S&DS 365 / 665

Intermediate Machine Learning

Convolutional Neural Networks

February 14

Yale

Reminders

- Assignment 1 is out, due a week from Wednesday
- Quiz 1 this Wednesday; 15 minutes, online, 24 hours
- OH schedule posted to Canvas/EdD
- Questions or concerns?

Topics for today

- Mechanics of convolutional networks
- Filters and pooling and flattening (oh my!)
- Example: Classifying Ca2+ brain scans
- Jumpstarting Problem 4 on Assn 1
- Other examples

Notes

- Animations from tutorial “Let’s Code Convolutional Neural Network in plain NumPy: Mysteries of Neural Networks” by Piotr Skalski
- `https://towardsdatascience.com/lets-code-convolutional-neural-network-in-plain-numpy-ce48e732f5d5`
- To see the animations, view this pdf using Adobe Acrobat

Convolution

Mathematically, a *convolution* sweeps a function $K(u)$ over the values of another function f:

Continuous:

$$K \star f(x) = \int K(x-u)\, f(u)\, du$$

- Same operation we saw with smoothing kernels
- If K is a Gaussian bump, this blurs or smooths out the values.
- For CNNs, K will have small support, encode features of the input

Convolution

Mathematically, a *convolution* sweeps a function $K(u)$ over the values of another function f:

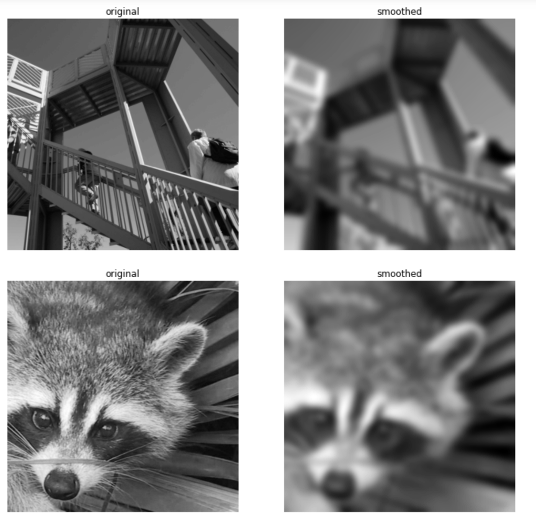
Discrete:

$$K \star f(x_j) = \sum_i K(x_j - x_i)\, f(x_i)$$

- Same operation we saw with smoothing kernels
- If K is a Gaussian bump, this blurs or smooths out the values.
- For CNNs, K will have small support, encode features of the input

Examples

`convolve_demo.ipynb` gives examples



Two principles

Two of the ideas behind convolutional neural networks (CNNs):

1. Parameter tying: Let neurons share the same weights
2. Kernel learning: The kernels should not be fixed, but rather *learned* from the data

CNNs are most commonly used for images; can be used whenever data have some kind of spatial structure (e.g. DNA)

Tensors

A tensor is a multidimensional array*—like a matrix, but with more than just a pair of indices for row and columns.

In Python, tensors is represented in `numpy` using the type `numpy.ndarray` ("*n*-dimensional array")

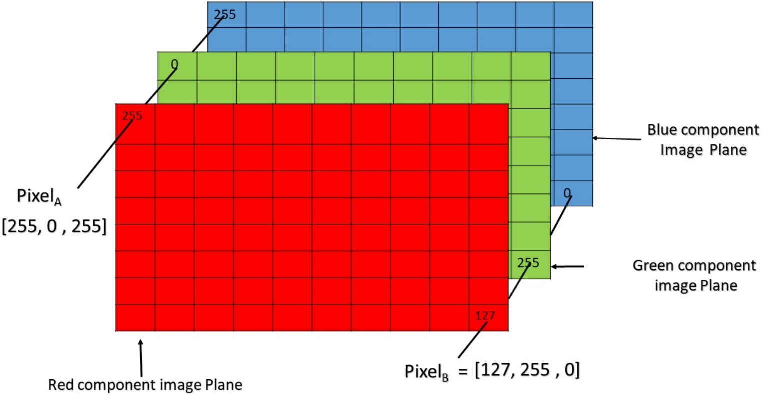
TensorFlow also has built-in types to represent tensors

* In mathematics, there is a little more structure to tensors.

