BST 261: Data Science II
Lecture 3

Feedforward networks in Python with Keras, Convolutional Neural Networks (CNNs)

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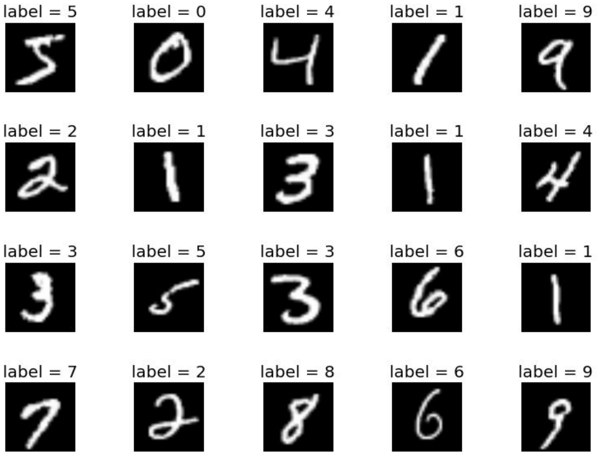
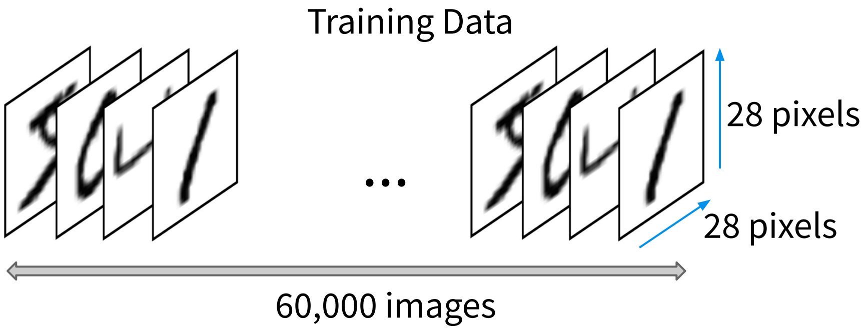
MNIST Data Example

- The MNIST data set includes handwritten digits with corresponding labels

- Training set: 60,000 images of handwritten digits and corresponding labels
    - Each digit is represented as a 28 x 28 matrix of grayscale values 0 - 255
    - The entire training set is stored in a 3D tensor of shape (60000, 28, 28)
    - The corresponding image values are stored as a 1D tensor of values 0 - 9

- Testing set: 10,000 images with the same set up as the training set





MNIST Data Example

Data wrangling

- We’ll get into RGB images later, but for grayscale images, we need to first transform the matrix of values into a vector of values, and then normalize them to be between 0 and 1. It is not strictly necessary to normalize your inputs, but smaller numbers help speed up training and avoid getting stuck in local minima. This also ensures the gradients don’t “explode” or “vanish”
  - Reshape each image from a 28 x 28 matrix of grayscale values 0 - 255 to a vector of length 28*28 = 784 of values 0 - 1 (divide each by 255)

- We now have 10 classes (categories; the digits 0-9)
  - We need to have multiclass labels that tell the network which digit the example is
  - Reshape each corresponding image label to a vector of length 10 of values 0 or 1
  - Example: the digit 3 would be represented as [0, 0, 0, 1, 0, 0, 0, 0, 0, 0]
  - You can think of this as “dummy coding” the labels

Activation and Loss Function Choices

Task	Last-layer activation	Loss function
Binary classification	sigmoid	Binary cross-entropy
Multiclass, single-label classification	softmax	Categorical cross-entropy
Multiclass, multilabel classification	sigmoid	Binary cross-entropy
Regression to arbitrary values	None	Mean square error (MSE)
Regression to values between 0 and 1	sigmoid	MSE or binary cross-entropy

Softmax function

$$\text{softmax}(\boldsymbol{z})_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

- Softmax units are used as outputs when predicting a discrete variable *y* with *k* possible values
- In this setting, which can be seen as a generalization of the Bernoulli distribution, we need to produce a vector $\hat{\mathbf{y}}$ with $\hat{y}_i = P(y = i|x)$
- We require that each $\hat{y}_i$ lie in the [0, 1] interval and that the entire vector sums to 1
- We first compute $z = w^T x + b$ as usual
- Here, $z_i = log[\tilde{P}(y = i|x)]$ represents an unnormalized log probability for class *i*
- The softmax function then exponentiates and normalizes *z* to obtain $\hat{\mathbf{y}}$

Softmax function

- In this case we want to maximize

$$log[P(y = i; z)] = log[\text{softmax}(z)_i] = z_i - log \sum_j exp(z_j)$$

- The first term shows that the input always has a direct contribution to the loss function

- Because $log \sum_j exp(z_j) \approx max_j z_j$, the negative log-likelihood loss function always strongly penalizes the most active incorrect prediction

MNIST Data Example

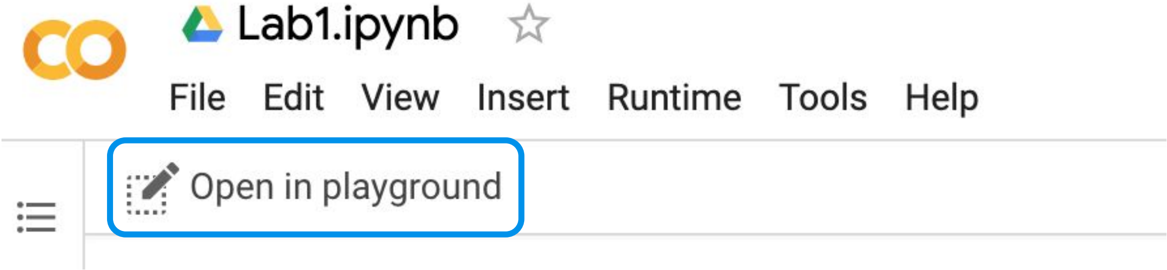
Network Architecture

- Let's start with 2 layers:
  - Hidden layer will have 512 hidden units and the **relu activation function**
  - Output layer with 10 units (one for each possible digit) and the **softmax activation function** (this produces a vector of length 10, where each element is a probability between 0 and 1 of the image being classified as that digit)
  - Example: [0, 0.3, 0, 0, 0, 0, 0, 0.7, 0, 0] - the highest probability corresponds to a label of 7, so the network would classify this image as a 7
  - **rmsprop optimization algorithm**
  - **categorical_crossentropy loss function**
  - **accuracy performance measure** (the proportion of times the correct class is chosen)

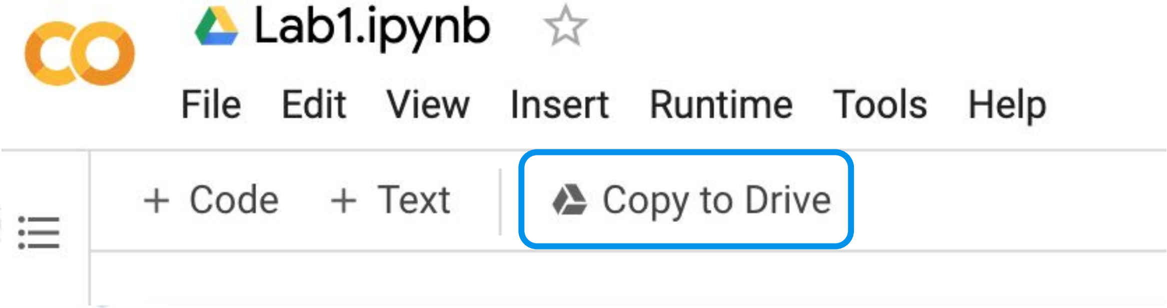
MNIST Data Example

Colab link

Step 1



Step 2



IMDb Data Example

The IMDb data set is a set of movie reviews that have been labeled as either positive or negative, based on the text content of the reviews

- Training set: 25,000 either positive or negative movie reviews that have each been turned into a vector of integers
  - We'll see how to actually do this later in the course
  - Each review can be of any length
  - Only the top 10,000 most frequently occurring words are kept i.e. rare words are discarded
  - Each review includes a label: 0 = negative review and 1 = positive review

- Testing set: 25,000 either positive or negative movie reviews, similar to the training set

IMDb Data Example

Data Wrangling

- Each review is of a varying length and is a list of integers - we need to turn this into a tensor with a common length for each review
- Create a 2D tensor of shape 25,000 x 10,000
  - 25,000 reviews and 10,000 possible words
- Use the **vectorize_sequences** function to turn a movie review list of integers into a vector of length 10,000 with 1s for each word that appears in the review and 0s for words that do not
- The labels are already 0s and 1s, so the only thing we need to do is make them float numbers

Activation and Loss Function Choices

Task	Last-layer activation	Loss function
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Multiclass, single-label classification	softmax	Categorical cross-entropy
Multiclass, multilabel classification	sigmoid	Binary cross-entropy
Regression to arbitrary values	None	Mean square error (MSE)
Regression to values between 0 and 1	sigmoid	MSE or binary cross-entropy

IMDb Data Example

Network Architecture

- 3 layers
  - 2 hidden layers and 1 output layer
  - Hidden layers have 16 hidden units each and a **relu activation function**
  - Output layer has 1 unit (the probability a review is positive)
- **Sigmoid activation function**
- **rmsprop optimization algorithm**
- **binary_crossentropy loss function**
- **accuracy performance measure** (proportion of times the correct class is chosen)

IMDb Data Example

Colab link

Regularization

Regularization

- One of the biggest problems with neural networks is overfitting.
- Regularization schemes combat overfitting in a variety of different ways

A perceptron represents the following optimization problem:

$$\text{argmin}_W l(y, f(X)) \quad \text{where} \quad f(X) = \frac{1}{1+\exp(-\phi(XW))}$$

Regularization

One way to regularize is to introduce penalties and change

$$\text{argmin}_W l(y, f(X))$$

to

$$\text{argmin}_W l(y, f(X)) + \lambda R(W)$$

where R(W) is often the L1 or L2 norm of W. These are the well-known ridge and LASSO penalties, and referred to as **weight decay** by the neural net community.

