Neural network architecture and learning

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Fully connected multi-layer Neural Networks

Computing gradients and learning weights

Automatic differentiation

Multi-class classification

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 $l \in \{1, \dots, L\}$ 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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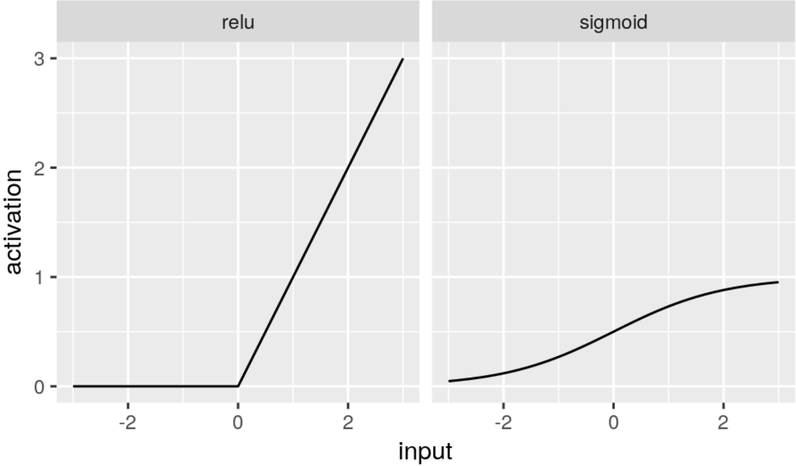
$$\sigma(z) = 1/(1 + \exp(-z))$$



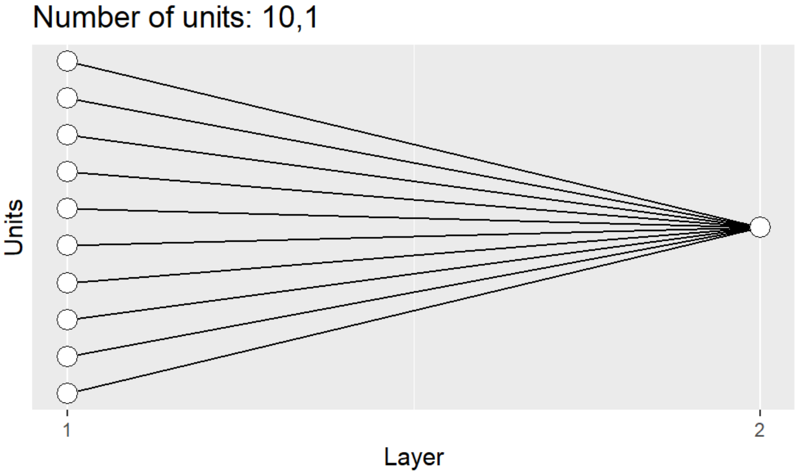
Network size

For binary classification with inputs $x \in \mathbb{R}^d$, the overall neural network architecture is $(u^{(0)} = d, u^{(1)}, \dots, u^{(L-1)}, u^{(L)} = 1)$, where $u^{(1)}, \dots, u^{(L-1)} \in \mathbb{Z}_+$ 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 $u^{(1)}, \dots, u^{(L-1)}$ 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.

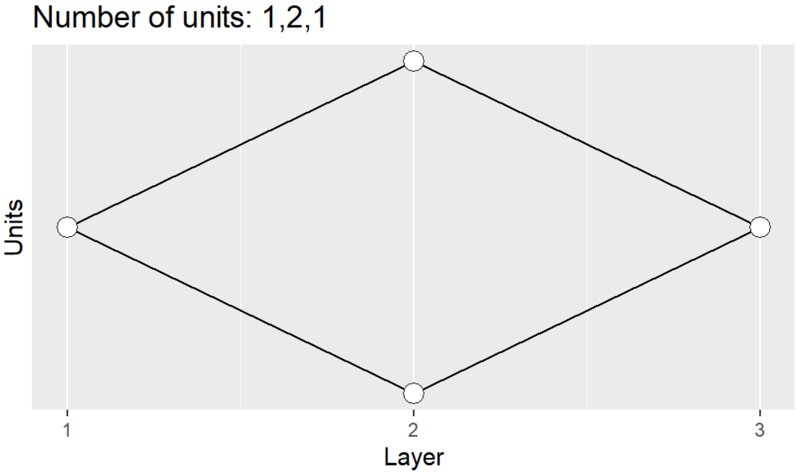
Network diagram for linear model with 10 inputs/features

