Convolutional Neural Networks

Recap: Goal of ML

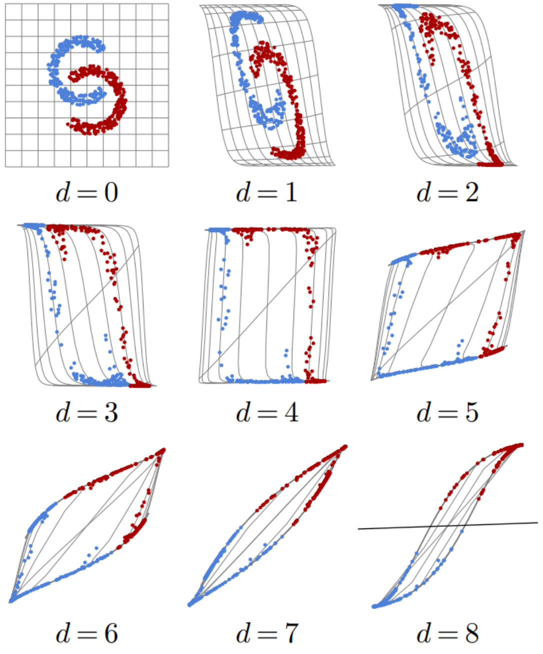
generalization from optimization on training data set (approximation of true data generating probability distribution by empirical risk minimization)

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

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

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

the deeper the better (accuracy, hierarchical representation)



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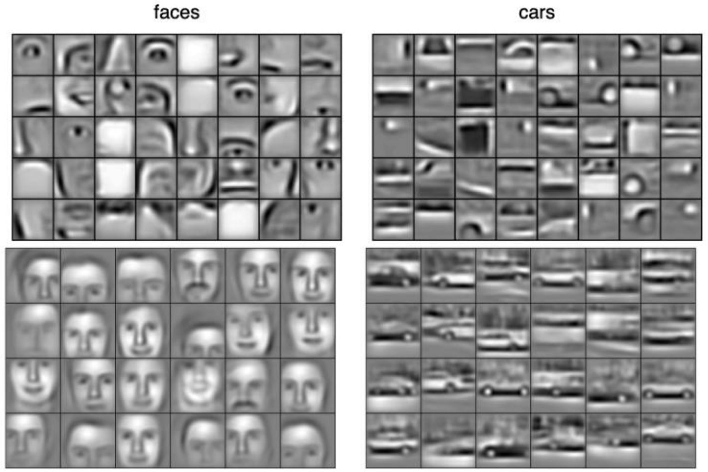

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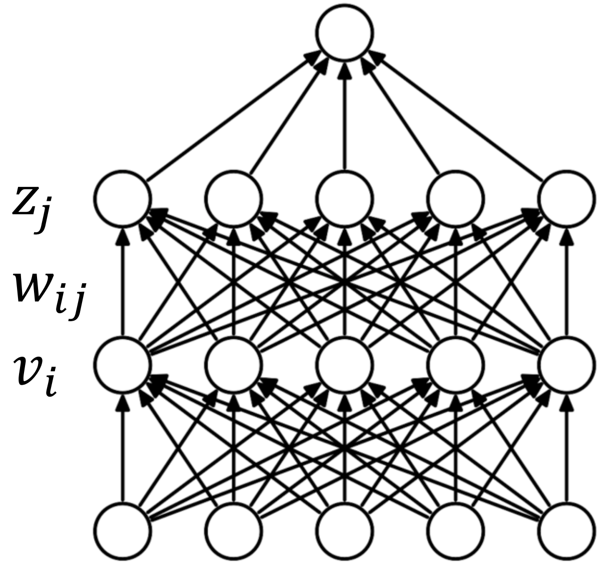
Recap: Feed-Forward Neural Networks

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

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

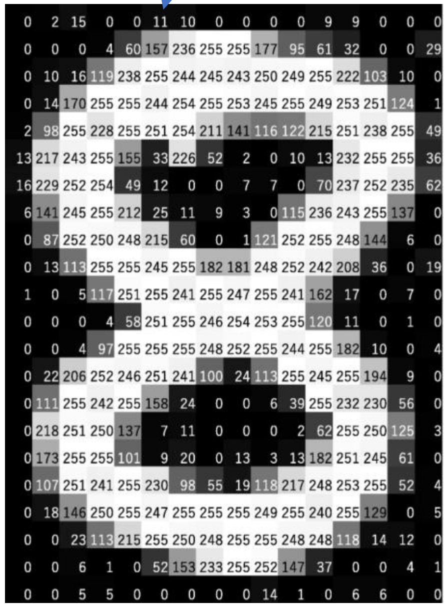
- time-series data: 1-D grid of data taken at regular time intervals (can also be done with recurrent neural networks or transformers)
- image data: 2-D grid of pixels (→ computer vision)

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

scalar value (like in usual feed-forward network)



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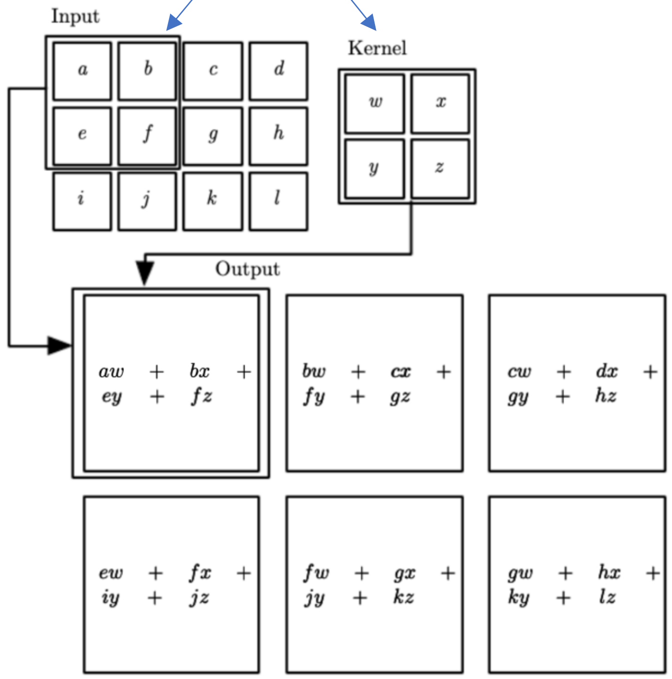
Convolution Operation

