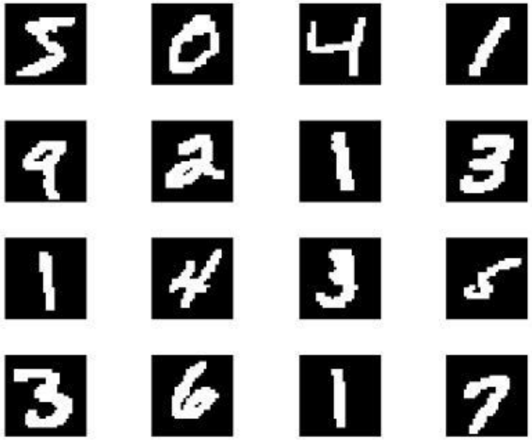
Neural Networks

Nicholas Ruozzi

University of Texas at Dallas

Handwritten Digit Recognition

- Given a collection of handwritten digits and their corresponding labels, we'd like to be able to correctly classify handwritten digits
  - A simple algorithmic technique can solve this problem with 95% accuracy
    - State-of-the-art methods can achieve near 99% accuracy (you've probably seen these in action if you've deposited a check recently)



Digits from the MNIST data set

Neural Networks

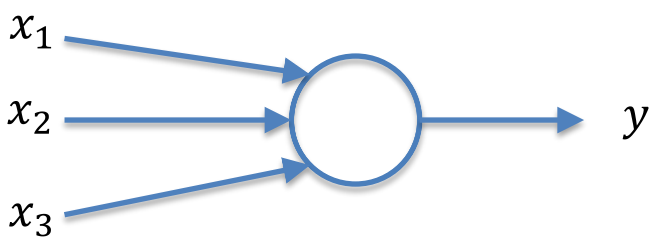
- The basis of neural networks was developed in the 1940s -1960s
  - The idea was to build mathematical models that might "compute" in the same way that neurons in the brain do
  - As a result, neural networks are biologically inspired, though many of the algorithms developed for them are not biologically plausible
  - Perform surprisingly well for the handwritten digit recognition task (and many others)

Neural Networks

- Neural networks consist of a collection of artificial neurons
- There are different types of neuron models that are commonly studied
  - The perceptron (one of the first studied)
  - The sigmoid neuron (one of the most common, but many more)
  - Rectified linear units
- A neural network is a directed graph consisting of a collection of neurons (the nodes), directed edges (each with an associated weight), and a collection of fixed binary inputs

The Perceptron

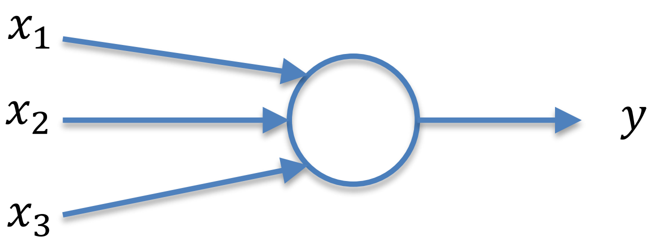
- A perceptron is an artificial neuron that takes a collection of binary inputs and produces a binary output
  - The output of the perceptron is determined by summing up the weighted inputs and thresholding the result: if the weighted sum is larger than the threshold, the output is one (and zero otherwise)



$$y = \begin{cases} 1 & w_1x_1 + w_2x_2 + w_3x_3 > threshold \\ 0 & otherwise \end{cases}$$

Perceptrons

- Perceptrons are usually expressed in terms of a collection of input weights and a bias b (which is the negative threshold)

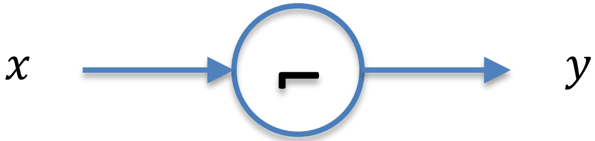


$$y = \begin{cases} 1 & w_1x_1 + w_2x_2 + w_3x_3 + b > 0 \\ 0 & otherwise \end{cases}$$

- A single node perceptron is just a linear classifier

- This is actually where the “perceptron algorithm” comes from

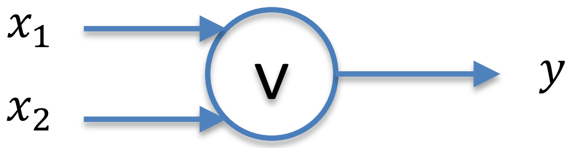
Perceptron for NOT



- Choose $w = -1$, threshold $= -.5$
- $y = \begin{cases} 1 & -x > -.5 \\ 0 & -x \leq -.5 \end{cases}$

Perceptron for OR

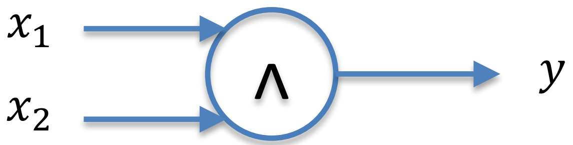
Perceptron for OR



- Choose $w_1 = w_2 = 1$, threshold $= 0$
- $y = \begin{cases} 1 & x_1 + x_2 > 0 \\ 0 & x_1 + x_2 \leq 0 \end{cases}$

Perceptron for AND

Perceptron for AND



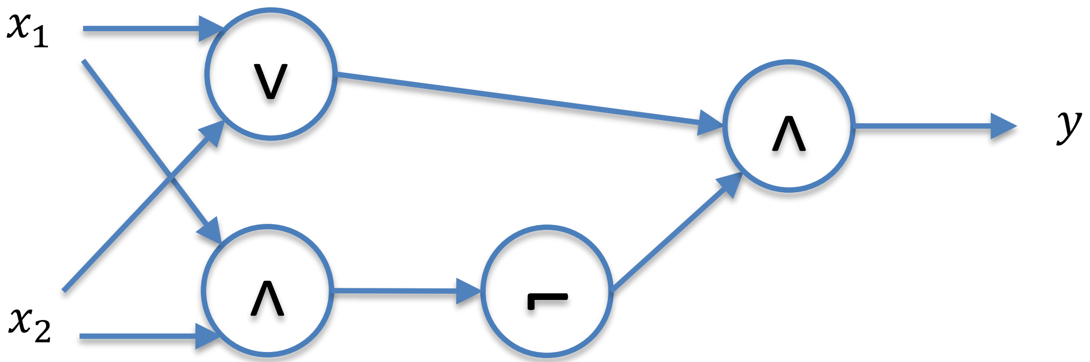
- Choose $w_1 = w_2 = 1$, threshold $= 1.5$

- $y = \begin{cases} 1 & x_1 + x_2 > 1.5 \\ 0 & x_1 + x_2 \leq 1.5 \end{cases}$

Perceptron for XOR

Perceptron for XOR

- Need more than one perceptron!



