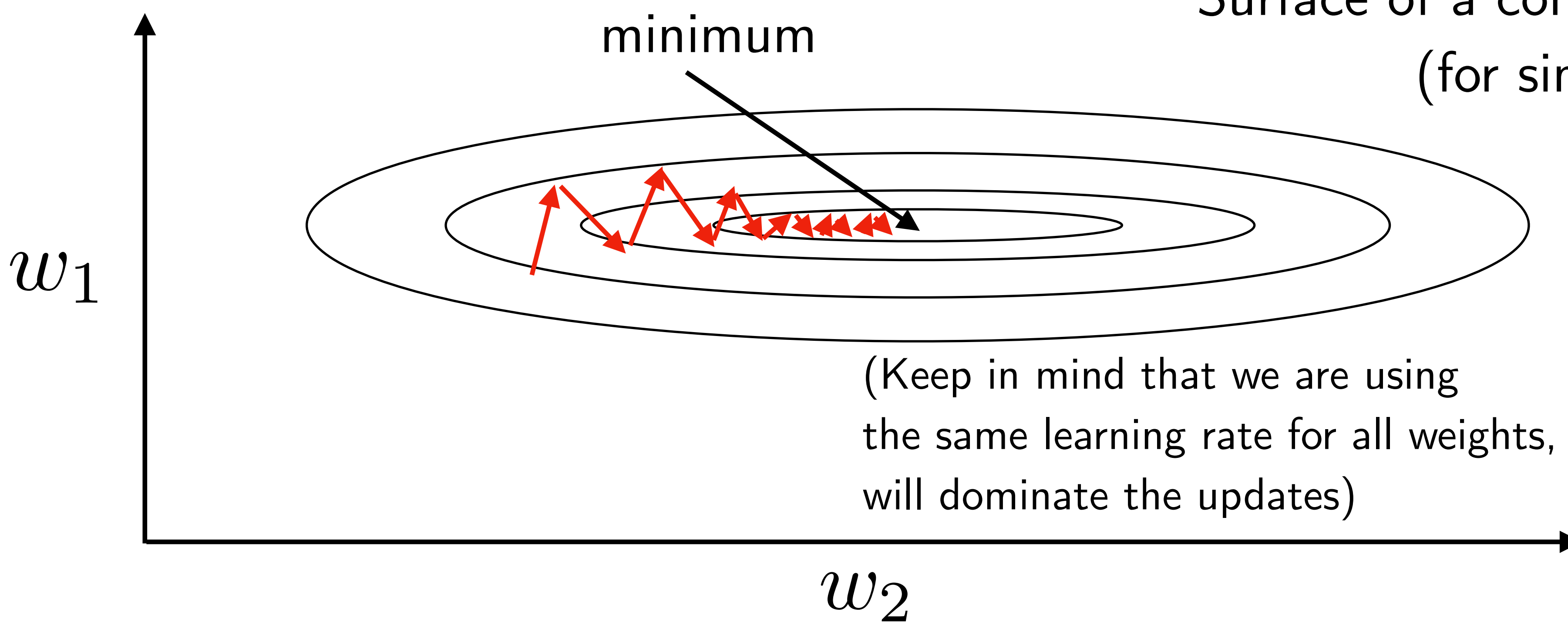
STATS 507: Data Analysis in Python

BatchNorm and Convolutional Neural Networks

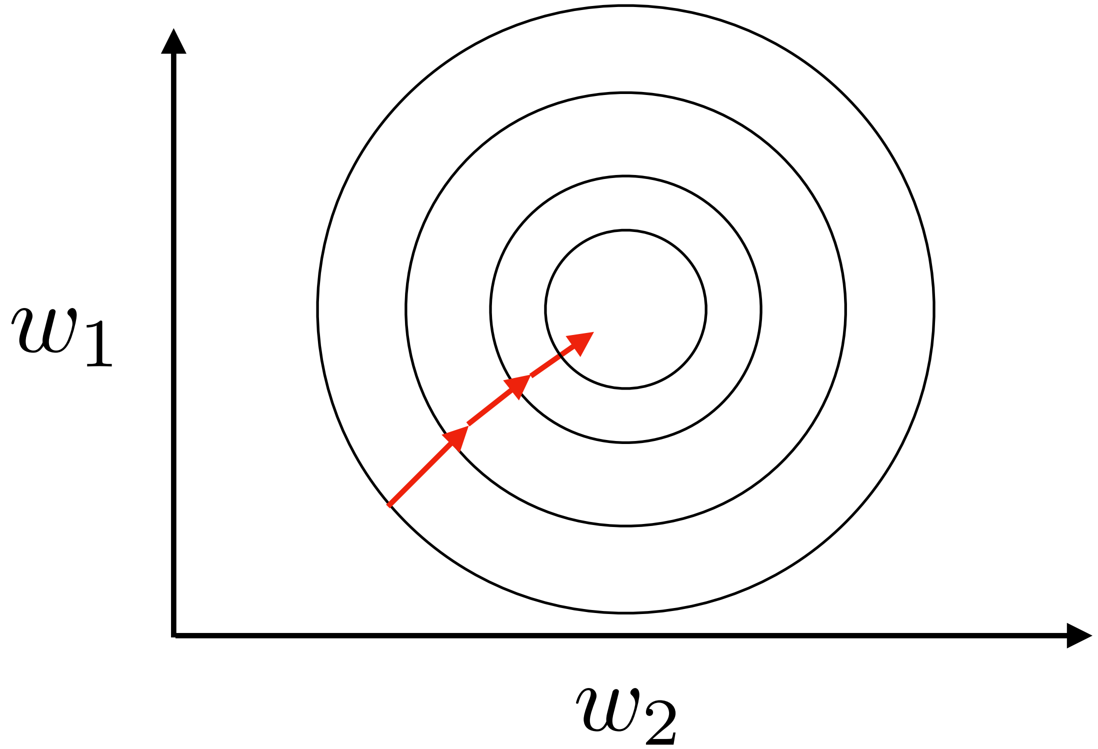
Adapted from slides by Sebastian Raschka.
Please do not distribute.

Why We Normalize Inputs for Gradient Descent

Surface of a convex cost function
(for simplicity)



(Keep in mind that we are using
the same learning rate for all weights, so large parameters
will dominate the updates)



"Standardization" of input features

$$x_j'^{[i]} = \frac{x_j^{[i]} - \mu_j}{\sigma_j}$$

(scaled feature will have
zero mean, unit variance)

Batch Normalization

Ioffe, S., & Szegedy, C. (2015, June). Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift. In *International Conference on Machine Learning* (pp. 448-456).

http://proceedings.mlr.press/v37/ioffe15.html

Batch Normalization

- Normalization of inputs for hidden layers
- Helps with exploding/vanishing gradient problems
- Can increase training stability and convergence rate
- Can be understood as additional normalization layers (with additional parameters)

