CONVOLUTIONAL NEURAL NETWORKS

Szabolcs Pável
(Ștefan Máthé)

BOSCH

Outline

- Math Refresher: Calculus
- Optimization for Deep Learning
- Convolutional Neural Networks
- Perspectives

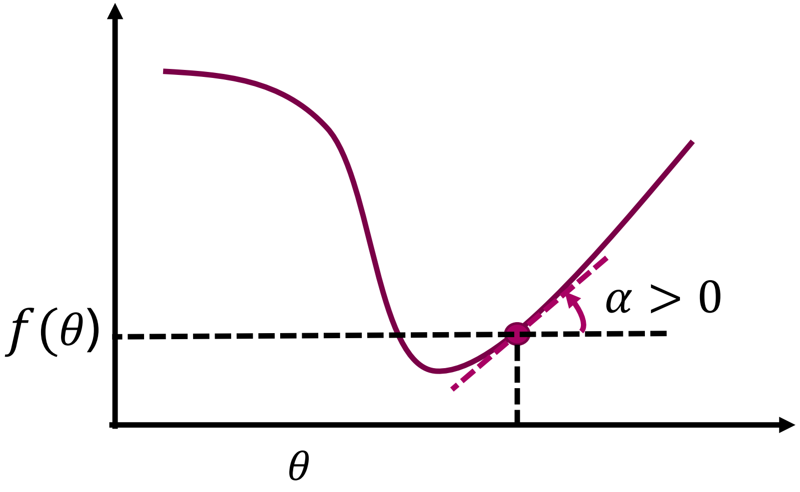
MATH REFRESHER: CALCULUS

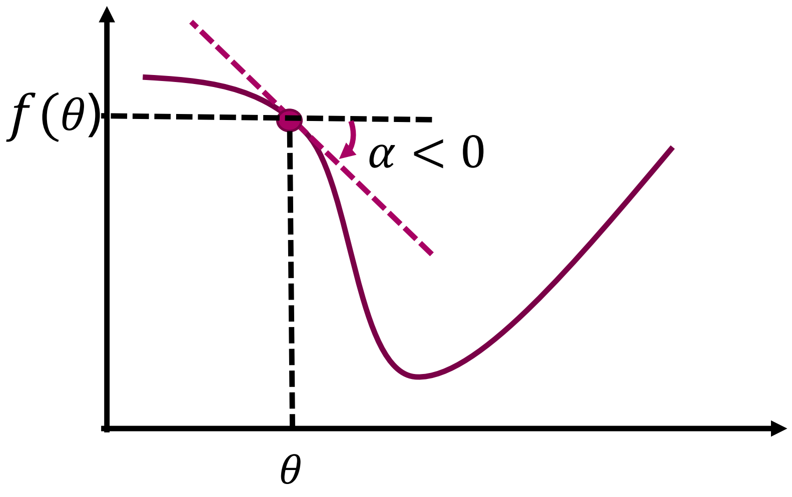
Quick Math Refresher
The Derivative

- Describes the sensitivity of a 1 dimensional scalar function to an infinitesimal change in input

$$f: \mathbb{R} \rightarrow \mathbb{R} \qquad f'(\theta) = \lim_{\varepsilon \to 0} \frac{f(\theta + \varepsilon) - f(\theta)}{\varepsilon} = \tan \alpha$$

- The derivative is a scalar
- Interpretation: the tangent of the slope of the function





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Quick Math Refresher
The Partial Derivative

- Assume we have a d-dimensional scalar function:

