Deep Learning

Lecture 9

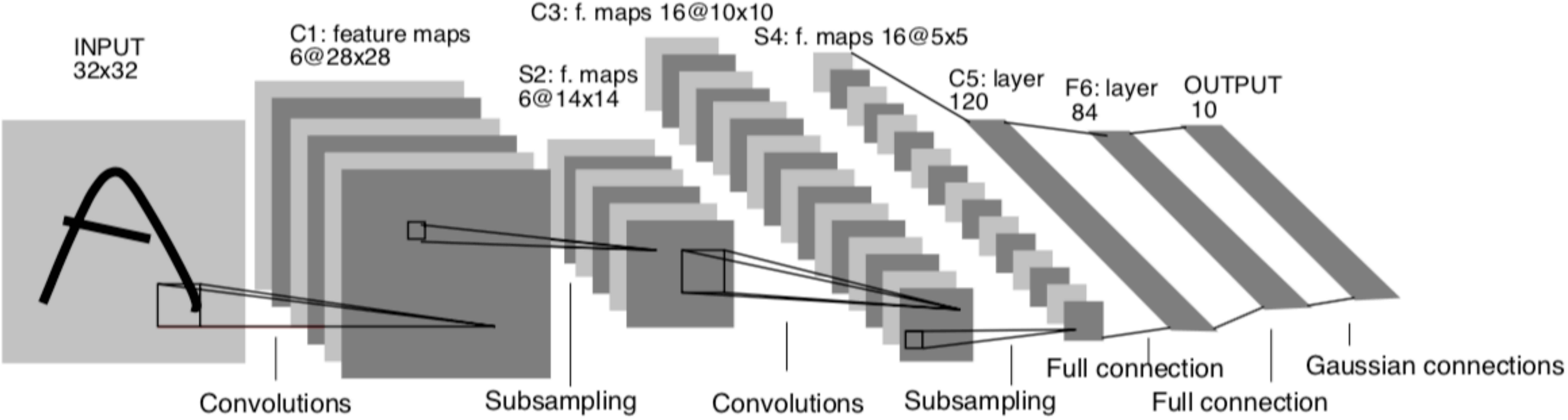
From LeNet to ResNet

A Brief History of CNNs

Part 2

Last time…LeNet-5

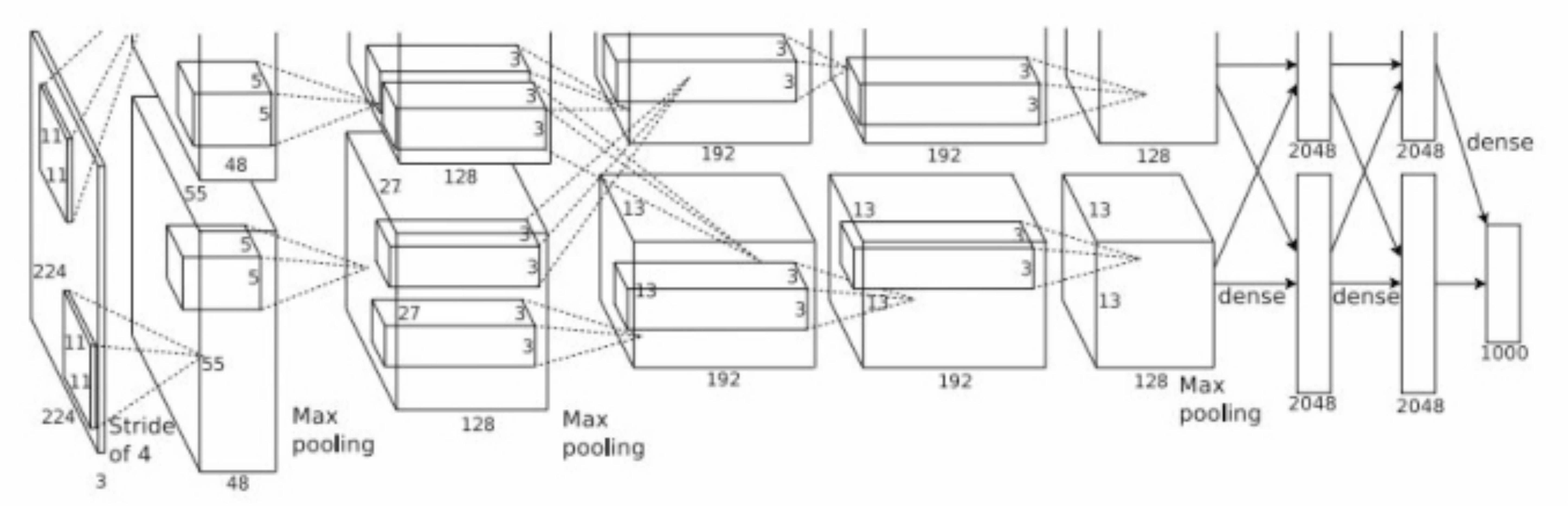
[LeCun et al., 1998]



Conv filters were 5x5, stride 1
Subsampling (Pooling) layers were 2x2, stride 2
Architecture is CONV-POOL-CONV-POOL-FC-FC
Fun fact: MNIST (modified NIST) hand-written digits dataset introduced in this paper!

Last time…AlexNet

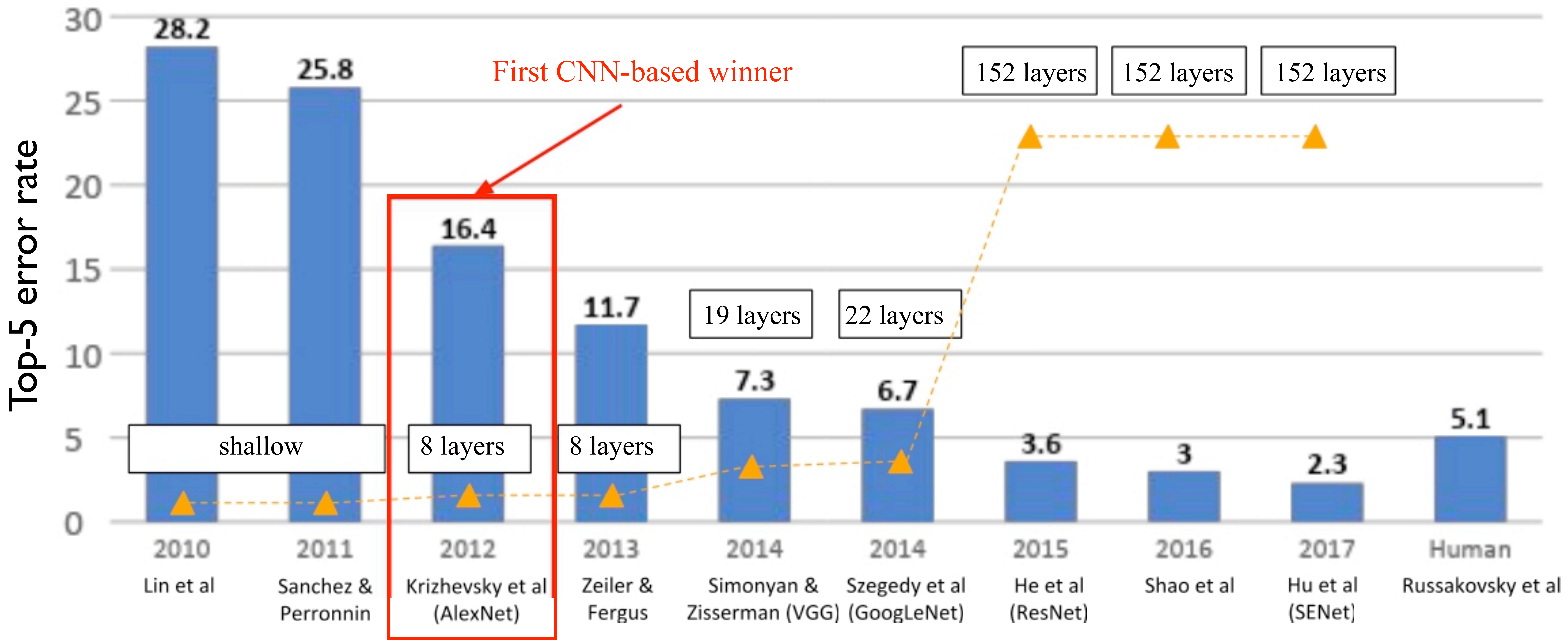
[Krizhevsky et al. 2012]



Full (simplified) AlexNet architecture:
[227x227x3] INPUT
[55x55x96] CONV1 : 96 11x11 filters at stride 4, pad 0
[27x27x96] MAX POOL1 : 3x3 filters at stride 2
[27x27x96] NORM1: Normalization layer
[27x27x256] CONV2 : 256 5x5 filters at stride 1, pad 2
[13x13x256] MAX POOL2: 3x3 filters at stride 2
[13x13x256] NORM2: Normalization layer
[13x13x384] CONV3 : 384 3x3 filters at stride 1, pad 1
[13x13x384] CONV4 : 384 3x3 filters at stride 1, pad 1
[13x13x256] CONV5 : 256 3x3 filters at stride 1, pad 1
[6x6x256] MAX POOL3 : 3x3 filters at stride 2
[4096] FC6: 4096 neurons
[4096] FC7: 4096 neurons
[1000] FC8: 1000 neurons (class scores)

Model	Top-1 (val)	Top-5 (val)	Top-5 (test)
SIFT + FVs [7]	—	—	*26.2%*
1 CNN	40.7%	18.2%	—
5 CNNs	38.1%	16.4%	**16.4%**
1 CNN*	39.0%	16.6%	—
7 CNNs*	36.7%	15.4%	**15.3%**

ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners



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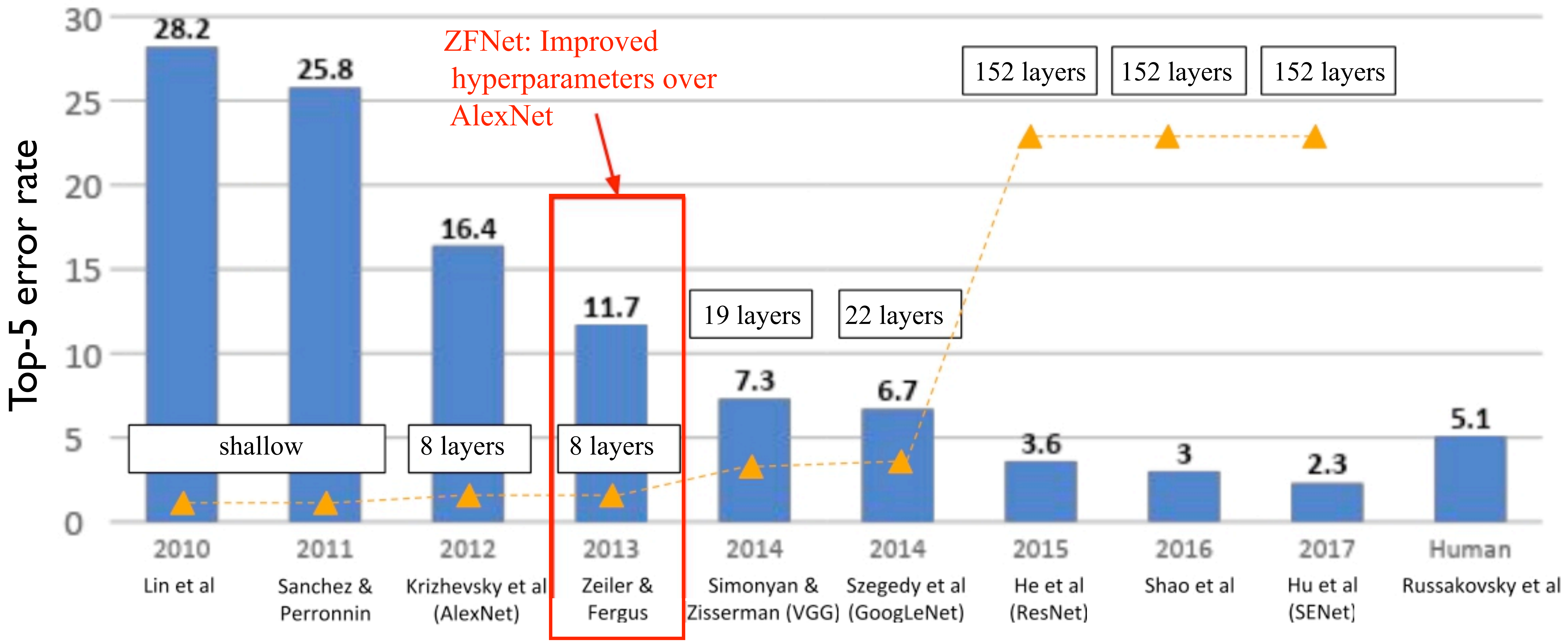
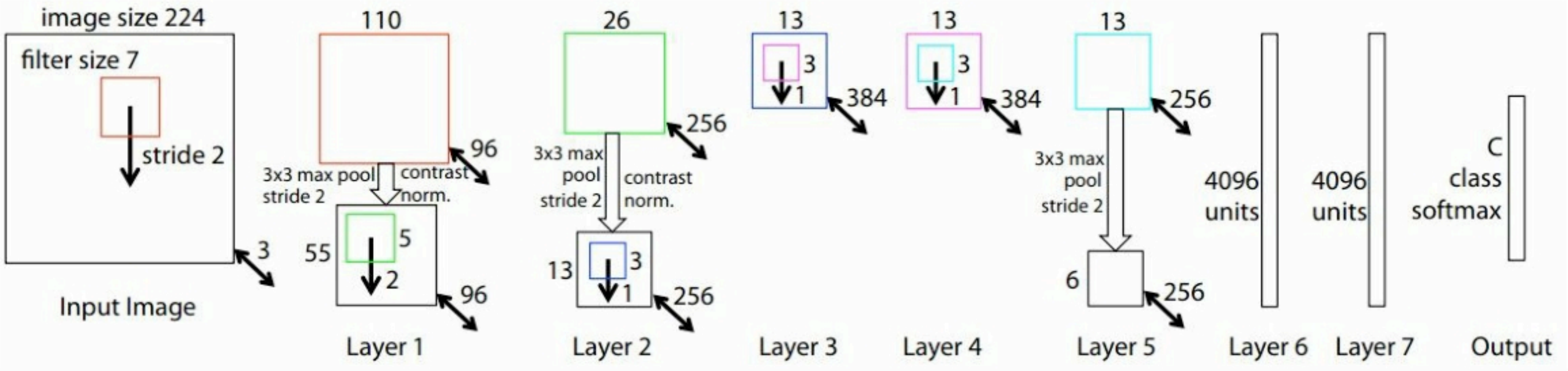


ZFNet

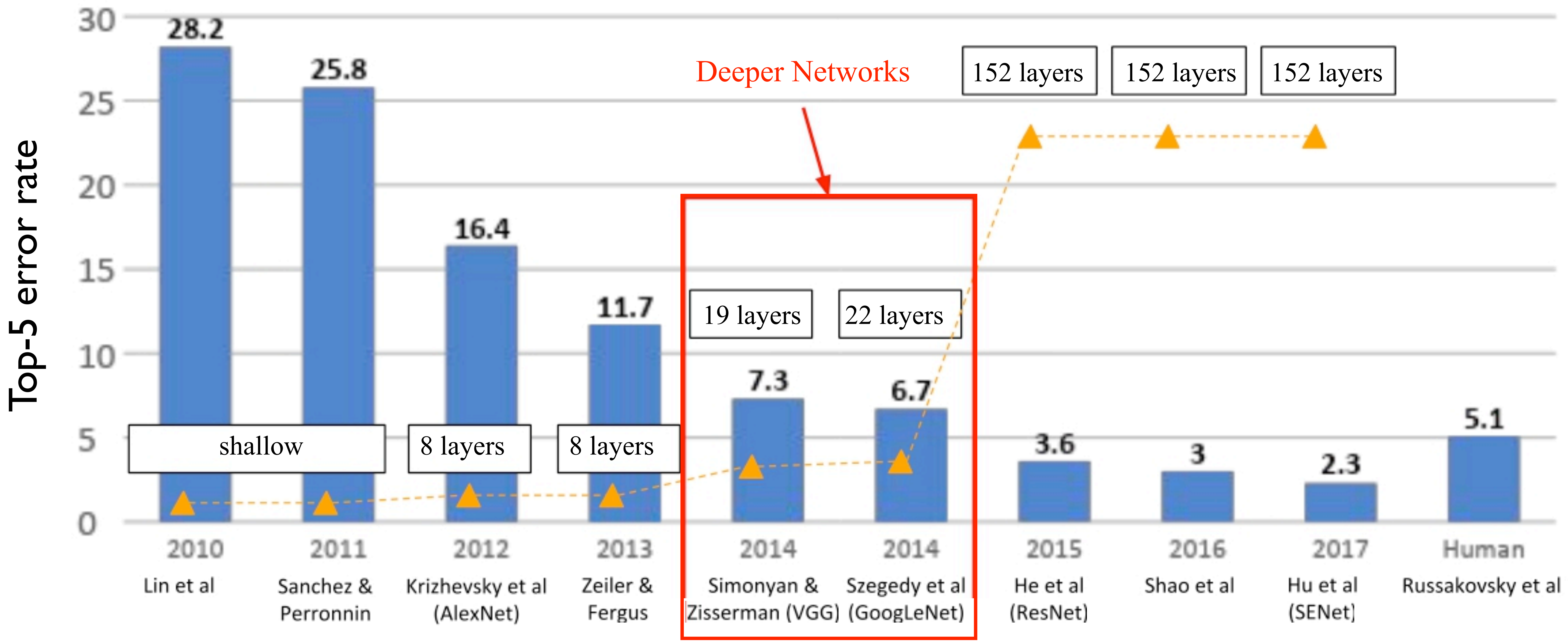
[Zeiler and Fergus, 2013]



AlexNet but:
CONV1: change from (11x11 stride 4) to (7x7 stride 2)
CONV3,4,5: instead of 384, 384, 256 filters use 512, 1024, 512

ImageNet top 5 error: 16.4% -> 11.7%

ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners



Used with permission from Justin Johnson

Case Study: VGGNet

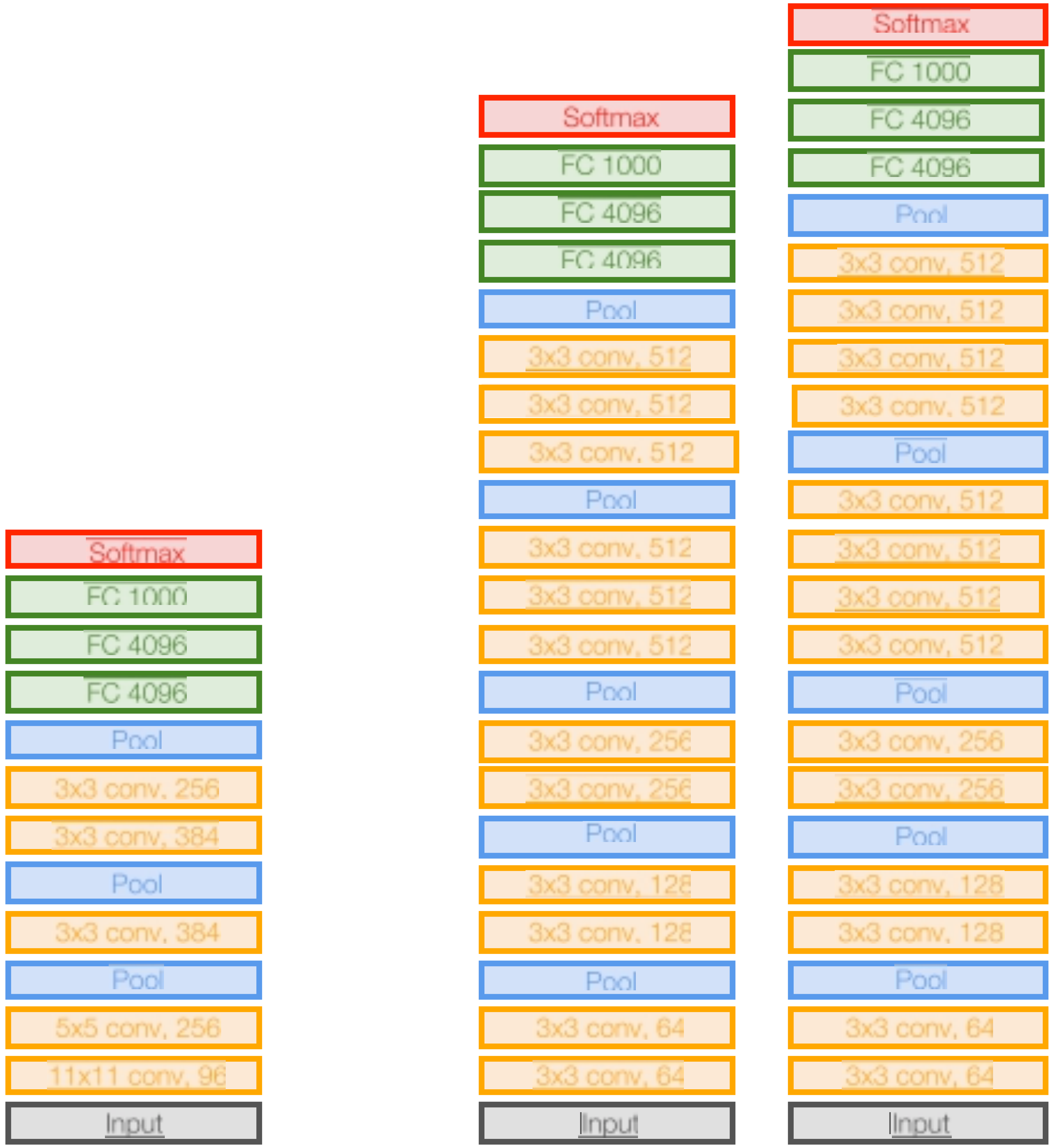
[Simonyan and Zisserman, 2014]

Small filters, Deeper networks

8 layers (AlexNet)
-> 16 - 19 layers (VGG16Net)

Only 3x3 CONV stride 1, pad 1
and 2x2 MAX POOL stride 2

11.7% top 5 error in ILSVRC'13
(ZFNet)
-> 7.3% top 5 error in ILSVRC'14

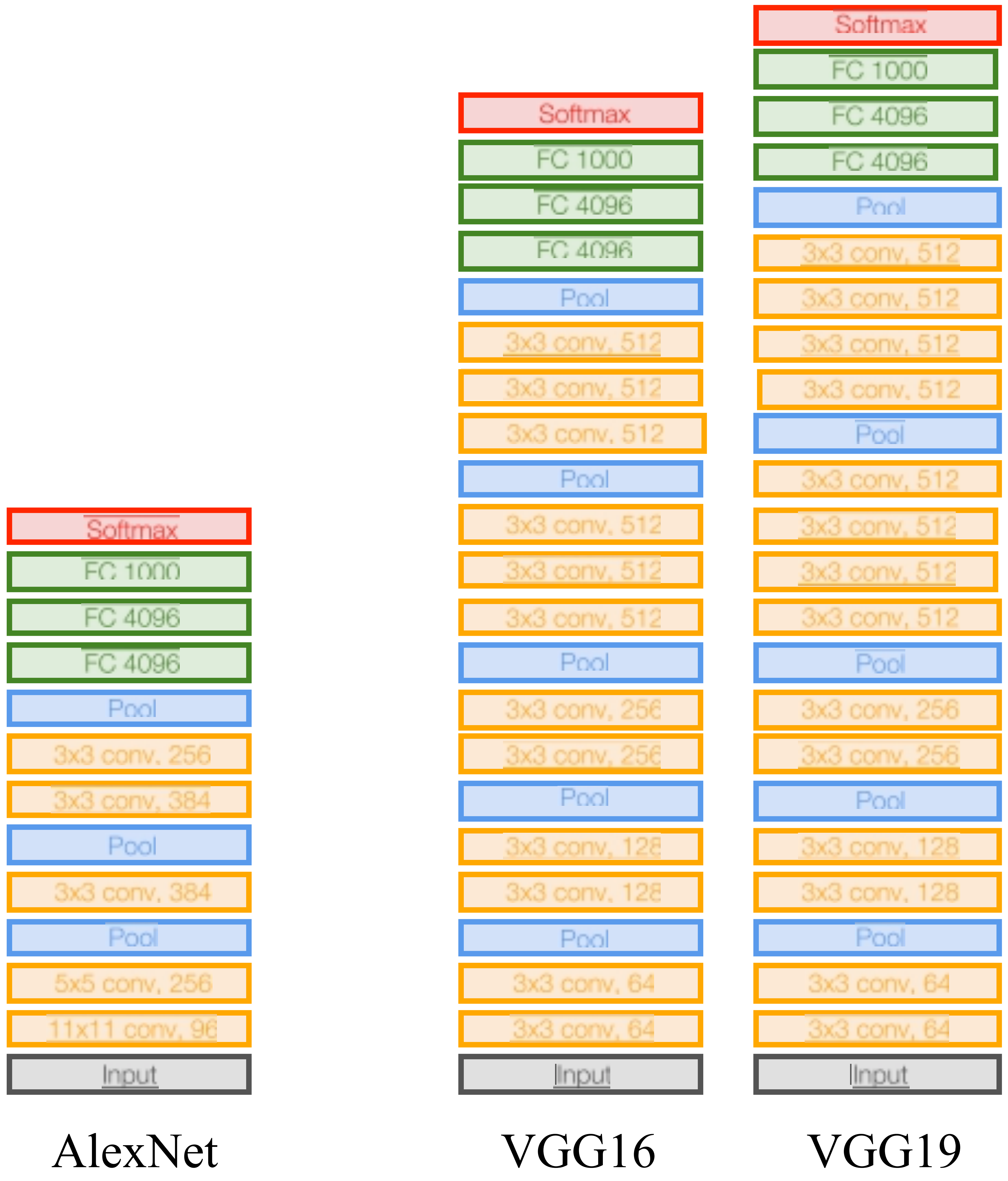


AlexNet VGG16 VGG19

Case Study: VGGNet

[Simonyan and Zisserman, 2014]

Q: Why use smaller filters? (3x3 conv)



Case Study: VGGNet

[Simonyan and Zisserman, 2014]

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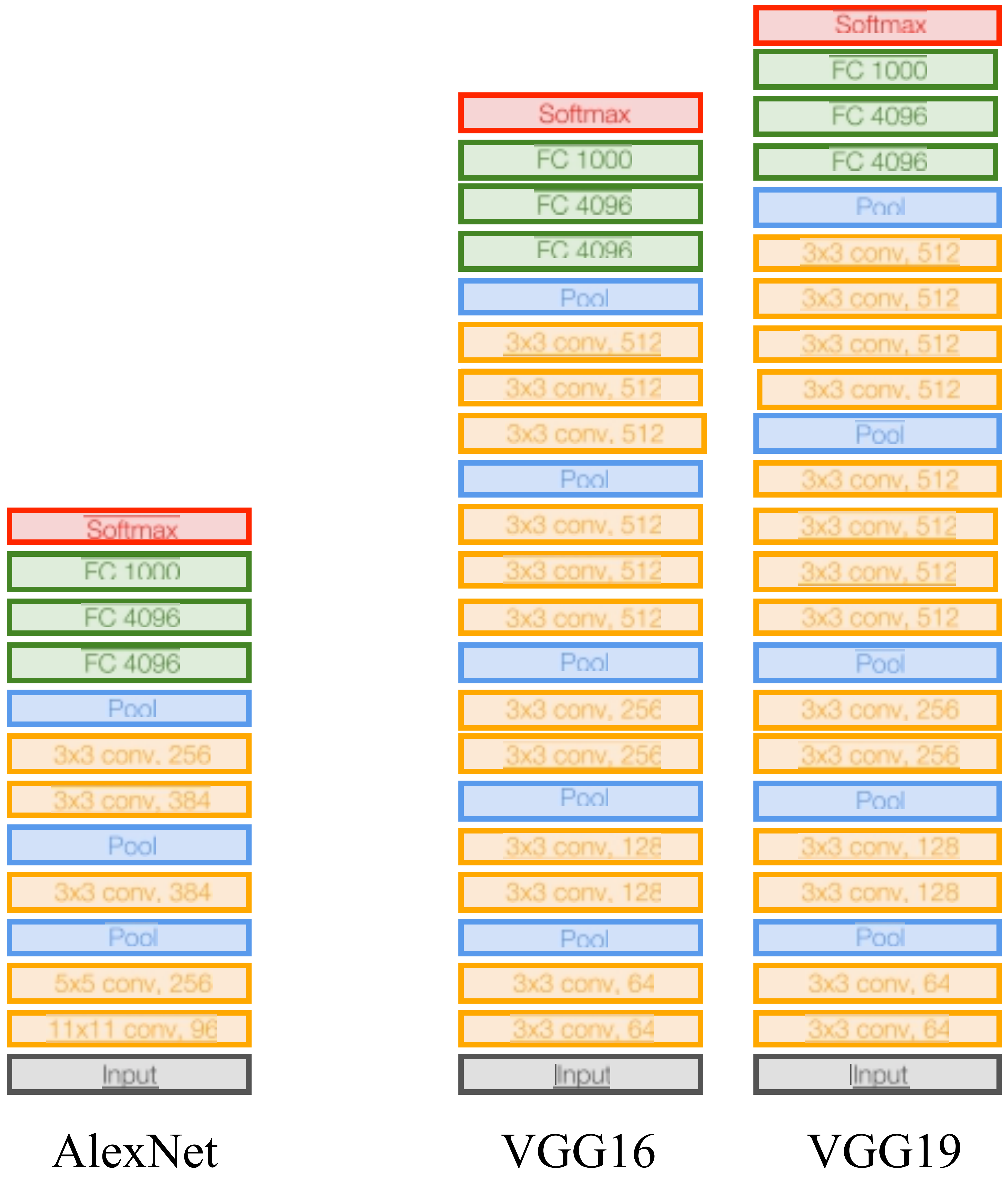
Smaller filters have fewer parameters.



Case Study: VGGNet

[Simonyan and Zisserman, 2014]

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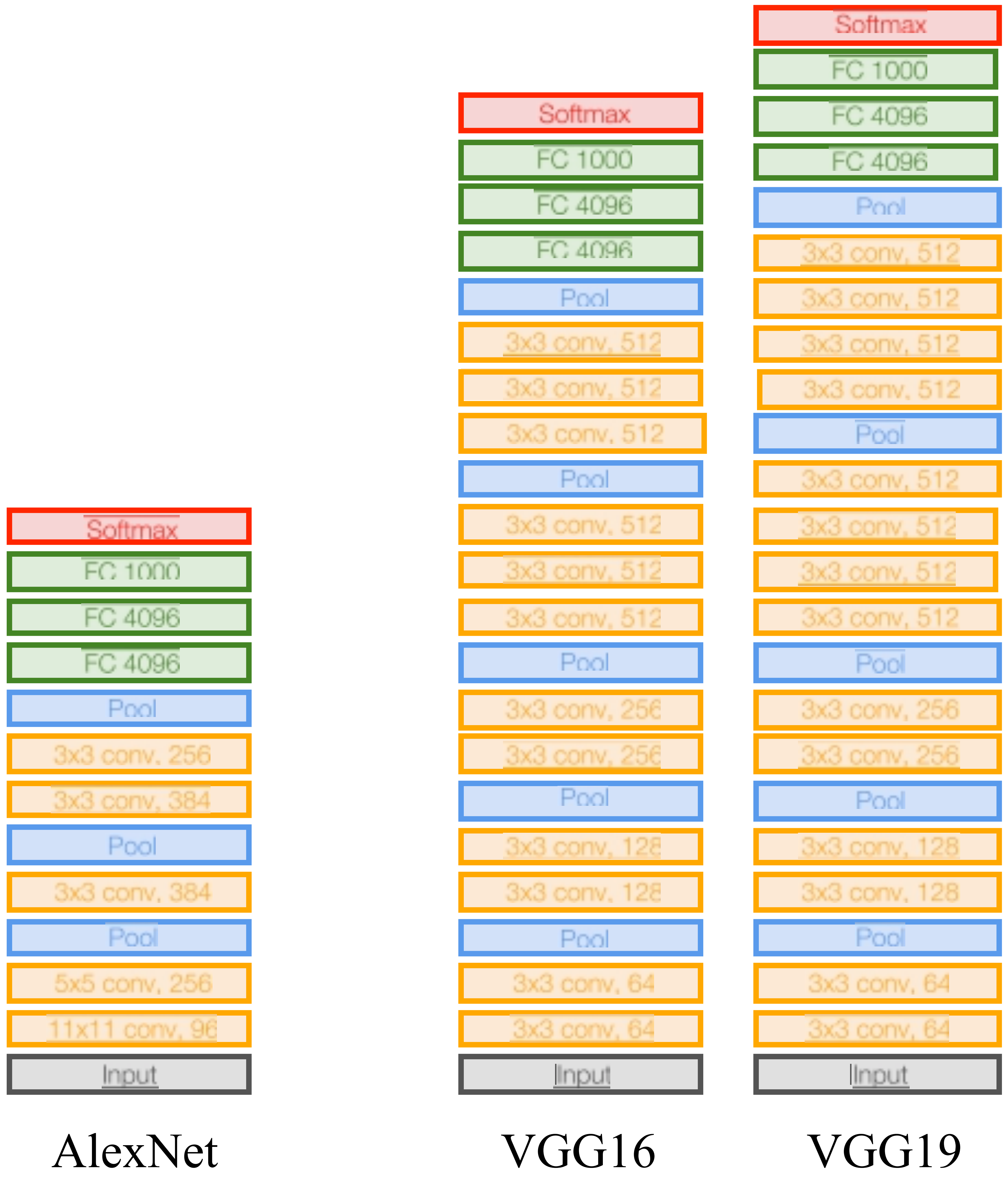
Smaller filters have fewer parameters.

Q: What is the effective receptive field of two 3x3 conv (stride 1) layers?