L2 Regularization

We can limit the size of the L2 norm of the weight vector:

$$\mathrm{argmin}_W l(y, f(X)) + \lambda \|W\|_2$$

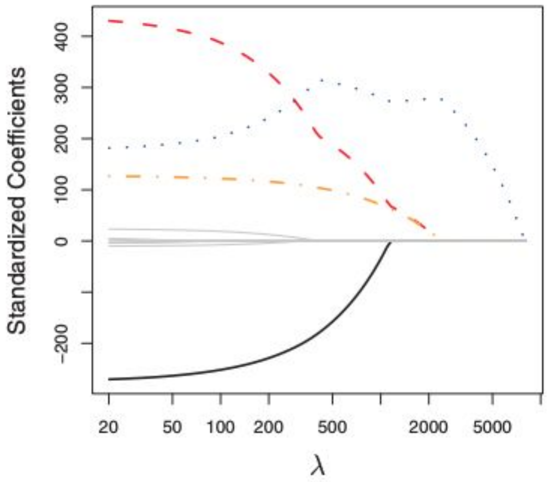
where

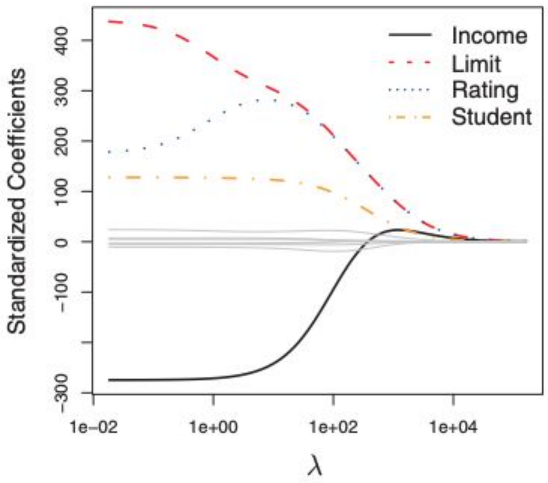
$$\|W\|_2 = \sum_{j=1}^{p} w_j^2$$

We can do the same for the L1 norm. What do the penalties do?

Shrinkage

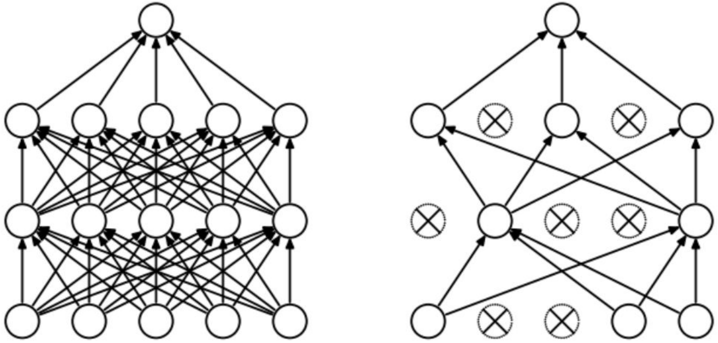
The L1 and L2 penalties shrink the weights to or towards 0.





Stochastic Regularization

- Why is this a good idea?
- One of the most popular ways to do this is **dropout**
- Given a hidden layer, we are going to set each element of the hidden layer to 0 with probability *p* each SGD update.



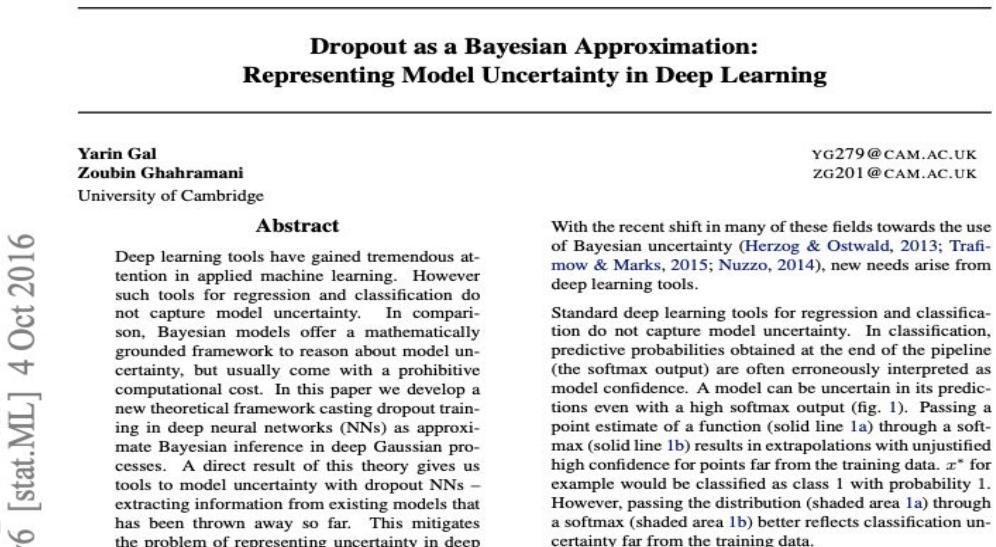
(a) Standard Neural Net

(b) After applying dropout.

https://medium.com/@amarbudhiraja/https-medium-com-amarbudhiraja-learning-less-to-learn-better-dropout-in-deep-machine-learning-74334da4bfc5

Stochastic Regularization

- One way to think of this is the network is trained by bagged versions of the network.
- **Bagging** reduces variance.
- Others have argued this is an approximate Bayesian model



Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning

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Abstract

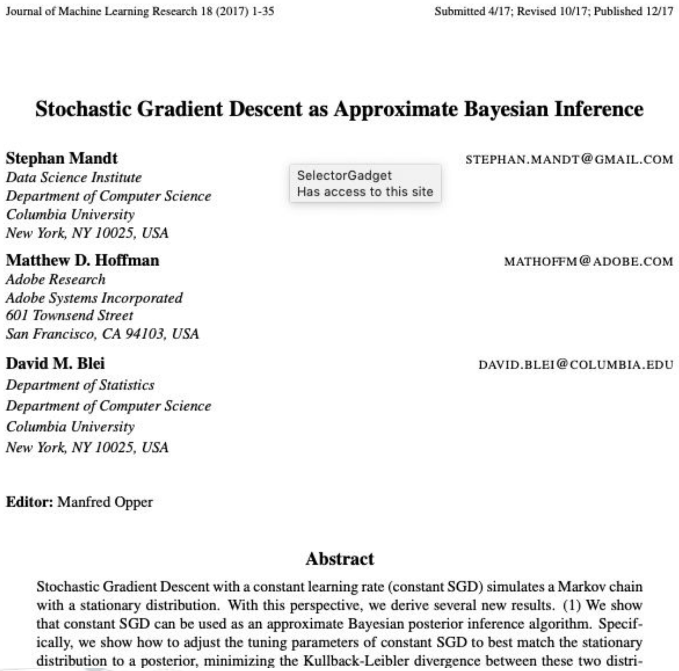
Deep learning tools have gained tremendous attention in applied machine learning. However such tools for regression and classification do not capture model uncertainty. In comparison, Bayesian models offer a mathematically grounded framework to reason about model uncertainty, but usually come with a prohibitive computational cost. In this paper we develop a new theoretical framework casting dropout training in deep neural networks (NNs) as approximate Bayesian inference in deep Gaussian processes. A direct result of this theory gives us tools to model uncertainty with dropout NNs – extracting information from existing models that has been thrown away so far. This mitigates the problem of representing uncertainty in deep

With the recent shift in many of these fields towards the use of Bayesian uncertainty (Herzog & Ostwald, 2013; Trafimow & Marks, 2015; Nuzzo, 2014), new needs arise from deep learning tools.

Standard deep learning tools for regression and classification do not capture model uncertainty. In classification, predictive probabilities obtained at the end of the pipeline (the softmax output) are often erroneously interpreted as model confidence. A model can be uncertain in its predictions even with a high softmax output (fig. 1). Passing a point estimate of a function (solid line 1a) through a softmax (solid line 1b) results in extrapolations with unjustified high confidence for points far from the training data. x^* for example would be classified as class 1 with probability 1. However, passing the distribution (shaded area 1a) through a softmax (shaded area 1b) better reflects classification uncertainty far from the training data.

Stochastic Regularization

- Many have argued that SGD itself provides regularization



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Stochastic Gradient Descent as Approximate Bayesian Inference

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Editor: Manfred Opper

Abstract

Stochastic Gradient Descent with a constant learning rate (constant SGD) simulates a Markov chain with a stationary distribution. With this perspective, we derive several new results. (1) We show that constant SGD can be used as an approximate Bayesian posterior inference algorithm. Specifically, we show how to adjust the tuning parameters of constant SGD to best match the stationary distribution to a posterior, minimizing the Kullback-Leibler divergence between these two distri-

Initialization Regularization

- The weights in a neural network are given random values initially.
- There is an entire literature on the best way to do this initialization
    - Normal
    - Truncated Normal
    - Uniform
    - Orthogonal
    - Scaled by number of connections
    - Etc.
- Try to “bias” the model into initial configurations that are easier to train

Initialization Regularization

- A popular way is to do **transfer learning**

Train the model on auxiliary task where lots of data is available → Use final weight values from previous task as initial values and “fine tune” on primary task

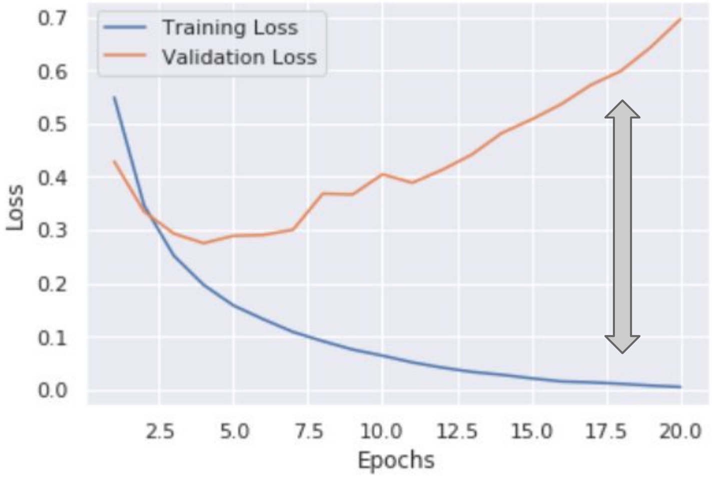
Structural Initialization

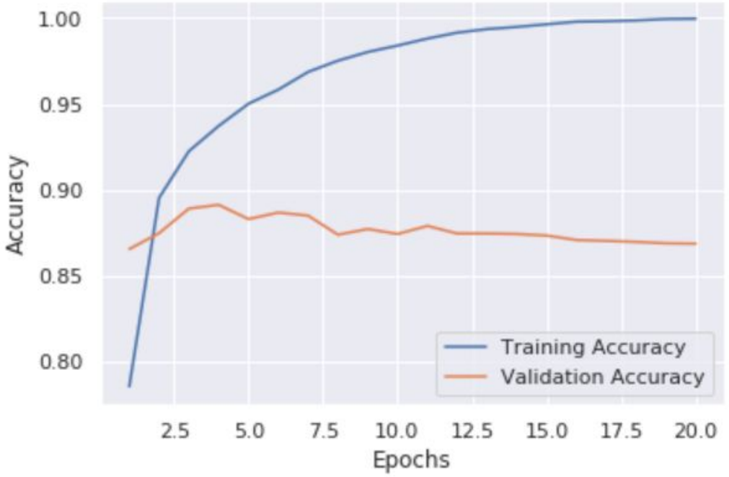
- The key advantage of neural nets is the ability to easily include properties of the data directly into the model through the network’s structure

- Convolutional neural networks (CNNs) are a prime example of this

IMDb Example

We saw overfitting in the IMDb example:





How do we make this model better?