BatchNorm Step 1: Normalize Net Inputs

$$\mu_j = \frac{1}{n} \sum_i z_j^{[i]}$$

$$\sigma_j^2 = \frac{1}{n} \sum_i (z_j^{[i]} - \mu_j)^2$$

$$z'^{[i]}_j = \frac{z_j^{[i]} - \mu_j}{\sigma_j}$$

BatchNorm Step 1: Normalize Net Inputs

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$$\sigma_j^2 = \frac{1}{n} \sum_i (z_j^{[i]} - \mu_j)^2$$

$$z'^{[i]}_j = \frac{z_j^{[i]} - \mu_j}{\sigma_j}$$

<u>In practice:</u>

$$z'^{[i]}_j = \frac{z_j^{[i]} - \mu_j}{\sqrt{\sigma_j^2 + \epsilon}}$$

For numerical stability, where epsilon is a small number like 1E-5

BatchNorm Step 2: Pre-Activation Scaling

$$z'^{[i]}_j = \frac{z^{[i]}_j - \mu_j}{\sqrt{\sigma^2_j + \epsilon}}$$

$$a'^{[i]}_j = \gamma_j \cdot z'^{[i]}_j + \beta_j$$

These are learnable parameters

BatchNorm Step 2: Pre-Activation Scaling

$$z'^{[i]}_j = \frac{z^{[i]}_j - \mu_j}{\sigma_j}$$

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Controls the mean

Controls the spread or scale

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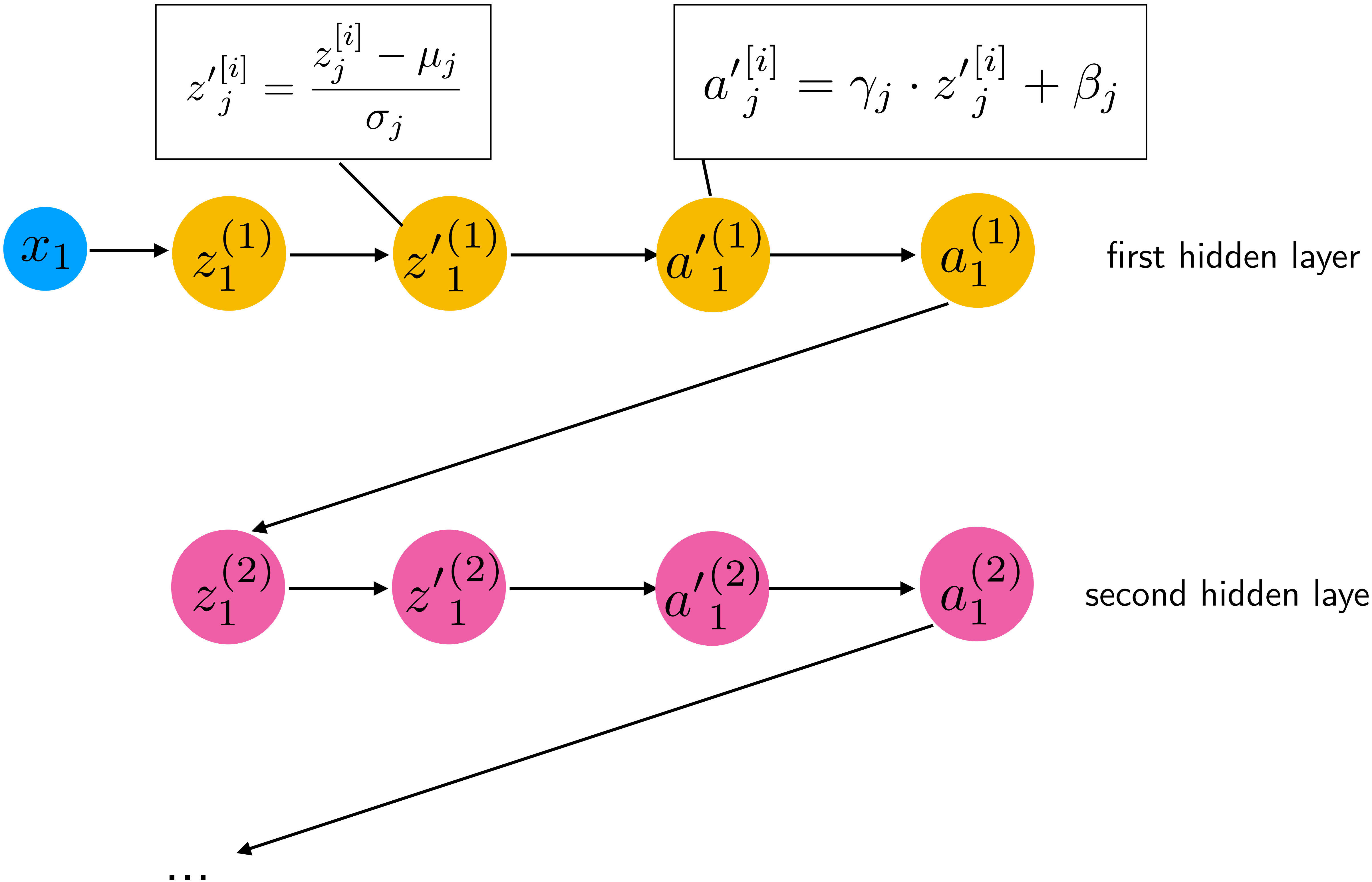
Controls the mean

Controls the spread or scale

Technically, a BatchNorm layer could learn to perform "standardization" with zero mean and unit variance

BatchNorm Step 1 & 2 Summarized



BatchNorm -- Additional Things to Consider

$$a'^{[i]}_j = \gamma_j \cdot z'^{[i]}_j + \beta_j$$

This parameter makes the bias units redundant

Also, note that the batchnorm parameters are vectors with the same number of elements as the bias vector

BatchNorm in PyTorch

```
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_features, num_hidden_1)
        self.linear_1_bn = torch.nn.BatchNorm1d(num_hidden_1)

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_hidden_1, num_hidden_2)
        self.linear_2_bn = torch.nn.BatchNorm1d(num_hidden_2)

        ### Output layer
        self.linear_out = torch.nn.Linear(num_hidden_2, num_classes)

    def forward(self, x):
        out = self.linear_1(x)
        # note that batchnorm is in the classic
        # sense placed before the activation
        out = self.linear_1_bn(out)
        out = F.relu(out)

        out = self.linear_2(out)
        out = self.linear_2_bn(out)
        out = F.relu(out)

        logits = self.linear_out(out)
        probas = F.softmax(logits, dim=1)
        return logits, probas
```

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        probas = F.softmax(logits, dim=1)
        return logits, probas
```

don't forget `model.train()`
and `model.eval()`
in training and test loops

BatchNorm During Prediction ("Inference")

- Use exponentially weighted average (moving average) of mean and variance

