)$
- Gradient is computed with respect to each parameter:

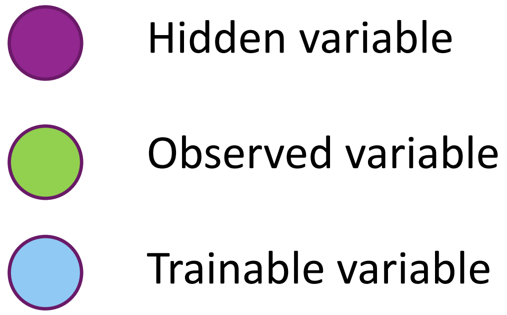
$$\nabla L(\theta) = [\nabla_{W_H} L(\theta), \nabla_{b_H} L(\theta), \nabla_{W_O} L(\theta), \nabla_{b_O} L(\theta)]$$

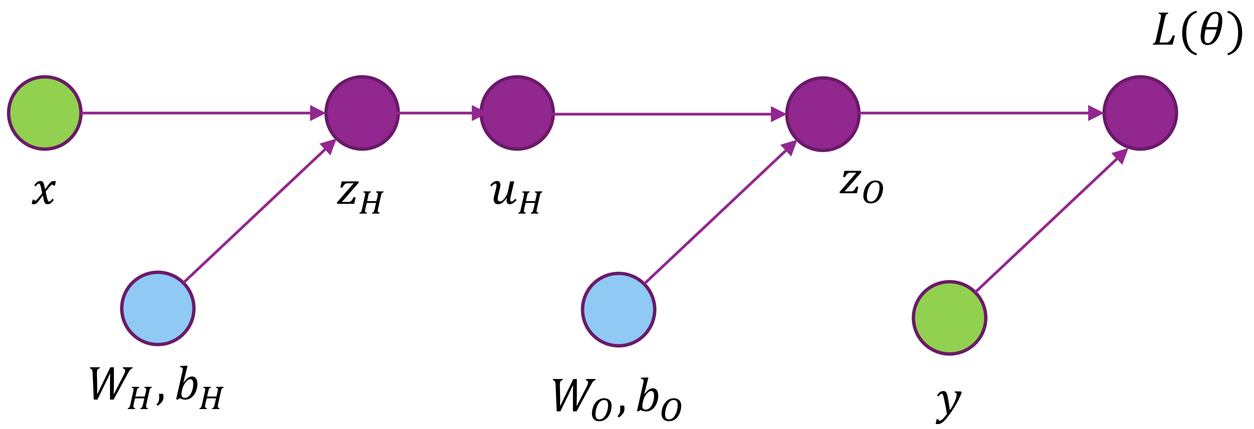
- Gradient descent is performed on each parameter:

$$W_H \leftarrow W_H - \alpha \nabla_{W_H} L(\theta),$$
$$b_H \leftarrow b_H - \alpha \nabla_{b_H} L(\theta),$$
$$\dots.$$

