# Neural network architecture and learning

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Fully connected multi-layer Neural Networks

Computing gradients and learning weights

Automatic differentiation

Torch

# Supervised learning setup

- Have an input $\mathbf{x} \in \mathbb{R}^d$ – a vector of $d$ real numbers.
- And an output $y$ (real number: regression, integer ID: classification, spam filtering, images of digits/clothing, etc).
- Want to learn a prediction function $f(\mathbf{x}) = y$ that will work on a new input.
- In a neural network (or multi-layer perceptron) with $L-1$ hidden layers, the function $f$ is defined using composition of $L$ functions, $f(x) = f^{(L)}[\cdots f^{(1)}[x]] \in \mathbb{R}$.
- Linear model is special case with $L = 1$ function, 0 hidden layers.
- "Deep" learning means $L \geq 3$ functions, at least 2 hidden layers.

# Each function is matrix multiplication and activation

- Prediction function $f(x) = f^{(L)}[\cdots f^{(1)}[x]] \in \mathbb{R}$.
- Each function $l \in \{1, \ldots, L\}$ is a matrix multiplication followed by an activation function: $f^{(l)}[z] = \sigma^{(l)}[W^{(l)}z]$ where $W^{(l)} \in \mathbb{R}^{u^{(l)} \times u^{(l-1)}}$ is a weight matrix to learn, and $z \in \mathbb{R}^{u^{(l-1)}}$ is the input vector to that layer.
- If the loss function is defined in terms of a real-valued predicted score (typical, like we did in linear models), then the last activation function is fixed to the identity $\sigma^{(L)}[z] = z$.
- The other activation functions must be non-linear, e.g. logistic/sigmoid $\sigma(z) = 1/(1 + \exp(-z))$ or rectified linear units (ReLU)

$$\sigma(z) = \begin{cases} z & \text{if } z > 0, \\ 0 & \text{else.} \end{cases}$$

# Non-linear activation functions

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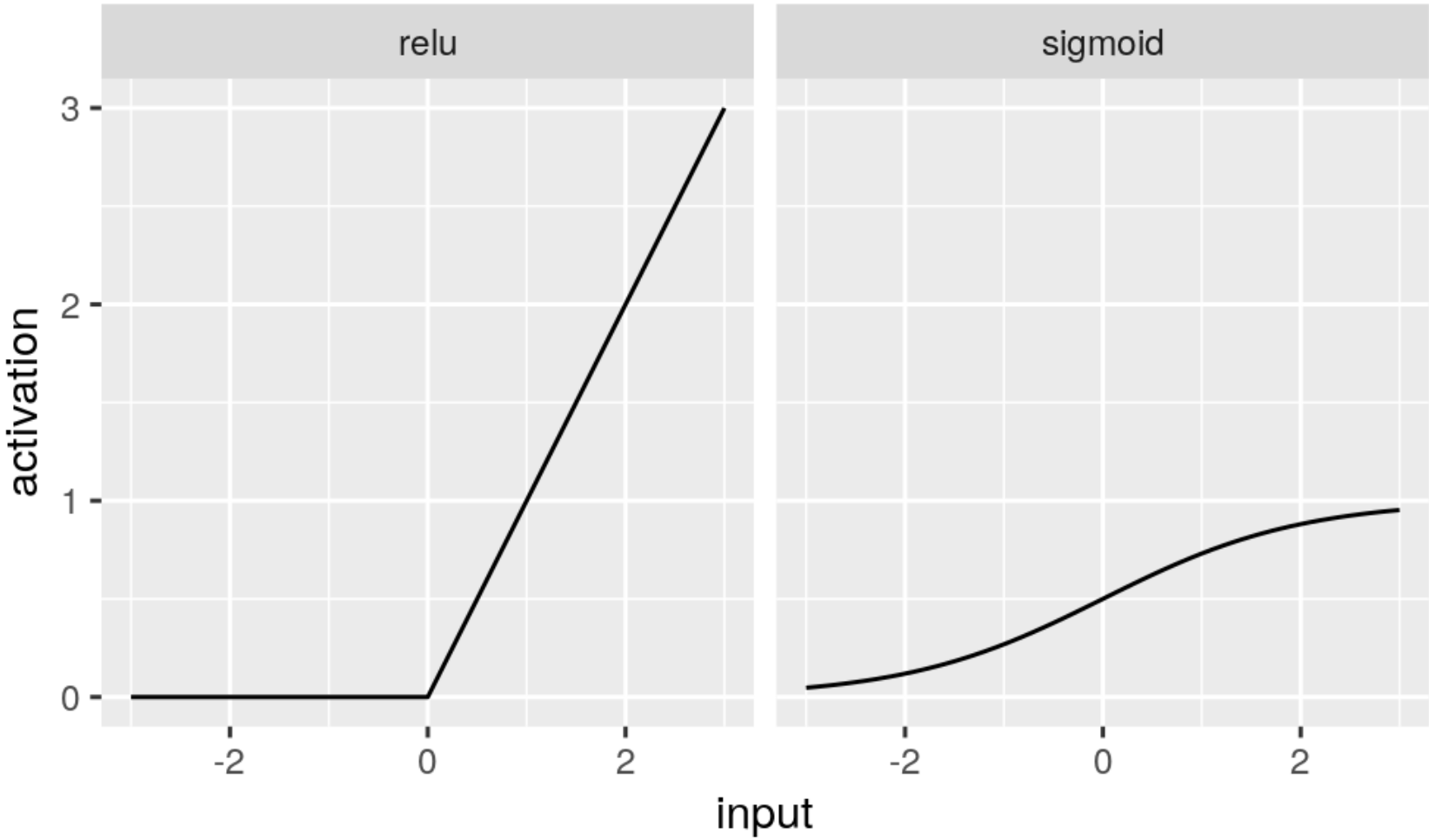