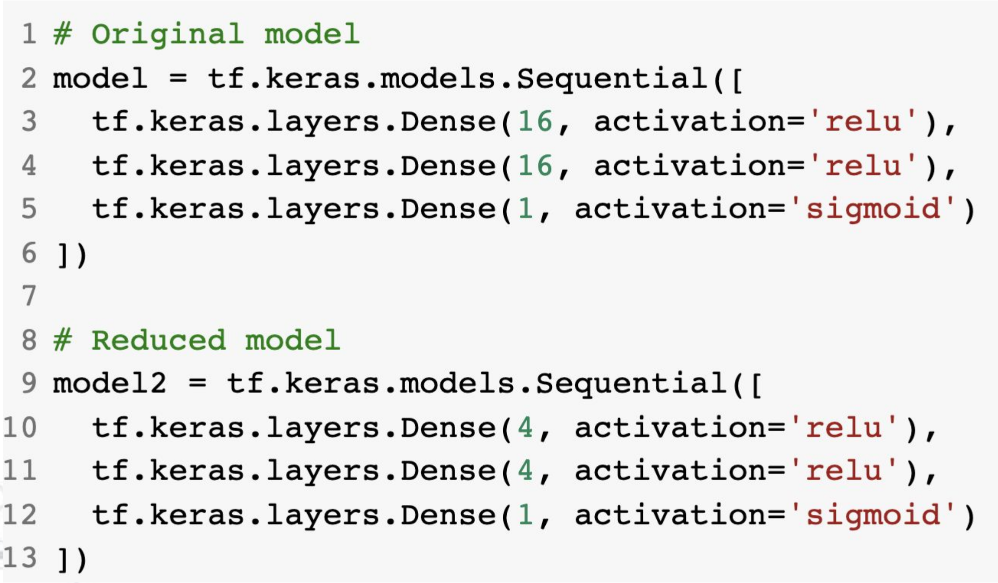
Regularization

1. Reduce network size
2. Weight regularization
3. Dropout

Back to the IMDb colab

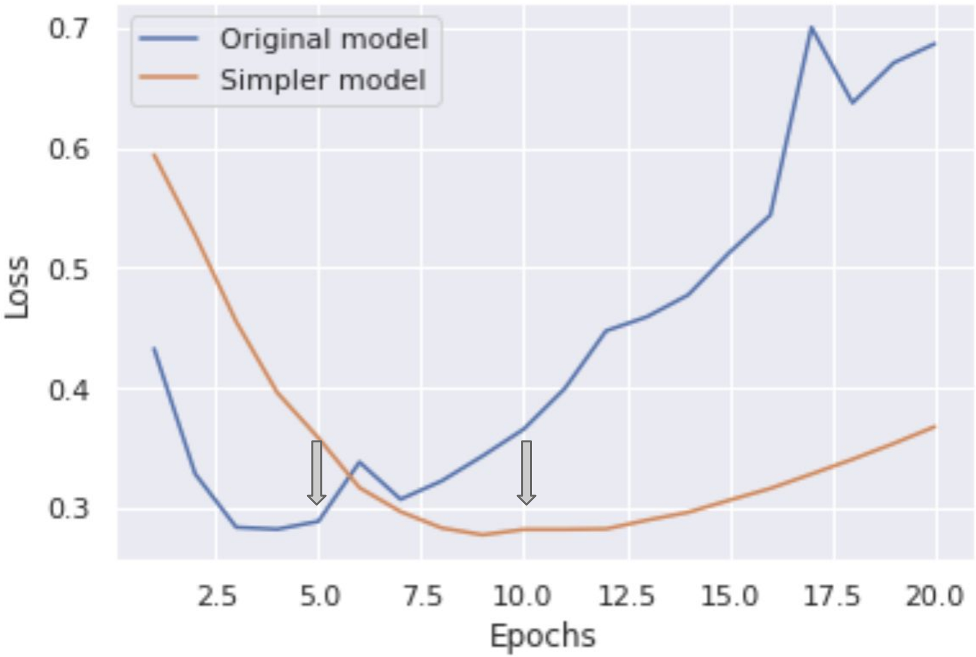
Regularization: reducing network size

When we are battling overfitting, one option is to simplify the model. Let’s compare the performance we get from a simpler model. Here we have simplified the model by reducing the number of hidden units in each hidden layer.



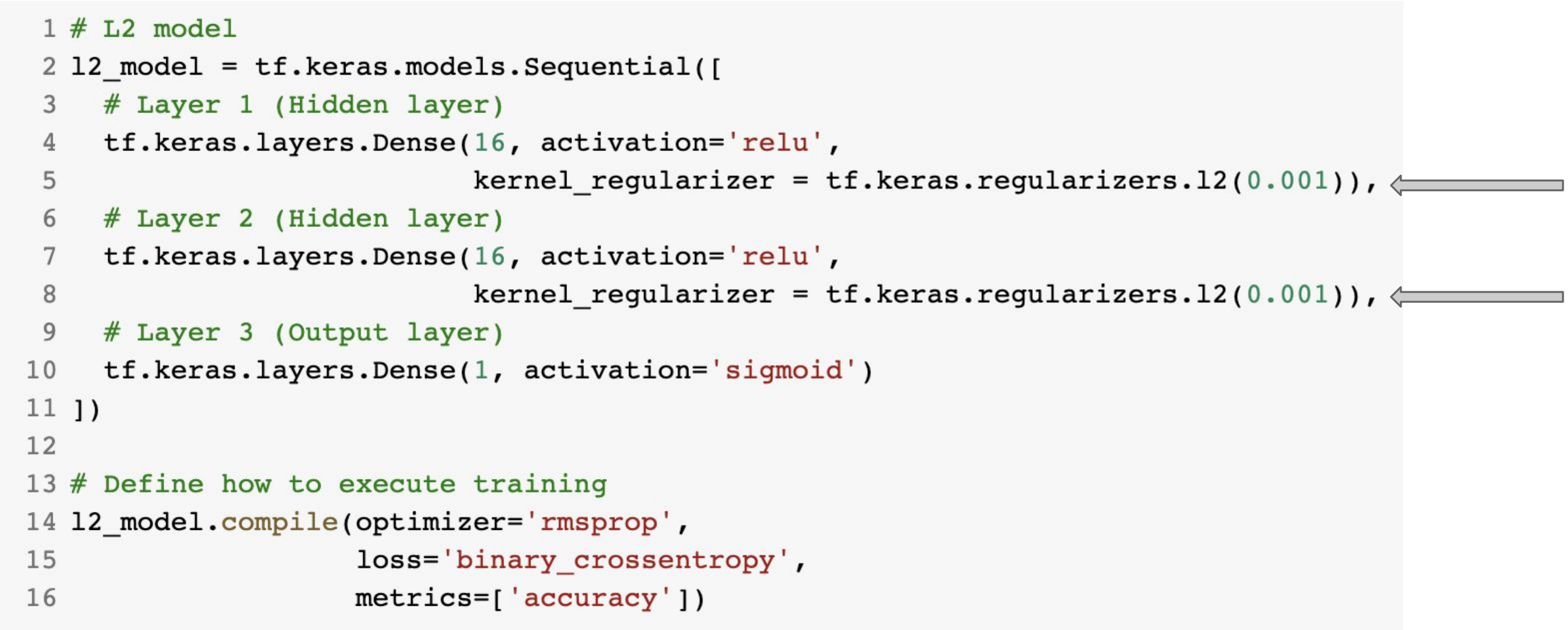
```
# Original model
model = tf.keras.models.Sequential([
  tf.keras.layers.Dense(16, activation='relu'),
  tf.keras.layers.Dense(16, activation='relu'),
  tf.keras.layers.Dense(1, activation='sigmoid')
])

# Reduced model
model2 = tf.keras.models.Sequential([
  tf.keras.layers.Dense(4, activation='relu'),
  tf.keras.layers.Dense(4, activation='relu'),
  tf.keras.layers.Dense(1, activation='sigmoid')
])
```

Regularization: reducing network size



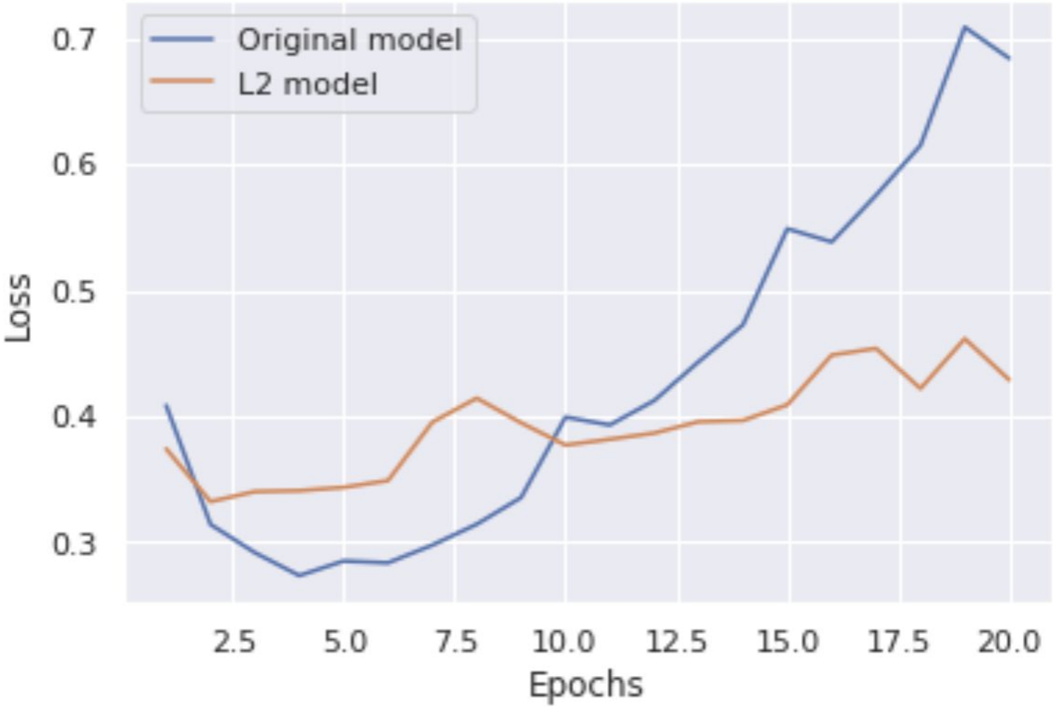
The smaller network performs better than the original model - it starts to overfit at epoch 10 rather than epoch 6. These values are when the validation loss starts to increase.