Computation Graph & Forward Pass

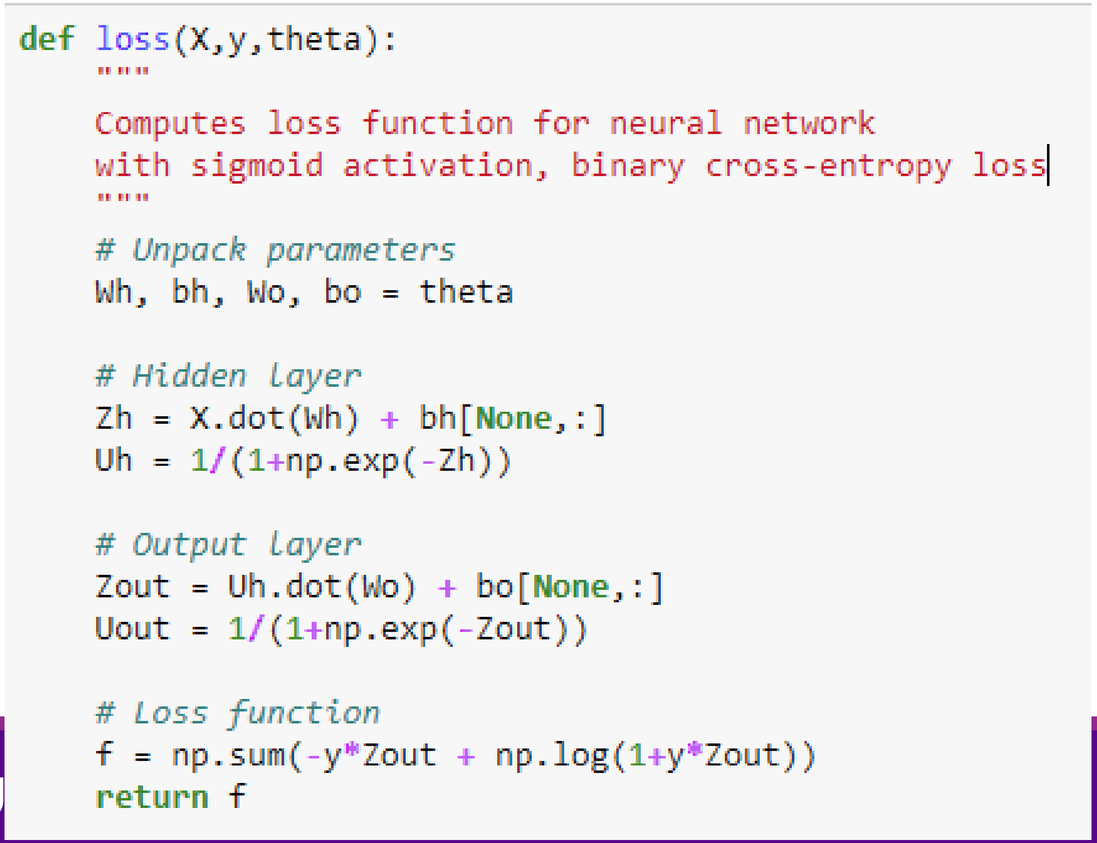
- Neural network loss function can be computed via a computation graph
- Sequence of operations starting from measured data and parameters
- Loss function computed via a forward pass in the computation graph
  - $z_{H,i} = W_H x_i + b_H$
  - $u_{H,i} = g_{act}(z_{H,i})$
  - $z_{O,i} = W_O u_{H,i} + b_O$
  - $L = \sum_i L_i(z_{O,i}, y_i)$