Case Study: VGGNet

[Simonyan and Zisserman, 2014]

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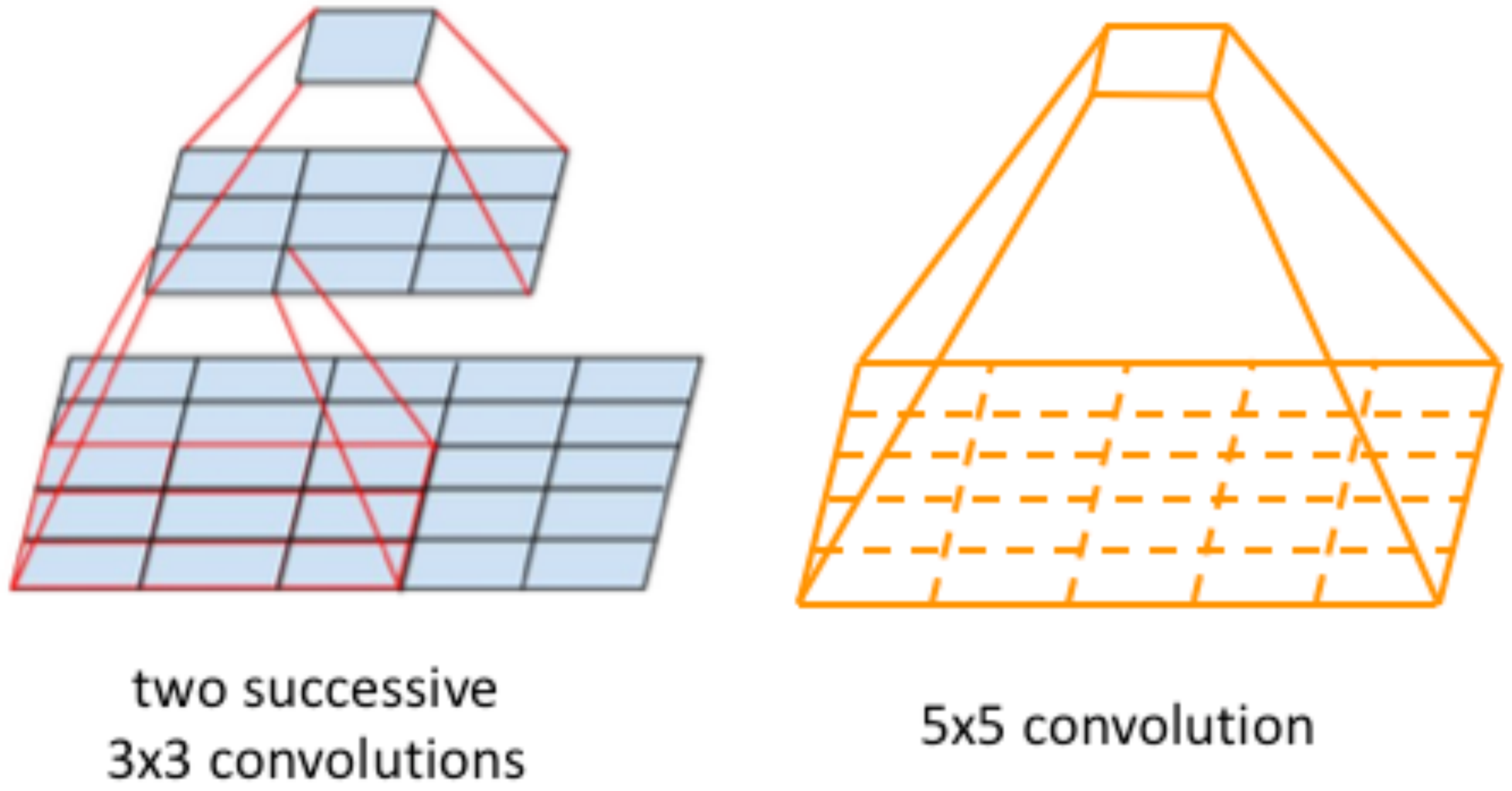
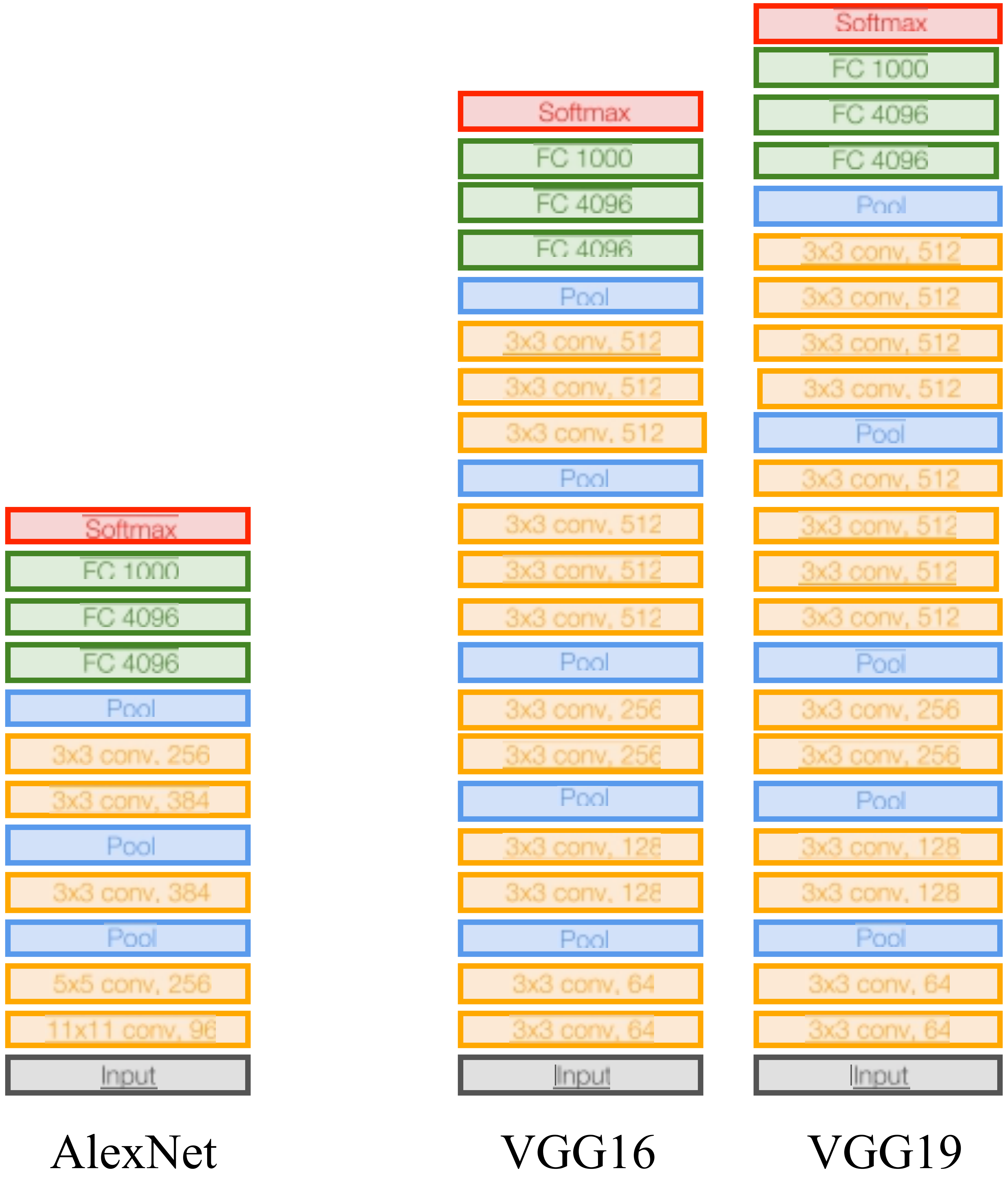
5x5





Case Study: VGGNet

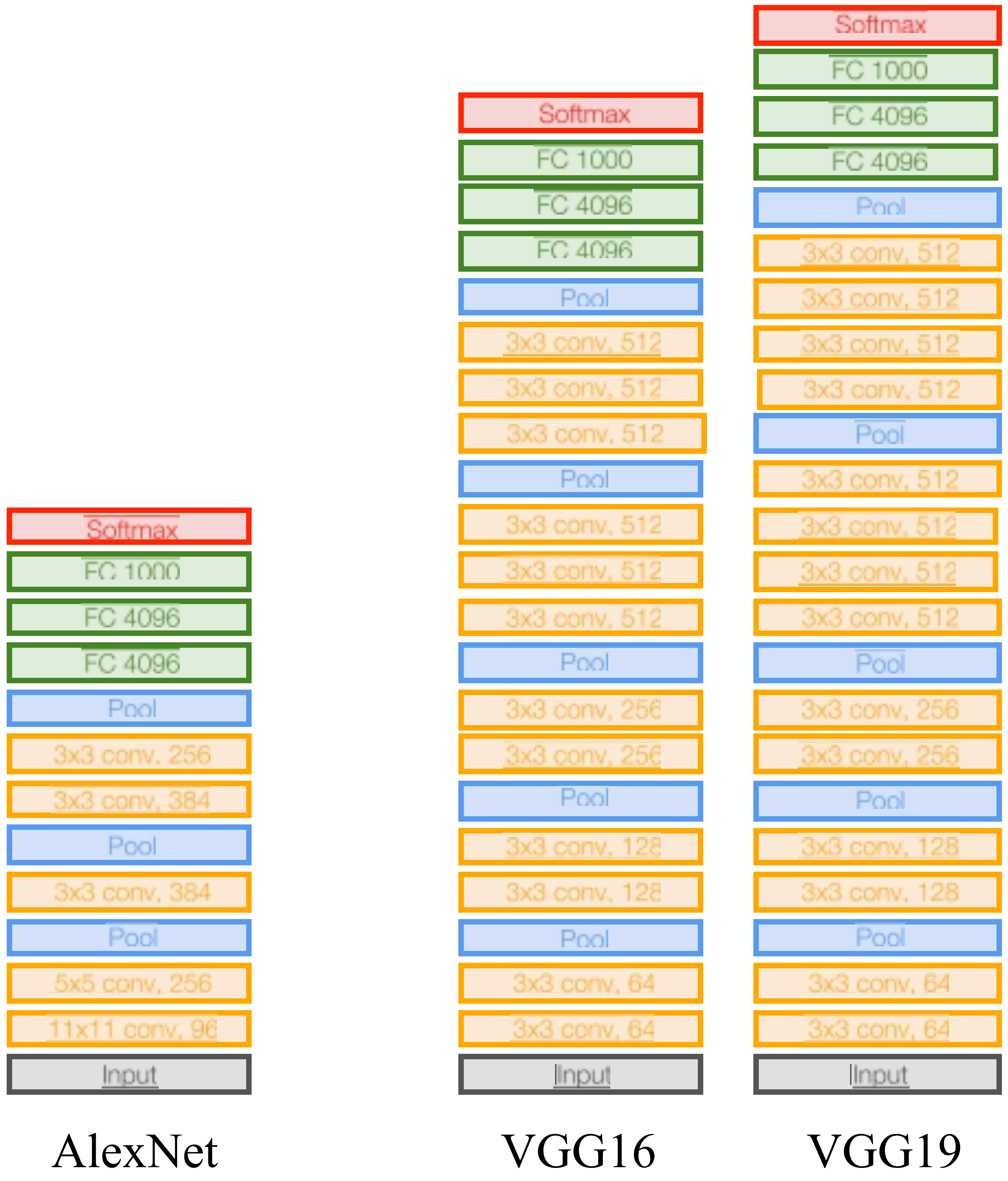
[Simonyan and Zisserman, 2014]

Q: Why use smaller filters? (3x3 conv)

Stack of three 3x3 conv (stride 1) layers has same **effective receptive field** as one 7x7 conv layer!

But deeper, more non-linearities.

And fewer parameters: $3 * (3^2C^2)$ vs. 7^2C^2 for C channels per layer



INPUT: [224x224x3] memory: 224*224*3=150K params: 0 (not counting biases)

CONV3-64: [224x224x64] memory: 224*224*64=3.2M params: (3*3*3)*64 = 1,728
CONV3-64: [224x224x64] memory: 224*224*64=3.2M params: (3*3*64)*64 = 36,864
POOL2: [112x112x64] memory: 112*112*64=800K params: 0
CONV3-128: [112x112x128] memory: 112*112*128=1.6M params: (3*3*64)*128 = 73,728
CONV3-128: [112x112x128] memory: 112*112*128=1.6M params: (3*3*128)*128 = 147,456
POOL2: [56x56x128] memory: 56*56*128=400K params: 0
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*128)*256 = 294,912
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*256)*256 = 589,824
CONV3-256: [56x56x256] memory: 56*56*256=800K params: (3*3*256)*256 = 589,824
POOL2: [28x28x256] memory: 28*28*256=200K params: 0
CONV3-512: [28x28x512] memory: 28*28*512=400K params: (3*3*256)*512 = 1,179,648
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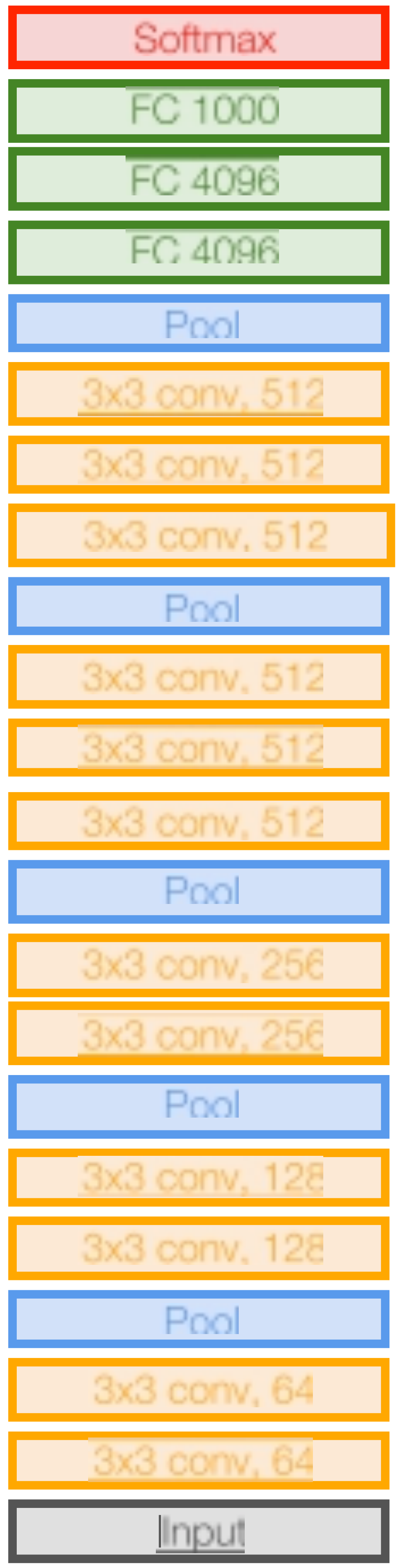
POOL2: [7x7x512] memory: 7*7*512=25K params: 0
FC: [1x1x4096] memory: 4096 params: 7*7*512*4096 = 102,760,448
FC: [1x1x4096] memory: 4096 params: 4096*4096 = 16,777,216
FC: [1x1x1000] memory: 1000 params: 4096*1000 = 4,096,000



VGG16

INPUT: [224x224x3] memory: 224*224*3=150K params: 0 (not counting biases)

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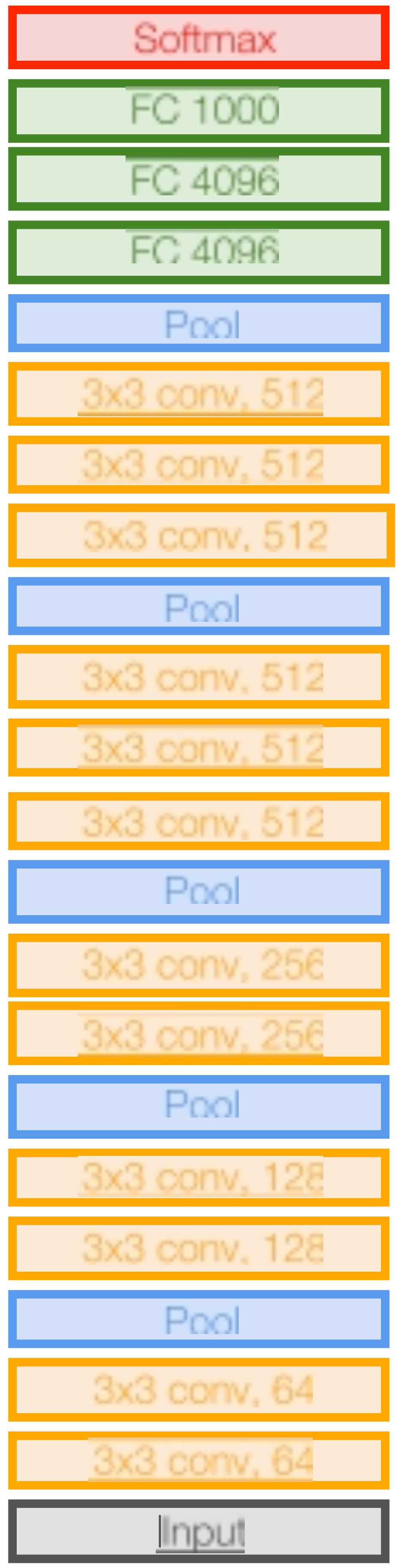

VGG16

TOTAL memory: 24M * 4 bytes ~= 96MB / image (for a forward pass)
TOTAL params: 138M parameters

INPUT: [224x224x3] memory: 224*224*3=150K params: 0 (not counting biases)

CONV3-64: [224x224x64] memory: **224*224*64=3.2M** params: (3*3*3)*64 = 1,728
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TOTAL memory: 24M * 4 bytes ~= 96MB / image (only forward! ~*2 for bwd)
TOTAL params: 138M parameters

Note:

Most memory is in early CONV

Most params are in late FC

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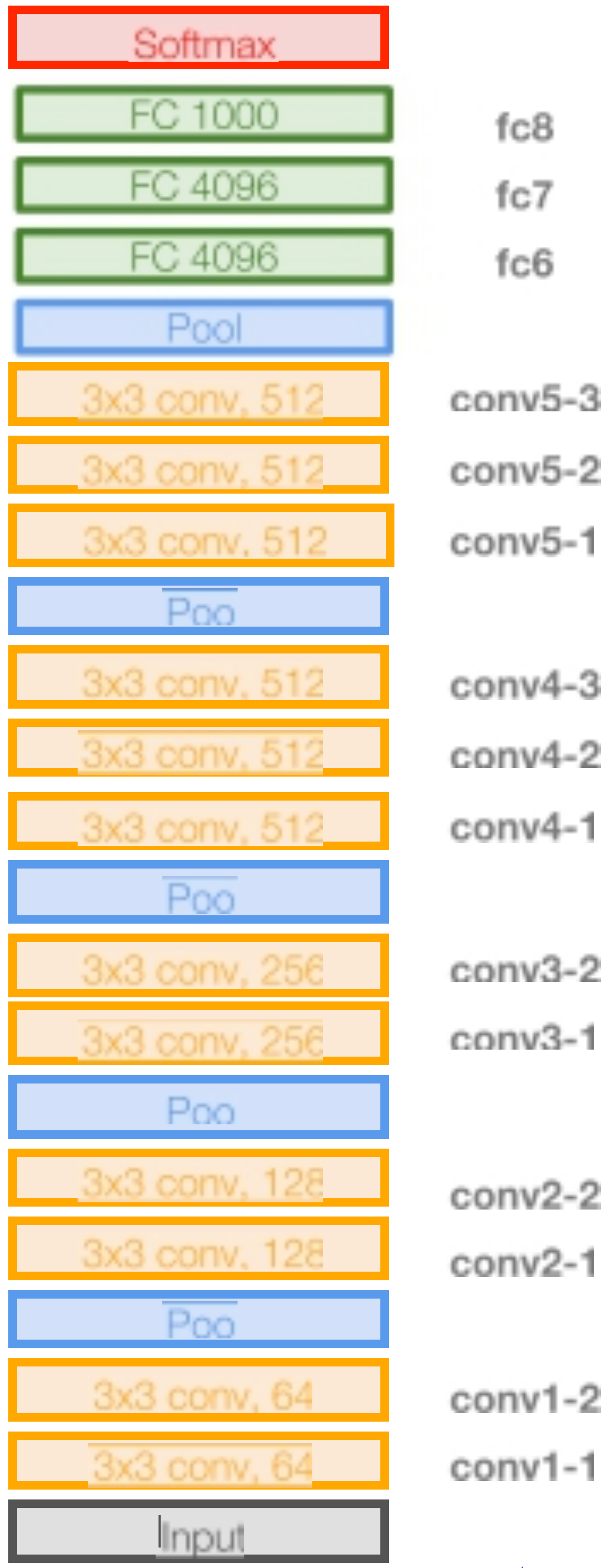


VGG16

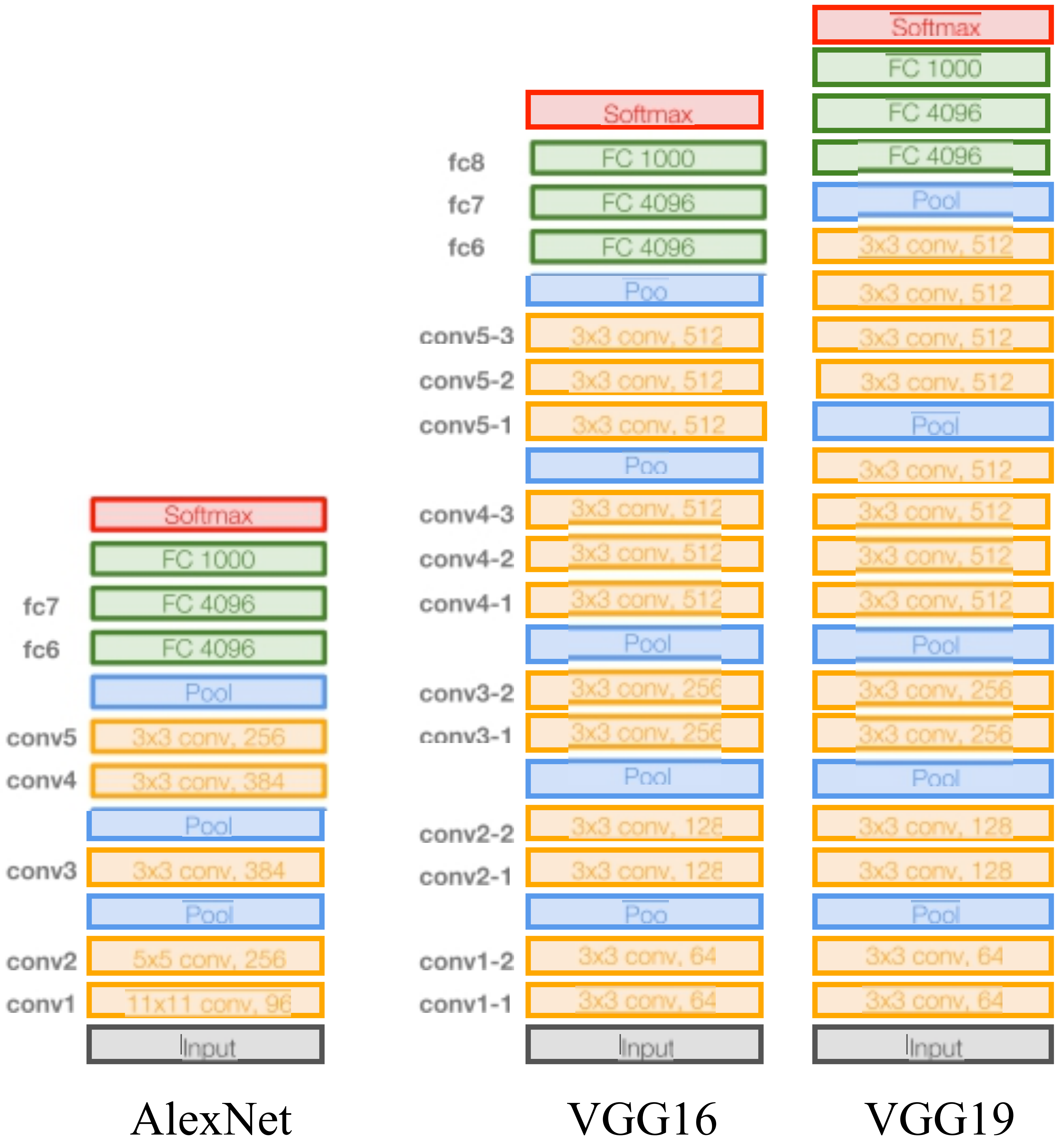
Common names

Case Study: VGGNet

[Simonyan and Zisserman, 2014]

Details:

- ILSVRC’14 2nd in classification, 1st in localization
- Similar training procedure as Krizhevsky 2012
- No Local Response Normalisation (LRN)
- Use VGG16 or VGG19 (VGG19 only slightly better, more memory)
- Use ensembles for best results
- FC7 features generalize well to other tasks
- (Sort of) used Xavier initialization



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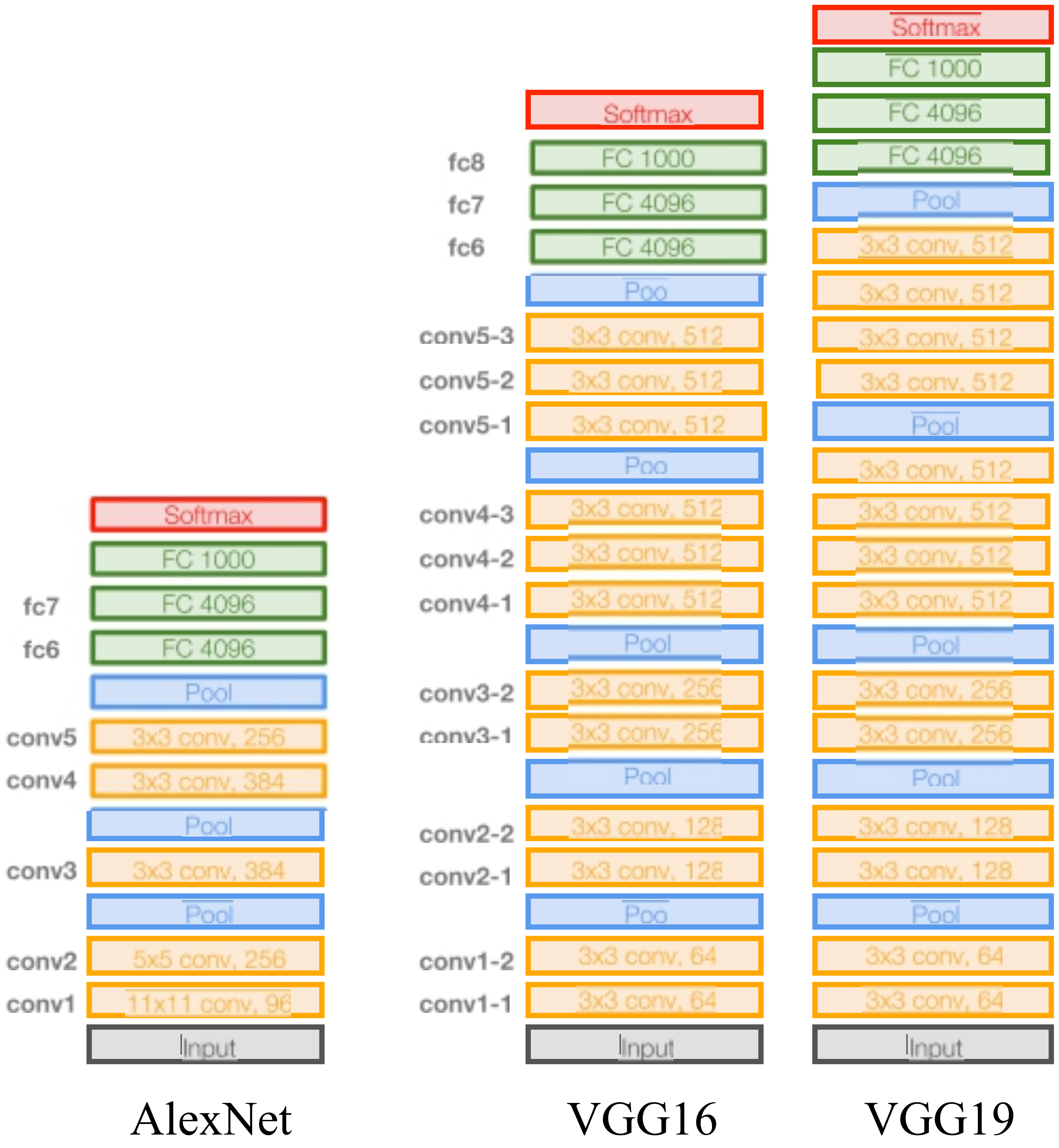
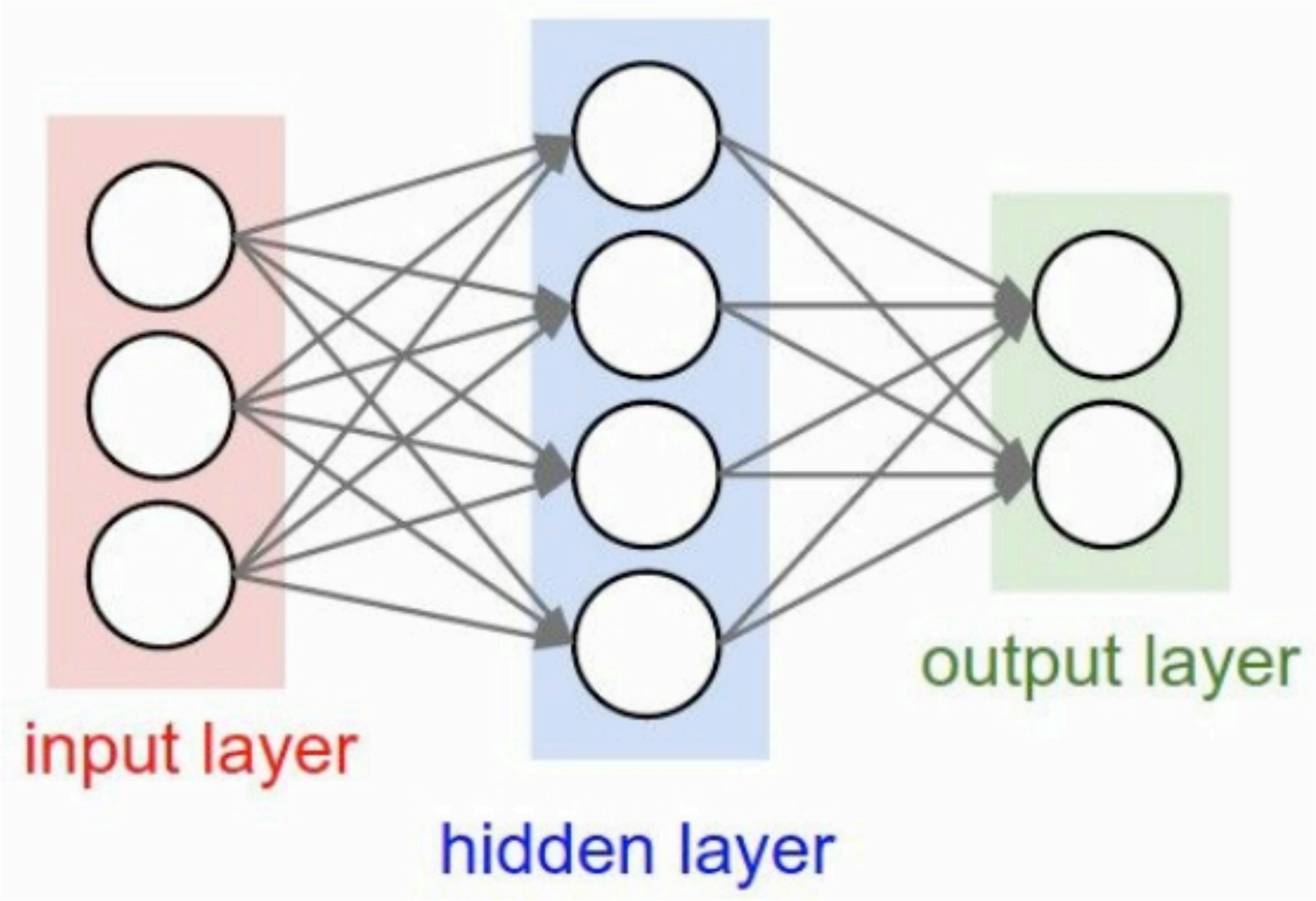


Weight initialization

Q: what happens when $W_{ij} = c$ is used?



Weight initialization

- First idea: **Small random numbers**

(gaussian with zero mean and 1e-2 standard deviation)

```
W = 0.01* np.random.randn(D,H)
```

Weight initialization

- First idea: **Small random numbers**
(gaussian with zero mean and 1e-2 standard deviation)

```
W = 0.01* np.random.randn(D,H)
```

Works ~okay for small networks, but problems with deeper networks.