Regularization: weight regularization



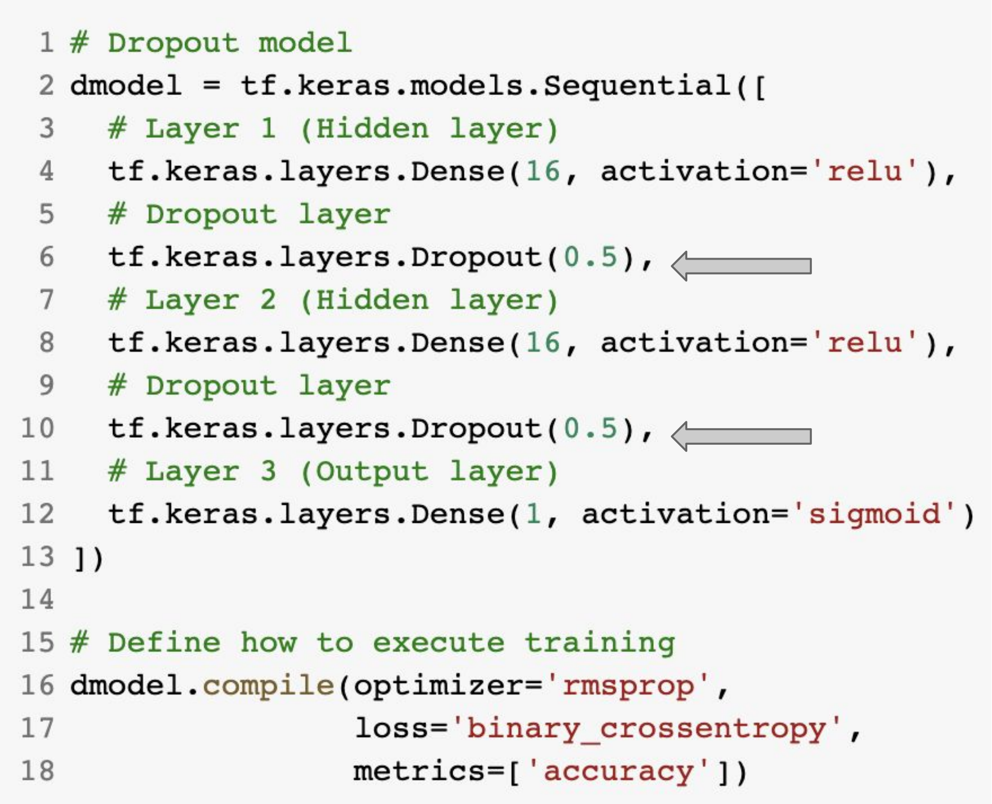
```
# L2 model
l2_model = tf.keras.models.Sequential([
  # Layer 1 (Hidden layer)
  tf.keras.layers.Dense(16, activation='relu',
                        kernel_regularizer = tf.keras.regularizers.l2(0.001)),
  # Layer 2 (Hidden layer)
  tf.keras.layers.Dense(16, activation='relu',
                        kernel_regularizer = tf.keras.regularizers.l2(0.001)),
  # Layer 3 (Output layer)
  tf.keras.layers.Dense(1, activation='sigmoid')
])

# Define how to execute training
l2_model.compile(optimizer='rmsprop',
                 loss='binary_crossentropy',
                 metrics=['accuracy'])
```

Regularization: weight regularization



The L2-regularized model is much more resistant to overfitting - the validation loss starts to increase at a much slower rate

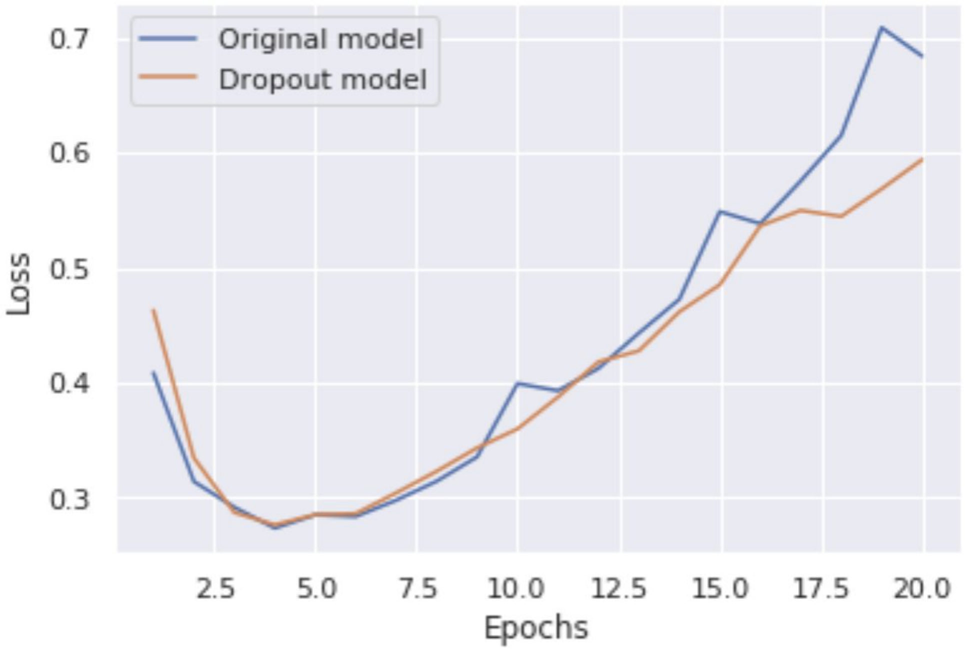
Regularization: adding dropout



```python
# Dropout model
dmodel = tf.keras.models.Sequential([
  # Layer 1 (Hidden layer)
  tf.keras.layers.Dense(16, activation='relu'),
  # Dropout layer
  tf.keras.layers.Dropout(0.5),
  # Layer 2 (Hidden layer)
  tf.keras.layers.Dense(16, activation='relu'),
  # Dropout layer
  tf.keras.layers.Dropout(0.5),
  # Layer 3 (Output layer)
  tf.keras.layers.Dense(1, activation='sigmoid')
])

# Define how to execute training
dmodel.compile(optimizer='rmsprop',
               loss='binary_crossentropy',
               metrics=['accuracy'])
```

The 0.5 indicates a 50% probability of dropping out a unit. Typically, 20% is used in practice but you can try different values and see what performs best.

Regularization: adding dropout



The dropout model is slightly better than the original model but does not control for overfitting as well as the L2 network

Convolutional Neural Networks (CNNs)

CNNs

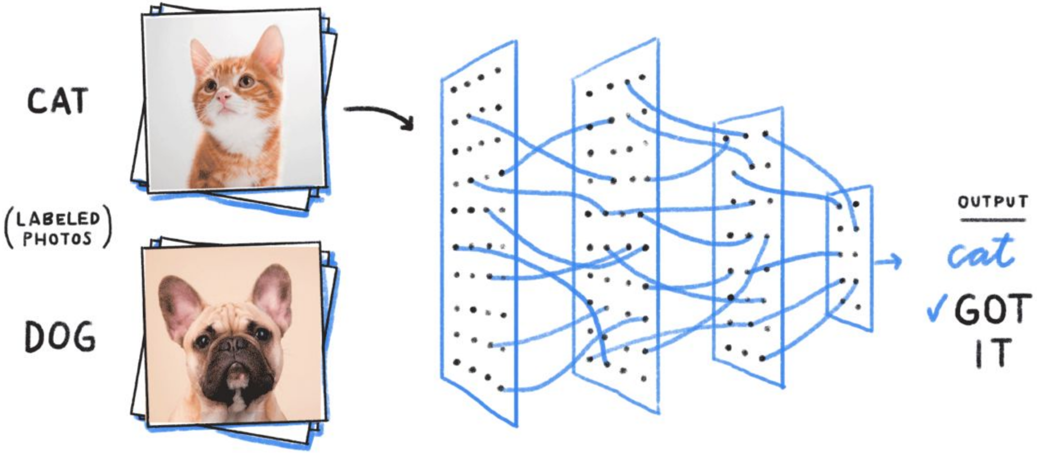
Convolutional neural networks = CNNs = convnets = (many times) computer vision

CNNs are at the heart of deep learning, emerging in recent years as the most prominent strain of neural networks in research. They have revolutionized computer vision, achieving state-of-the-art results in many fundamental tasks, as well as making strong progress in natural language processing, computer vision, reinforcement learning, and many other areas. CNNs have been widely deployed by tech companies for many of the new services and features we see today. They have numerous and diverse applications, including:

◎ Detecting and labeling objects, locations, and people in images
◎ Converting speech into text and synthesizing audio of natural sounds
◎ Describing images and videos with natural language
◎ Tracking roads and navigating around obstacles in autonomous vehicles
◎ Analyzing video game screens to guide autonomous agents playing them