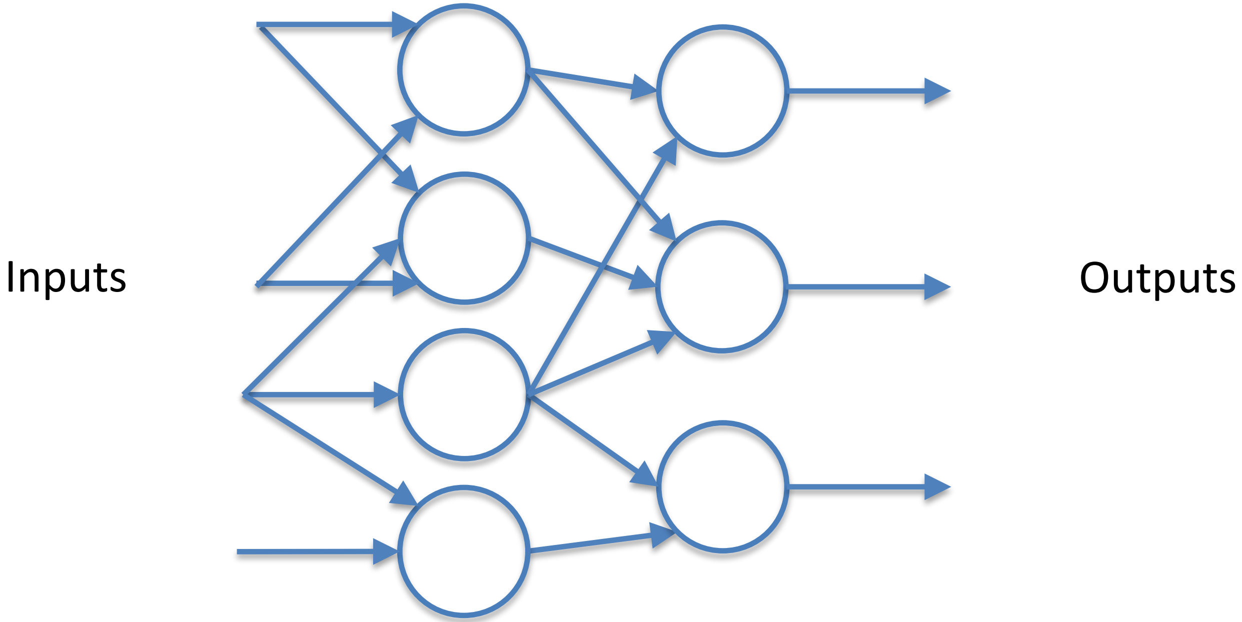
- Weights for incoming edges are chosen as before

- Networks of perceptrons can encode any circuit!

Neural Networks

- Gluing a bunch of perceptrons together gives us a neural network

- In general, neural nets have a collection of binary inputs and a collection of binary outputs

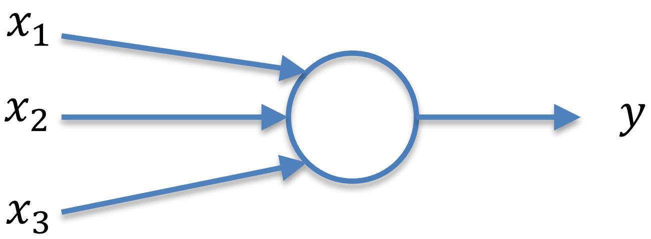


Beyond Perceptrons

- Given a collection of input-output pairs, we'd like to learn the weights of the neural network so that we can correctly predict the output of an unseen input
  - We could try learning via gradient descent (e.g., by minimizing the Hamming loss)
    - This approach doesn't work so well: small changes in the weights can cause dramatic changes in the output
    - This is a consequence of the discontinuity of sharp thresholding (same problem we saw with perceptron alg.)

The Sigmoid Neuron

- A sigmoid neuron is an artificial neuron that takes a collection of real inputs and produces an output in the interval [0,1]
  - The output is determined by summing up the weighted inputs plus the bias and applying the sigmoid function to the result



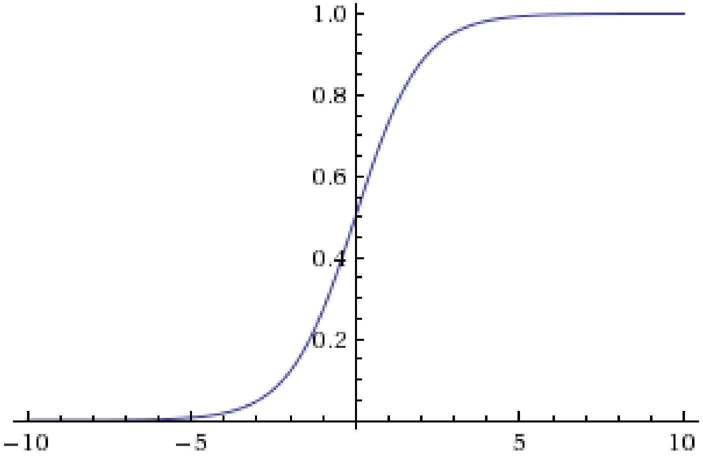
$$y = \sigma(w_1 x_1 + w_2 x_2 + w_3 x_3 + b)$$

where σ is the sigmoid function

The Sigmoid Function

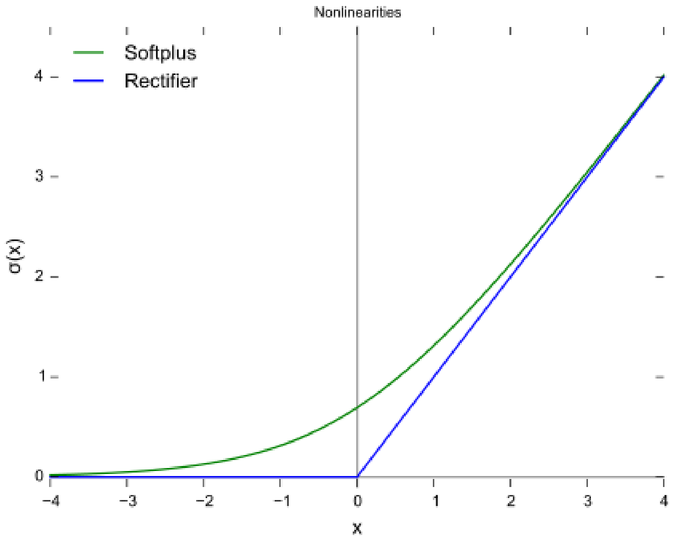
- The sigmoid function is a continuous function that approximates a step function

$$\sigma(z) = \frac{1}{1+e^{-z}}$$



Rectified Linear Units

- The sigmoid neuron approximates a step function as a smooth function
- The relu is given by $\max(0, x)$ which can be approximated as a smooth continuous function $\ln(1 + e^{x})$



Softmax

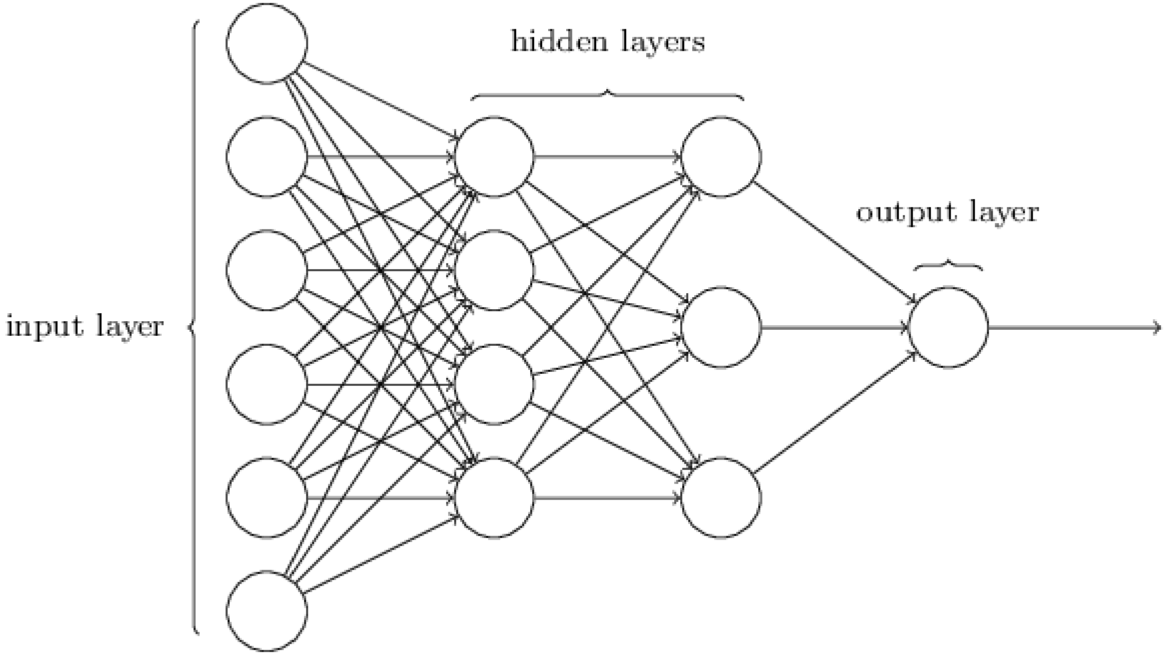
- The softmax function maps a vector of real numbers to a vector of probabilities as