Lets look at some activation statistics

E.g. 10-layer net with 500 neurons on each layer, using tanh non-linearities, and initializing as described in last slide.

```
# assume some unit gaussian 10-D input data
D = np.random.randn(1000, 500)
hidden_layer_sizes = [500]*10
nonlinearities = ['tanh']*len(hidden_layer_sizes)
```

```
act = {'relu':lambda x:np.maximum(0,x), 'tanh':lambda x:np.tanh(x)}
Hs = {}
for i in xrange(len(hidden_layer_sizes)):
    X = D if i == 0 else Hs[i-1] # input at this layer
    fan_in = X.shape[1]
    fan_out = hidden_layer_sizes[i]
    W = np.random.randn(fan_in, fan_out) * 0.01 # layer initialization

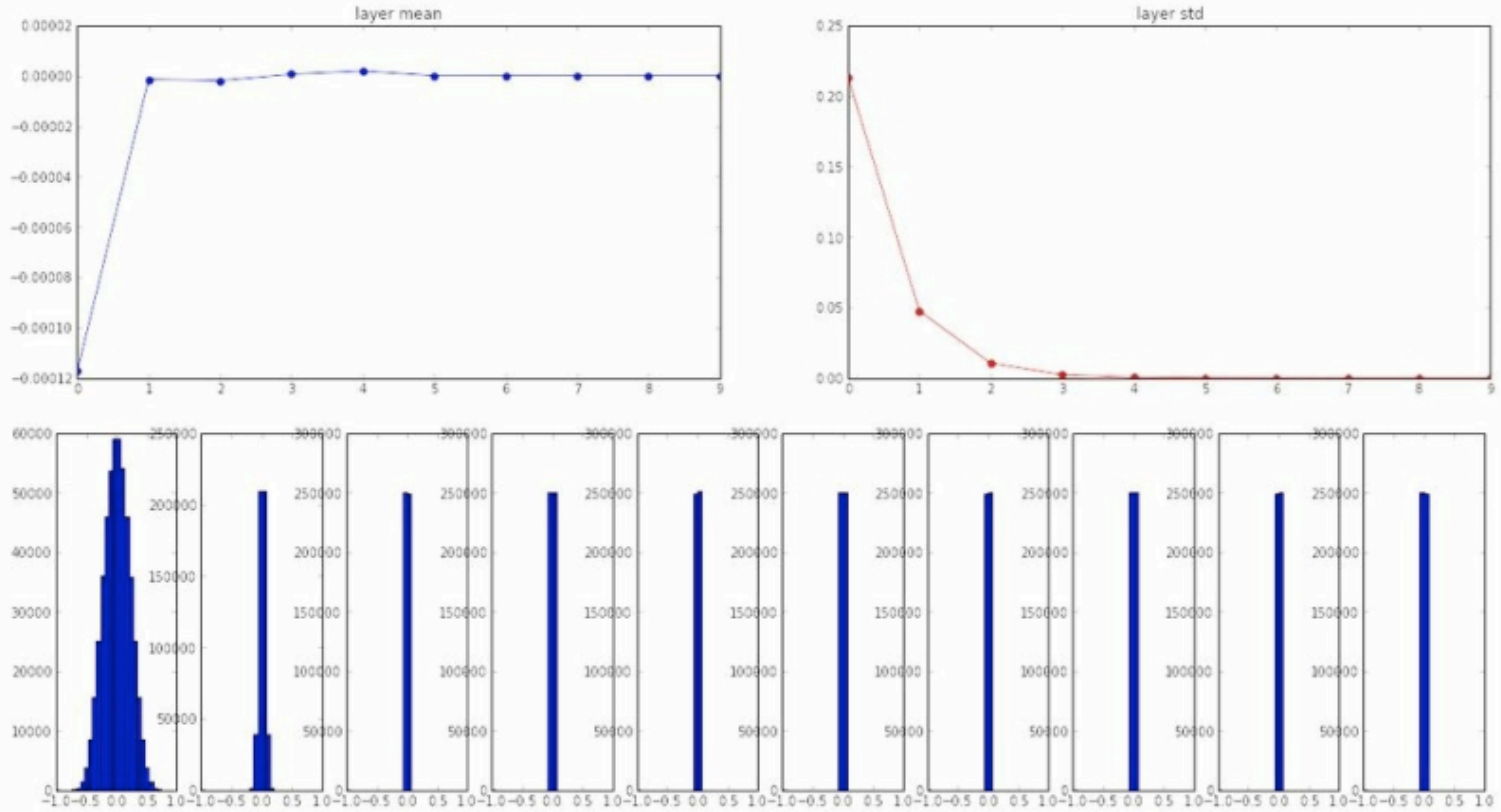
    H = np.dot(X, W) # matrix multiply
    H = act[nonlinearities[i]](H) # nonlinearity
    Hs[i] = H # cache result on this layer
```

```
# look at distributions at each layer
print 'input layer had mean %f and std %f' % (np.mean(D), np.std(D))
layer_means = [np.mean(H) for i,H in Hs.iteritems()]
layer_stds = [np.std(H) for i,H in Hs.iteritems()]
for i,H in Hs.iteritems():
    print 'hidden layer %d had mean %f and std %f' % (i+1, layer_means[i], layer_stds[i])

# plot the means and standard deviations
plt.figure()
plt.subplot(121)
plt.plot(Hs.keys(), layer_means, 'ob-')
plt.title('layer mean')
plt.subplot(122)
plt.plot(Hs.keys(), layer_stds, 'or-')
plt.title('layer std')

# plot the raw distributions
plt.figure()
for i,H in Hs.iteritems():
    plt.subplot(1,len(Hs),i+1)
    plt.hist(H.ravel(), 30, range=(-1,1))
```

```
input layer had mean 0.000927 and std 0.998388
hidden layer 1 had mean -0.000117 and std 0.213081
hidden layer 2 had mean -0.000001 and std 0.047551
hidden layer 3 had mean -0.000002 and std 0.010630
hidden layer 4 had mean 0.000001 and std 0.002378
hidden layer 5 had mean 0.000002 and std 0.000532
hidden layer 6 had mean -0.000000 and std 0.000119
hidden layer 7 had mean 0.000000 and std 0.000026
hidden layer 8 had mean -0.000000 and std 0.000006
hidden layer 9 had mean 0.000000 and std 0.000001
hidden layer 10 had mean -0.000000 and std 0.000000
```



Used with permission from Justin Johnson

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input layer had mean 0.000927 and std 0.998388
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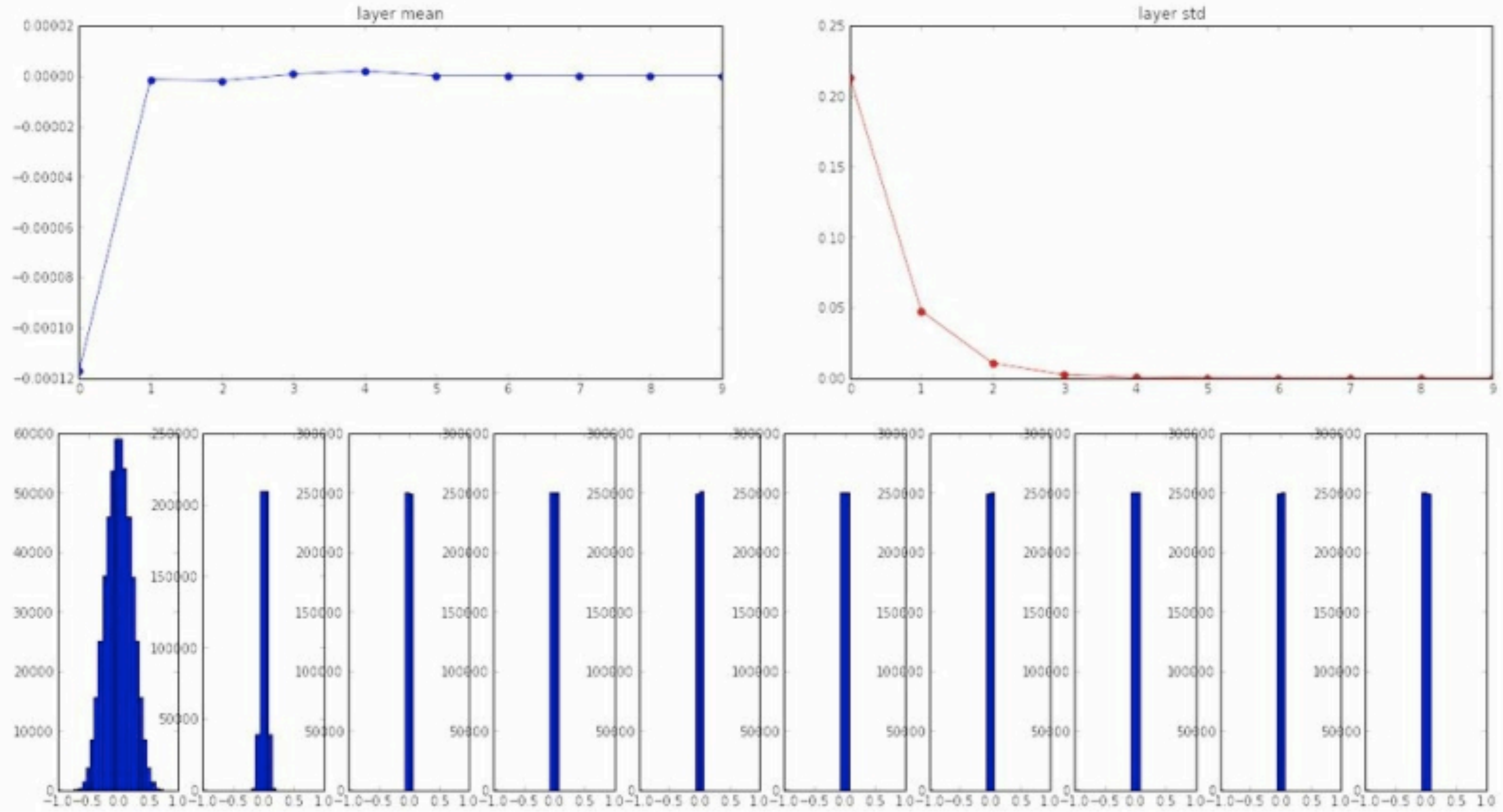
hidden layer 7 had mean 0.000000 and std 0.000026
hidden layer 8 had mean -0.000000 and std 0.000006
hidden layer 9 had mean 0.000000 and std 0.000001
hidden layer 10 had mean -0.000000 and std 0.000000
```



All activations become zero!

Q: think about the backward pass. What do the gradients look like?

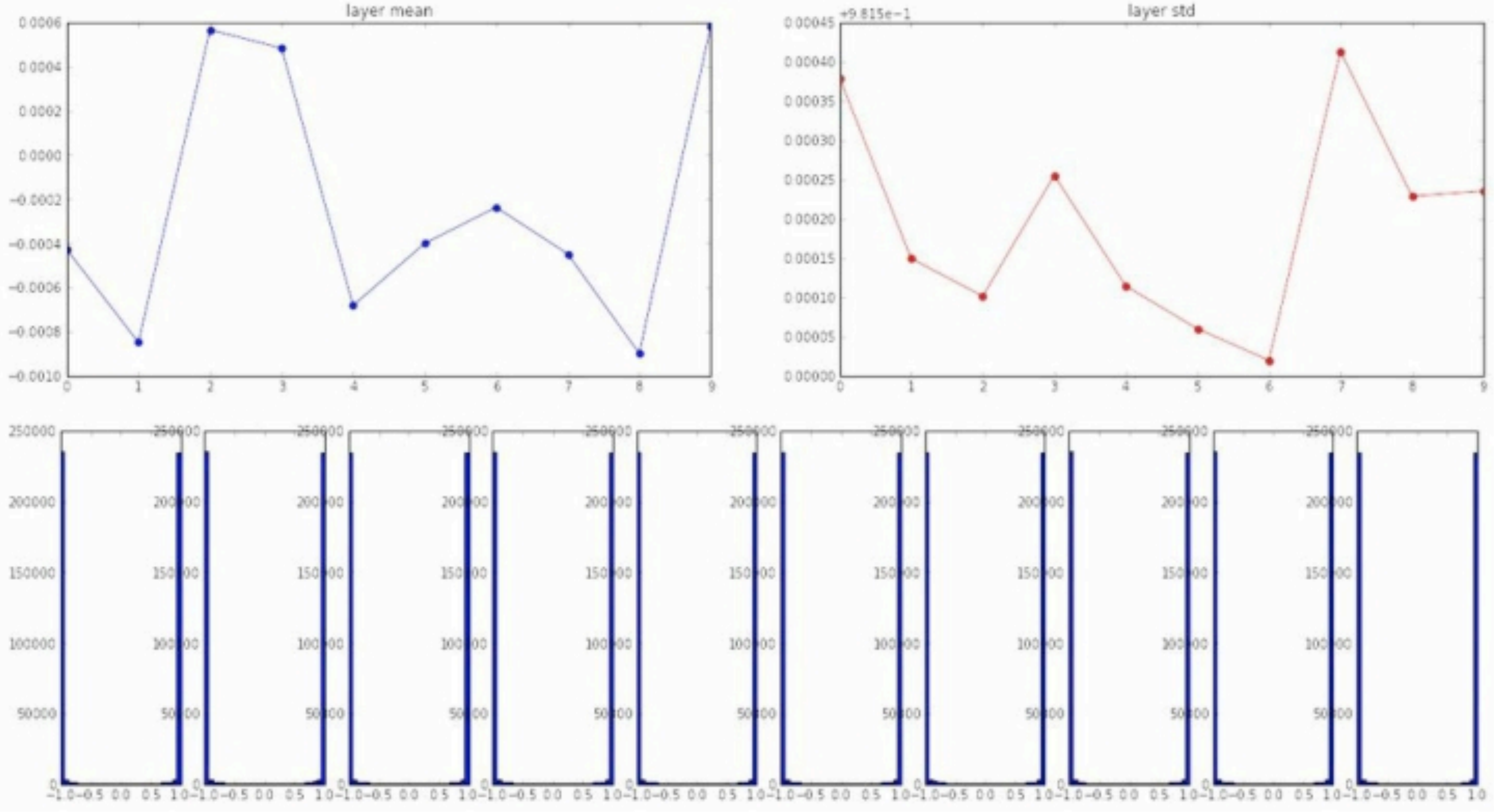
Hint: think about backward pass for a W*X gate.

Used with permission from Justin Johnson

```
W = np.random.randn(fan_in, fan_out) * 1.0 # layer initialization
```

*1.0 instead of *0.01

```
input layer had mean 0.001800 and std 1.001311
hidden layer 1 had mean -0.000430 and std 0.981879
hidden layer 2 had mean -0.000849 and std 0.981649
hidden layer 3 had mean 0.000566 and std 0.981601
hidden layer 4 had mean 0.000483 and std 0.981755
hidden layer 5 had mean -0.000682 and std 0.981614
hidden layer 6 had mean -0.000401 and std 0.981560
hidden layer 7 had mean -0.000237 and std 0.981520
hidden layer 8 had mean -0.000448 and std 0.981913
hidden layer 9 had mean -0.000899 and std 0.981728
hidden layer 10 had mean 0.000584 and std 0.981736
```

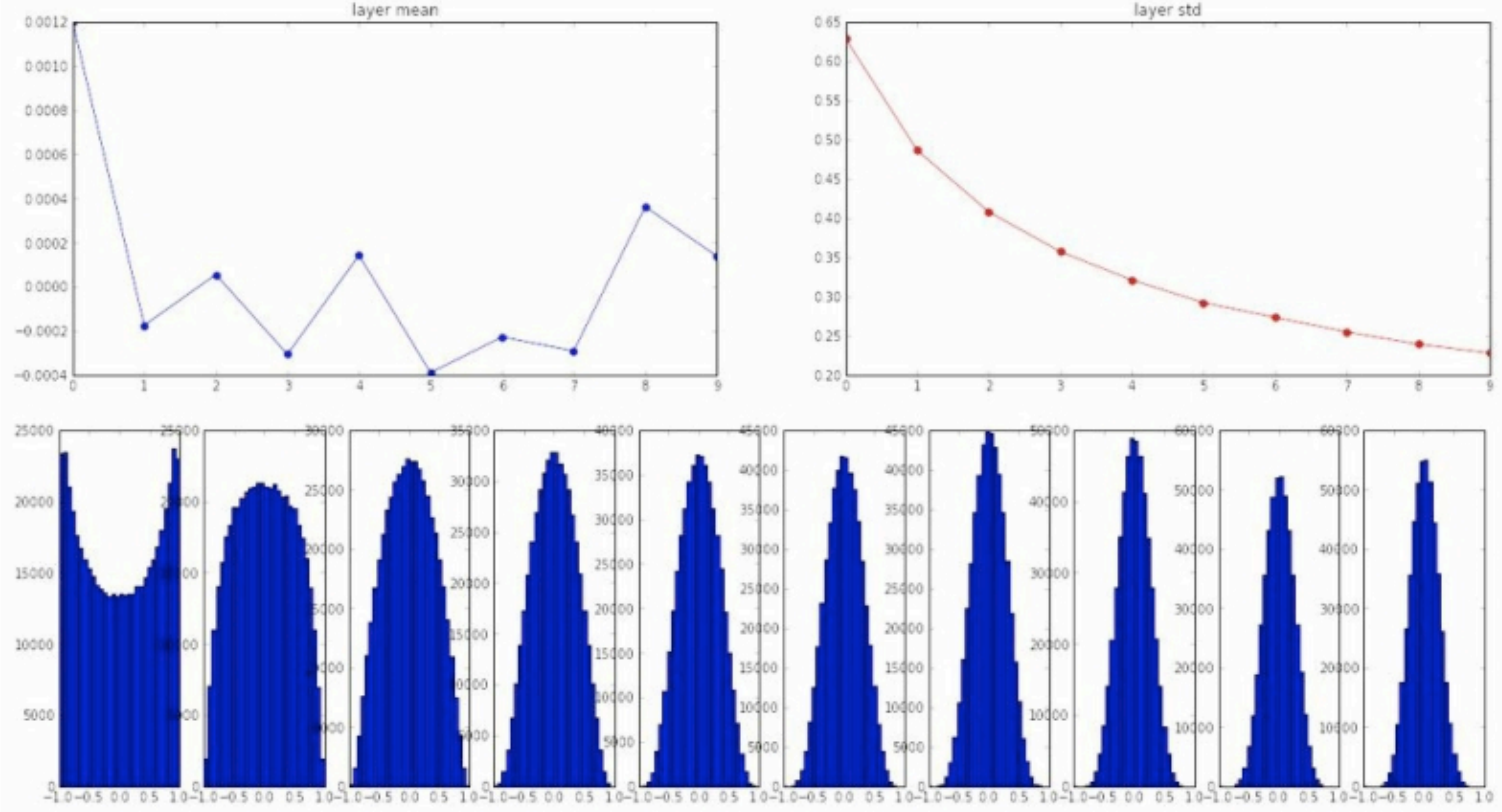


Almost all neurons completely saturated, either -1 and 1. Gradients will be all zero.

```
input layer had mean 0.001800 and std 1.001311
hidden layer 1 had mean 0.001198 and std 0.627953
hidden layer 2 had mean -0.000175 and std 0.486051
hidden layer 3 had mean 0.000055 and std 0.407723
hidden layer 4 had mean -0.000306 and std 0.357108
hidden layer 5 had mean 0.000142 and std 0.320917
hidden layer 6 had mean -0.000389 and std 0.292116
hidden layer 7 had mean -0.000228 and std 0.273387
hidden layer 8 had mean -0.000291 and std 0.254935
hidden layer 9 had mean 0.000361 and std 0.239266
hidden layer 10 had mean 0.000139 and std 0.228008
```

