3 - Training Neural Networks

Ludwig Krippahl

FACULDADE DE CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA

Summary

- Algebra (revisions)
- The computational graph and AutoDiff
- Training with Stochastic Gradient Descent

Algebra

Algebra

Basic concepts:

- Scalar: A number
- Vector: An ordered array of numbers
- Matrix: A 2D array of numbers
- Tensor: A relation between sets of algebraic objects
  - (numbers, vectors, etc)
  - **For our purposes**: an N-dimensional array of numbers
- We will be using tensors in our models (hence Tensorflow)

Tensor operations

- Adition and subtraction:

- In algebra, we can add or subtract tensors with the same dimensions
- The operation is done element by element

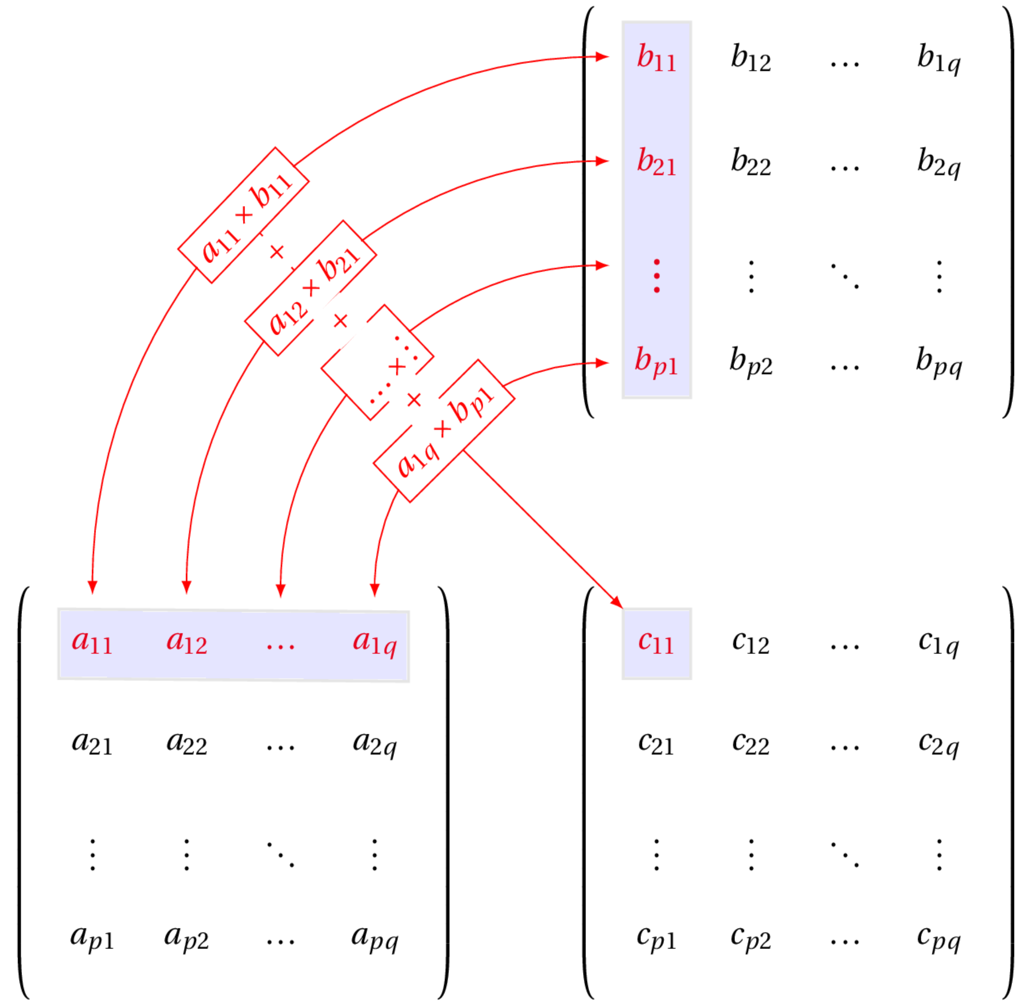
$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1q} \\ a_{21} & a_{22} & \cdots & a_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1} & a_{p2} & \cdots & a_{pq} \end{pmatrix} \quad \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1q} \\ b_{21} & b_{22} & \cdots & b_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ b_{p1} & b_{p2} & \cdots & b_{pq} \end{pmatrix} \quad \begin{pmatrix} a_{11}+b_{11} & a_{12}+b_{12} & \ldots+\ldots & a_{1q}+b_{1q} \\ a_{21}+b_{21} & a_{22}+b_{22} & \ldots+\ldots & a_{2q}+b_{2q} \\ \vdots+\vdots & \vdots+\vdots & \ddots+\ddots & \vdots+\vdots \\ a_{p1}+b_{p1} & a_{p2}+b_{p2} & \ldots+\ldots & a_{pq}+b_{pq} \end{pmatrix}$$

Tensor operations

- Matrix multiplication (2D)
  - Follows algebra rules:

$$\mathbf{C} = \mathbf{AB}$$

$\mathbf{A}$ columns same as $\mathbf{B}$ rows



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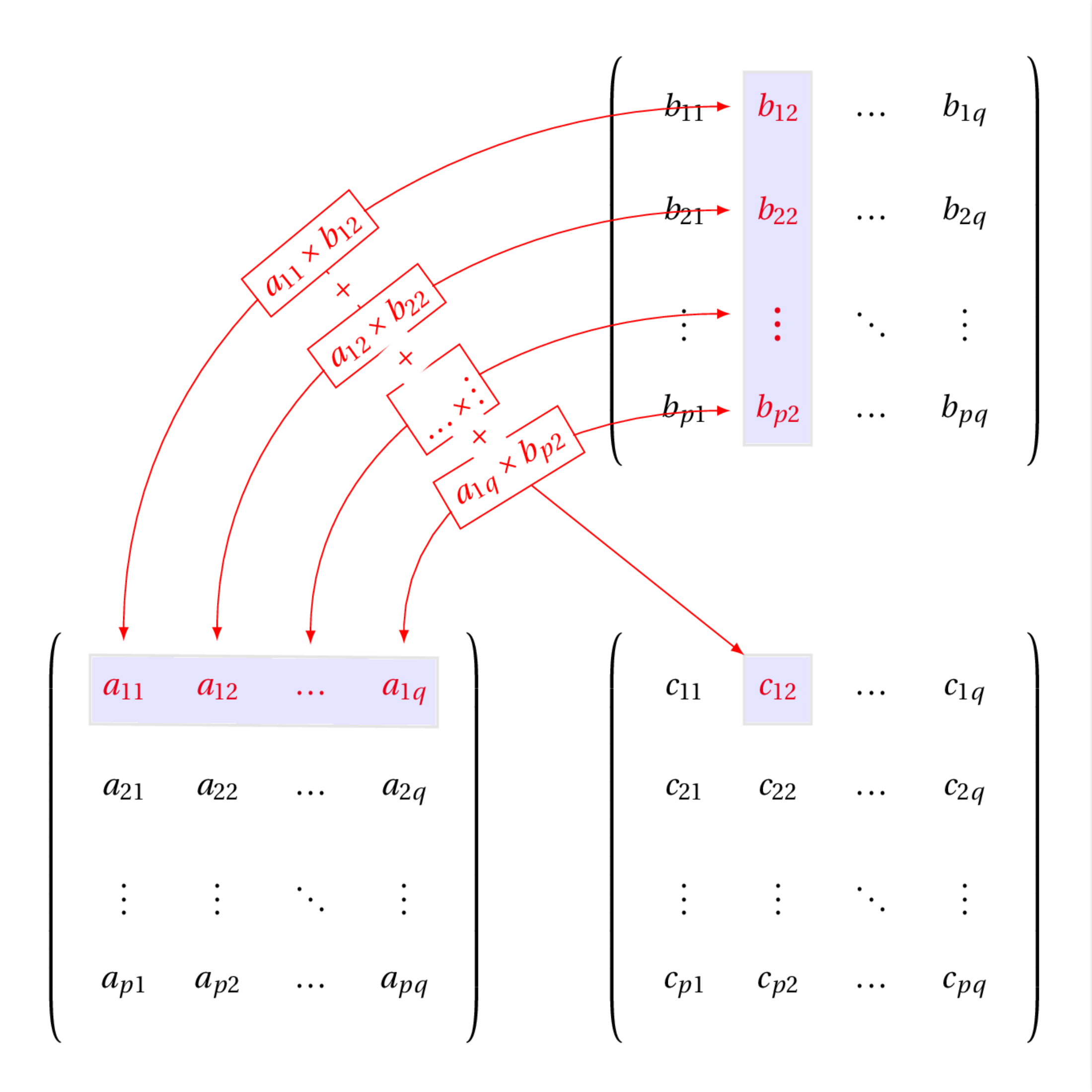

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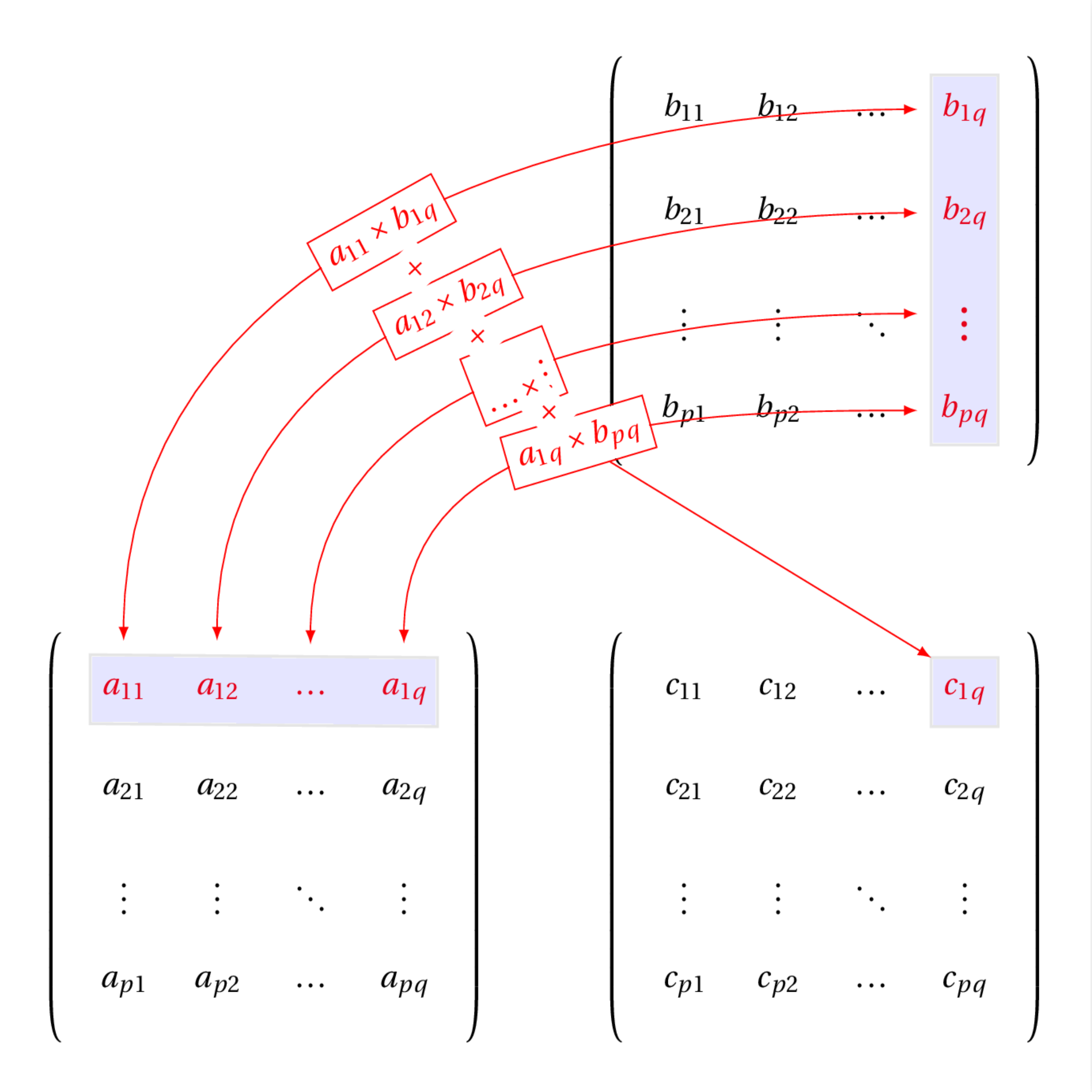