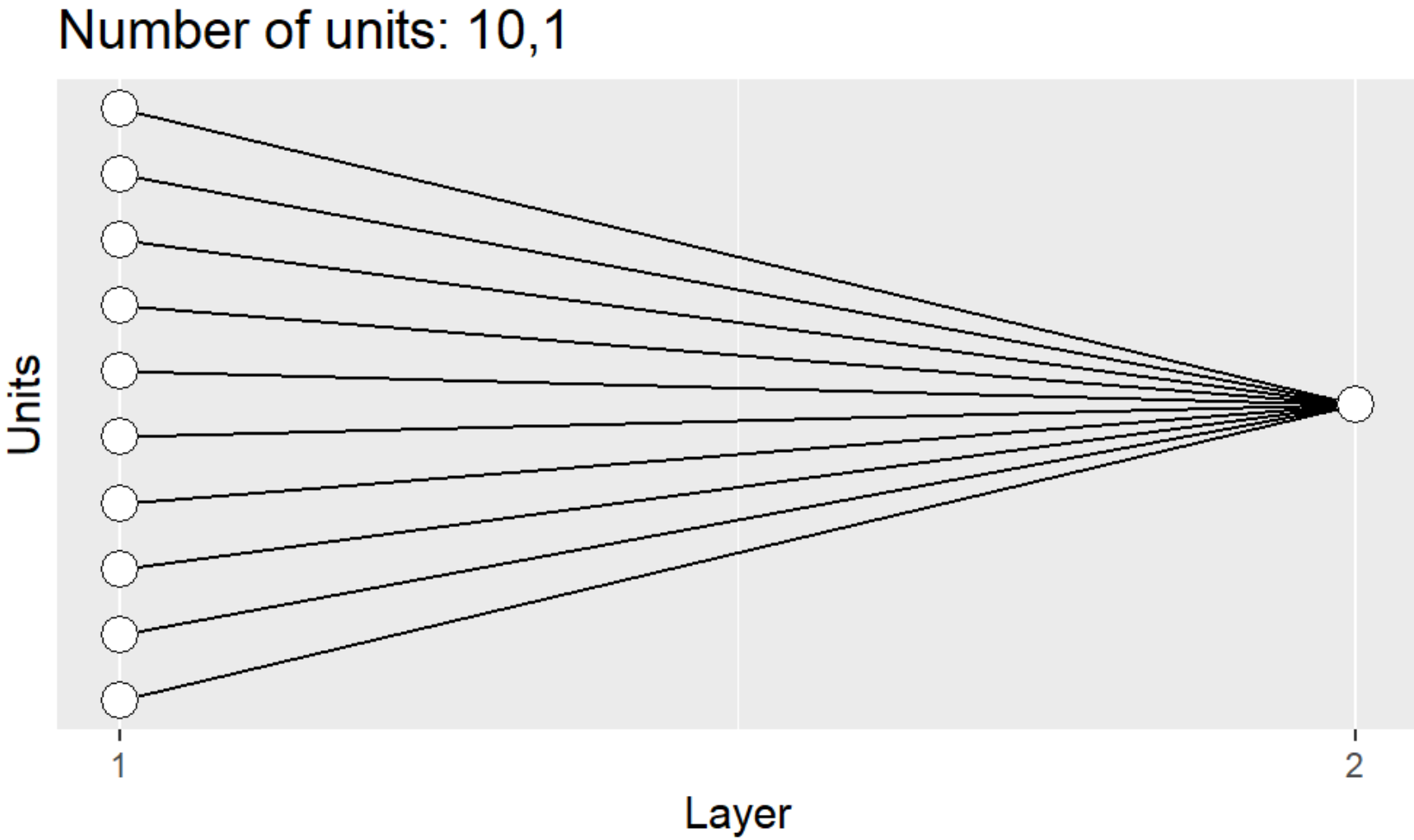
# Network size

For binary classification with inputs $x \in \mathbb{R}^d$, the overall neural network architecture is $(u^{(0)} = d, u^{(1)}, \ldots, u^{(L-1)}, u^{(L)} = 1)$, where $u^{(1)}, \ldots, u^{(L-1)} \in \mathbb{Z}_+$ are positive integers (hyper-parameters that control the number of units in each hidden layer, and the size of the parameter matrices $W^{(l)}$).

- "Units" is a synonym for "features" and "variables."
- First and last layer are "visible" others are "hidden."
- First layer size $u^{(0)}$ is fixed to input size.
- Last layer size $u^{(L)}$ is fixed to output size.
- Number of layers and hidden layer sizes $u^{(1)}, \ldots, u^{(L-1)}$ must be chosen (by you).
- No hidden layers/units means $L = 1$, linear model.
- "Deep" learning means $L \geq 3$ functions, at least 2 hidden layers.

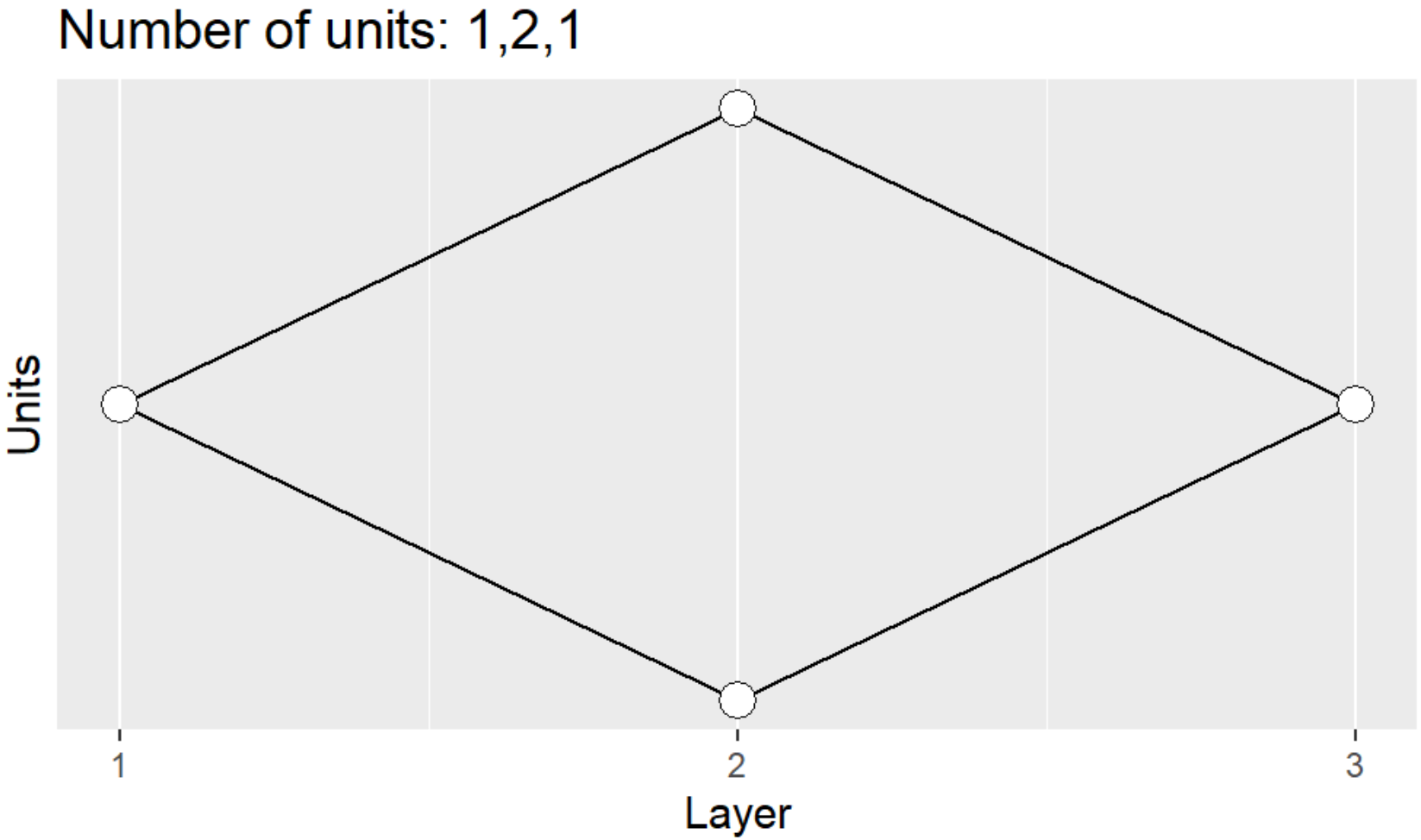
# Network diagram for linear model with 10 inputs/features

Neural network diagrams show how each unit (node) is computed by applying the weights (edges) to the values of the units at the previous layer.



# Network diagram for single hidden layer with 2 units

Neural network diagrams show how each unit (node) is computed by applying the weights (edges) to the values of the units at the previous layer.