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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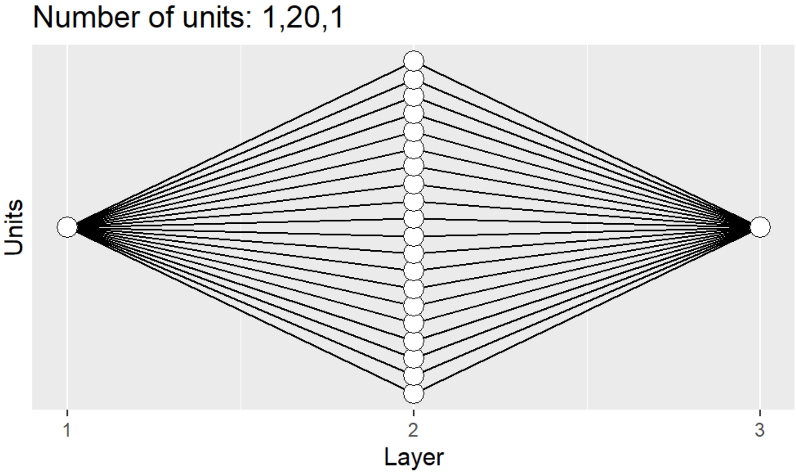

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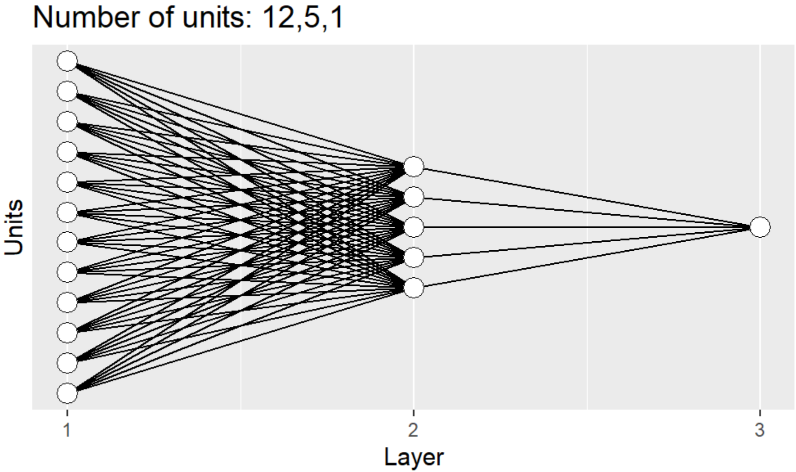

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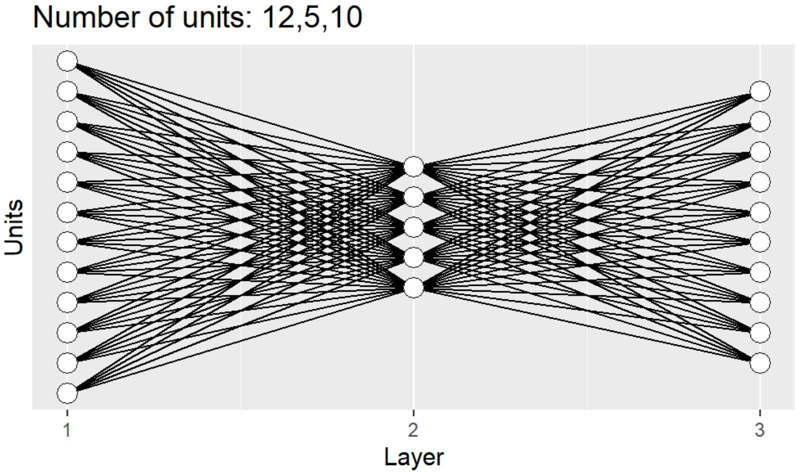