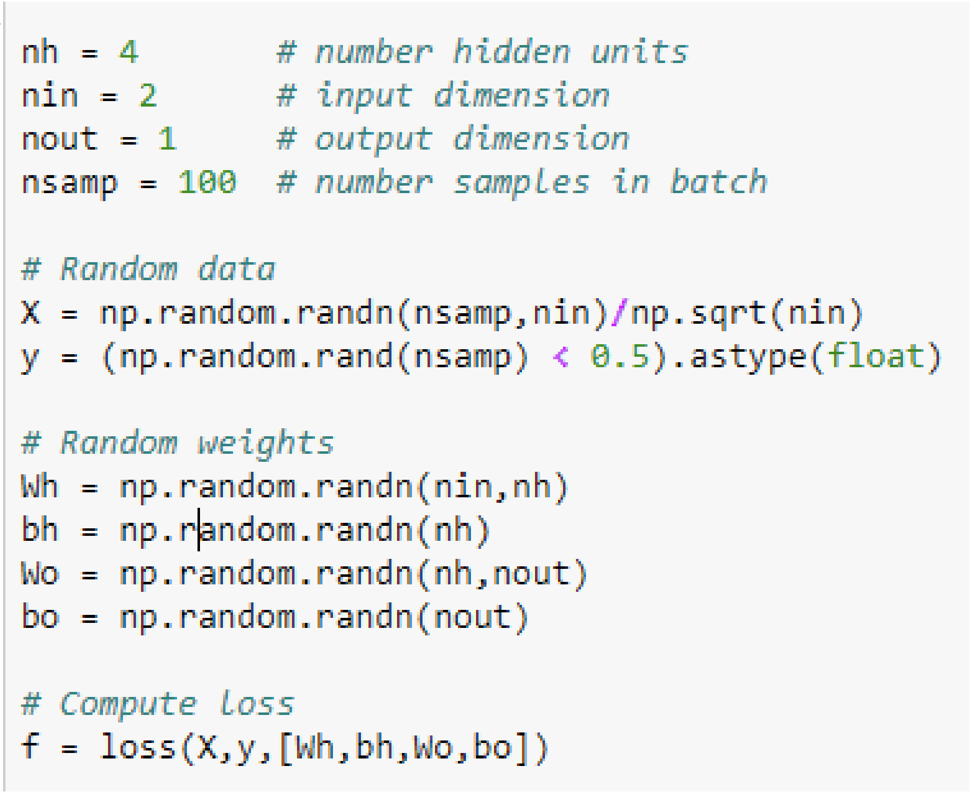


Forward Pass Example in Numpy

- Example network:
  - Single hidden layer with N_H hidden units, single output unit
  - Sigmoid activation, binary cross entropy loss



```python
def loss(X,y,theta):
    """
    Computes loss function for neural network
    with sigmoid activation, binary cross-entropy loss
    """
    # Unpack parameters
    Wh, bh, Wo, bo = theta

    # Hidden layer
    Zh = X.dot(Wh) + bh[None,:]
    Uh = 1/(1+np.exp(-Zh))

    # Output layer
    Zout = Uh.dot(Wo) + bo[None,:]
    Uout = 1/(1+np.exp(-Zout))

    # Loss function
    f = np.sum(-y*Zout + np.log(1+y*Zout))
    return f
```

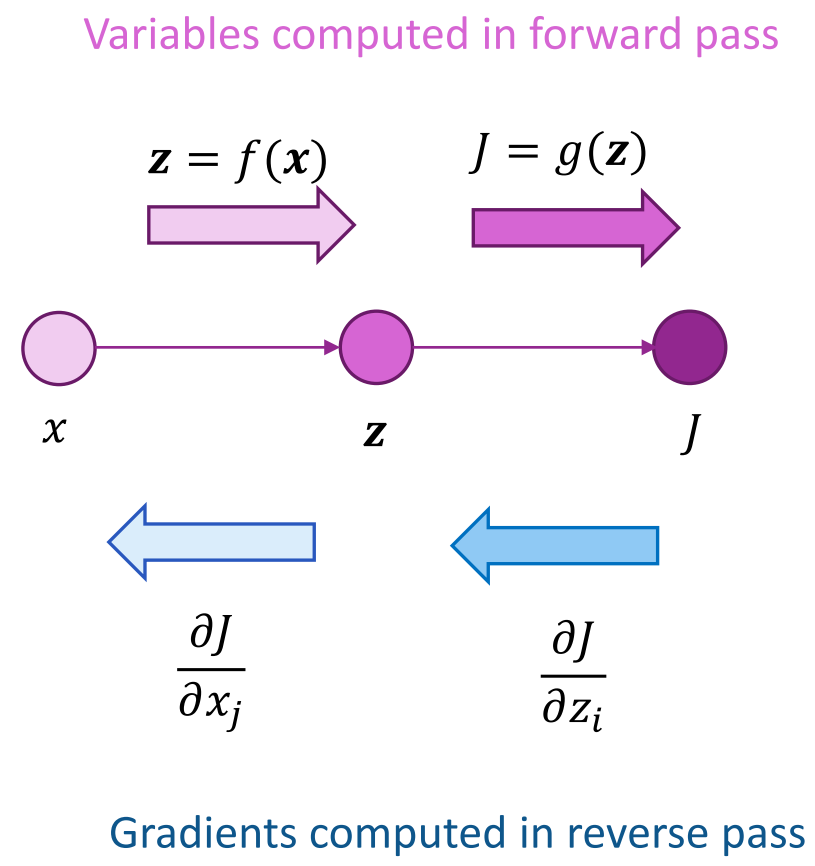


```python
nh = 4        # number hidden units
nin = 2       # input dimension
nout = 1      # output dimension
nsamp = 100   # number samples in batch

# Random data
X = np.random.randn(nsamp,nin)/np.sqrt(nin)
y = (np.random.rand(nsamp) < 0.5).astype(float)

# Random weights
Wh = np.random.randn(nin,nh)
bh = np.random.randn(nh)
Wo = np.random.randn(nh,nout)
bo = np.random.randn(nout)

# Compute loss
f = loss(X,y,[Wh,bh,Wo,bo])
```