Tensors

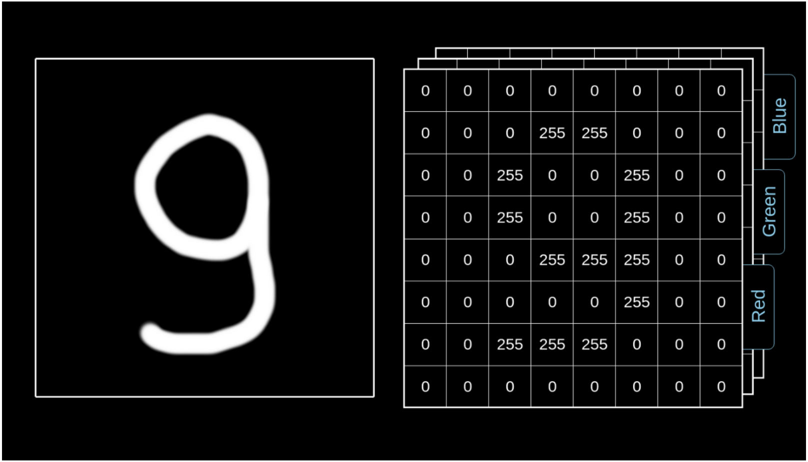
```
x = np.array(np.arange(24)).reshape(2,3,4)
print(x)
print(x[:,:,0])

[[[ 0  1  2  3]
  [ 4  5  6  7]
  [ 8  9 10 11]]

 [[12 13 14 15]
  [16 17 18 19]
  [20 21 22 23]]]

[[ 0  4  8]
 [12 16 20]]
```

Images as tensors: Channels



Pixel of an RGB image are formed from the corresponding pixel of the three component images

Images as tensors: Channels



Convolutional layer

- In a convolutional layer, a set of *kernels* are “swept over” or convolved over the input
- The kernels are themselves tensors with entries that are trained weights
- The result of convolving the kernel over the input tensor is called a *feature map*
- A convolutional layer is equivalent to a standard fully connected layer, but where the weights are constrained to be sparse and “tied” (constrained to be equal) across different neurons

Convolutional layer

$$\begin{array}{ccccc}
\text{Input Image} & & \text{Kernel} & & \text{Feature Map} \\
\begin{bmatrix}
10 & 10 & 10 & 10 & 10 & 10 \\
10 & 10 & 10 & 10 & 10 & 10 \\
10 & 10 & 10 & 10 & 10 & 10 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
& * &
\begin{bmatrix}
1 & 2 & 1 \\
0 & 0 & 0 \\
-1 & -2 & -1
\end{bmatrix}
& = &
\begin{bmatrix}
 & & & \\
 & & & \\
 & & & \\
 & & &
\end{bmatrix}
\end{array}$$

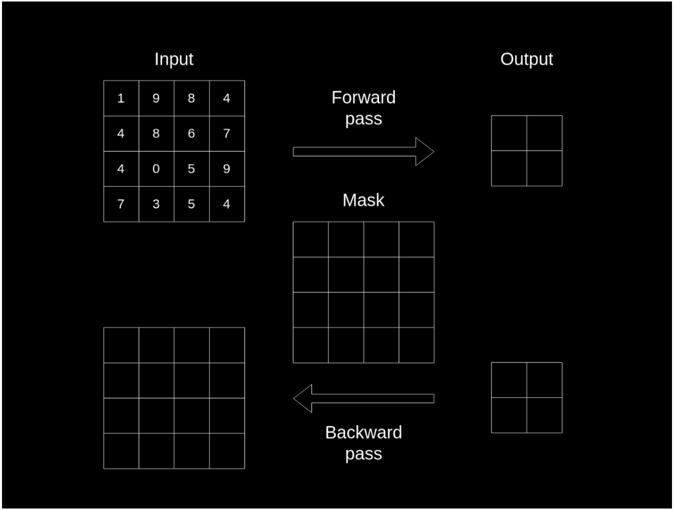
Adding a nonlinearity

- So far everything is linear
- An activation function is used to add a nonlinearity
- Each filter also has an intercept (a single number), added before applying the activation function
- The same activation function is used for all of the kernels in a layer