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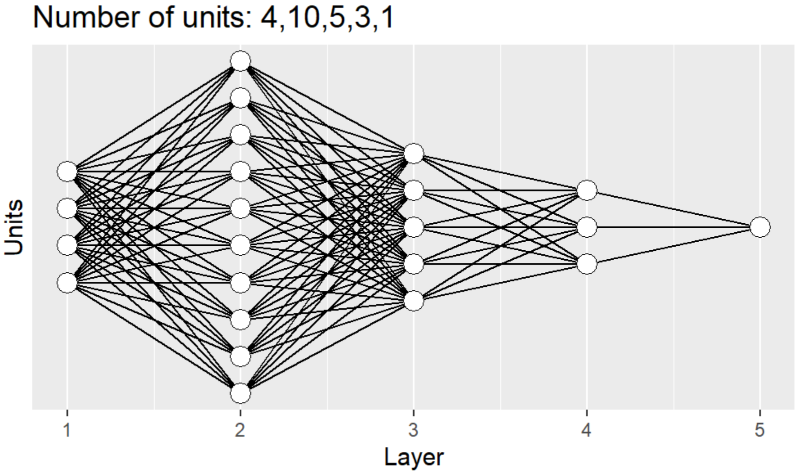

Units in each layer

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 $\mathbf{W} = [W^{(1)}, \dots, W^{(L)}]$ to improve predictions on the subtrain set.

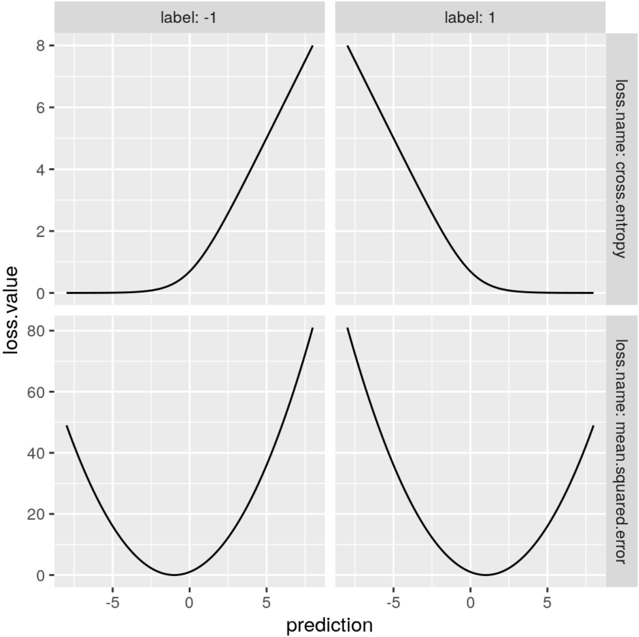
- Need to define a loss function $\mathcal{L}(\mathbf{W})$ which is differentiable, and takes small values for good predictions.
- Typically for regression we use the mean squared error, and for binary classification we use the mean logistic loss (sometimes called cross entropy).
- The mean loss $\mathcal{L}(\mathbf{W})$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