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

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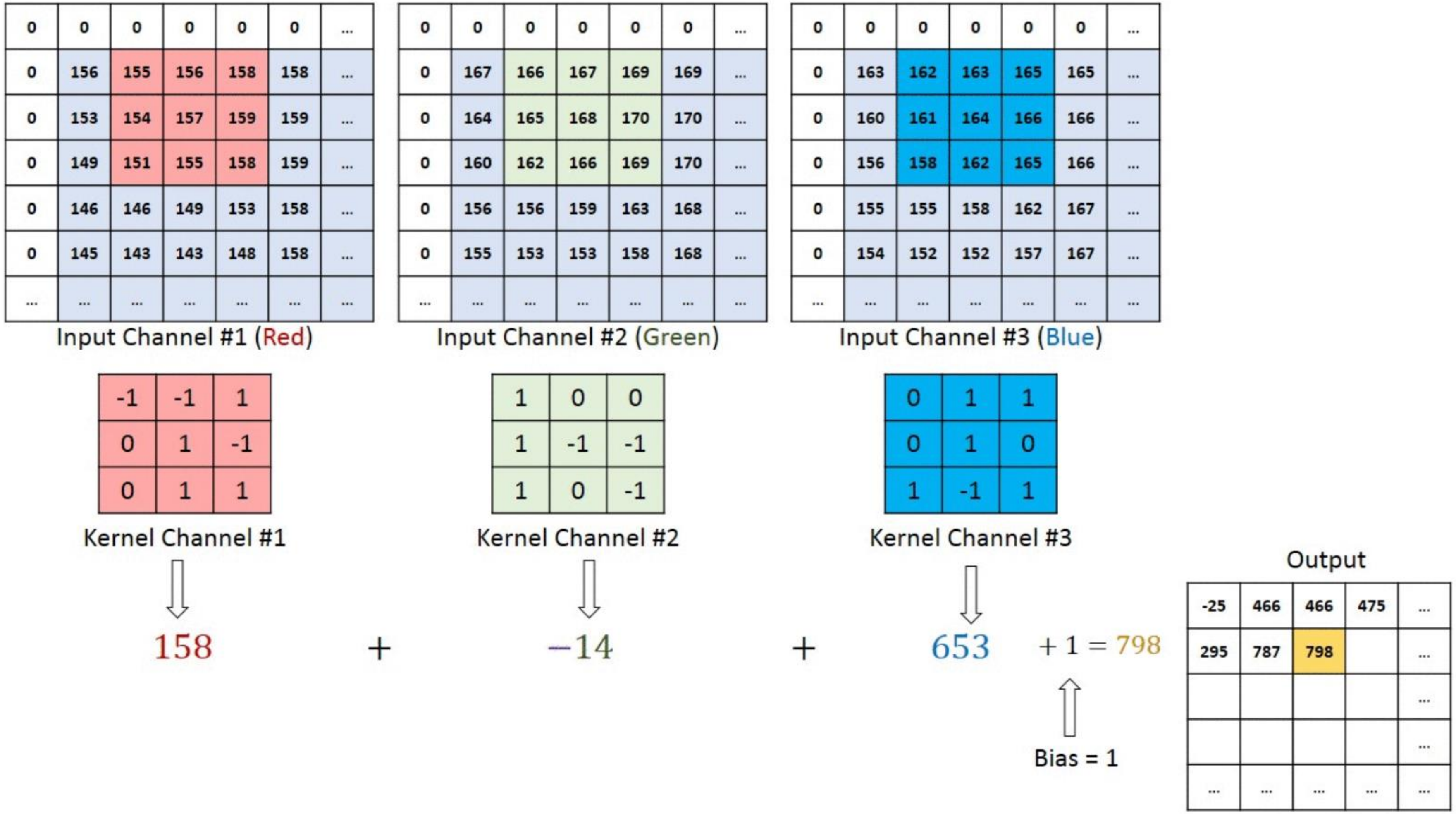
again, dropping dimension of different training observations