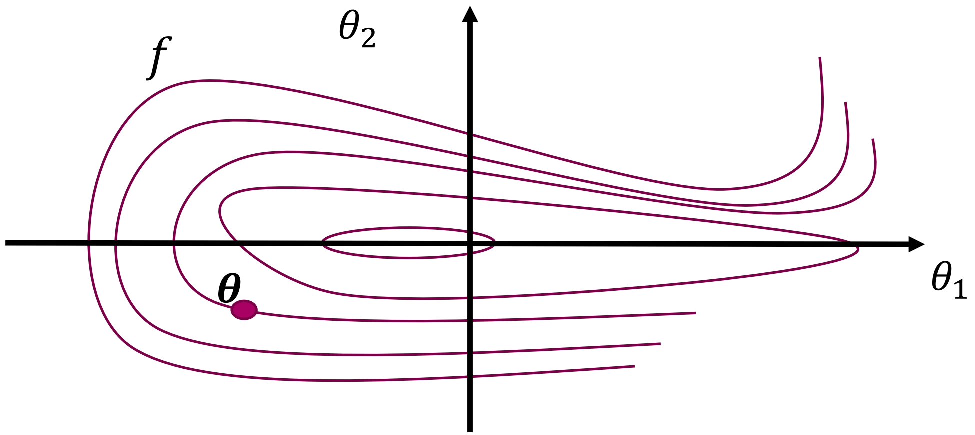
$$f: \mathbb{R}^d \to \mathbb{R}$$

- The partial derivative for dimension i describes how sensitive f is to infinitesimal changes along dimension i

θ_2

$$\frac{\partial f}{\partial \theta_i}(\theta) = \lim_{\varepsilon \to 0} \frac{f(\theta + \varepsilon \Delta_i) - f(\theta)}{\varepsilon}$$

where: $\Delta_i = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ i-th dimension



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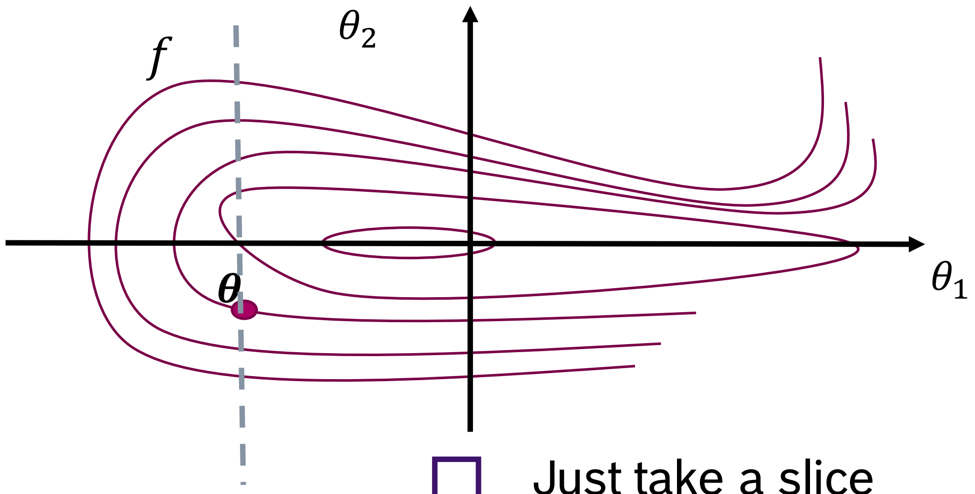
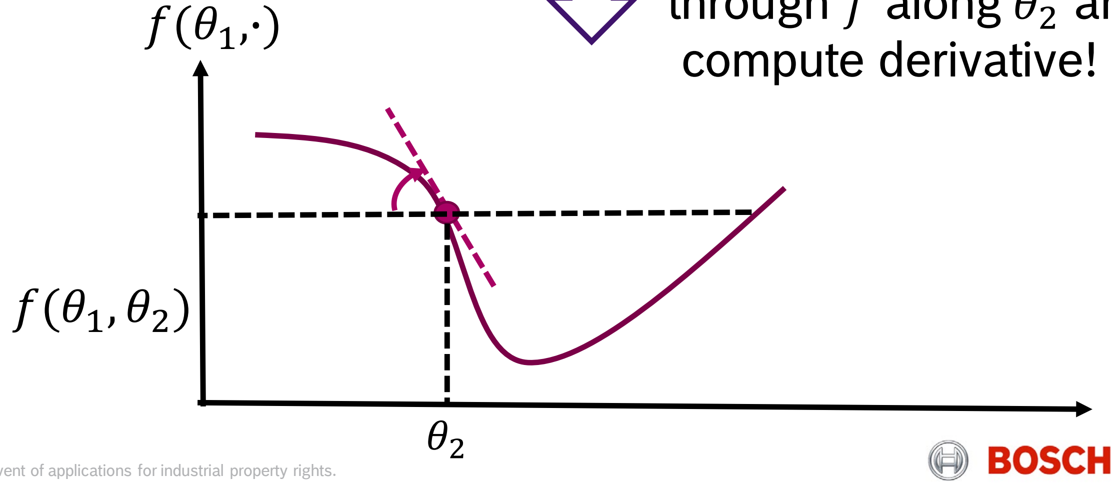