$$\text{softmax}(z)_j = \frac{e^{z_j}}{\sum_k e^{z_k}}$$

- If there is a dominant value in z, then it will become one under the softmax

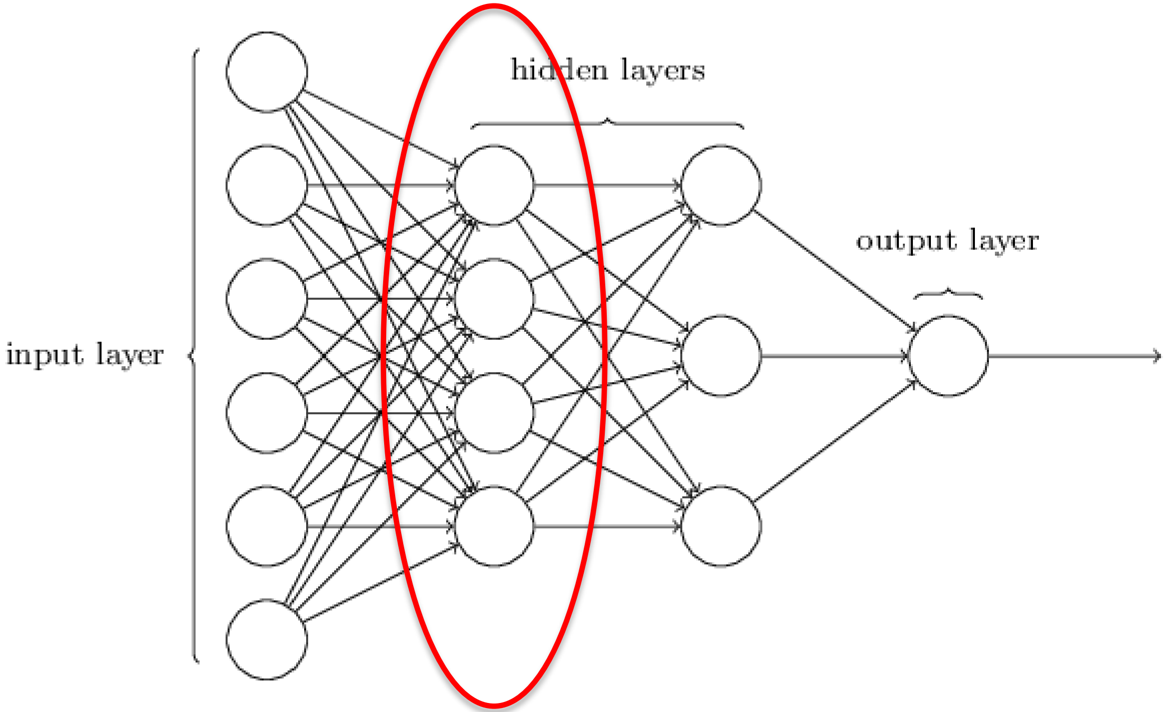
- Often used as the final layer of a neural network

Multilayer Neural Networks



from Neural Networks and Deep Learning by Michael Nielson

Multilayer Neural Networks



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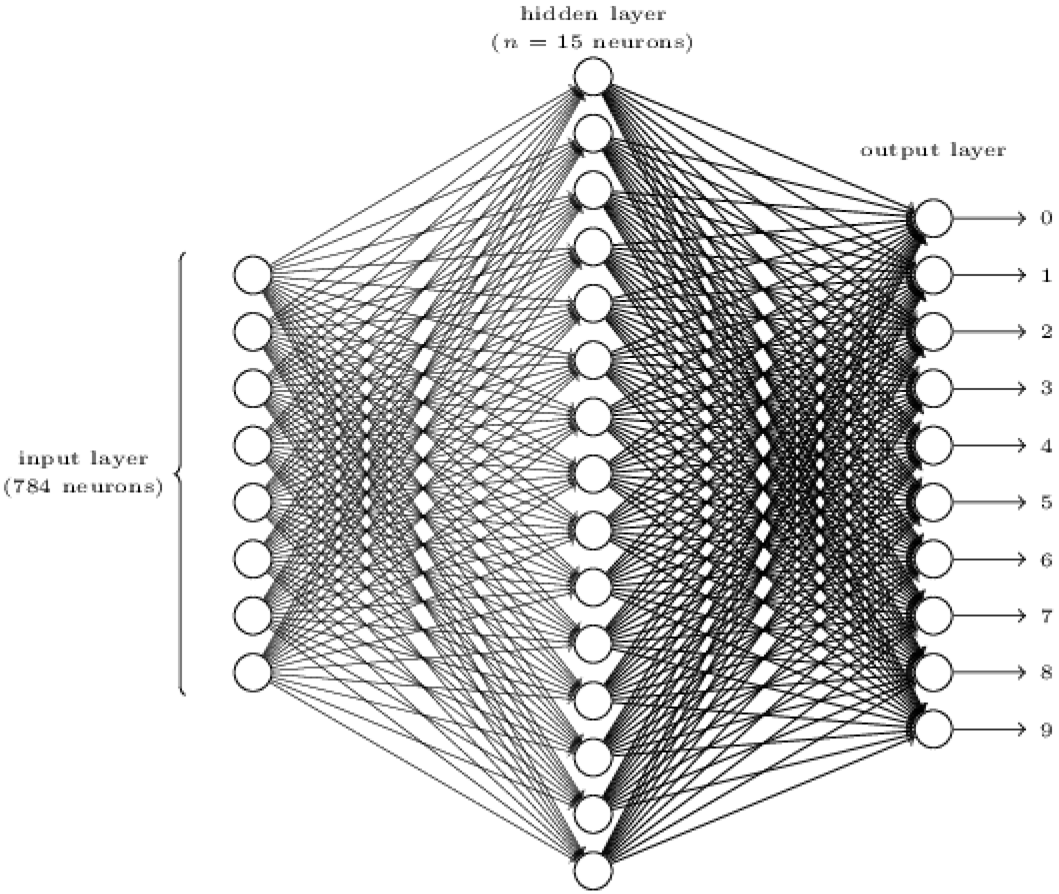
Neural Network for Digit Classification