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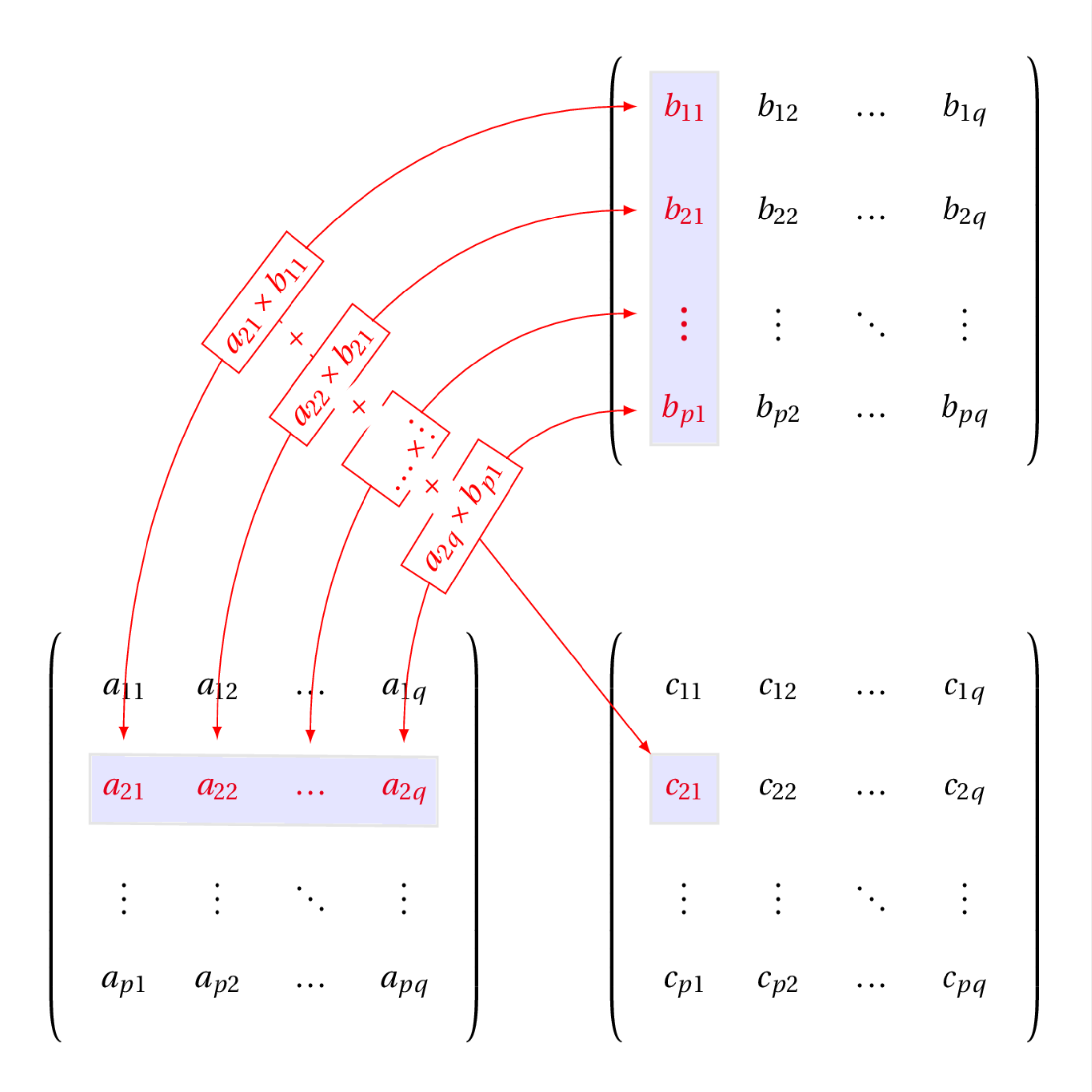

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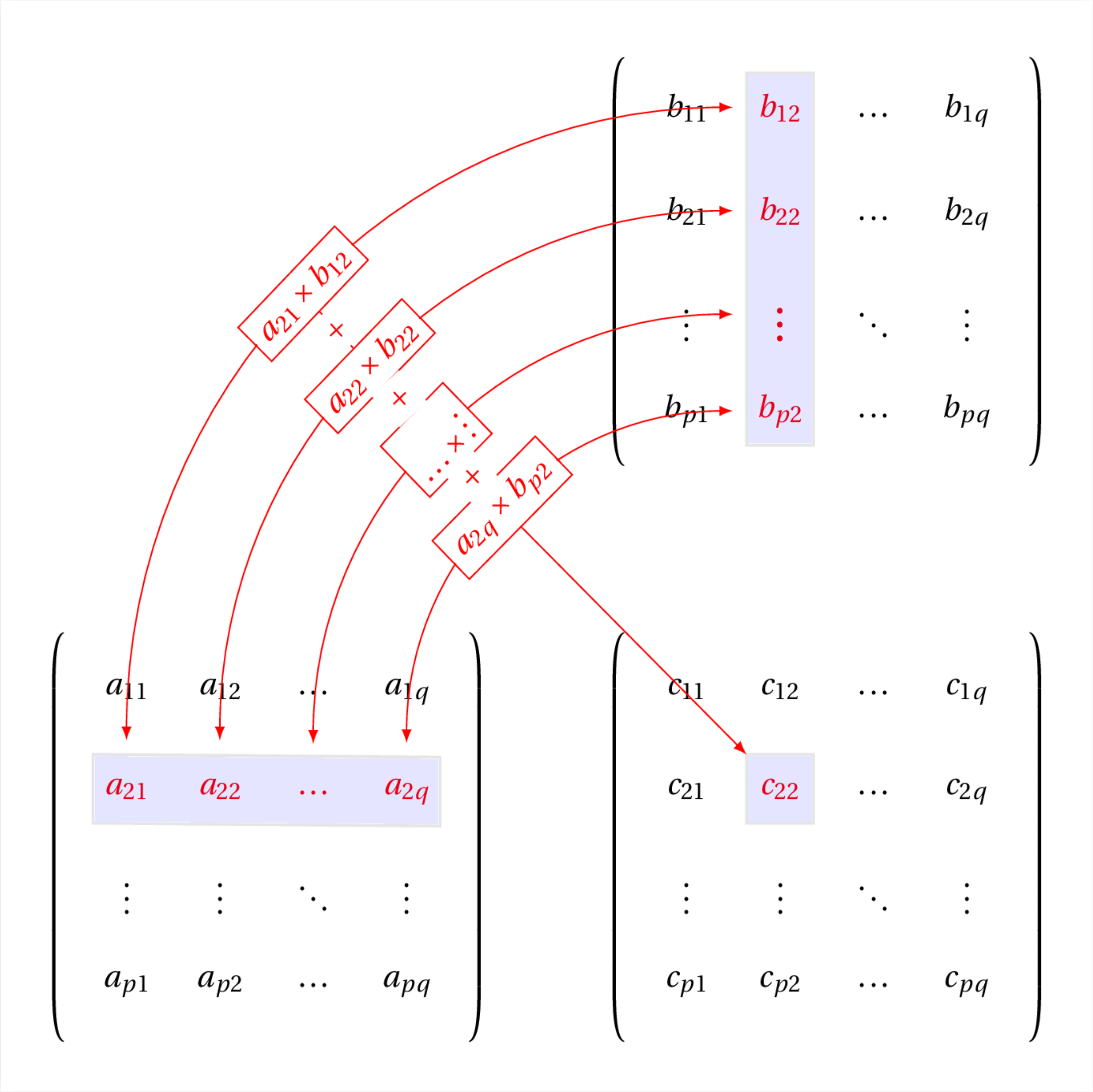

Algebra

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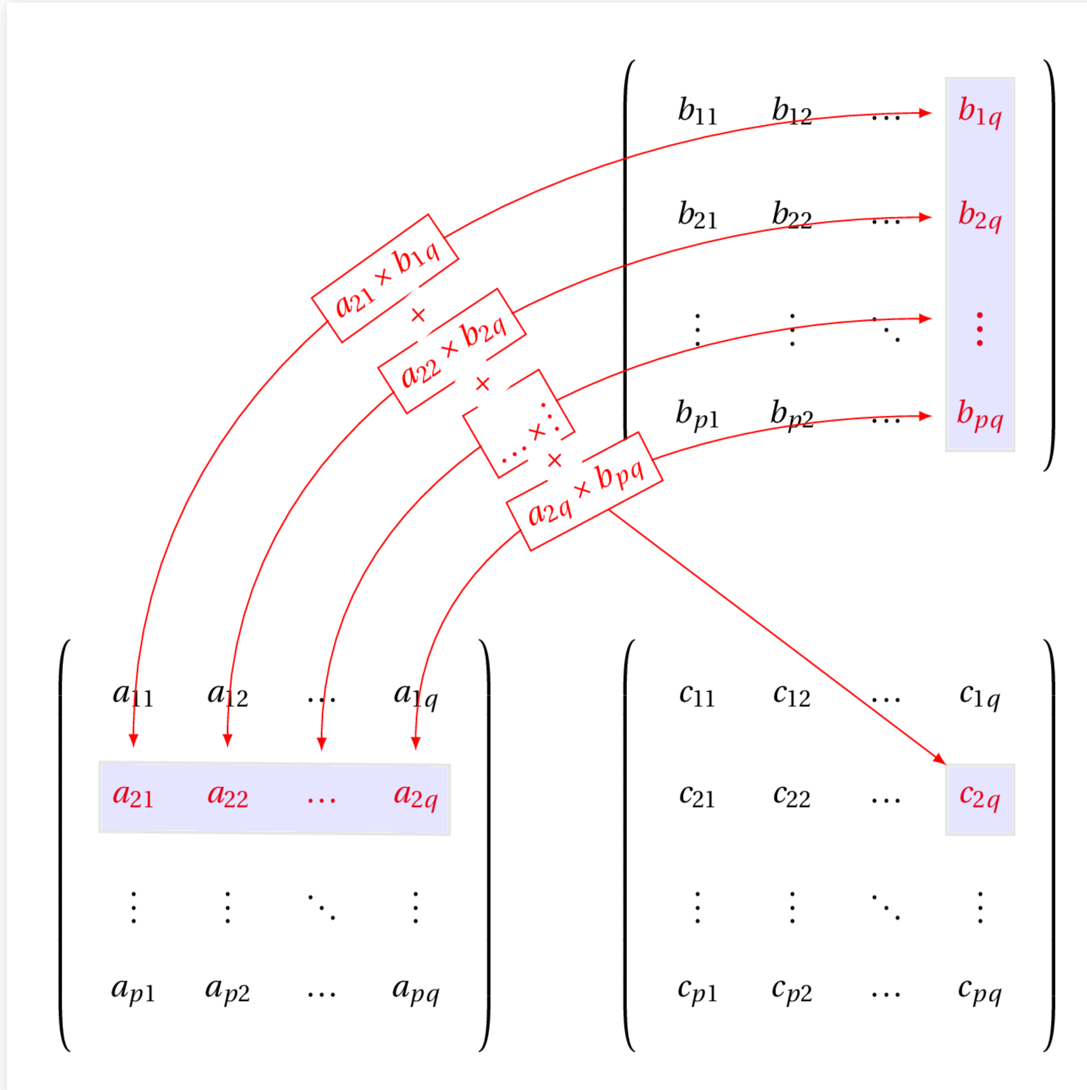

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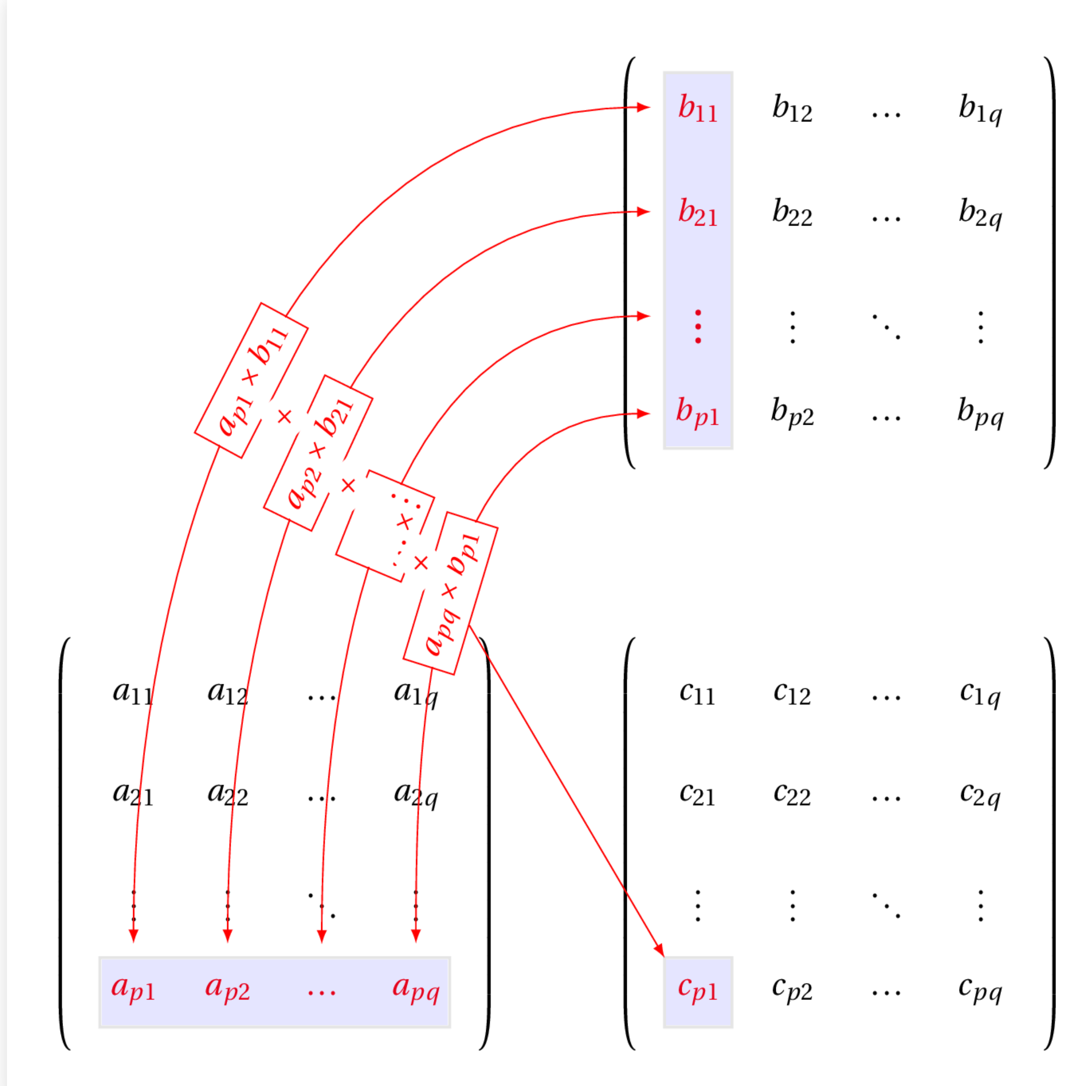