```
running_mean = momentum * running_mean
               + (1 - momentum) * sample_mean
```

(where momentum is typically ~0.1; and same for variance)

- Alternatively, can also use global training set mean and variance

How Does Batch Normalization Help Optimization?

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Abstract

Batch Normalization (BatchNorm) is a widely adopted technique that enables faster and more stable training of deep neural networks (DNNs). Despite its pervasiveness, the exact reasons for BatchNorm's effectiveness are still poorly understood. The popular belief is that this effectiveness stems from controlling the change of the layers' input distributions during training to reduce the so-called "internal covariate shift". In this work, we demonstrate that such distributional stability of layer inputs has little to do with the success of BatchNorm. Instead, we uncover a more fundamental impact of BatchNorm on the training process: it makes the optimization landscape significantly smoother. This smoothness induces a more predictive and stable behavior of the gradients, allowing for faster training.

BatchNorm Enables Faster Convergence By Allowing Larger Learning Rates

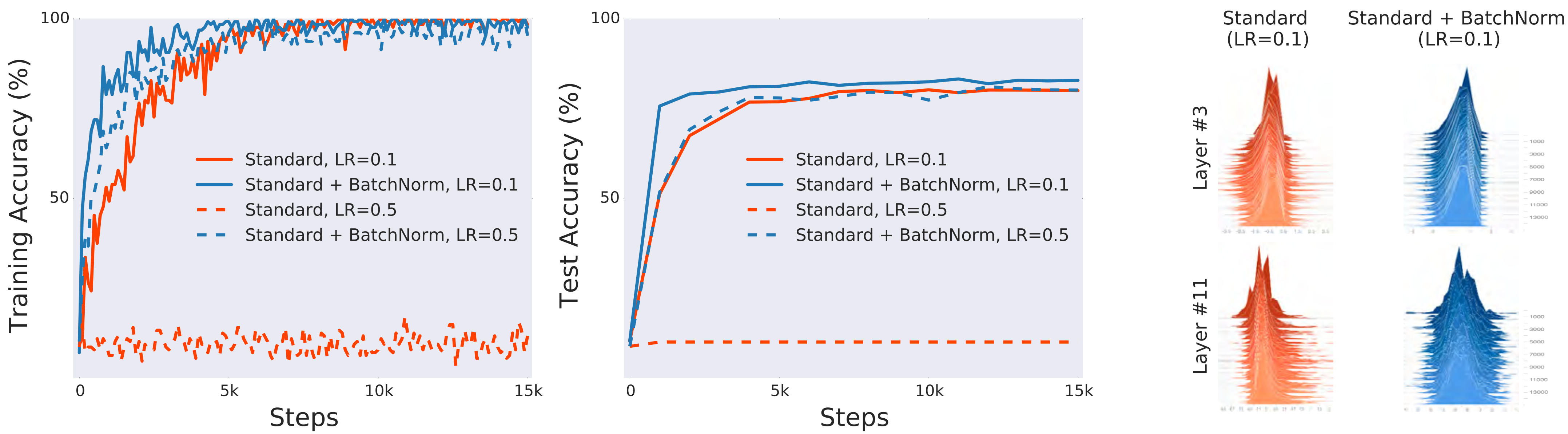


Figure 1: Comparison of (a) training (optimization) and (b) test (generalization) performance of a standard VGG network trained on CIFAR-10 with and without BatchNorm (details in Appendix A). There is a consistent gain in training speed in models with BatchNorm layers. (c) Even though the gap between the performance of the BatchNorm and non-BatchNorm networks is clear, the difference in the evolution of layer input distributions seems to be much less pronounced. (Here, we sampled activations of a given layer and visualized their distribution over training steps.)

Santurkar, S., Tsipras, D., Ilyas, A., & Madry, A. (2018). How does batch normalization help optimization?.
In *Advances in Neural Information Processing Systems* (pp. 2488-2498).

Practical Consideration

BatchNorm become more stable with larger minibatch sizes

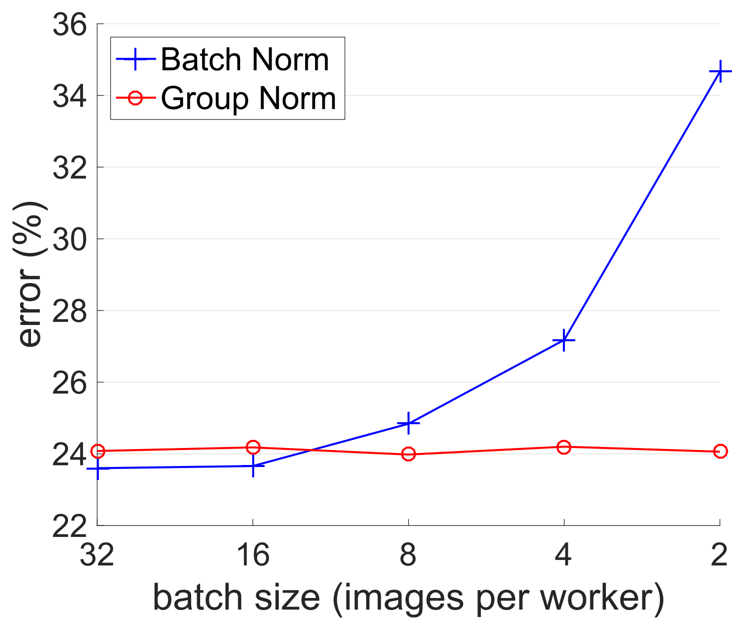


Figure 1. ImageNet classification error *vs*. batch sizes. The model is ResNet-50 trained in the ImageNet training set using 8 workers (GPUs) and evaluated in the validation set. BN's error increases rapidly when reducing the batch size. GN's computation is independent of batch sizes, and its error rate is stable despite the batch size changes. GN has substantially lower error (by 10%) than BN with a batch size of 2.