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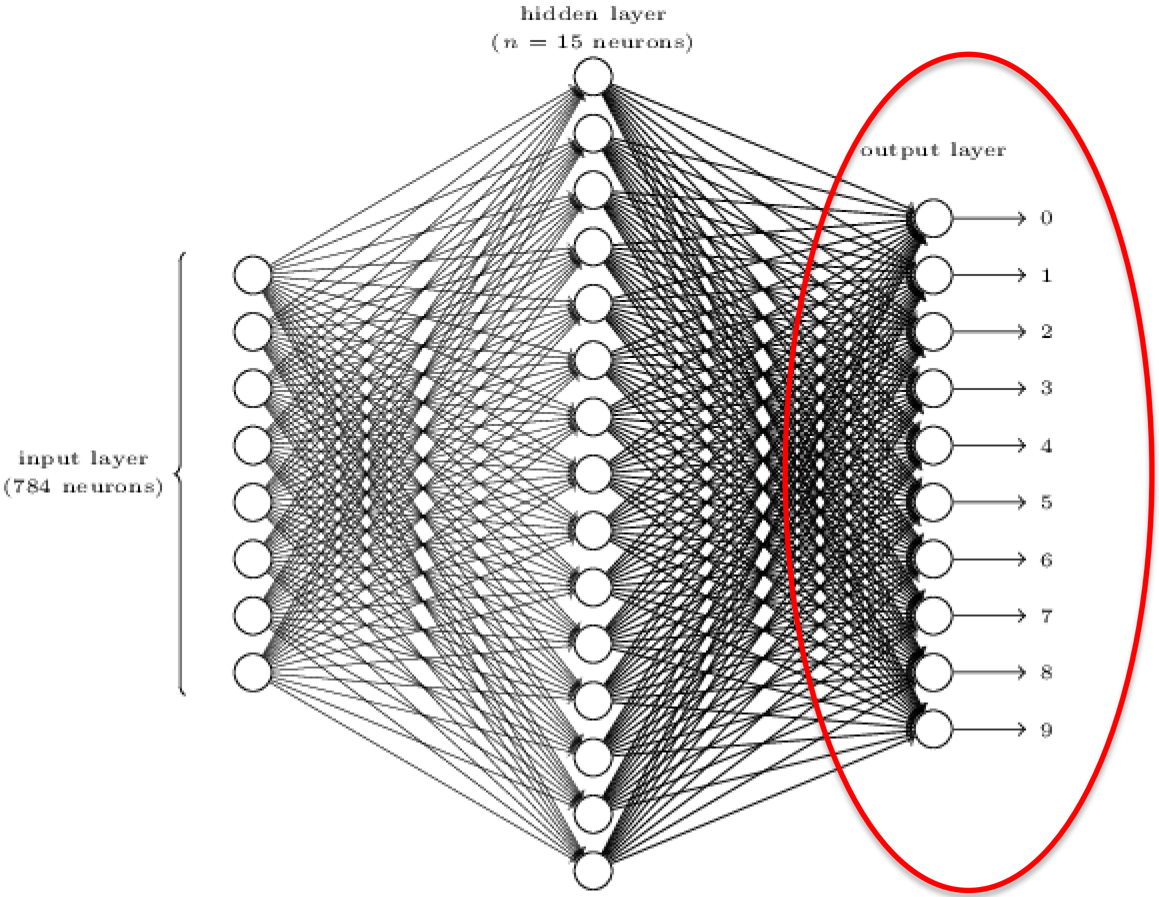


Why 10
instead of 4?

from Neural Networks and Deep Learning by Michael Nielson

Expressiveness of NNs

- Boolean functions
  - Every Boolean function can be represented by a network with a single hidden layer consisting of possibly exponentially many hidden units
- Continuous functions
  - Every bounded continuous function can be approximated up to arbitrarily small error by a network with one hidden layer
  - Any function can be approximated to arbitrary accuracy with two hidden layers

Expressiveness of NNs

- **Theorem [Zhang et al. 2016]:** There exists a two-layer neural network with ReLU activations and $2n + d$ weights that can represent any function on a sample of size n in d dimensions
  - This should mean that it is very easy to overfit with neural networks
  - Generalization performance of networks is difficult to assess theoretically

Training Neural Networks

- To do the learning, we first need to define a loss function to minimize

$$C(w, b) = \frac{1}{2M} \sum_{m} \| y^m - a(x^m, w, b) \|^2$$

- The training data consists of input output pairs $(x^1, y^1), \ldots, (x^M, y^M)$
- $a(x^m, w, b)$ is the output of the neural network for the m^{th} sample
- w and b are the weights and biases

Gradient of the Loss

- The derivative of the loss function is calculated as follows

$$\frac{\partial C(w,b)}{\partial w_k} = \frac{1}{M}\sum_m [y^m - a(x^m,w,b)]\frac{\partial a(x^m,w,b)}{\partial w_k}$$

  - To compute the derivative of a, use the chain rule and the derivative of the sigmoid function

$$\frac{d\sigma(z)}{dz} = \sigma(z)\cdot(1-\sigma(z))$$

  - This gets complicated quickly with lots of layers of neurons

Stochastic Gradient Descent

- To make the training more practical, stochastic gradient descent is used instead of standard gradient descent

- Recall, the idea of stochastic gradient descent is to approximate the gradient of a sum by sampling a few indices and averaging

$$\nabla_x \sum_{i=1}^{n} f_i(x) \approx \frac{1}{K} \sum_{k=1}^{K} \nabla_x f_{i^k}(x)$$

here, for example, each i^k is sampled uniformly at random from $\{1, \dots, n\}$

Computing the Gradient

- We'll compute the gradient for a single sample

$$C(w,b) = \frac{1}{2}\|y - a(x,w,b)\|^2$$

- Some definitions:
  - L is the number of layers
  - a_j^l is the output of the j^{th} neuron on the l^{th} layer
  - z_j^l is the weighted input of the j^{th} neuron on the l^{th} layer

$$z_j^l = \sum_k w_{jk}^l a_k^{l-1} + b_j^l$$

  - δ_j^l is defined to be $\frac{\partial C}{\partial z_j^l}$

Computing the Gradient

For the output layer, we have the following partial derivative

$$\frac{\partial C}{\partial z_j^L} = -\left(y_j - a_j^L\right)\frac{\partial a_j^L}{\partial z_j^L}$$

$$= -\left(y_j - a_j^L\right)\frac{\partial \sigma\left(z_j^L\right)}{\partial z_j^L}$$

$$= -\left(y_j - a_j^L\right)\sigma\left(z_j^L\right)\left(1 - \sigma\left(z_j^L\right)\right)$$

$$= \delta_j^L$$

- For simplicity, we will denote the vector of all such partials for each node in the l^{th} layer as δ^l

Computing the Gradient

For the $L-1$ layer, we have the following partial derivative

$$
\begin{aligned}
\frac{\partial C}{\partial z_k^{L-1}} &= \sum_j \left(a_j^L - y_j\right) \frac{\partial a_j^L}{\partial z_k^{L-1}} \\
&= \sum_j \left(a_j^L - y_j\right) \frac{\partial \sigma\left(z_j^L\right)}{\partial z_k^{L-1}} \\
&= \sum_j \left(a_j^L - y_j\right) \sigma\left(z_j^L\right) \left(1 - \sigma\left(z_j^L\right)\right) \frac{\partial z_j^L}{\partial z_k^{L-1}} \\
&= \sum_j \left(a_j^L - y_j\right) \sigma\left(z_j^L\right) \left(1 - \sigma\left(z_j^L\right)\right) \frac{\partial \sum_{k'} w_{jk'}^L a_{k'}^{L-1} + b_j^L}{\partial z_k^{L-1}} \\
&= \sum_j \left(a_j^L - y_j\right) \sigma\left(z_j^L\right) \left(1 - \sigma\left(z_j^L\right)\right) \sigma\left(z_k^{L-1}\right) \left(1 - \sigma\left(z_k^{L-1}\right)\right) w_{jk}^L \\
&= \left(\left(\delta^L\right)^T w_{*k}^L\right) \left(1 - \sigma\left(z_k^{L-1}\right)\right) \sigma\left(z_k^{L-1}\right)
\end{aligned}
$$

Computing the Gradient

- We can think of w^l as a matrix
- This allows us to write

$$\delta^{L-1} = \left((\delta^L)^T w^L\right)^T \circ \left(1 - \sigma(z^{L-1})\right) \circ \sigma(z^{L-1}\ )$$

where $\sigma(z^{L-1})$ is the vector whose k^{th} component is $\sigma\left(z_k^{L-1}\right)$

- Applying the same strategy, for $l < L$

$$\delta^l = \left(\left(\delta^{l+1}\right)^T w^{l+1}\right)^T \circ \left(1 - \sigma\left(z^l\right)\right) \circ \sigma\left(z^l\ \right)$$

Computing the Gradient

- Now, for the partial derivatives that we care about

$$\frac{\partial C}{\partial b_j^l} = \frac{\partial C}{\partial z_j^l} \cdot \frac{\partial z_j^l}{\partial b_j^l} = \delta_j^l$$

$$\frac{\partial C}{\partial w_{jk}^l} = \frac{\partial C}{\partial z_j^l} \cdot \frac{\partial z_j^l}{\partial w_{jk}^l} = \delta_j^l a_k^{l-1}$$

- We can compute these derivatives one layer at a time!