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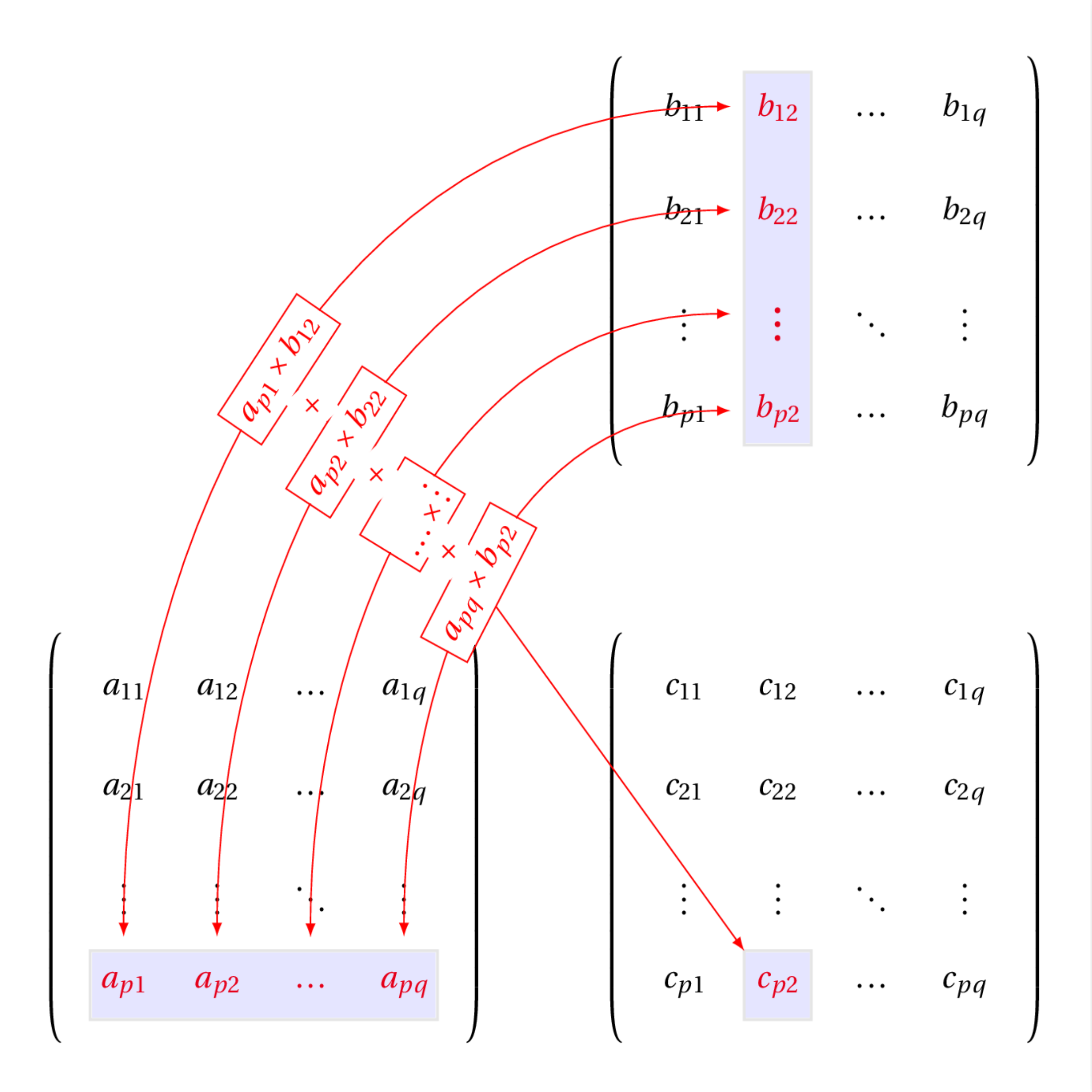

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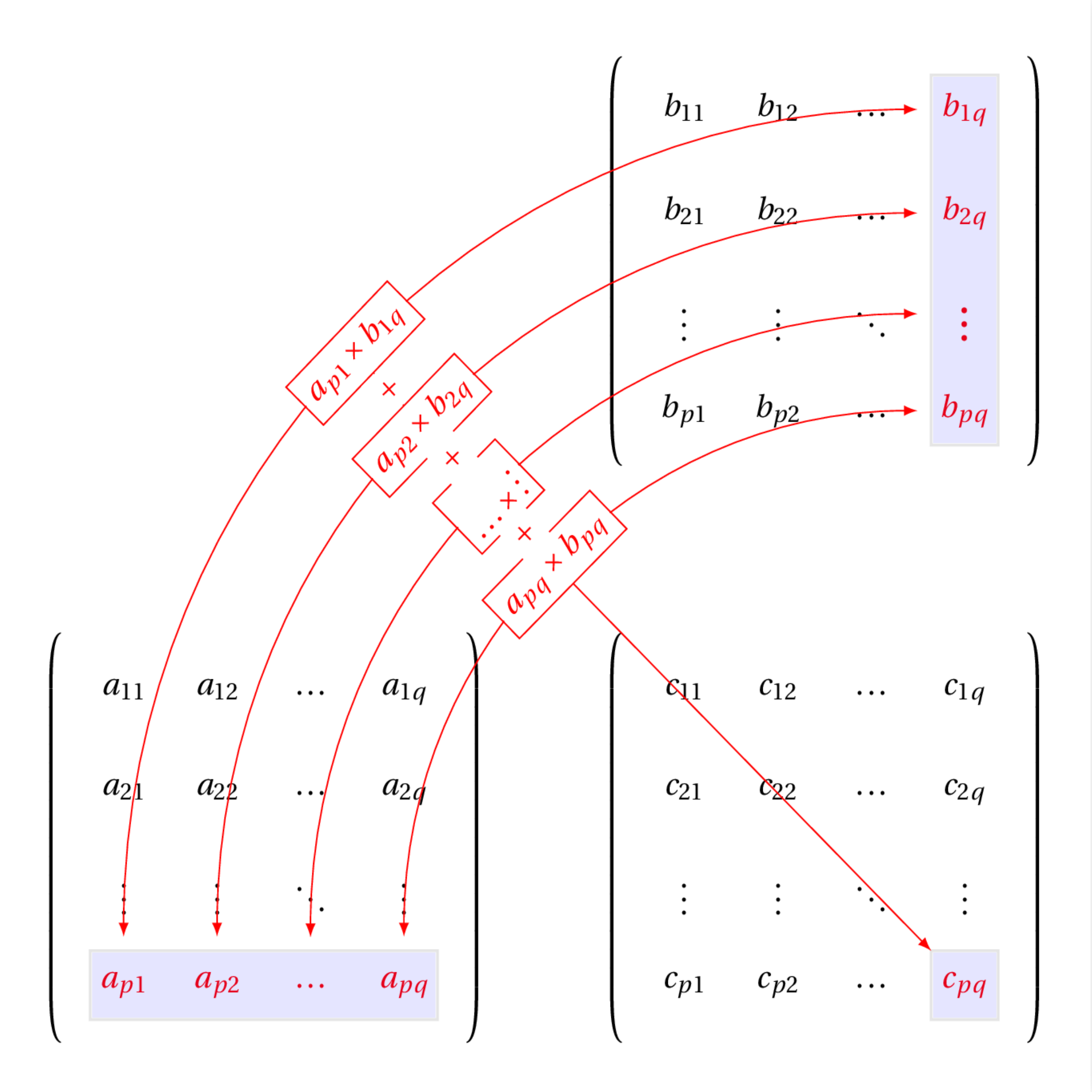
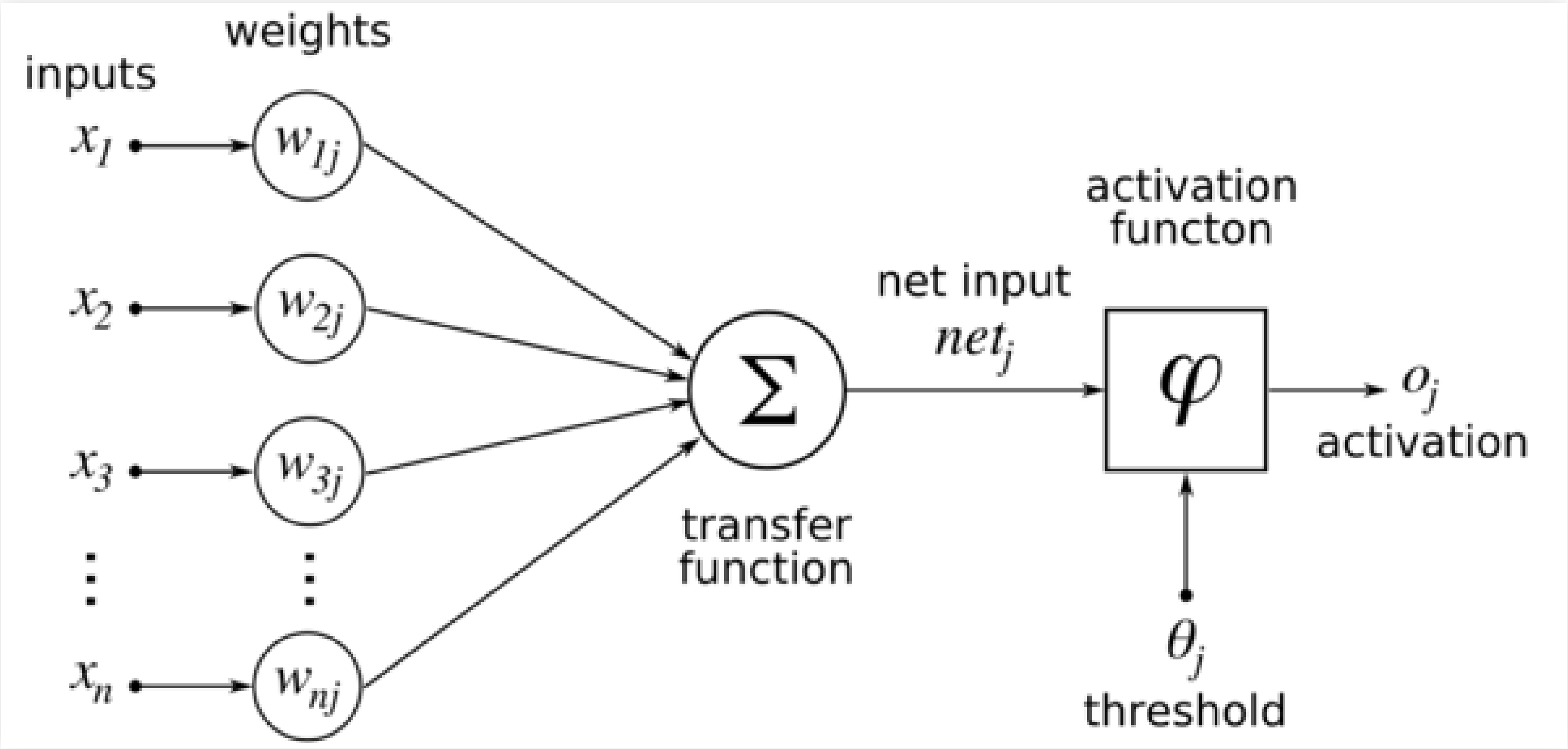


$\mathbf{A}$ columns same as $\mathbf{B}$ rows

Algebra

- Neuron: linear combination of inputs with non-linear activation



Algebra

Tensor operations

- Tensorflow also allows **broadcasting** like `numpy`

• Element-wise operations aligned by the last dimensions

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1q} \\ a_{21} & a_{22} & \dots & a_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1} & a_{p2} & \dots & a_{pq} \end{pmatrix} \quad \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1q} \end{pmatrix} \quad \begin{pmatrix} a_{11}+b_{11} & a_{12}+b_{12} & \dots+\dots & a_{1q}+b_{1q} \\ a_{21}+b_{11} & a_{22}+b_{12} & \dots+\dots & a_{2q}+b_{1q} \\ \vdots+b_{11} & \vdots+b_{12} & \ddots+\dots & \vdots+b_{1q} \\ a_{p1}+b_{11} & a_{p2}+b_{12} & \dots+\dots & a_{pq}+b_{1q} \end{pmatrix}$$

Tensor operations

- Tensorflow also allows **broadcasting** like `numpy`
  - Element-wise operations aligned by the last dimensions
- `tf.matmul()` also works on 3D tensors, in batch
  - Can be used to compute the product of a batch of 2D matrices
  - Example (from Tensorflow `matmul` documentation):

```
In : a = tf.constant(np.arange(1, 13, dtype=np.int32), shape=[2, 2, 3])
In : b = tf.constant(np.arange(13, 25, dtype=np.int32), shape=[2, 3, 2])
In : c = tf.matmul(a, b) # or a * b
Out: <tf.Tensor: id=676487, shape=(2, 2, 2), dtype=int32, numpy=
array([[[ 94, 100],
        [229, 244]],

       [[508, 532],
        [697, 730]]], dtype=int32)>
```

Algebra

Why is this important?