```
W = np.random.randn(fan_in, fan_out) / np.sqrt(fan_in) # layer initialization
```

"Xavier initialization"
[Glorot et al., 2010]



Reasonable initialization.
(Mathematical derivation assumes linear activations)

Used with permission from Justin Johnson

Case Study: VGGNet

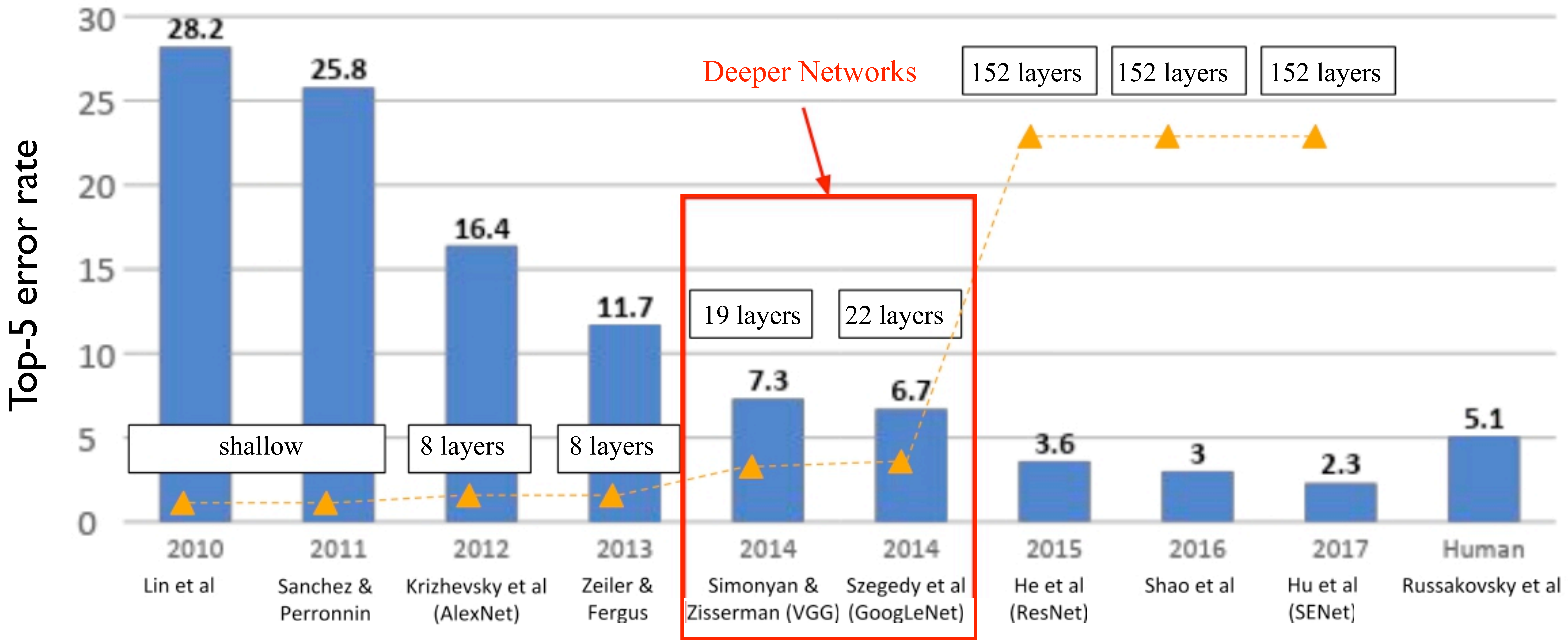
[Simonyan and Zisserman, 2014]

Table 6: **Multiple ConvNet fusion results.**

Combined ConvNet models	Error		
	top-1 val	top-5 val	top-5 test
ILSVRC submission			
(D/256/224,256,288), (D/384/352,384,416), (D/[256;512]/256,384,512) (C/256/224,256,288), (C/384/352,384,416) (E/256/224,256,288), (E/384/352,384,416)	24.7	7.5	7.3
post-submission			
(D/[256;512]/256,384,512), (E/[256;512]/256,384,512), dense eval.	24.0	7.1	7.0
(D/[256;512]/256,384,512), (E/[256;512]/256,384,512), multi-crop	23.9	7.2	-
(D/[256;512]/256,384,512), (E/[256;512]/256,384,512), multi-crop & dense eval.	**23.7**	**6.8**	**6.8**

Method	top-1 val. error (%)	top-5 val. error (%)	top-5 test error (%)
VGG (2 nets, multi-crop & dense eval.)	**23.7**	**6.8**	**6.8**
VGG (1 net, multi-crop & dense eval.)	24.4	7.1	7.0
VGG (ILSVRC submission, 7 nets, dense eval.)	24.7	7.5	7.3
GoogLeNet (Szegedy et al., 2014) (1 net)	-	7.9	
GoogLeNet (Szegedy et al., 2014) (7 nets)	-	**6.7**	

ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners



Used with permission from Justin Johnson

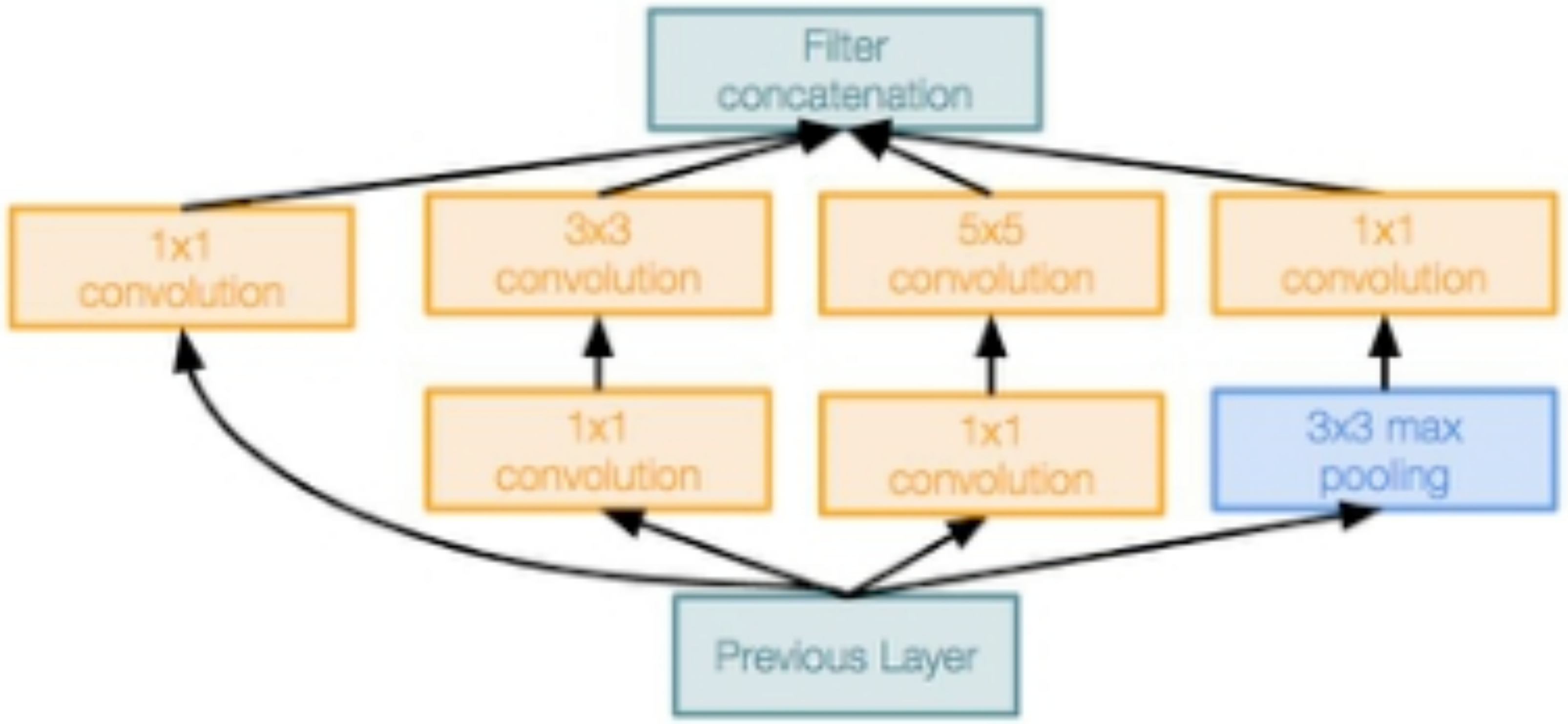

WE NEED TO GO
DEEPER

Case Study: GoogLeNet

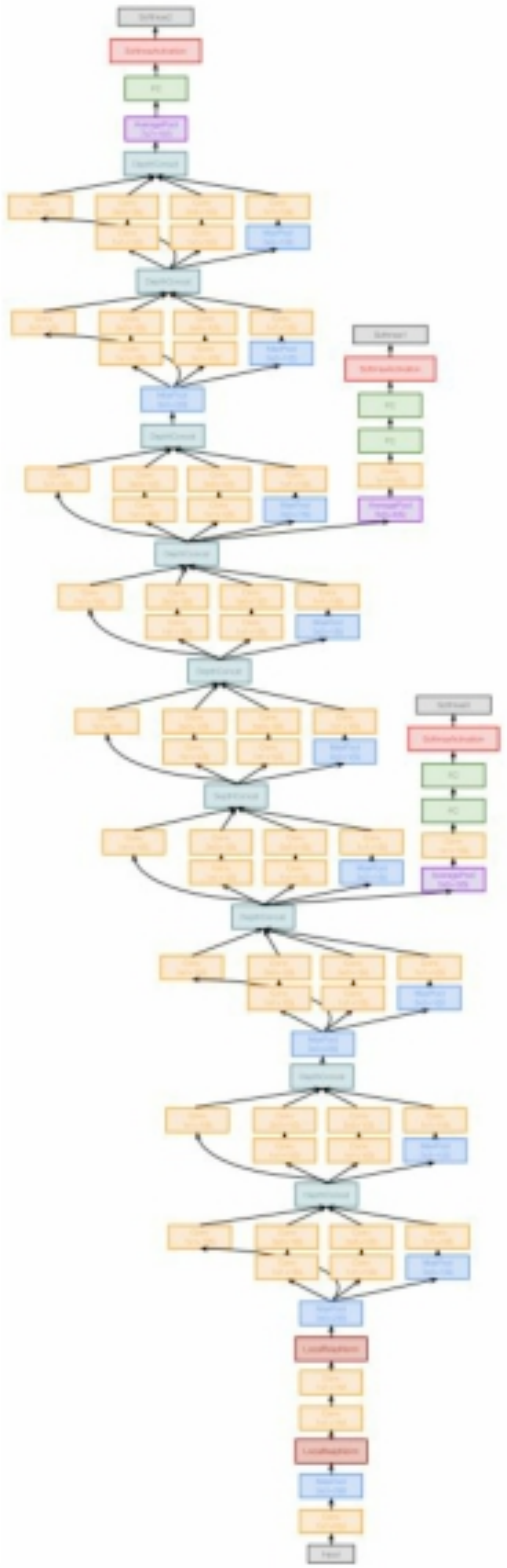
[Szegedy et al., 2014]

Deeper networks, with computational efficiency

- 22 layers
- Efficient "Inception" module
- No FC layers
- Only 5 million parameters!
  12x less than AlexNet
- ILSVRC'14 classification winner (6.7% top 5 error)



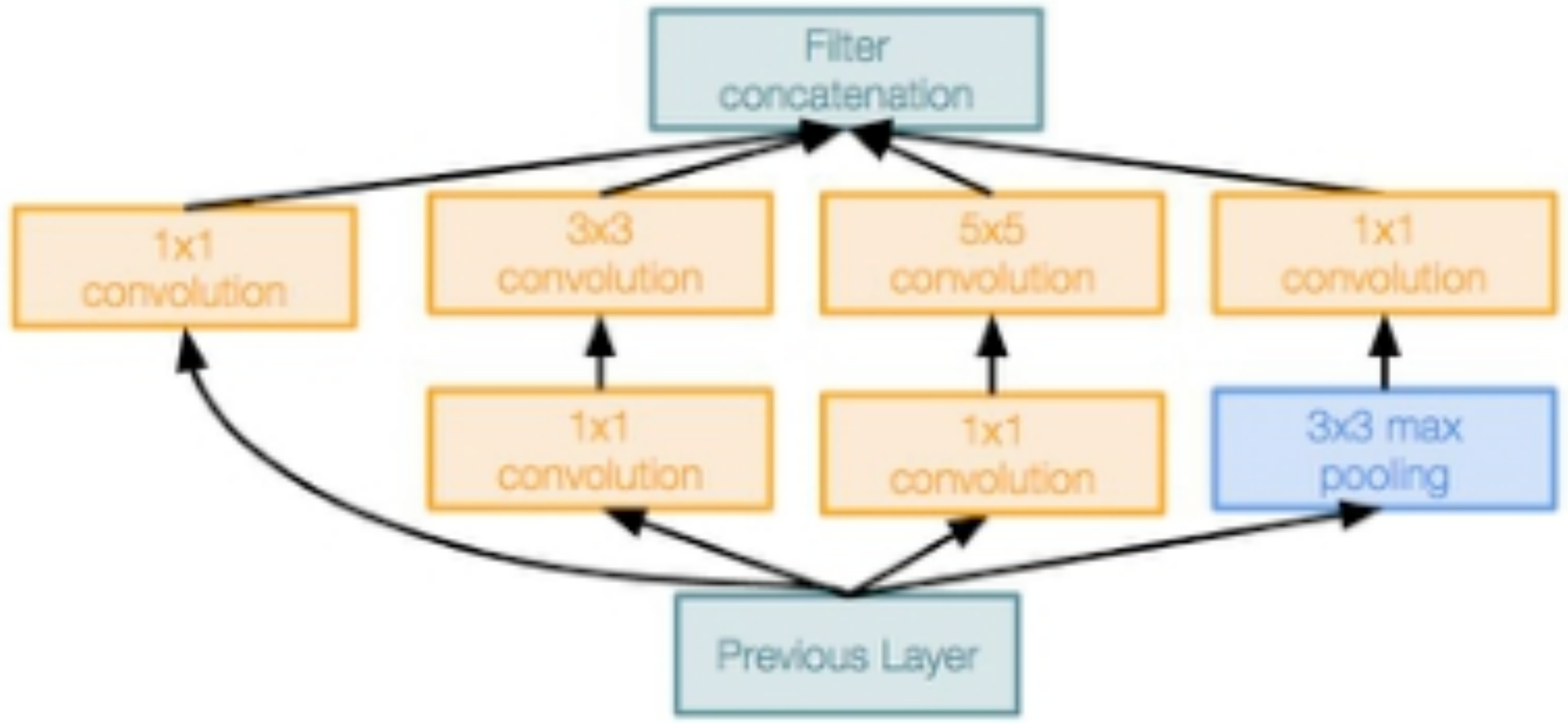
Inception module



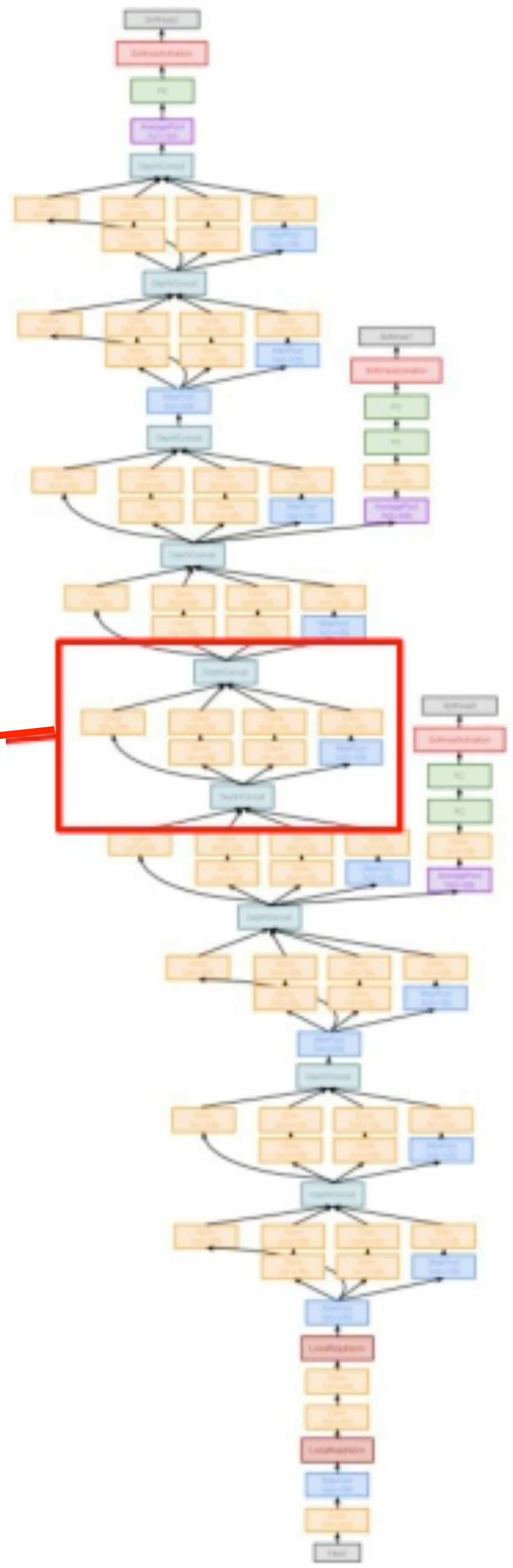
Case Study: GoogLeNet

[Szegedy et al., 2014]

“Inception module”: design a good local network topology (network within a network) and then stack these modules on top of each other

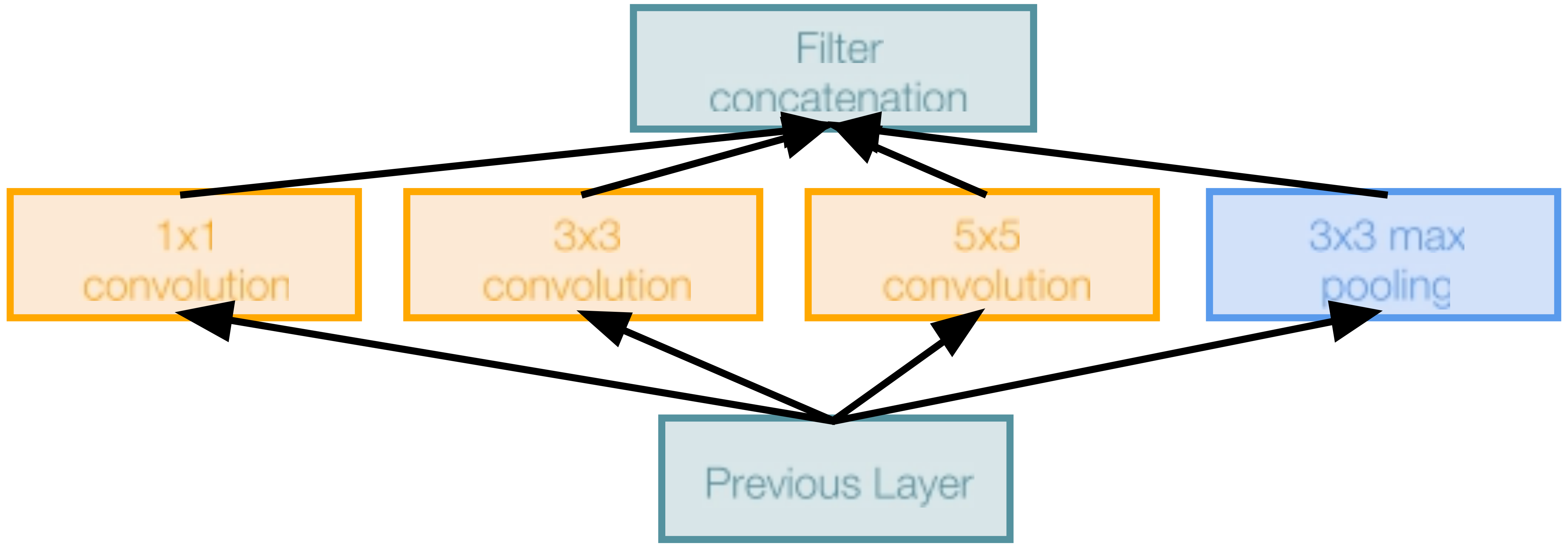


Inception module



Case Study: GoogLeNet

[Szegedy et al., 2014]



Naive Inception module

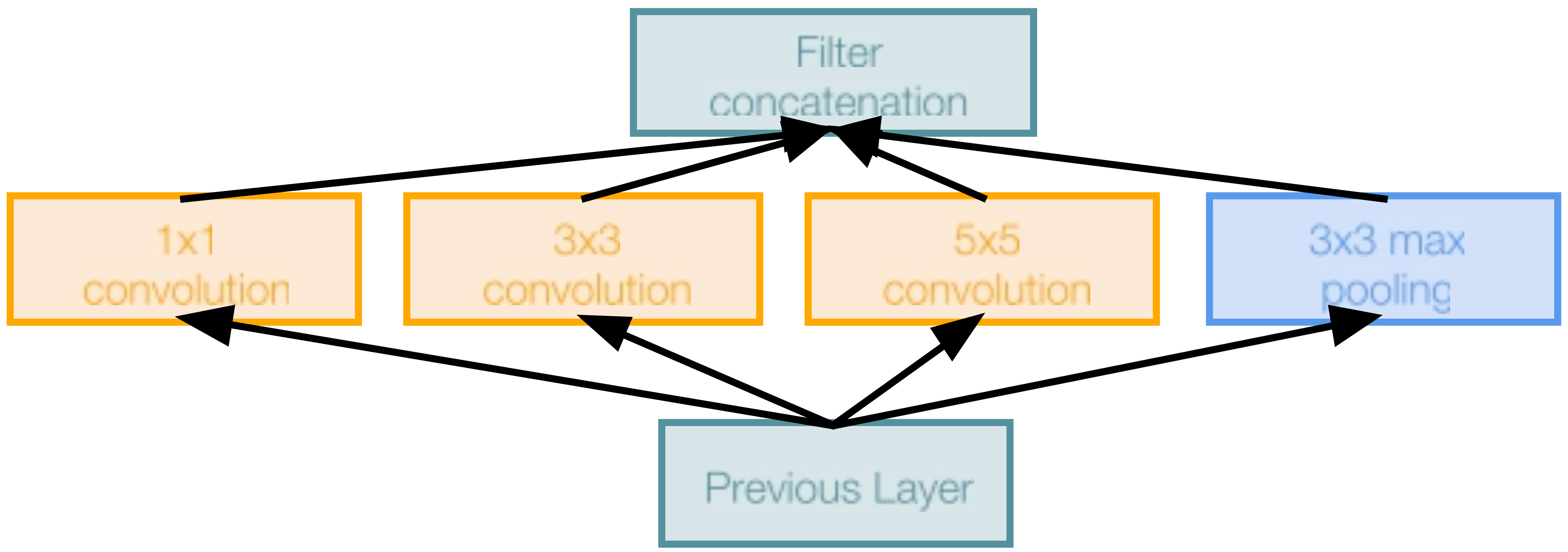
Apply parallel filter operations on the input from previous layer:

- Multiple receptive field sizes for convolution (1x1, 3x3, 5x5)
- Pooling operation (3x3)

Concatenate all filter outputs together depth-wise

Case Study: GoogLeNet

[Szegedy et al., 2014]



Naive Inception module

Apply parallel filter operations on the input from previous layer:

- Multiple receptive field sizes for convolution (1x1, 3x3, 5x5)
- Pooling operation (3x3)

Concatenate all filter outputs together depth-wise

Q: What is the problem with this?
[Hint: Computational complexity]

Case Study: GoogLeNet

[Szegedy et al., 2014]

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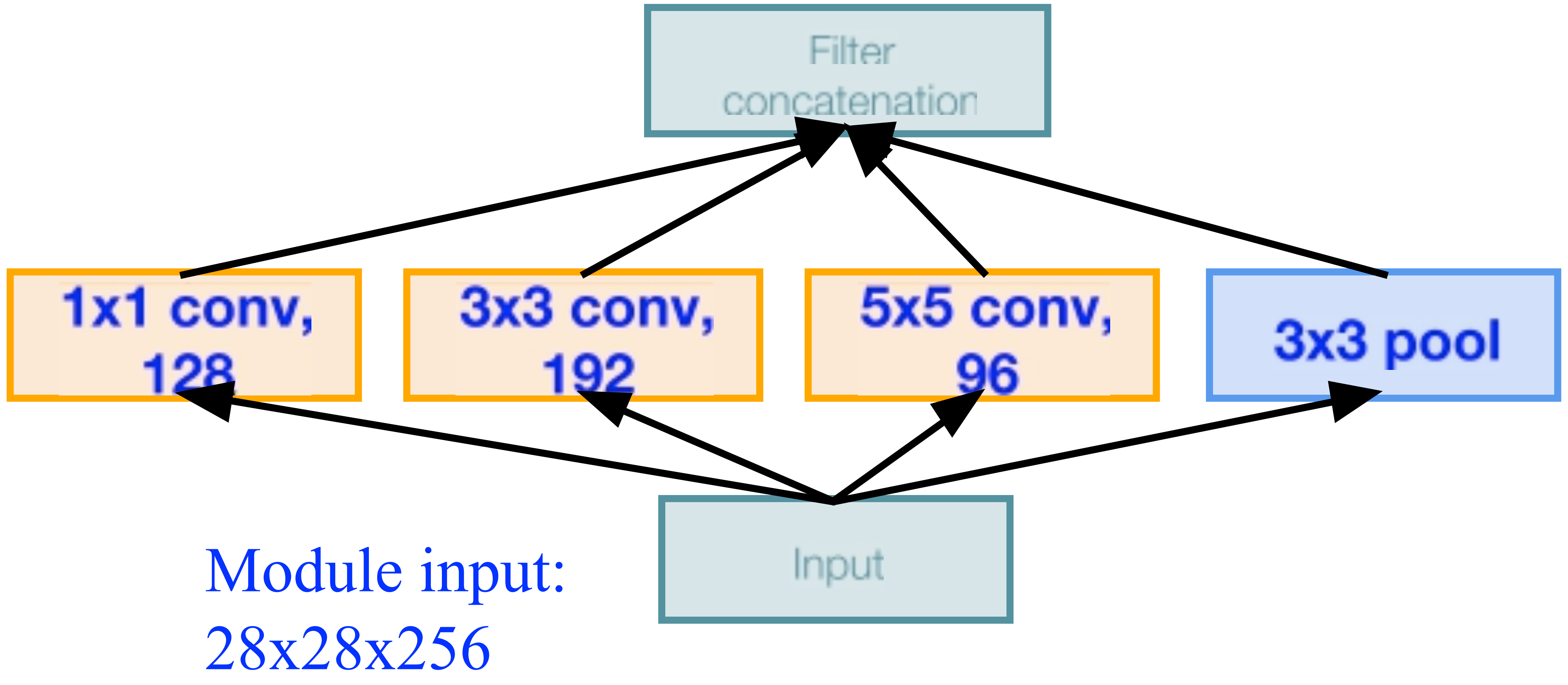
[Hint: Computational complexity]

Example:



Naive Inception module

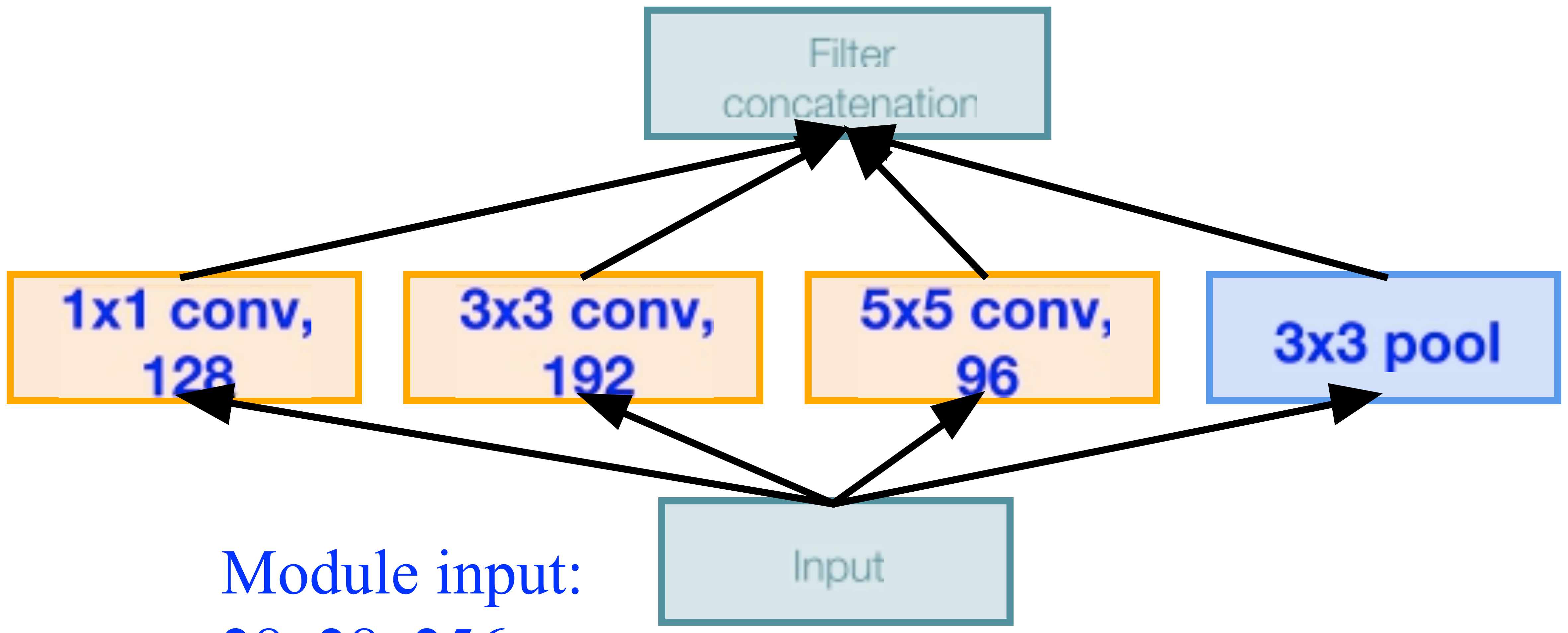
Case Study: GoogLeNet

[Szegedy et al., 2014]

Q: What is the problem with this?
[Hint: Computational complexity]

Example:

Q1: What is the output size of the 1x1 conv, with 128 filters?



Module input: 28x28x256

Naive Inception module

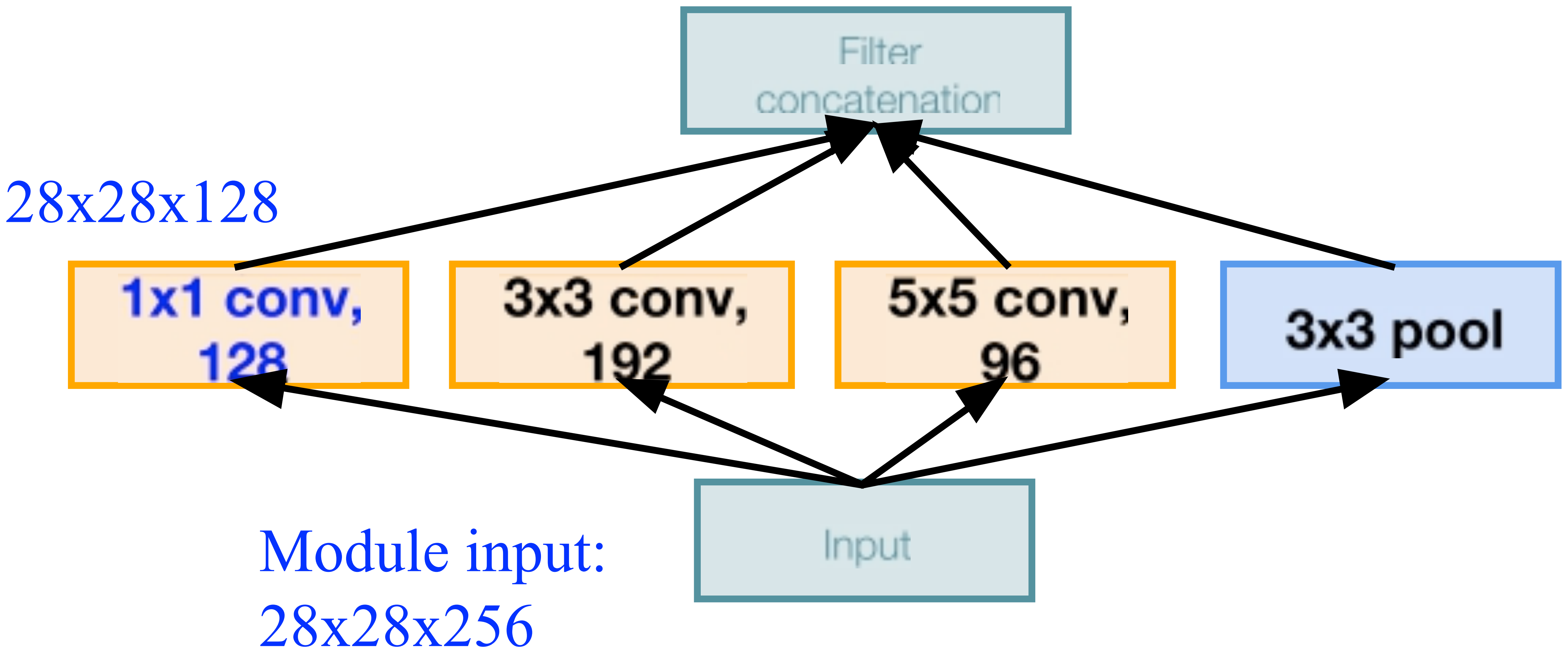
Case Study: GoogLeNet

[Szegedy et al., 2014]

Q: What is the problem with this?
[Hint: Computational complexity]

Example:

Q1: What is the output size of the 1x1 conv, with 128 filters?



Naive Inception module