Backpropagation

- Compute the inputs/outputs for each layer by starting at the input layer and applying the sigmoid functions

- Compute δ^L for the output layer

$$\delta_j^L = -(y_j - a_j^L)\,\sigma(z_j^L)\left(1 - \sigma(z_j^L)\right)$$

- Starting from $l = L - 1$ and working backwards, compute

$$\delta^l = \left(\left(\delta^{l+1}\right)^T w^{l+1}\right)^T \circ \sigma(z^l) \circ \left(1 - \sigma(z^l)\right)$$

- Perform gradient descent

$$b_j^l = b_j^l - \gamma \cdot \delta_j^l$$

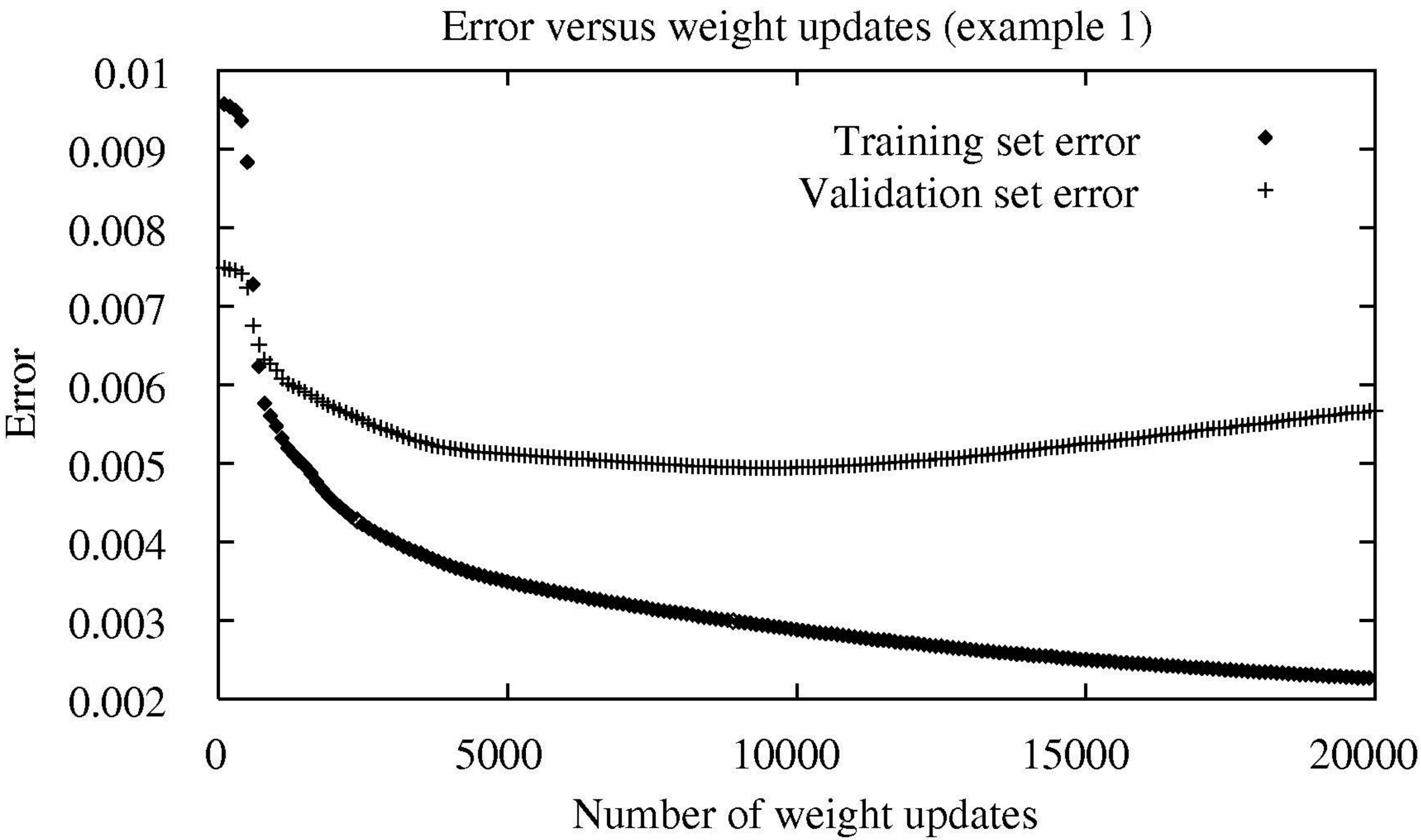
$$w_{jk}^l = w_{jk}^l - \gamma \cdot \delta_j^l a_k^{l-1}$$

Backpropagation

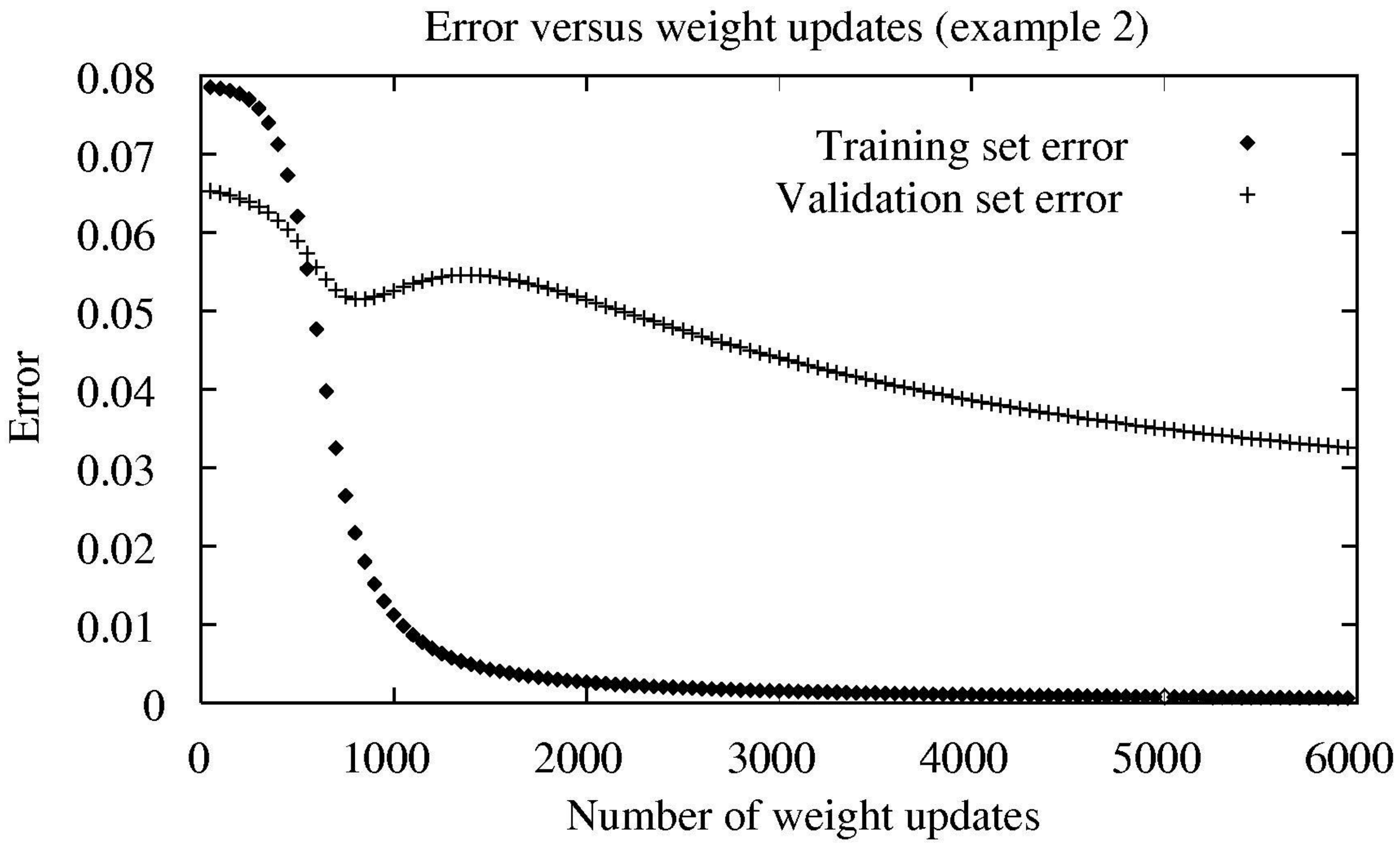
- Backpropagation converges to a local minimum (loss is not convex in the weights and biases)
  - Like EM, can just run it several times with different initializations
  - Training can take a very long time (even with stochastic gradient descent)
  - Prediction after learning is fast
  - Sometimes include a momentum term α in the gradient update

$$w(t) = w(t-1) - \gamma \cdot \nabla_w C(t-1) + \alpha(-\gamma \cdot \nabla_w C(t-2))$$

Overfitting



Overfitting



Neural Networks in Practice

- Many ways to improve weight learning in NNs
  - Use a regularizer!   (better generalization?)