- Our models will be based on this type of operations
- Example batches will be tensors (2D or more)
- Network layers can be matrices of weights (several neurons)
- Loss functions will operate and aggregate on activations and data

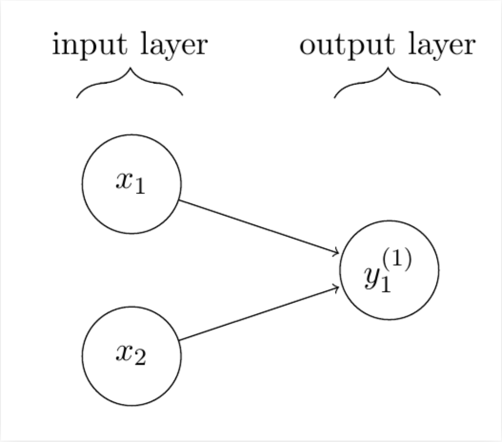
In practice mostly hidden

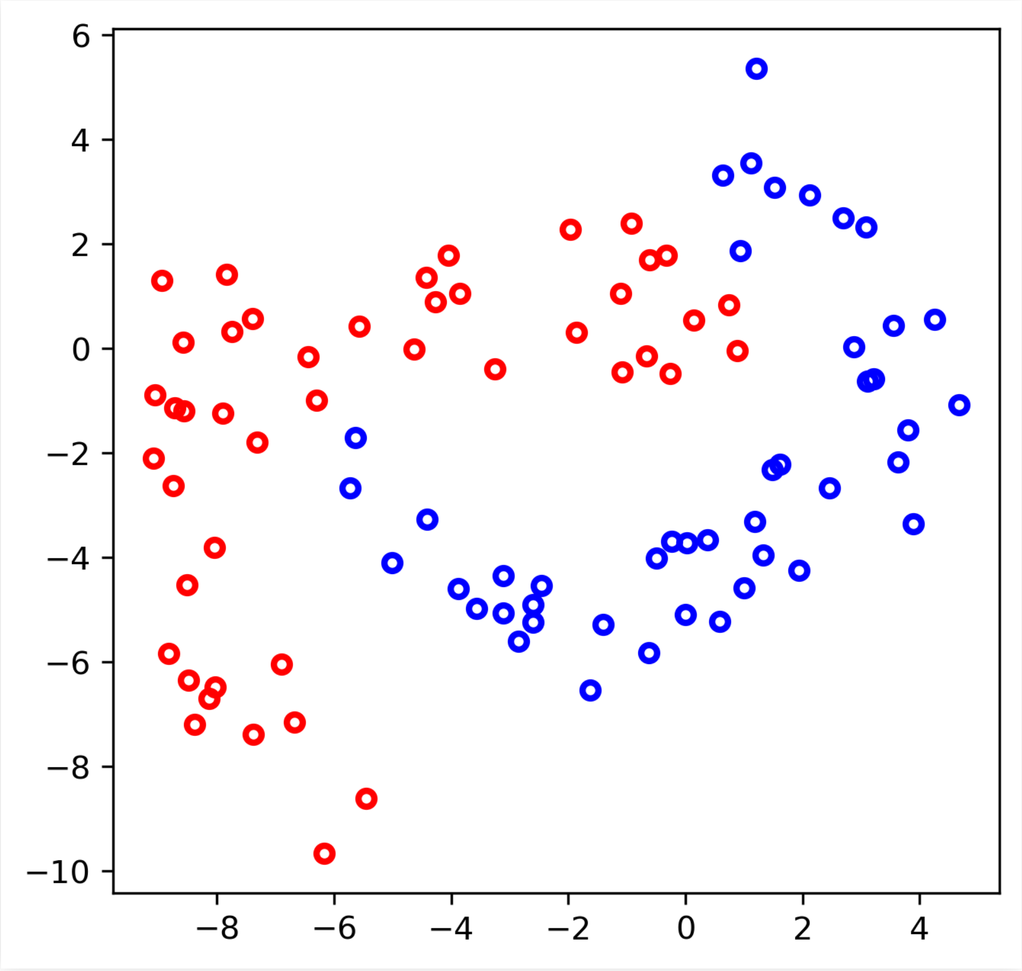
- When we use the `keras` API we don't need to worry about this
- But it's important to understand how things work
- And necessary to work with basic Tensorflow operations

Basic Example

Basic Example

- Classify these data with two weights, sigmoid activation





Computing activation

- Input is a matrix with data, two columns for the features, N rows
- To compute $\sum_{j=1}^{2} w_j x_j$ use matrix multiplication

$$\begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \\ \vdots & \vdots \\ x_{n1} & x_{n2} \end{pmatrix}$$

$$\begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

$$\begin{pmatrix} x_{11} & * & w_1 & + & x_{12} & * & w_2 \\ x_{21} & * & w_1 & + & x_{22} & * & w_2 \\ x_{31} & * & w_1 & + & x_{32} & * & w_2 \\ \vdots & * & w_1 & + & \vdots & * & w_2 \\ x_{n1} & * & w_1 & + & x_{n2} & * & w_2 \end{pmatrix}$$

Computing activation

- Input is a matrix with data, two columns for the features, N rows
- To compute $\sum_{j=1}^{2} w_j x_j$ use matrix multiplication
- For each example with 2 features we get one weighted sum
- Then apply sigmoid function, one activation value per example
- Thus, we get activations for a batch of examples

Training (Backpropagation)

Training

Backpropagation

- For weight m on hidden layer i, propagate error backwards
  - Gradient of error w.r.t. weight of output neuron:

$$\frac{\delta E_{kn}^j}{\delta s_{kn}^j} \frac{\delta s_{kn}^j}{\delta net_{kn}^j} \frac{\delta net_{kn}^j}{\delta w_{mkn}}$$

- Chain derivatives through the network:

$$\Delta w_{min}^j = -\eta \left(\sum_p \frac{\delta E_{kp}^j}{\delta s_{kp}^j} \frac{\delta s_{kp}^j}{\delta net_{kp}^j} \frac{\delta net_{kp}^j}{\delta s_{in}^j} \right) \frac{\delta s_{in}^j}{\delta net_{in}^j} \frac{\delta net_{in}^j}{\delta w_{min}}$$

$$= \eta (\sum_p \delta_{kp} w_{mkp}) s_{in}^j (1 - s_{in}^j) x_i^j = \eta \delta_{in} x_i^j$$

- Backpropagation is a special case of Reverse mode Automatic Differentiation

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Computing derivatives

Symbolic differentiation:

- Compute the expression for the derivatives given the function.
- Difficult, especially with flow control (`if`, `for`)

$$\Delta w_i^j = -\eta \frac{\delta E^j}{\delta w_i} = \eta(t^j - s^j)s^j(1 - s^j)x_i^j$$

Numerical differentiation:

- Use finite steps to compute deltas and approximate derivatives.
- Computationally inefficient and prone to convergence problems.

Automatic differentiation:

- Apply the chain rule to basic operations that compose complex functions
- product, sum, sine, cosine, etc
- Applicable in general provided we know the derivative of each basic operation

Training

Automatic differentiation in `tensorflow`

- Reverse-mode automatic differentiation
- Forward pass keeping intermediate results of operations
- Backwards pass using the derivatives of operations in the computation graph
  - Graph with operations as nodes and tensors as edges

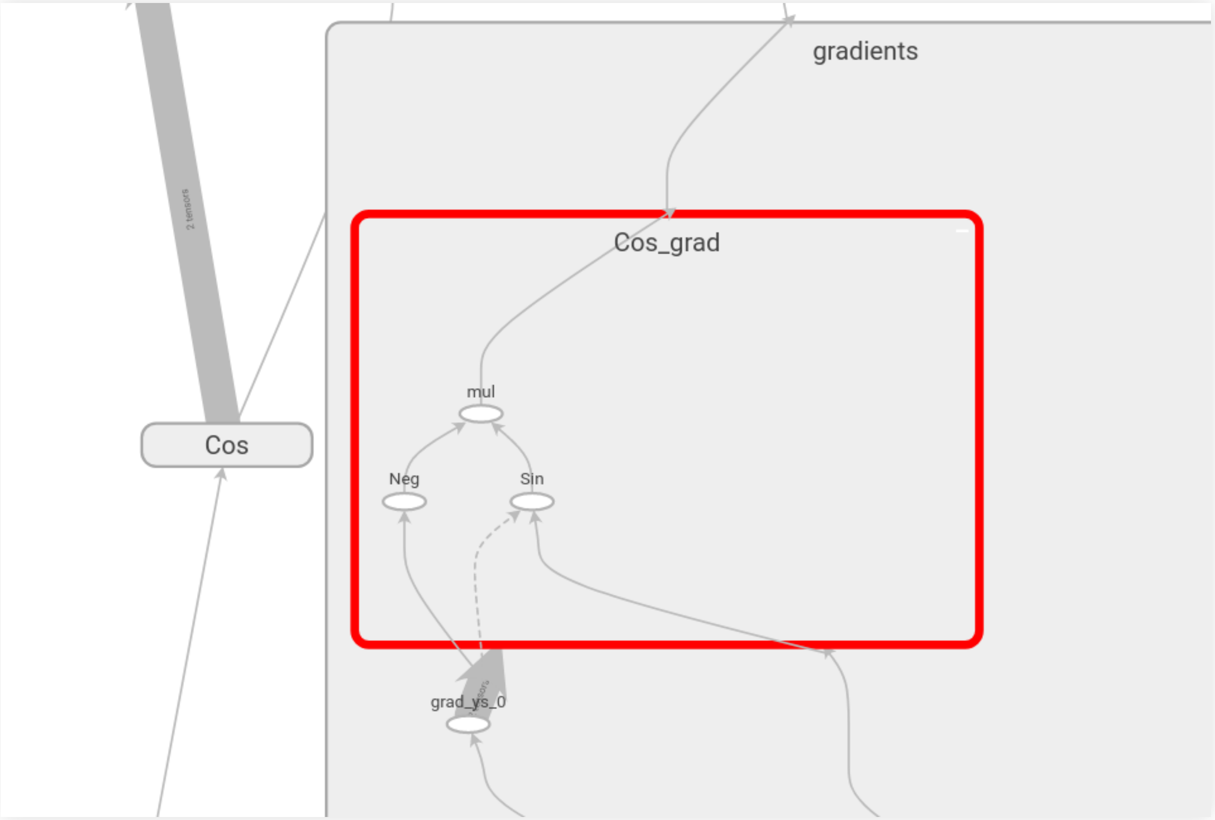
Tutorial, simpler example

- Forward-mode automatic differentiation
- Uses dual numbers to keep track of function and derivative values
- But the idea is the same:
  - Use the analytical derivatives of elementary operations to compute the derivative of the composition

Training

- Automatic differentiation example:

$$\operatorname*{argmin}_x (\cos x) \qquad \frac{d \cos x}{dx} = -\sin x$$



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Training

- Automatic differentiation example:

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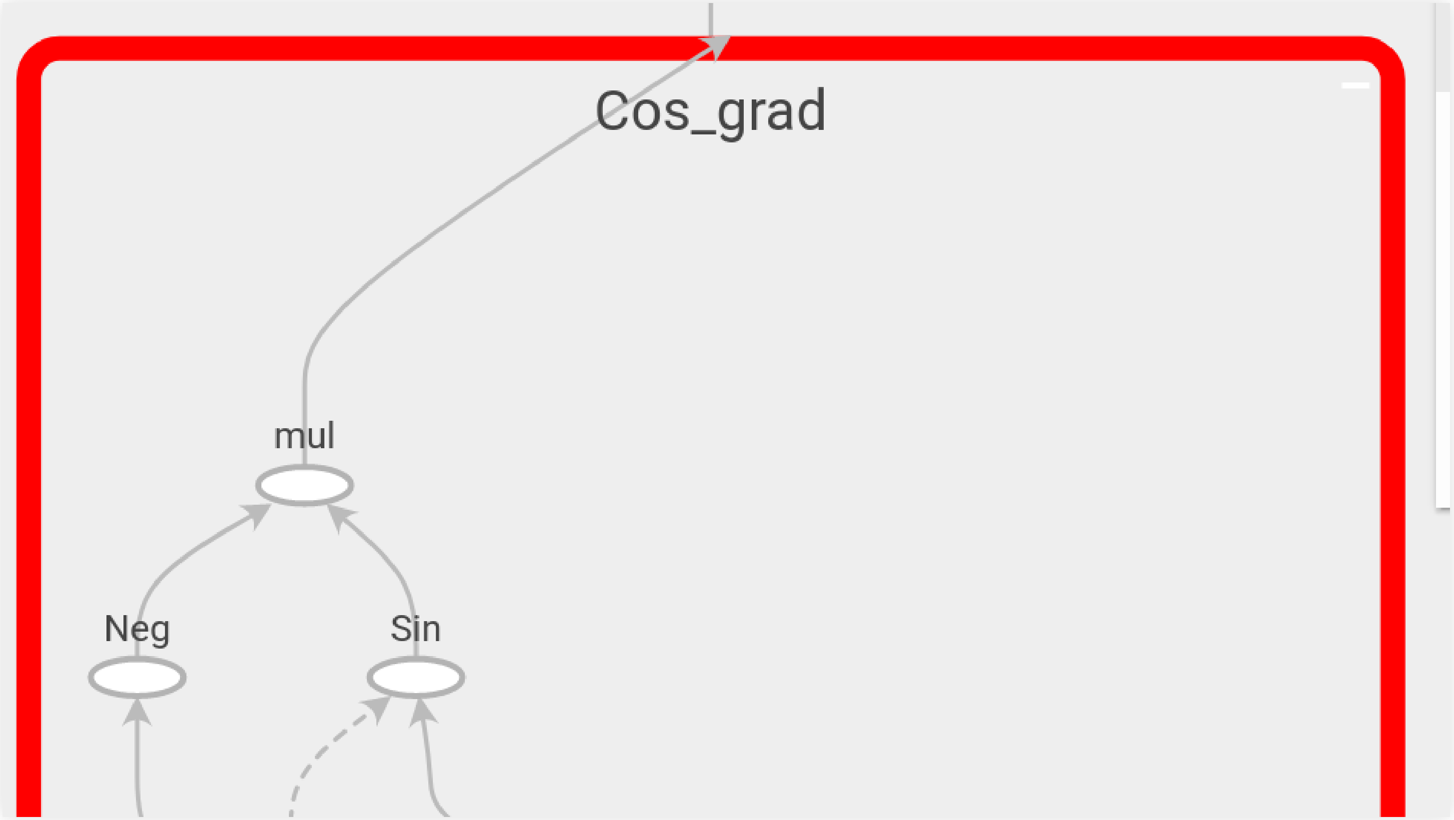
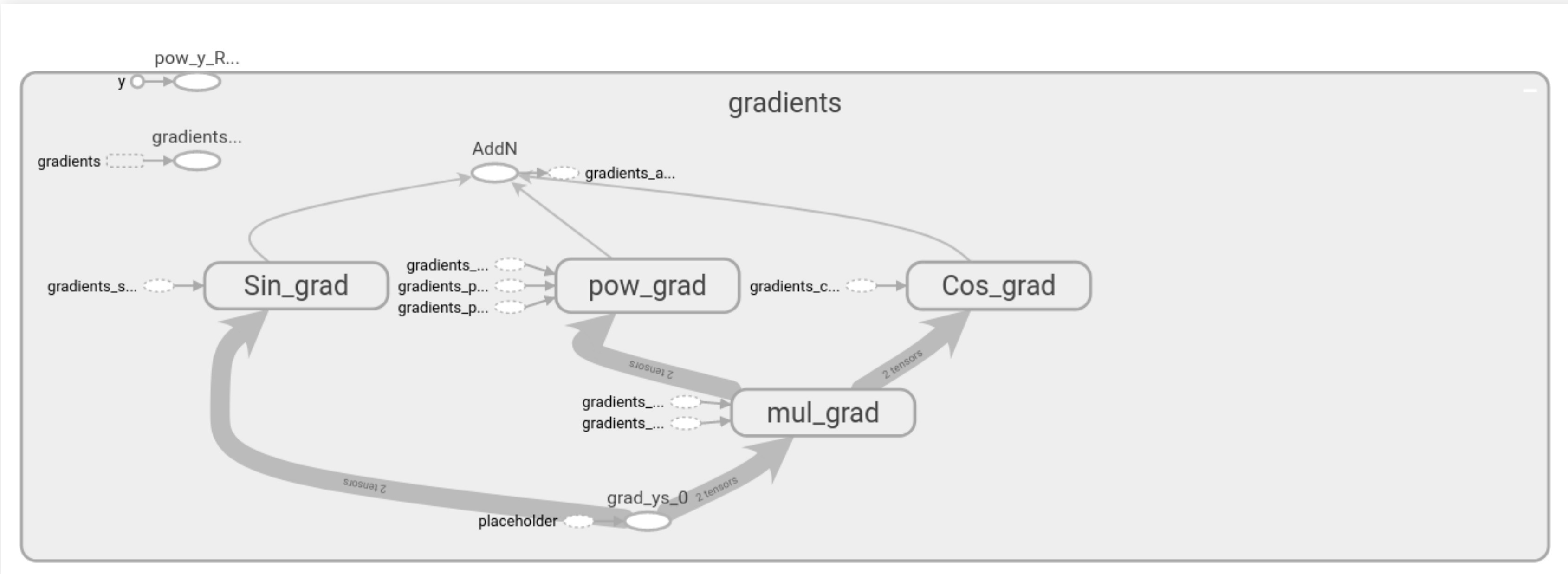


Training

- Automatic differentiation example:

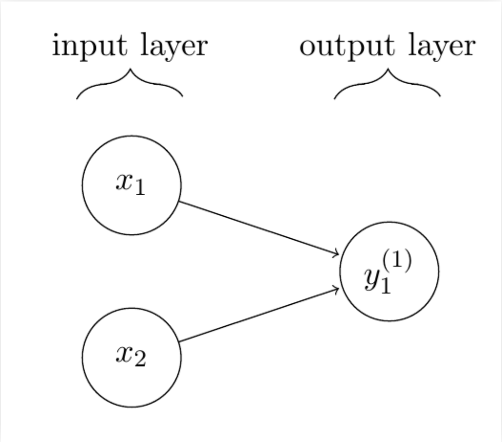
$$\underset{x}{\operatorname{argmin}} \left(x^2 \cos x + \sin x \right)$$

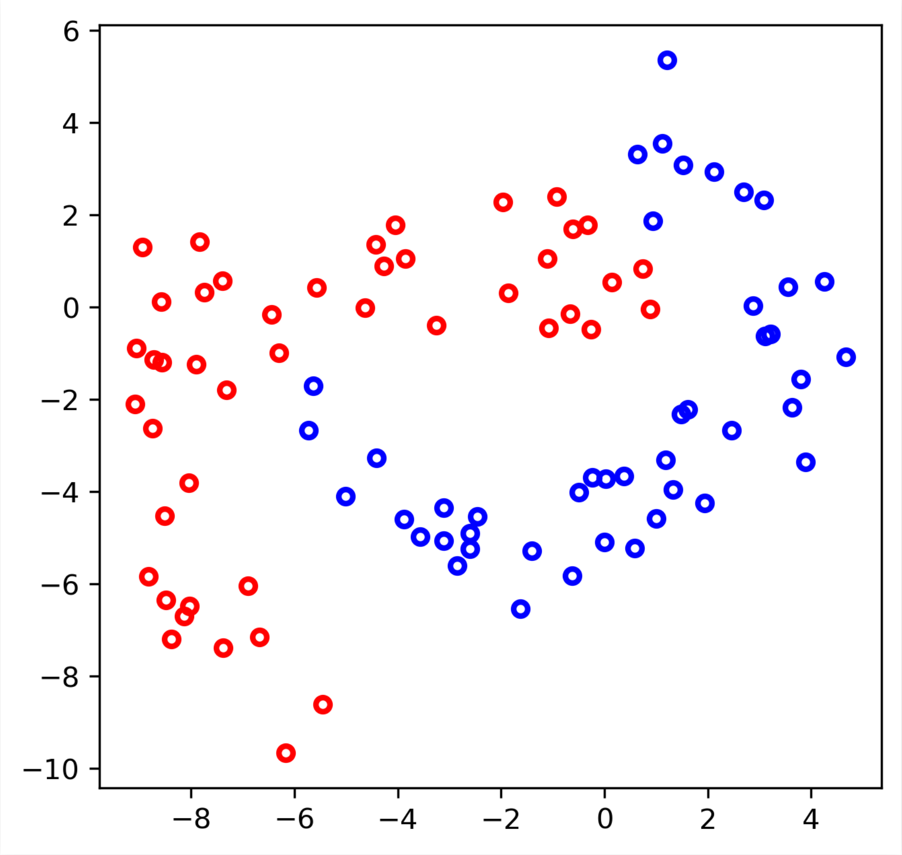


- Tensorflow operators include gradient information

Stochastic Gradient Descent

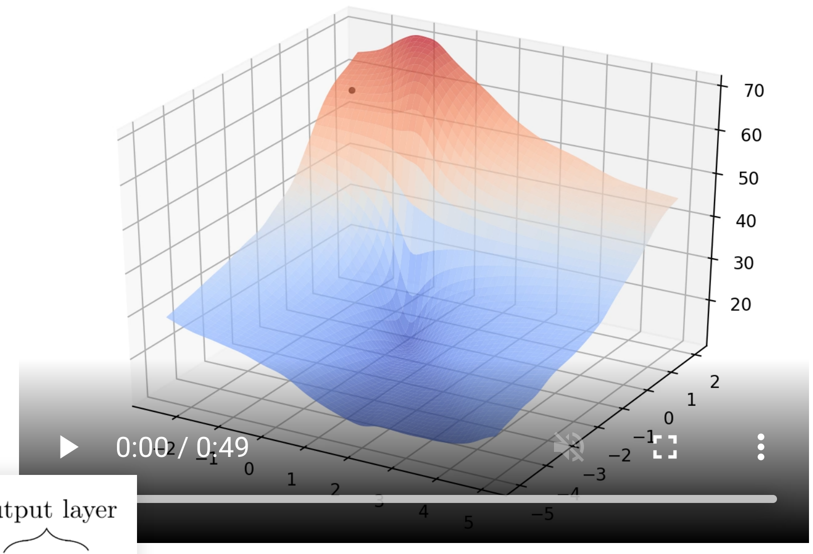
- Going back to our simple model:

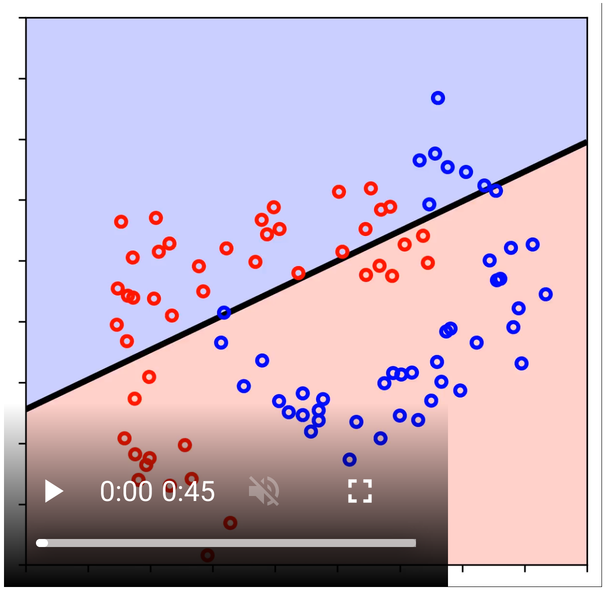


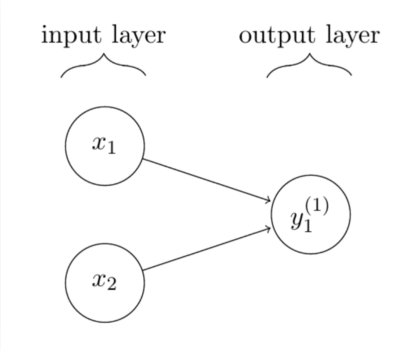


Stochastic Gradient Descent

- Since we can compute the derivatives, we can "slide" down the loss function

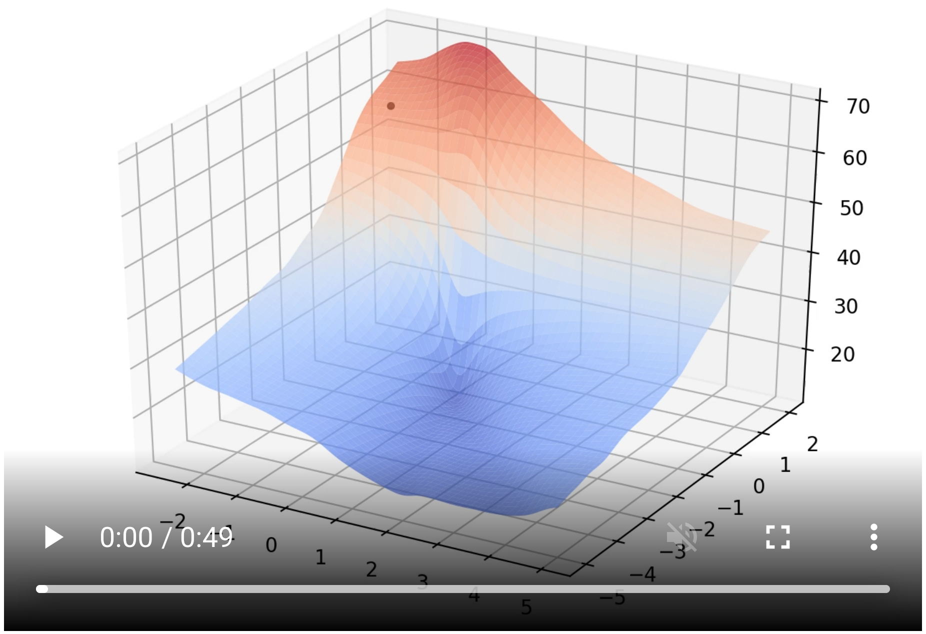


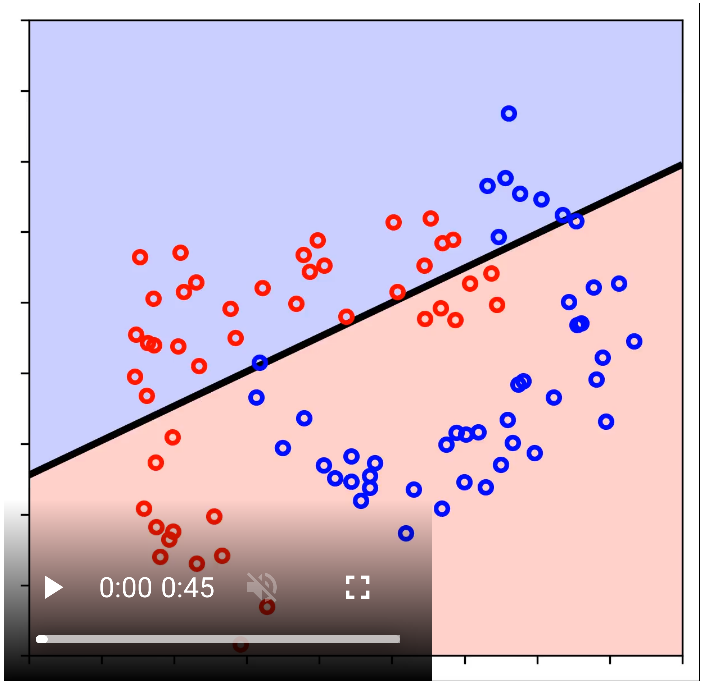




Stochastic Gradient Descent

- Gradient Descent because of sliding down the gradient
- Stochastic because we are presenting a random minibatch of examples at a time