Just take a slice through f along θ_2 and compute derivative!

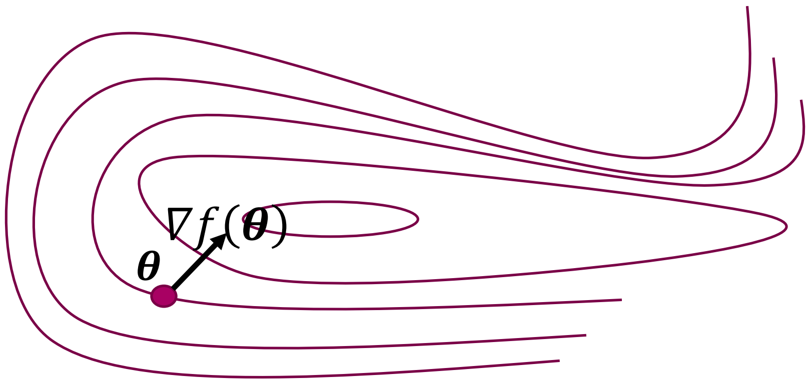


Quick Math Refresher
The Gradient

- Generalizes the gradient to a d-dimensional scalar function
- Just stack together the partial derivatives along each axis
- The gradient is a vector
- Interpretation: the direction of steepest ascent

$$f : \mathbb{R}^d \rightarrow \mathbb{R}$$

$$\nabla f(\theta) = \begin{bmatrix} \frac{\partial f}{\partial \theta_1} \\ \frac{\partial f}{\partial \theta_2} \\ \vdots \\ \frac{\partial f}{\partial \theta_d} \end{bmatrix}$$



OPTIMIZATION

Optimization
Problem Formulation

- Almost all machine learning problems are a form of (constrained / approximate) minimization of an **objective function** (*e.g.* training negative log likelihood)

$$\boxed{\boldsymbol{\theta}^* = \operatorname{argmin}_{\boldsymbol{\theta}} J(\boldsymbol{\theta})}$$

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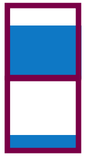

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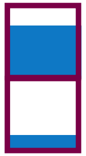

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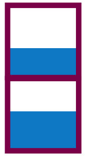