Wu, Y., & He, K. (2018). Group normalization. In *Proceedings of the European Conference on Computer Vision (ECCV)* (pp. 3-19).

Also note: BatchNorm can make Dropout unnecessary.

Other Normalization Methods for Hidden Activations

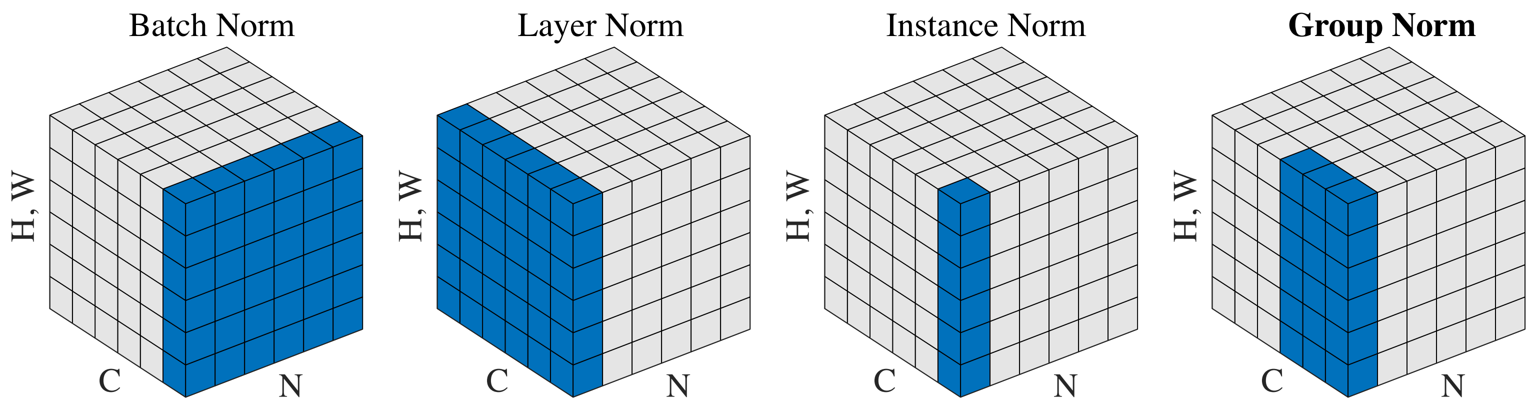


Figure 2. Normalization methods. Each subplot shows a feature map tensor. The pixels in blue are normalized by the same mean and variance, computed by aggregating the values of these pixels. Group Norm is illustrated using a group number of 2.

Wu, Y., & He, K. (2018). Group normalization. In *Proceedings of the European Conference on Computer Vision (ECCV)* (pp. 3-19).

Adaptive Learning Rates

There are many different flavors of adapting the learning rate (bit out of scope for this course to review them all)

Key take-aways:

- decrease learning if the gradient changes its direction
- increase learning if the gradient stays consistent

Adaptive Learning Rate via ADAM

$$m_t := \alpha \cdot m_{t-1} + (1-\alpha) \cdot \frac{\partial \mathcal{L}}{\partial w_{i,j}}(t)$$

$$r := \beta \cdot MeanSquare(w_{i,j}, t-1) + (1-\beta)\left(\frac{\partial \mathcal{L}}{\partial w_{i,j}(t)}\right)^2$$

CLASS `torch.optim.Adam(params, lr=0.001, betas=(0.9, 0.999), eps=1e-08, weight_decay=0, amsgrad=False)` [SOURCE]

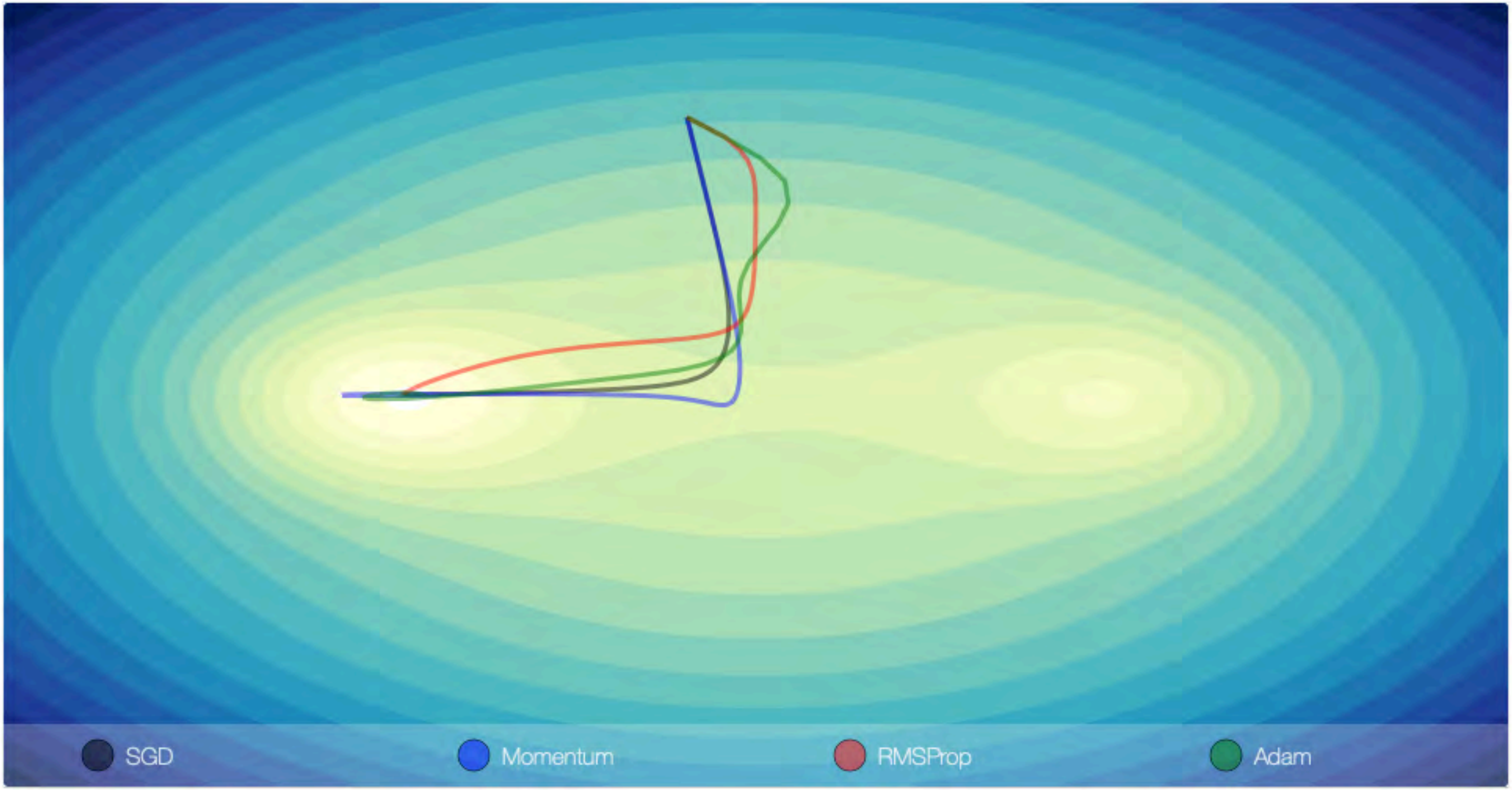
Implements Adam algorithm.

It has been proposed in Adam: A Method for Stochastic Optimization.

Parameters:
- **params** (*iterable*) – iterable of parameters to optimize or dicts defining parameter groups
- **lr** (*float*, *optional*) – learning rate (default: 1e-3)
- **betas** (*Tuple[float, float]*, *optional*) – coefficients used for computing running averages of gradient and its square (default: (0.9, 0.999))
- **eps** (*float*, *optional*) – term added to the denominator to improve numerical stability (default: 1e-8)
- **weight_decay** (*float*, *optional*) – weight decay (L2 penalty) (default: 0)

The default settings for the "betas" work usually just fine

Source: https://pytorch.org/docs/stable/optim.html



https://bl.ocks.org/EmilienDupont/aaf429be5705b219aaaf8d691e27ca87

Using Different Optimizers in PyTorch

Usage is the as for vanilla SGD, which we used before,

you can find an overview at: https://pytorch.org/docs/stable/optim.html