Stochastic Gradient Descent

- Gradient Descent because of sliding down the gradient
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Algorithm:

- Estimate the gradient of $L\left(f\left(x,\theta\right),y\right)$ given m examples:

$$\hat{g}_t = \nabla_\theta \left(\frac{1}{m} \sum_{i=1}^{m} L\left(f\left(x^{(i)},\theta\right),y^{(i)}\right)\right)$$

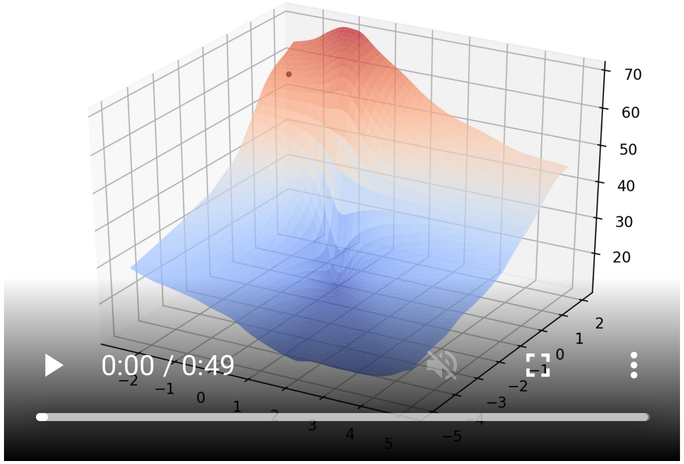
- Update θ with a learning rate ϵ

$$\theta_{t+1} = \theta_t - \epsilon \hat{g}_t$$

Training

SGD can be improved with momentum

- If we are rolling down the surface we could pick up speed



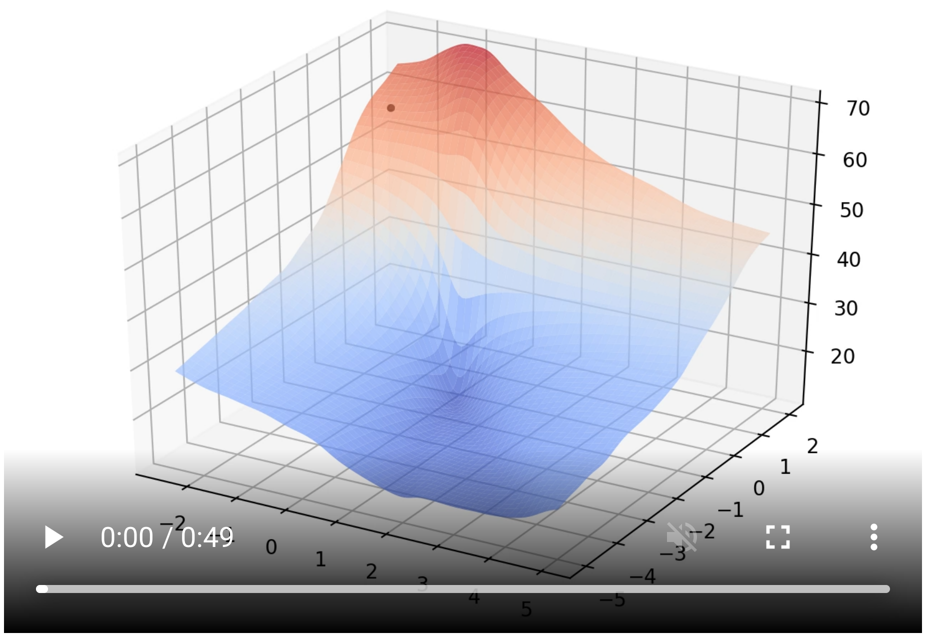
- Use gradients as an "acceleration", with

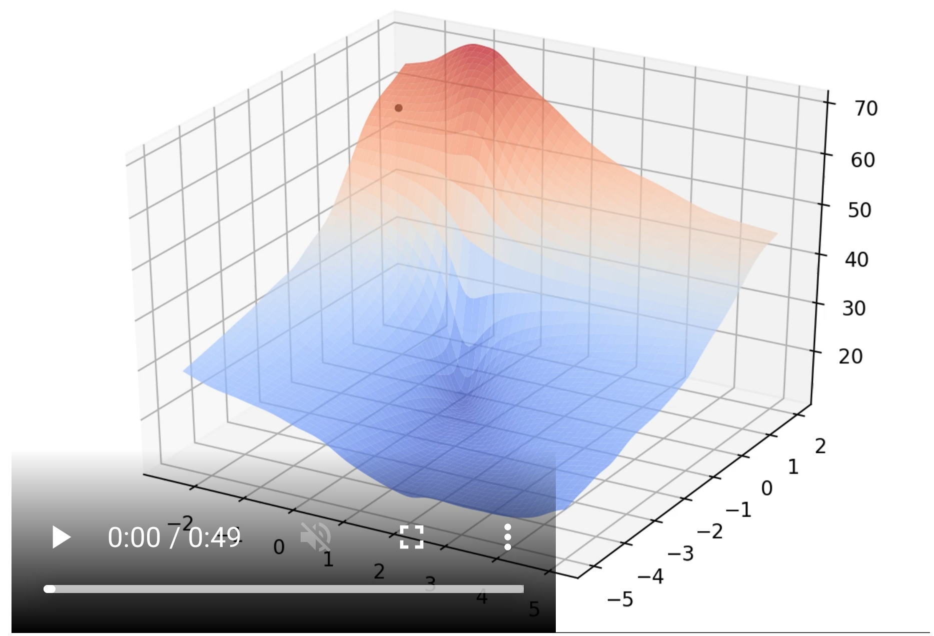
$$v_{t+1} = \alpha v_t - \nabla_\theta \left(\frac{1}{m} \sum_{i=1}^{m} L\left(f\left(x^{(i)}, \theta\right), y^{(i)}\right) \right)$$

$$\theta_{t+1} = \theta_t + \epsilon v_{t+1}$$

SGD can be improved with momentum

- SGD
- SGD + 0.9 momentum





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Nesterov momentum

- Compute gradients where we will be after the momentum step:

$$v_{t+1} = \alpha v_t - \nabla_\theta \left(\frac{1}{m} \sum_{i=1}^{m} L\left(f\left(x^{(i)}, \theta + \alpha v_t \right), y^{(i)} \right) \right)$$

$$\theta_{t+1} = \theta_t + \epsilon v_{t+1}$$

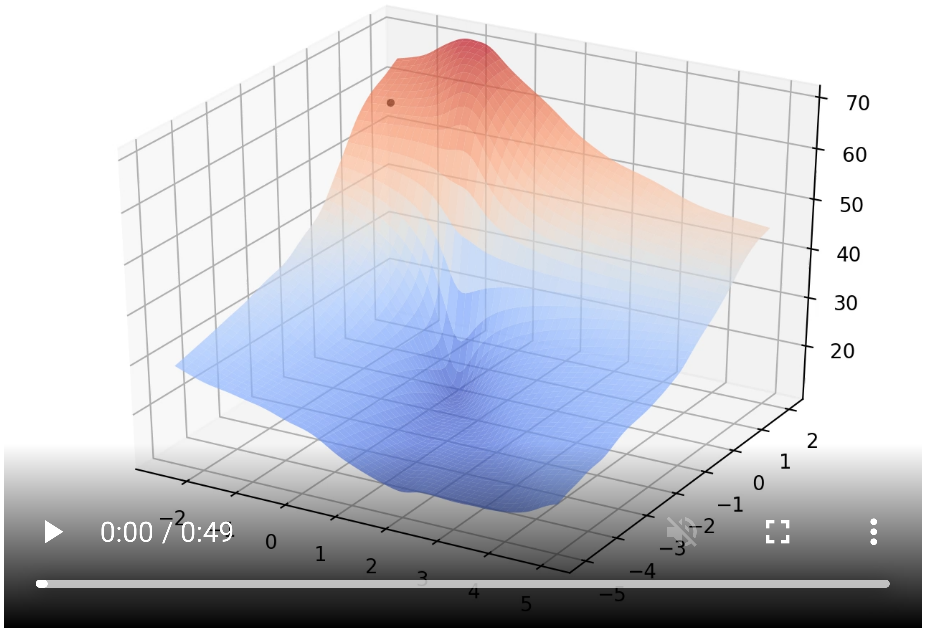
- This works great for optimizing convex functions (Nesterov, 1983)
- But with stochastic gradient descent it's not as effective
  - (due to random sampling)

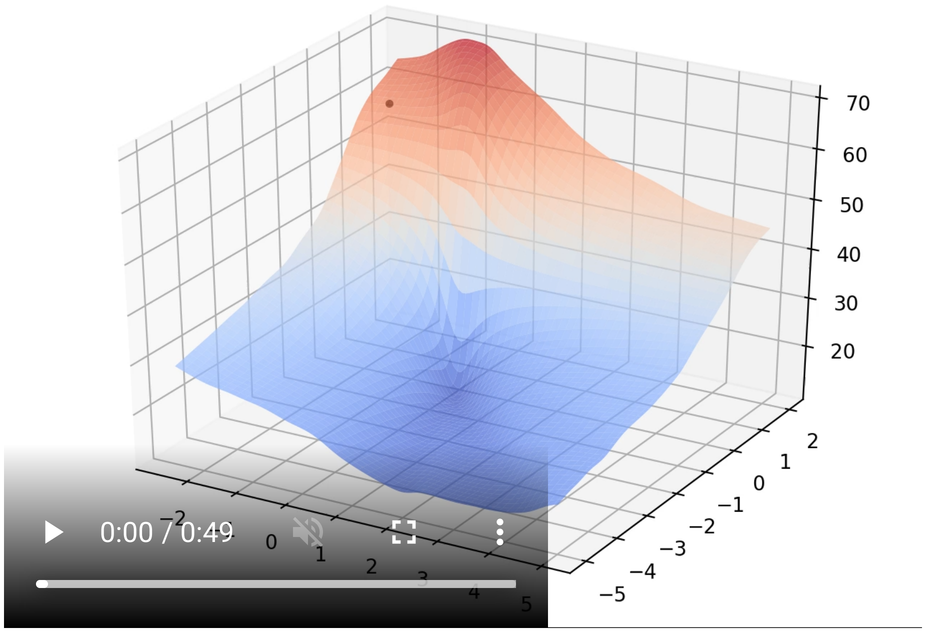
"Unfortunately, in the stochastic gradient case, Nesterov momentum does not improve the rate of convergence."

Goodfellow et al. 2016

Nesterov momentum

- SGD + 0.9 momentum
- SGD + 0.9 Nesterov m.



