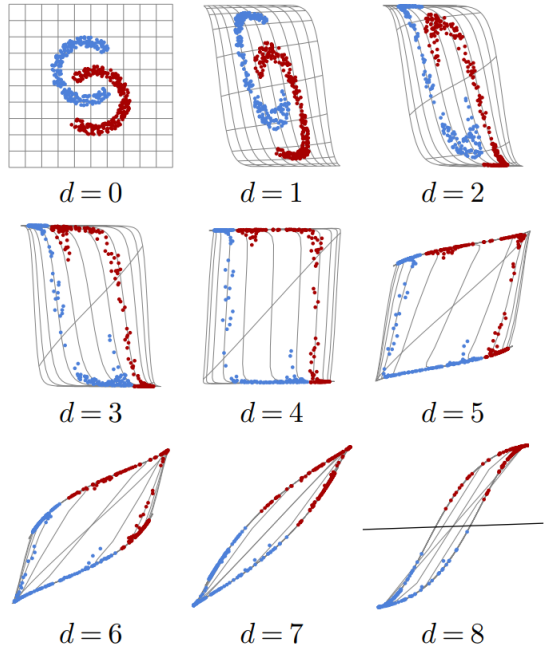
Convolutional Neural Networks

Recap: Goal of ML

generalization from optimization on training data set
(approximation of true data generating probability distribution by empirical risk minimization)

- fitting: complex function approximation
- for generalization: learning of good abstraction/representation of data/concepts

→ deep learning methods (MLP, CNN, …) optimal candidates



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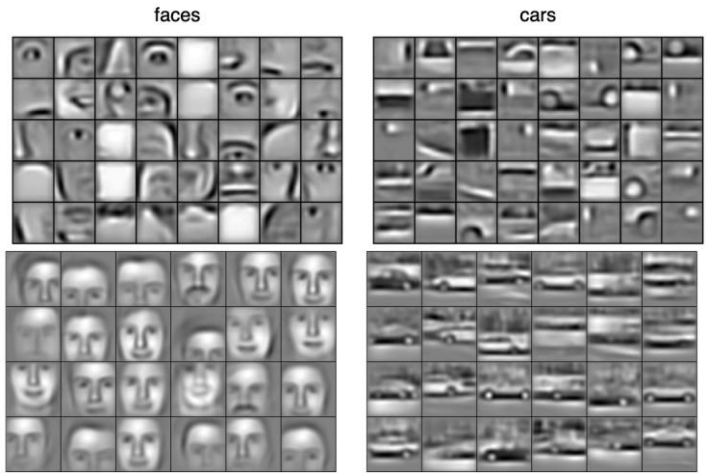
e.g., CNNs can learn hierarchical representation by means of many convolutional and pooling layers



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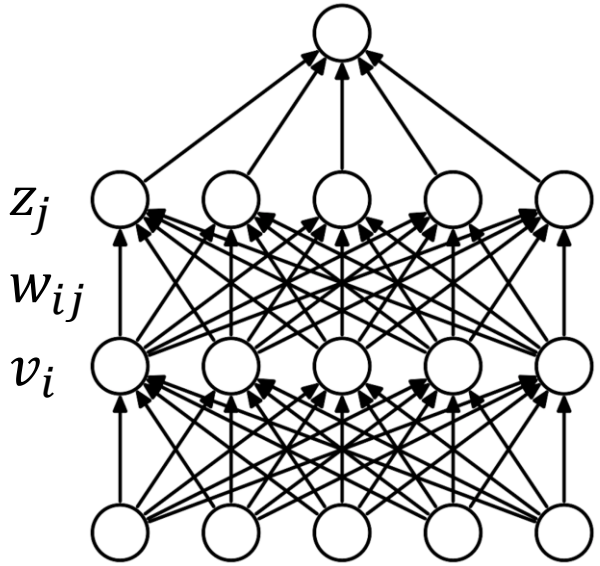
the deeper the better (accuracy, hierarchical representation)

Recap: Feed-Forward Neural Networks

computation in usual feed-forward network:

scalar input values z_j to activation function of nodes j in hidden or output layer as matrix multiplication of scalar output values v_i from activation function of nodes i from previous layer with connecting weights $w_{i,j}$

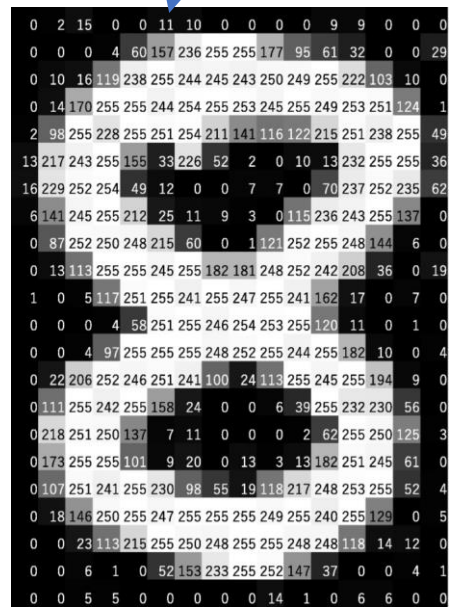
$$z_j = \sum_i v_i \, w_{i,j}$$



dropping dimension of different training observations in this view → loading full batch or mini-batches

Grid-Like Data

scalar value (like in usual feed-forward network)



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data with grid-like topology (spatial structures), e.g.:

- time-series data: 1-D grid of data taken at regular time intervals (can also be done with recurrent neural networks or transformers)
- image data: 2-D grid of pixels (→ computer vision)

convolutional networks:

neural networks using convolutions with kernels (local groups of values, e.g., pixels from an object, highly correlated) in place of general matrix multiplications in at least one of their layers