Case Study: GoogLeNet

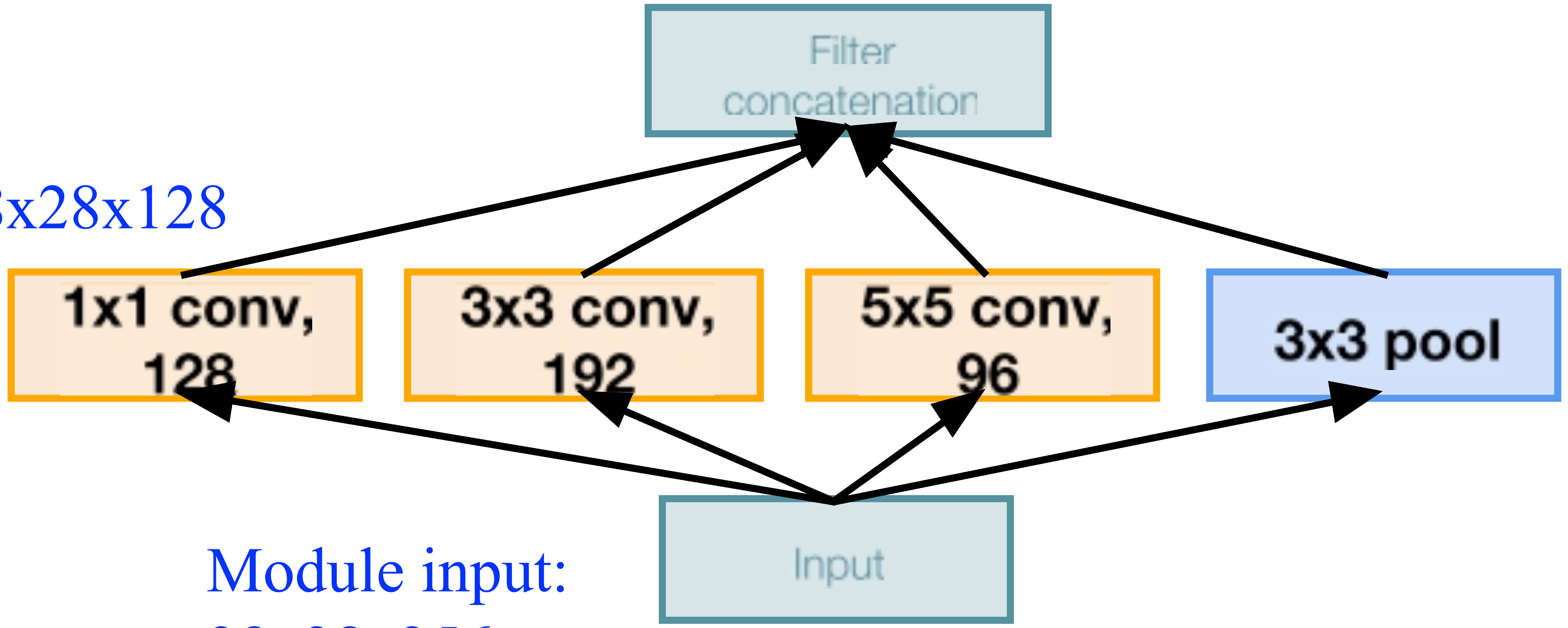
[Szegedy et al., 2014]

Q: What is the problem with this?
[Hint: Computational complexity]

Example:

Q2: What are the output sizes of all different filter operations?

28x28x128



Module input:
28x28x256

Naive Inception module

Case Study: GoogLeNet

[Szegedy et al., 2014]

Q: What is the problem with this?
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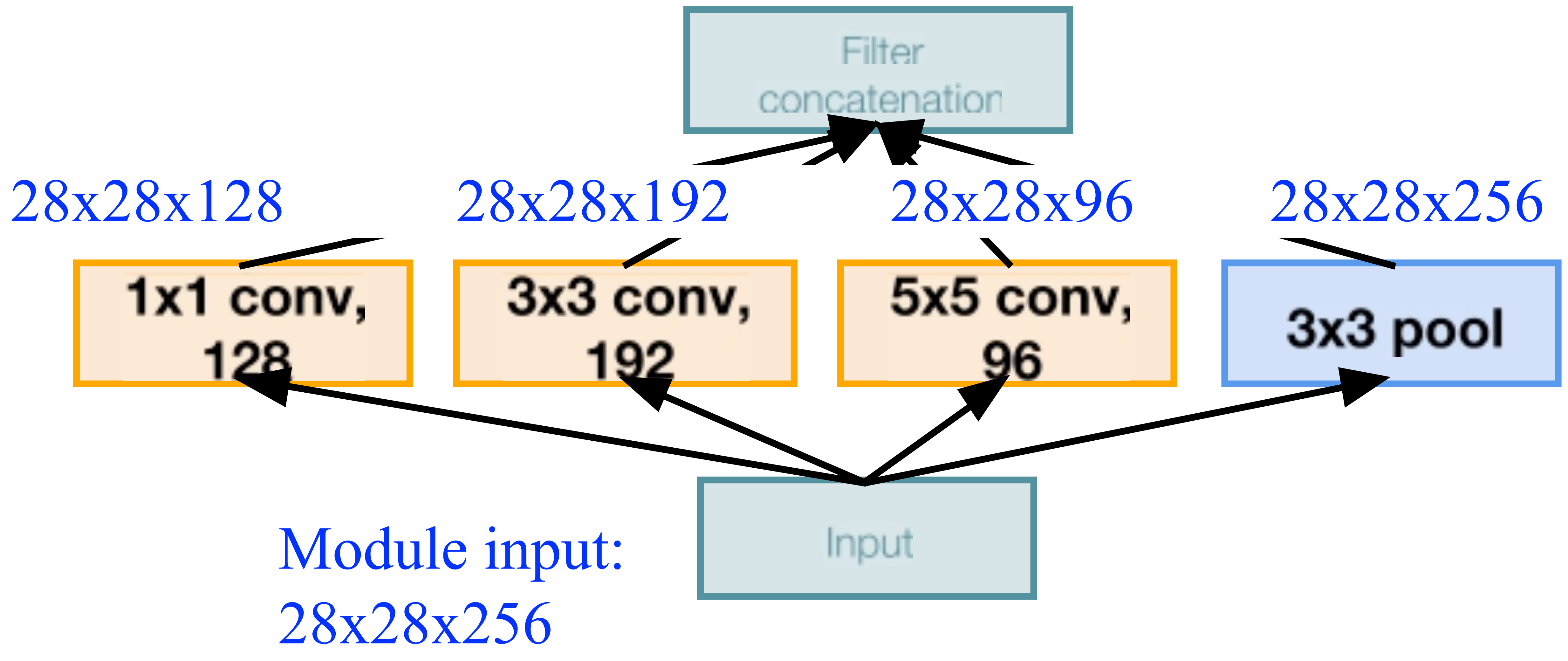


Naive Inception module

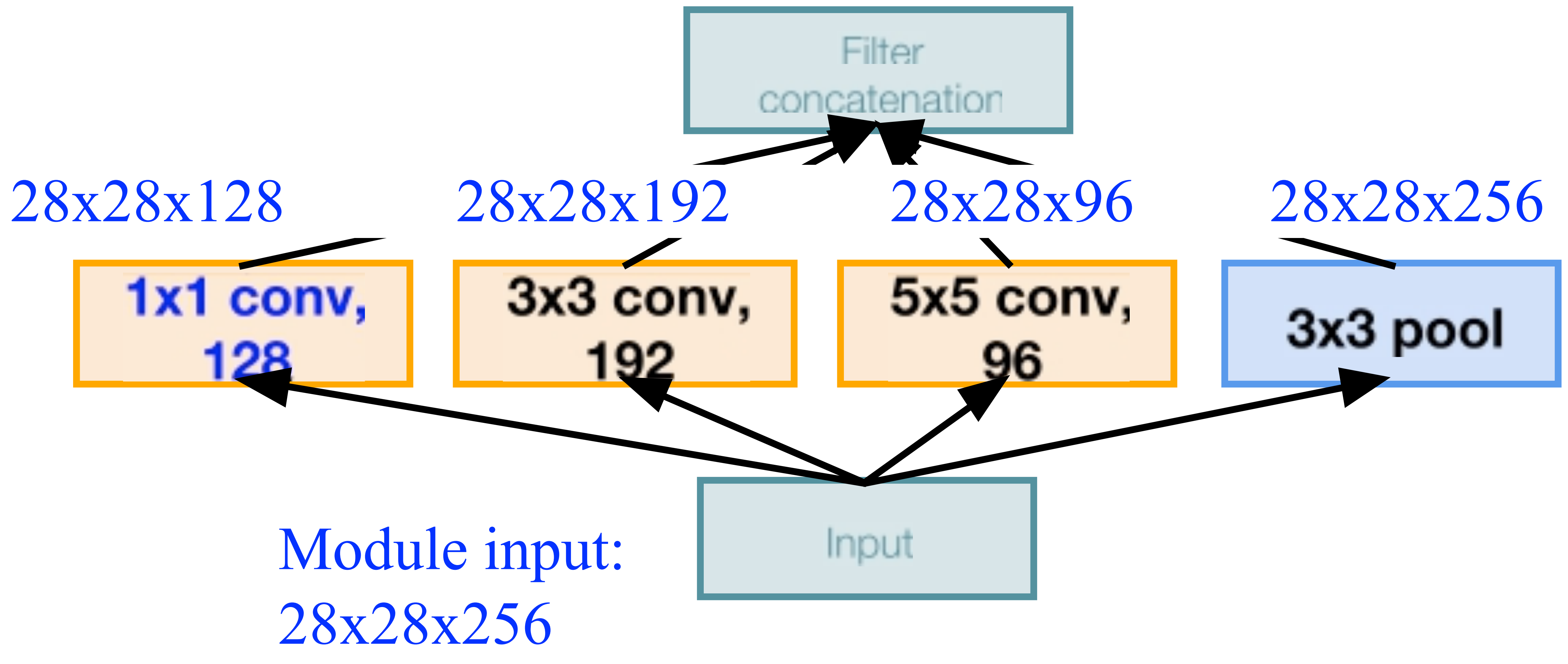
Case Study: GoogLeNet

[Szegedy et al., 2014]

Q: What is the problem with this?
[Hint: Computational complexity]

Example:

Q3:What is output size after filter concatenation?



Naive Inception module

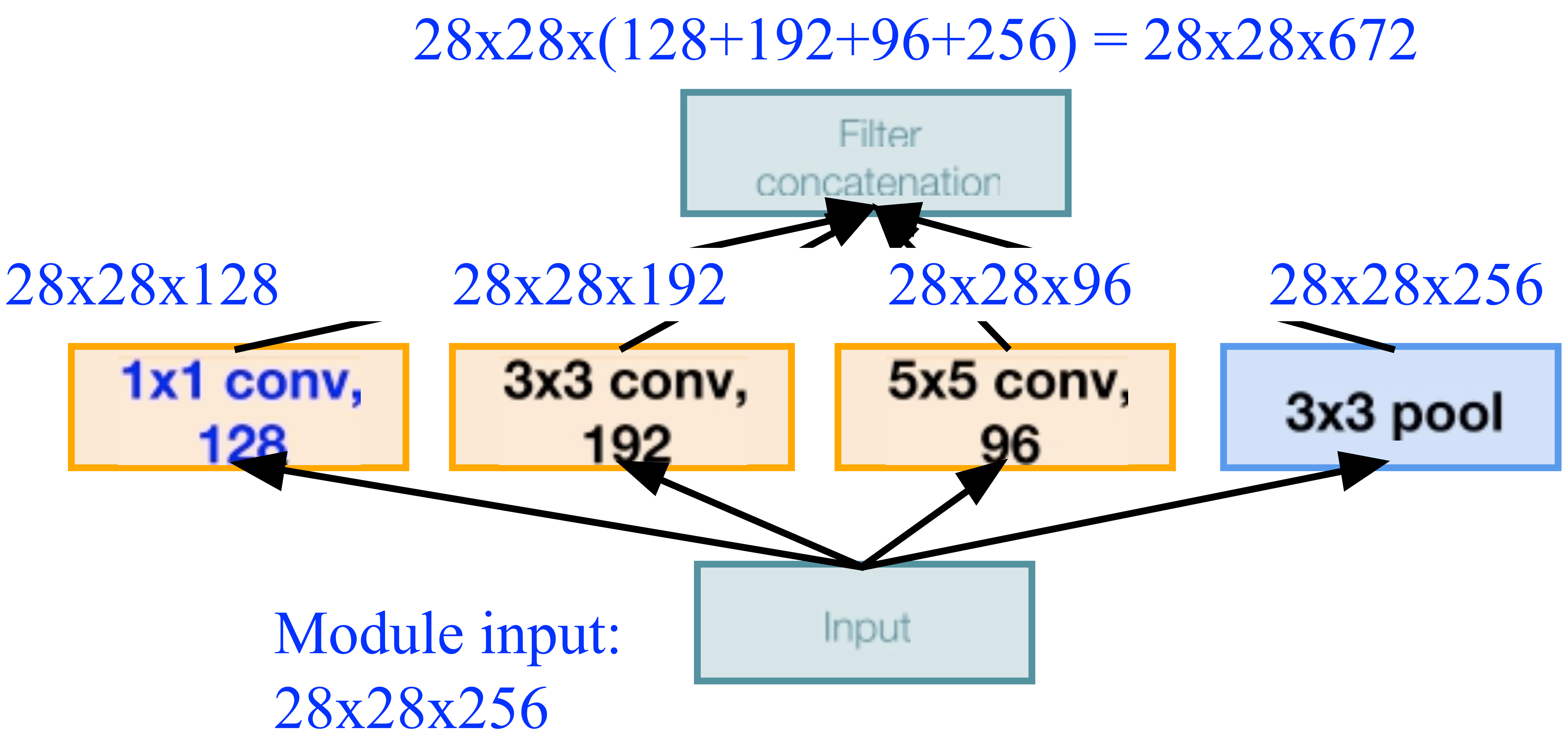
Case Study: GoogLeNet

[Szegedy et al., 2014]

Q: What is the problem with this?
[Hint: Computational complexity]

Example:

Q3:What is output size after
filter concatenation?



Naive Inception module

Case Study: GoogLeNet

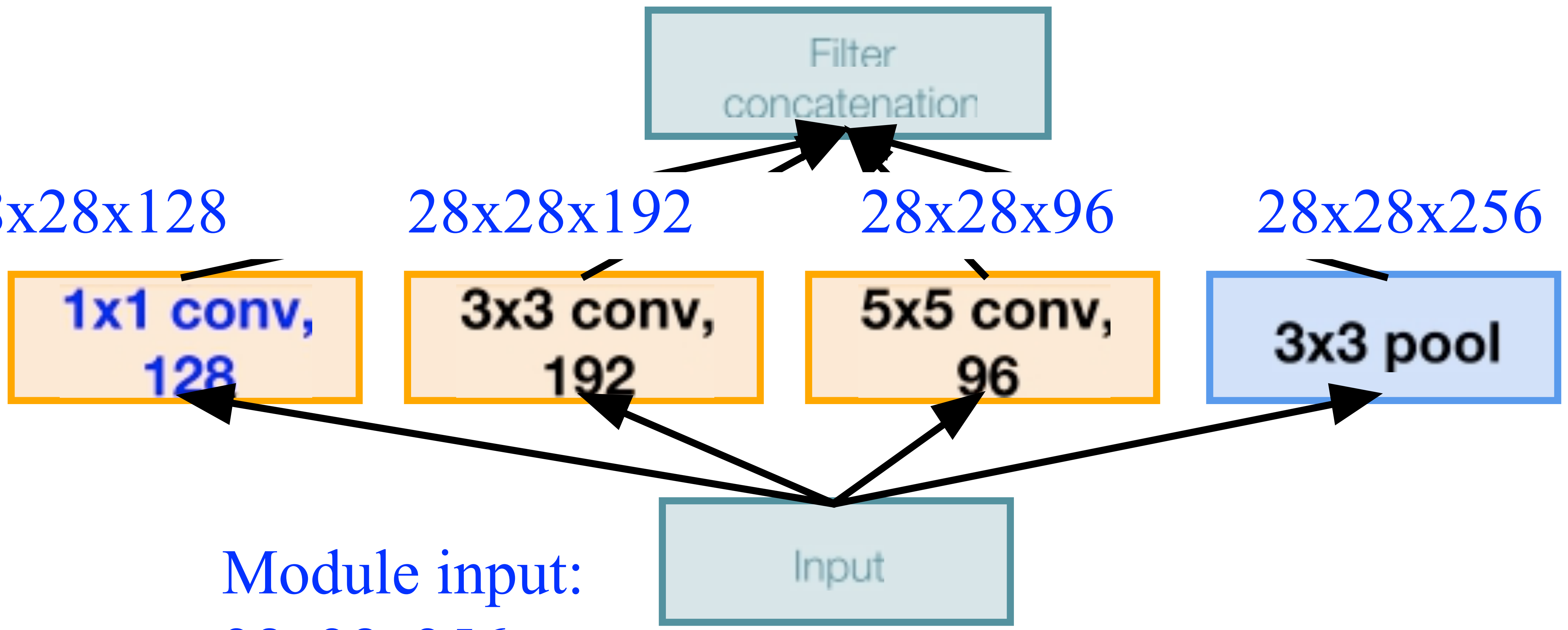
[Szegedy et al., 2014]

Example:

Q3:What is output size after filter concatenation?

28x28x(128+192+96+256) = 28x28x672

28x28x128 28x28x192 28x28x96 28x28x256



Module input: 28x28x256

Naive Inception module

Q: What is the problem with this?
[Hint: Computational complexity]

Conv Ops:

[1x1 conv, 128] 28x28x128x1x1x256

[3x3 conv, 192] 28x28x192x3x3x256

[5x5 conv, 96] 28x28x96x5x5x256

Total: 854M ops

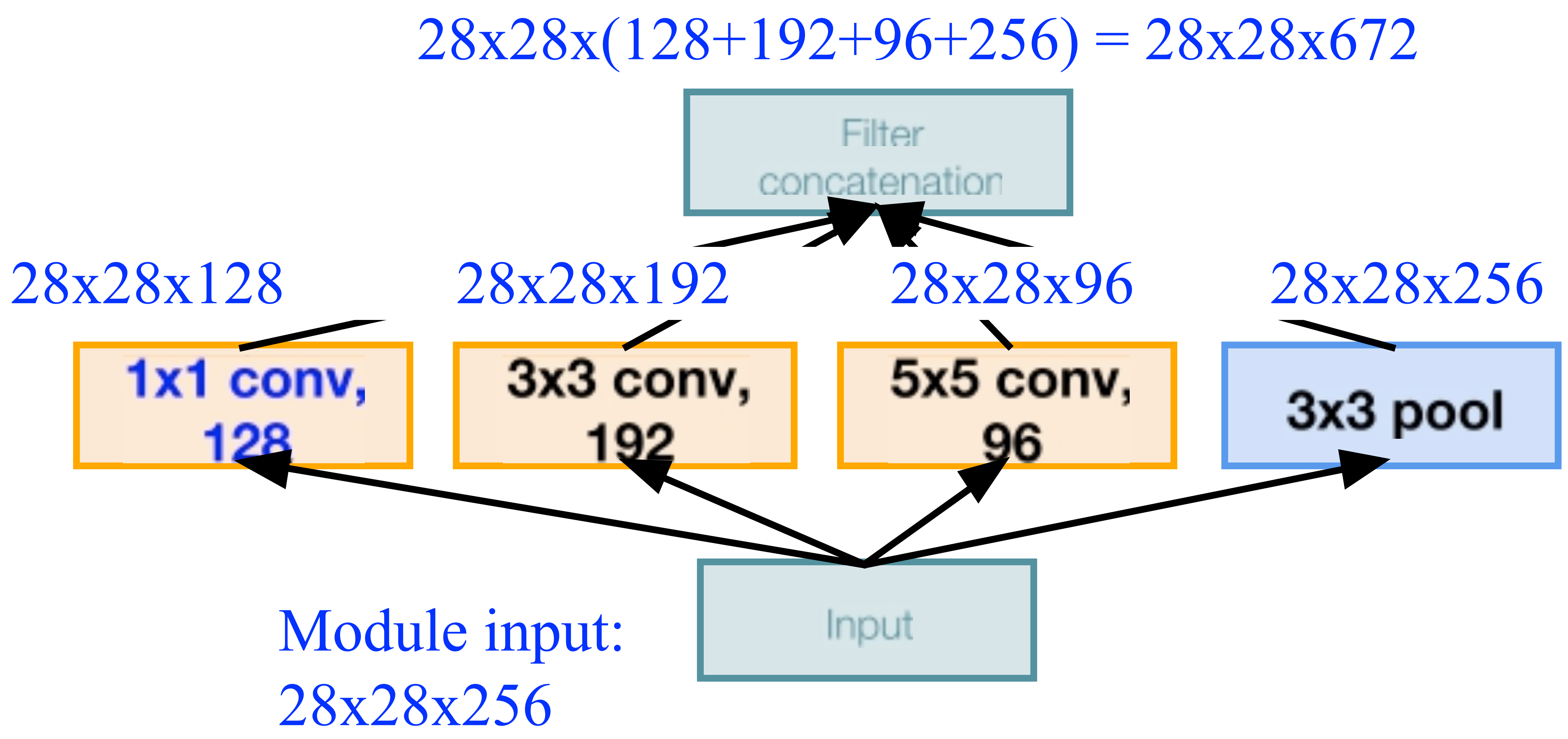
Case Study: GoogLeNet

[Szegedy et al., 2014]

Q: What is the problem with this?
[Hint: Computational complexity]

Example:

Q3:What is output size after filter concatenation?



Naive Inception module

Conv Ops:
[1x1 conv, 128] 28x28x128x1x1x256
[3x3 conv, 192] 28x28x192x3x3x256
[5x5 conv, 96] 28x28x96x5x5x256
Total: 854M ops

Very expensive compute

Pooling layer also preserves feature depth, which means total depth after concatenation can only grow at every layer!

Case Study: GoogLeNet

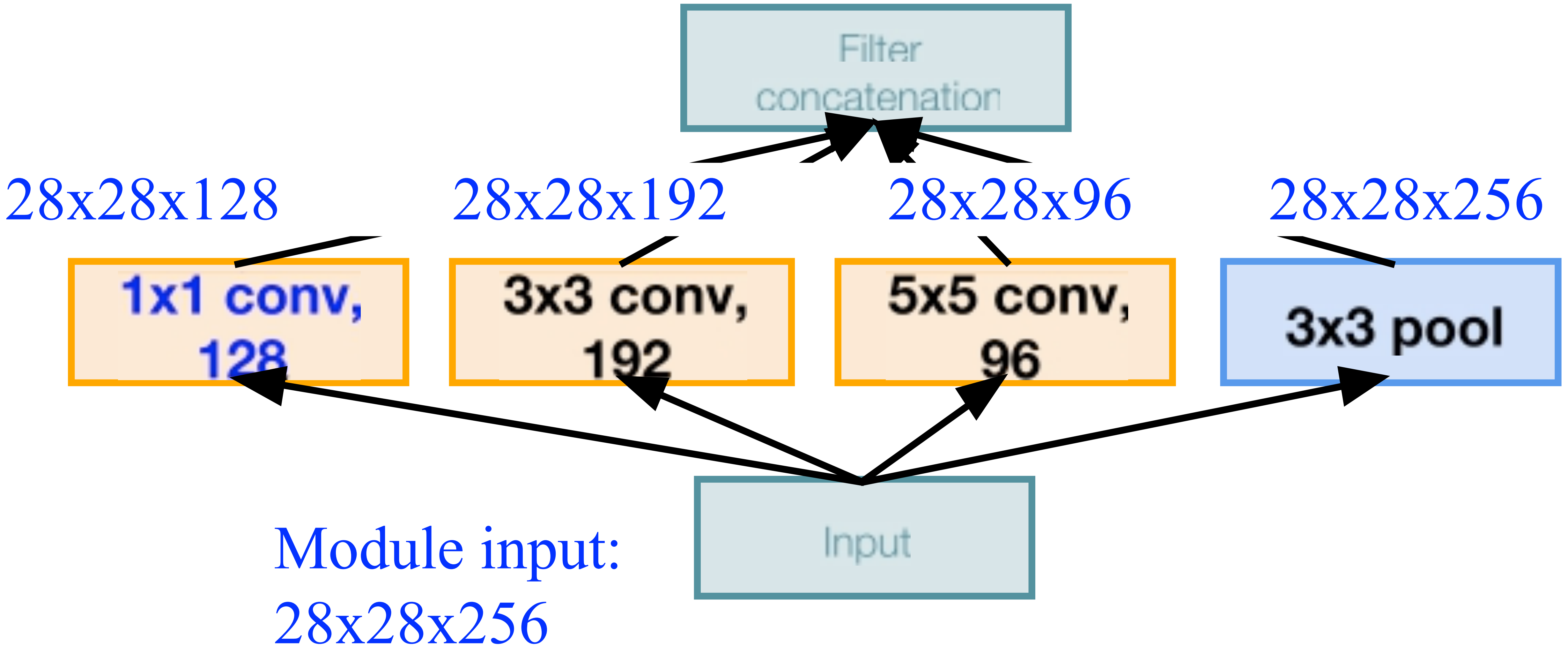
[Szegedy et al., 2014]

Q: What is the problem with this?
[Hint: Computational complexity]

Example:

Q3:What is output size after filter concatenation?

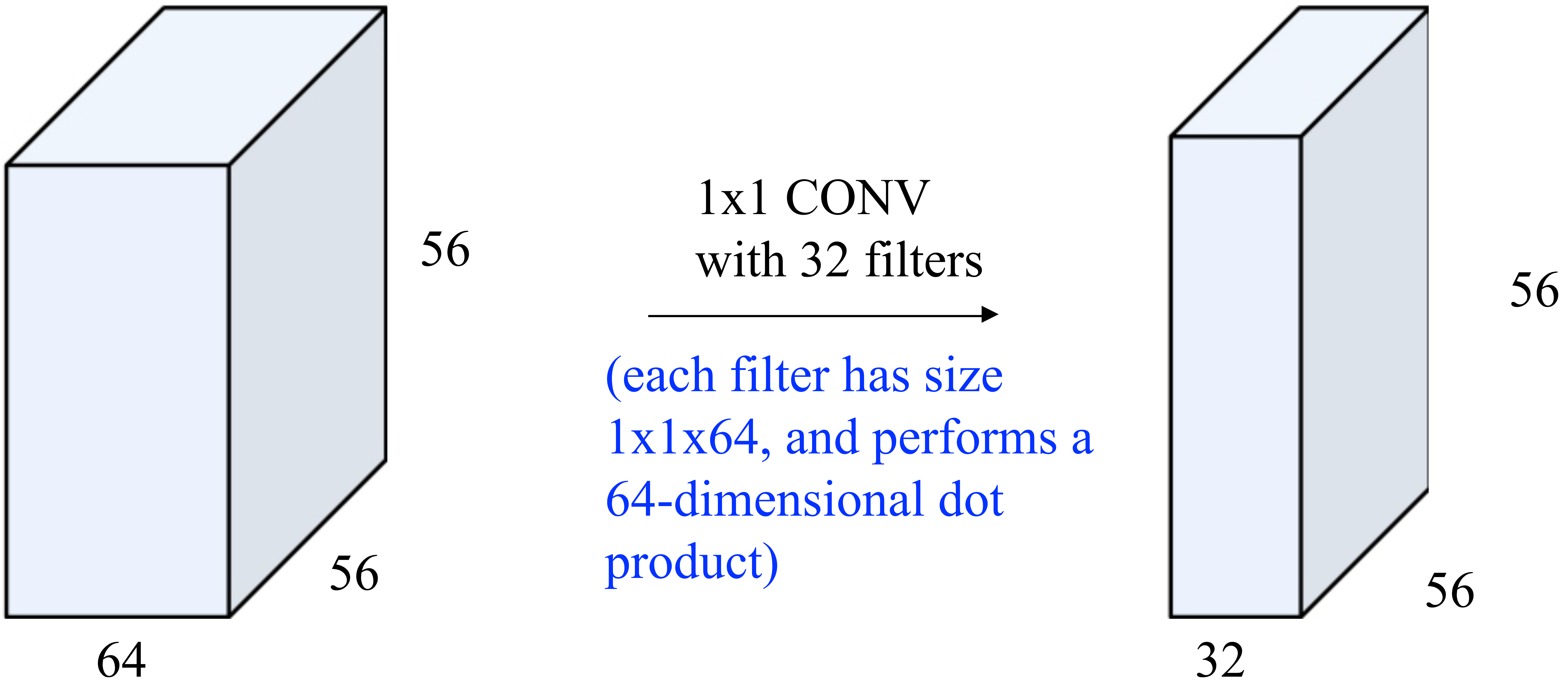
28x28x(128+192+96+256) = **529k**



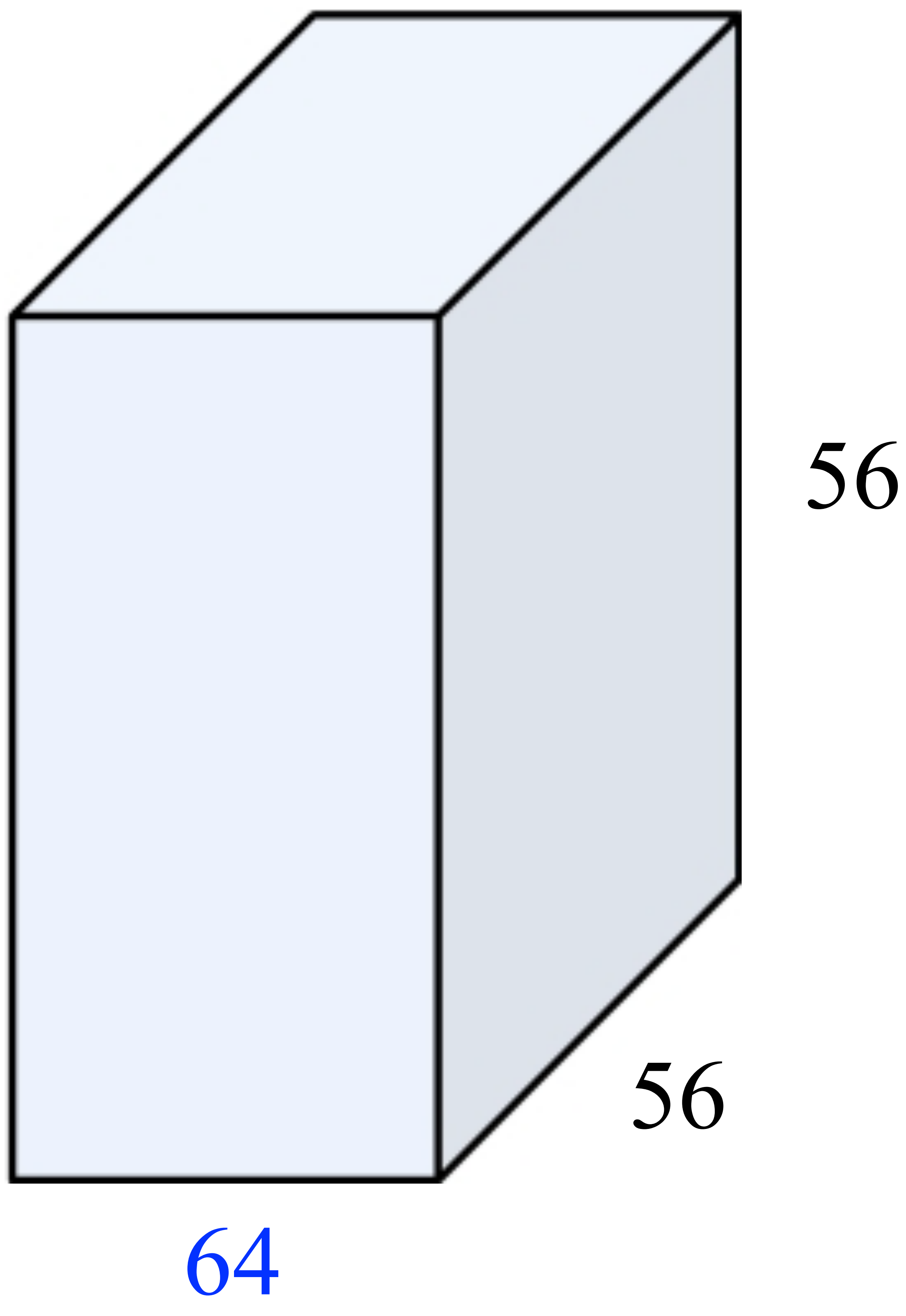
Naive Inception module

Solution: "bottleneck" layers that use 1x1 convolutions to reduce feature depth

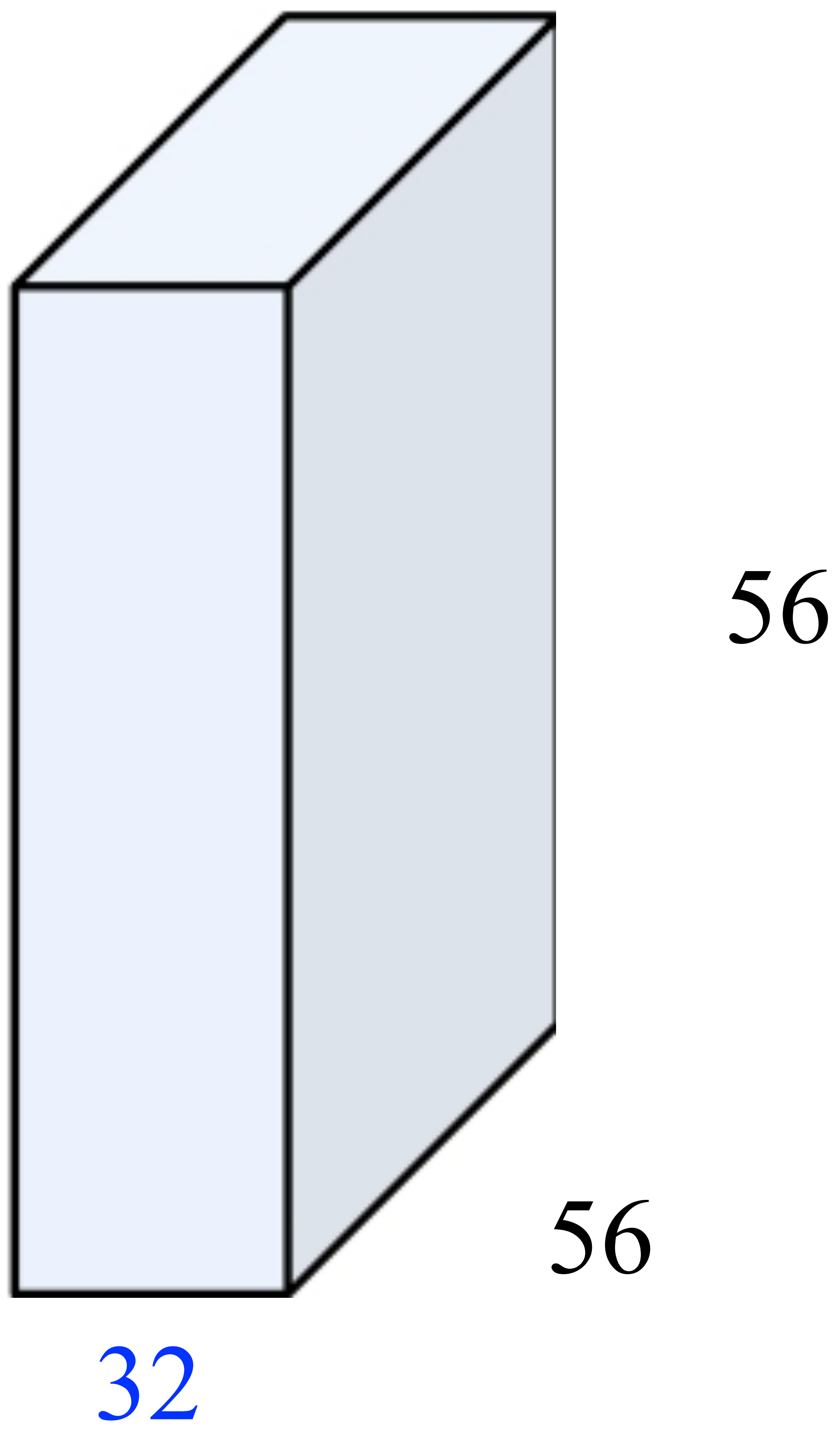
Reminder: 1x1 convolutions



Reminder: 1x1 convolutions



1x1 CONV
with 32 filters

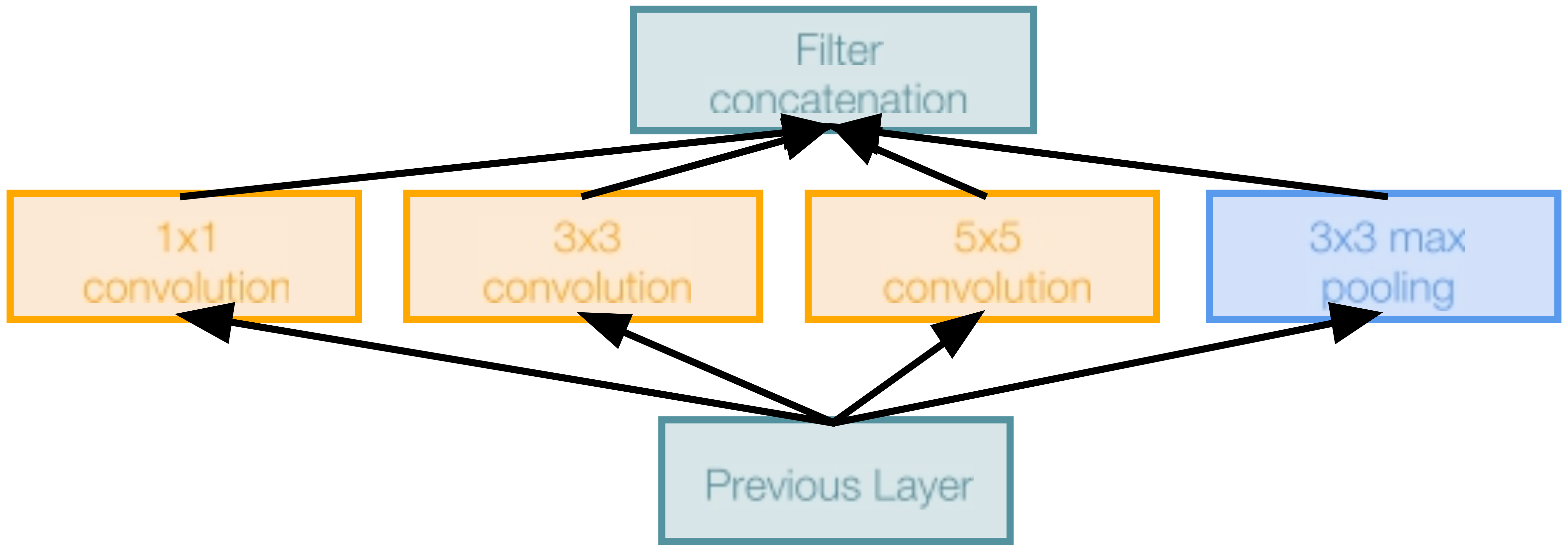


preserves spatial dimensions, reduces depth!

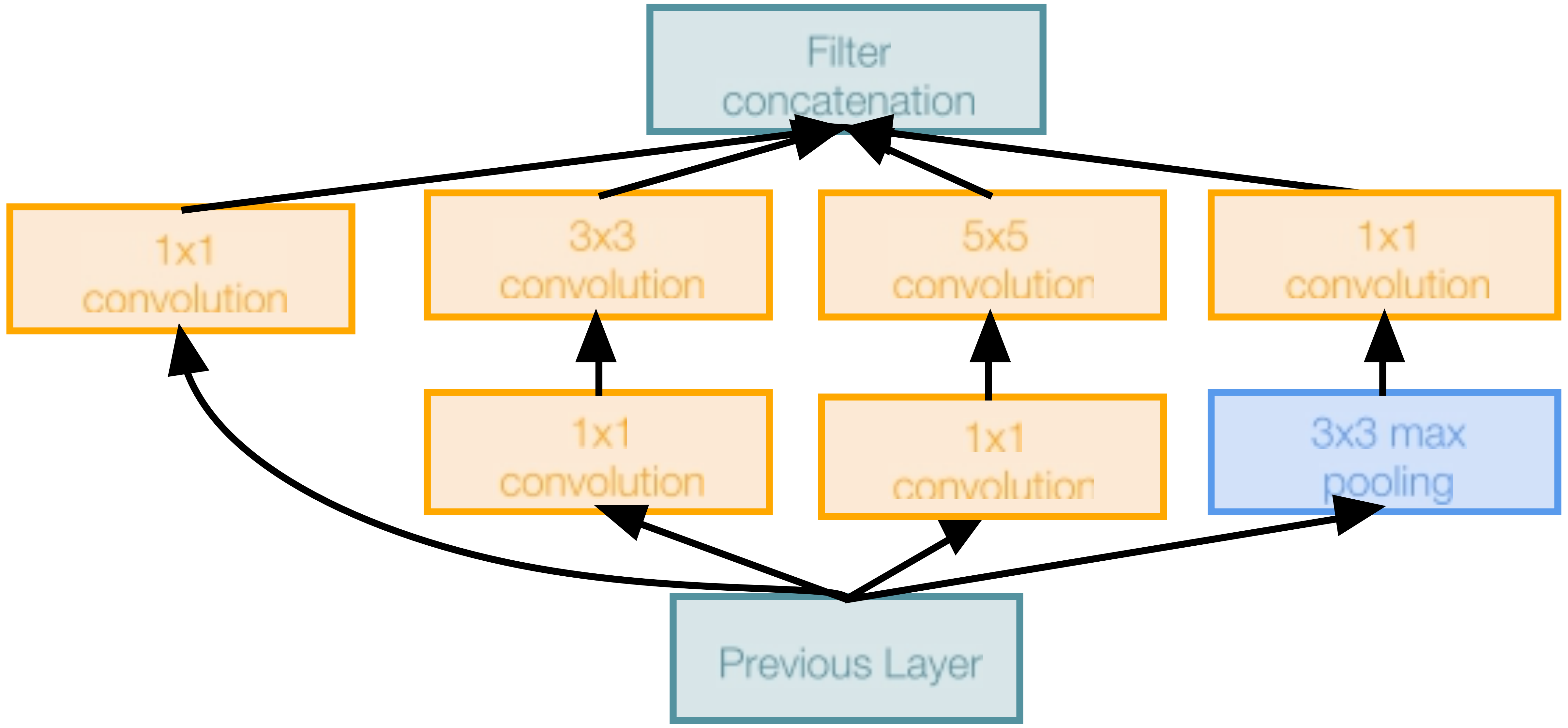
Projects depth to lower dimension (combination of feature maps)

Case Study: GoogLeNet

[Szegedy et al., 2014]



Naive Inception module

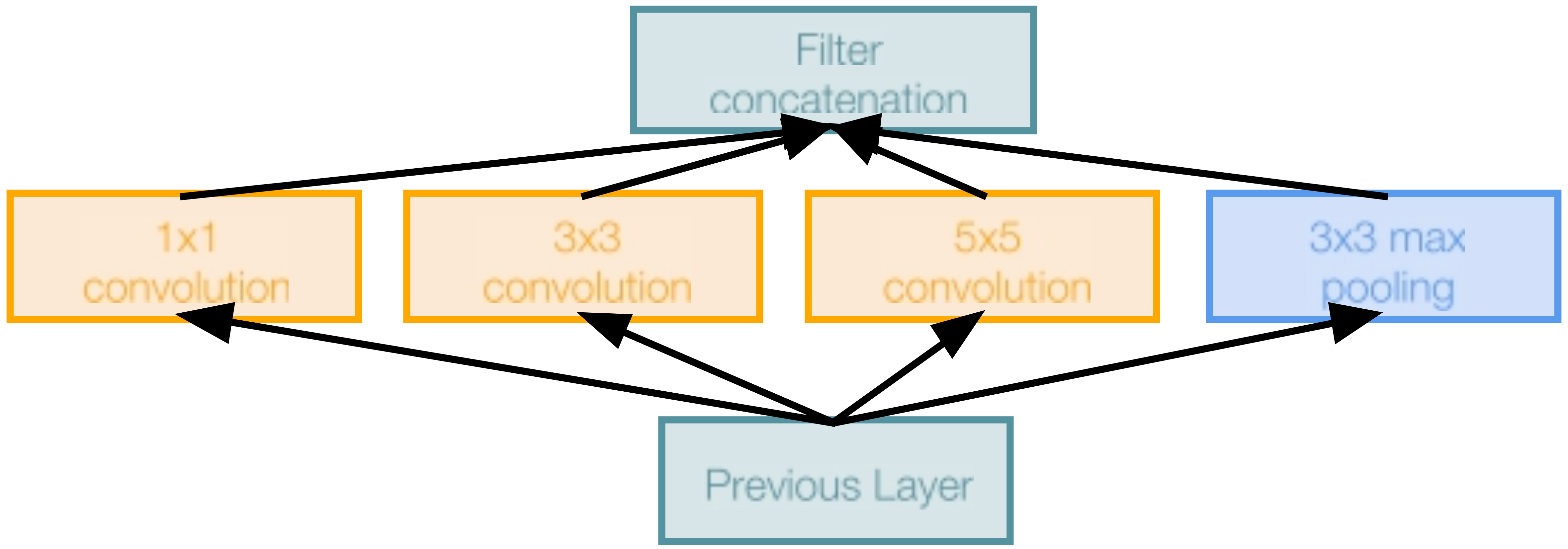


Inception module with dimension reduction

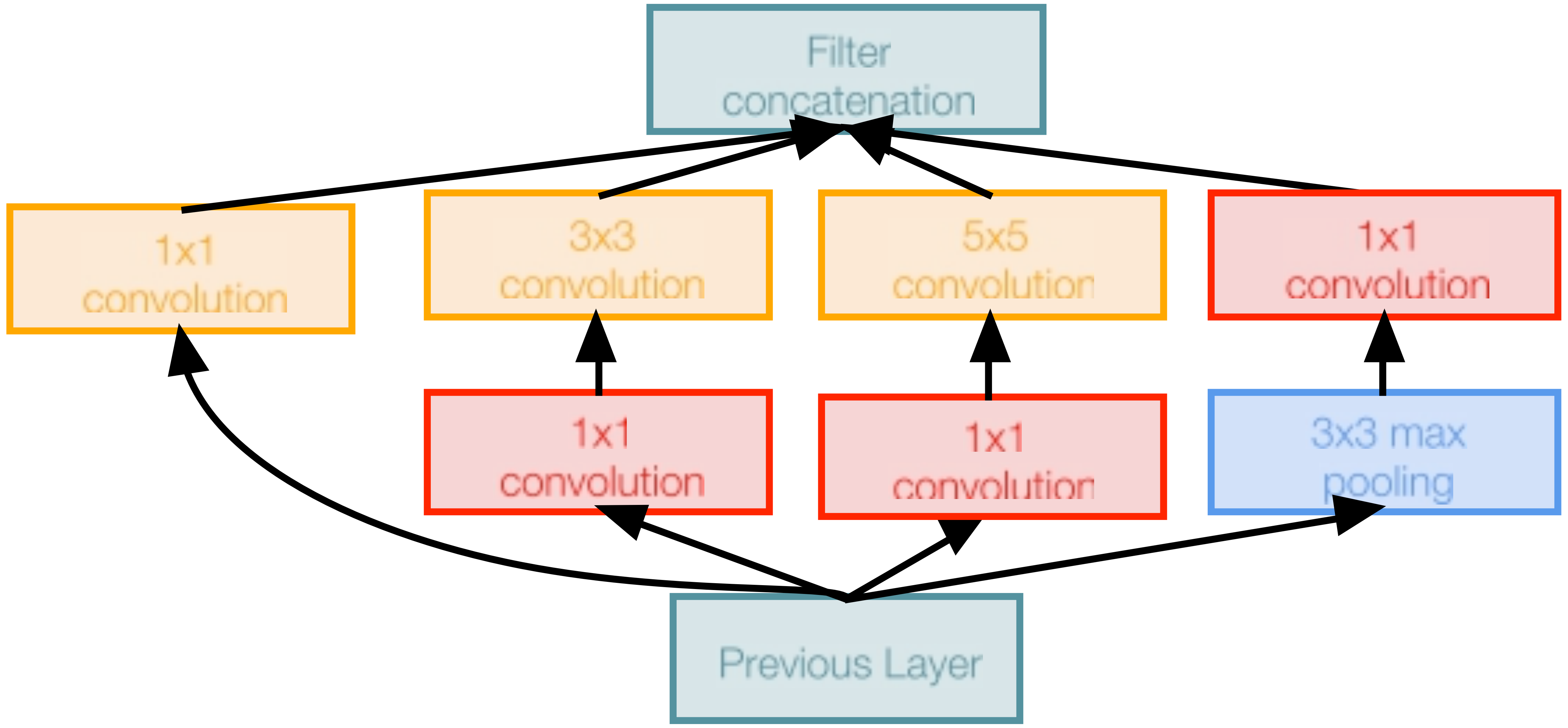
Case Study: GoogLeNet

[Szegedy et al., 2014]

1x1 conv “bottleneck”
layers



Naive Inception module

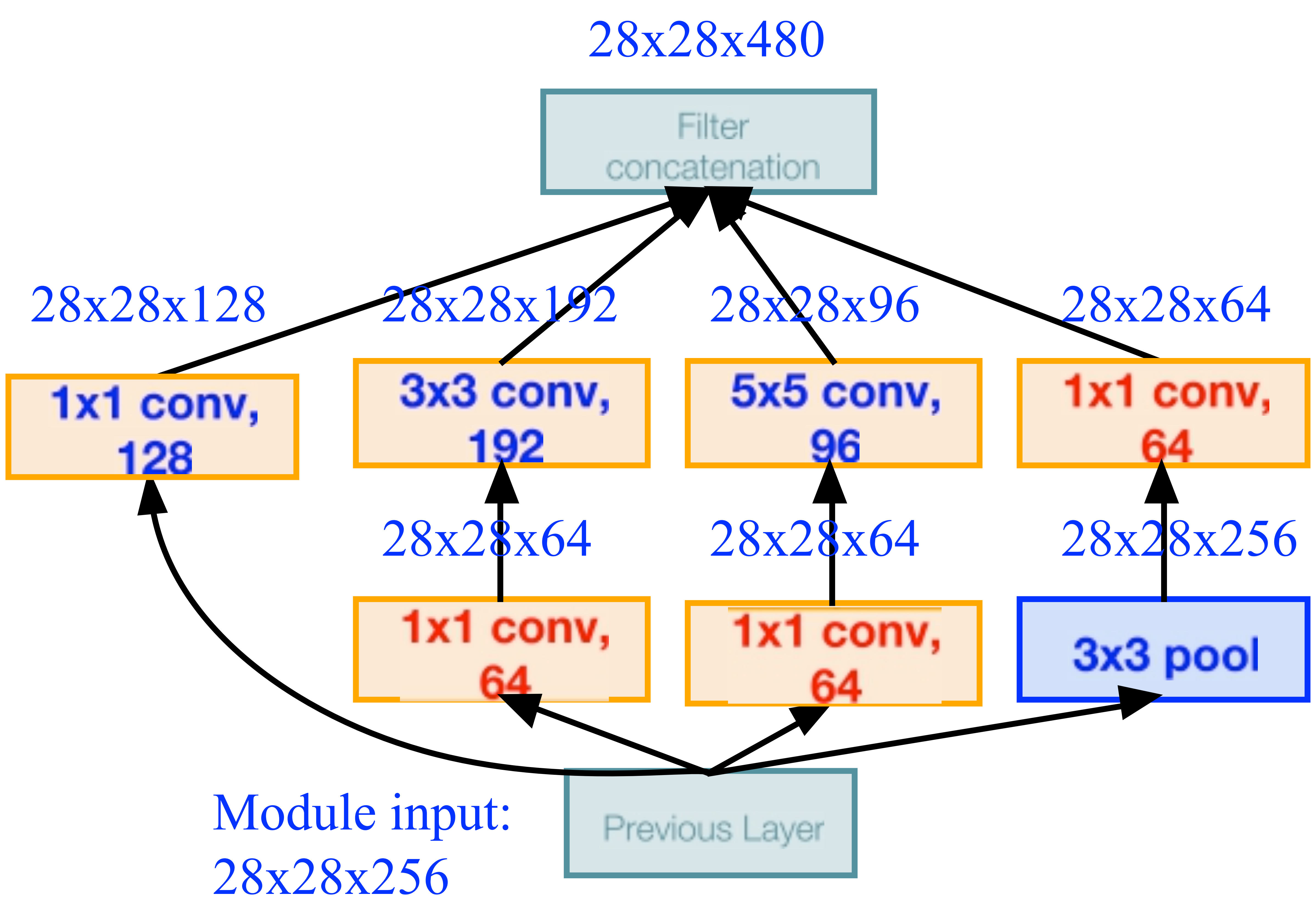


Inception module with dimension reduction

Used with permission from Justin Johnson

Case Study: GoogLeNet

[Szegedy et al., 2014]



Inception module with dimension reduction

Using same parallel layers as naive example, and adding "1x1 conv, 64 filter" bottlenecks:

Conv Ops:

[1x1 conv, 64] 28x28x64x1x1x256

[1x1 conv, 64] 28x28x64x1x1x256

[1x1 conv, 128] 28x28x128x1x1x256

[3x3 conv, 192] 28x28x192x3x3x64

[5x5 conv, 96] 28x28x96x5x5x64