```
optimizer = torch.optim.SGD(model.parameters(), lr=0.01, momentum=0.9)
optimizer = torch.optim.Adam(model.parameters(), lr=0.0001)
```

Convolutional Neural Networks (a.k.a. ConvNets; a.k.a. CNNs)

Adapted from slides by Alex Smola (UC Berkeley and Amazon Web Services)

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Classifying Dogs and Cats in Images

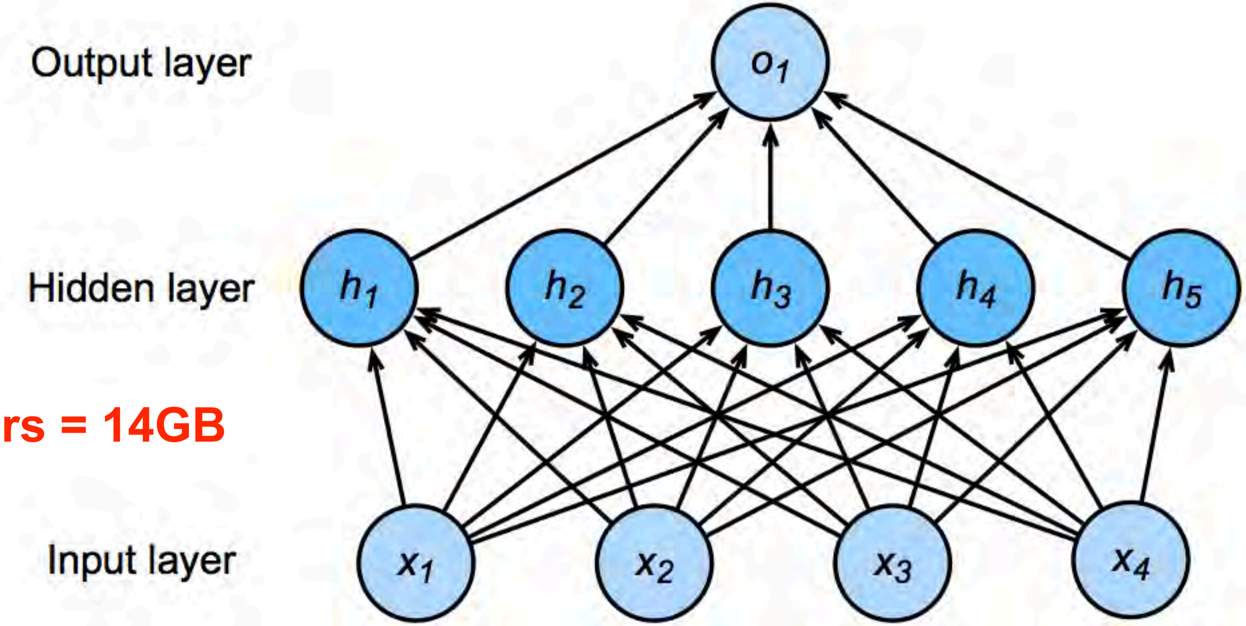
- Use a good camera
- RGB image has 36M elements
- The model size of a single hidden layer MLP with a 100 hidden size is 3.6 Billion parameters
- Exceeds the population of dogs and cats on earth (900M dogs + 600M cats)

Flashback - Network with one hidden layer

100 neurons

3.6B parameters = 14GB

36M features



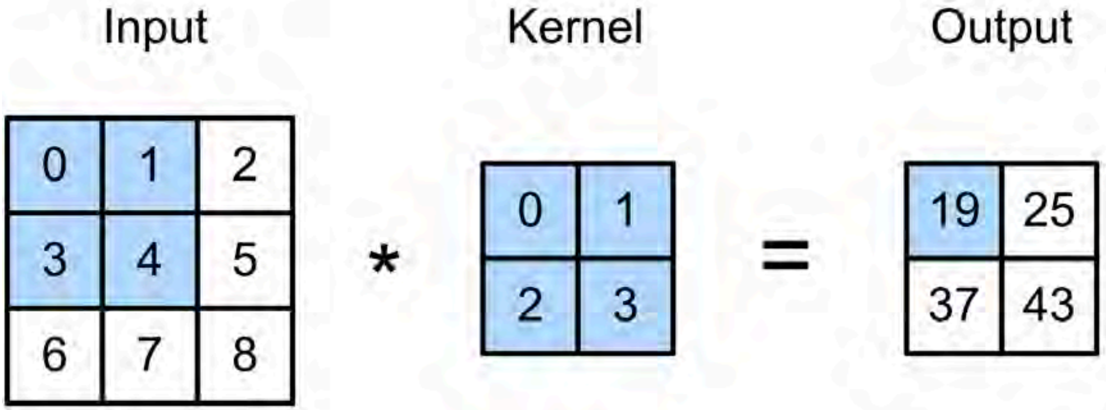
$$\mathbf{h} = \sigma\left(\mathbf{W}\mathbf{x} + \mathbf{b}\right)$$

Where is Waldo?

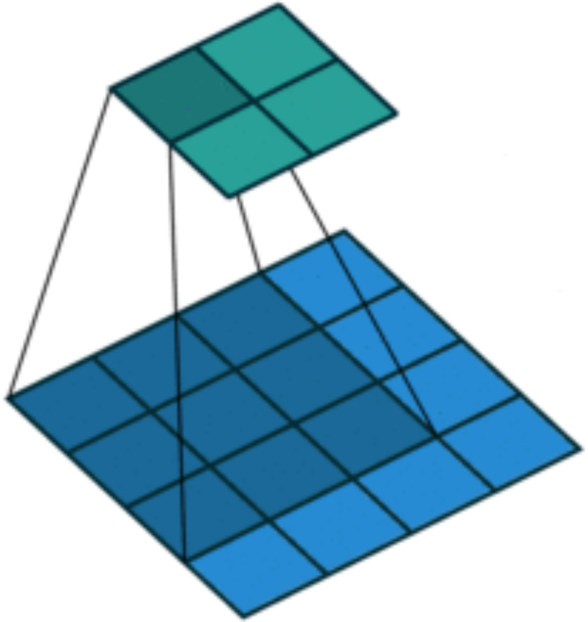
Two Principles

- Translation Invariance
- Locality

2-D Convolution



$$
\begin{aligned}
0 \times 0 + 1 \times 1 + 3 \times 2 + 4 \times 3 &= 19, \\
1 \times 0 + 2 \times 1 + 4 \times 2 + 5 \times 3 &= 25, \\
3 \times 0 + 4 \times 1 + 6 \times 2 + 7 \times 3 &= 37, \\
4 \times 0 + 5 \times 1 + 7 \times 2 + 8 \times 3 &= 43.
\end{aligned}
$$



(vdumoulin@ Github)

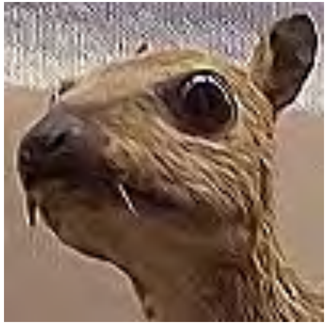
Examples

(wikipedia)

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

Edge Detection

$$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$



Sharpen

$$\frac{1}{16}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$$

Gaussian Blur

2-D Convolution Layer

$$\begin{bmatrix}0&1&2\\3&4&5\\6&7&8\end{bmatrix} * \begin{bmatrix}0&1\\2&3\end{bmatrix} = \begin{bmatrix}19&25\\37&43\end{bmatrix}$$

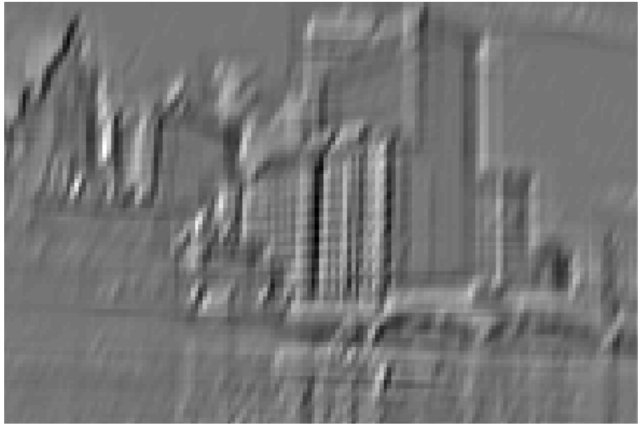
- $\mathbf{X} : n_h \times n_w$ input matrix
- $\mathbf{W} : k_h \times k_w$ kernel matrix
- b: scalar bias
- $\mathbf{Y} : (n_h - k_h + 1) \times (n_w - k_w + 1)$ output matrix

$$\mathbf{Y} = \mathbf{X} \star \mathbf{W} + b$$

- **W** and *b* are learnable parameters

Examples

(Rob Fergus)



1-D and 3-D Cross Correlations

- 1-D

$$y_i = \sum_{a=1}^{h} w_a x_{i+a}$$