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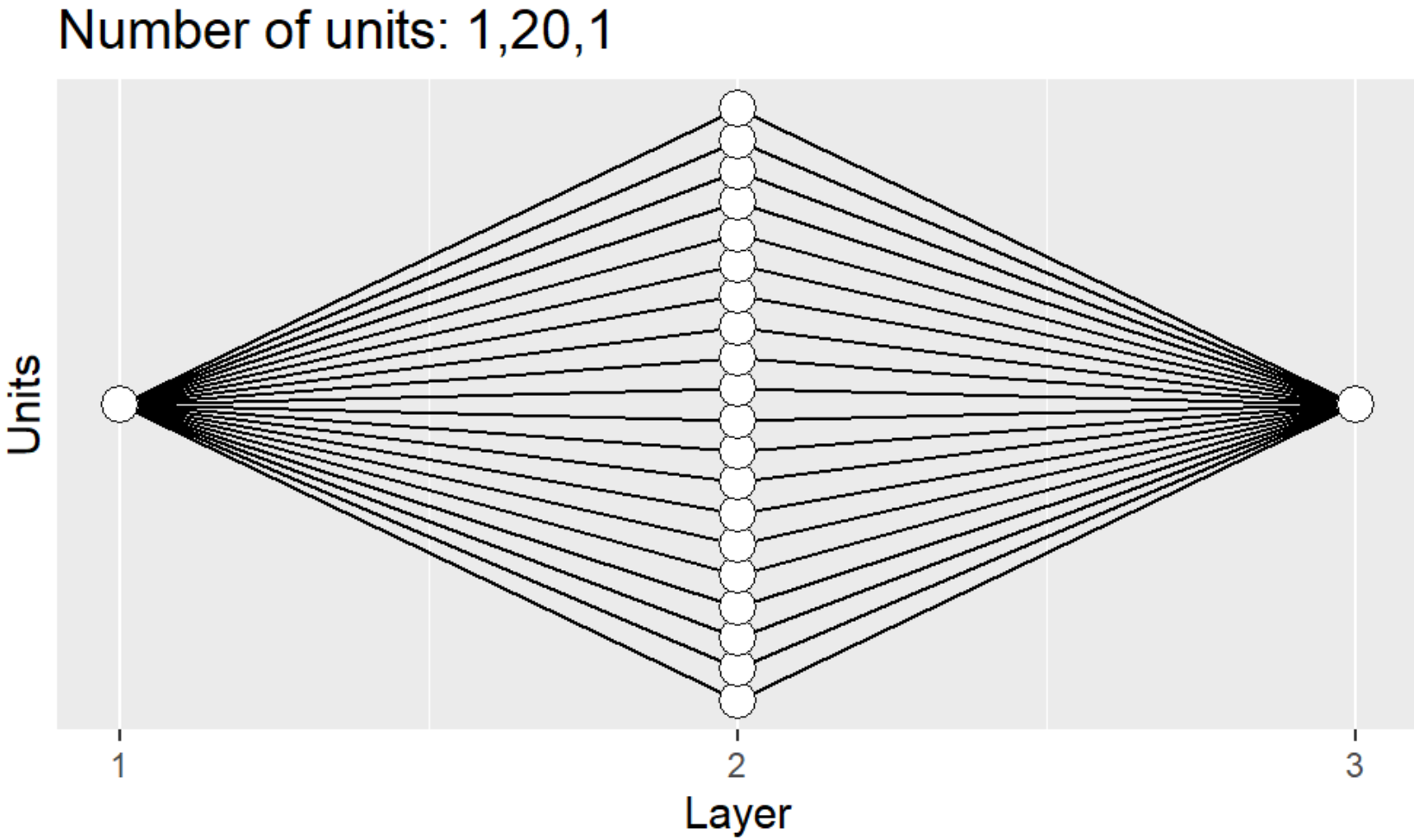

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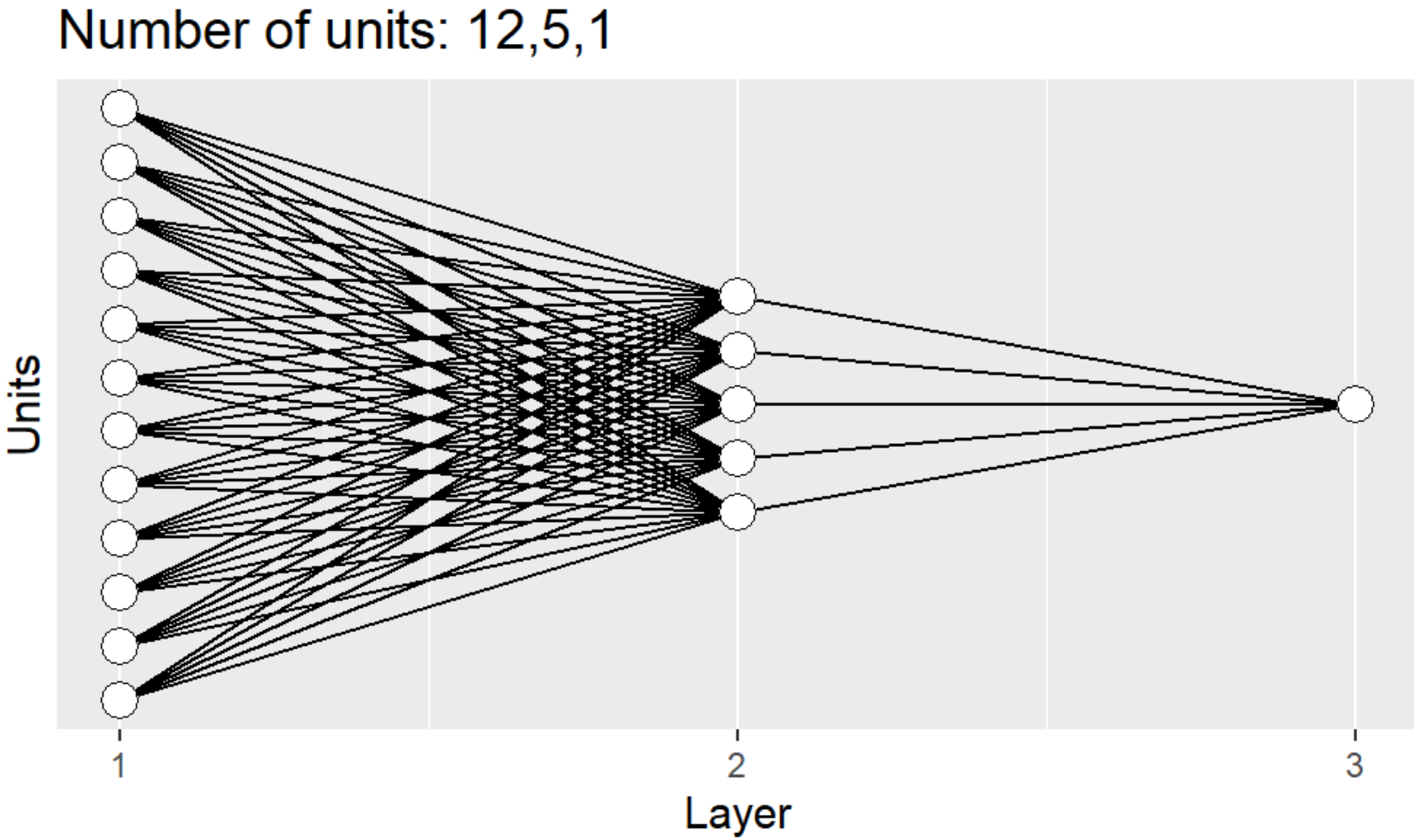

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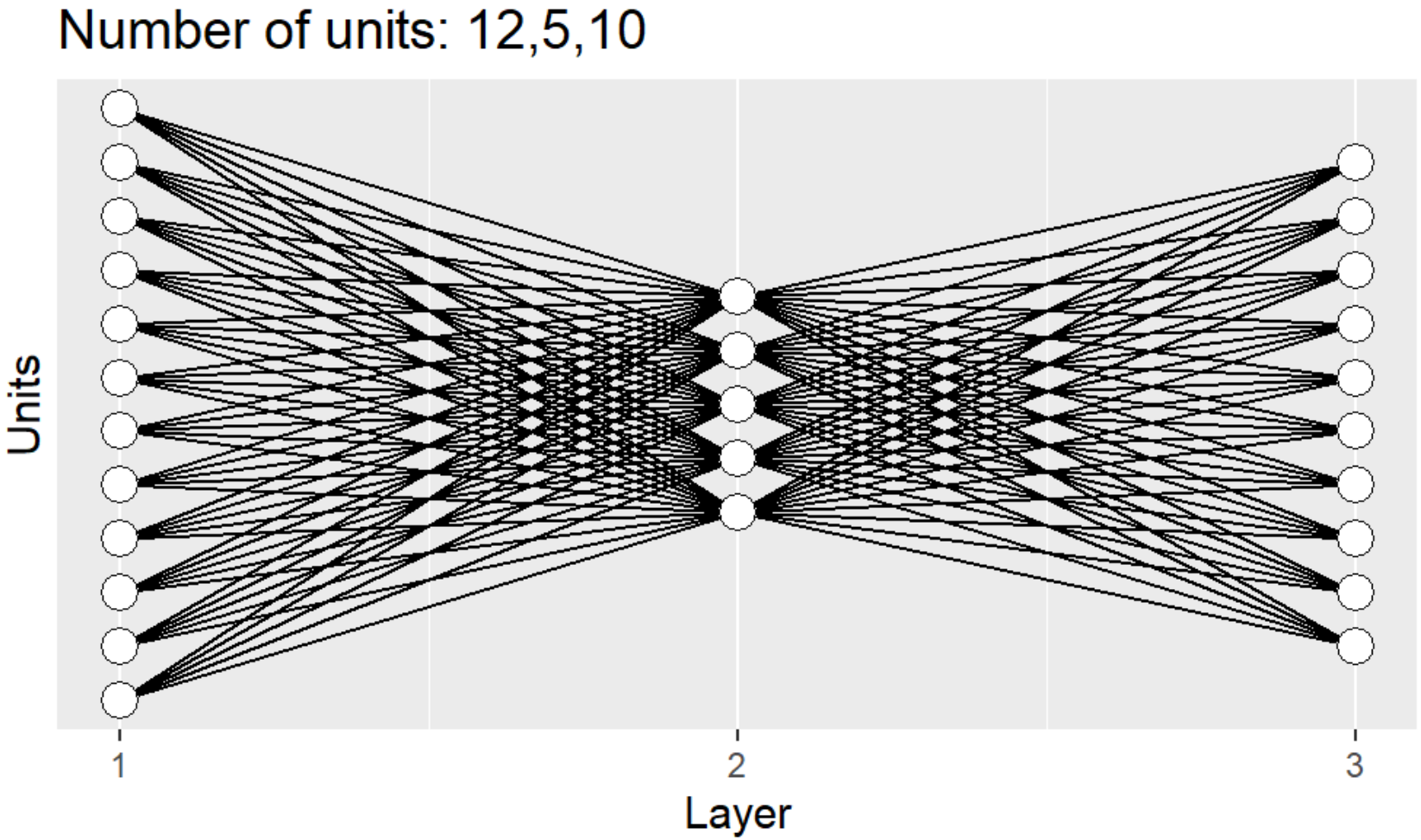