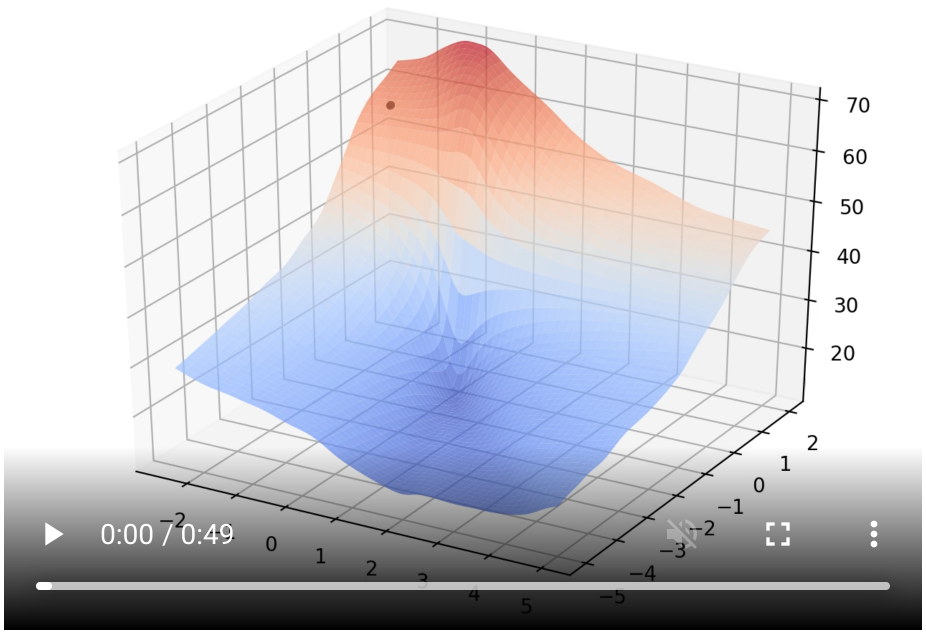


Minibatch size

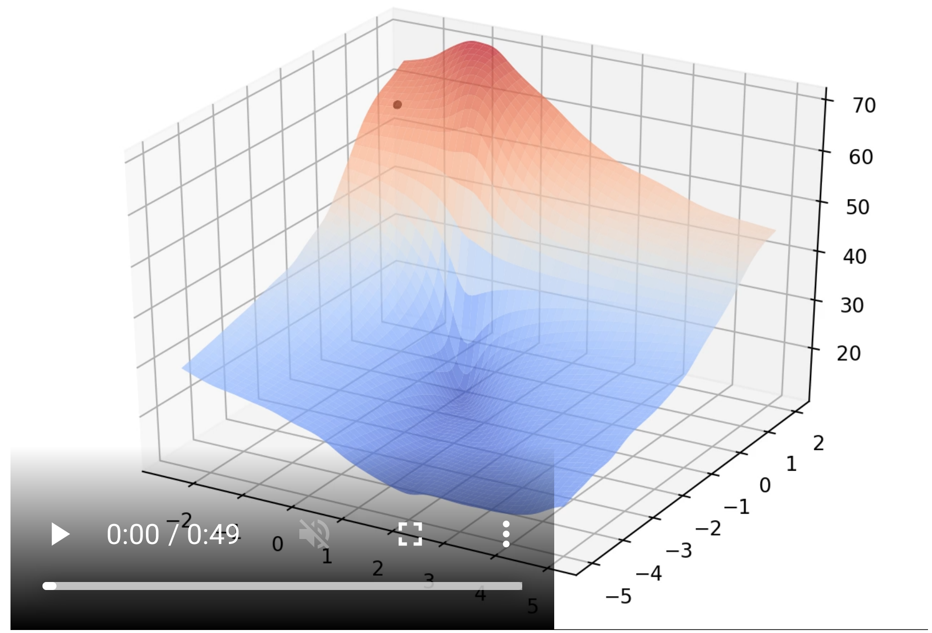
- Averaging over a set of examples gives a (slightly) better estimate of the gradient, improving convergence
  - (Note that the true gradient is for the mean loss over all points)
- The main advantage of batches is in using multicore hardware (GPU, for example)
  - This is also the reason for power of 2 minibatch sizes (8, 16, 32, ...)
- Smaller minibatches improve generalization because of the random error
  - The best for this is a minibatch of 1, but this takes much longer to train
- In practice, minibatch size will probably be limited by RAM.

Training

- Minibatch of 10



- Minibatch of 1



- Note: the actual time is much longer for minibatch of 1

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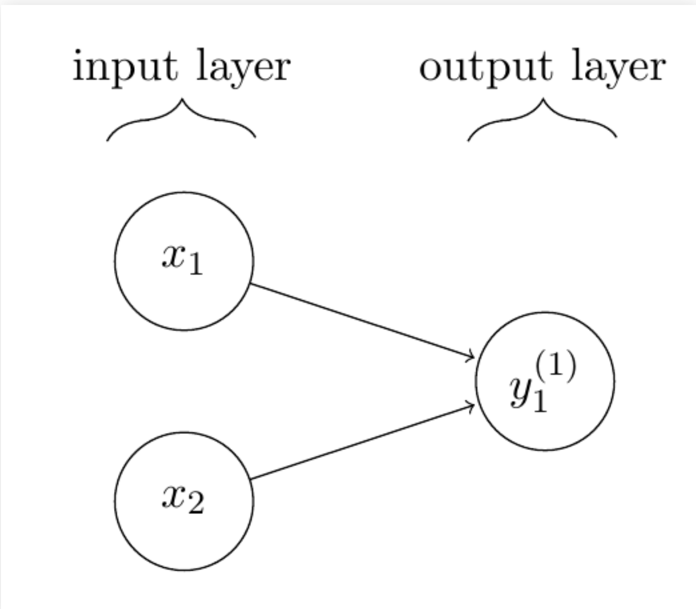
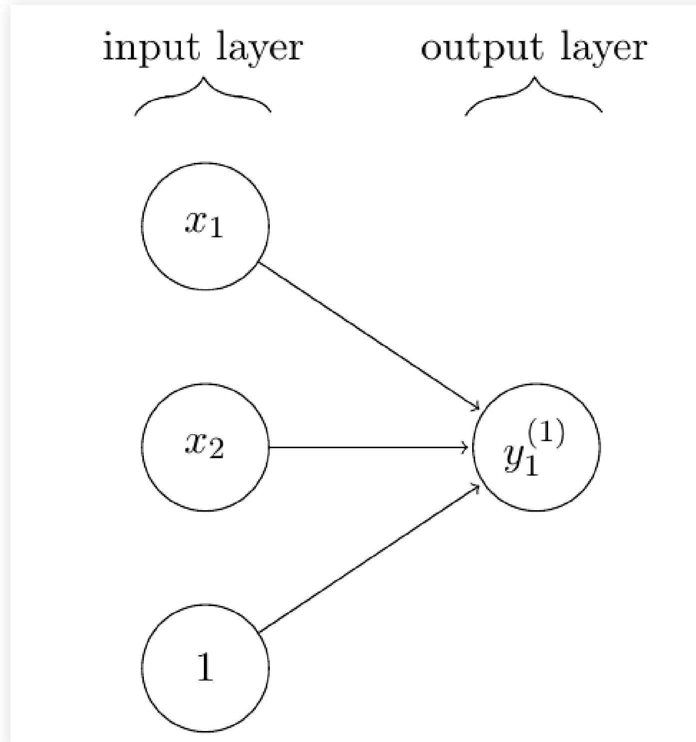
Improving the model