Pooling

- The point of a convolutional layer is to learn “features” of the input
- We don’t care too much exactly where they appear
- *Pooling* the feature map reduces the dimension and encodes the approximate location of features
- Two common types: max pooling and average pooling
- When using max pooling, to update weights in backpropagation, the locations of the features can be noted

Pooling



Input
Output
1 9 8 4
4 8 6 7
4 0 5 9
7 3 5 4
Forward pass
Mask
Backward pass

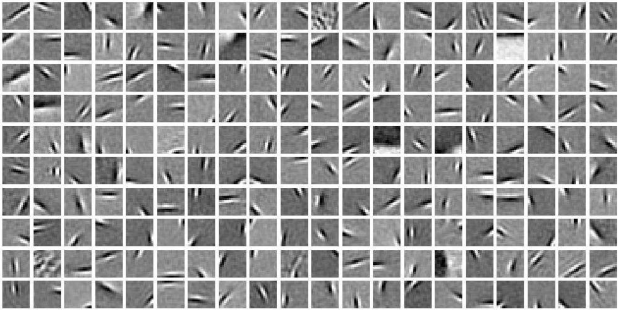
How features are built up

- Each kernel has a weight for each spatial position and channel
- Features from previous layers are recorded in the channels
- So the next layer can have a kernel that says

  "Oh, I see that feature 17 from the previous layer is active in position (1,1), feature 42 is in position (1,2), feature 5 is in position (2,1), and feature 11 is in position (2,2)"
- This enables compound features to be built up

How features are built up

- Filters in the first layer may look like this:



- Filters in second layer can then capture more complex shapes

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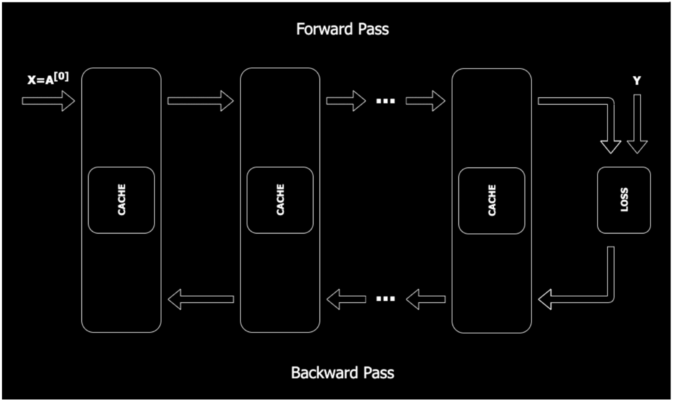
Filter is synonomous with kernel in today's discussion

Pooling and backpropagation

- A forward pass through the layers is used to make predictions, and store intermediate results to be used later
- A backward pass propagates the errors in prediction back through the layers, and computes changes to the weights for the gradient step

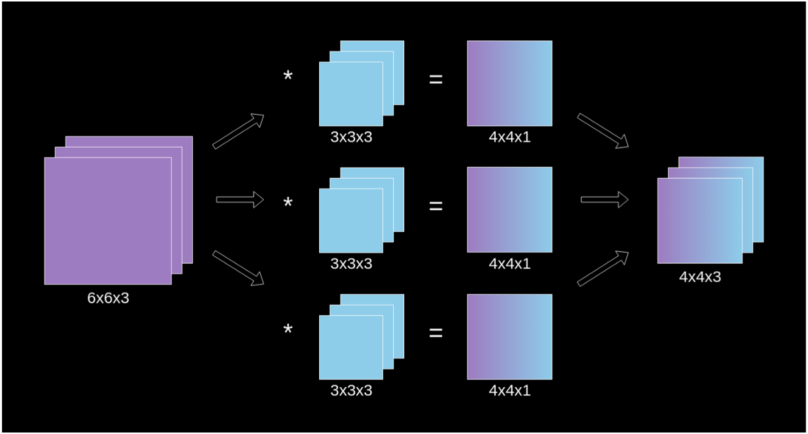
Forward and backward passes



Applying kernels across channels

- Typically each kernel (filter) has the same number of channels as the input tensor
- A kernel is applied at each location by multiplying component-wise and then summing
- The feature map for each kernel is then one channel in the output tensor
- So, the number of channels in the output is the number of kernels