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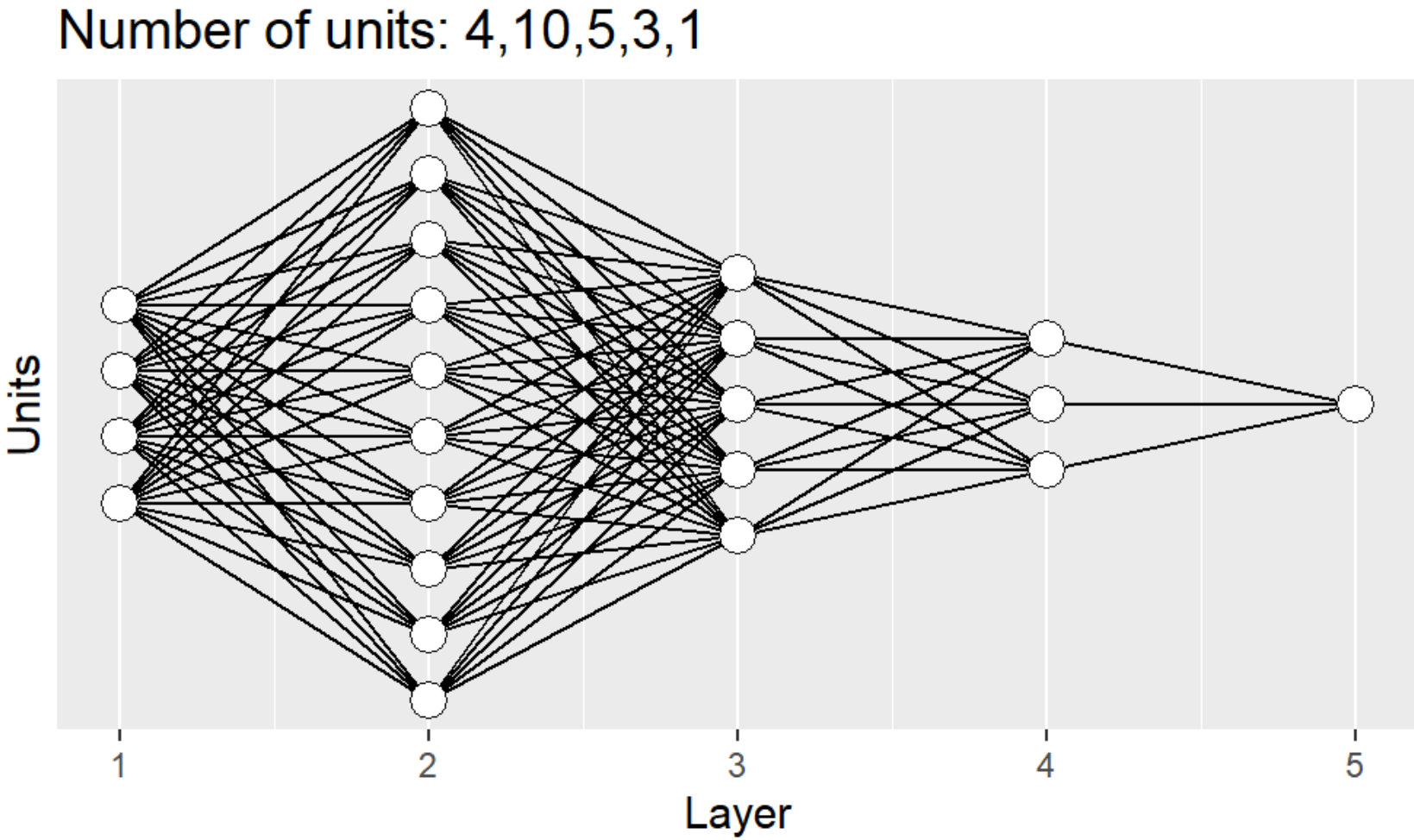

# Units in each layer

We can write the units at each layer as $h^{(0)}, h^{(1)}, \ldots, h^{(L-1)}, h^{(L)}$ where

- $h^{(0)} = x \in \mathbb{R}^d$ is an input feature vector,
- and $h^{(L)} \in \mathbb{R}$ is the predicted output.

For each layer $l \in \{1, \ldots, L\}$ we have:

$$h^{(l)} = f^{(l)}\left[h^{(l-1)}\right] = \sigma^{(l)}\left[W^{(l)} h^{(l-1)}\right].$$

Total number of parameters to learn is $\sum_{l=1}^{L} u^{(l)} u^{(l-1)}$.
Quiz: how many parameters in a neural network for $d = 10$ inputs/features with one hidden layer with $u = 100$ units? (one output unit, ten output units)

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# Gradient descent learning

Basic idea of gradient descent learning algorithm is to iteratively update weights $\mathbf{W} = [W^{(1)}, \ldots, W^{(L)}]$ to improve predictions on the subtrain set.