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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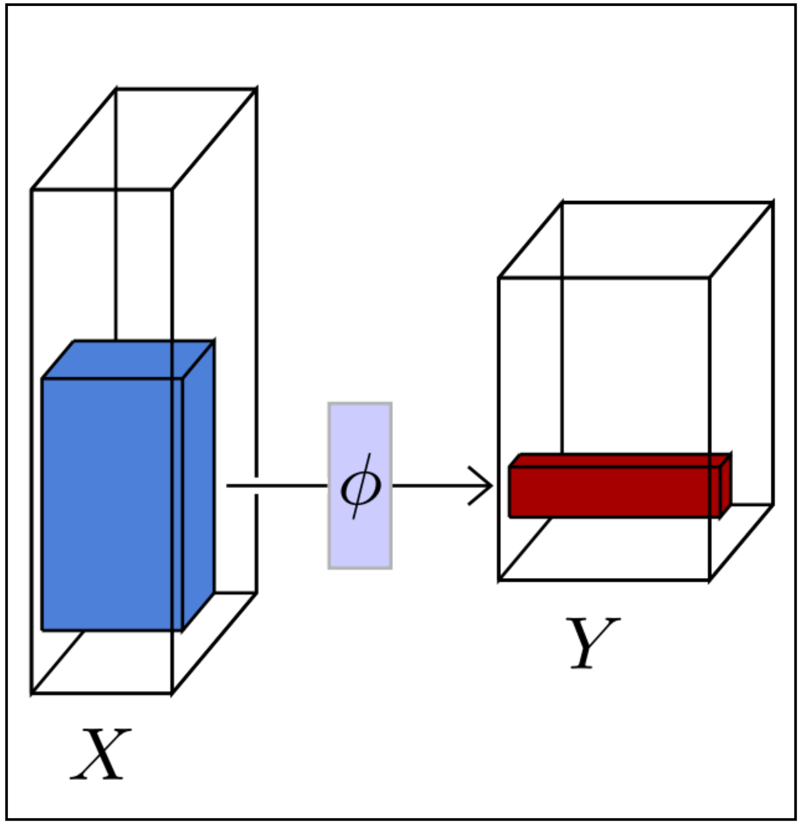
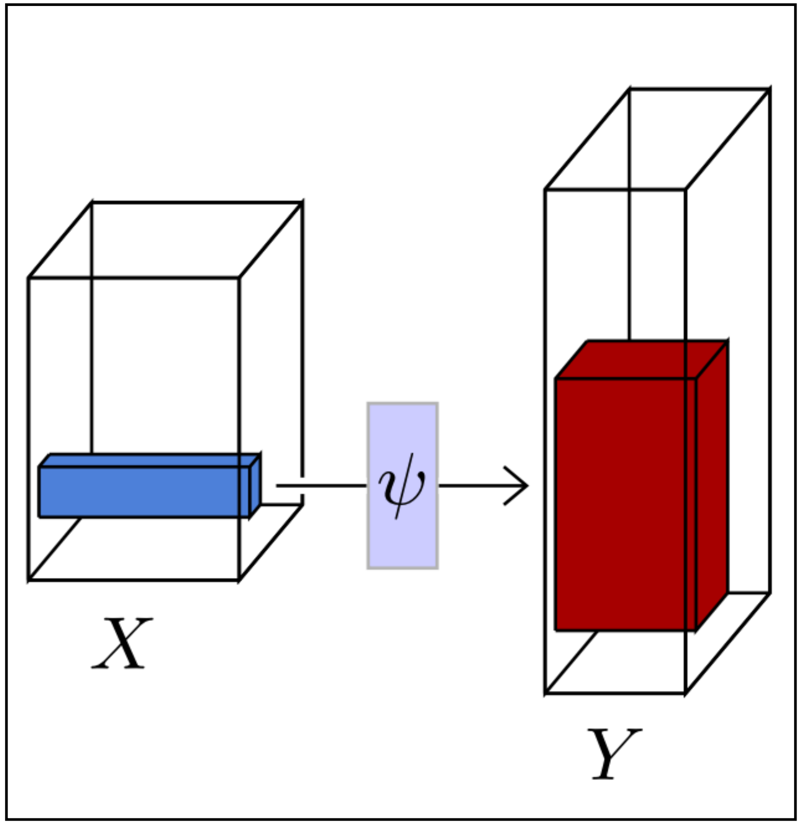
Decrease or Increase Dimensionality

typical use cases discussed here



2D convolution



2D transposed convolution

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

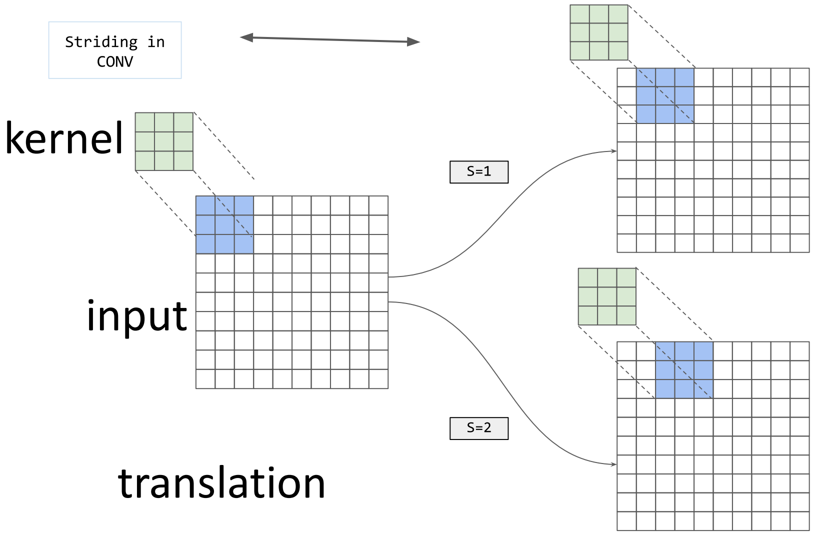
Important Details: Striding and Padding

need to define how to stride over image

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

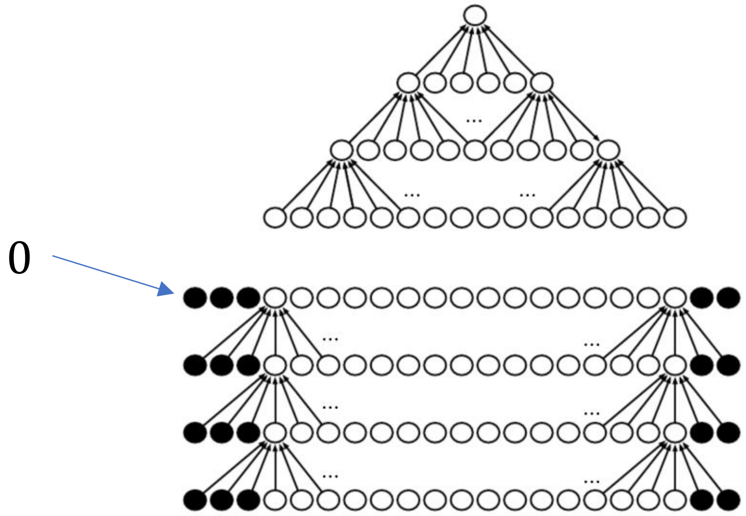
$s > 1$ corresponds to down-sampling

→ 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

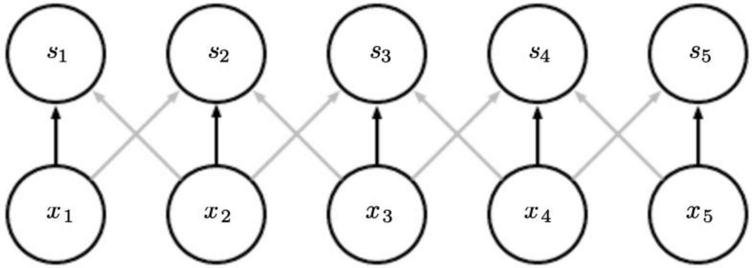
- sparse interactions: much less weights
- parameter sharing: use same weights for different connections

effect of receptive field over several layers:

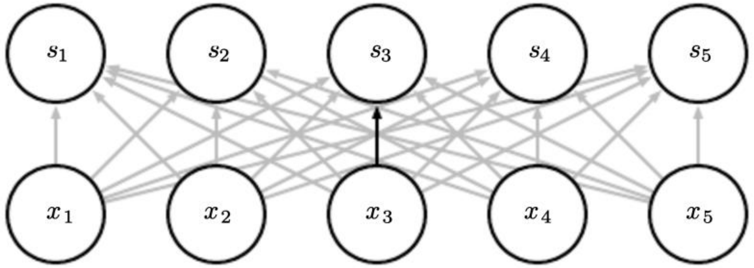
- consider only locally restricted number of input values from previous layer
- grows for earlier layers (indirect interactions)

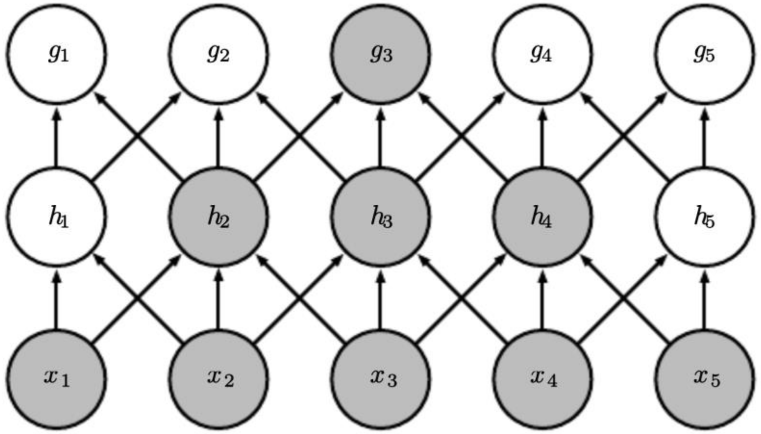
→ hierarchical patterns from simple building blocks (many aspects of nature hierarchical)

convolutional layer:



fully-connected layer:





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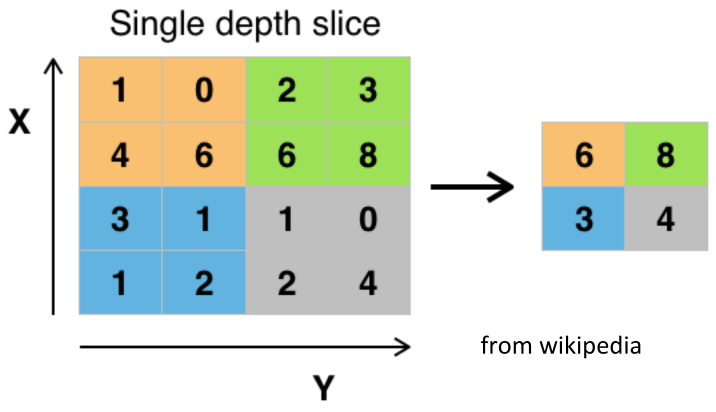
Another Ingredient: Pooling

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

→ non-linear down-sampling (regularization)

max pooling:

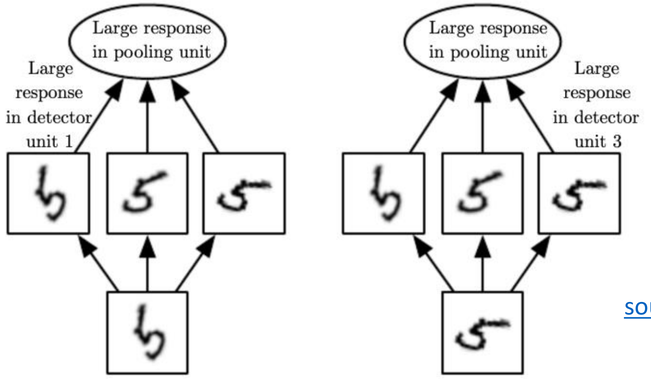


from wikipedia

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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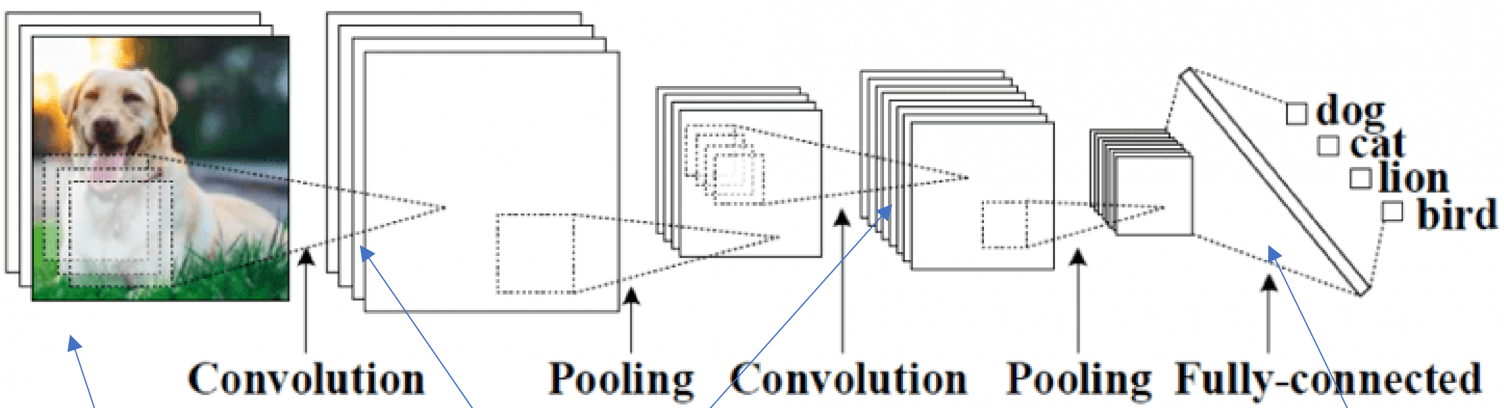
Putting It All Together