Applying kernels across channels

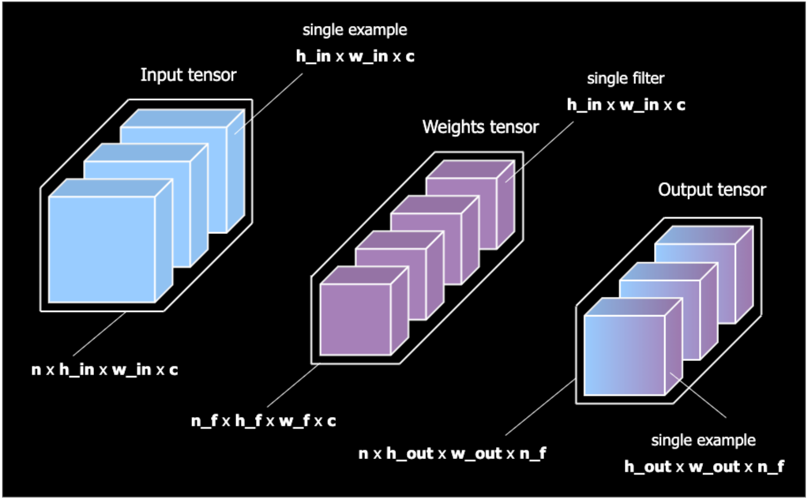


Convolutional layer: Tensor shapes

- Data points are processed in “mini-batches” of n items
- The first dimension of the input and output tensors at each layer is always n
- The last dimension of the output is the number of kernels (filters)

Can you find the typo in the next figure?

Convolutional layer: Tensor shapes



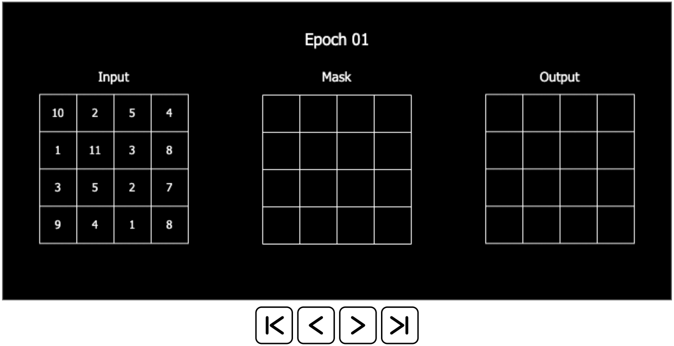
Can you find the typo in this figure?

Dropout

- "Dropout" is a type of regularization that is easy to incorporate
- Idea: Randomly zero out entries in a tensor
- Helps guard against overfitting
- Usual form:
  - Independently zero out each entry with probability ε
  - Divide by $(1 - \varepsilon)$