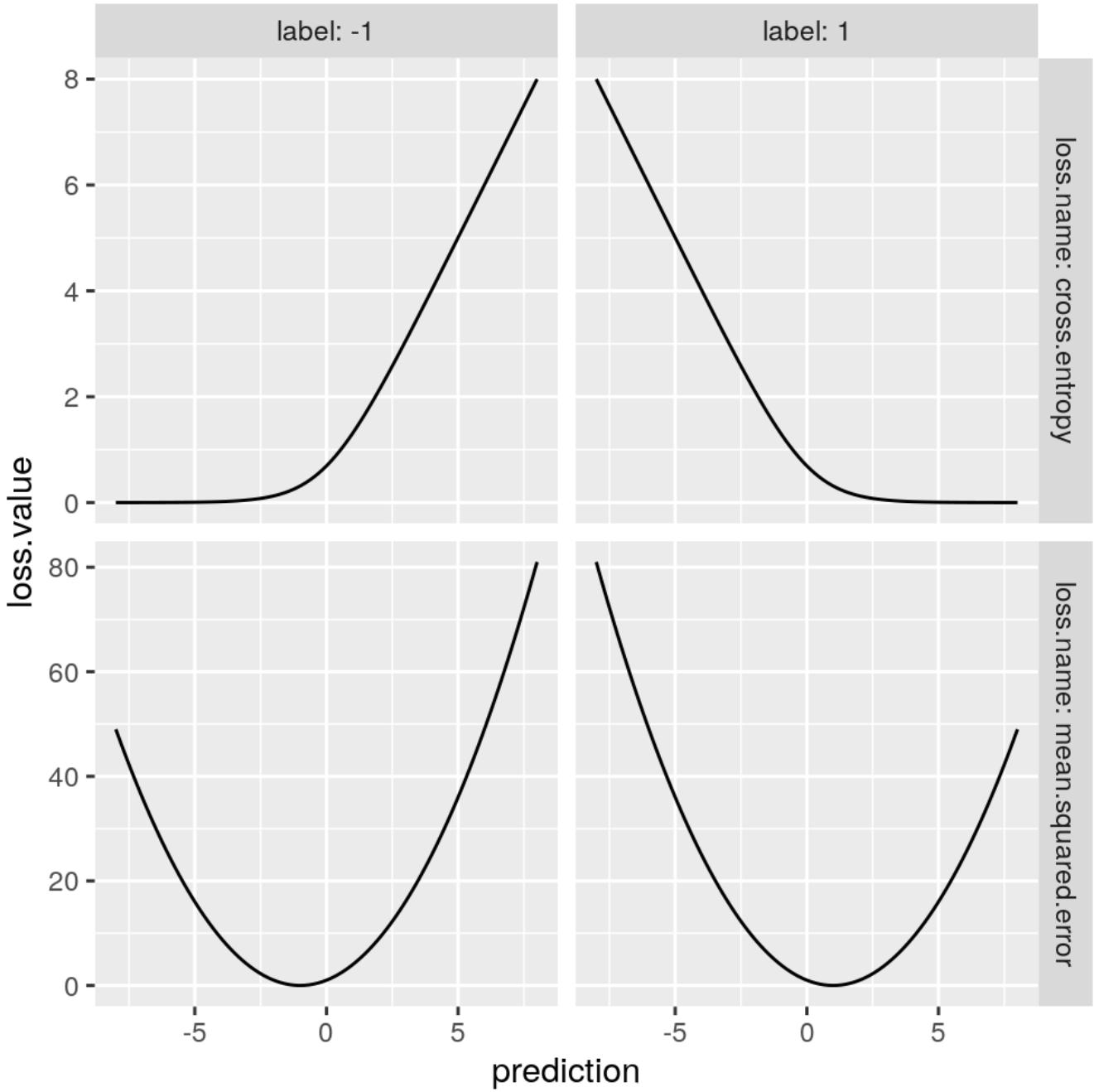
- Need to define a loss function $\mathcal{L}(\mathbf{W})$ which is differentiable, and takes small values for good predictions.
- Typically for regression we use the mean squared error, and for binary classification we use the mean logistic loss (sometimes called cross entropy).
- The mean loss $\mathcal{L}(\mathbf{W})$ is averaged over all $N$ observations or batches $i$:

$$\mathcal{L}(\mathbf{W}) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(\mathbf{W}, \mathbf{X}_i, \mathbf{y}_i)$$

- The mean full gradient $\nabla\mathcal{L}(\mathbf{W})$ is a function which tells us the local direction where the loss is most increasing:

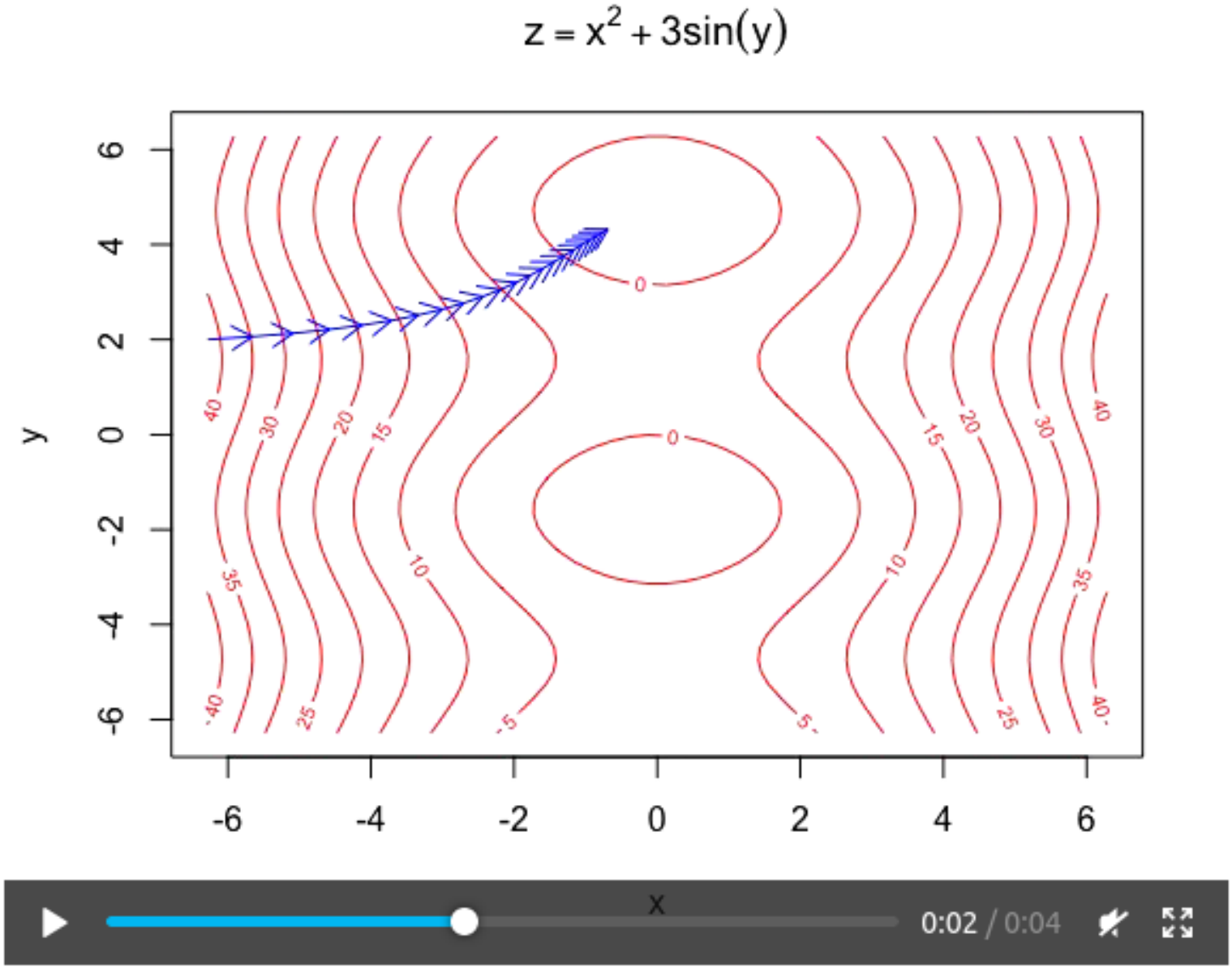
$$\nabla\mathcal{L}(\mathbf{W}) = \frac{1}{N} \sum_{i=1}^{N} \nabla\mathcal{L}(\mathbf{W}, \mathbf{X}_i, \mathbf{y}_i)$$

# Loss functions



# Gradient descent animations

https://yihui.org/animation/example/grad-desc/



# Basic full gradient descent algorithm

- Initialize weights $\mathbf{W}_0$ at some random values near zero (more complicated initializations possible).
- Since we want to decrease the loss, we take a step $\alpha > 0$ in the opposite direction of the mean full gradient,

$$\mathbf{W}_t = \mathbf{W}_{t-1} - \alpha \nabla \mathcal{L}(\mathbf{W}_{t-1})$$

- This is the **full** gradient method (same as we did for linear models): batch size $= n =$ subtrain set size, so 1 step per epoch/iteration.
- An **epoch** is the time/iterations to go through the subtrain set (computing gradient for each observation once).

# Stochastic gradient descent algorithm

- Initialize weights $\mathbf{W}$ at some random values near zero (more complicated initializations possible).
- for each epoch $t$ from 1 to max epochs:
- for each batch $i$ from 1 to $n$:
- Let $\mathcal{L}(\mathbf{W}, \mathbf{X}_i, \mathbf{y}_i)$ be the loss with respect to the single observation in batch $i$.

$$\mathbf{W} \leftarrow \mathbf{W} - \alpha \nabla \mathcal{L}(\mathbf{W}, \mathbf{X}_i, \mathbf{y}_i)$$

- This is the **stochastic** gradient method: batch size $= 1$, so there are $n$ steps per epoch.