Regularized Loss

- Penalize learning large weights

$$C'^{(w,b)} = \frac{1}{2M}\sum_m \|y^m - a(x^m, w, b)\|^2 + \frac{\lambda}{2}\|w\|_2^2$$

- Can still use the backpropagation algorithm in this setting
- ℓ_1 regularization can also be useful
- Regularization can help with convergence, λ should be chosen with a validation set

Neural Networks in Practice

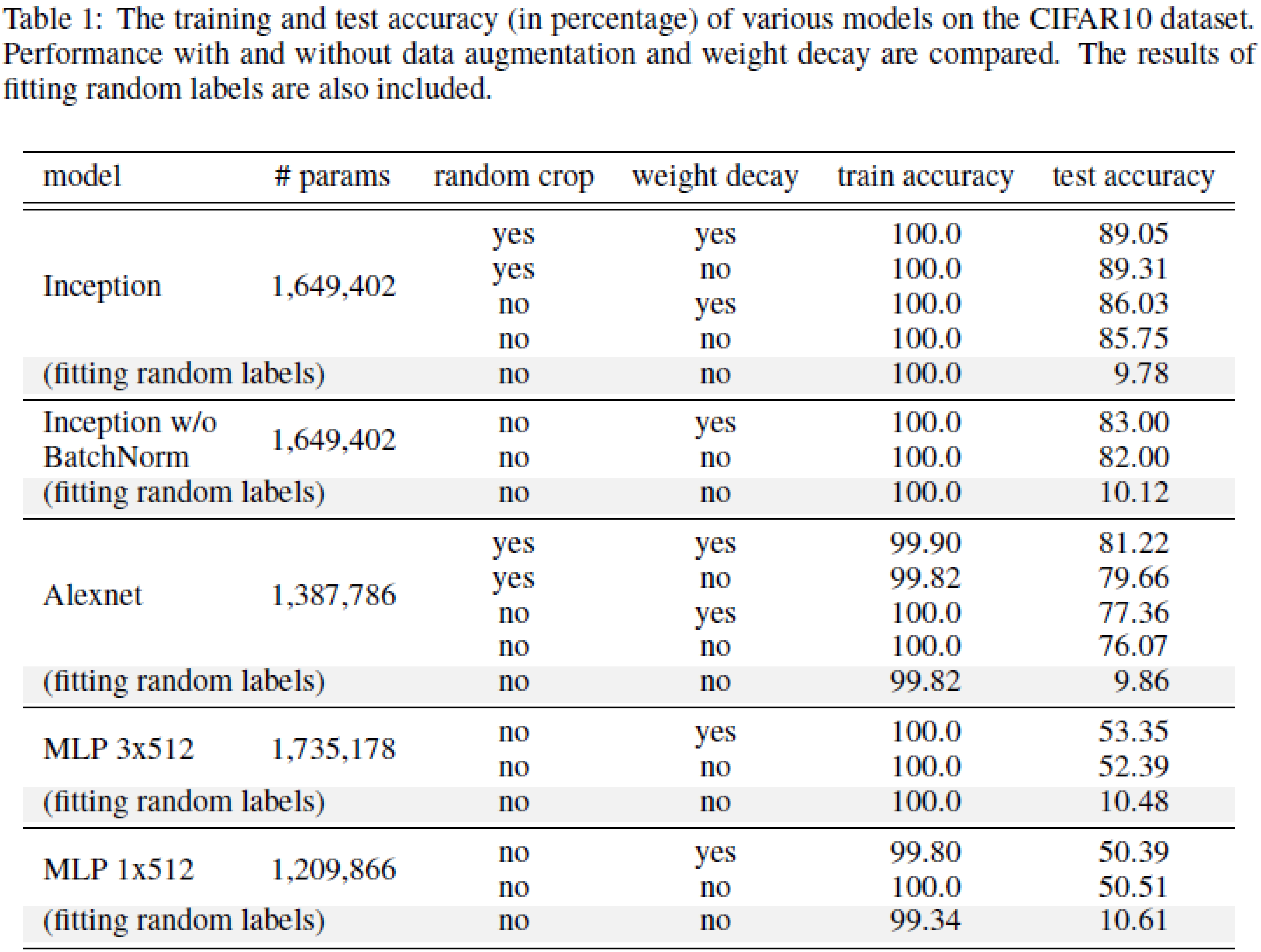


Table 1: The training and test accuracy (in percentage) of various models on the CIFAR10 dataset. Performance with and without data augmentation and weight decay are compared. The results of fitting random labels are also included.

model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61

Zhang et al. 2016

Neural Networks in Practice

- Many ways to improve weight learning in NNs
  - Use a regularizer! (better generalization?)
  - Try other loss functions, e.g., the cross entropy

$$-y \log a(x, w, b) - (1 - y) \log(1 - a(x, w, b))$$

  - Initialize the weights of the network more cleverly
    - Random initializations are likely to be far from optimal
- The learning procedure can have numerical difficulties if there are a large number of layers