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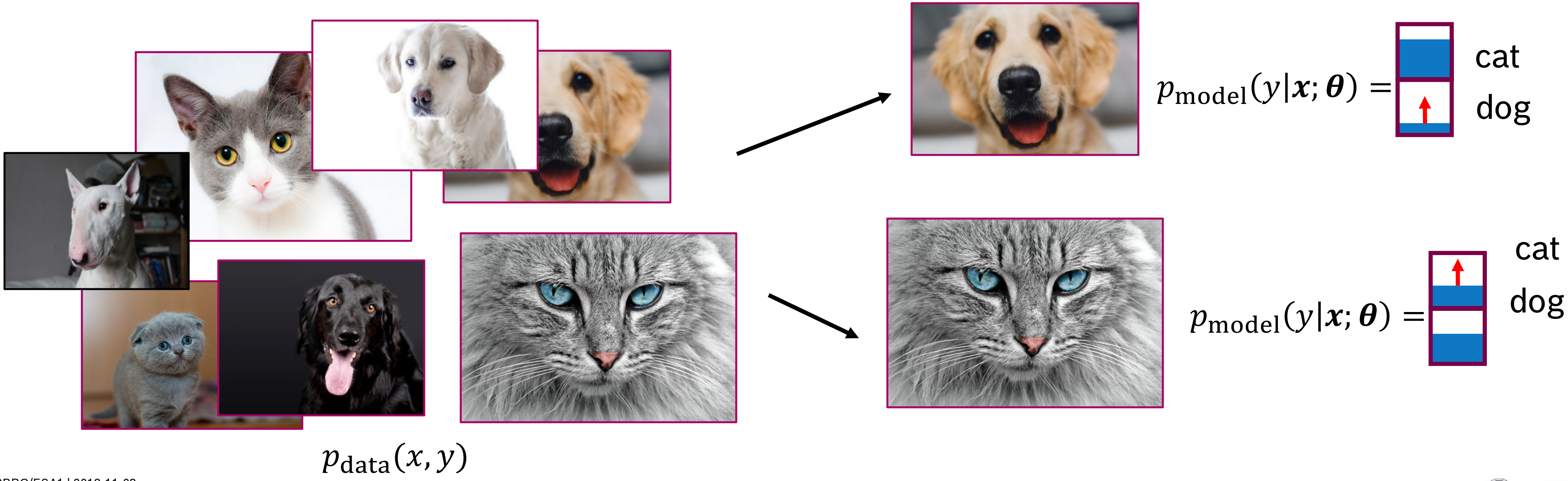

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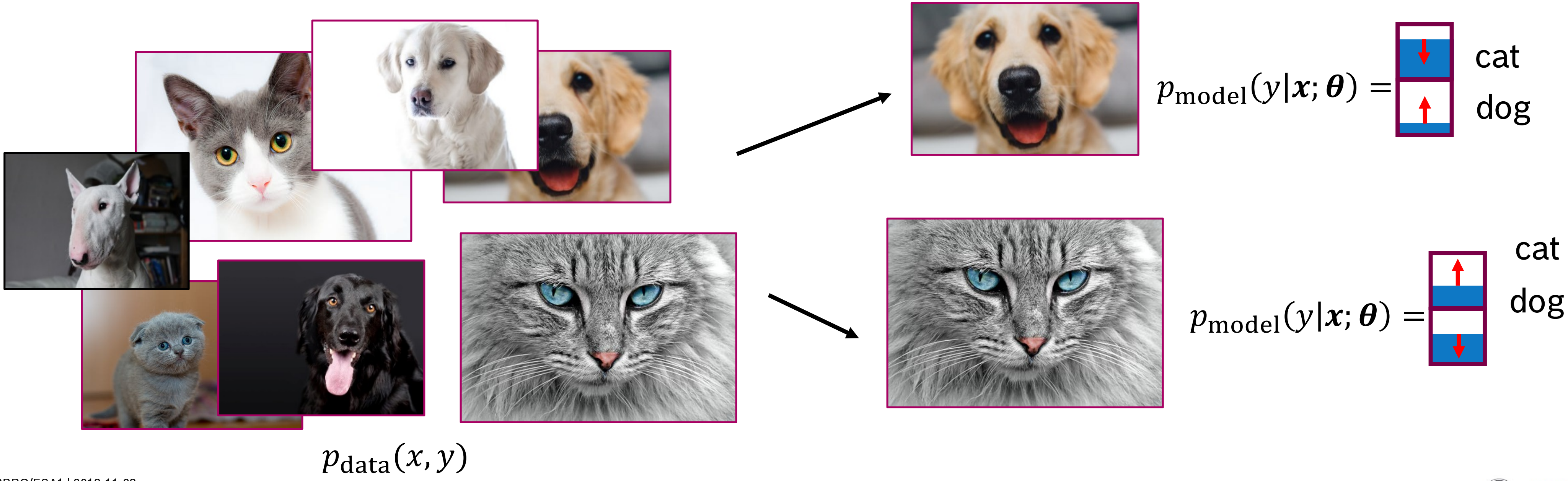