Equivalent to a type of ridge penalization: https://arxiv.org/abs/1307.1493

Dropout

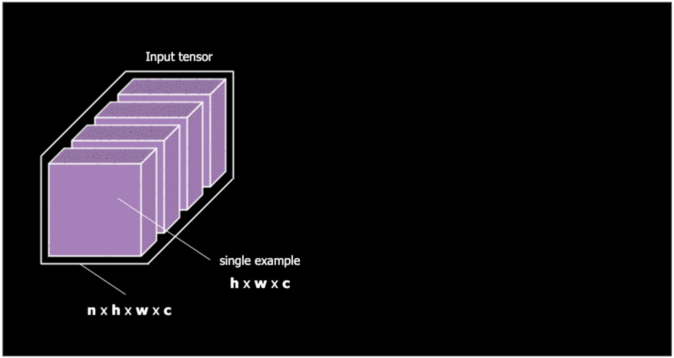


This illustrates something a bit different than the standard dropout

Flattening

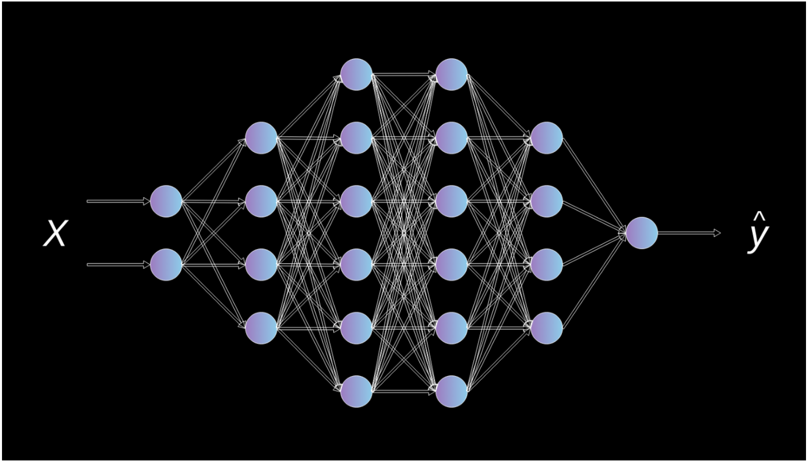
- After one or more convolutional layers, we usually add “dense” layers
- These are the standard types of layers in a neural network, with each output neuron connected to each input neuron, with a tuneable weight
- In CNNs, the convolutional layers build up a set of “features” and then these features are used to make a prediction

Flattening

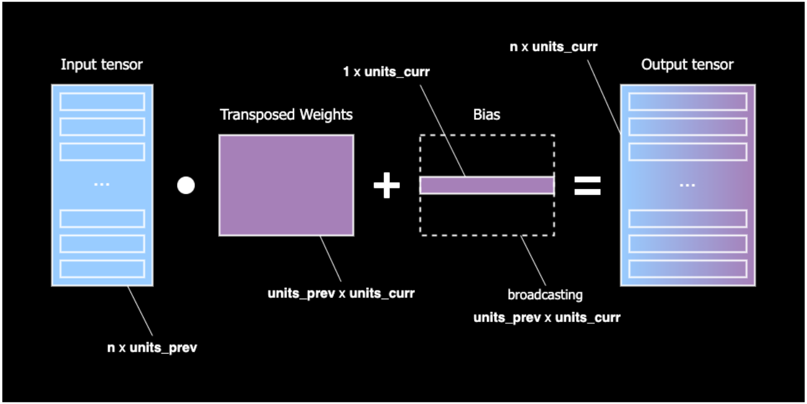


This is the same as the `numpy.flatten()` operation

Dense layers



Dense operations

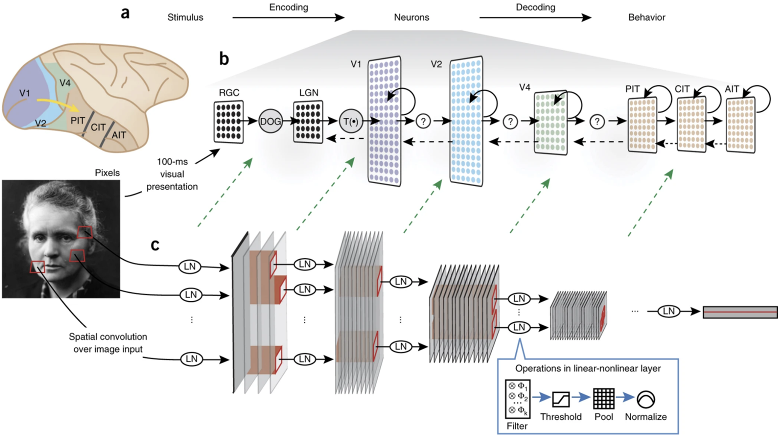


Again, this is not showing the use of an activation function

CNNs: Biological analogies

- It has been argued that common architectures for CNNs used for image processing mirror the organization and function of visual cortex in many species

CNNs: Biological analogies



Using goal-driven deep learning models to understand sensory cortex, Yamins and DiCarlo, 2016, https://www.nature.com/articles/nn.4244

Problem 4: Brain food (20 points)

This problem gives you some experience with convolutional neural networks for image classification using TensorFlow.