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

kernels

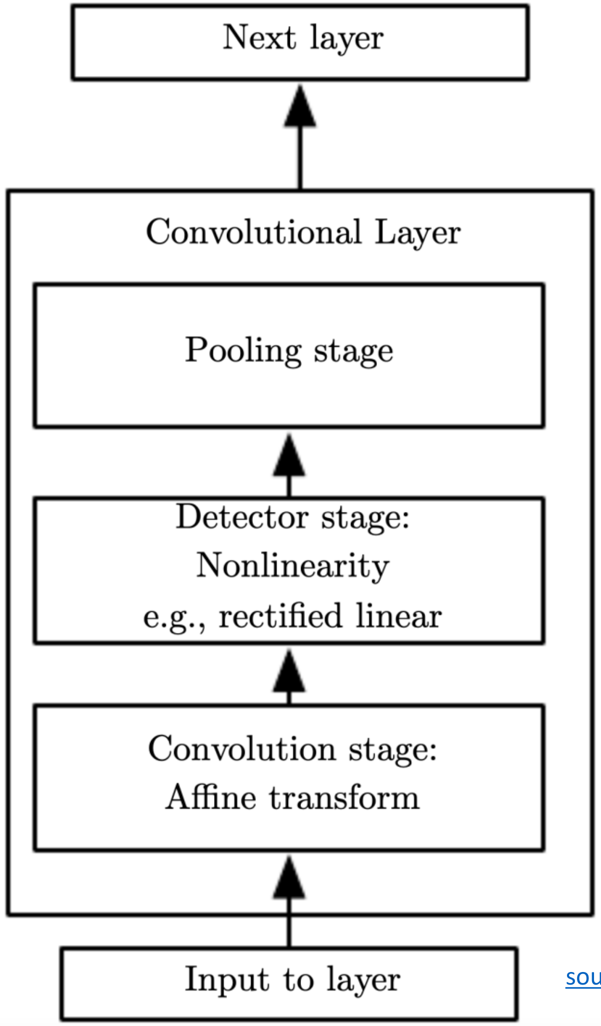


many images (training examples), potentially with several channels

several kernels producing several feature maps

down-sampling by convolutions and pooling

flatten dimensions for final classification or regression



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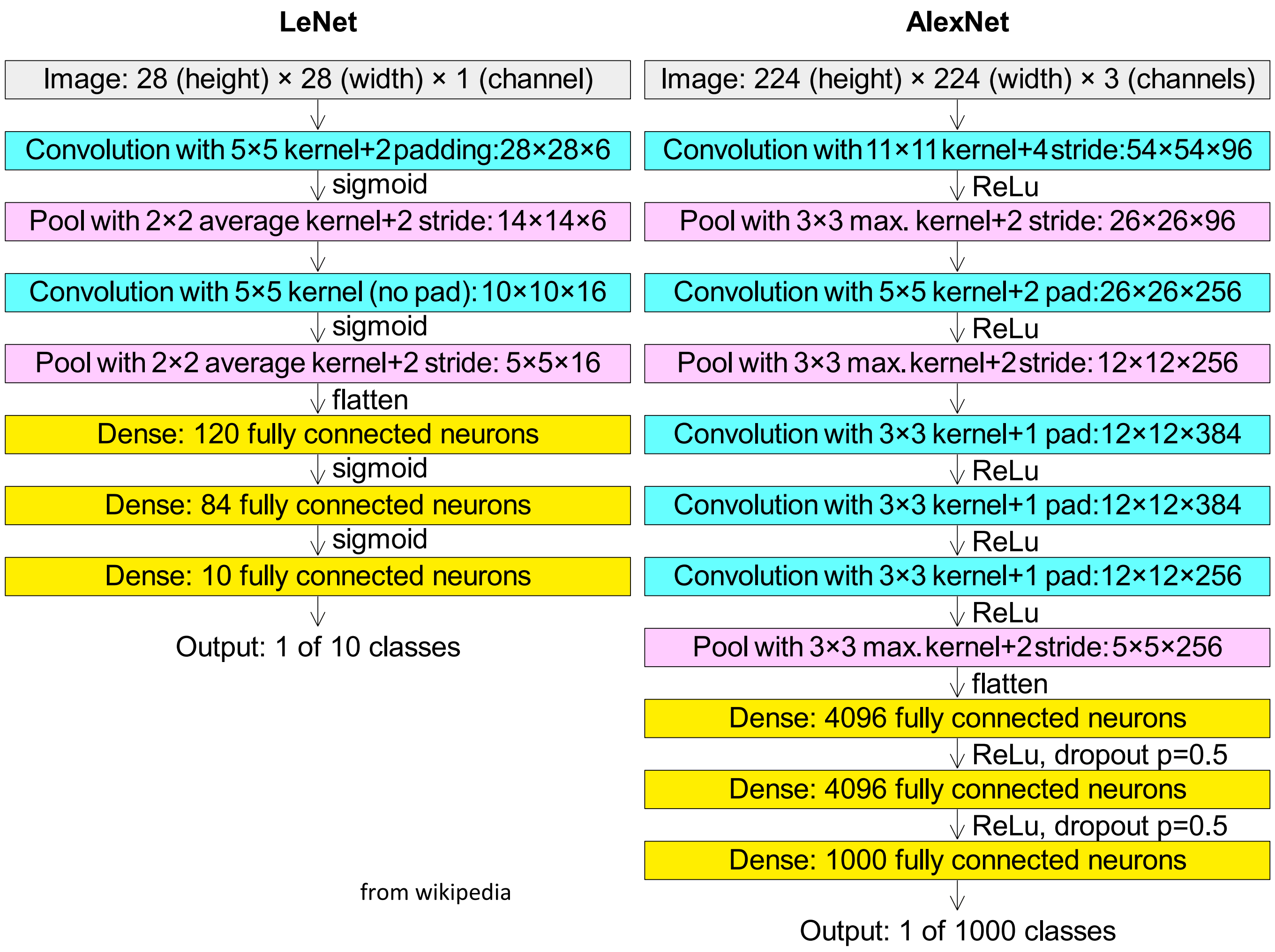
Going Deeper



from wikipedia

AlexNet finally started the deep learning hype.