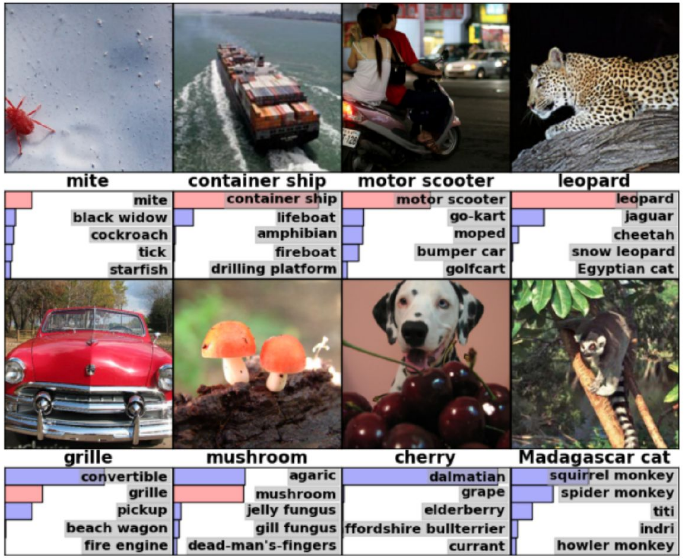
CNN Applications

Image classification



CNN Applications

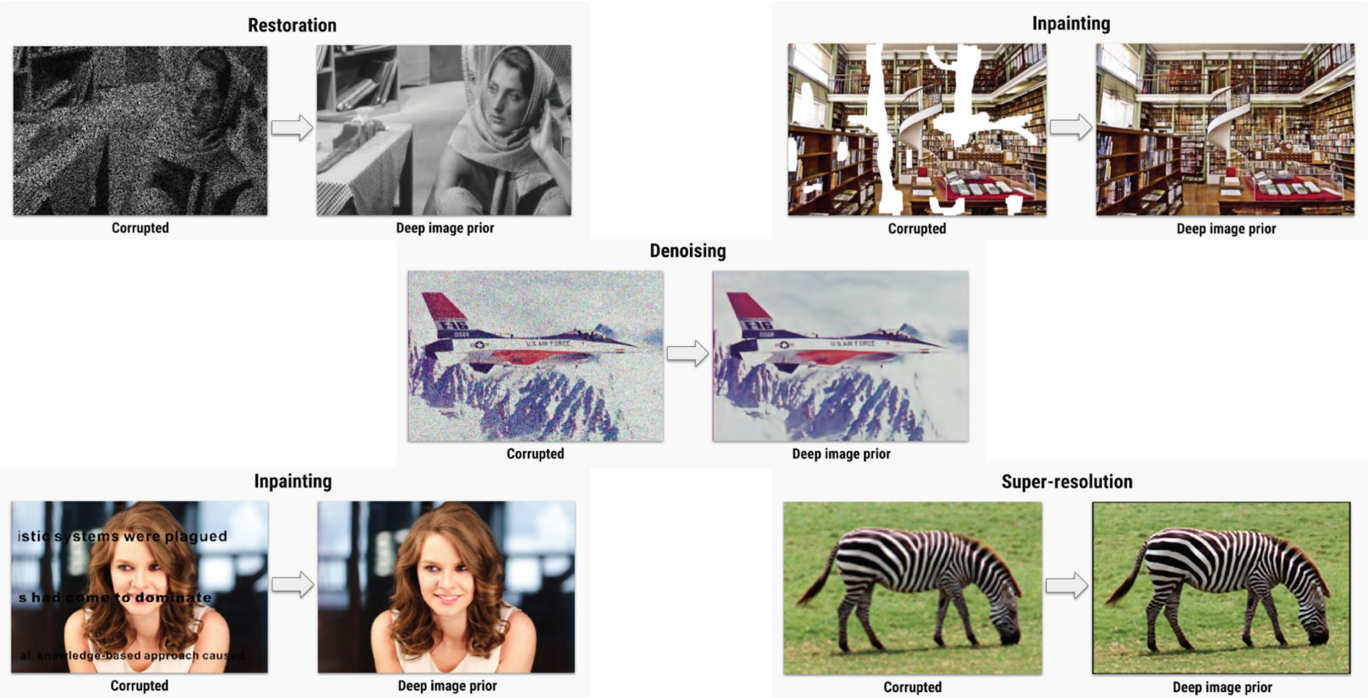
Computer vision



Top: 4 correctly classified examples. Bottom: 4 incorrectly classified examples. Each example has an image, followed by its label, followed by the top 5 guesses with probabilities. From Krizehvsky *et al.* (2012).

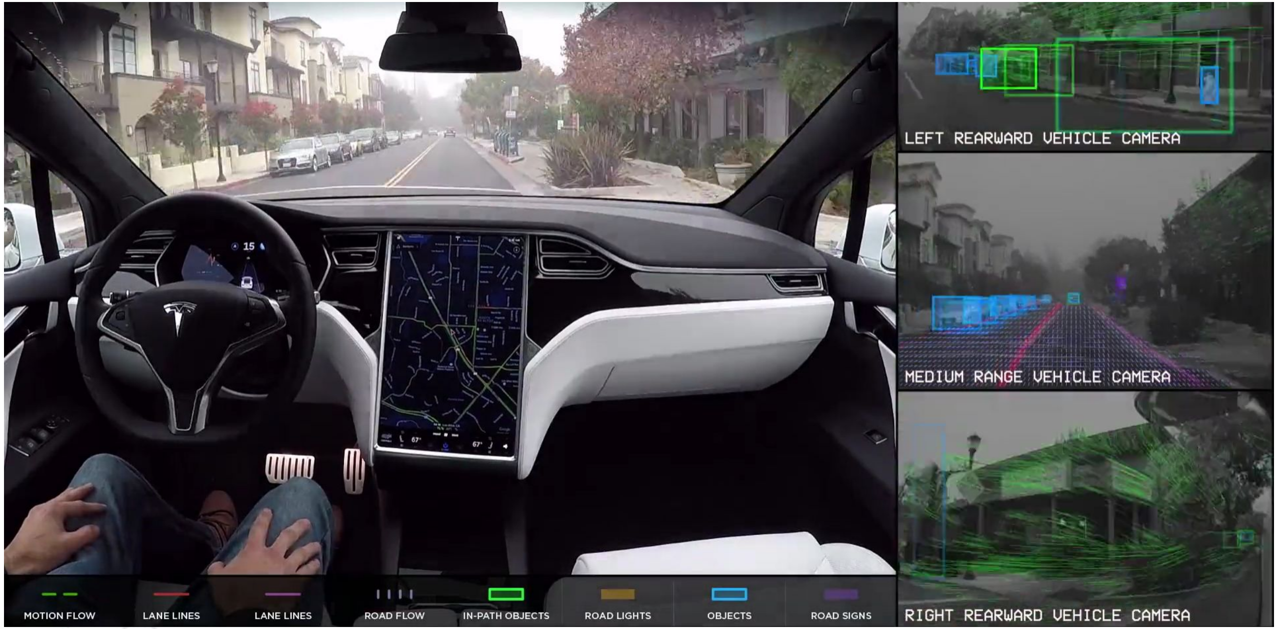
CNN Applications

Restoration, inpainting, denoising and super-resolution



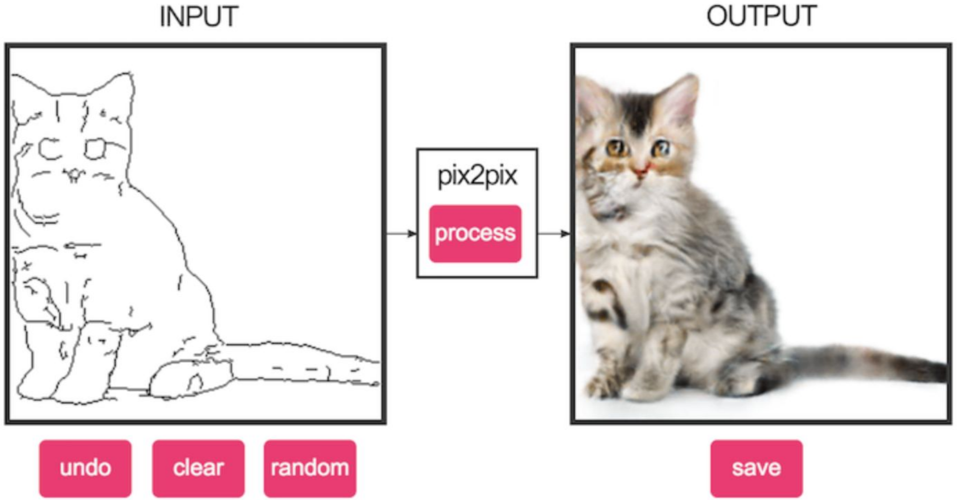
CNN Applications

Self-driving cars


LEFT REARWARD VEHICLE CAMERA
MEDIUM RANGE VEHICLE CAMERA
RIGHT REARWARD VEHICLE CAMERA
MOTION FLOW
LANE LINES
LANE LINES
ROAD FLOW
IN-PATH OBJECTS
ROAD LIGHTS
OBJECTS
ROAD SIGNS

CNN Applications

Generating realistic pictures from drawn edges

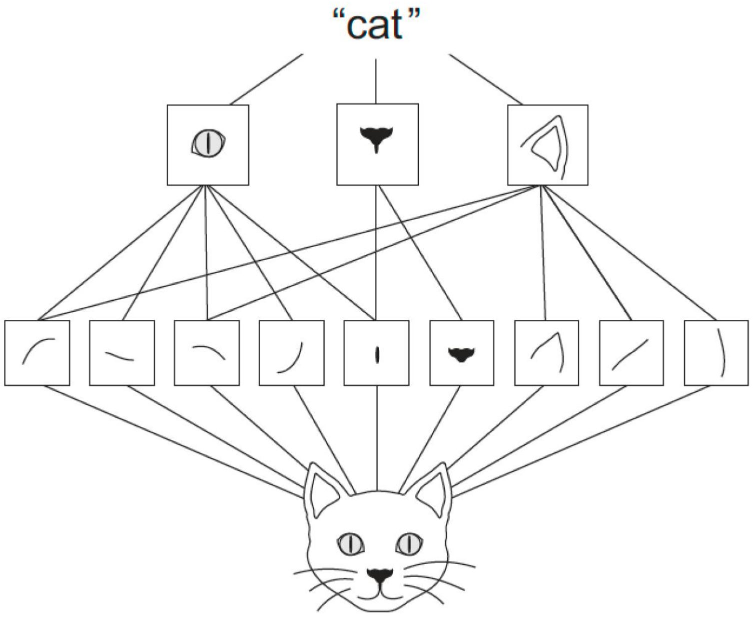


Dense vs Convolutional Layers

- Dense layers learn **global** patterns

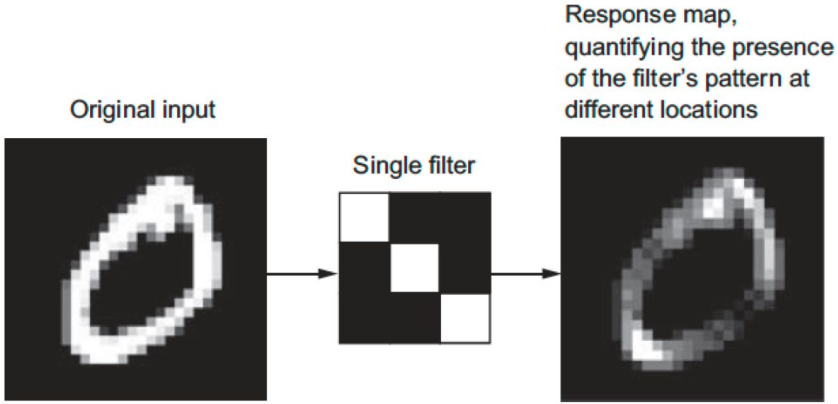
- Convolutional layers learn **local** patterns

- CNNs learn **spatial hierarchies of patterns**: one convolutional layer will learn small patterns and the next larger patterns made of the features of the layer before, and so on