Optimization
Gradient Descent Algorithm (1D Case)

function *gradient-descent-1d*
input: a function J
output: a local optimum θ^* of J

// Start from a random initial guess.
$\theta(0) \leftarrow rand(\mathbb{R});$

// Take steps in the direction of negative slope until
// convergence.
$t \leftarrow 0;$
do {
$\quad \theta(t+1) \leftarrow \theta(t) - \eta\, J'(\theta(t));$
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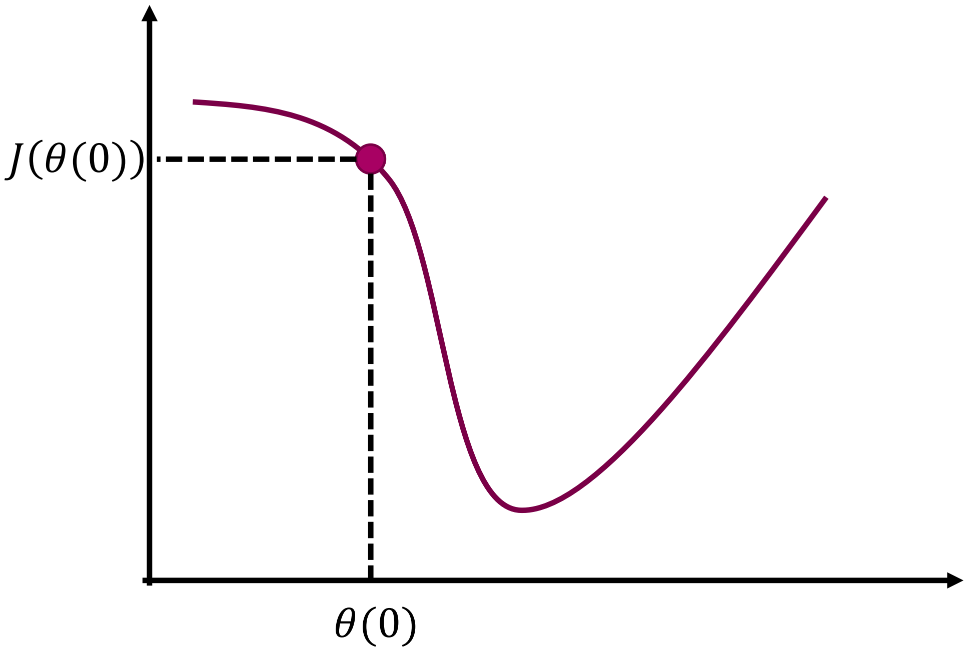