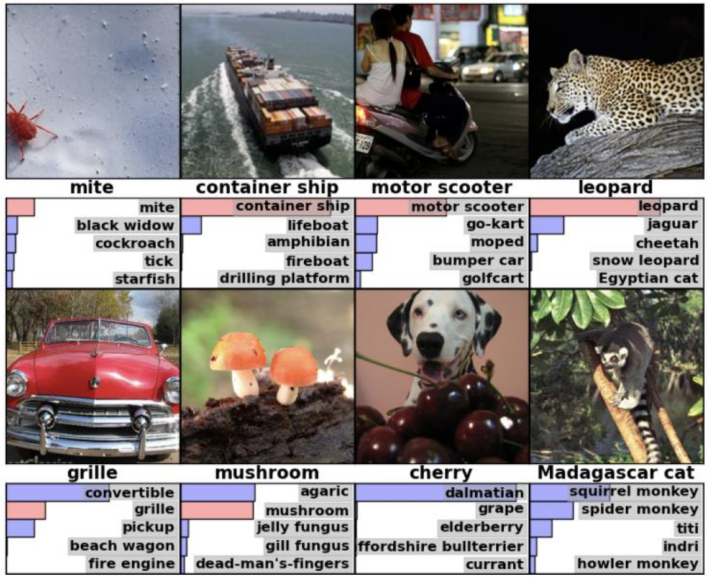
(winning the ImageNet challenge in 2012)

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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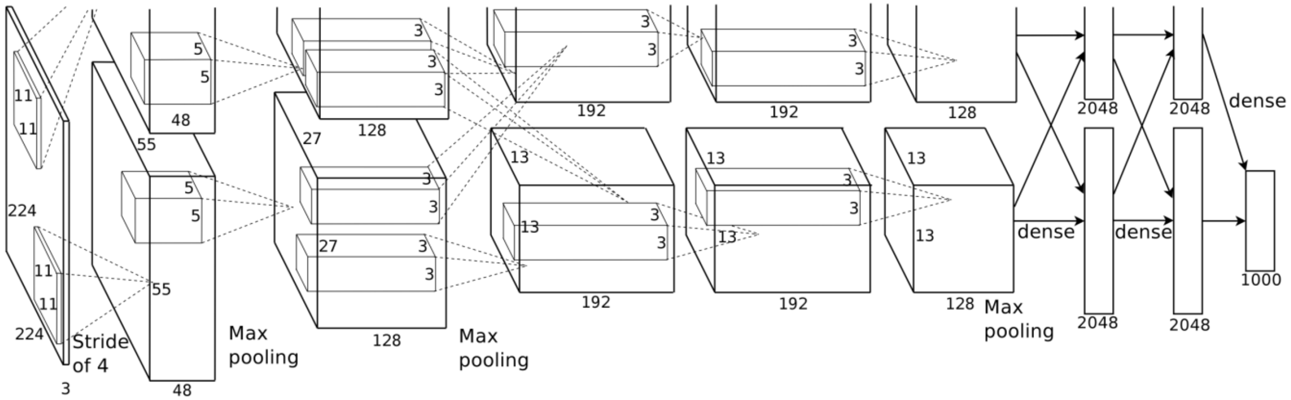
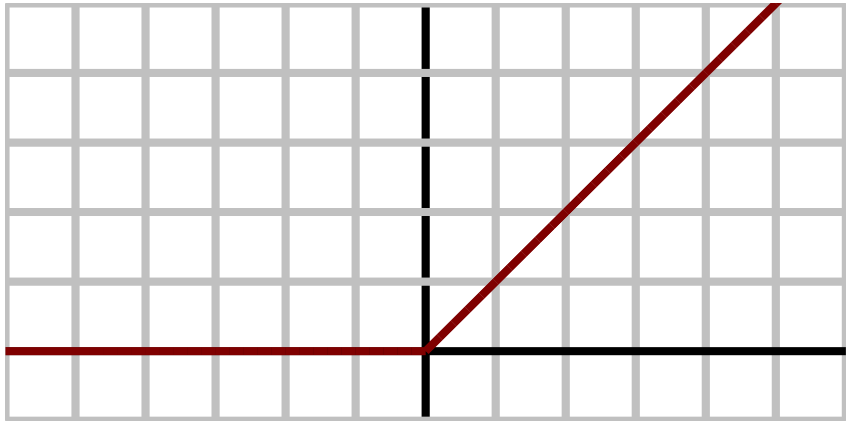


Rectified Linear Unit (ReLU)



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

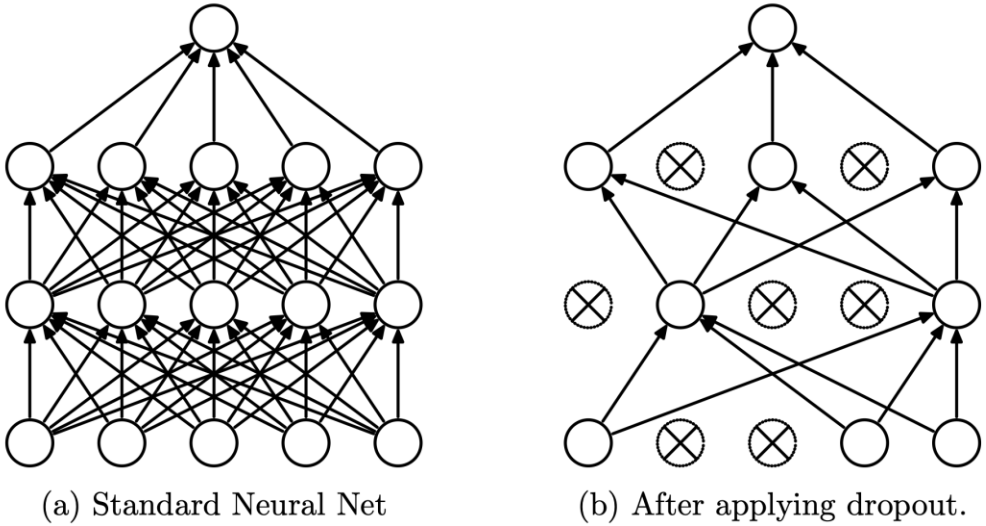
Dropout in Neural Networks

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

- 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



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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