Back-Propagation on A Two Node Graph

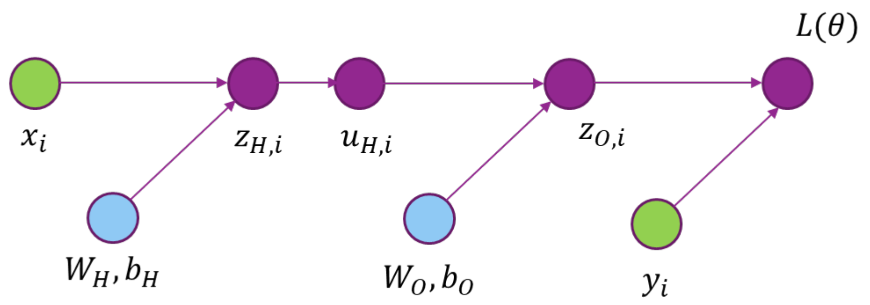
- Back Propagation:
  - A way to compute gradients
  - Iterative procedure that works in reverse
- Consider a simple 2 node computation graph
- Each component is a vector:
  - $\boldsymbol{x} = (x_1, \dots, x_N), \quad \boldsymbol{z} = (z_1, \dots, z_M)$
- First we compute $\frac{\partial J}{\partial z_i}$
- Then compute $\frac{\partial J}{\partial x_j}$ from multi-variable chain rule:

$$\frac{\partial J}{\partial x_j} = \sum_{i=1}^{n} \frac{\partial J}{\partial z_i} \frac{\partial z_i}{\partial x_j}$$


Variables computed in forward pass
$\boldsymbol{z} = f(\boldsymbol{x})$
$J = g(\boldsymbol{z})$
x
$\boldsymbol{z}$
J
$\frac{\partial J}{\partial x_j}$
$\frac{\partial J}{\partial z_i}$
Gradients computed in reverse pass

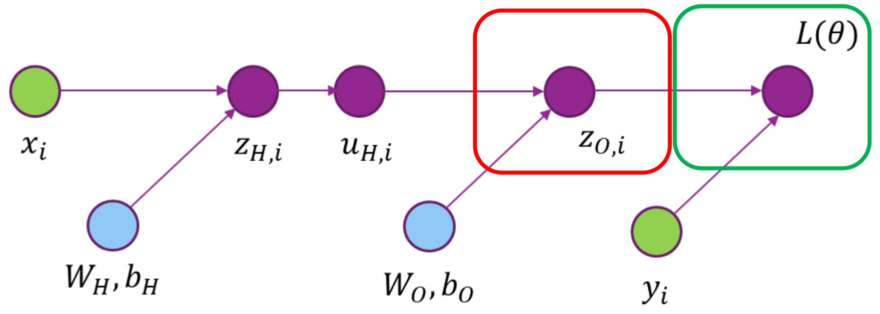
Back-Prop on a General Computation Graph

- Backpropagation:
  - Compute gradients backwards
  - Work one node at a time
- First compute all derivatives of all the variables
  - $\partial L/\partial z_O$
  - $\partial L/\partial u_H$ from $\partial L/\partial z_O$, $\partial z_O/\partial u_H$
  - $\partial L/\partial z_H$ from $\partial L/\partial u_H$, $\partial u_H/\partial z_H$
- Then compute gradient of parameters:
  - $\partial L/\partial W_O$ from $\partial L/\partial z_O$, $\partial z_O/\partial W_O$
  - $\partial L/\partial b_O$ from $\partial L/\partial z_O$, $\partial z_O/\partial b_O$
  - $\partial L/\partial W_H$ from $\partial L/\partial z_H$, $\partial z_H/\partial W_H$
  - $\partial L/\partial b_H$ from $\partial L/\partial z_H$, $\partial z_H/\partial b_H$
  -