# Batch (stochastic) gradient descent algorithm

- Input: batch size $b$.
- Initialize weights $\mathbf{W}$ at some random values near zero (more complicated initializations possible).
- for each epoch $t$ from 1 to max epochs:
- for each batch $i$ from 1 to $\lceil n/b \rceil$:
- Let $\mathcal{L}(\mathbf{W}, \mathbf{X}_i, \mathbf{y}_i)$ be the mean loss with respect to the $b$ observations in batch $i$.

$$\mathbf{W} \leftarrow \mathbf{W} - \alpha \nabla \mathcal{L}(\mathbf{W}, \mathbf{X}_i, \mathbf{y}_i)$$

- This is the **(mini)batch** stochastic gradient method: batch size $= b$, so there are $\lceil n/b \rceil$ steps per epoch.

# Forward propagation

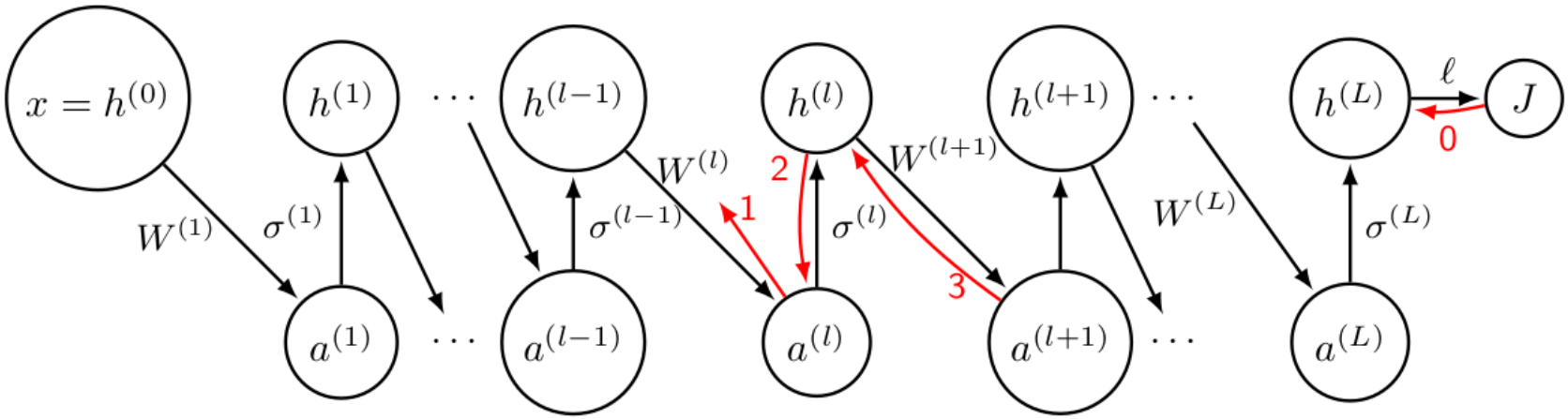
- Forward propagation is the computation of hidden units $h^{(1)}, \ldots, h^{(L)}$ given the inputs $x$ and current parameters $W^{(1)}, \ldots, W^{(L)}$.
- Start from input, apply weights and activation in each layer until predicted output is computed.
- In the code this should be a for loop from first to last layer.

# Back propagation

Back propagation is the computation of gradients given current parameters and hidden units.

- Start from loss function, compute gradient, send it to last layer, use chain rule, send gradient to previous layer, finally end up at first layer.
- Result is gradients with respect to all weights in all layers.
- Deep learning libraries like torch/keras do this using automatic differentiation based on your definition of the forward method and the loss function.
- We will code the gradient computation from scratch to see how it works.
- In the code this should be a for loop from last layer to first layer.

# Computation graph




For each layer $l \in \{1, \ldots, L\}$ we have:

$$\begin{aligned} a^{(l)} &= W^{(l)} h^{(l-1)}, \\ h^{(l)} &= \sigma^{(l)} \left[ a^{(l)} \right]. \end{aligned}$$

There are essentially four rules for computing gradients during backpropagation (0-3).

# Backprop rules

The rules 0–3 for backprop (from loss backwards):

Rule 0 computes $\nabla_{h^{(L)}} J$, which depends on the choice of the loss function $\ell$.

Rule 1 computes $\nabla_{W^{(l)}} J$ using $\nabla_{a^{(l)}} J$, for any $l \in \{1, \ldots, L\}$

$$\nabla_{W^{(l)}} J = \left(h^{(l-1)}\right)^T (\nabla_{a^{(l)}} J) \tag{1}$$

Rule 2 computes $\nabla_{a^{(l)}} J$ using $\nabla_{h^{(l)}} J$, for any $l \in \{1, \ldots, L\}$.

$$\nabla_{a^{(l)}} J = (\nabla_{h^{(l)}} J) \odot \left(\nabla_{a^{(l)}} h^{(l)}\right) \tag{2}$$

Rule 3 computes $\nabla_{h^{(l)}} J$ using $\nabla_{a^{(l+1)}} J$, for any $l \in \{1, \ldots, L-1\}$.

$$\nabla_{h^{(l)}} J = (\nabla_{a^{(l+1)}} J) \left(W^{(l+1)}\right)^T \tag{3}$$

# Implementation details

- Previous slides explained computations for a single observation, here we explain for a batch.
- Each $h^{(l)}, a^{(l)}$ and their gradients can be stored as a matrix (nrow=batch size, ncol=$u^{(l)}$=number units in this layer).
- Each $W^{(l)}$ and its gradient is a $u^{(l-1)} \times u^{(l)}$ matrix.
- You may want to code assertions to make sure each matrix is the correct shape.
- Matrix multiply features by weights to get next layer, $a^{(l)} = h^{(l-1)} W^{(l)}$.
- Use np.where to implement relu activation (output is non-negative).
- Make sure last activation is identity — final predicted values should be real numbers (both positive and negative).

# Computation exercises (gradient descent learning)

Now assume we have used backpropagation to compute gradients with respect to four observations $i$:

$$\nabla_{\mathbf{v}} \mathcal{L}(\mathbf{v}, \mathbf{X}_i, \mathbf{y}_i) = \begin{cases} [-1, 1] & i = 1 \\ [-2, 2] & i = 2 \\ [-3, 2] & i = 3 \\ [-1, 2] & i = 4 \end{cases}$$

Starting at current weights $\mathbf{v} = [-2, 1]$ and using gradient descent with step size $\alpha = 0.5$, ($\mathcal{L}$ is total loss, show your work!)

1. For the full gradient method, there is one step. What is the new weight vector $\mathbf{v}$ after that step?
2. For a batch size of 2, there are two steps. Assume batch 1 is observations $i = 1, 2$ and batch 2 is observations $i = 3, 4$. What is the new weight vector $\mathbf{v}$ after the batch 1 step? After the batch 2 step?
3. For the stochastic gradient method, there are four steps $i = 1, 2, 3, 4$. What is $\mathbf{v}$ after each of those steps?