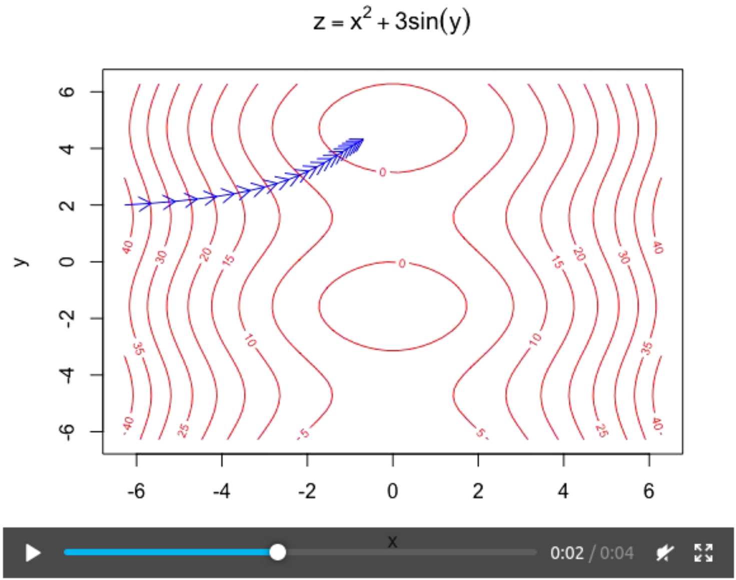
$$\nabla \mathcal{L}(\mathbf{W}) = \frac{1}{N} \sum_{i=1}^{N} \nabla \mathcal{L}(\mathbf{W}, \mathbf{x}_i, \mathbf{y}_i)$$

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

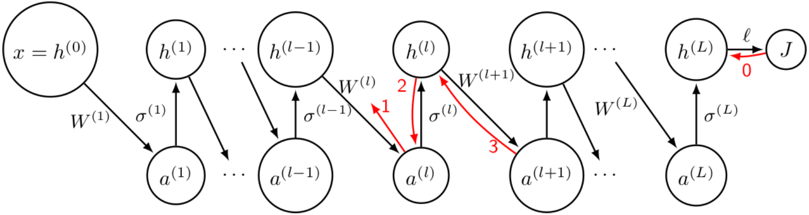
- Forward propagation is the computation of hidden units $h^{(1)}, \ldots, h^{(L)}$ given the inputs x and current parameters $W^{(1)}, \ldots, W^{(L)}$.
- Start from input, apply weights and activation in each layer until predicted output is computed.
- In the code this should be a for loop from first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

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

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

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

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

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

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

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?

Fully connected multi-layer Neural Networks

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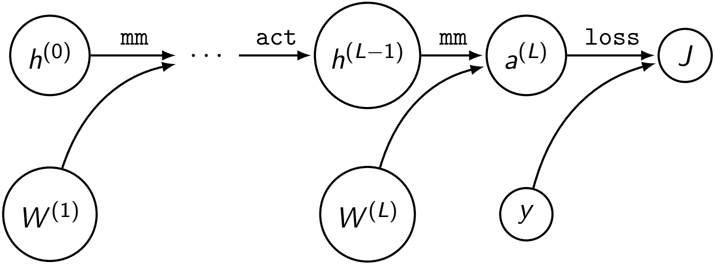
Why automatic differentiation?

- 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 $a^{(L)}$.

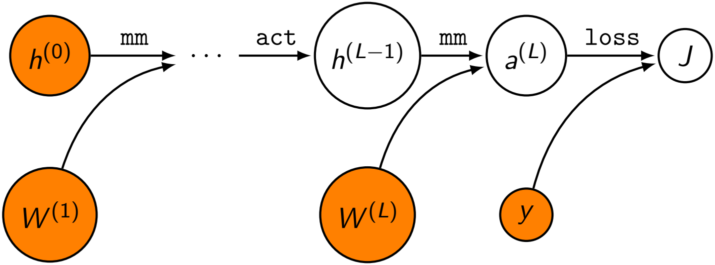


Nodes in the computation graph

- 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

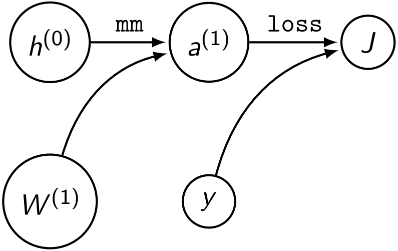
- `Operation` class represents a node in the computation graph which is computed using other nodes.
- On instantiation, stores input nodes and does forward propagation.
- Method backward() computes gradient and recursively calls backward() on input nodes.
- `Operation` is virtual so we only instantiate 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.