Back-Propagation Example (Part 1)

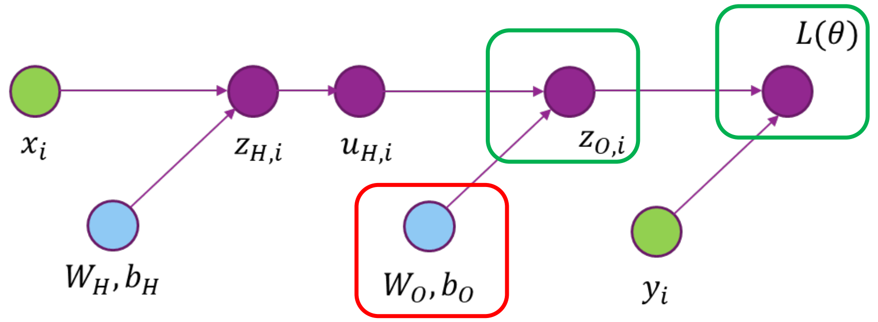
- Continue our example:
  - Single hidden layer with M hidden units, single output unit
  - Sigmoid activation, binary cross entropy loss
  - N samples, D input dimension



- Loss node:
  - $L = \sum_i L_i(z_{O,i}, y_i)$
  - $L_i(z_{oi}) = -(y_i \ln P(y_i = 1|x_i, \theta) + (1 - y_i) \ln P(y_i = 0|x_i, \theta)) = y_i z_{oi} - \ln[1 + e^{y_i z_{oi}}]$
  - $\frac{\partial L}{\partial z_{O,i}} = y_i - \frac{e^{y_i z_{oi}}}{1+e^{y_i z_{oi}}}$

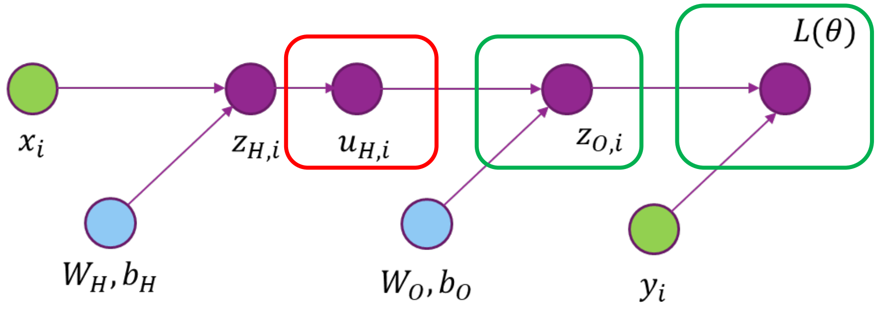
Back-Propagation Example (Part 2)

- Node z_O
  - $z_O = u_H W_O + b_O$
  - $z_{Oi} = \sum_m u_{H,im} W_{Om} + b_O$
- Gradient:
  - $\frac{\partial z_{O,i}}{\partial W_{O,m}} = u_{H,i,m}$
  - $\frac{\partial z_{O,i}}{\partial b_O} = 1$
  - Other partial derivatives are zero
- Apply chain rule:
  - $\frac{\partial L}{\partial W_{O,m}} = \sum_i \frac{\partial L}{\partial z_{O,i}} \frac{\partial z_{O,i}}{\partial W_{O,m}} = \sum_i \frac{\partial L}{\partial z_{O,i}} u_{H,im}$
  - $\frac{\partial L}{\partial b_O} = \sum_i \frac{\partial L}{\partial z_{O,i}} \frac{\partial z_{O,i}}{\partial b_O} = \sum_i \frac{\partial L}{\partial z_{O,i}}$