→ highly regularized feed-forward networks

Convolution Operation

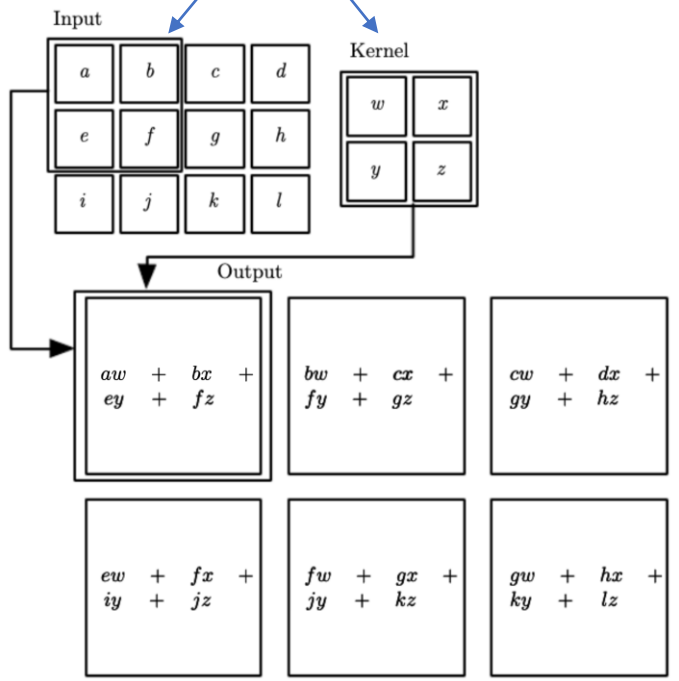
learned parameters:

- connection to **local patches** of previous layer's feature maps
- shared over entire image (common learning across image)

to be exact, usually rather cross-correlation instead of convolution operation (what would have – here):

$$Z_{i,j} = (K * V)_{i,j} = \sum_{m,n} V_{i+m,j+n}\, K_{m,n}$$

feature map — input (matrix) — kernel (matrix)



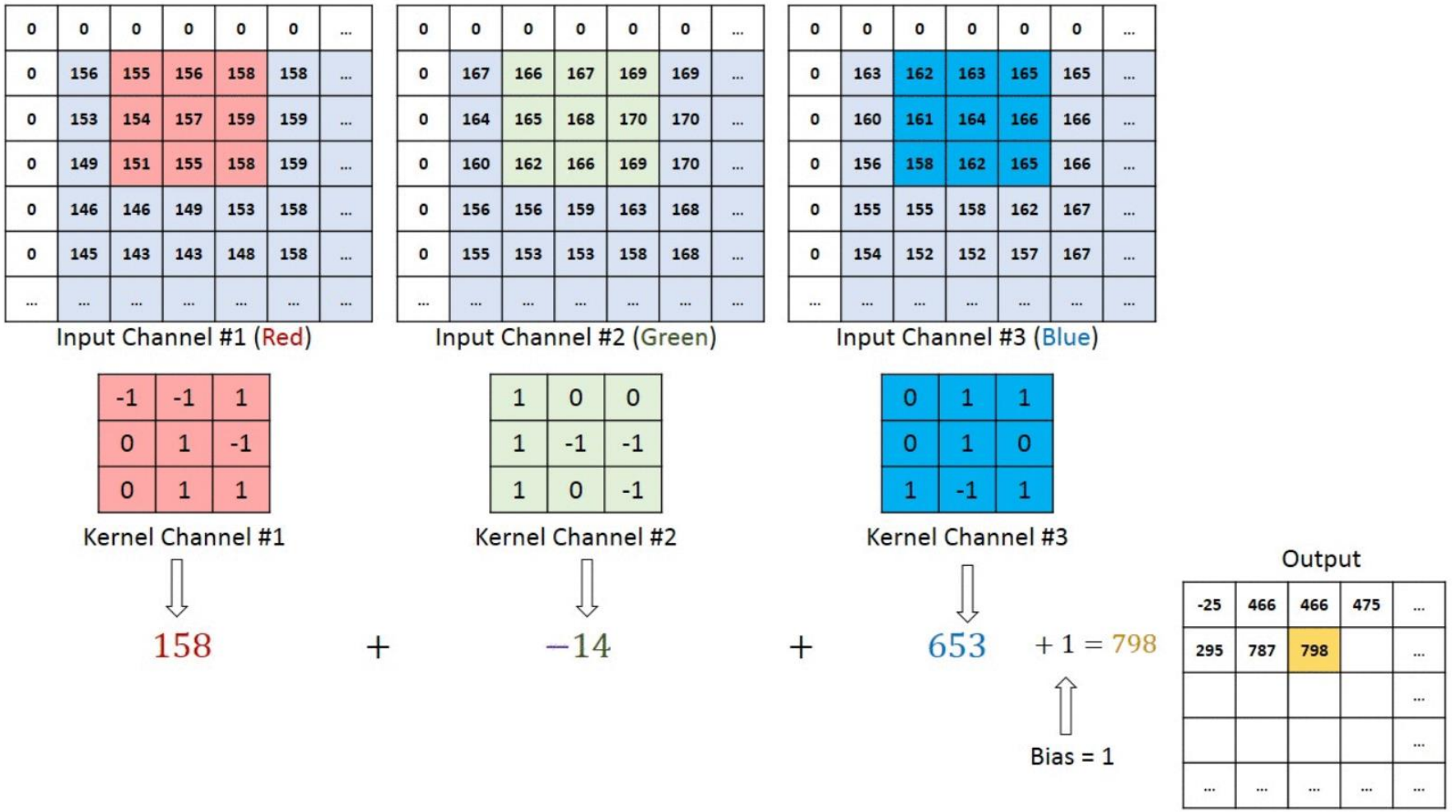
translation source

again, dropping dimension of different training observations

matrices → tensors: several input channels c (e.g., RGB) and several output channels f (different feature maps, e.g., vertical edge, nose, ear, …)