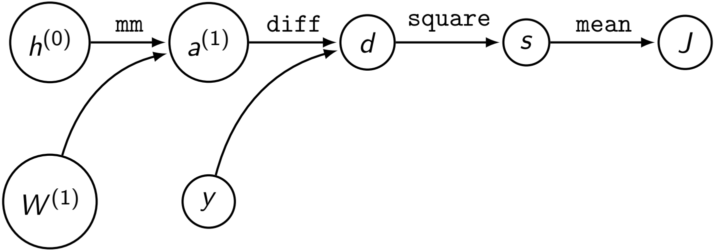
Simple computation graph for linear model

- 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 for regression

- 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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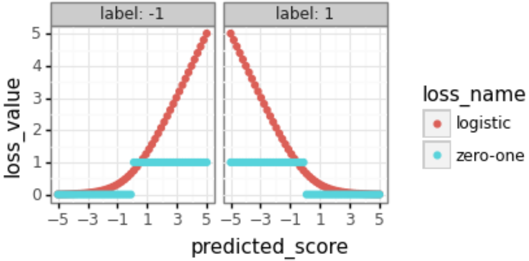
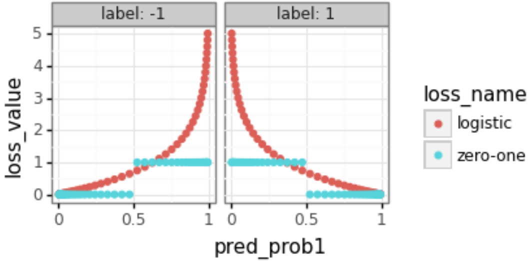
Review of logistic loss for binary classification



- For binary classification we have labels $\underline{y} \in \{-1, 1\}$ (underline for label coded as -1 or 1).
- Let $f(x) = \hat{y} \in \mathbb{R}$ be the predicted score (output of neural network).
- The logistic loss is $\ell(\hat{y}, \underline{y}) = \log[1 + \exp(\hat{y}\underline{y})]$.
- Minimizing the logistic loss is equivalent to maximizing the binomial likelihood (sometimes called Bernoulli, special case when there is 1 trial), ex: flipping coins or rolling dice.
- The binomial distribution (two classes) is a special case of the multinomial distribution (two or more classes).

Probabilistic interpretation of logistic loss



- Let $y \in \{0, 1\}$ be the binary class label (non-negative integer).
- Let $\hat{p}_1 = 1/(1 + \exp(-\hat{y})) \in (0, 1)$ be the predicted probability of class 1 (positive), output by the neural network.
- Then $\hat{p}_0 = 1 - \hat{p}_1$ is the predicted probability of negative class.
- Then the logistic loss is the negative log probability/likelihood of the label class,

$$
\begin{aligned}
\ell(\hat{y}, y) &= \begin{cases} -\log[\hat{p}_1] & \text{if label is positive, } y = 1 \\ -\log[\hat{p}_0] & \text{if label is negative, } y = 0 \end{cases} \\
&= -\log[\hat{p}_y].
\end{aligned}
$$