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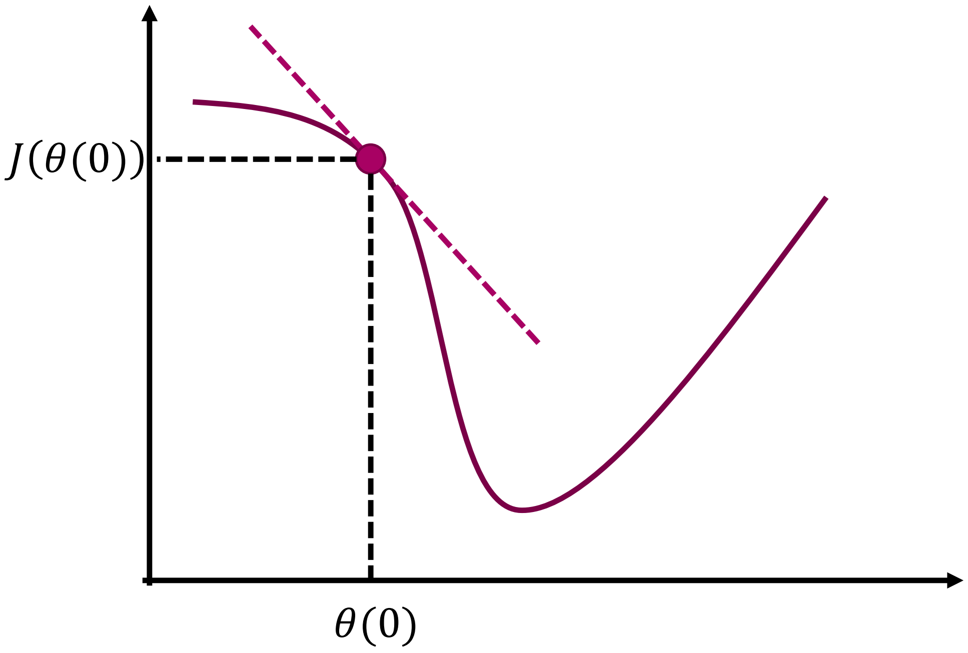

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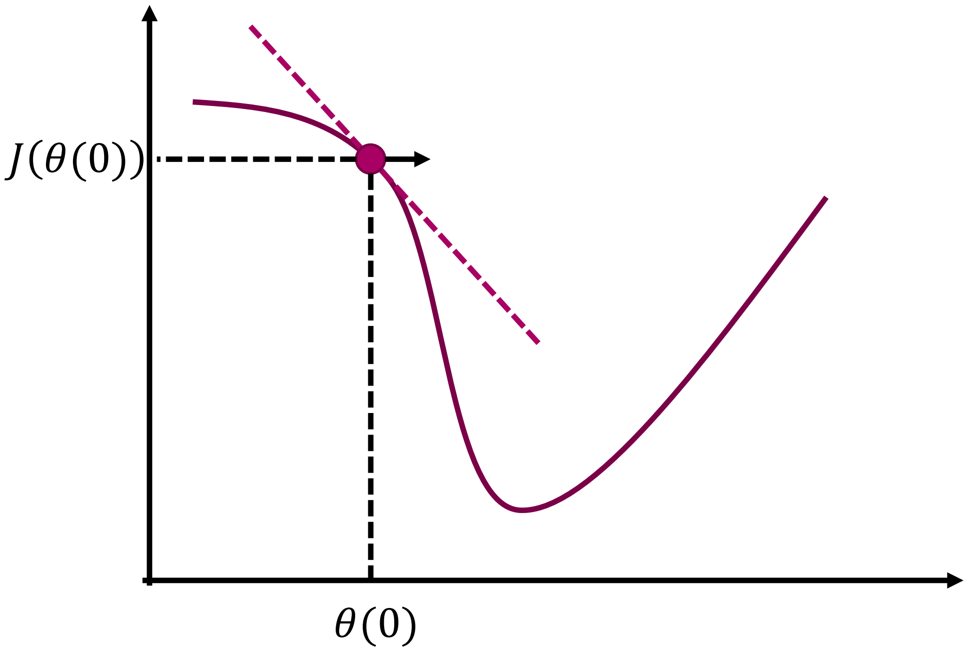