$$Z_{f,i,j} = \sum_{c,m,n} V_{c,i+m,j+n}\, K_{f,c,m,n}$$

Channel Mixing



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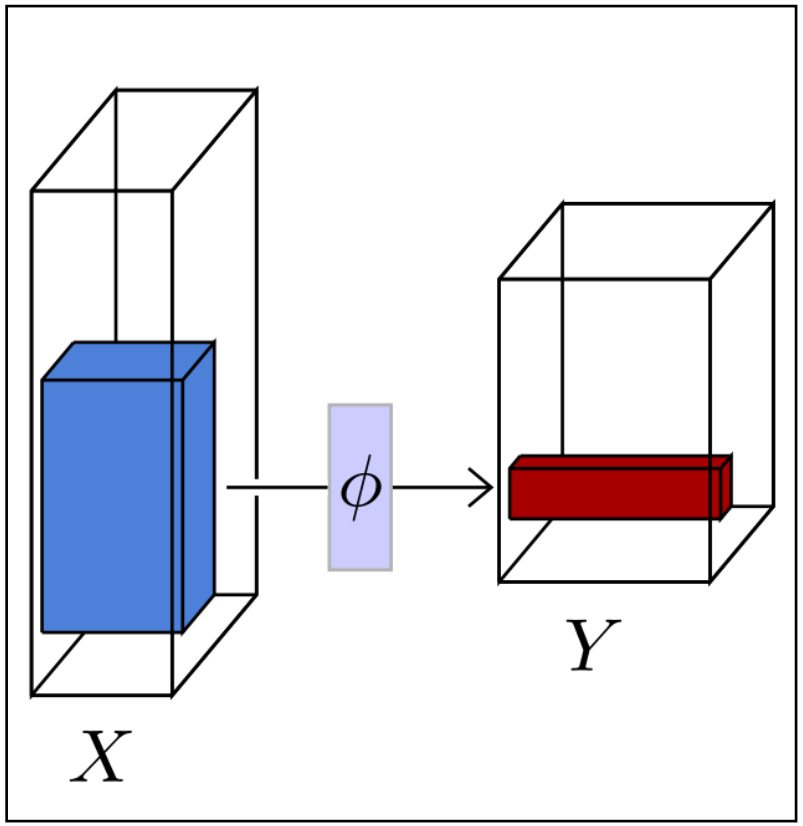
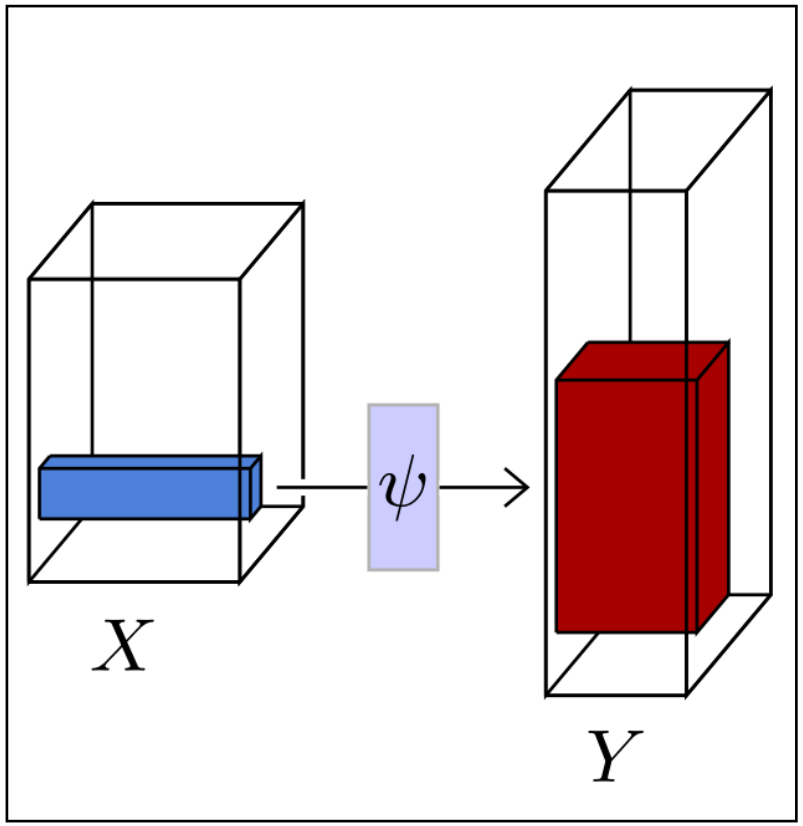
Decrease or Increase Dimensionality

typical use cases discussed here



2D convolution



2D transposed convolution

e.g., decoder side of autoencoders or U-nets in diffusion models

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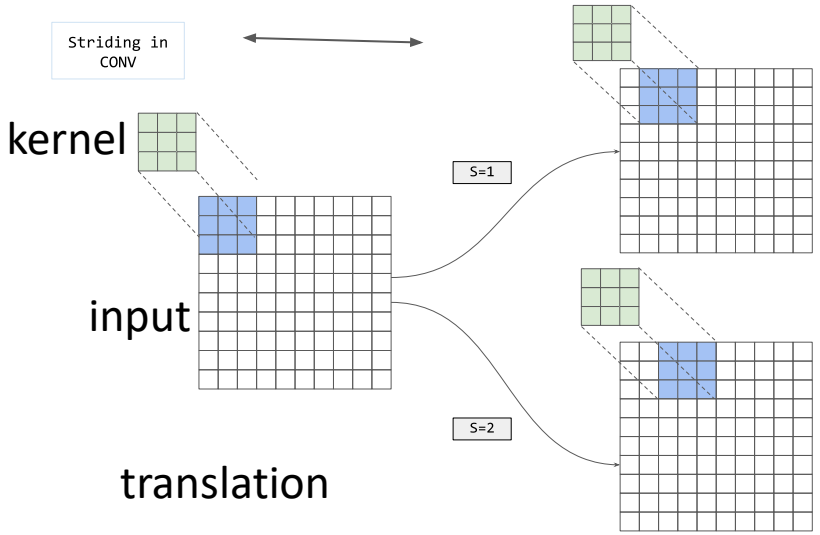
Important Details: Striding and Padding