  - Text
  - Voice
  - Time series

- 3-D

$$y_{i,j,k} = \sum_{a=1}^{h} \sum_{b=1}^{w} \sum_{c=1}^{d} w_{a,b,c} x_{i+a,j+b,k+c}$$

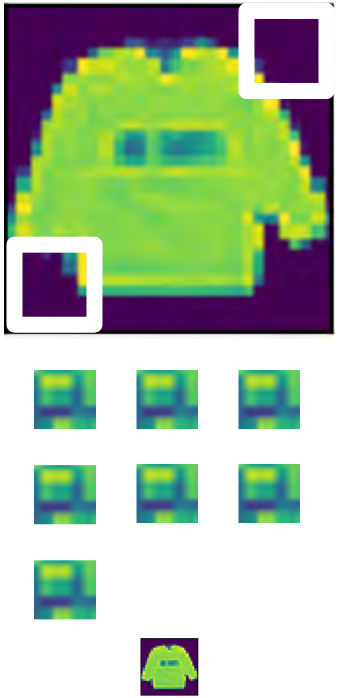
  - Video
  - Medical images

Padding and Stride

Padding

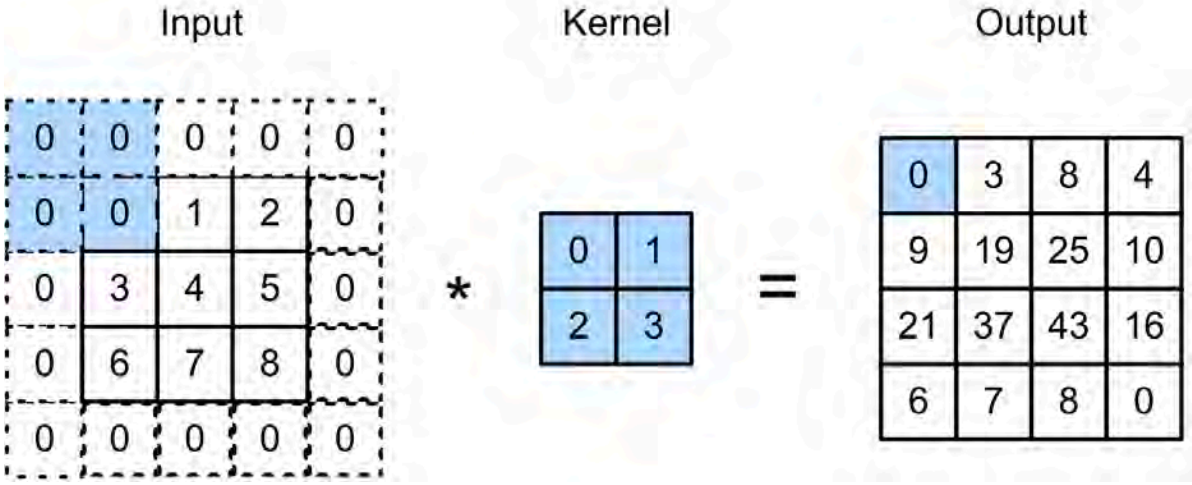
- Given a 32 x 32 input image
- Apply convolutional layer with 5 x 5 kernel
  - 28 x 28 output with 1 layer
  - 4 x 4 output with 7 layers
- Shape decreases faster with larger kernels
  - Shape reduces from $n_h \times n_w$ to

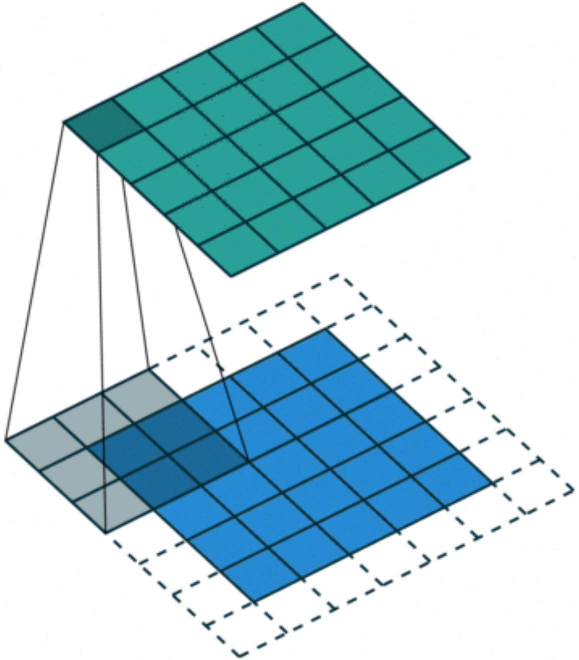
$$(n_h - k_h + 1) \times (n_w - k_w + 1)$$



Padding

Padding adds rows/columns around input

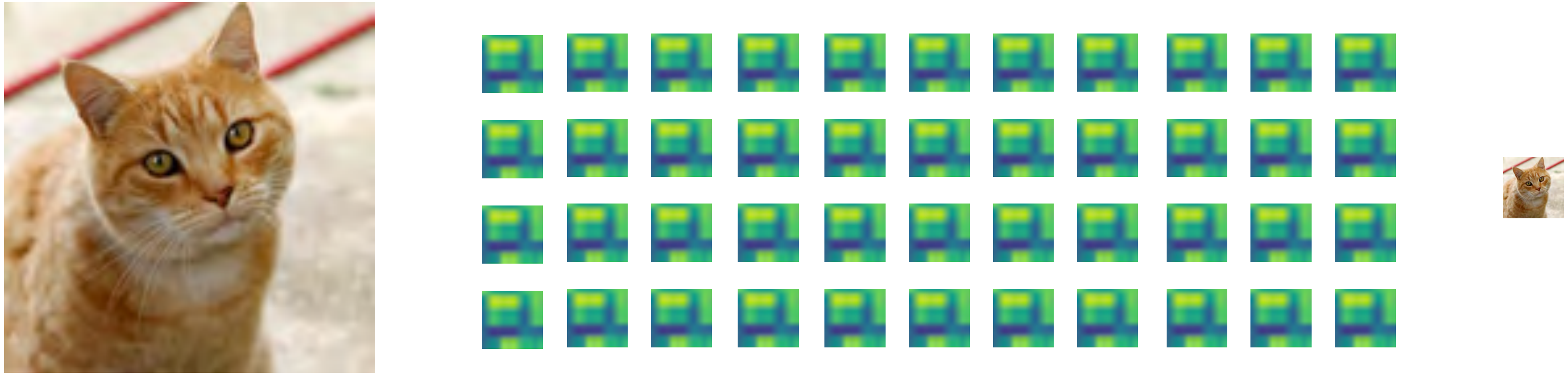




$$0 \times 0 + 0 \times 1 + 0 \times 2 + 0 \times 3 = 0$$

Stride

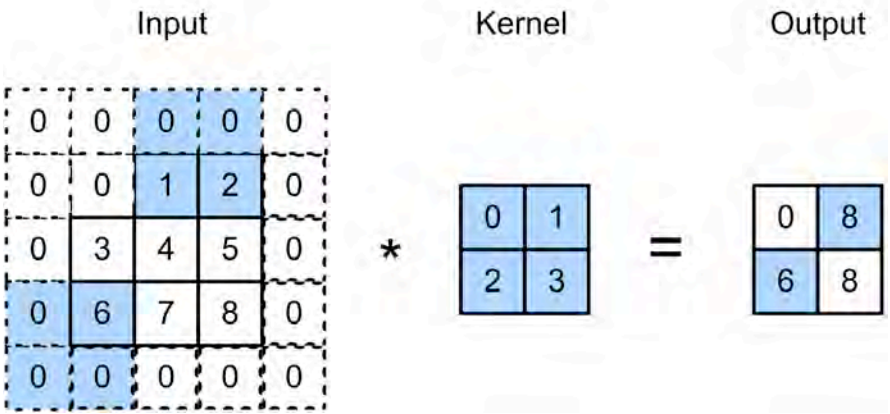
- Convolution reduces shape linearly with #layers
  - Given a 224 x 224 input with a 5 x 5 kernel, needs 44 layers to reduce the shape to 4 x 4
  - Requires a large amount of computation



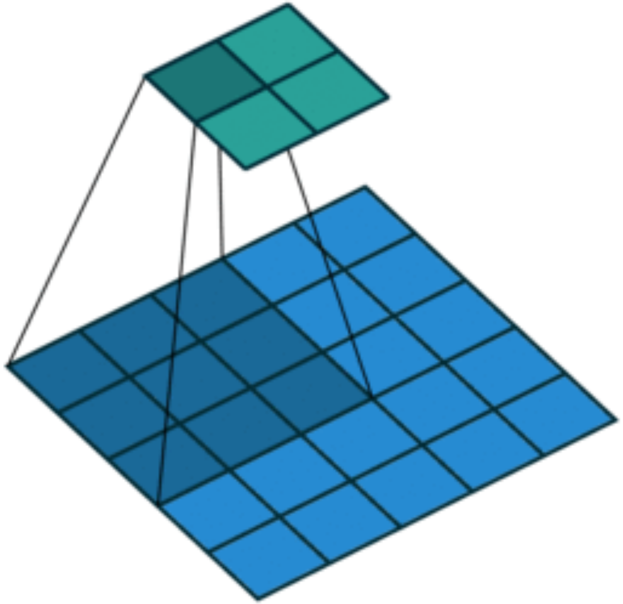
Stride

- Stride is the #rows/#columns per slide

Strides of 3 and 2 for height and width



$$0 \times 0 + 0 \times 1 + 1 \times 2 + 2 \times 3 = 8$$
$$0 \times 0 + 6 \times 1 + 0 \times 2 + 0 \times 3 = 6$$



Stride

- Given stride s_h for the height and stride s_w for the width, the output shape is

$$\lfloor (n_h - k_h + p_h + s_h)/s_h \rfloor \times \lfloor (n_w - k_w + p_w + s_w)/s_w \rfloor$$

- With $p_h = k_h - 1$ and $p_w = k_w - 1$

$$\lfloor (n_h + s_h - 1)/s_h \rfloor \times \lfloor (n_w + s_w - 1)/s_w \rfloor$$

- If input height/width are divisible by strides

$$(n_h/s_h) \times (n_w/s_w)$$

Multiple Input and Output Channels

Multiple Input Channels

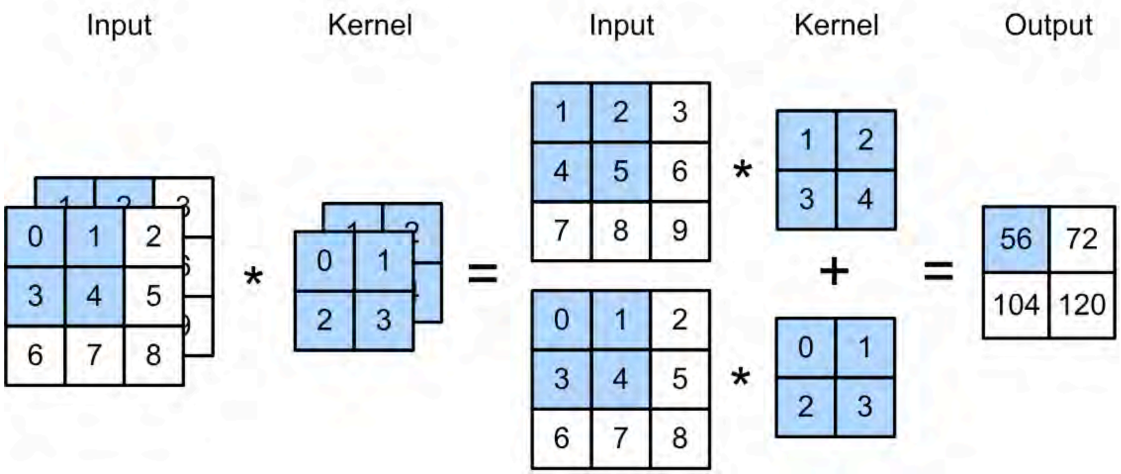
- Color image may have three RGB channels
- Converting to grayscale loses information

Multiple Input Channels

- Color image may have three RGB channels
- Converting to grayscale loses information

Multiple Input Channels

- Have a kernel for each channel, and then sum results over channels



$$(1\times1+2\times2+4\times3+5\times4)$$
$$+(0\times0+1\times1+3\times2+4\times3)$$