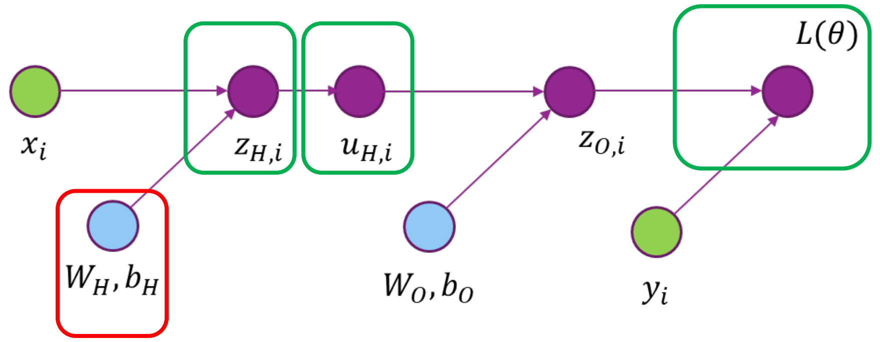
Back-Propagation Example (Part 3)

- Node z_O
  - $z_O = u_H W_O + b_O$
  - $z_{Oi} = \sum_m u_{H,im} W_{Om} + b_O$
- Gradient:
  - $\frac{\partial z_{O,i}}{\partial u_{H,ij}} = W_{O,j}$, m=1,…,M
  - Other partial derivatives are zero
- Apply chain rule:
  - $\frac{\partial L}{\partial u_{H,ij}} = \frac{\partial L}{\partial z_{O,i}} \frac{\partial z_{O,i}}{\partial u_{H,ij}} = \frac{\partial L}{\partial z_{O,i}} W_{O,j}$



Back-Propagation Example (Part 4,…)

- Compute $\frac{\partial L}{\partial W_H}, \frac{\partial L}{\partial b_H}$
- Following previous procedures, in class



- Summary:
  - Forward pass: Compute hidden nodes and loss
  - Backward pass: Compute gradients

Initialization and Data Normalization

- ❑Solution by gradient descent algorithm depends on the initial solution
- ❑Typically weights are set to random values near zero.
- ❑Small weights make the network behave like linear classifier.
  - Hence model starts out nearly linearly
  - Becomes nonlinear as weights increase during the training process.
- ❑Starting with large weights often lead to poor results.
- ❑Normalizing data to zero mean and unit variance
  - Allows all input dimensions be treated equally and facilitate better convergence.
- ❑With normalized data, it is typical to initialize the weights to be uniform in [-0.7, 0.7] [ESL]

Regularization

- ❑ To avoid the weights get too large, can add a penalty term explicitly, with regularization level λ
- ❑ Ridge penalty