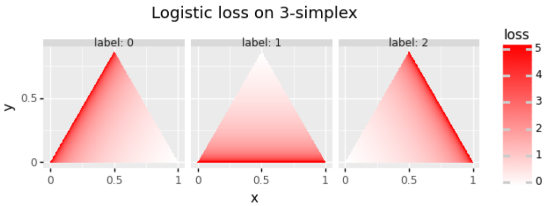
Multi-class loss and softmax function

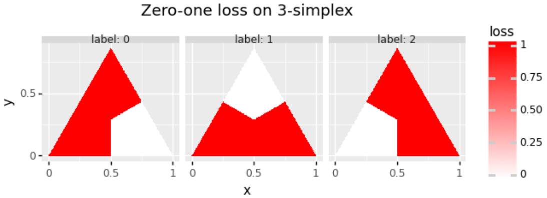
- We assume there are $K \geq 2$ classes of labels, $y \in \{0, 1, \ldots, K-1\}$.
- The neural network can output a probability for each class, $\hat{p} = [\hat{p}_0, \hat{p}_1, \ldots, \hat{p}_{K-1}]$, with $\hat{p}_j \in [0, 1]$ and $\sum_j \hat{p}_j = 1$.
- The loss function to minimize via gradient descent is the negative log likelihood of the label class, $\ell[\hat{p}, y] = -\log \hat{p}_y$.
- The neural network last linear layer outputs K units/features (real numbers from matrix multiplication, possibly negative), one for each class: $\hat{y}_0, \hat{y}_1, \ldots, \hat{y}_{K-1} \in \mathbb{R}$.
- To convert to a vector of probability values, we use the softmax function,

$$\hat{p} = \text{softmax}(\hat{y}_0, \ldots, \hat{y}_{K-1}) = \left[\frac{\exp \hat{y}_0}{\sum_{j=0}^{K-1} \exp \hat{y}_j}, \ldots, \frac{\exp \hat{y}_{K-1}}{\sum_{j=0}^{K-1} \exp \hat{y}_j} \right].$$

- (exp converts to positive, division normalizes to one)

Visualization of loss functions for 3 class problem





- Each point in 3-simplex is a probability triple (p_0, p_1, p_2).
- Corners: max prob. for one class (1,0,0) or (0,1,0) or (0,0,1).
- Midpoint when classes have equal probability $(1/3, 1/3, 1/3)$.
- Zero-one loss $=0$ when label class most probable.

Note about over-parameterization

- A neural network for K classes which outputs K features is actually over-parameterized (but easy to code).
- For K classes, we only need $K - 1$ outputs (fewer parameters in last weight matrix, more computationally efficient).
- For example, binary classification, $K = 2$, we only need 1 output (higher values mean more likely positive class).
- For example, $K = 3$ classes, $f(x) = [\hat{p}_1, \hat{p}_2]$ only needs parameters for two outputs, and the third class probability can be derived from the other two, $\hat{p}_0 = 1 - \hat{p}_1 - \hat{p}_2$.

Predicted probability and loss

- Let $z \in \mathbb{R}^K$ be a vector of real-valued predictions (inputs to softmax), same as neural network outputs if over-parameterized with K outputs $\hat{y}_0, \hat{y}_1, \ldots, \hat{y}_{K-1}$.
- Otherwise if neural network only has $K - 1$ outputs $\hat{y}_1, \ldots, \hat{y}_{K-1}$ then $z = [0, \hat{y}_1, \ldots, \hat{y}_{K-1}]$.
- Then the predicted probability vector is $\hat{p} = \text{softmax}(z_0, \ldots, z_{K-1})$.
- The loss function is the negative log probability of the label class,

$$-\log \hat{p}_y = -\log \left[\frac{\exp(z_y)}{\sum_{j=0}^{K-1} \exp(z_j)} \right] = \log \left[\sum_{j=0}^{K-1} \exp(z_j) \right] - z_y.$$

Binary classification is a special case 1

- For label y and real-valued predictions $z_0, \dots, z_{K-1}$, loss is $\log \left[\sum_{j=0}^{K-1} \exp(z_j) \right] - z_y$.
- In binary classification, $K = 2$ classes, the neural network outputs a single score $\hat{y} \in \mathbb{R}$, larger values mean more likely to be positive class.
- Let $z = [0, \hat{y}]$, then $\sum_{j=0}^{K-1} \exp(z_j) = 1 + \exp(\hat{y})$.
- If label is positive, $y = 1$, then $z_y = \hat{y}$ and loss is

$$\log \left[1 + \exp(\hat{y})\right] - \hat{y} = \log \left[\frac{1 + \exp(\hat{y})}{\exp(\hat{y})} \right] = \log[1 + \exp(-\hat{y})].$$