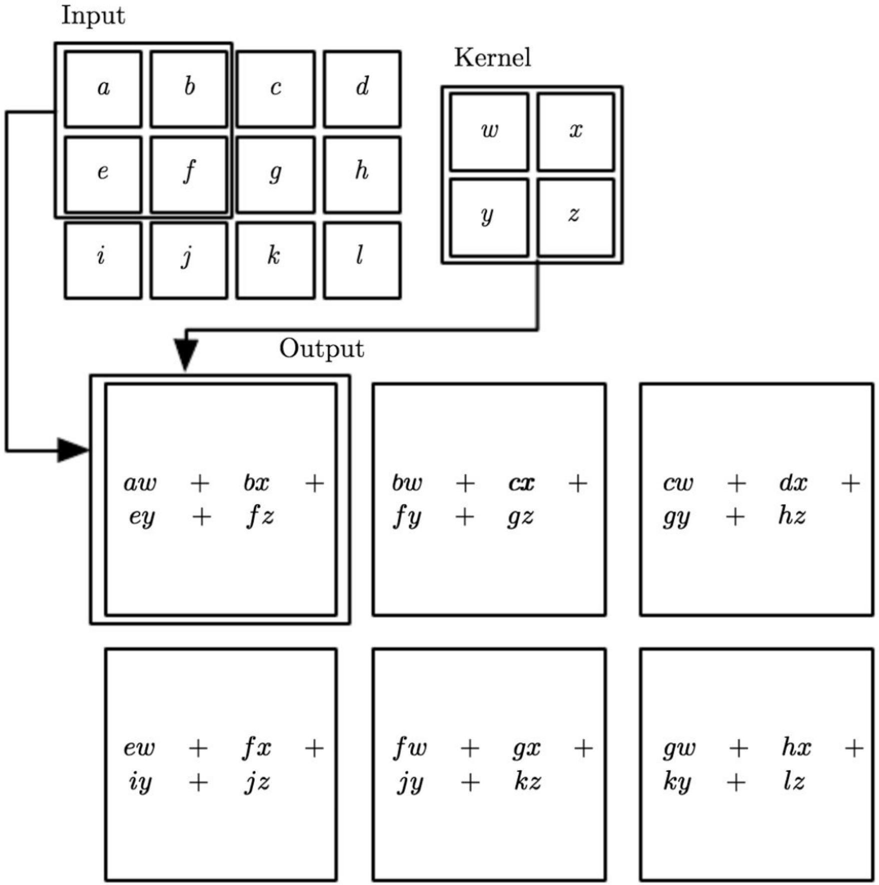


Convolution Layers

- The primary purpose of the convolution operation is to extract features from the input
- To do this, the input is split into several different areas, and the convolution operation applied to each area
- A summary value is then calculated and kept as part of the output
- Here, *I* is the input image (sometimes called **feature map**), *K* is a two-dimensional **kernel**, or more commonly, **filter**, and is a weighting function
- The output resulting from this operation is called the **response map**


Original input
Single filter
Response map, quantifying the presence of the filter's pattern at different locations

The Convolution Operation



Input

a	b	c	d
e	f	g	h
i	j	k	l

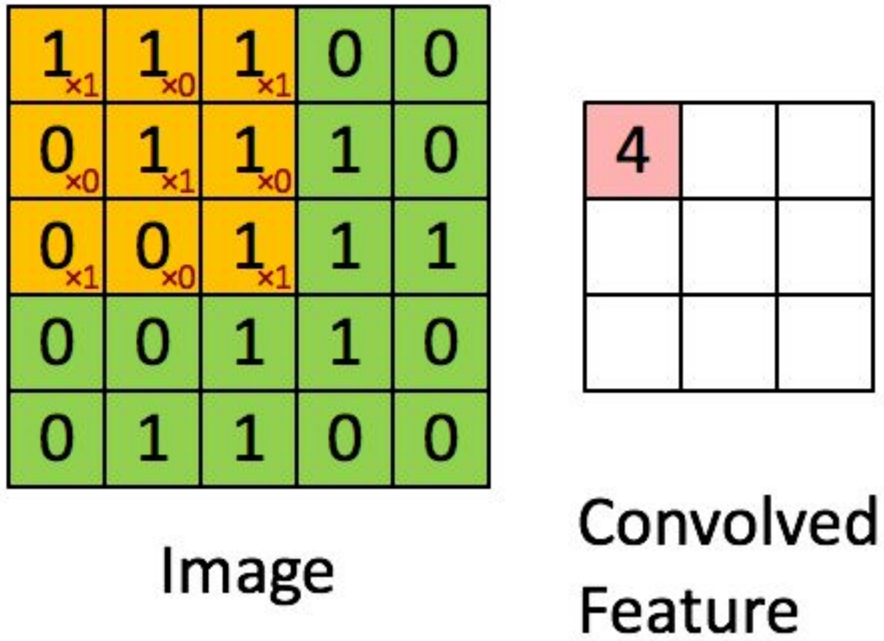
Kernel

w	x
y	z

Output

$aw + bx + ey + fz$	$bw + cx + fy + gz$	$cw + dx + gy + hz$
$ew + fx + iy + jz$	$fw + gx + jy + kz$	$gw + hx + ky + lz$

The Convolution Operation



1 ×1	1 ×0	1 ×1	0	0
0 ×0	1 ×1	1 ×0	1	0
0 ×1	0 ×0	1 ×1	1	1
0	0	1	1	0
0	1	1	0	0

4		

Filters

- The most common filter sizes are 3 x 3 and 5 x 5
- Sometimes 7 x 7 filters are also used
- A 1 x 1 filter is a special case that we will see later in the course when talking about RNNs
- Odd dimension filters are preferred for computer vision
  - Provide natural padding (we'll see this in the following slides)
  - Ensures a central position or pixel of the filter

Convolution

- Convolution leverages 3 important ideas that can help improve a machine learning system:
  - **Sparse interactions** / sparse connectivity / sparse weights
    - Filters are smaller than the input images and thus fewer parameters (weights) need to be stored
    - This reduces computational expense and improves statistical efficiency
  - **Parameter sharing**
    - The same parameter is used for more than one function in the model
    - In a CNN, each each element of the filter is applied to every position of the input

Convolution

- **Equivariant representations**
  - Parameter sharing causes equivariance to translation: if the input changes, the output changes in the same way
  - A function f(x) is invariant to a function g if f(g(x)) = g(f(x))
  - When processing time-series data, this means that convolution produces a sort of timeline that shows when different features appear in the input
  - Note that convolution is not equivariant to some other transformations, such as changes in the scale or rotation of an image

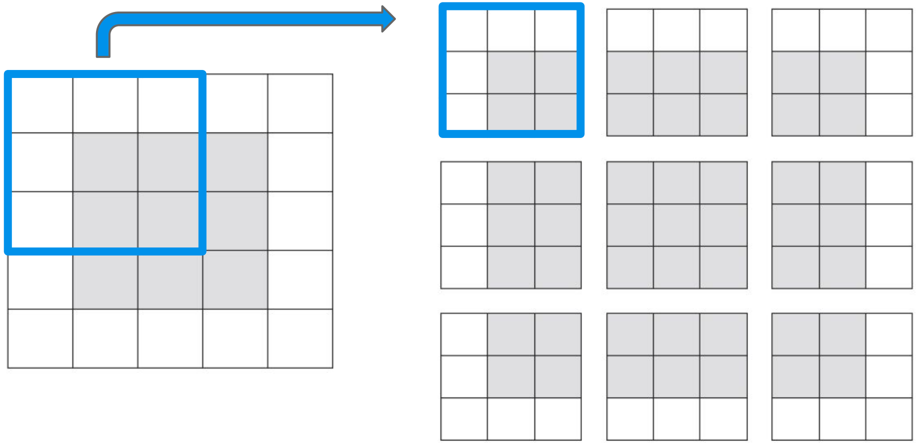
- **Translation invariant**: After learning a certain pattern from one part of an image, it can recognize it anywhere
- Convolution also provides a way to work with inputs of different size

Padding

- Applying a filter to an input image shrinks it - the output dimensions are smaller than the input dimensions
- Additionally, when we perform the convolution operation on an input, the pixels on the edges aren't used as much as the pixels in the middle
- To make the amount of information used more equal across pixels, you can use **padding**
- Padding consists of adding an appropriate number of rows and columns to each side of the image (think a border of pixels)
- **This enables an output with the same dimensions as the input**

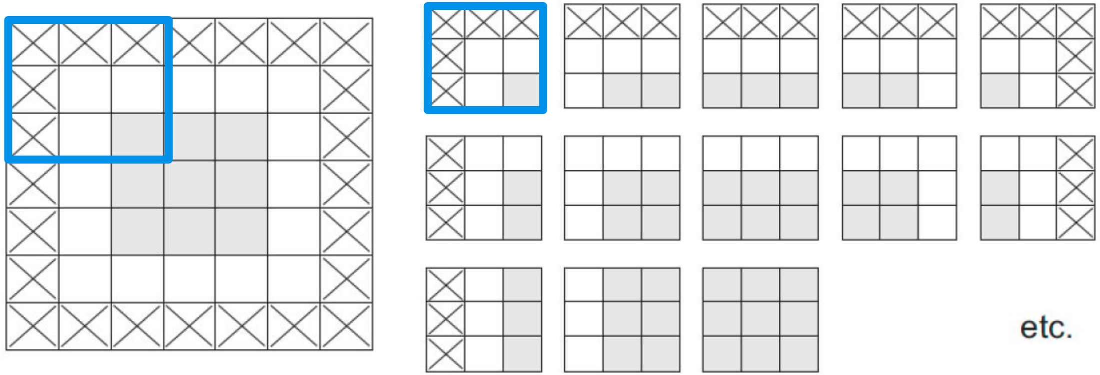
Valid Padding

- In Keras, the default is no padding, or **“valid” padding**
- This means the output will not be the same dimension as the input, and will instead depend on the dimension of the input and the size of the filter
- On the right is a 5 x 5 image
- If we apply a 3 x 3 filter, the output will also be 3 x3



Same Padding

- On the right is the same 5 x 5 image, but with an added border
- If we use a 3 x 3 filter, we need to add $p = 1$ padding - here, p is the number of rows to add to the border of an image
- The output will then be 5 x 5
- Because the input and output have the same dimensions, this is called **“same” padding**



General Padding Formula

- There is a general formula that can help you decide how much padding you need or want
  - Let the input be *n* x *m* and the filter *f* x *f*
  - Without padding, the output would be:

$$(n - f + 1) \times (m - f + 1)$$

- For an output with the same dimension as the input, need *p* such that:

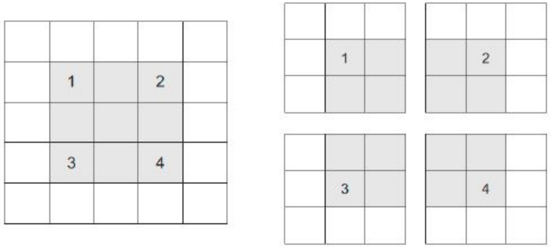
$$n \times m = (n + 2p - f + 1) \times (m + 2p - f + 1)$$

which boils down to $p = \dfrac{f - 1}{2}$

Convolutional Strides

- Another factor that can influence output size is convolution **strides**
- So far we have assumed that we slide the filter over a single space to extract a new patch - but what if we wanted to slide over 2 spaces, 3 spaces, or more?
- Convolutional strides are convolutions with a stride greater than 1
- If your stride is set equal to 2, you will downsample the width and height of the input image by a factor of 2
- If *s* is the size of the stride, the output will have dimensions

$$\left\lfloor \frac{n+2p-f}{s}+1 \right\rfloor \times \left\lfloor \frac{m+2p-f}{s}+1 \right\rfloor$$