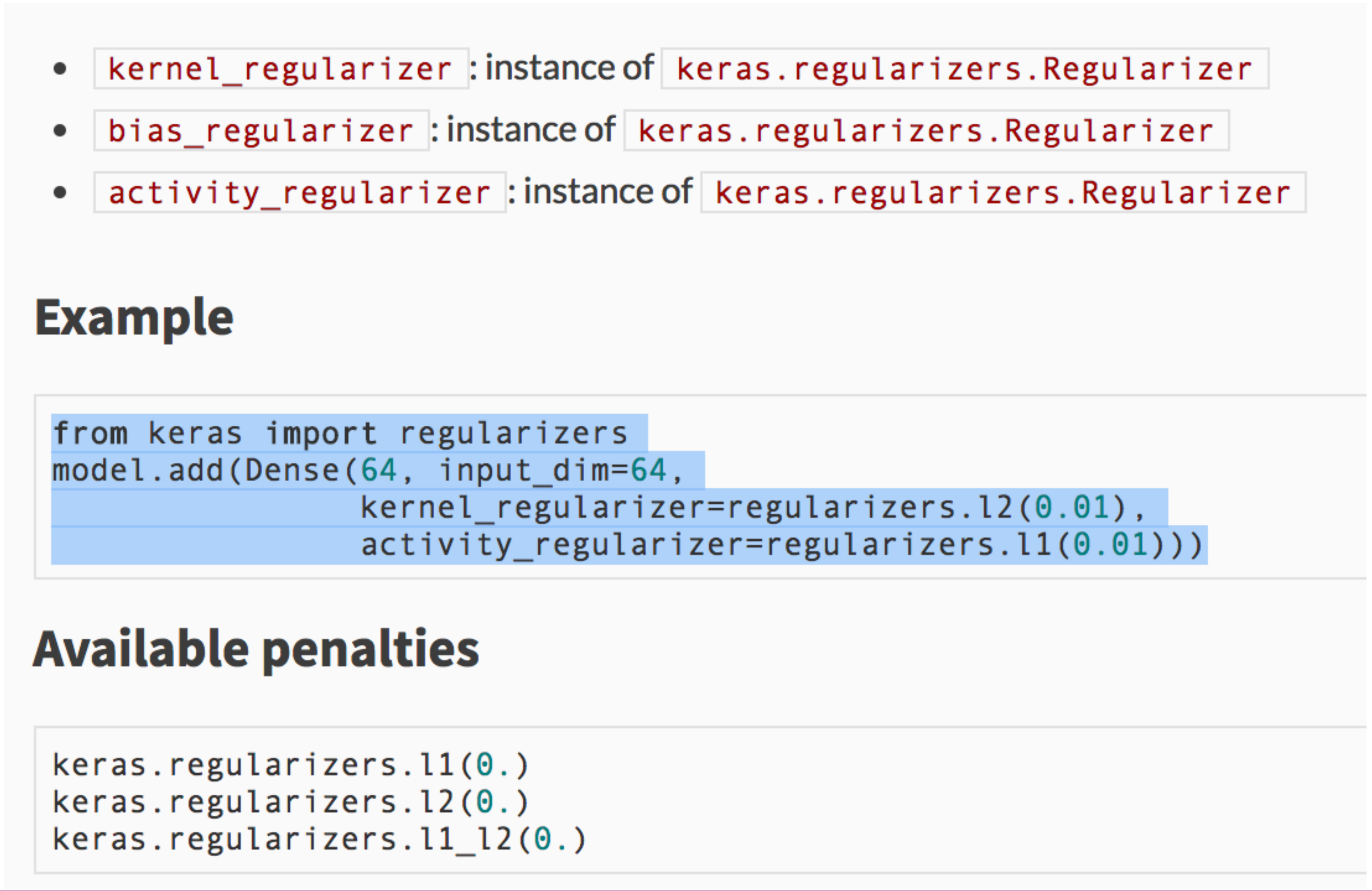
$$R(\theta) = \sum_{d,m} w_{H,d,m}^2 + \sum_{m,k} w_{O,m,k}^2 = \|w_H\|^2 + \|w_O\|^2$$

- ❑ Total loss

$$L_{reg}(\theta) = L(\theta) + \lambda R(\theta)$$

- ❑ Change in gradient calculation
- ❑ Typically used regularization
  - L2 = Ridge: Shrink the sizes of weights
  - L1: Prefer sparse set of weights
  - L1-L2: use a combination of both

Regularization in Keras



- `kernel_regularizer` : instance of `keras.regularizers.Regularizer`
- `bias_regularizer` : instance of `keras.regularizers.Regularizer`
- `activity_regularizer` : instance of `keras.regularizers.Regularizer`

Example

```
from keras import regularizers
model.add(Dense(64, input_dim=64,
                kernel_regularizer=regularizers.l2(0.01),
                activity_regularizer=regularizers.l1(0.01)))
```

Available penalties

```
keras.regularizers.l1(0.)
keras.regularizers.l2(0.)
keras.regularizers.l1_l2(0.)
```

Activity regularization tries to make the output at each layer small or sparse.

Choice of network parameters

- ❑Number of layers (typically not more than 2)
- ❑Number of hidden units in the hidden layer
- ❑Regularization level
- ❑Learning rate
- ❑Determined by maximizing the cross validation error through typically exhaustive search

Learning Objectives

- ❑ Mathematically describe a neural network with a single hidden layer
  - Describe mappings for the hidden and output units
- ❑ Manually compute output regions for very simple networks
- ❑ Select the loss function based on the problem type
- ❑ Build and train a simple neural network in Keras
- ❑ Write the formulas for gradients using backpropagation
- ❑ Describe mini-batches in stochastic gradient descent
- ❑ Importance of regularization
- ❑ Hyperparameter optimization

Lab for this unit

- ❑Music instrument classification based on music signals
- ❑Use hand-crafted features for audio (MFCC)
- ❑Train a neural net
- ❑Optimize the learning rate