- If label is negative, $y = 0$, then $z_y = 0$ and loss is $\log \left[1 + \exp(\hat{y})\right]$.
- Both cases agree with our previous logistic loss formula, $\log[1 + \exp(-\underline{y}\hat{y})]$, with $\underline{y} \in \{-1, 1\}$.

Note about numerical stability

- For label y and real-valued predictions $z_0, \ldots, z_{K-1}$, loss is

$$\log \left[\sum_{j=0}^{K-1} \exp(z_j) \right] - z_y = L - z_y.$$

- exp may overflow to ∞ if z_j values are too large (bad).
- Numerical issues can be limited by using the log-sum-exp trick: let $M = \max_j z_j$, then

$$L = \log \left[\sum_{j=0}^{K-1} \exp(z_j) \right] = M + \log \left[\sum_{j=0}^{K-1} \exp(z_j - M) \right].$$

Gradient computation

- For label y and real-valued predictions $z_0, \ldots, z_{K-1}$, loss is $\log\left[\sum_{j=0}^{K-1} \exp(z_j)\right] - z_y = L - z_y$.
- Partial derivative with respect to prediction for class $k \in \{0, \ldots, K-1\}$ can be written in terms of indicator function I (1 if argument is true, otherwise 0):

$$\frac{\partial}{\partial z_k}(L - z_y) = \frac{\exp(z_k)}{\sum_{j=0}^{K-1} \exp(z_j)} - I[y = k].$$

- We compute L during forward pass to get loss and then use it again in backward pass, since $\exp(L) = \sum_{j=0}^{K-1} \exp(z_j)$,

$$\frac{\partial}{\partial z_k}(L - z_y) = \frac{\exp(z_k)}{\exp(L)} - I[y = k] = \underbrace{\exp(z_k - L)}_{\hat{p}_k} - I[y = k].$$

Binary classification is a special case 2

- For label y and real-valued predictions $z_0, \dots, z_{K-1}$, partial derivative for class $k \in \{0, \dots, K-1\}$ is

$$\frac{\partial}{\partial z_k} (L - z_y) = \frac{\exp(z_k)}{\sum_{j=0}^{K-1} \exp(z_j)} - I[y = k].$$

- In binary classification, $K = 2$ classes, the neural network outputs a single score $\hat{y} \in \mathbb{R}$, larger values mean more likely to be positive class.
- Let $z = [0, \hat{y}]$, then $\sum_{j=0}^{K-1} \exp(z_j) = 1 + \exp(\hat{y})$.
- Partial derivative with respect to predictions $\hat{y}$ is

$$\frac{\partial}{\partial \hat{y}} (L - z_y) = \frac{\exp(\hat{y})}{1 + \exp(\hat{y})} - I[y = 1] = \frac{1}{1 + \exp(-\hat{y})} - I[y = 1].$$

- If label is positive, $y = 1$, then gradient is $-1/[1 + \exp(\hat{y})]$.
- If label is negative, $y = 0$, then gradient is $1/[1 + \exp(-\hat{y})]$.
- Both cases agree with our previous logistic loss gradient formula, $(-\underline{y})/[1 + \exp(\underline{y}\hat{y})]$, with $\underline{y} \in \{-1, 1\}$.

Gradient example, very bad prediction

```
label=9
   pred_prob  neg_grad
0        0.0      -0.0
1        0.0      -0.0
2        0.0      -0.0
3        0.0      -0.0
4        0.0      -0.0
5        0.0      -0.0
6        1.0      -1.0
7        0.0      -0.0
8        0.0      -0.0
9        0.0       1.0
```

Predicted 100% class 6, label class 9, gradient says to decrease prob for class 6 and increase prob for class 9.