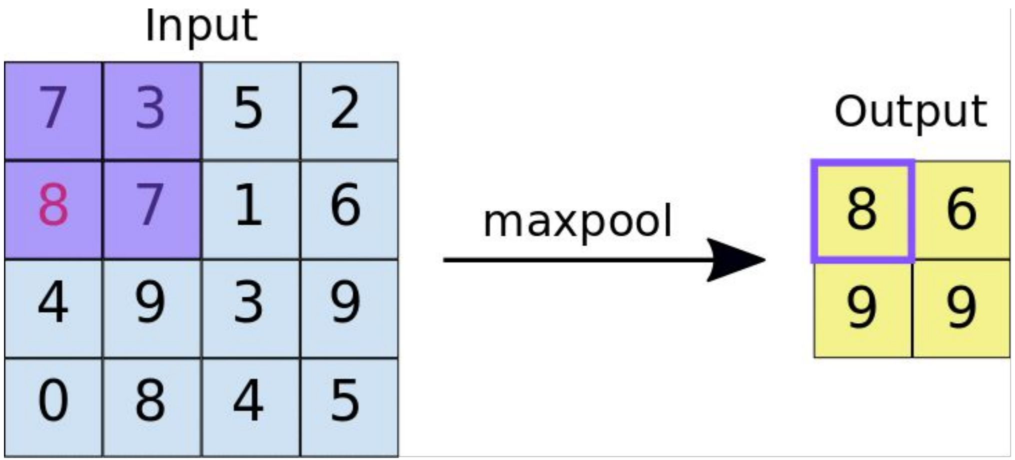
Pooling

- Strided convolutions are rarely used in practice - **max-pooling** is more common
- A typical layer of a CNN consists of 3 stages:
  - **Convolution stage** - linear transformation of the input
  - **Detector stage** - Nonlinear activation (ex: relu activation function is applied)
  - **Pooling stage** - further modification (downsizing) of the output
- A pooling function replaces the output at a certain location with a summary statistic of the nearby outputs
- Pooling greatly reduces the computational expense of the network by decreasing the number of parameters to be learned

Pooling

- There are different types of pooling
  - **Max Pooling**
    - Outputs the maximum value from a patch for each channel
    - Similar to convolution, but instead of transforming patches via a learned linear transformation, they're transformed via a hardcoded max tensor operation
    - Very common
    - Usually done with 2 x 2 windows
  - **Average Pooling**
  - **Weighted Pooling**
    - Based on the distance from the central pixel
- Max pooling tends to work better than other pooling functions and convolutional strides

Max Pooling



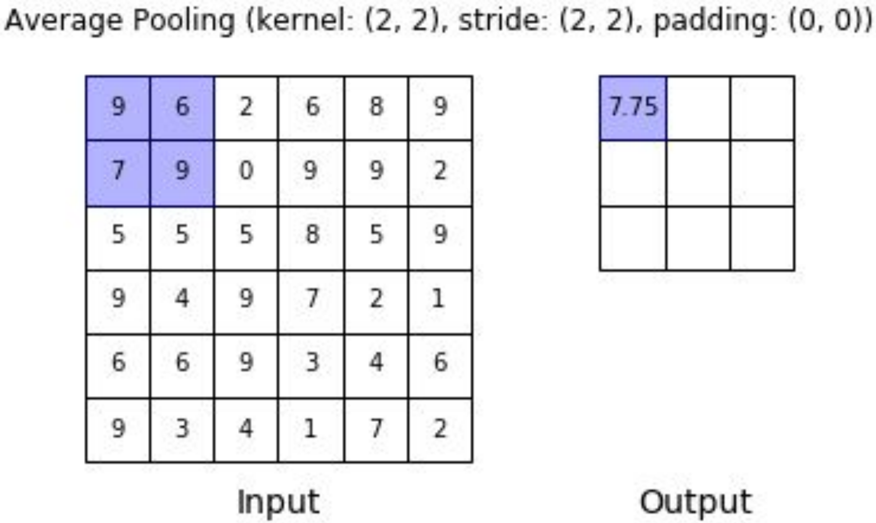
Input

7	3	5	2
8	7	1	6
4	9	3	9
0	8	4	5

Output

8	6
9	9

Average Pooling



Average Pooling (kernel: (2, 2), stride: (2, 2), padding: (0, 0))

9	**6**	2	6	8	9
7	**9**	0	9	9	2
5	5	5	8	5	9
9	4	9	7	2	1
6	6	9	3	4	6
9	3	4	1	7	2

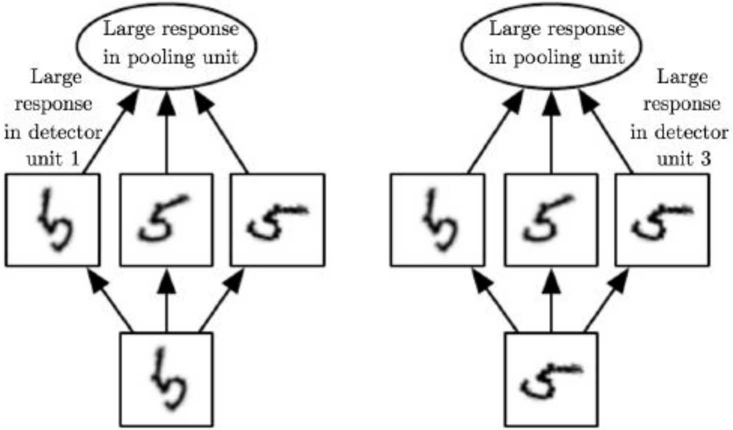
Input

7.75		

Output

Pooling and Invariance

- A pooling unit that pools over multiple features that are learned with separate parameters can learn to be invariant to transformations of the input
- Here, a set of 3 learned filters and a max pooling unit can learn to become invariant to rotation



Large response in pooling unit
Large response in detector unit 1
Large response in pooling unit
Large response in detector unit 3

Terminology

- Convolutions operate over 3D tensors with two spatial axes, **height** and **width**, as well as a **depth** axis (or **channels** axis)
- For a color (RGB) image, the depth is equal to 3
- For black and white (grayscale) images, the depth is equal to 1
- The convolution operation extracts different **patches** from the input image and applies the same transformation to to each of them, resulting in a response map that is also a 3D tensor

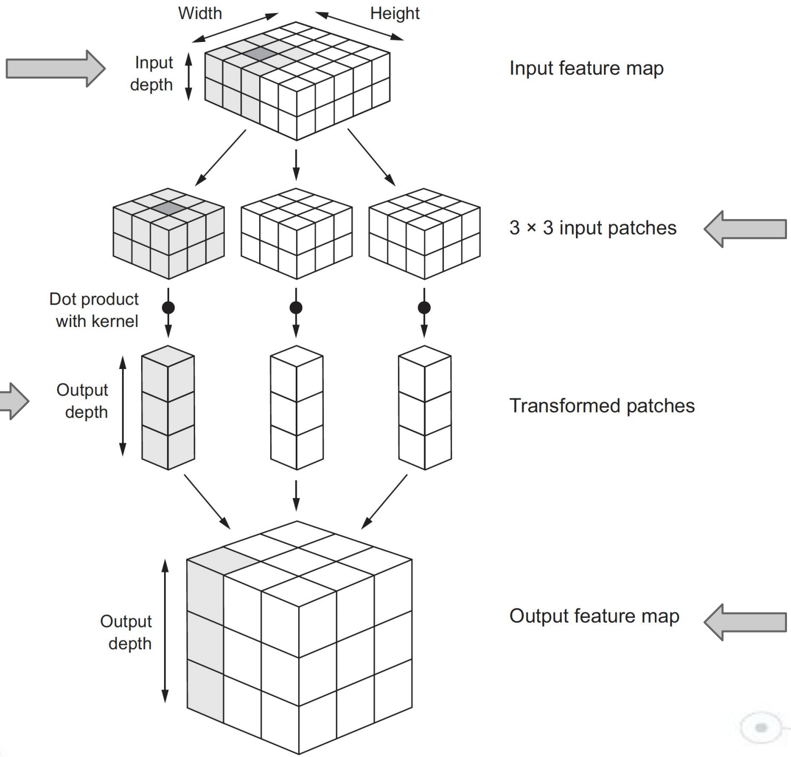
Terminology

- The response map has a width, height, and depth, all of which depend on the input image, filter, padding and stride
- Convolutions are defined by 2 key parameters:
  - Size of the filter
  - Depth of the output response map, i.e., how many filters are applied to the input
- Convolution works by sliding the filter over the 3D input image, stopping at every possible location, and extracting the 3D patch at each location
  - Each 3D patch is transformed into a 1D vector
  - All 1D vectors are then reassembled into a 3D output map

Convolution Schematic

Input image has shape 5x5x2

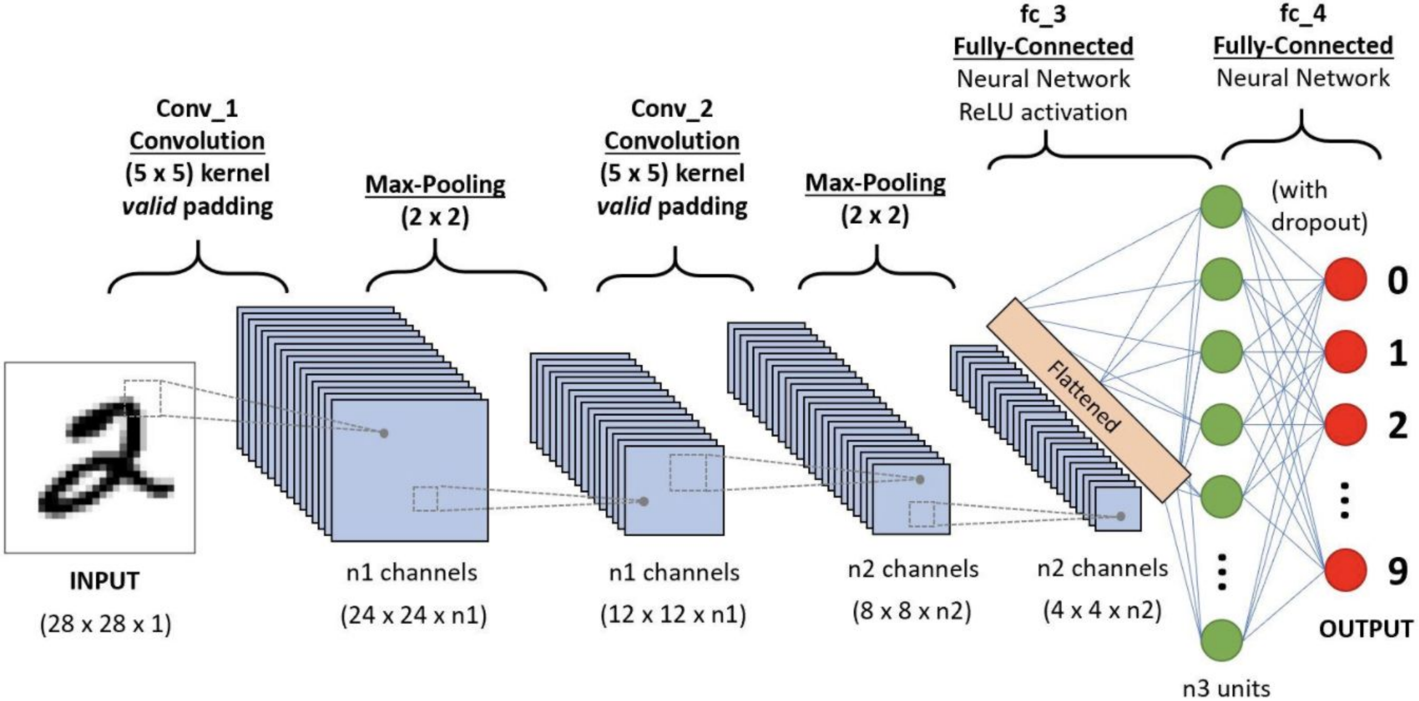
There are 3 filters (not shown) which results in a depth of 3 for each patch.