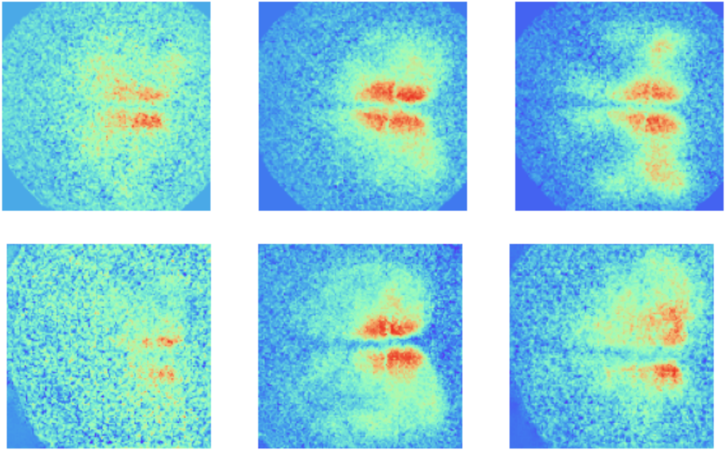
The classification task is to discriminate real optical images of brain activity in mice from fake images that were constructed using a generative adversarial network (GAN). A paper on the underlying imaging technologies developed by Yale researchers is here.

For this problem we'll walk you through the following steps:

- Downloading the data
- Loading the data
- Displaying some sample images
- Building a classification model using a simple CNN

After this, your task will be to improve upon this baseline model by building, training, and evaluating two more CNNs.

Task: Real or Fake?



Task: Real or Fake?

- The real images are optical images of neural activity at the surface of the cortex in transgenic mice
- The fake images were generated by a “deconvolutional” neural network trained as part of a GAN
- The discriminator network is similar to the networks you’ll train

Baseline model

```
model = models.Sequential()
model.add(layers.Conv2D(32, (5, 5), activation='relu', input_shape=(128, 128, 1)))
model.add(layers.MaxPooling2D((4, 4)))
model.add(layers.Flatten())
model.add(layers.Dense(2))
model.summary()
```

```
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d (Conv2D)              (None, 124, 124, 32)      832
_________________________________________________________________
max_pooling2d (MaxPooling2D) (None, 31, 31, 32)        0
_________________________________________________________________
flatten (Flatten)            (None, 30752)             0
_________________________________________________________________
dense (Dense)                (None, 2)                 61506
=================================================================
Total params: 62,338
Trainable params: 62,338
Non-trainable params: 0
_________________________________________________________________
```

Baseline model

First layer:

- Input: 128×128 images, 1 channel
- First layer: 32 filters, each of size 5×5
- Output of first layer: tensor of shape $124 \times 124 \times 32$
- Number of parameters: $(5 \times 5 + 1) \times 32 = 832$
- Activation function: ReLU
- Output of first layer: tensor of shape $124 \times 124 \times 32$

Baseline model

Second layer:

- Maximum of 4×4 regions in feature map
- Output: Tensor of shape $31 \times 31 \times 32$ since $124/4 = 31$
- Number of parameters: None!

Baseline model

Third layer:

- Flattened version of previous layer
- Number of neurons: $31 \times 31 \times 32 = 30{,}752$
- Number of parameters: None!

Baseline model

Final layer:

- Dense connections
- Two neurons in output (“fake” and “real”)
- Number of parameters: 30,752 $\times$ 2 $=$ 61,506

Baseline model

Overall:

- Number of parameters: $832 + 61{,}506 = 62{,}338$
- Most come from dense layer (98.7%)

Let's build another model

```
model = models.Sequential()
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```

Summary

- A convolutional layer applies a set of kernels (filters) across the input
- Each kernel is a tensor of smaller dimension than the input
- The values of the kernels are learned by backpropagation
- The convolutional layers define a set of features that are then used to make predictions in one or more dense layers
- CNNs are attractive whenever the data have “spatial” structure where the same features might appear at many different locations