Gradient example, very bad prediction

```
label=9
   pred_prob  neg_grad
0        0.0      -0.0
1        0.0      -0.0
2        0.0      -0.0
3        0.7      -0.7
4        0.0      -0.0
5        0.0      -0.0
6        0.3      -0.3
7        0.0      -0.0
8        0.0      -0.0
9        0.0       1.0
```

Predicted 70% class 3, 30% class 6, label class 9, gradient says to decrease prob for classes 3 and 6 (but by different amounts), and increase prob for class 9.

Gradient example, bad prediction

```
label=3
   pred_prob  neg_grad
0        0.0      -0.0
1        0.0      -0.0
2        0.0      -0.0
3        0.1       0.9
4        0.0      -0.0
5        0.0      -0.0
6        0.9      -0.9
7        0.0      -0.0
8        0.0      -0.0
9        0.0      -0.0
```

Predicted 10% class 3 and 90% class 6, label class 3, gradient says to increase prob for class 3 and decrease prob for class 6 (note gradient smaller than for predicting 0% label class).

Gradient example, decent but incorrect prediction

```
label=3
   pred_prob  neg_grad
0        0.0      -0.0
1        0.3      -0.3
2        0.0      -0.0
3        0.3       0.7
4        0.0      -0.0
5        0.4      -0.4
6        0.0      -0.0
7        0.0      -0.0
8        0.0      -0.0
9        0.0      -0.0
```

Predicted 30% class 1, 30% class 3, 40% class 5, label class 3, gradient says to decrease prob for class 1, increase prob for class 3, and decrease prob for class 5.

Gradient example, good prediction

```
label=1
   pred_prob  neg_grad
0        0.0      -0.0
1        0.6       0.4
2        0.0      -0.0
3        0.0      -0.0
4        0.0      -0.0
5        0.0      -0.0
6        0.0      -0.0
7        0.4      -0.4
8        0.0      -0.0
9        0.0      -0.0
```

Predicted 60% class 1, 40% class 7, label class 1, gradient says to decrease prob for class 7 and increase prob for class 1.

Gradient example, very good prediction

```
label=6
   pred_prob  neg_grad
0        0.0      -0.0
1        0.0      -0.0
2        0.0      -0.0
3        0.0      -0.0
4        0.0      -0.0
5        0.0      -0.0
6        1.0       0.0
7        0.0      -0.0
8        0.0      -0.0
9        0.0      -0.0
```

Predicted 100% class 6, label class 6, gradient zero indicates that predictions should not be updated.

Fully connected multi-layer Neural Networks

Computing gradients and learning weights

Automatic differentiation

Multi-class classification

Torch

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)
```

Neural network for regression: square loss

```
net = Net()
loss_fun = torch.nn.MSELoss() #The only change!
optimizer = torch.optim.SGD(net.parameters(), lr=0.03)

# to do in a loop:
optimizer.zero_grad()
loss_value = loss_fun(net(inputs), outputs)
# outputs are real numbers, not 0/1 binary classes.
loss_value.backward() # auto grad
optimizer.step() # learning
```

Neural network for multiple classes, cross entropy loss

```
class Net(torch.nn.Module):
    def __init__(self, n_features, n_hidden, n_classes):
        super(Net, self).__init__()
        self.stack = torch.nn.Sequential(
          torch.nn.Linear(n_features, n_hidden),
          torch.nn.ReLU(),
          torch.nn.Linear(n_hidden, n_classes))
    def forward(self, feature_mat):
        return self.stack(feature_mat)
net = Net()
loss_fun = torch.nn.CrossEntropyLoss()
loss_value = loss_fun(net(inputs), outputs)
```

No need to explicitly compute predicted probability.

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.
- Request a GPU on Monsoon via –gres=gpu:tesla:1 flag to srun/sbatch.

```
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.