Here, each filter has a shape of 3x3x2, which results in a total of 9 patches from the original input. Only 3 of those patches are shown here.

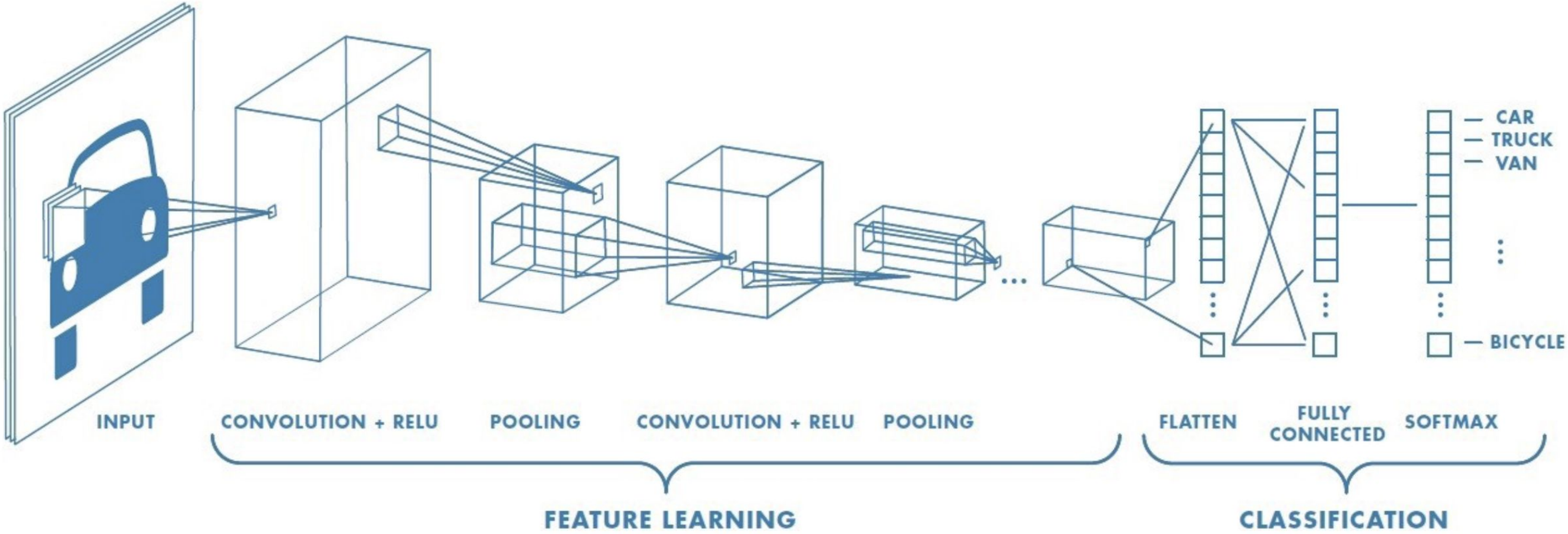
9 total patches, each with a depth of 3 (one number for each filter), resulting in an output shape of 3x3x2.

CNN Schematic



https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53

CNN Schematic

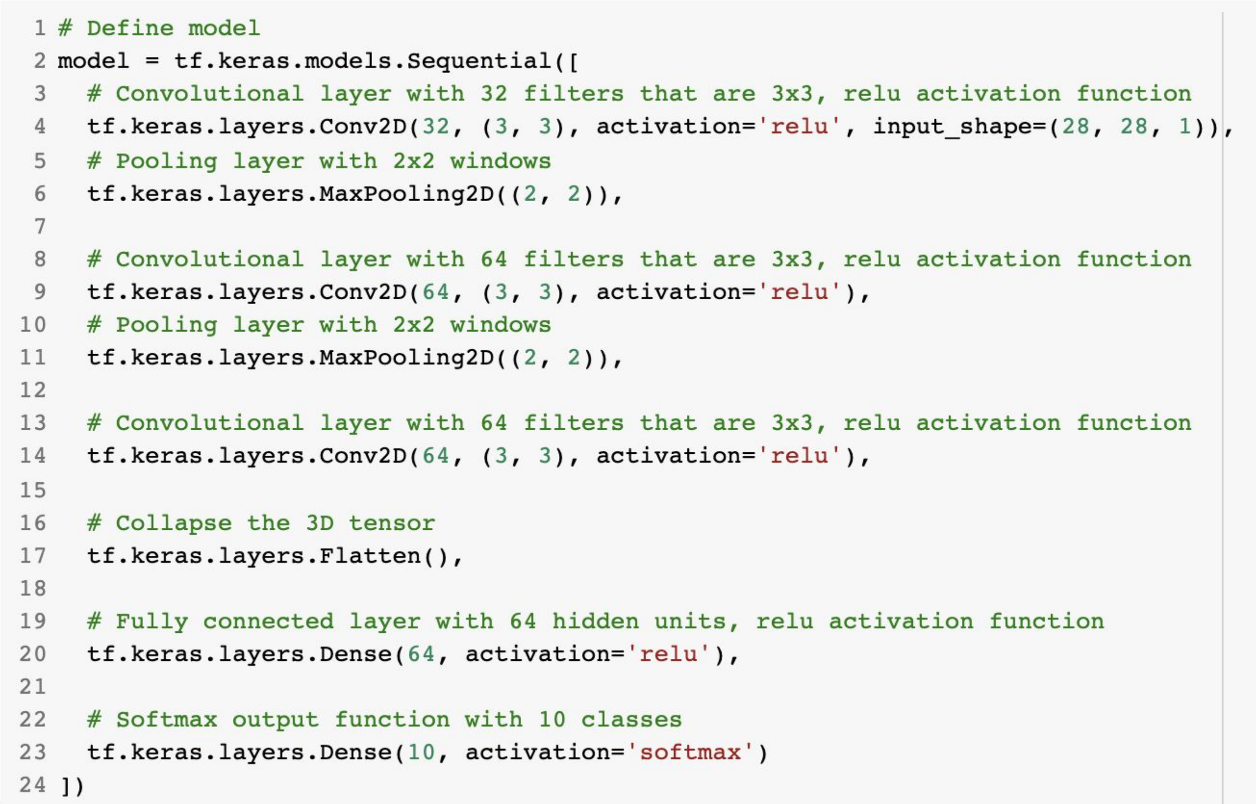


https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53

MNIST Example

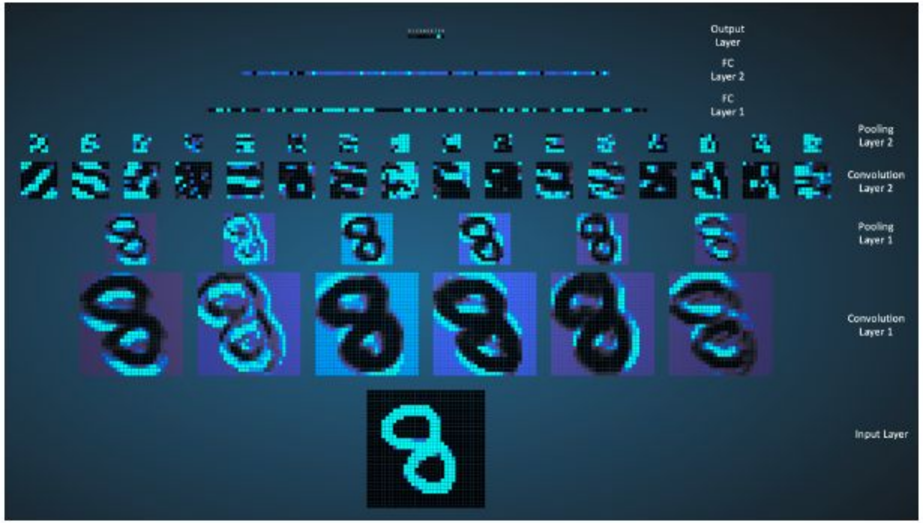
Colab notebook

MNIST Example



```python
# Define model
model = tf.keras.models.Sequential([
  # Convolutional layer with 32 filters that are 3x3, relu activation function
  tf.keras.layers.Conv2D(32, (3, 3), activation='relu', input_shape=(28, 28, 1)),
  # Pooling layer with 2x2 windows
  tf.keras.layers.MaxPooling2D((2, 2)),

  # Convolutional layer with 64 filters that are 3x3, relu activation function
  tf.keras.layers.Conv2D(64, (3, 3), activation='relu'),
  # Pooling layer with 2x2 windows
  tf.keras.layers.MaxPooling2D((2, 2)),

  # Convolutional layer with 64 filters that are 3x3, relu activation function
  tf.keras.layers.Conv2D(64, (3, 3), activation='relu'),

  # Collapse the 3D tensor
  tf.keras.layers.Flatten(),

  # Fully connected layer with 64 hidden units, relu activation function
  tf.keras.layers.Dense(64, activation='relu'),

  # Softmax output function with 10 classes
  tf.keras.layers.Dense(10, activation='softmax')
])
```

MNIST Example



Output Layer
FC Layer 2
FC Layer 1
Pooling Layer 2
Convolution Layer 2
Pooling Layer 1
Convolution Layer 1
Input Layer