Dropout

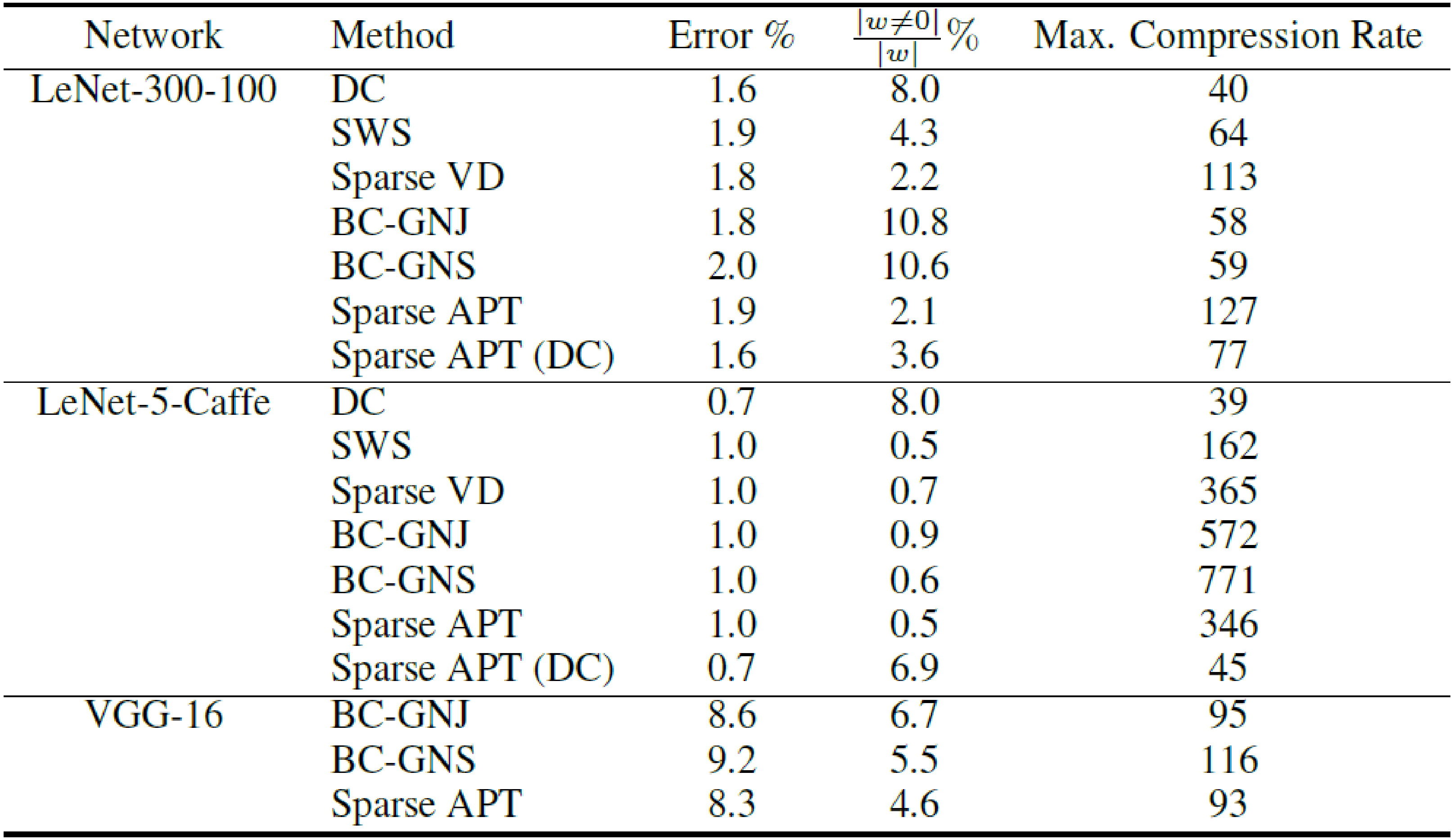
- A heuristic bagging-style approach applied to neural networks to counteract overfitting
  - Randomly remove a certain percentage of the neurons from the network and then train only on the remaining neurons
  - The networks are recombined using an approximate averaging technique (keeping around too many networks and doing proper bagging can be costly in practice)

Other Techniques

- Early stopping
    - Stop the learning early in the hopes that this prevents overfitting
- Parameter tying
    - Assume some of the weights in the model are the same to reduce the dimensionality of the learning problem
    - Also a way to learn “simpler” models
    - Can lead to significant compression in neural networks (i.e., >90%)

Other Techniques

Table 1: Comparison of sparse APT with other compression and/or sparsity-inducing methods.



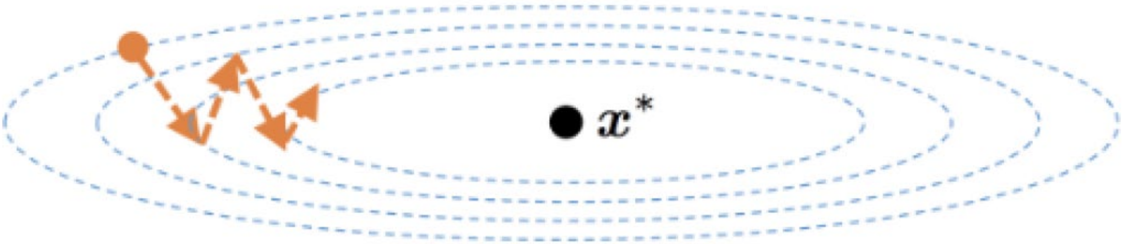
Network	Method	Error %	$\frac{\lvert w \neq 0 \rvert}{\lvert w \rvert}\%$	Max. Compression Rate
LeNet-300-100	DC	1.6	8.0	40
	SWS	1.9	4.3	64
	Sparse VD	1.8	2.2	113
	BC-GNJ	1.8	10.8	58
	BC-GNS	2.0	10.6	59
	Sparse APT	1.9	2.1	127
	Sparse APT (DC)	1.6	3.6	77
LeNet-5-Caffe	DC	0.7	8.0	39
	SWS	1.0	0.5	162
	Sparse VD	1.0	0.7	365
	BC-GNJ	1.0	0.9	572
	BC-GNS	1.0	0.6	771
	Sparse APT	1.0	0.5	346
	Sparse APT (DC)	0.7	6.9	45
VGG-16	BC-GNJ	8.6	6.7	95
	BC-GNS	9.2	5.5	116
	Sparse APT	8.3	4.6	93

Other Ideas

- Convolutional neural networks
  - Instead of the output of every neuron at layer l being used as an input to every neuron at layer $l + 1$, the edges between layers are chosen more locally
  - Many tied weights and biases (i.e., convolution nets apply the same process to many different local chunks of neurons)
  - Often combined with pooling layers (i.e., layers that, say, half the number of neurons by replacing small regions of neurons with their maximum output)
  - Used extensively for image classification tasks

Momentum

- Standard gradient descent does not adjust its step size based on local function information, e.g., curvature of the function
  - This can result in slow convergence



gradient descent

Momentum

- Gradient descent with momentum adds an inertia term

$$x^{(t+1)} = x^{(t)} - \gamma \nabla f\left(x^{(t)}\right) + \beta\left(x^{(t)} - x^{(t-1)}\right)$$

Momentum

- Gradient descent with momentum adds an inertia term

$$x^{(t+1)} = x^{(t)} - \gamma \nabla f\left(x^{(t)}\right) + \beta\left(x^{(t-1)} - \gamma \nabla f\left(x^{(t-1)}\right) - x^{(t-1)}\right)$$

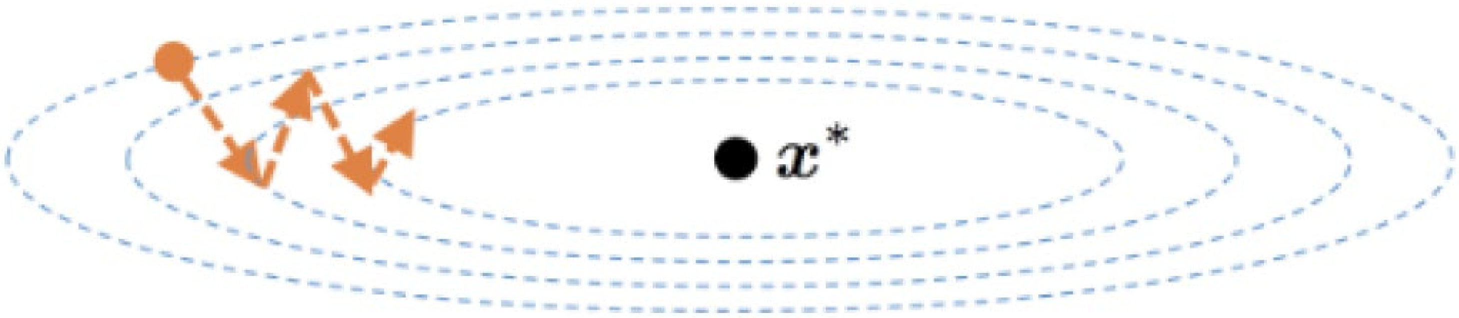
Momentum

- Gradient descent with momentum adds an inertia term

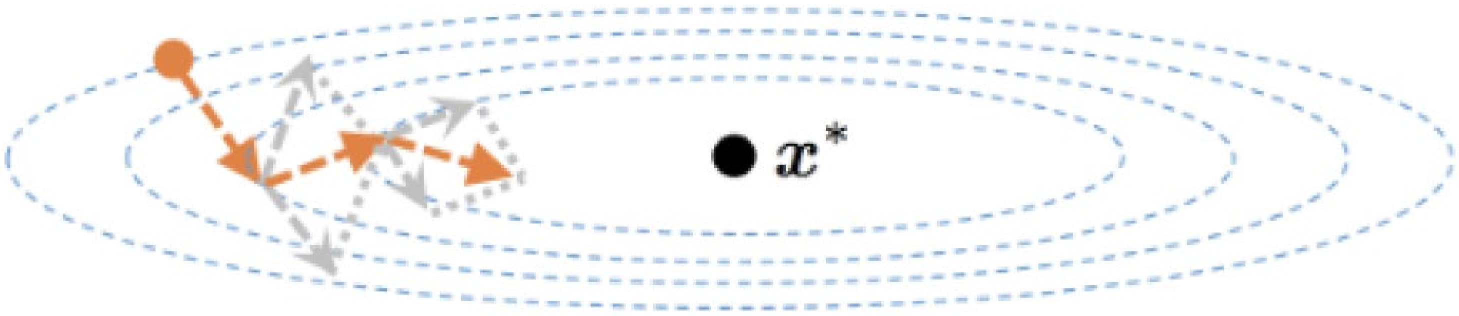
$$x^{(t+1)} = x^{(t)} - \gamma \nabla f\left(x^{(t)}\right) - \gamma \beta \nabla f\left(x^{(t-1)}\right)$$

  - If the gradients are similar in two consecutive times steps you get an extra boost!