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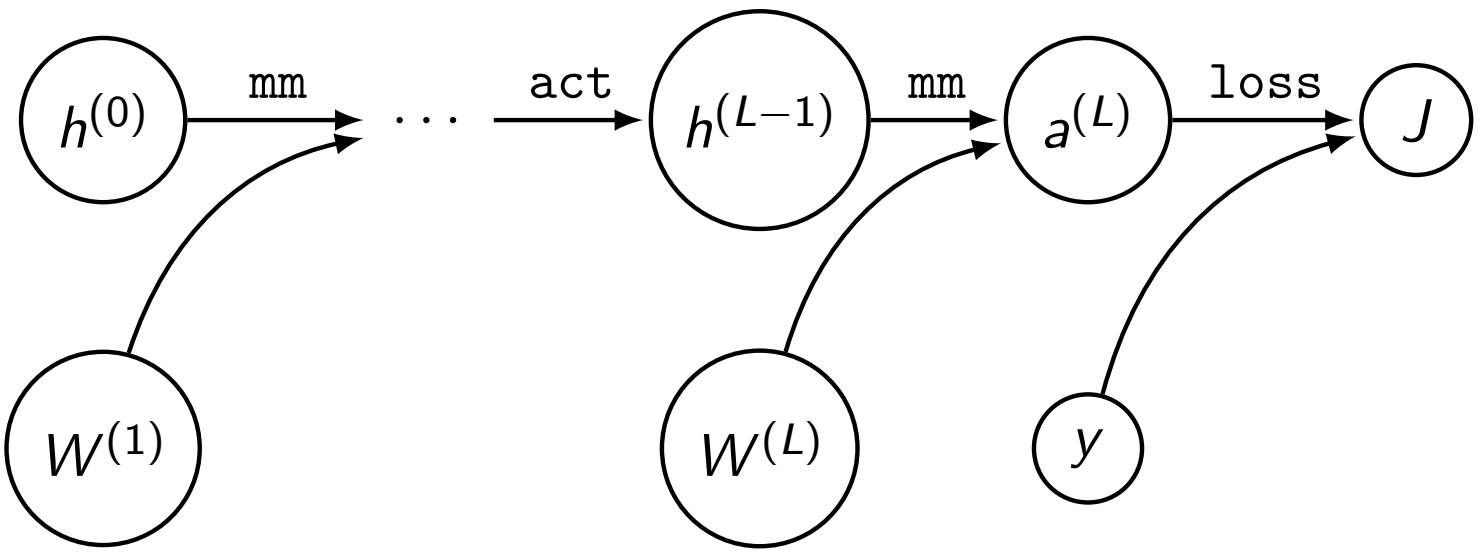
# Why automatic differentiation?

- Also called "auto-grad," short for automatic gradient.
- People who design new neural network architectures and loss functions (fit method of learner class) do not necessarily have the expertise to compute the gradients.
- Automatic differentiation allows "separation of concerns."
- People who know how to compute gradients can implement classes which encapsulate forward/backward computations for individual operations (matrix multiplication, log, exp, etc).
- Other people can use these classes to implement their neural network, without having to know about the details of the forward/backward computations (and no worries about coding buggy/incorrect gradients).

# Computation graph for multi-layer perceptron

- Each node in the computation graph is a tensor (0d=scalar, 1d=vector, 2d=matrix, etc).
- Each edge in the computation graph is an operation (with methods for forward/back-prop).
- Only three operations needed: matrix multiply (`mm`), non-linear activation (`act`), and computing `loss` given labels $y$ and predicted scores $a^{(L)}$.

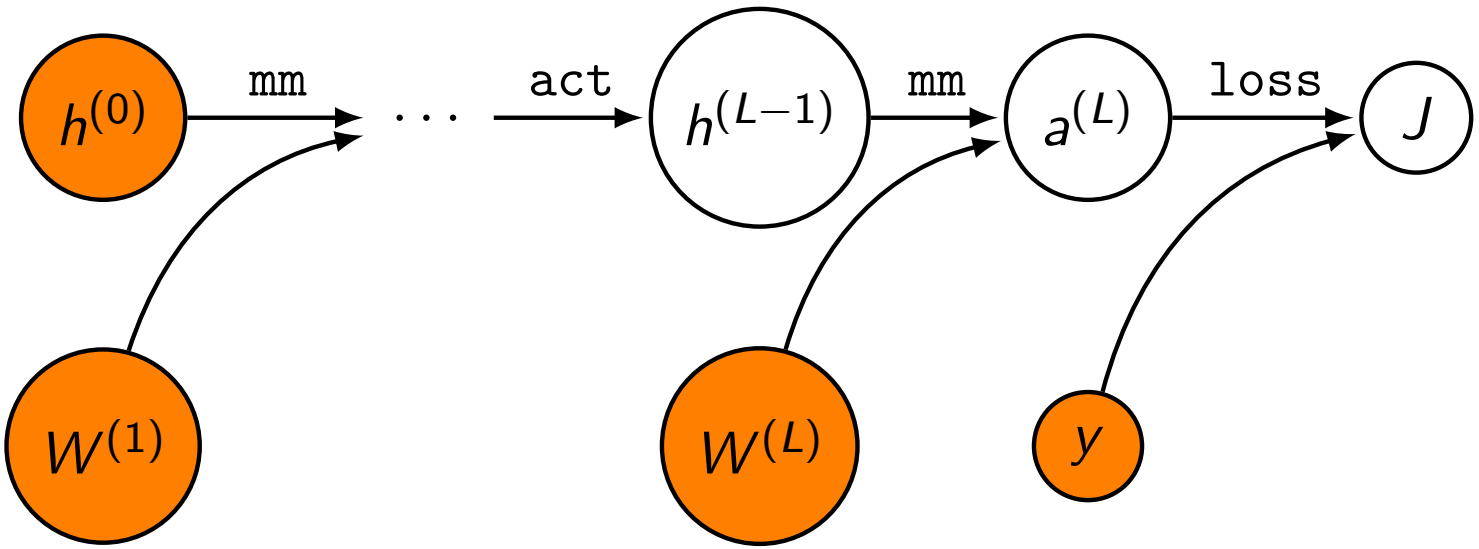


# Nodes in the computation graph

- Each node in the computation graph can be represented by an instance of a python class.
- `value` attribute is a numpy array, result of forward propagation, computed during instantiation.
- `grad` attribute is a numpy array of same size, gradient of loss with respect to this node, result of back-propagation.
- Main idea is to link these instances together to form a computation graph and `value` (forward pass), then recursively compute `grad` (backward pass).

# Initial nodes in the computation graph

- Initial node in the computation graph can be represented by an instance of `InitialNode` class.
- `value` attribute is a numpy array, stored on instantiation.
- Main uses are wrapping training data and neural network weights: `InitialNode(weight_mat)`, `InitialNode(feature_mat)`, `InitialNode(label_vec)`.



# Derived nodes in the computation graph

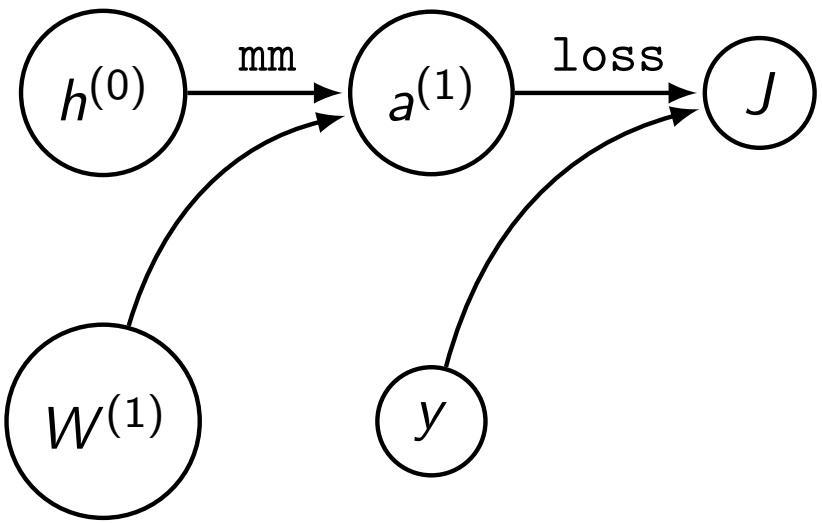
- `Operation` class represents a node in the computation graph which is computed using other nodes.
- On instantiation, stores input nodes and does forward propagation.
- Method backward() computes gradient and recursively calls backward() on input nodes.
- `Operation` is virtual so we only instantiate sub-classes: `mm(features, weights)`, `relu(a_mat)`, `logistic_loss(a_mat, label_vec)`.
- Sub-classes should define `forward` and `gradient` methods which implement details of forward/back-prop, results are stored as `value`/`grad` attributes.
- Don't get confused! Parent class (sub-classes of `Operation` inherit methods/attributes) not the same as parent node (child node is an instance of an `Operation` sub-class, and has parent nodes as attributes).