need to define how to stride over image

$$Z_{f,i,j} = \sum_{c,m,n} V_{c,i\times s+m,j\times s+n}\, K_{f,c,m,n}$$

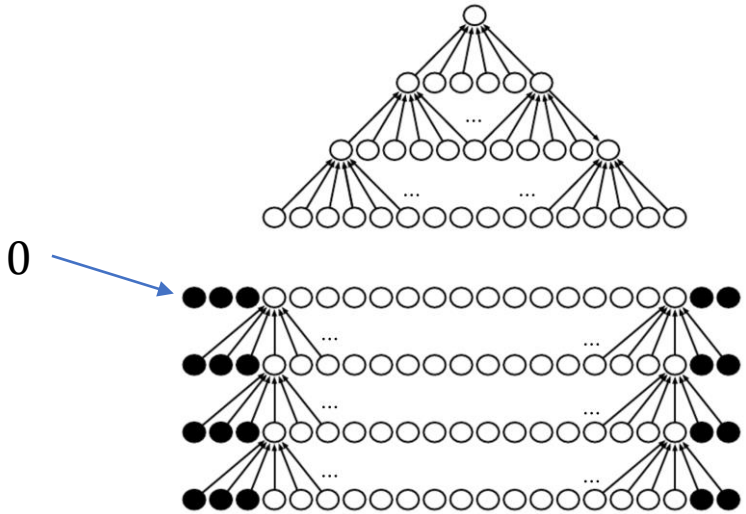
$s > 1$ corresponds to down-sampling

→ fewer nodes after convolutional layer



zero-padding of input to make it wider:

otherwise shrinking of represenation with each layer (depending on kernel size) → allowing large kernels and slow shrinkage



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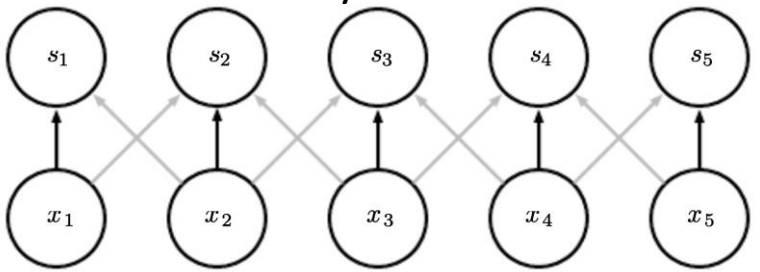
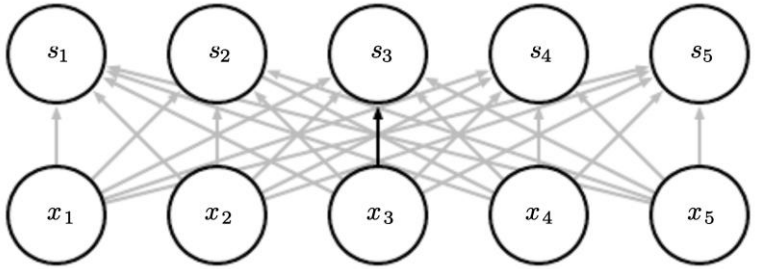
Regularization Effects

- sparse interactions: much less weights
- parameter sharing: use same weights for different connections

convolutional layer:



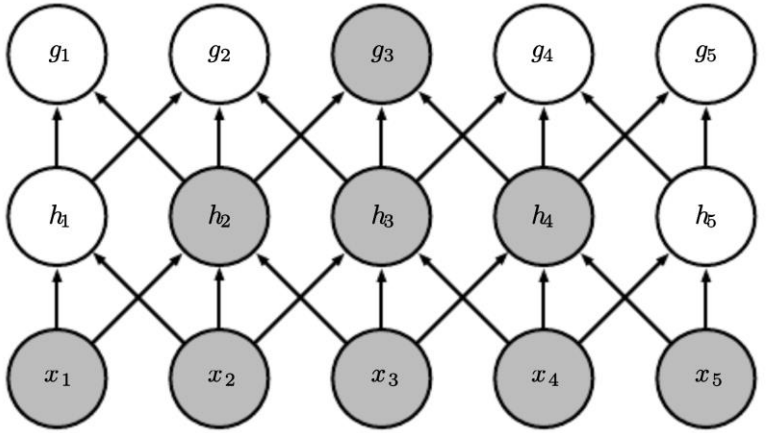
fully-connected layer:



effect of receptive field over several layers:

- consider only locally restricted number of input values from previous layer
- grows for earlier layers (indirect interactions)

→ hierarchical patterns from simple building blocks (many aspects of nature hierarchical)



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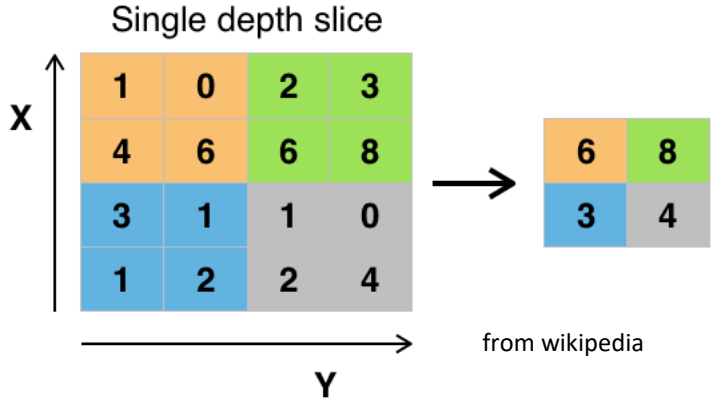
Another Ingredient: Pooling

replacing outputs of neighboring nodes with summary statistic (e.g., maximum or average value of nodes)