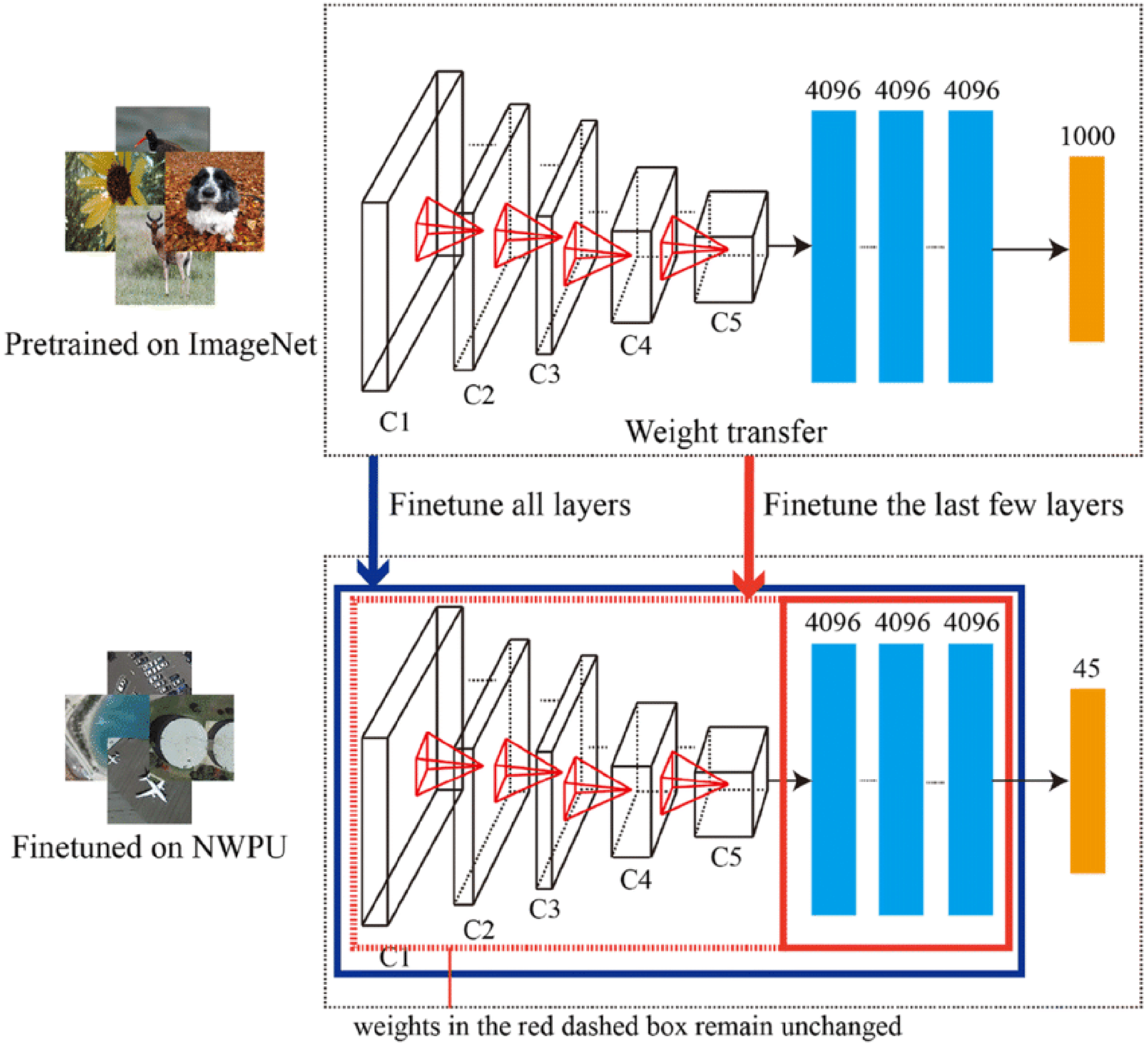
All optimization/ML algorithms (both sophisticated and simple ones) perform equally well when their performance is averaged across all possible problems.

(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

CNN Fine-Tuning



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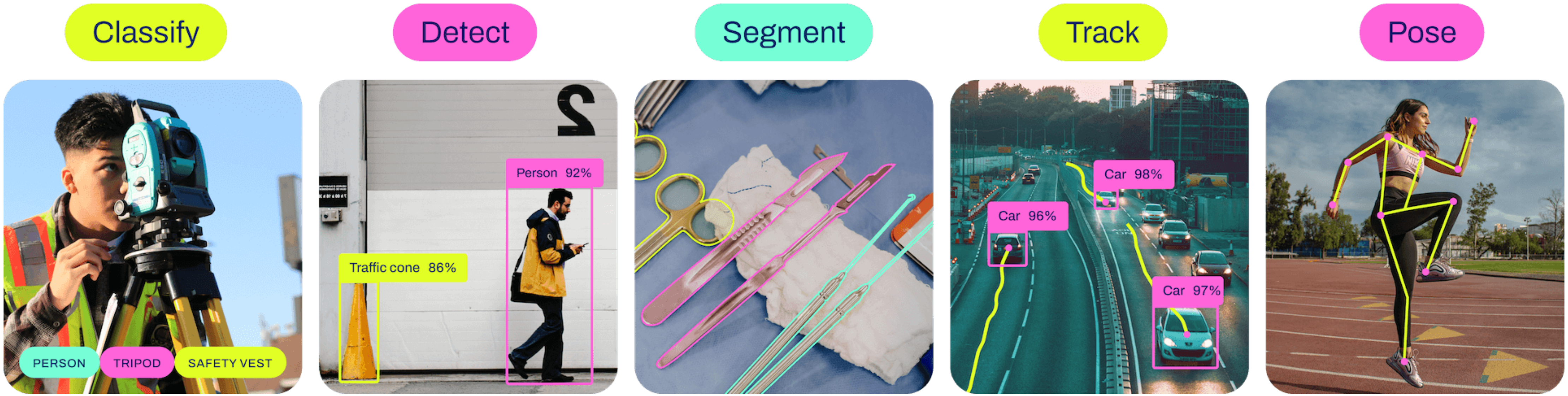
Object Detection and Image Segmentation