# Functions and gradients

- $J = \text{logistic\_loss}(A, y) \in \mathbb{R}^{b \times 1}$ is same as in linear models. Values are $J_i = \log[1 + \exp(-y_i A_i)]$ and gradient is $(\nabla_A J)_i = -y_i/(1 + \exp(y_i A_i))$.
- $A = \texttt{mm}(X, W) = XW \in \mathbb{R}^{b \times u}$ where $X$ is a $b \times p$ matrix ($b$ =number of samples in batch, $p$ =number of units/features in this layer), and $W$ is a $p \times u$ matrix ($u$ =number of units/features in next layer). Gradient of linear function is constant: $\nabla_X J = (\nabla_A J)(W^T)$, $\nabla_W J = X^T(\nabla_A J)$.
- $H = \texttt{relu}(A) \in \mathbb{R}^{b \times u}$ where each element $H_i = A_i$ if $A_i > 0$ else 0. Gradient $\nabla_A J = \nabla_A H \nabla_H J$ is piecewise constant, $(\nabla_A J)_i = (\nabla_H J)_i$ if $A_i > 0$ else 0.

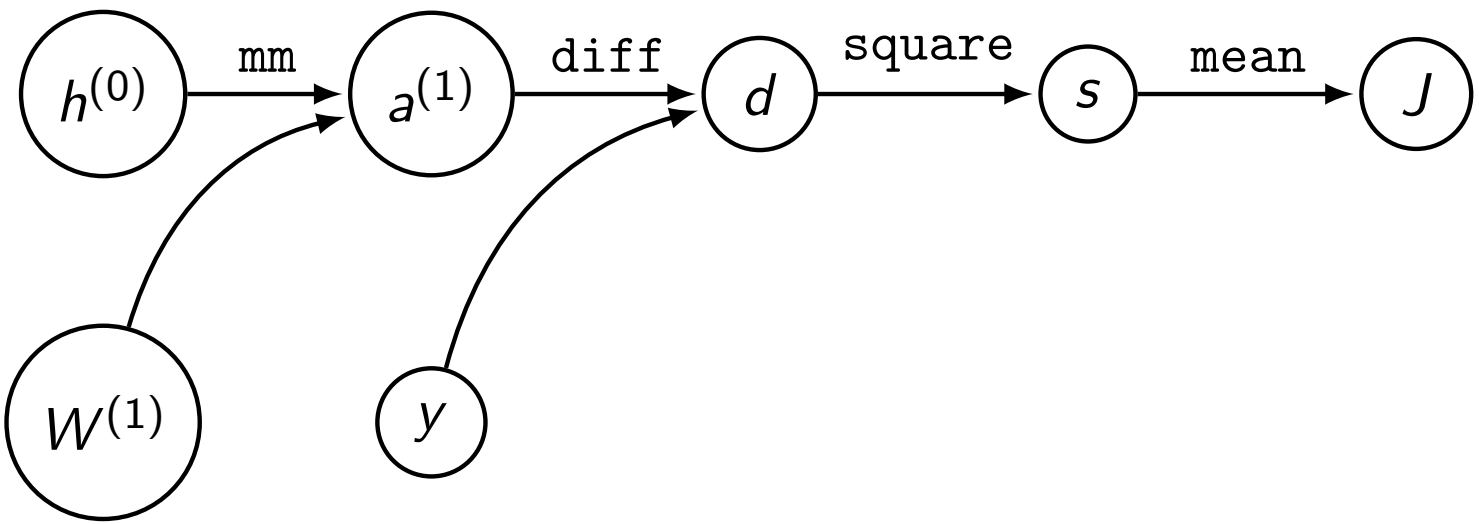
# Simple computation graph for linear model

- Only two operations needed: matrix multiply (`mm`) and computing loss given predicted scores (`loss`).
- To implement the `loss` operation/class, you need to know how to compute the gradient of the loss (maybe difficult for complex loss functions).



# Detailed computation graph for linear model

- Example: square loss $\ell(a^{(1)}, y) = (a^{(1)} - y)^2 = d^2$,
- Mean squared error: $J = \sum_{i=1}^{n} \ell(a_i^{(1)}, y_i)/n = \sum_{i=1}^{n} s_i/n$.
- More operations needed: matrix multiply (`mm`), subtraction (`diff`), `square`, `mean`.
- Each operation has a simple gradient (demo).



# Possible exam questions

- Given a computation graph, and values for initial nodes, compute `value` in each derived node by hand (forward propagation), then compute `grad` (back-prop).
- In linear models we used scaling inside of the fit method — make sure each feature/column has mean=0 and sd=1 before running gradient descent. What would you have to change in your neural network class to use scaling?
- In linear models we used gradient descent to learn an intercept parameter (a constant added to each real-valued prediction). We discussed two methods: (1) adding a column of ones to the feature matrix and an entry to the weight vector, or (2) adding a separate node representing the intercept in the computation graph. How would you modify your neural network class, using each method? (each hidden/output unit/feature in the neural network should have its own intercept parameter)

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# torch

- Machine learning library/module for python (and R, C++).
- Lots of standard neural network architectures and loss functions supported out of the box.
- Supports automatic differentiation! (easy to experiment with new models and loss functions without having to worry about gradient computations)

# torch code for linear model for binary classification

```
import torch
class LinearModel(torch.nn.Module):
    def __init__(self):
        super(LinearModel, self).__init__()
        self.weight_vec = torch.nn.Linear(n_features, 1)
    def forward(self, features):
        return self.weight_vec(features)
```

- Linear is a matrix multiplication, with optional intercept (present by default, bias=False to suppress).
- One output because we are doing binary classification (want to predict a single real-valued score).
- Linear and other objects with weight parameters to learn must be assigned to an attribute of self (so torch.optim algorithms can find weights to update).

# torch code for neural network with one hidden layer

```
class OneHiddenLayer(torch.nn.Module):
    def __init__(self, n_features, n_hidden):
        super(OneHiddenLayer, self).__init__()
        self.hidden_weights = torch.nn.Linear(
          n_features, n_hidden)
        self.activation = torch.nn.ReLU()
        self.out_weights = torch.nn.Linear(n_hidden, 1)
    def forward(self, feature_mat):
        a_mat = self.hidden_weights(feature_mat)
        h_mat = self.activation(a_mat)
        return self.out_weights(h_mat)
```

Use activation after each Linear layer except for last.

# torch code for stack of hidden layers

```
class Net(torch.nn.Module):
    def __init__(self, n_features, n_hidden):
        super(Net, self).__init__()
        self.stack = torch.nn.Sequential(
          torch.nn.Linear(n_features, n_hidden),
          torch.nn.ReLU(),
          torch.nn.Linear(n_hidden, 1))
    def forward(self, feature_mat):
        return self.stack(feature_mat)
```

# Differences between gradient descent algorithm variants

```
net = Net()
loss_fun = torch.nn.BCEWithLogitsLoss()
optimizer = torch.optim.SGD(net.parameters(), lr=0.03)

# to do in a loop:
optimizer.zero_grad()
loss_value = loss_fun(net(inputs), outputs) # last node
loss_value.backward() # auto grad
optimizer.step() # learning

# stochastic, batch, full gradient descent variants:
loss_one = loss_fun(
  net(one_input), one_output)
loss_batch = loss_fun(
  net(batch_inputs), batch_outputs)
loss_subtrain = loss_fun(
  net(subtrain_inputs), subtrain_outputs)
```

# Copy data from numpy and onto GPU

- Torch is very similar to numpy (tensor data types, vectorized functions and methods).
- Can easily run on GPU for speedups, but need to copy neural network weights and data to GPU memory.

```
device = "cuda" if torch.cuda.is_available() else "cpu"
# features and labels to torch and GPU
cpu_features = torch.from_numpy(numpy_features).float()
dev_features = cpu_features.to(device)
cpu_labels = torch.from_numpy(numpy_labels).float()
dev_labels = cpu_labels.to(device)
# weights to GPU
cpu_net = Net()
dev_net = cpu_net.to(device)
```

# torch Dataset/DataLoader helpers for batching

```
class CSV(torch.utils.data.Dataset):
    def __init__(self, features, labels):
        self.features = features
        self.labels = labels
    def __getitem__(self, item):
        return self.features[item,:], self.labels[item]
    def __len__(self):
        return len(self.labels)
ds = CSV(feature_mat, set_labels["subtrain"])
dl = torch.utils.data.DataLoader(
  ds, batch_size=1000, shuffle=True)
for batch_features, batch_labels in dl:
    # gradient descent code here.
```

Not necessary (you can do your own batching), but can be useful.