→ non-linear down-sampling (regularization)

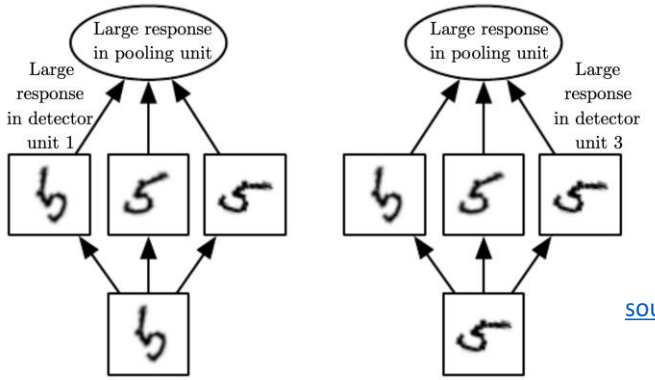
max pooling:



pooling is translation invariant: no interest in exact position of, e.g., maximum value

pooling over features learned by separate kernels (cross-channel pooling) can also learn other transformation invariances, like rotation or scale

(convolutions can detect same translated motif across entire image, but not rotated or scaled versions of it)



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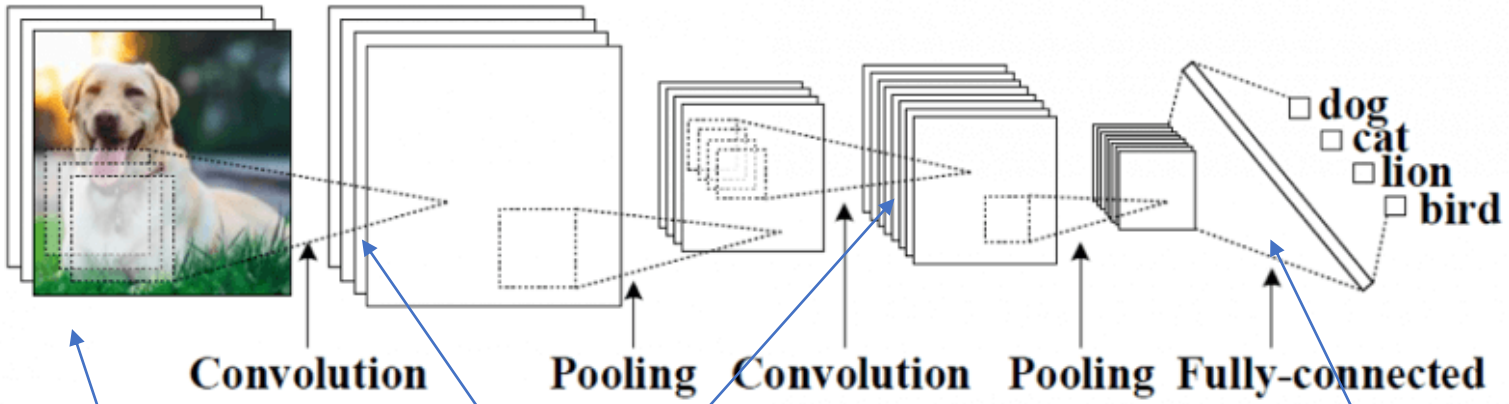
Putting It All Together