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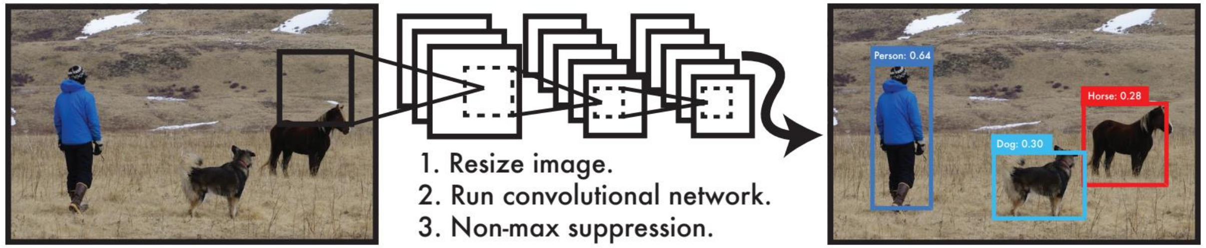
coding example: object detection and image segmentation with YOLO

→ homogenous data (like images) and deep learning allow to use one model for different problems

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

You Only Look Once (YOLO)



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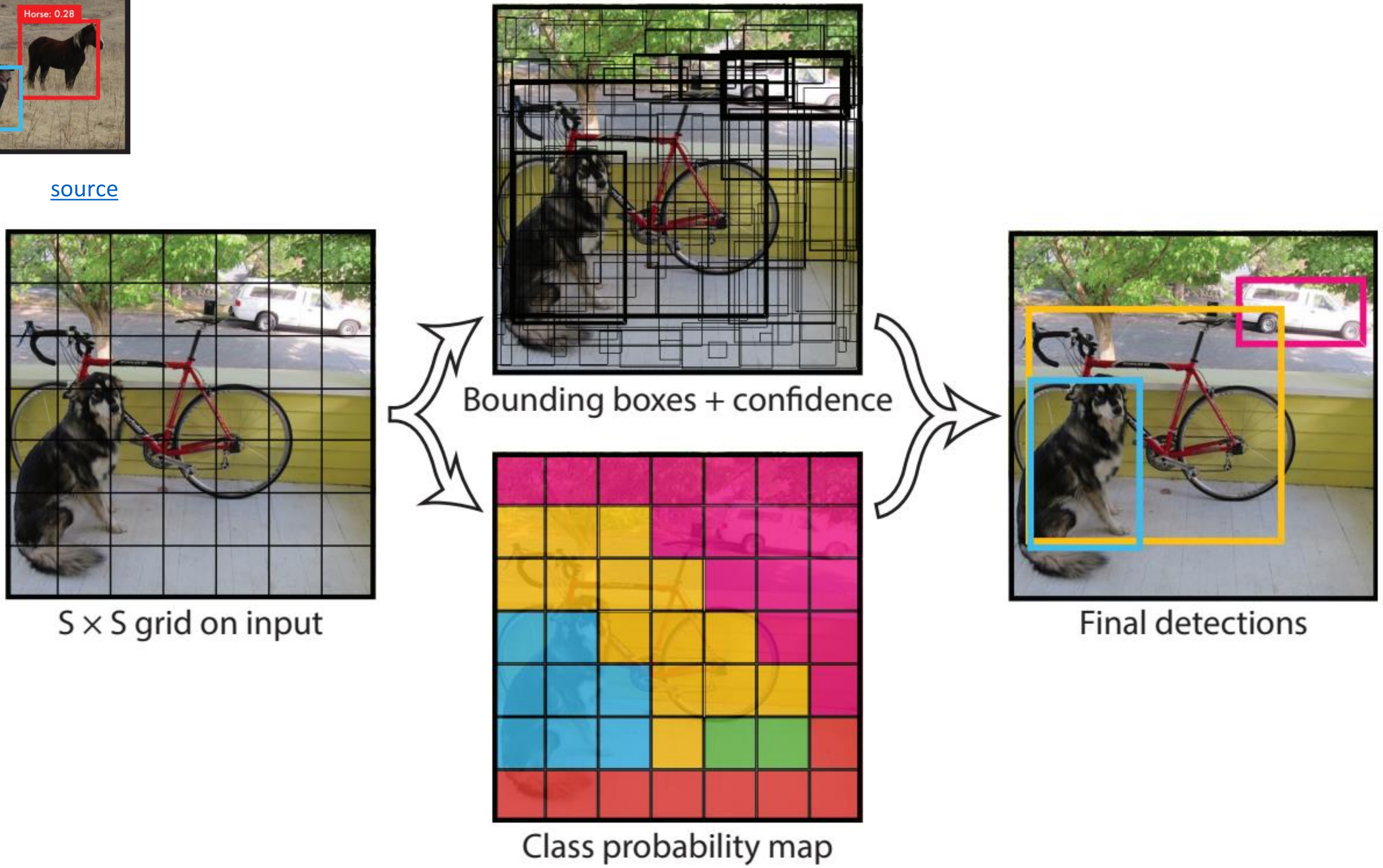
prediction of bounding boxes and class probabilities in one go:
partition image into grid and label each



Assignments

- handwritten digit classification: Kaggle Digit Recognizer

(build PyTorch CNN)

- image classification: Kaggle Intel Image Classification

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