[1x1 conv, 64] 28x28x64x1x1x256

Total: 358M ops

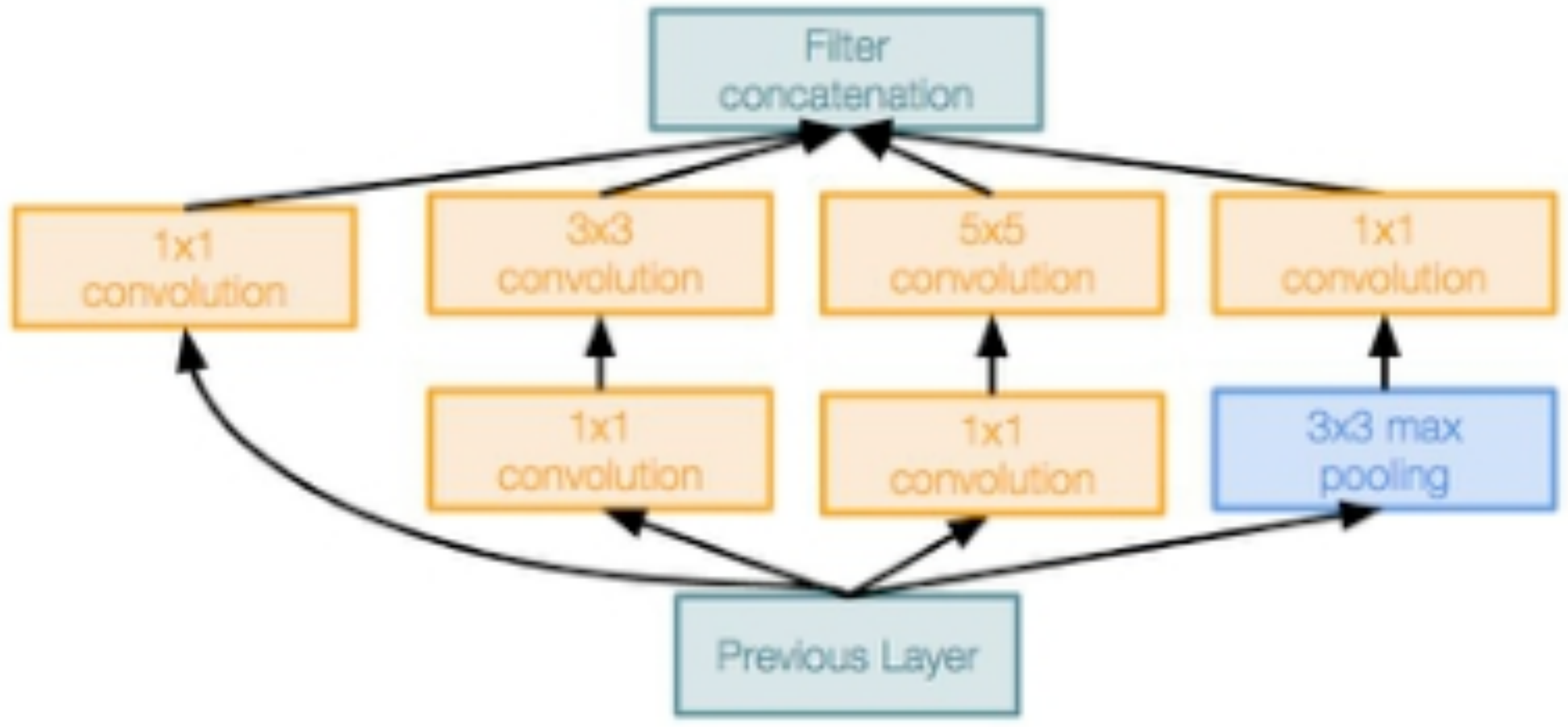
Compared to 854M ops for naive version

Bottleneck can also reduce depth after pooling layer

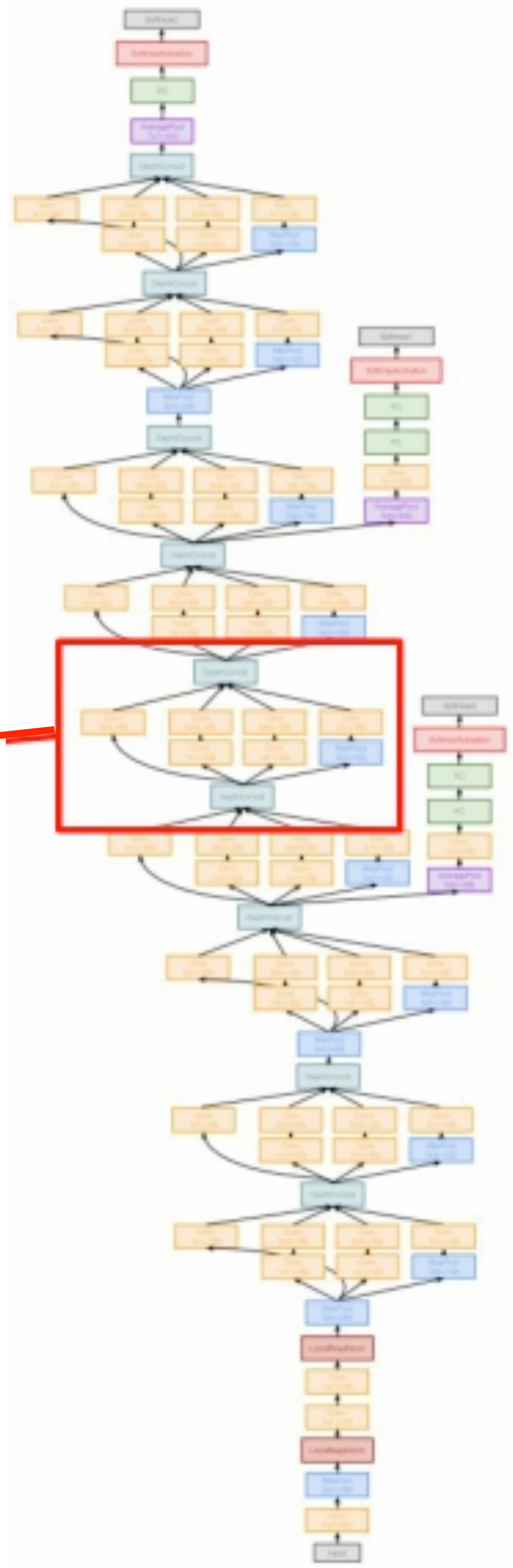
Case Study: GoogLeNet

[Szegedy et al., 2014]

Stack Inception modules
with dimension reduction
on top of each other



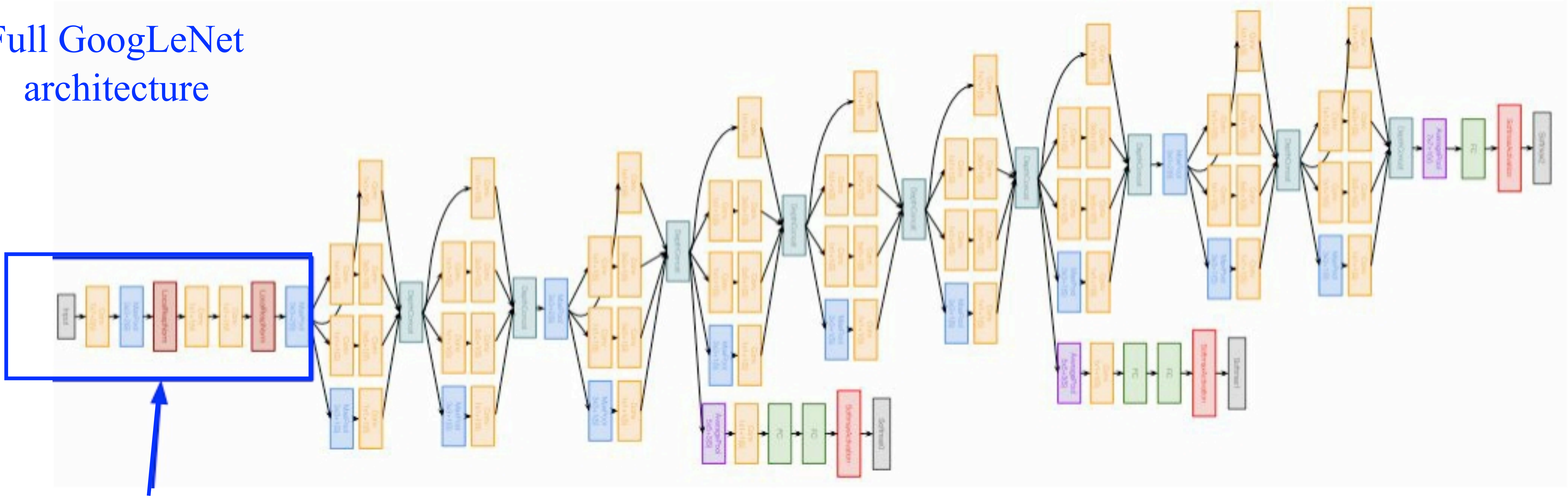
Inception module



Case Study: GoogLeNet

[Szegedy et al., 2014]

Full GoogLeNet architecture

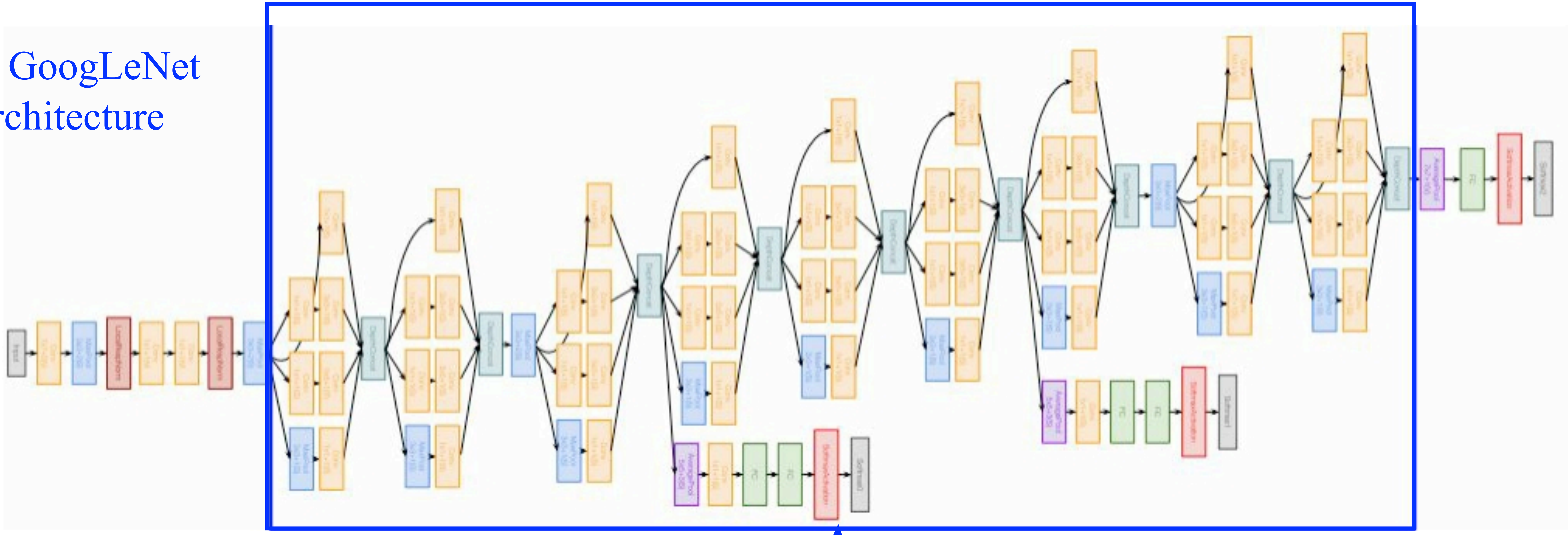


Stem Network:
Conv-Pool-
2x Conv-Pool

Case Study: GoogLeNet

[Szegedy et al., 2014]

Full GoogLeNet architecture

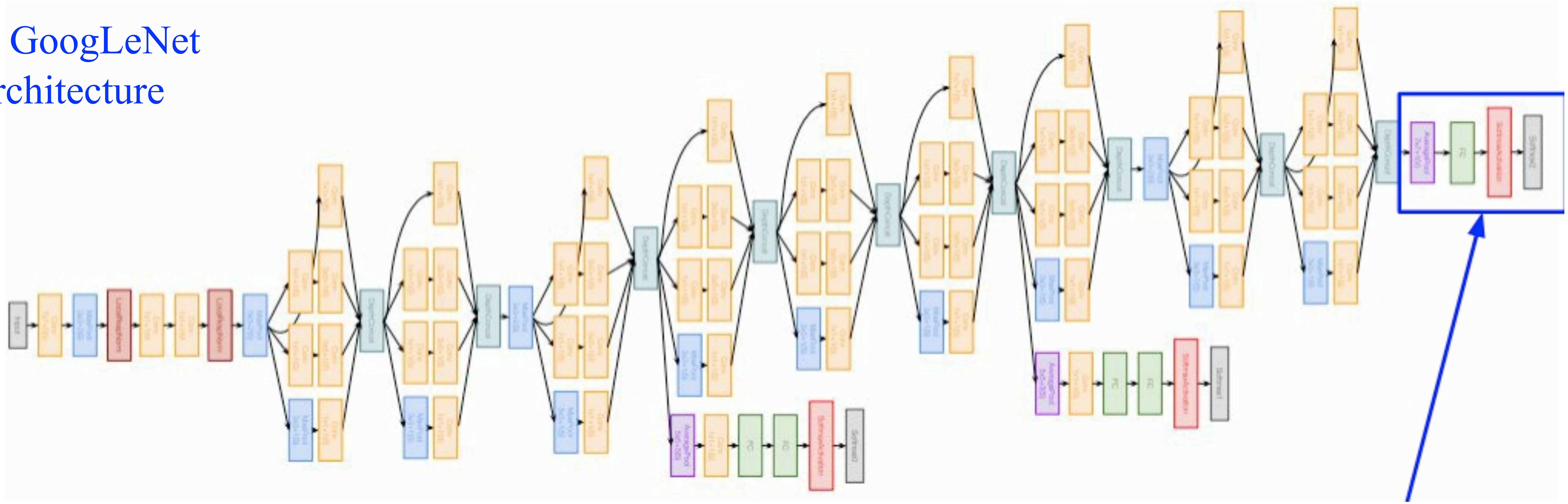


Stacked Inception Modules

Case Study: GoogLeNet

[Szegedy et al., 2014]

Full GoogLeNet architecture



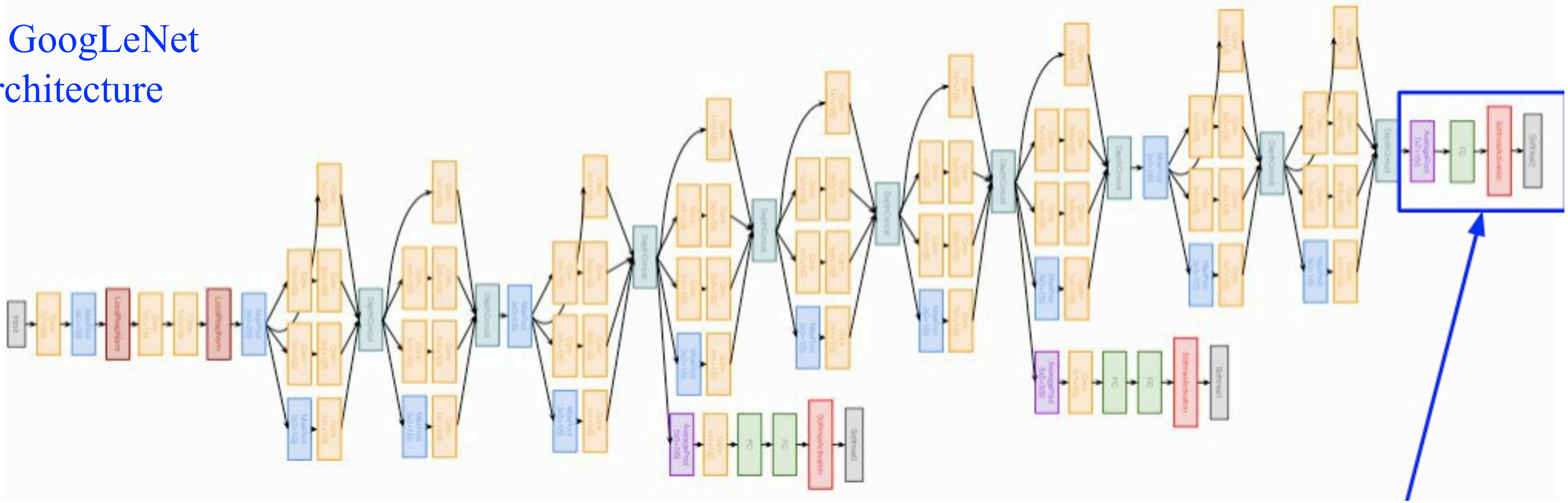
Classifier output

Used with permission from Justin Johnson

Case Study: GoogLeNet

[Szegedy et al., 2014]

Full GoogLeNet architecture

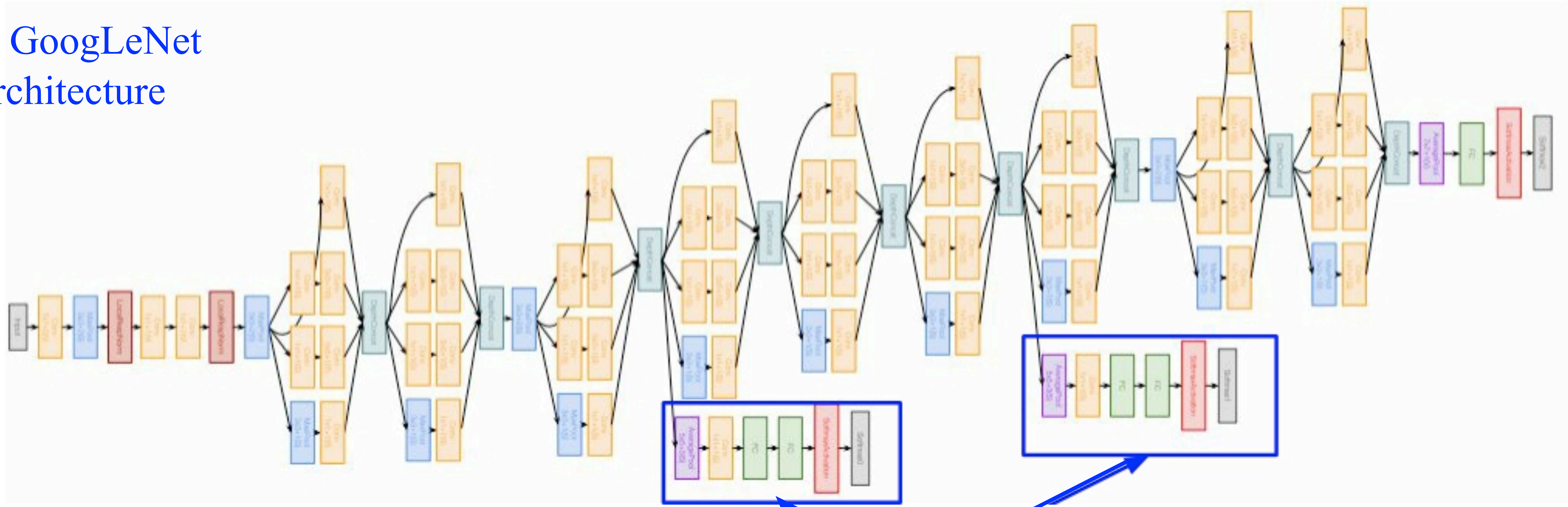


Classifier output
(removed expensive FC layers!)

Case Study: GoogLeNet

[Szegedy et al., 2014]

Full GoogLeNet architecture

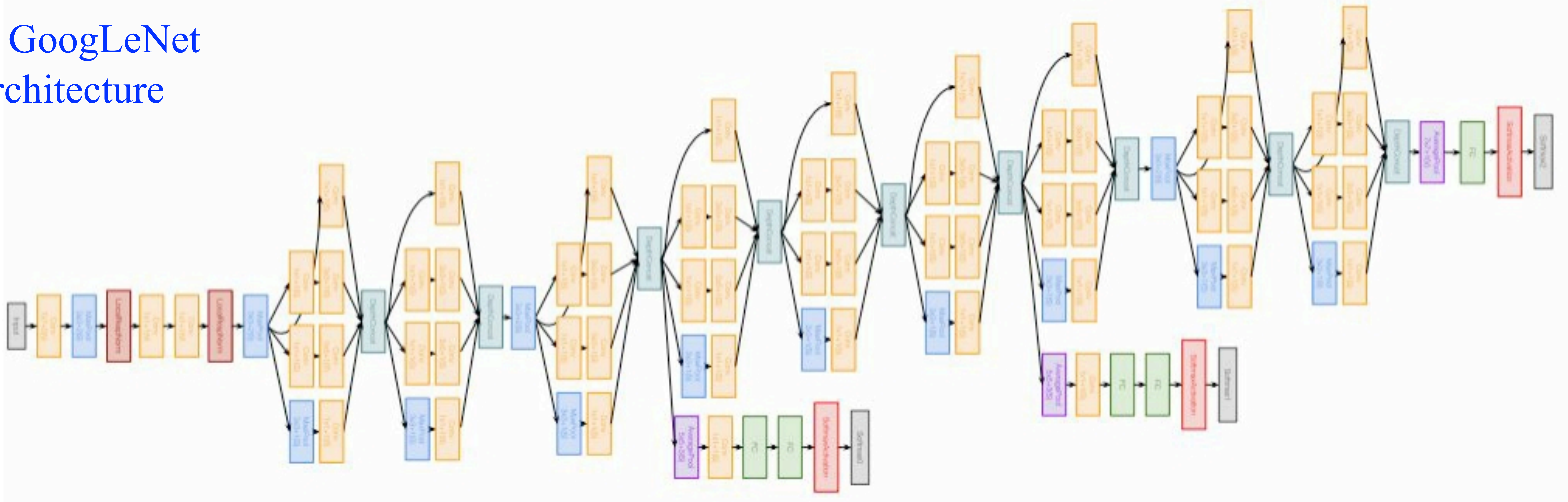


Auxiliary classification outputs to inject additional gradient at lower layers
(AvgPool-1x1Conv-FC-FC-Softmax)

Case Study: GoogLeNet

[Szegedy et al., 2014]

Full GoogLeNet
architecture



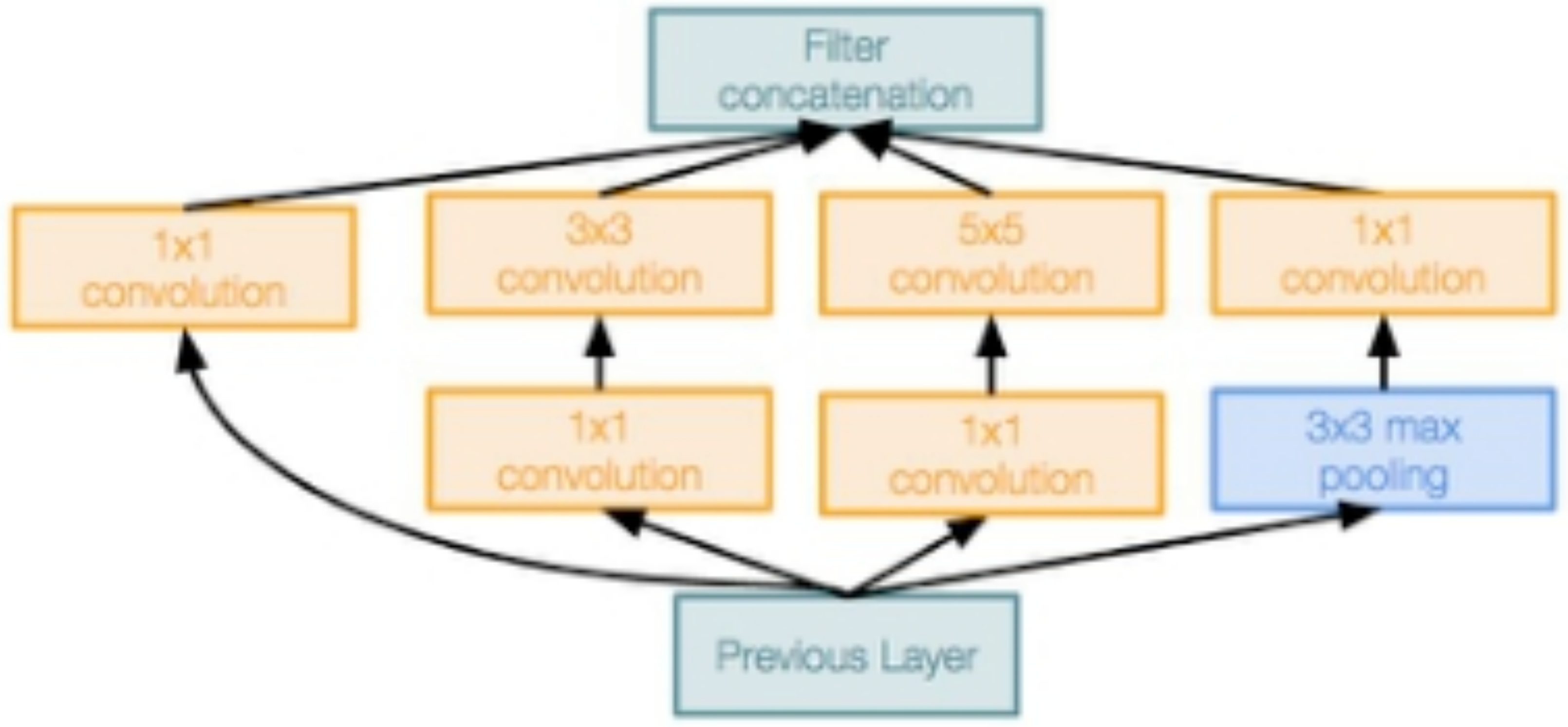
22 total layers with weights
(parallel layers count as 1 layer => 2 layers per Inception module. Don't count auxiliary output layers)

Case Study: GoogLeNet

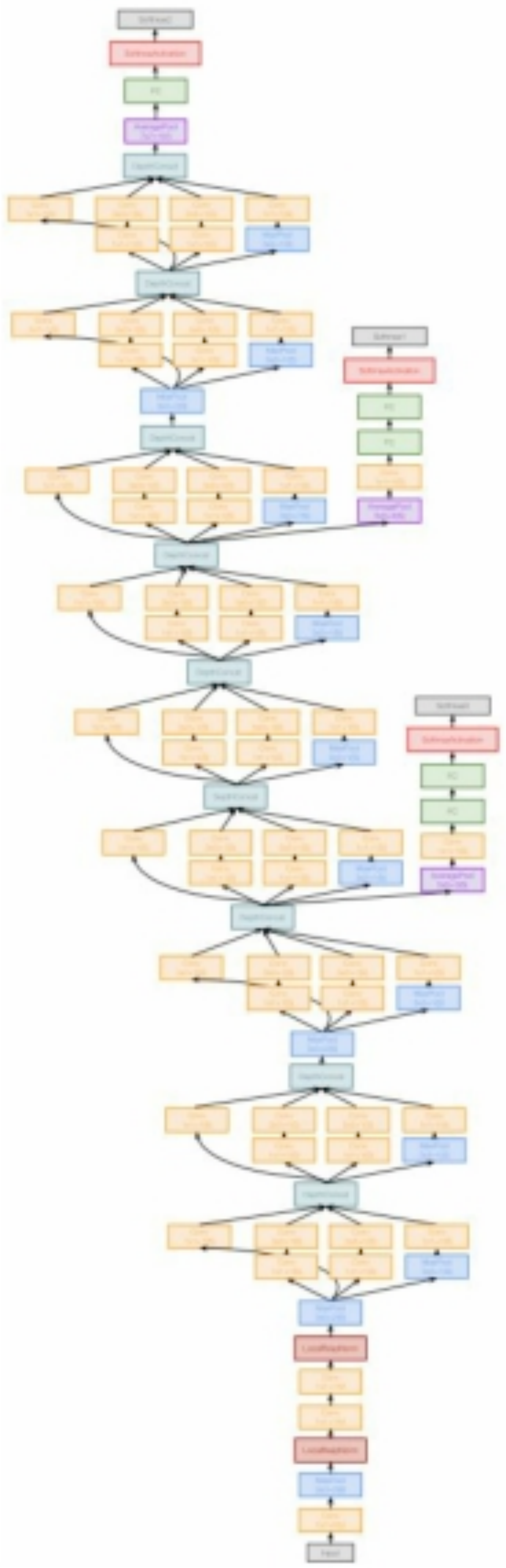
[Szegedy et al., 2014]

Deeper networks, with computational efficiency

- 22 layers
- Efficient "Inception" module
- No FC layers
- 12x less params than AlexNet
- ILSVRC'14 classification winner (6.7% top 5 error)



Inception module



Inception v2, v3

- Regularize training with batch normalization, reducing importance of auxiliary classifiers

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \text{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \text{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

C. Szegedy et al., Rethinking the inception architecture for computer vision, CVPR 2016

Batch Normalization

[Ioffe and Szegedy, 2015]

"you want zero-mean unit-variance activations? just make them so."

consider a batch of activations at some layer. To make each dimension zero-mean unit-variance, apply:

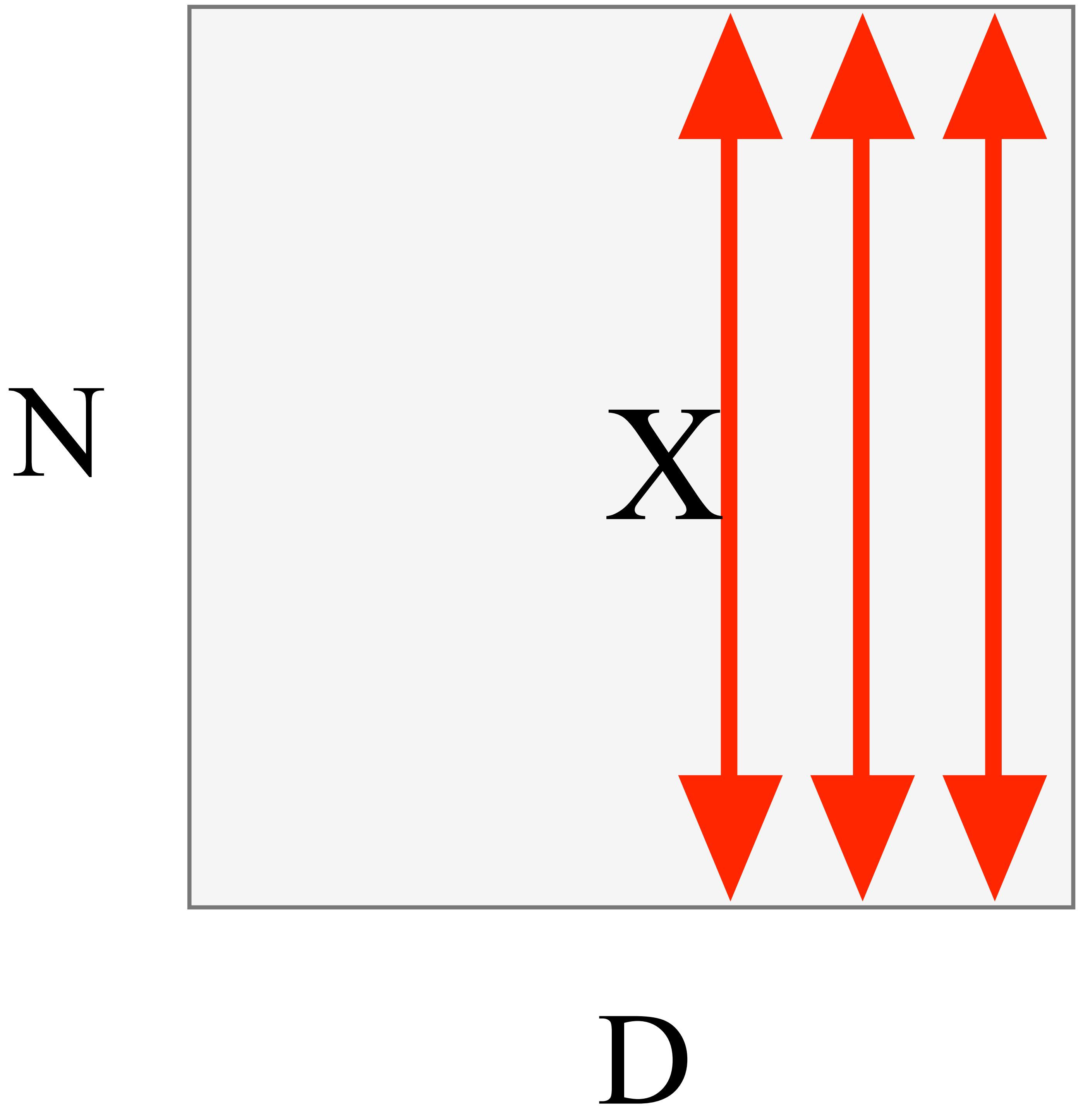
$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

this is a vanilla differentiable function...

Batch Normalization

[Ioffe and Szegedy, 2015]

"you want zero-mean unit-variance activations? just make them so."



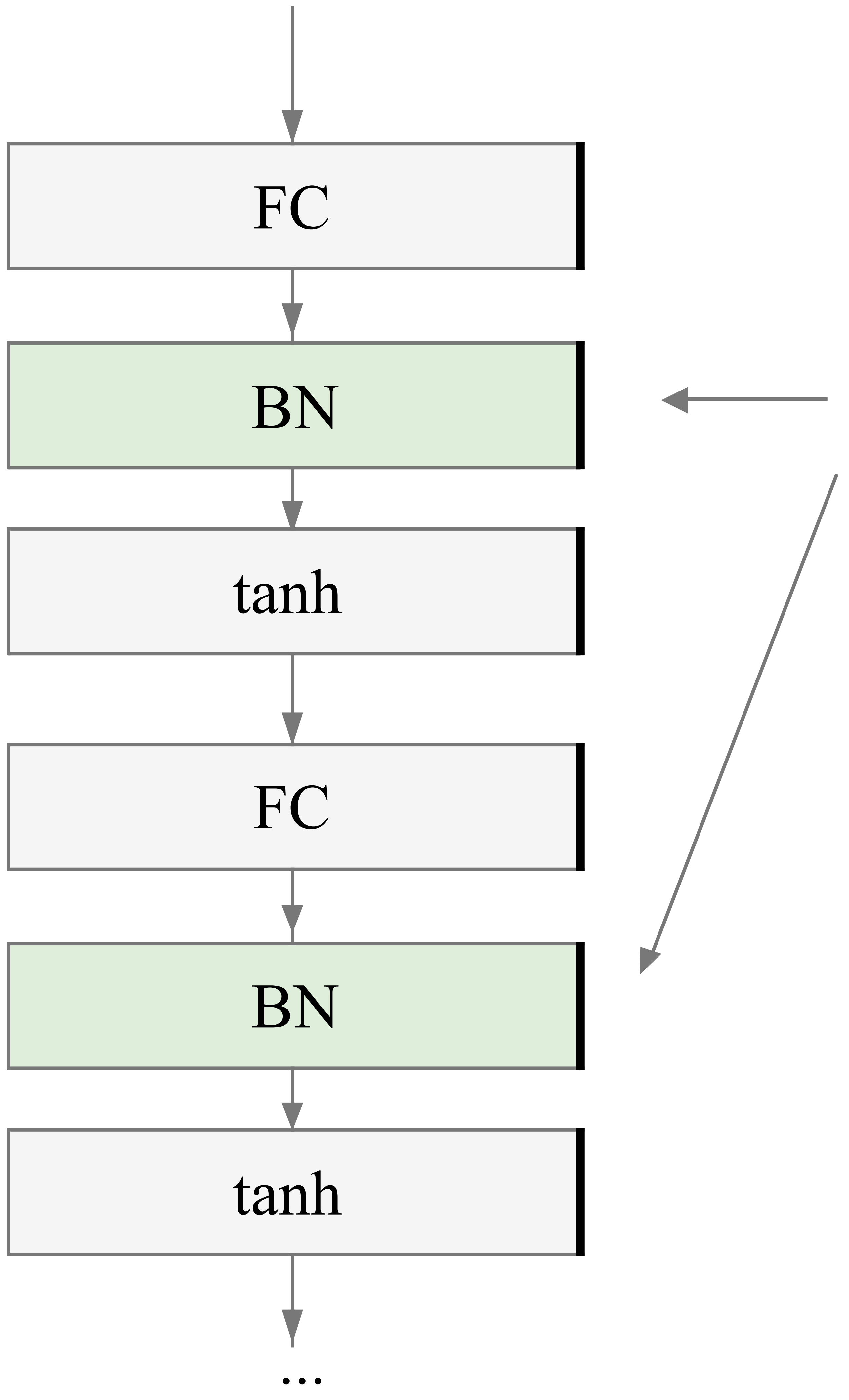
1. compute the empirical mean and variance independently for each dimension.

2. Normalize

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

Batch Normalization

[Ioffe and Szegedy, 2015]

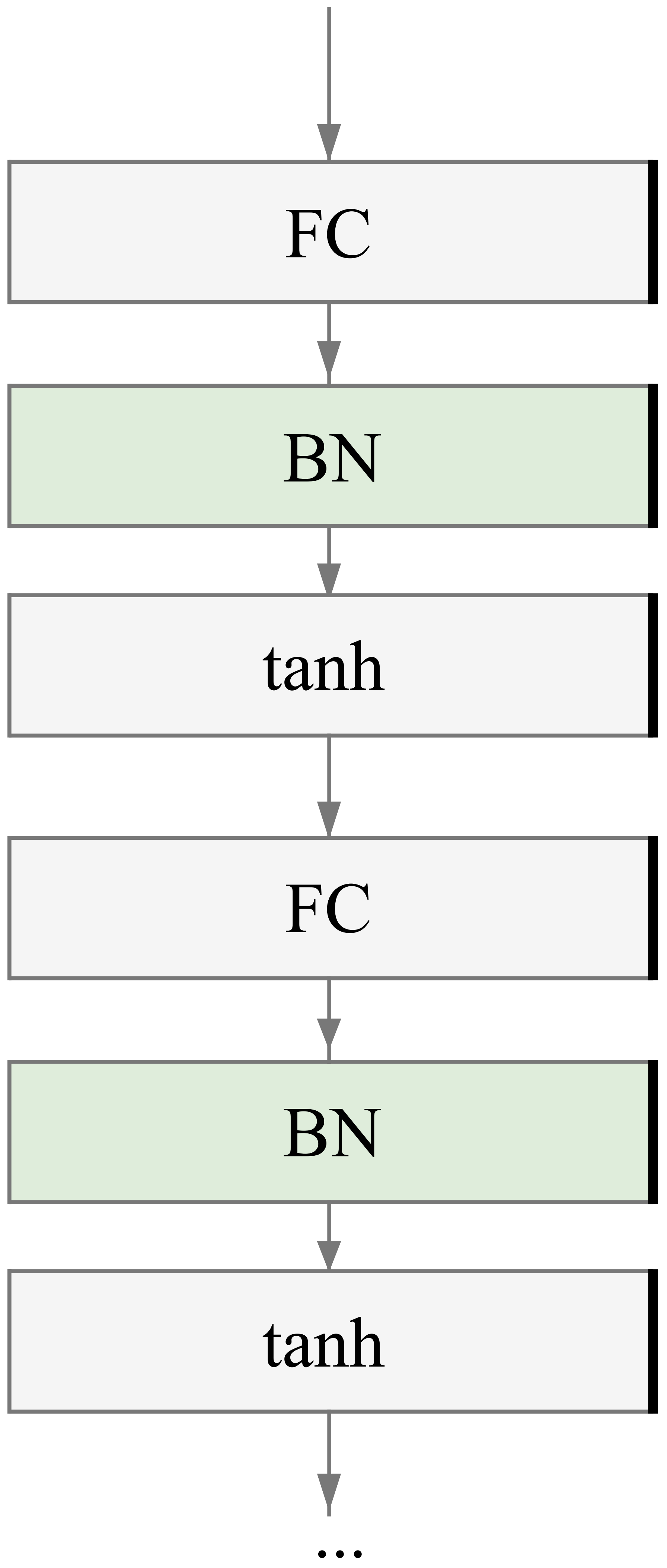


Usually inserted after Fully Connected or Convolutional layers, and before nonlinearity.

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

Batch Normalization

[Ioffe and Szegedy, 2015]



Usually inserted after Fully Connected or Convolutional layers, and before nonlinearity.

Problem: do we necessarily want a zero-mean unit-variance input?

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

Batch Normalization

[Ioffe and Szegedy, 2015]

Normalize:

$$\boxed{\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}}$$