$$=56$$

Multiple Input Channels

- $\mathbf{X} : c_i \times n_h \times n_w$ input
- $\mathbf{W} : c_i \times k_h \times k_w$ kernel
- $\mathbf{Y} : m_h \times m_w$ output

$$\mathbf{Y} = \sum_{i=0}^{c_i} \mathbf{X}_{i,:,:} \star \mathbf{W}_{i,:,:}$$

Multiple Output Channels

- No matter how many inputs channels, so far we always get single output channel
- We can have multiple 3-D kernels, each one generates a output channel
- Input $\mathbf{X} : c_i \times n_h \times n_w$
- Kernel $\mathbf{W} : c_o \times c_i \times k_h \times k_w$
- Output $\mathbf{Y} : c_o \times m_h \times m_w$

$$\mathbf{Y}_{i,:,:} = \mathbf{X} \star \mathbf{W}_{i,:,:,:}$$

$$\text{for } i = 1,\ldots,c_o$$

Multiple Input/Output Channels

- Each output channel may recognize a particular pattern

- Input channels kernels recognize and combines patterns in inputs

2-D Convolution Layer Summary

- Input $\mathbf{X} : c_i \times n_h \times n_w$
- Kernel $\mathbf{W} : c_o \times c_i \times k_h \times k_w$
- Bias $\mathbf{B} : c_o \times c_i$
- Output $\mathbf{Y} : c_o \times m_h \times m_w$

$$\mathbf{Y} = \mathbf{X} \star \mathbf{W} + \mathbf{B}$$

- Complexity (number of floating point operations FLOP)

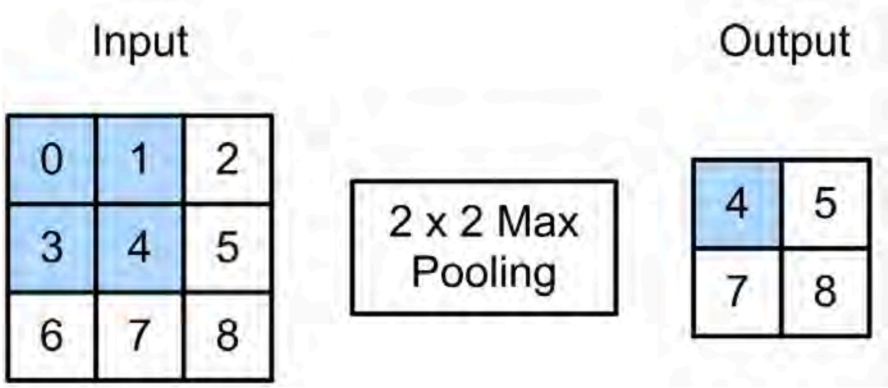
$$c_i = c_o = 100$$
$$k_h = h_w = 5 \qquad O(c_i c_o k_h k_w m_h m_w) \qquad \text{1GFLOP}$$
$$m_h = m_w = 64$$

- 10 layers, 1M examples: 10PF
(CPU: 0.15 TF = 18h, GPU: 12 TF = 14min)

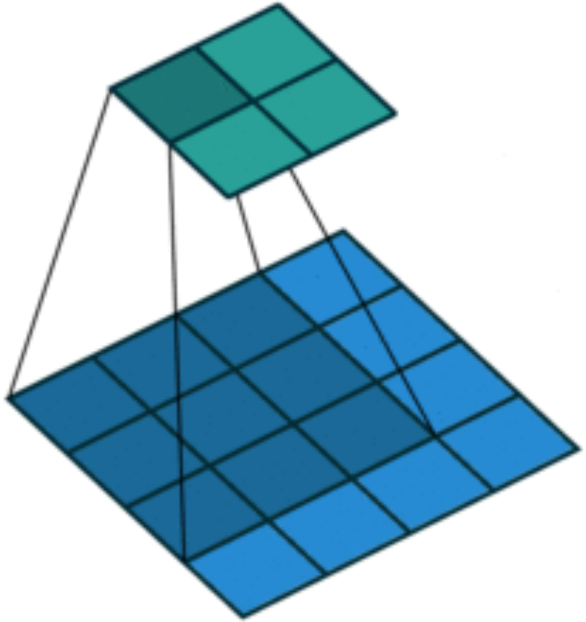
Pooling Layer

2-D Max Pooling

- Returns the maximal value in the sliding window



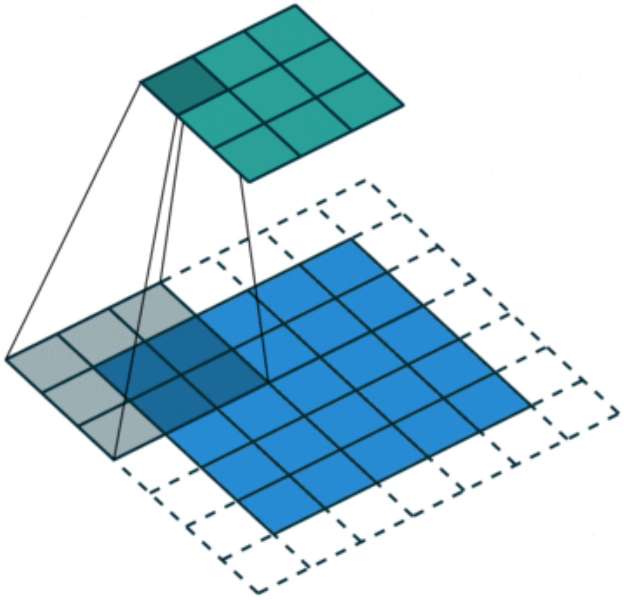
$$\max(0,1,3,4) = 4$$



Padding, Stride, and Multiple Channels

- Pooling layers have similar padding and stride as convolutional layers
- No learnable parameters
- Apply pooling for each input channel to obtain the corresponding output channel

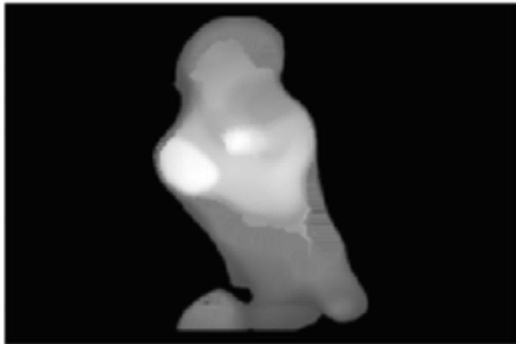
  #output channels = #input channels



Average Pooling

- Max pooling: the strongest pattern signal in a window
- Average pooling: replace max with mean in max pooling
  - The average signal strength in a window

Max pooling



Average pooling