CNN in short:
local connections, shared weights, pooling, many layers

kernels

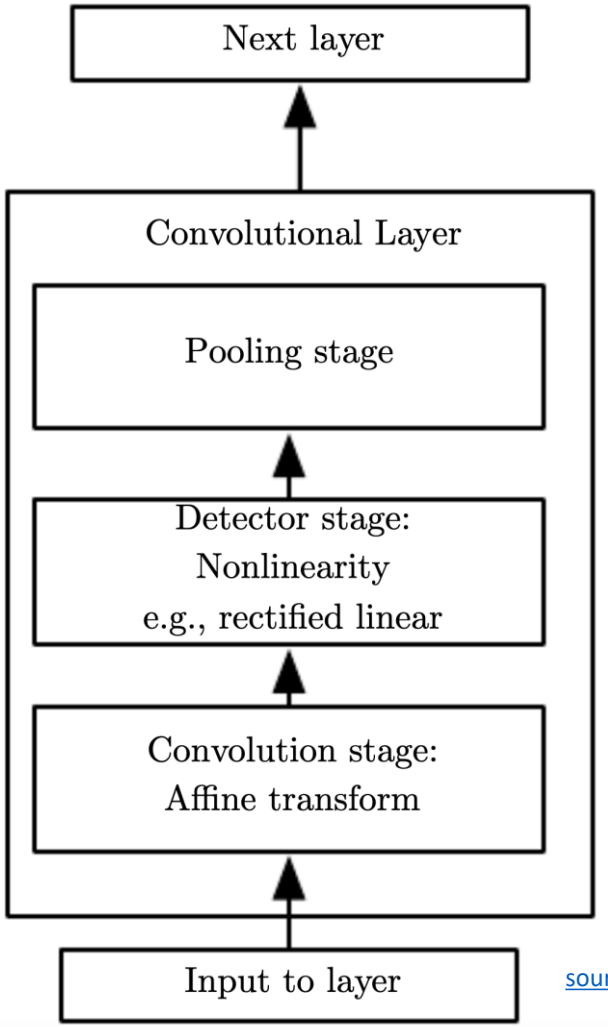


many images (training examples), potentially with several channels

several kernels producing several feature maps

down-sampling by convolutions and pooling

flatten dimensions for final classification or regression



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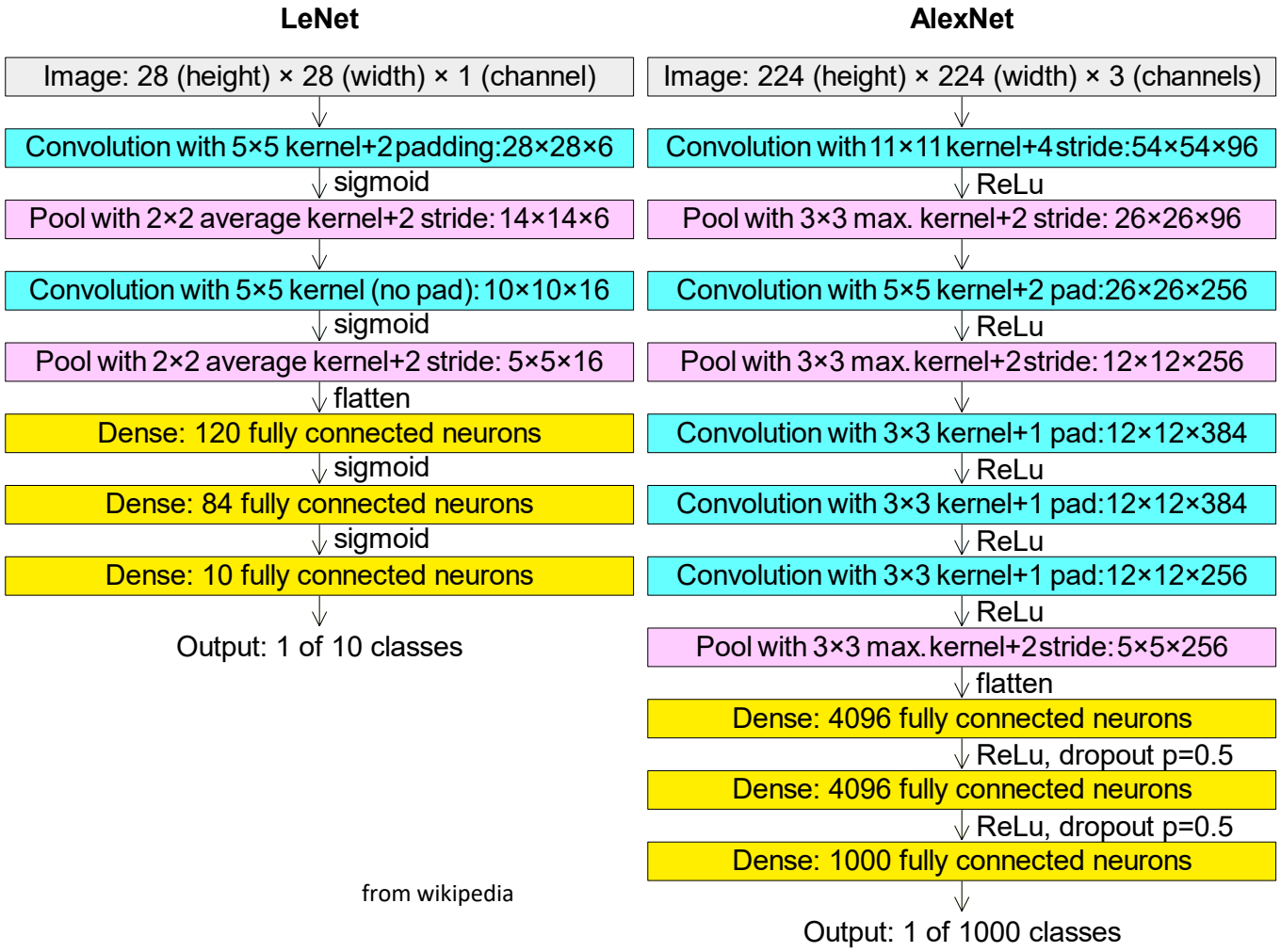
Going Deeper



from wikipedia

AlexNet finally started the deep learning hype.

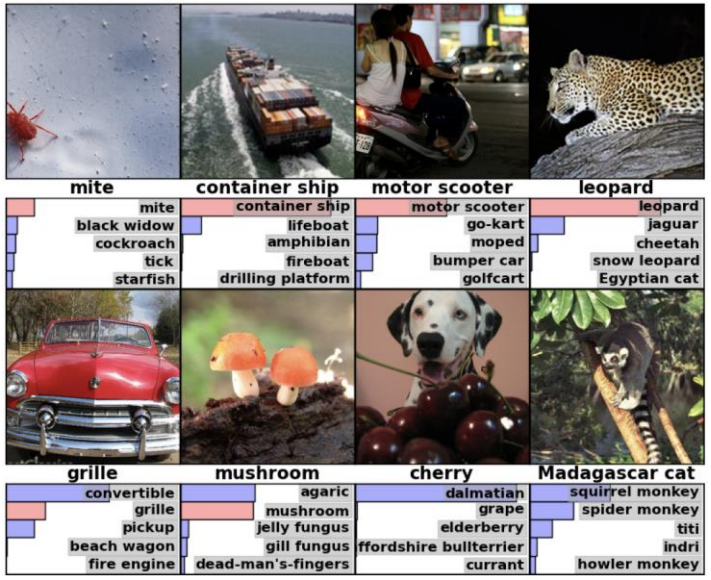
(winning the ImageNet challenge in 2012)