And then allow the network to squash the range if it wants to:

$$\boxed{y^{(k)} = \gamma^{(k)} \widehat{x}^{(k)} + \beta^{(k)}}$$

$$\gamma^{(k)} = \sqrt{\mathrm{Var}[x^{(k)}]}$$

$$\beta^{(k)} = \mathrm{E}[x^{(k)}]$$

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
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$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \text{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization in a funny way, and slightly reduces the need for dropout, maybe

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

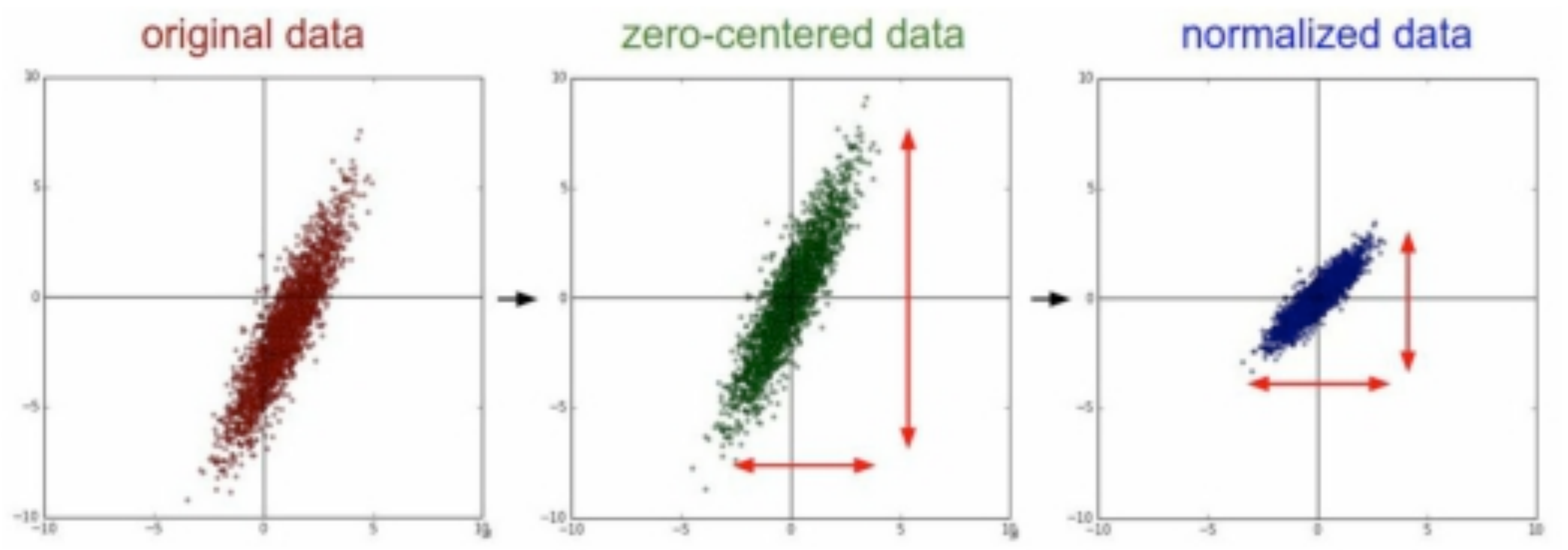
Note: at test time BatchNorm layer functions differently:

The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations during training is used.

(e.g. can be estimated during training with running averages)

Decorrelated Batch Normalization

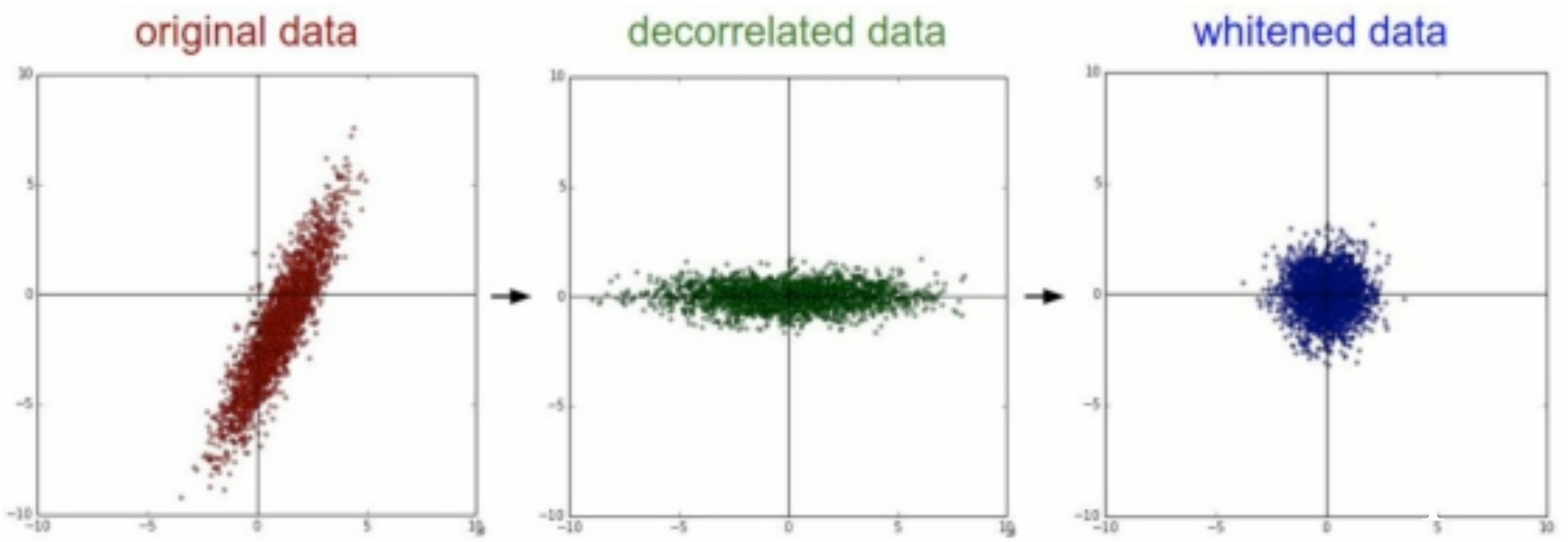
Batch Normalization



$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

BatchNorm normalizes the data, but cannot correct for correlations among the input features

Decorrelated Batch Normalization



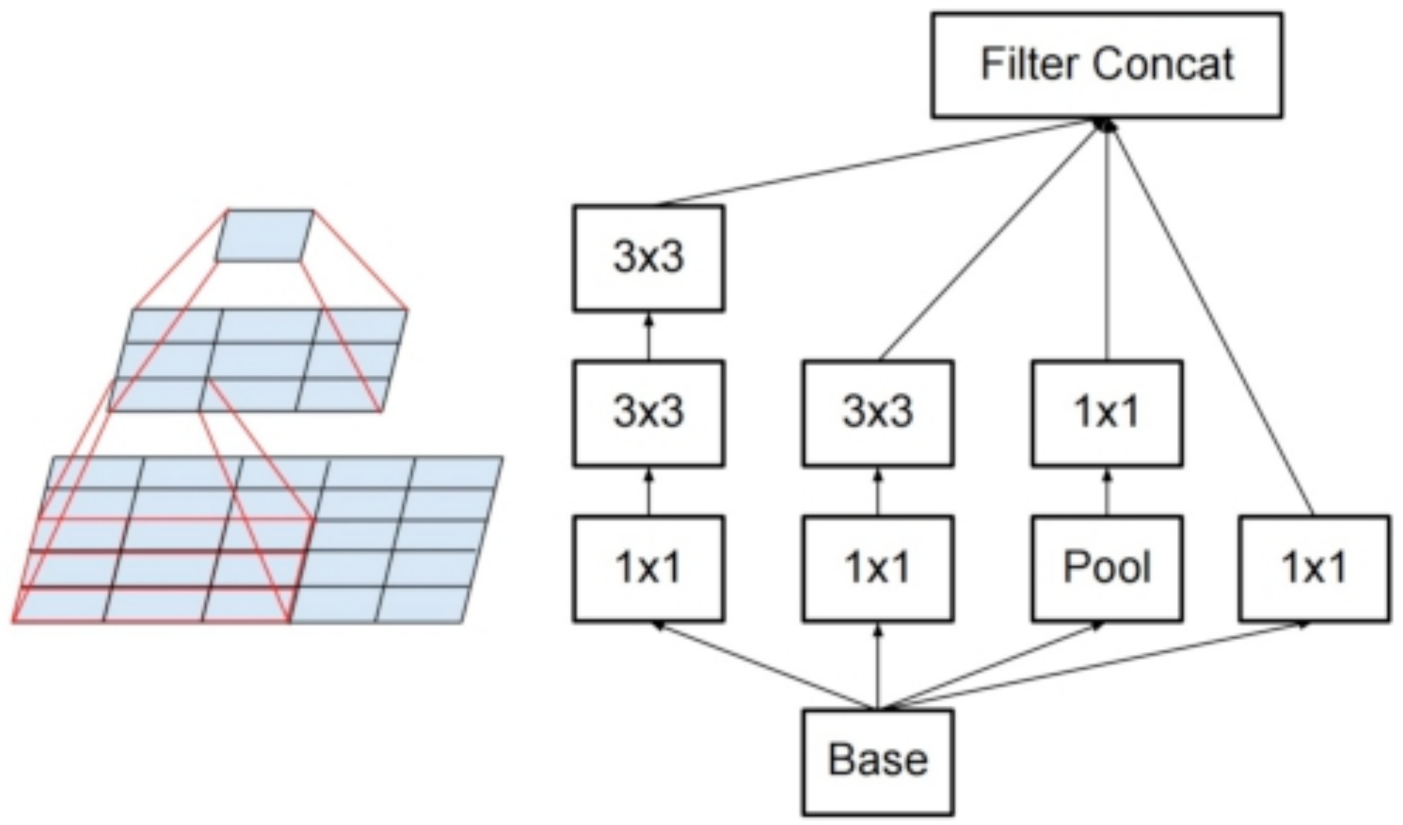
$$\hat{x}_i = \Sigma^{-\frac{1}{2}}(x_i - \mu)$$

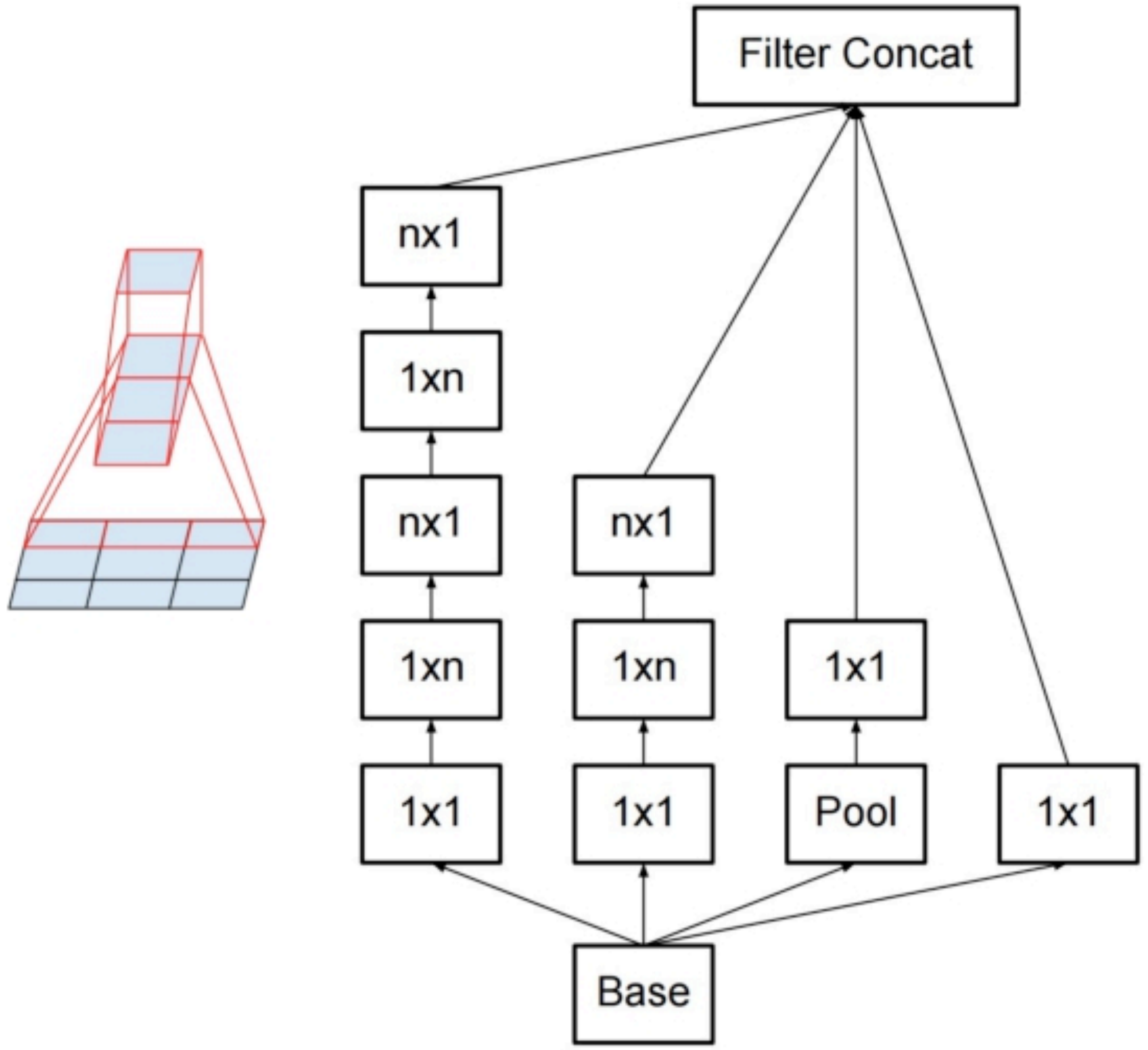
DBN **whitens** the data using the full covariance matrix of the minibatch; this corrects for correlations

Huang et al, "Decorrelated Batch Normalization", arXiv 2018 (Appeared 4/23/2018)

Inception v2, v3

- Regularize training with batch normalization, reducing importance of auxiliary classifiers
- More variants of inception modules with aggressive factorization of filters





C. Szegedy et al., Rethinking the inception architecture for computer vision, CVPR 2016

Inception v2, v3

- Regularize training with batch normalization, reducing importance of auxiliary classifiers
- More variants of inception modules with aggressive factorization of filters
- Increase the number of feature maps while decreasing spatial resolution (pooling)

Network	Models Evaluated	Crops Evaluated	Top-1 Error	Top-5 Error
VGGNet [18]	2	-	23.7%	6.8%
GoogLeNet [20]	7	144	-	6.67%
PReLU [6]	-	-	-	4.94%
BN-Inception [7]	6	144	20.1%	4.9%
Inception-v3	4	144	**17.2%**	**3.58%***

C. Szegedy et al., Rethinking the inception architecture for computer vision, CVPR 2016

MOAR Optimization!

AdaGrad

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

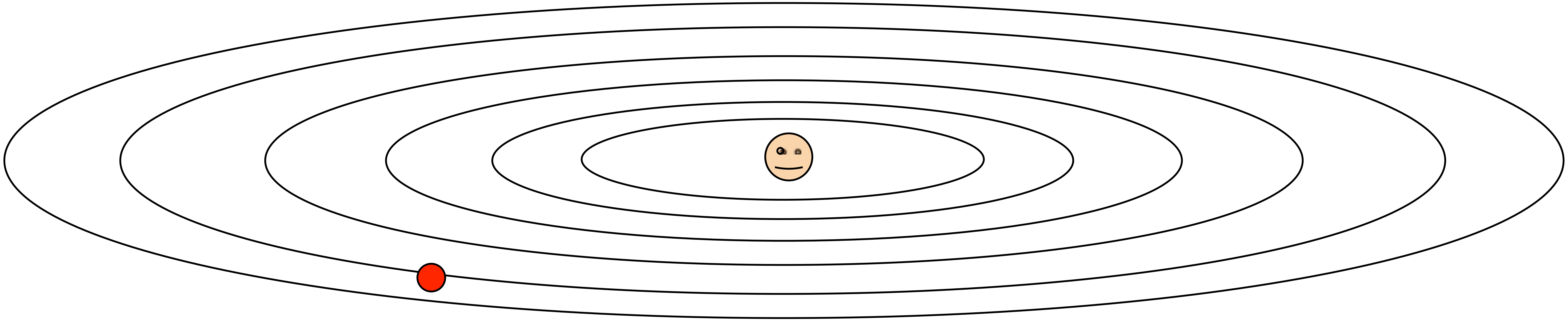
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

"Per-parameter learning rates"
or "adaptive learning rates"

Duchi et al, "Adaptive subgradient methods for online learning and stochastic optimization", JMLR 2011

AdaGrad

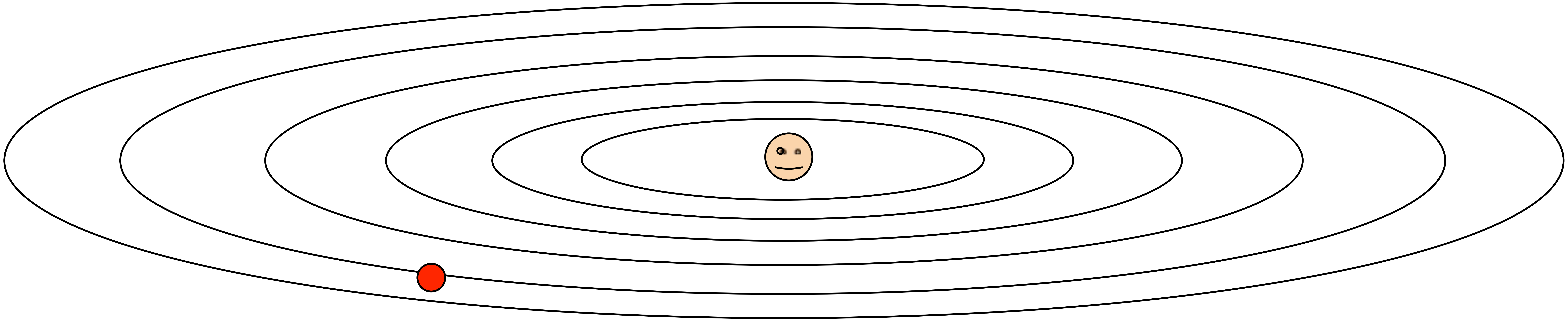
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q: What happens with AdaGrad?

AdaGrad

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

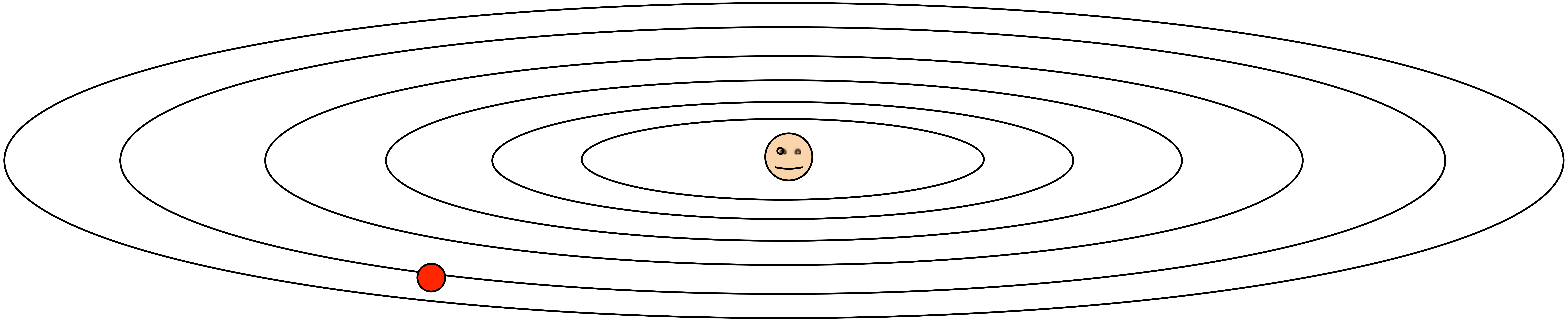


Q: What happens with AdaGrad?

Progress along "steep" directions is damped;
Progress along "flat" directions is accelerated

AdaGrad

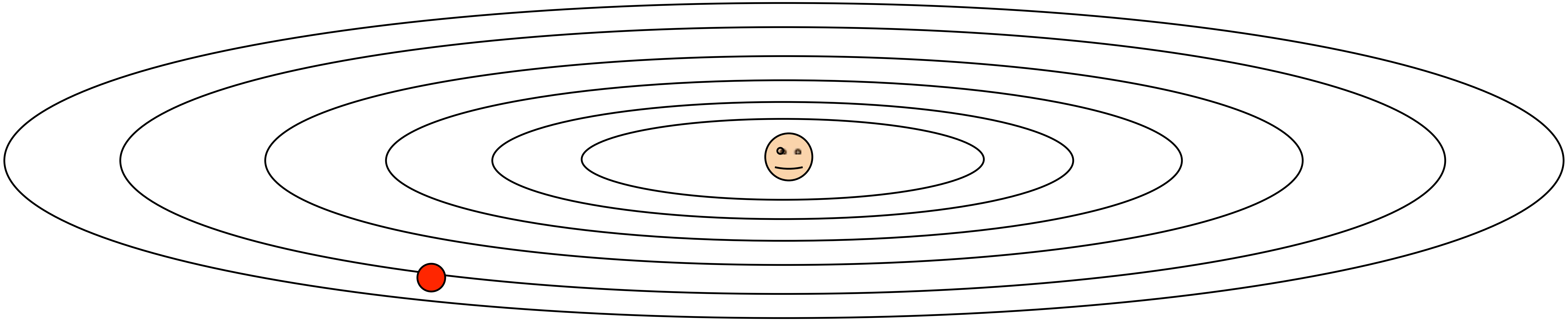
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q2: What happens to the step size over long time?

AdaGrad

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q2: What happens to the step size over long time?

Decays to zero

RMSProp

AdaGrad

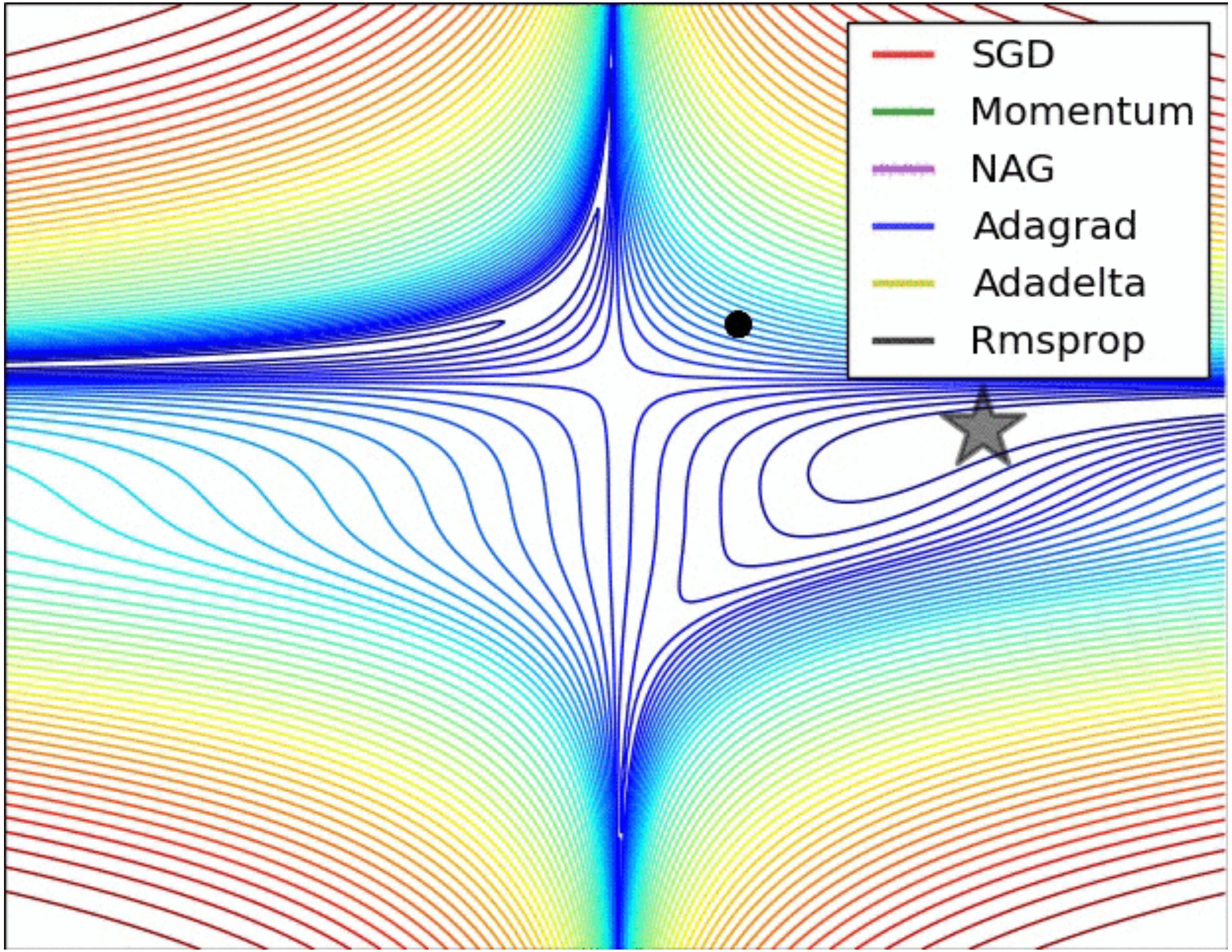
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

RMSProp

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

Tieleman and Hinton, 2012

AdaGrad vs RMSProp



Adam (almost)