```python
class LeNet5(nn.Module):

    def __init__(self, num_classes, grayscale=False):
        super(LeNet5, self).__init__()

        self.grayscale = grayscale
        self.num_classes = num_classes

        if self.grayscale:
            in_channels = 1
        else:
            in_channels = 3

        self.features = nn.Sequential(
            nn.Conv2d(in_channels, 6, kernel_size=5),
            nn.Tanh(),
            nn.MaxPool2d(kernel_size=2),
            nn.Conv2d(6, 16, kernel_size=5),
            nn.Tanh(),
            nn.MaxPool2d(kernel_size=2)
        )

        self.classifier = nn.Sequential(
            nn.Linear(16*5*5, 120),
            nn.Tanh(),
            nn.Linear(120, 84),
            nn.Tanh(),
            nn.Linear(84, num_classes),
        )

    def forward(self, x):
        x = self.features(x)
        x = torch.flatten(x, 1)
        logits = self.classifier(x)
        probas = F.softmax(logits, dim=1)
        return logits, probas
```

LeNet-5 in PyTorch

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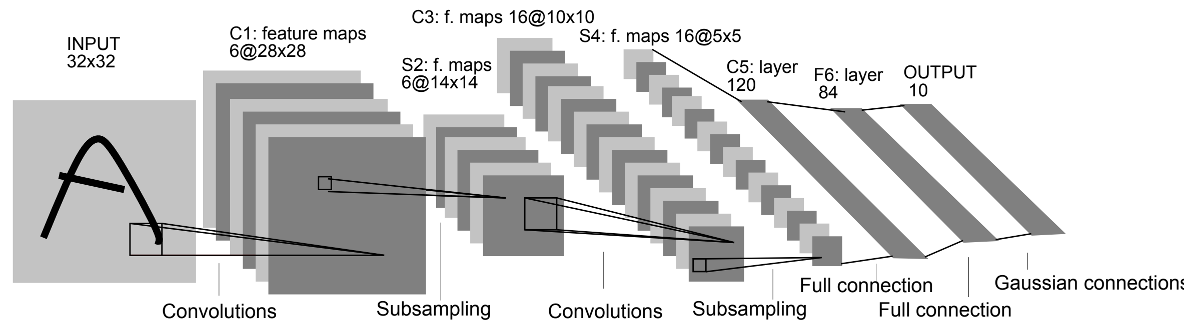

Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

slide credit: Sebastian Raschka