Rise of Deep Learning

a little bit oversimplified:

deep learning = lots of training data + parallel computation + smart algorithms

AlexNet: ImageNet (with data augmentation) + GPUs + ReLU, dropout, SGD



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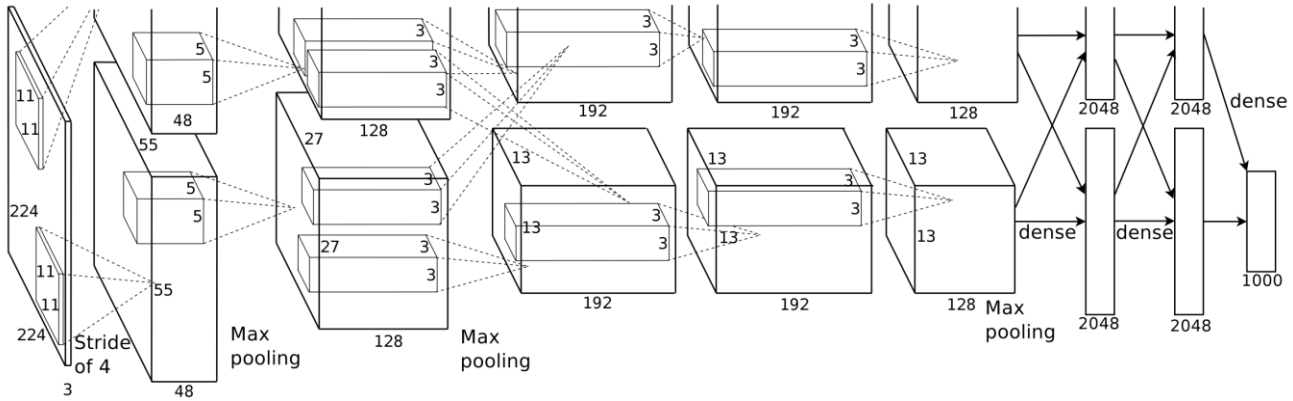
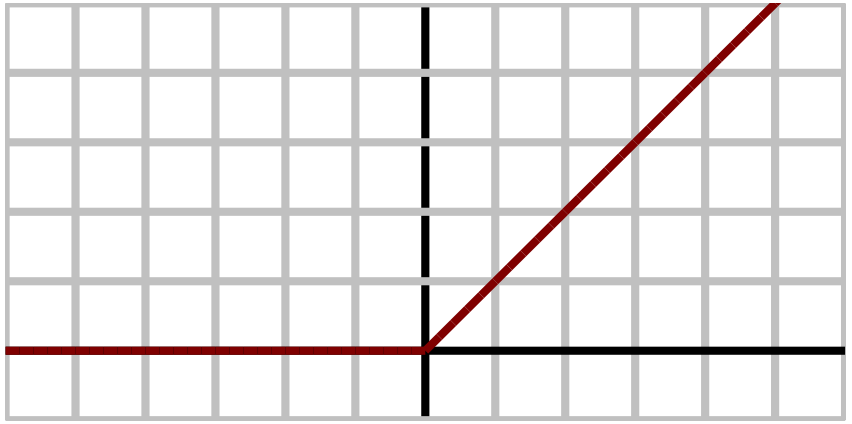


Rectified Linear Unit (ReLU)



reminder: activation function non-linear transformation of summed weighted input of a node (linear), output to be used as input for nodes of subsequent layer

needs to be differentiable for back-propagation (ReLU at 0 no issue, just set to 0 or 1)

neural network model with ReLU activation can be interpreted as exponential number of linear models that share parameters

main advantages (leading to enablement of deeper networks by better optimization):

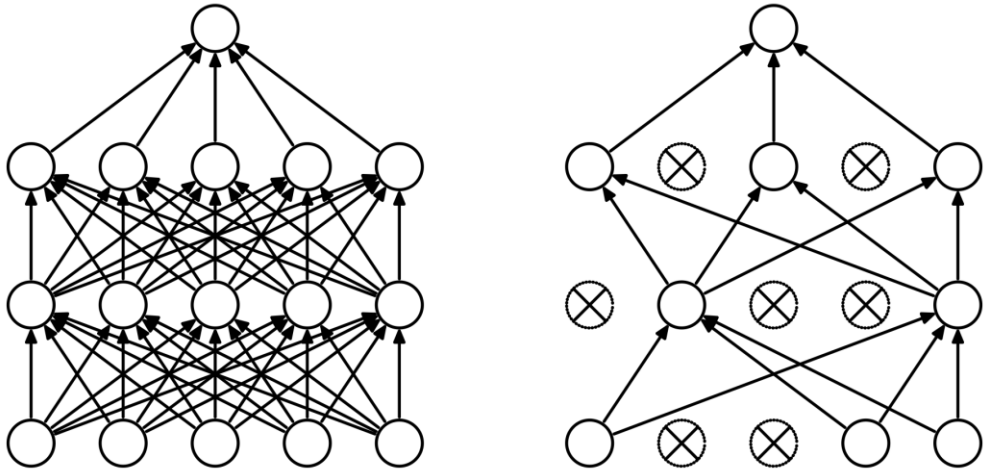
- unlike sigmoid or $\tanh$ (predominantly used before) activation, no issue with vanishing gradients from saturation effects
- very efficient computation: constant gradients of 0 and 1 below and above input of zero
- sparse activation: many hidden nodes deactivated (output 0) → information disentangling

Dropout in Neural Networks

goal: prevent overfitting of large neural networks

idea: randomly drop non-output nodes (along with their connections) during training (not prediction)

→ adaptability: regularizing each hidden node to perform well regardless of which other hidden nodes are in the model



(a) Standard Neural Net (b) After applying dropout.

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- for each mini-batch, randomly sample independent binary masks for the nodes
- much less computation than bagging (training many different neural networks)
- destroying extracted features rather than input values

dropout for 2D structures, such as images, usually drops entire channels instead of individual nodes (because locality nullifies the effect of standard dropout → neighboring nodes step in)

Inductive Bias (aka Learning Bias)

set of assumptions that a learning algorithm uses to predict outputs of inputs that it has not encountered during training

examples: linear response (linear regression), maximum margin (SVM), nearest neighbors (kNN), spatial structure (CNN)

but also: different regularization and optimization methods

crucial piece of generalization

data in disguise (replacement for missing information on specific situations in limited training data sets)

No Free Lunch Theorem

All optimization/ML algorithms (both sophisticated and simple ones) perform equally well when their performance is averaged across all possible problems.