Our simple (pseudo) neuron lacks a bias

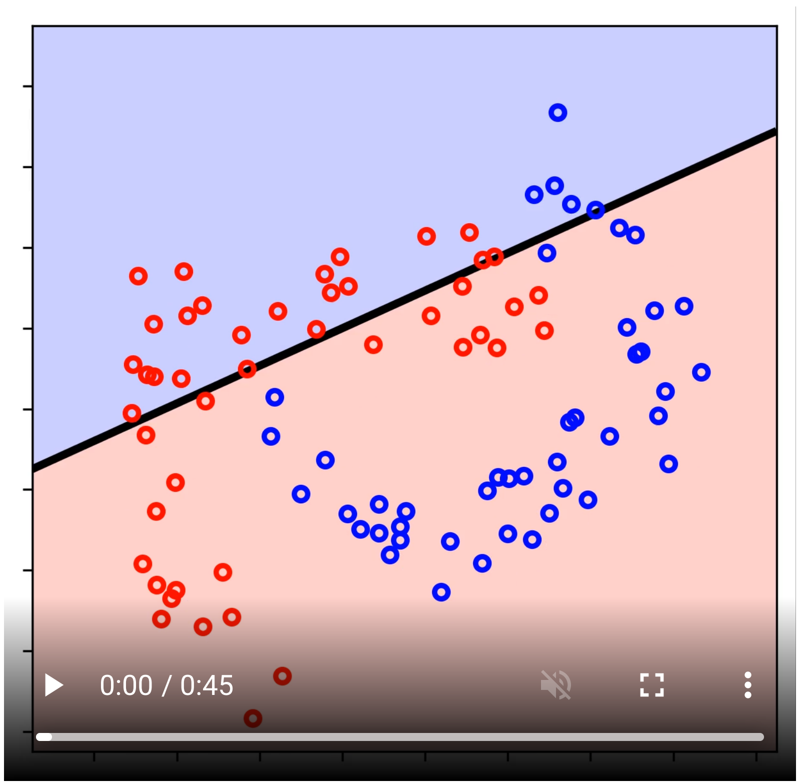
$$y = \sum_{j=1}^{2} w_j x_j + bias$$



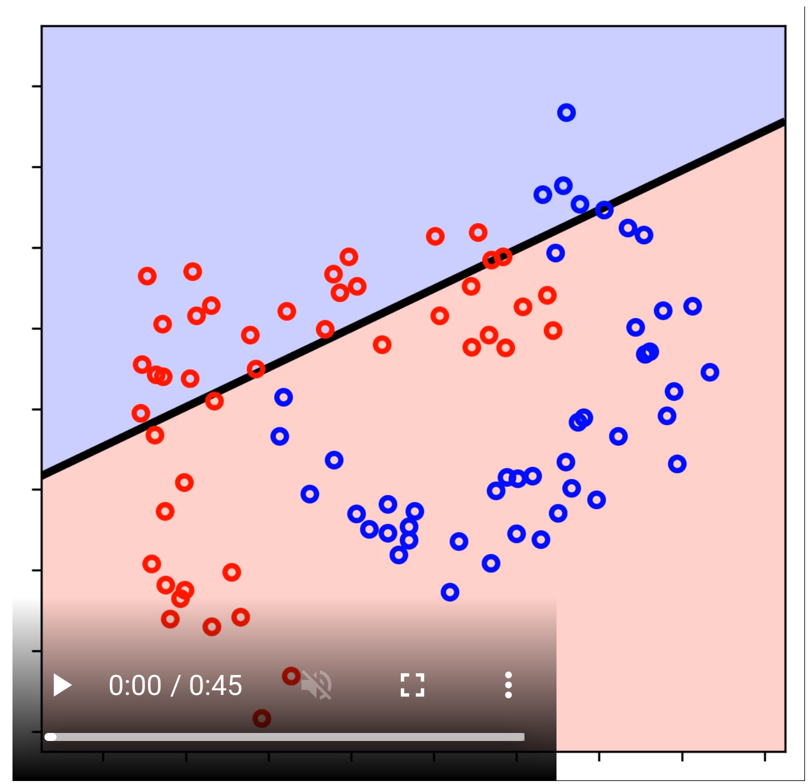


Our simple (pseudo) neuron lacks a bias

- This means that it is stuck a (0,0)
  - No bias input

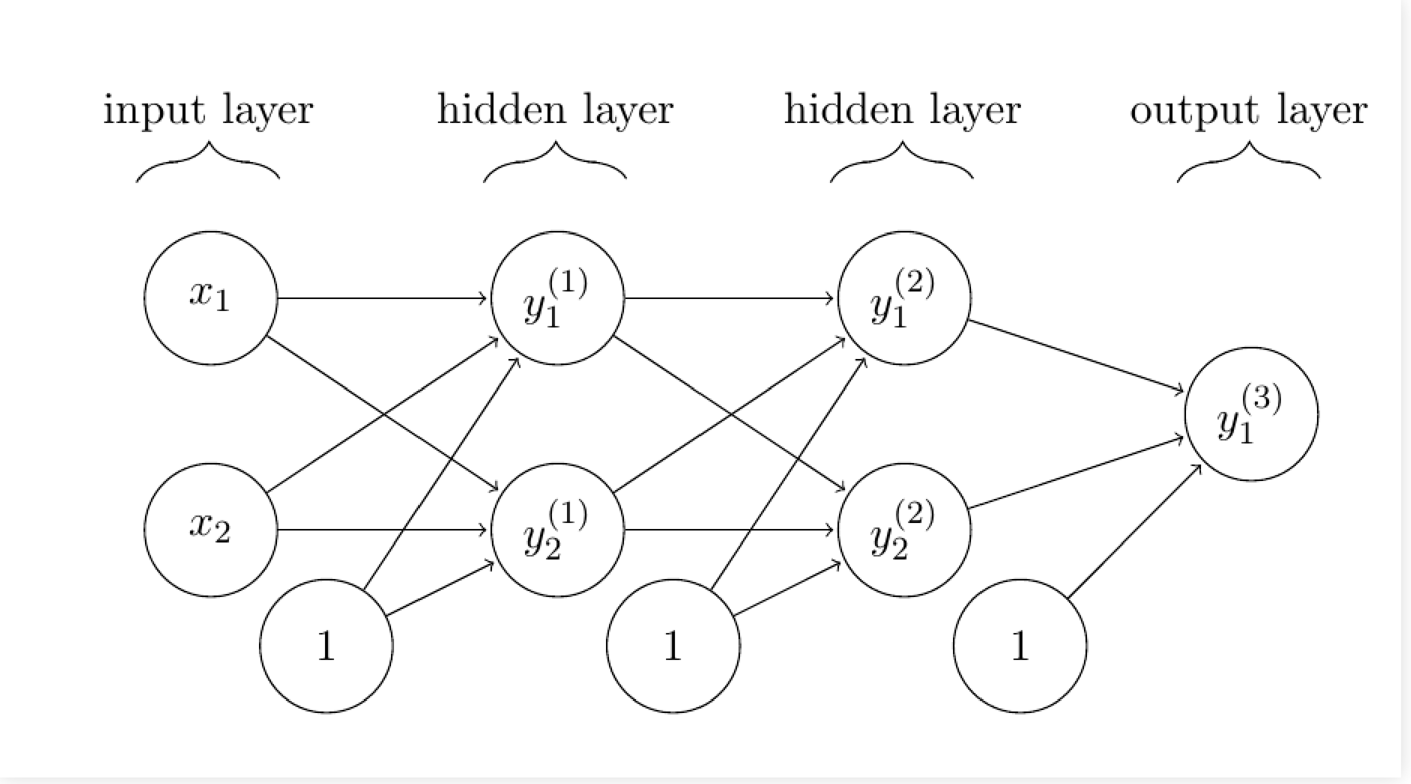


  - With bias input

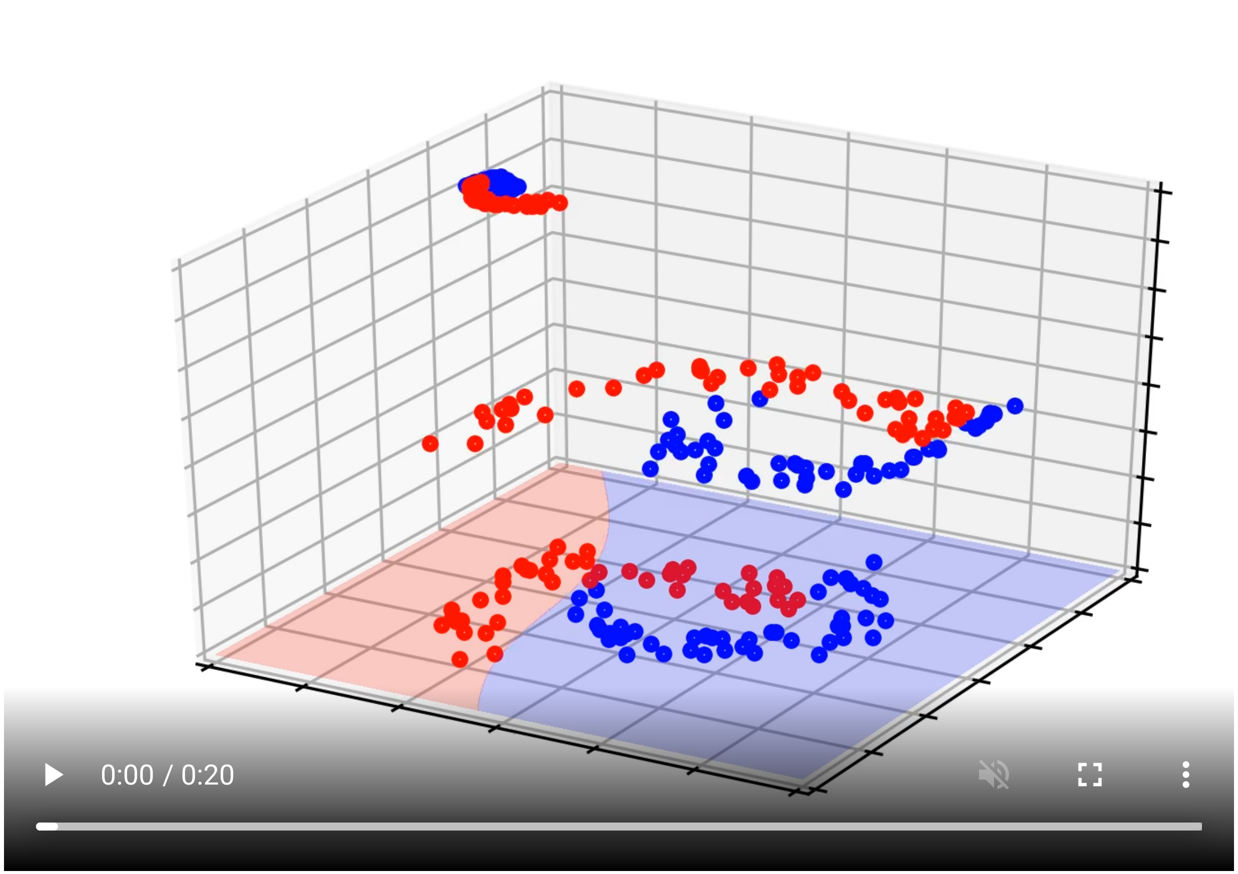


And one neuron cannot properly separate these set

- We need a better model:



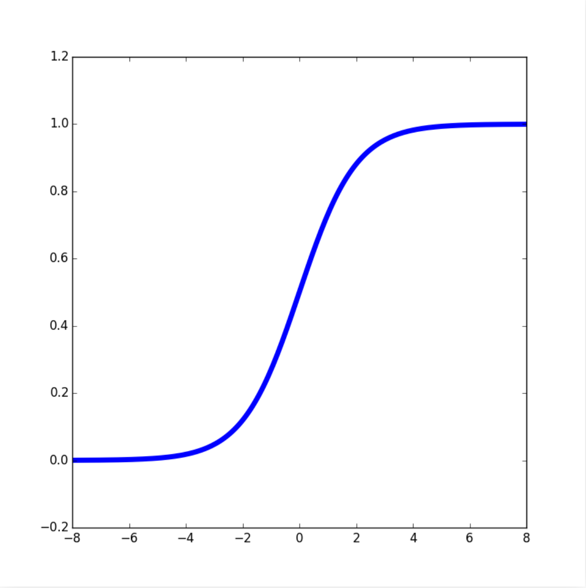
With two hidden layers it works better



Other Details

Initialization

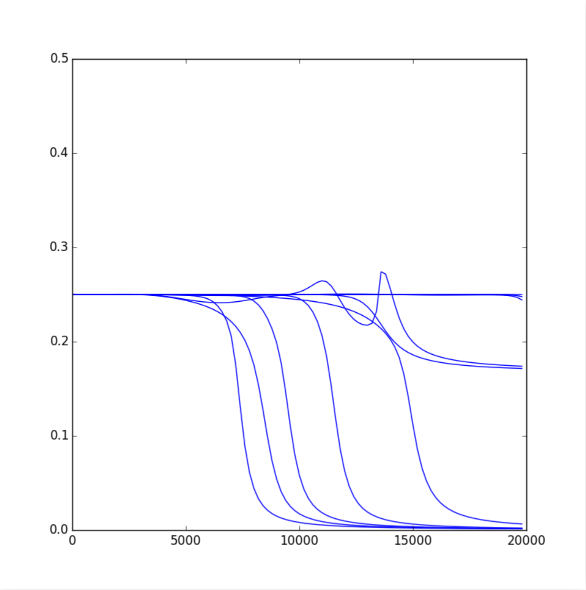
- Weights: random values close to zero (Gaussian or uniform p.d)
  - Need to break symmetry between neurons (but bias can start the same)
  - Some activations (e.g. sigmoid) saturate rapidly away from zero



- (There are other, more sophisticated, methods)

Convergence

- Since weight initialization and order of examples is random, expect different runs to converge at different epochs

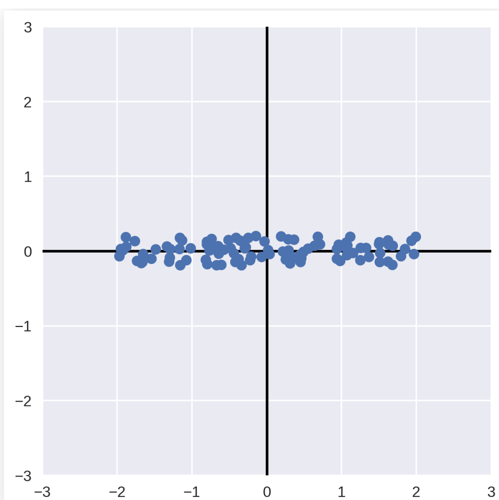


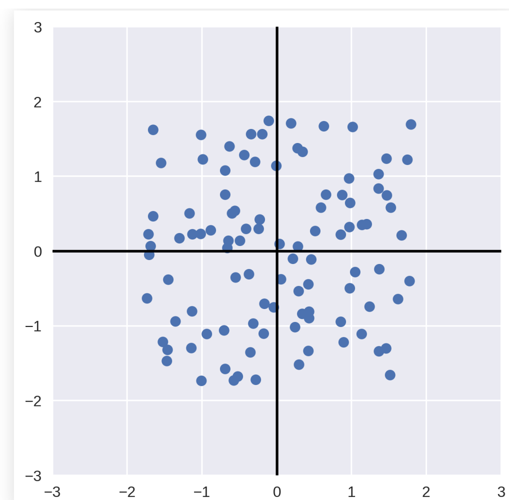
Other Details

Convergence

- Standardize the inputs: $x_{new} = \frac{x - \mu(X)}{\sigma(X)}$

- It is best to avoid different features weighing differentely
- It is also best to avoid very large or tiny values due to numerical problems
- Shifting the mean of the inputs to 0 and scaling the different dimensions also improves the loss function "landscape"





Other Details

Training schedules

- Epoch: one full pass through the training data
- Mini-batch: one batch with part of the training data

Generally needs many epochs to train

- (the greater the data set, the fewer the epochs, other things being equal)

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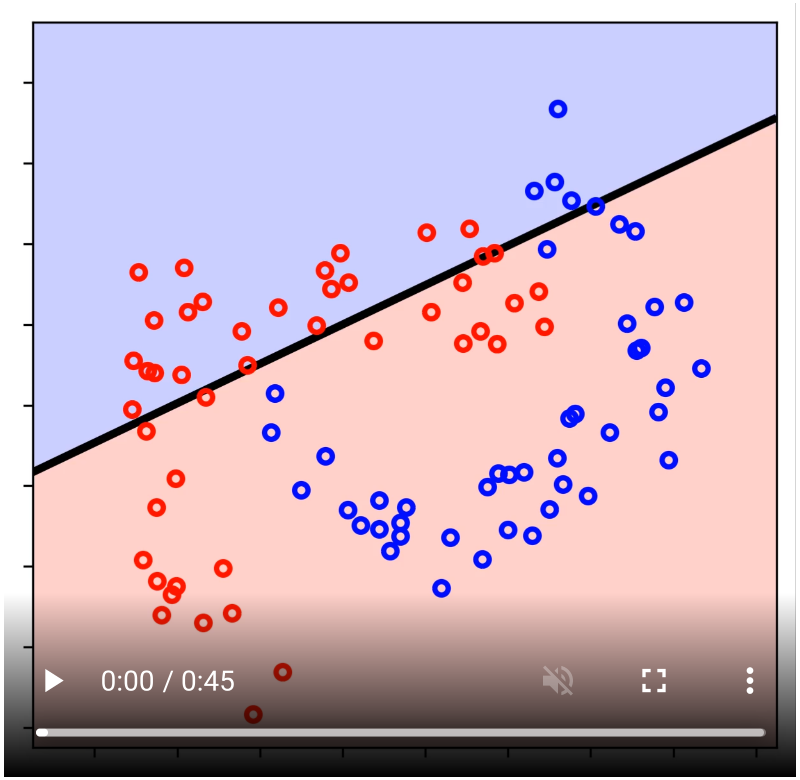
Shuffle the data in each epoch

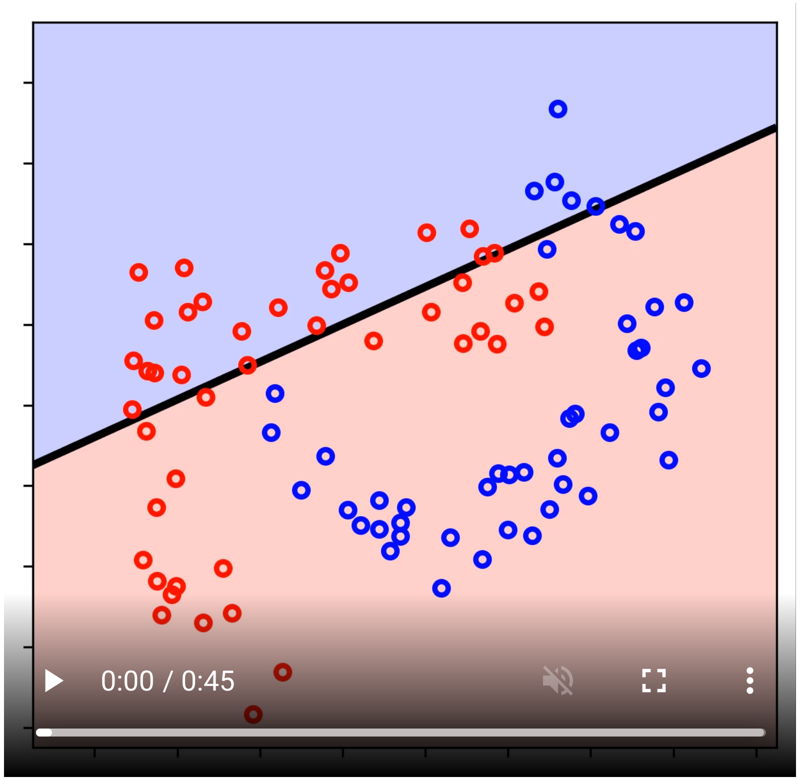
- Otherwise some patterns will repeat



Other Details

Take care with the learning rate

- Too small and training takes too long
- But if it is too large convergence is poor at the end



Summary

Training Neural Networks

Summary

- Matrix algebra
- Automatic Differentiation
- Layers and nonlinear transformations
- Training multilayer feedforward neural networks
  - MLP is a special case, fully connected

Further reading:

- Goodfellow, chapters 2 (algebra), 4 (calculus) and 8 (optimization)