Momentum



gradient descent



heavy-ball method

Accelerated Gradient Methods

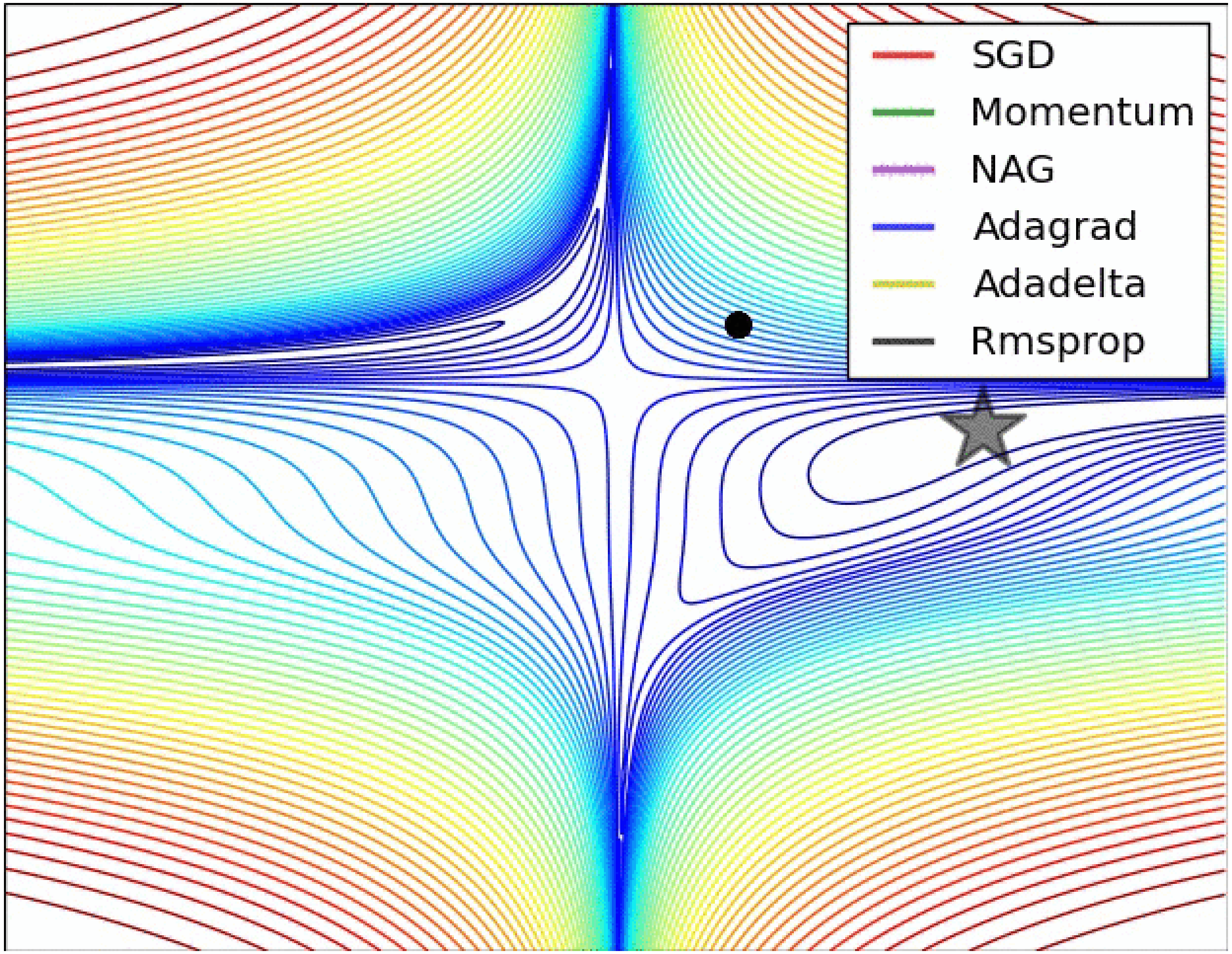


Image: Sebastian Ruder

Neural Networks in Practice

- Oftentimes you have a small amount of labeled training data for your real domain
  - It might not be enough to train a deep NN for the task
  - Can you still apply NNs?

Neural Networks in Practice

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  - Can you still apply NNs?

Yes! Use transfer learning!

Transfer Learning

- Idea: take a model trained in a domain with lots of training data and transfer it to a smaller, data-limited domain
  - The ML task may or may not be the same in both domains
  - Lots of ways to do this… one way is to fine-tune a pretrained model
- Example: Bounding box detection using a pretrained model

Bounding Box Detection

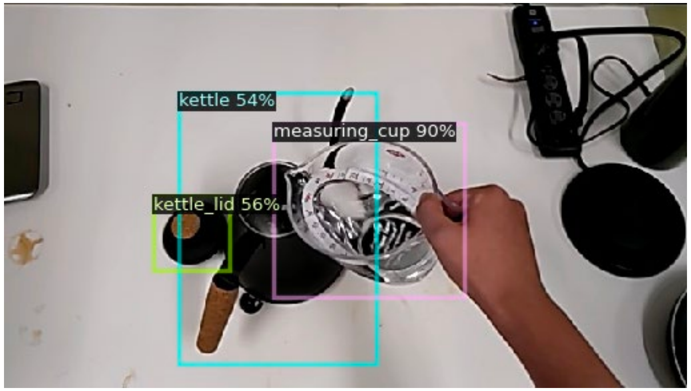
- After 15 training epochs on new training data…
- Confidence threshold = 0.0
  - Ap50 without Training (pretrained weights) = 0.0004
  - Ap50 with Training (trained weights) = 31.64

- Confidence threshold = 0.05
  - Ap50 without Training (pretrained weights) = 0.0002
  - Ap50 with Training (trained weights) = 30.975

- Confidence threshold = 0.3
  - Ap50 without Training (pretrained weights) = nan
  - Ap50 with Training (trained weights) = 28.21

Bounding Box Detection (.3)

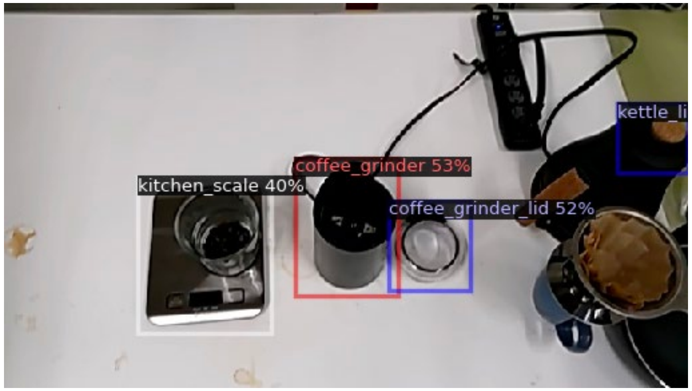
Input image



Trained weights output

Bounding Box Detection (.3)

Input image



Trained weights output