(But deep learning is trying to solve many problems with very general-purpose forms of regularization.)

Particularly, model complexity doesn't reflect if inductive bias is appropriate for problem at hand.

→ choose right ML method for learning task at hand

Object Detection and Image Segmentation

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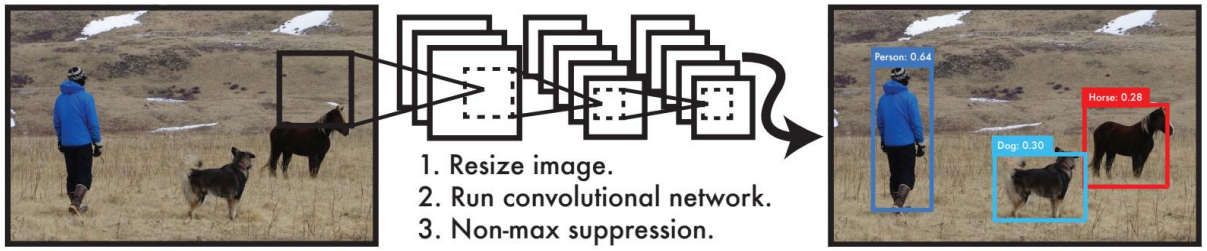
coding example: object detection and image segmentation with YOLO

see also image and video segmentation with Segment Anything Model (SAM, SAM 2)

You Only Look Once (YOLO)



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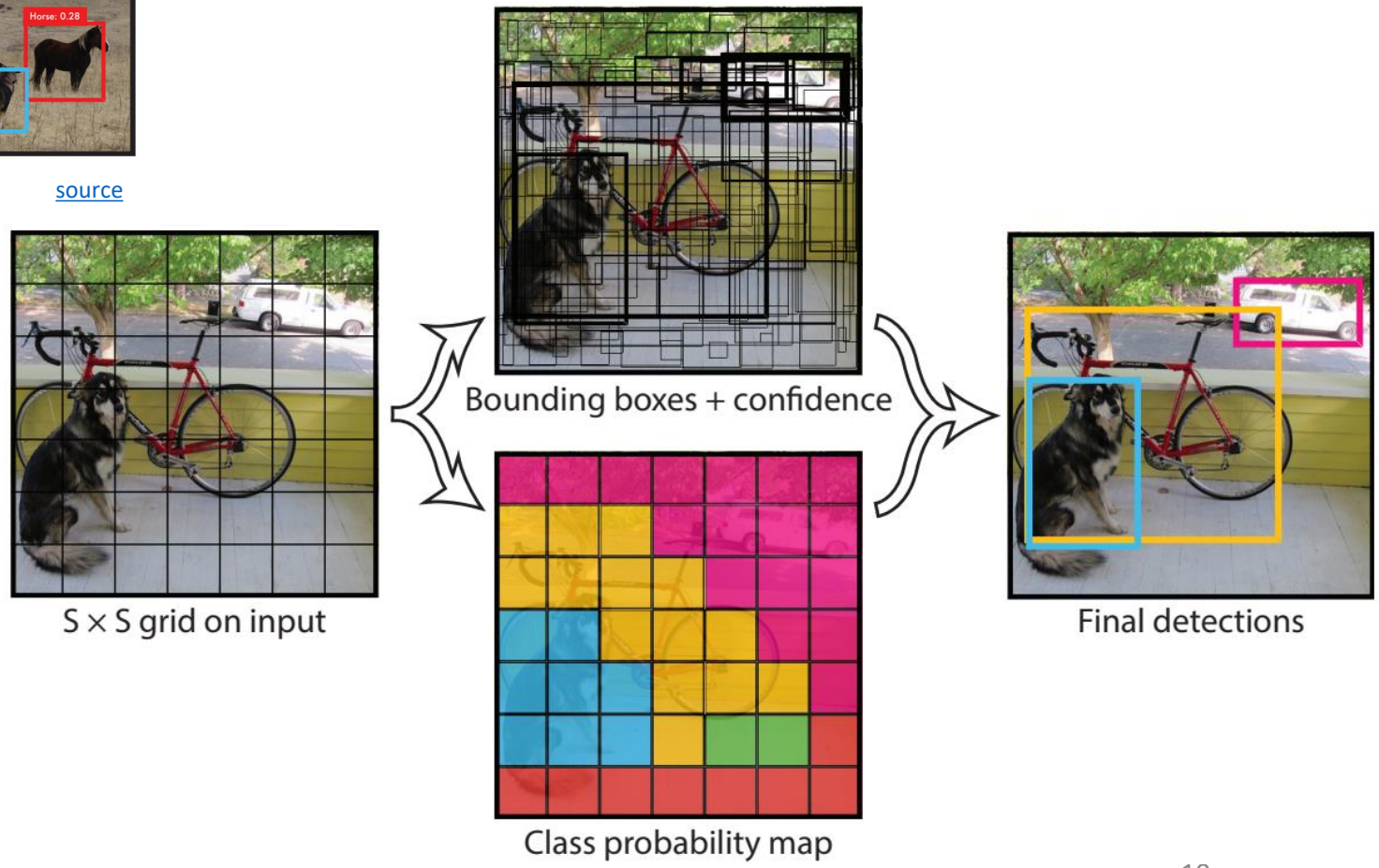
prediction of bounding boxes and class probabilities in one go:
partition image into grid and label each



Assignments

- handwritten digit classification: Kaggle Digit Recognizer

(build PyTorch CNN)

- image classification: Kaggle Intel Image Classification

(fine-tune a torchvision model, e.g., AlexNet)