```
first_moment = 0
second_moment = 0
while True:
  dx = compute_gradient(x)
  first_moment = beta1 * first_moment  + (1 - beta1) * dx
  second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
  x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

Kingma and Ba, “Adam: A method for stochastic optimization”, ICLR 2015

Adam (almost)

```
first_moment = 0
second_moment = 0
while True:
  dx = compute_gradient(x)
  first_moment = beta1 * first_moment  + (1 - beta1) * dx
  second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
  x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

Momentum

AdaGrad / RMSProp

Sort of like RMSProp with momentum

Q: What happens at first timestep?

Kingma and Ba, “Adam: A method for stochastic optimization”, ICLR 2015

Adam (full form)

```
first_moment = 0
second_moment = 0
for t in range(1, num_iterations):
  dx = compute_gradient(x)
  first_moment = beta1 * first_moment  + (1 - beta1) * dx
  second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
  first_unbias = first_moment / (1 - beta1 ** t)
  second_unbias = second_moment / (1 - beta2 ** t)
  x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))
```

Momentum

Bias correction

AdaGrad / RMSProp

Bias correction for the fact that first and second moment estimates start at zero

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam (full form)

```
first_moment = 0
second_moment = 0
for t in range(1, num_iterations):
  dx = compute_gradient(x)
  first_moment = beta1 * first_moment  + (1 - beta1) * dx
  second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
  first_unbias = first_moment / (1 - beta1 ** t)
  second_unbias = second_moment / (1 - beta2 ** t)
  x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))
```

Momentum

Bias correction

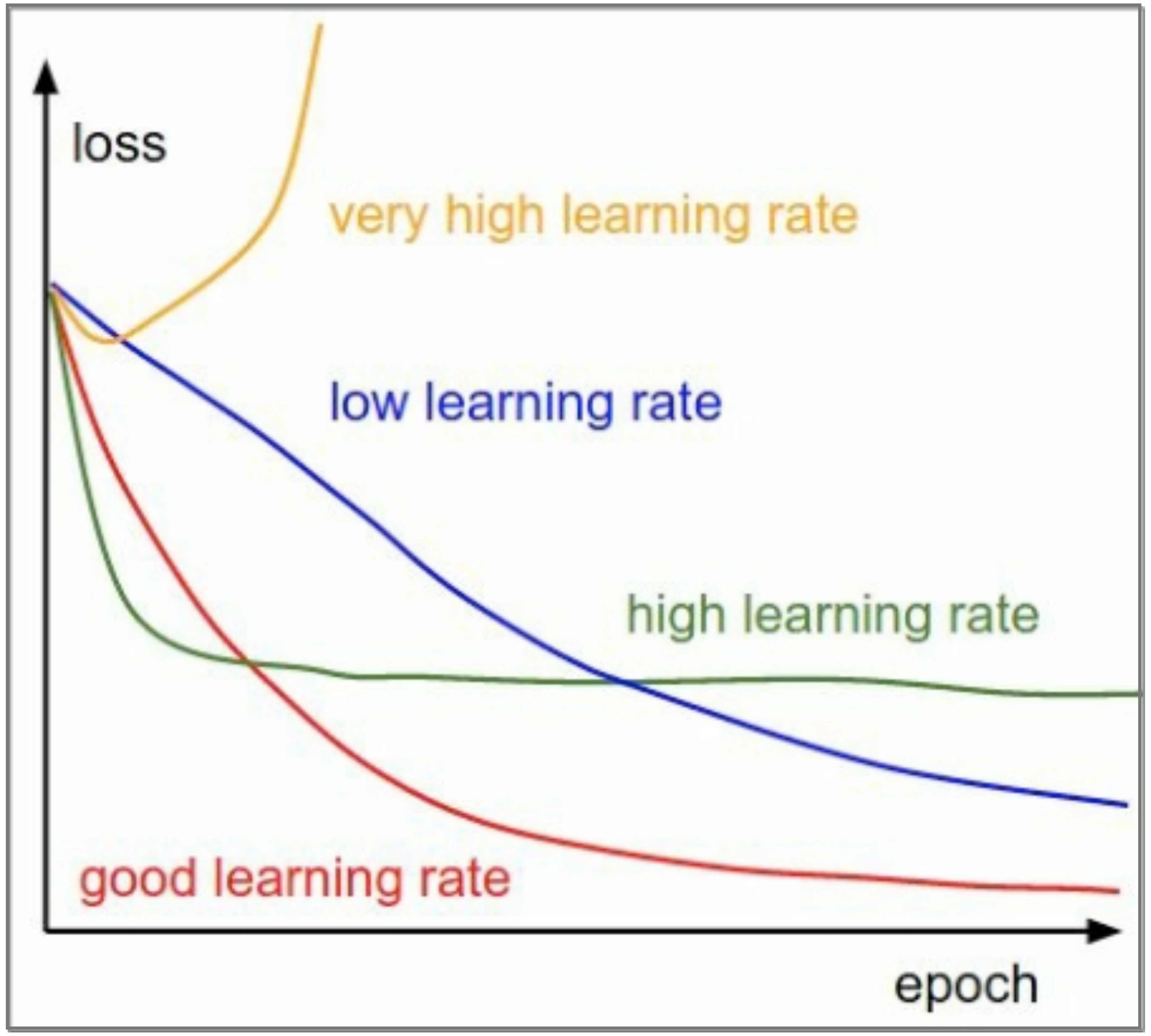
AdaGrad / RMSProp

Bias correction for the fact that first and second moment estimates start at zero

Adam with beta1 = 0.9, beta2 = 0.999, and learning_rate = 1e-3 or 5e-4 is a great starting point for many models!

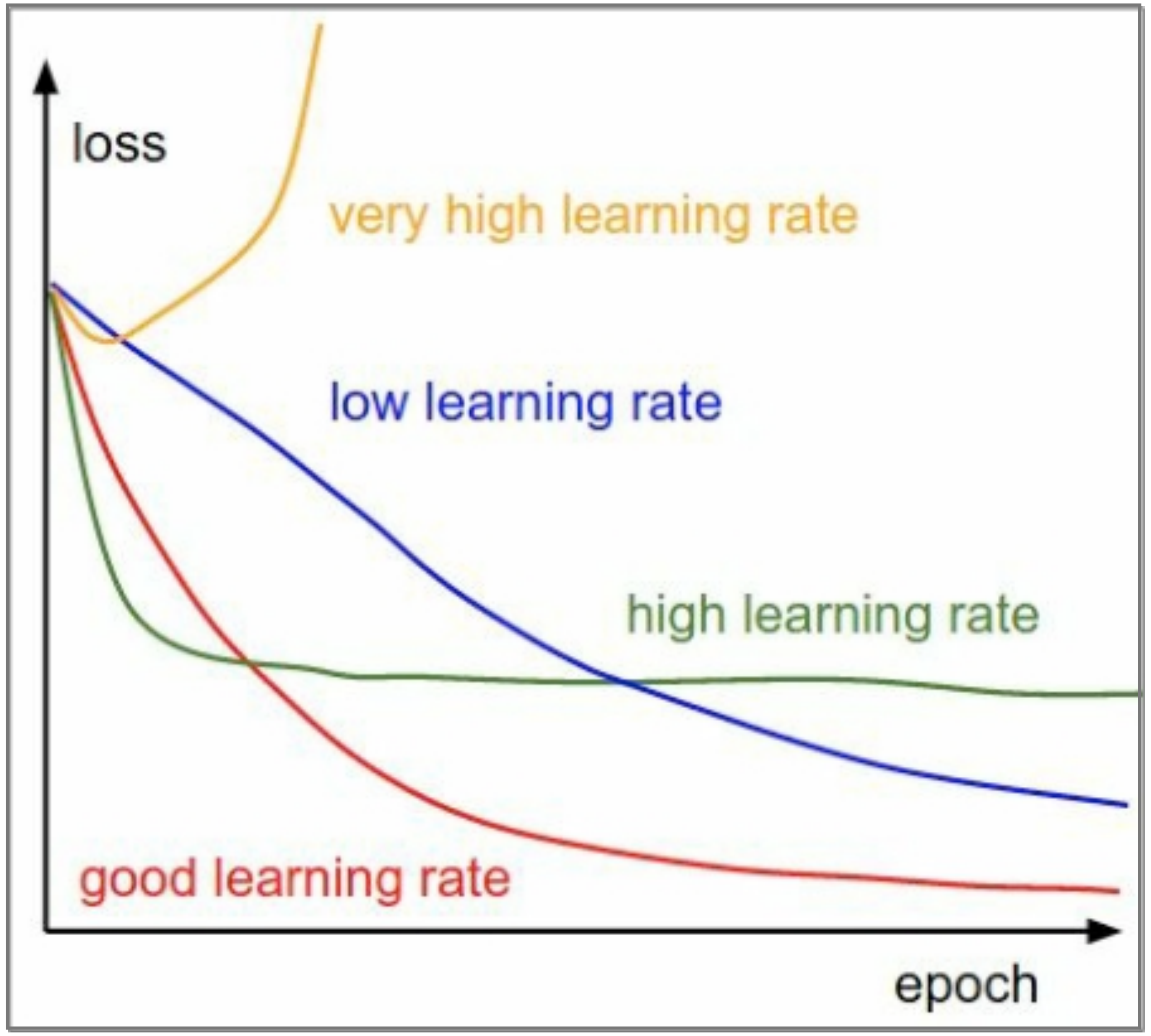
Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



Q: Which one of these learning rates is best to use?

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



=> Learning rate decay over time!

step decay:
e.g. decay learning rate by half every few epochs.

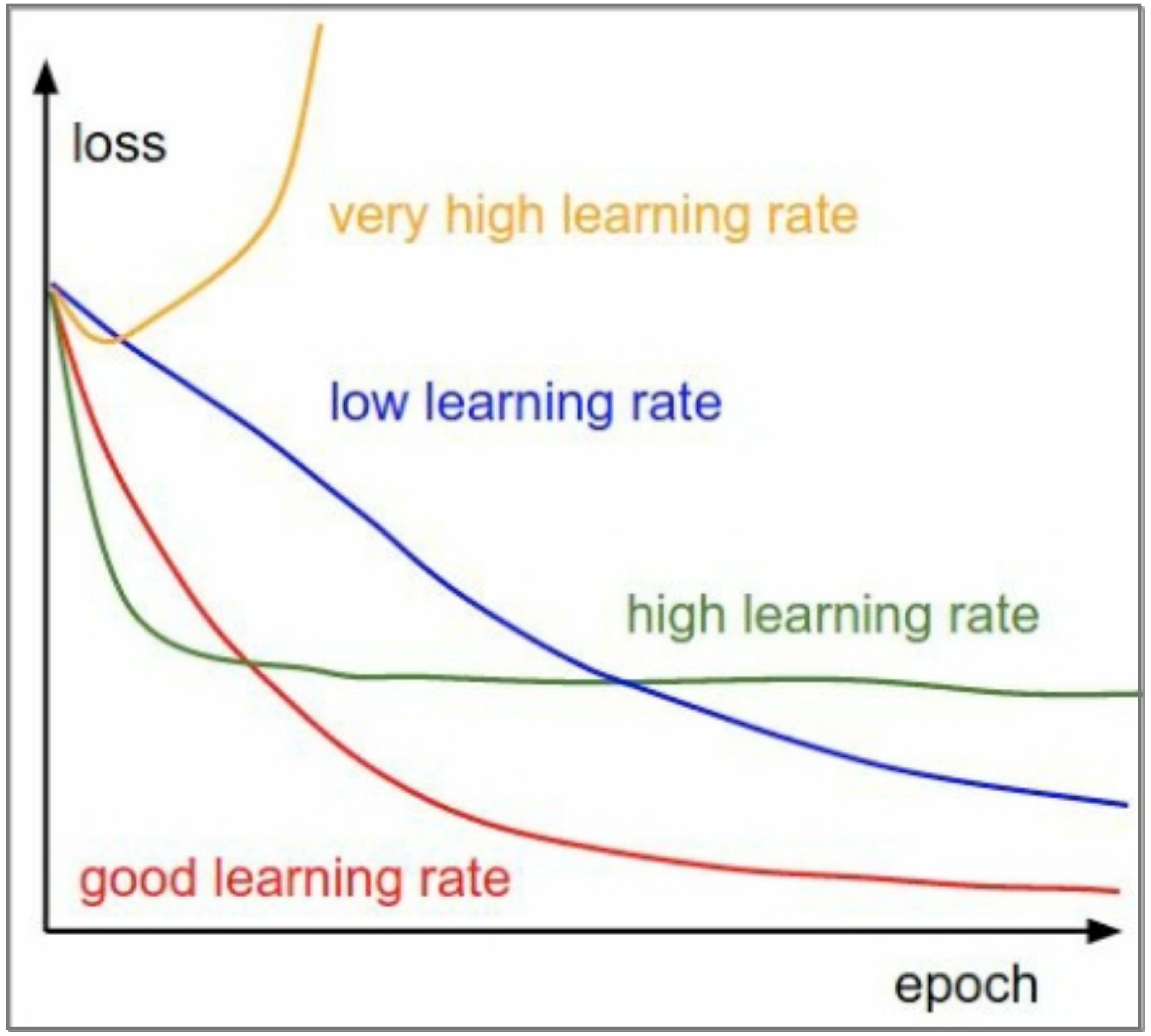
exponential decay:

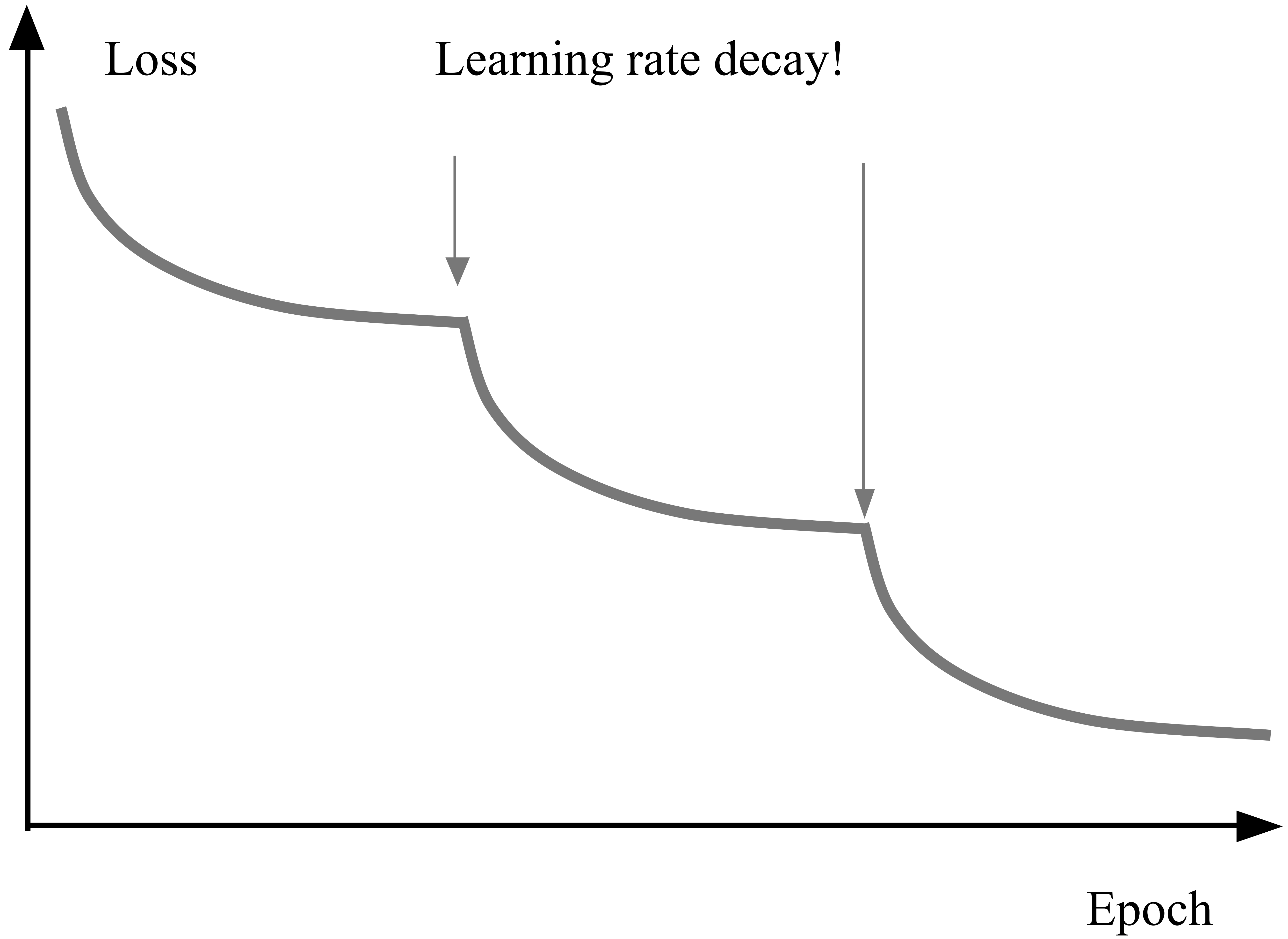
$$\alpha = \alpha_0 e^{-kt}$$

1/t decay:

$$\alpha = \alpha_0 / (1 + kt)$$

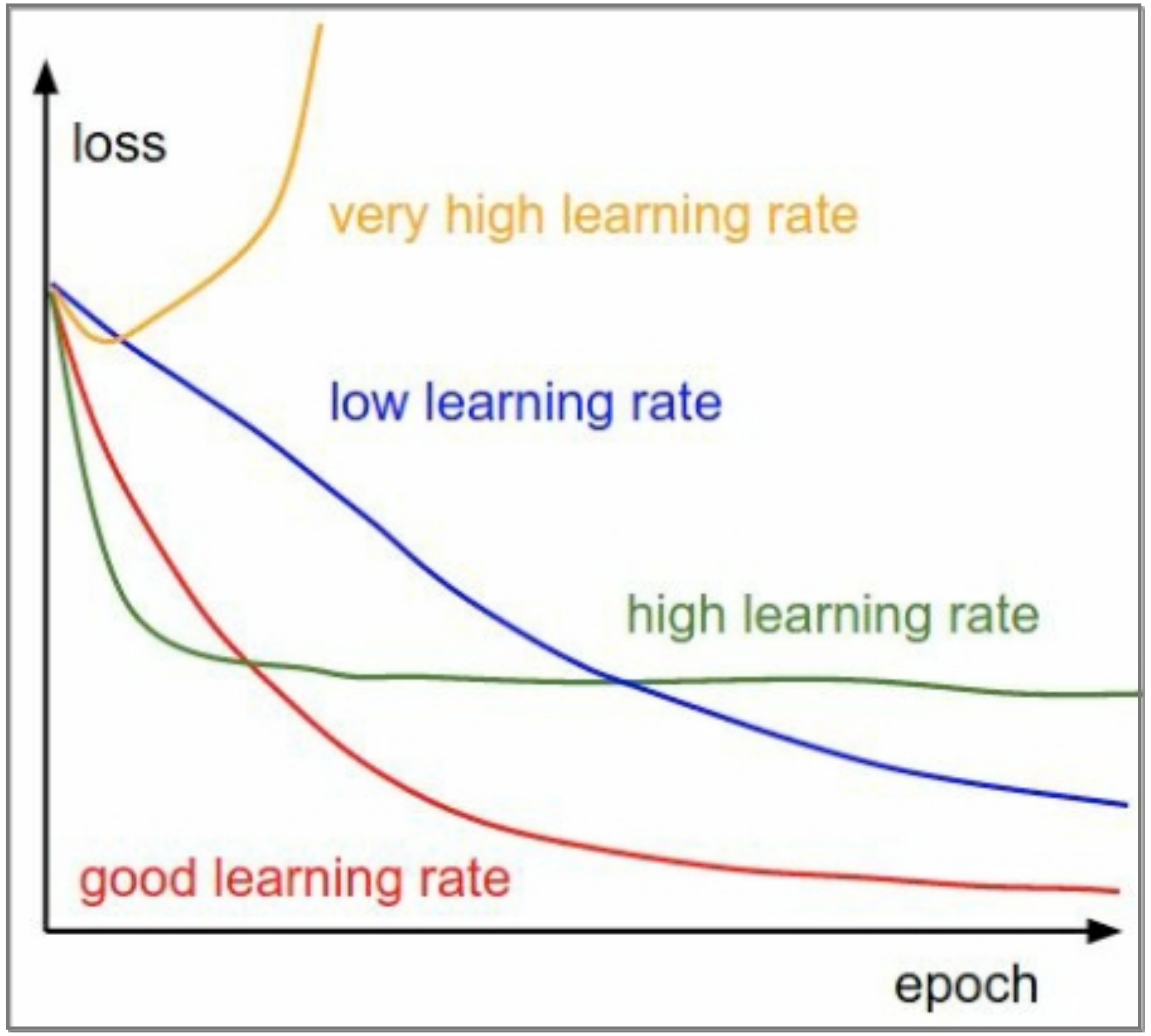
SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.

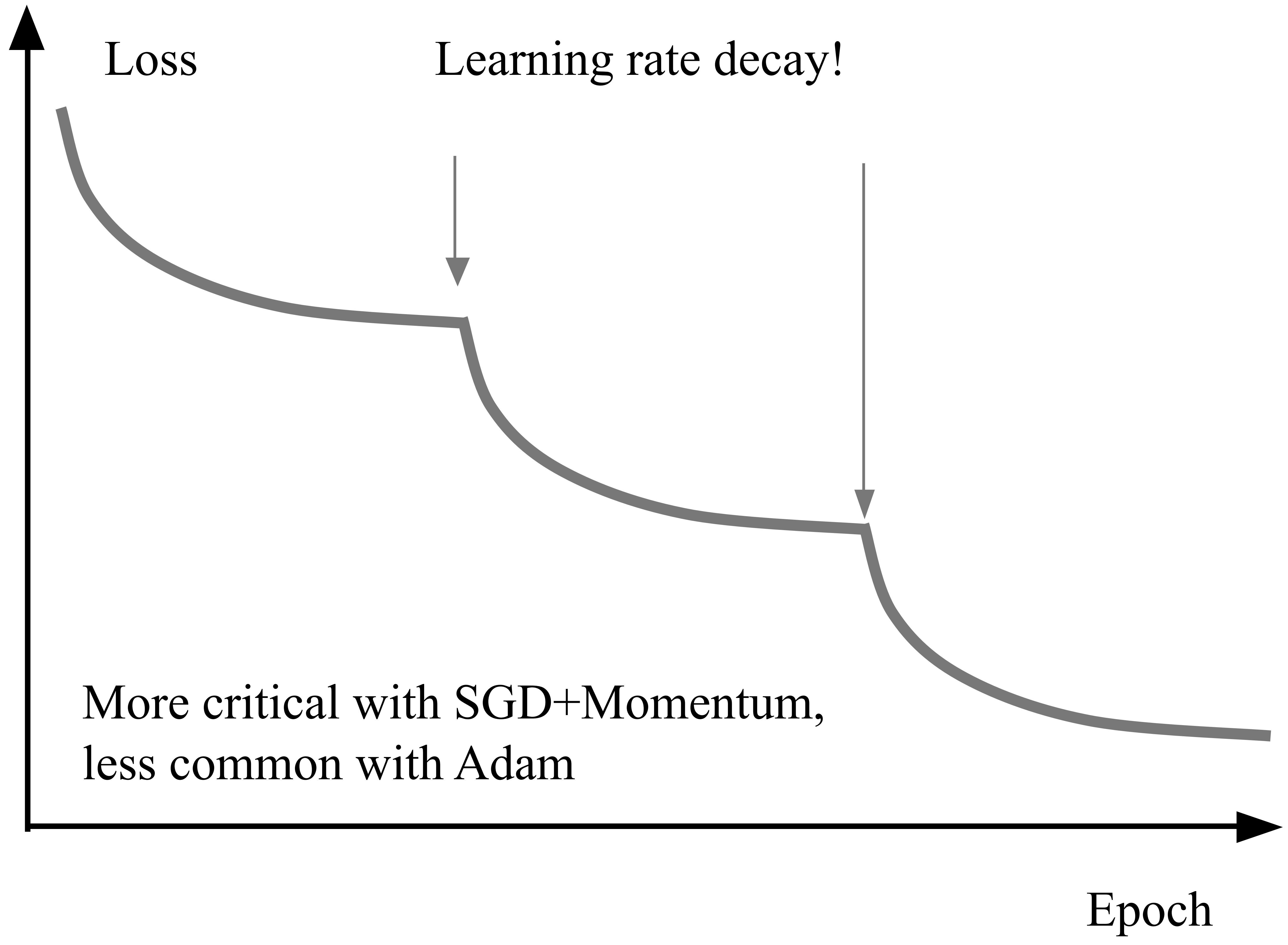




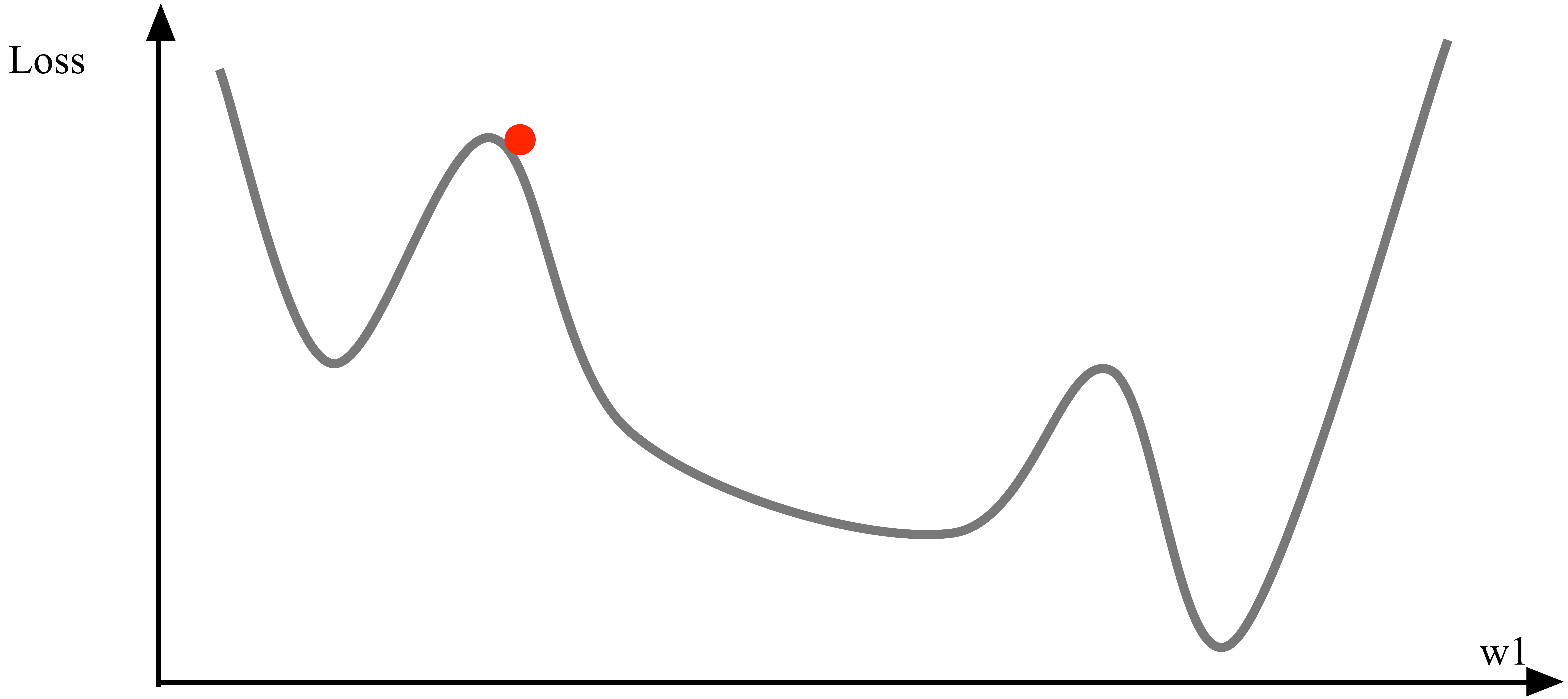
Used with permission from Justin Johnson

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



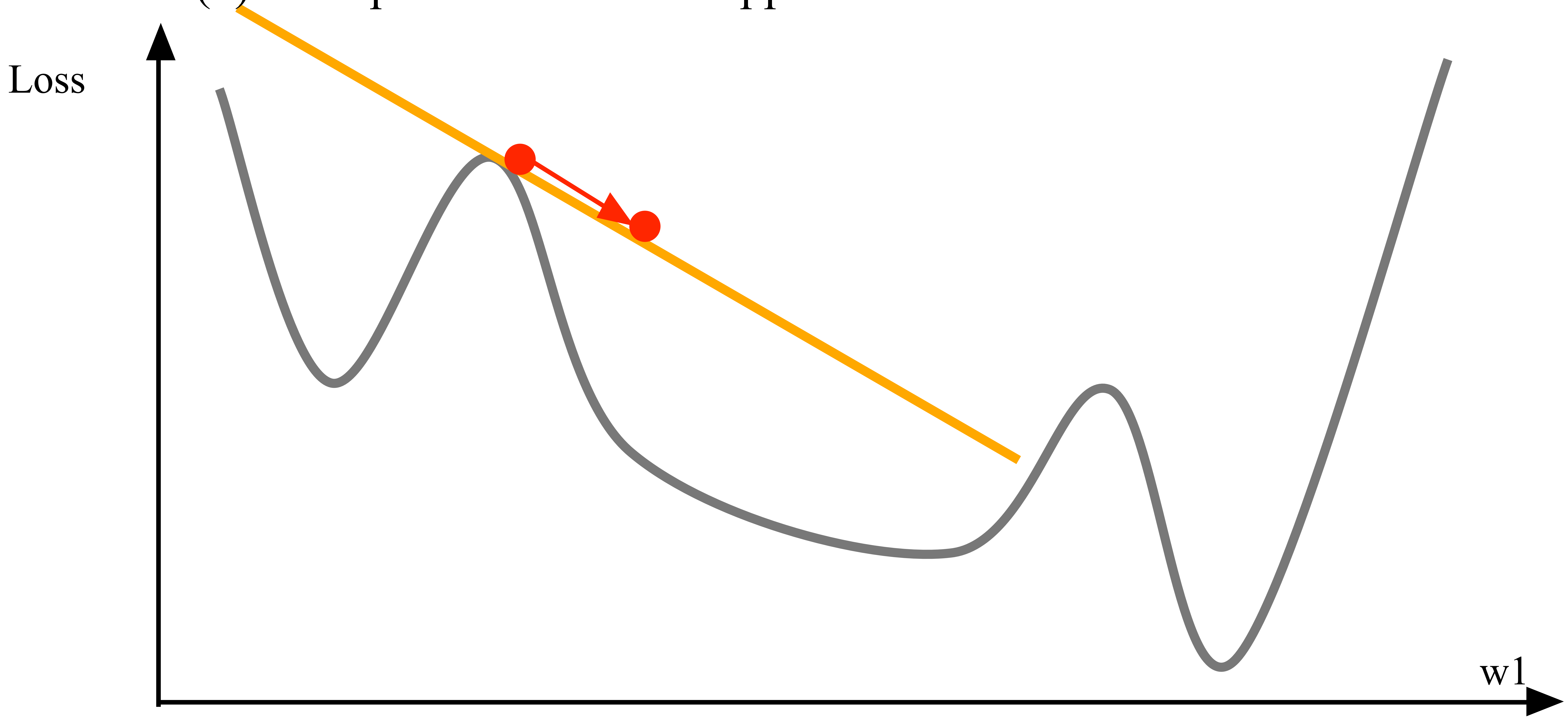


First-Order Optimization



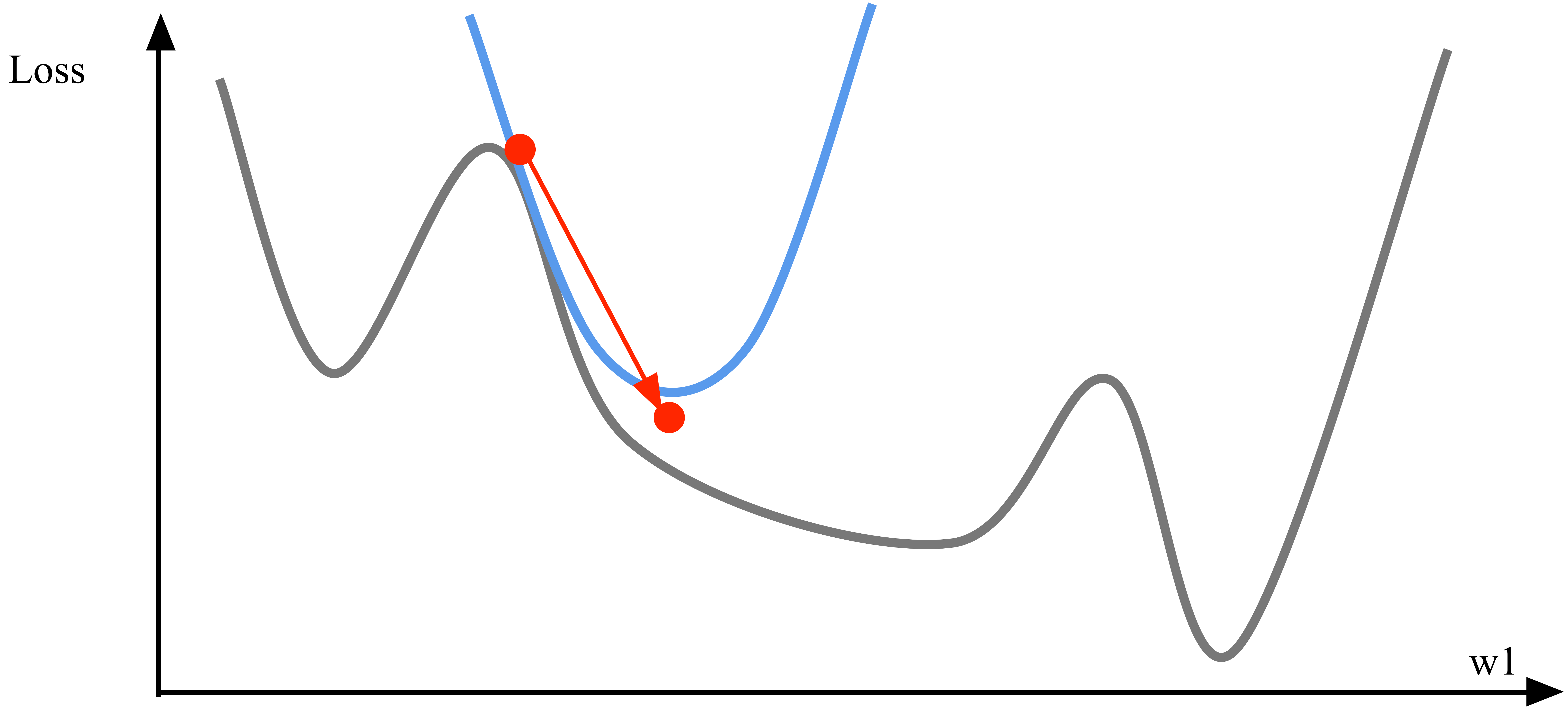
First-Order Optimization

(1) Use gradient form linear approximation
(2) Step to minimize the approximation



Second-Order Optimization

(1) Use gradient **and Hessian** to form **quadratic** approximation
(2) Step to the **minima** of the approximation



Second-Order Optimization

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Q: What is nice about this update?

Second-Order Optimization

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H} (\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

No hyperparameters!
No learning rate!
(Though you might use one in practice)

Q: What is nice about this update?

Second-Order Optimization

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Q2: Why is this bad for deep learning?

Second-Order Optimization

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Hessian has O(N^2) elements
Inverting takes O(N^3)
N = (Tens or Hundreds of) Millions

Q2: Why is this bad for deep learning?

Second-Order Optimization

$$\theta^* = \theta_0 - H^{-1} \nabla_\theta J(\theta_0)$$

- Quasi-Newton methods (**BFGS** most popular):
  instead of inverting the Hessian (O(n^3)), approximate inverse Hessian with rank 1 updates over time (O(n^2) each).

- **L-BFGS** (Limited memory BFGS):
  Does not form/store the full inverse Hessian.

L-BFGS

- **Usually works very well in full batch, deterministic mode**
  i.e. if you have a single, deterministic f(x) then L-BFGS will probably work very nicely

- **Does not transfer very well to mini-batch setting** . Gives bad results. Adapting second-order methods to large-scale, stochastic setting is an active area of research.

Le et al, "On optimization methods for deep learning, ICML 2011"
Ba et al, "Distributed second-order optimization using Kronecker-factored approximations", ICLR 2017

In practice:

- **Adam** is a good default choice in many cases
- **SGD+Momentum** with learning rate decay often outperforms Adam by a bit, but requires more tuning

- If you can afford to do full batch updates then try out **L-BFGS** (and don't forget to disable all sources of noise)