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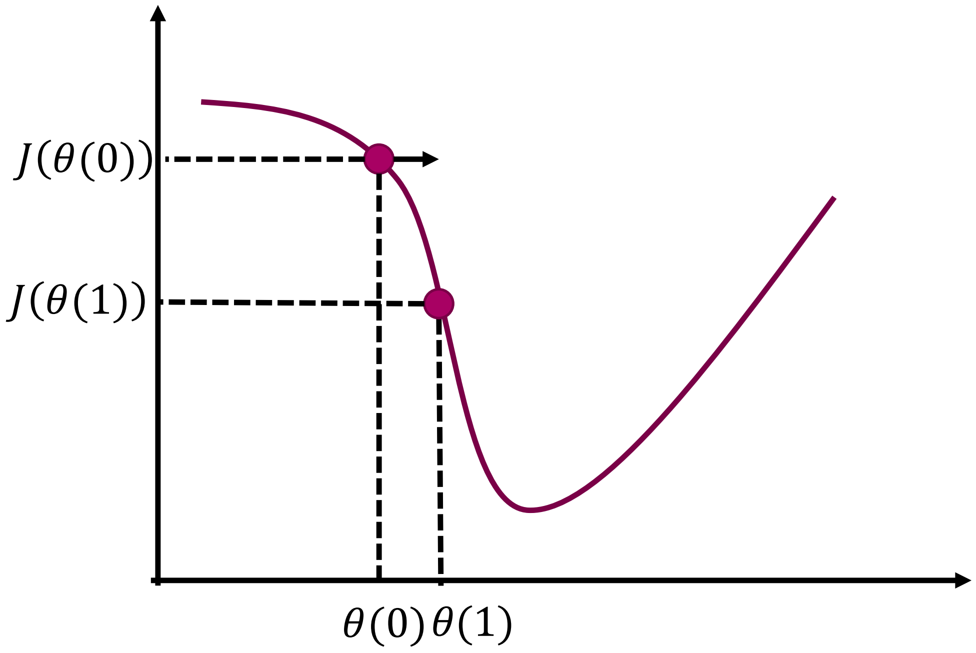

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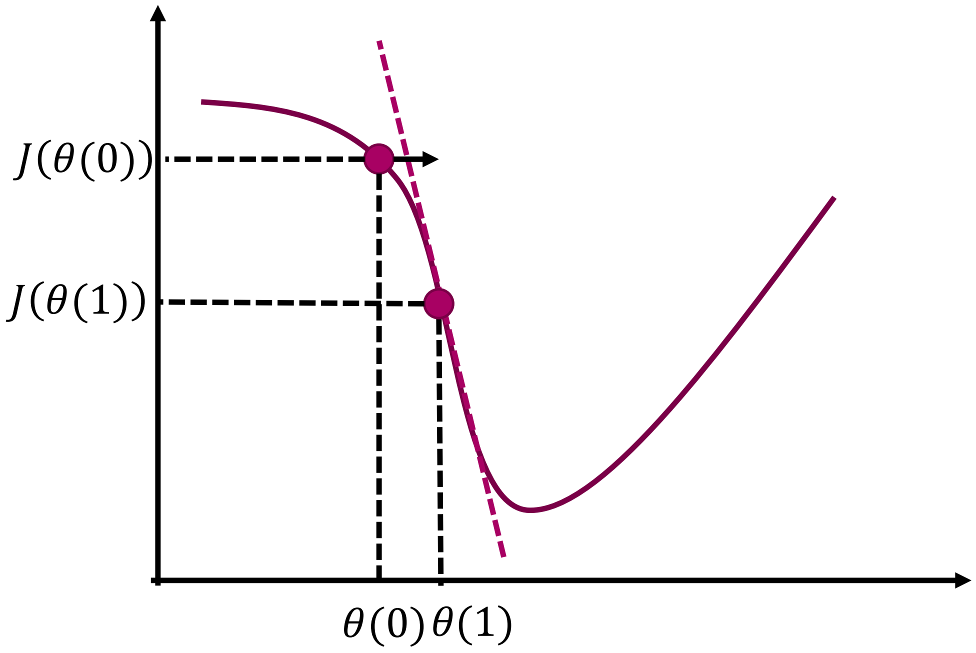

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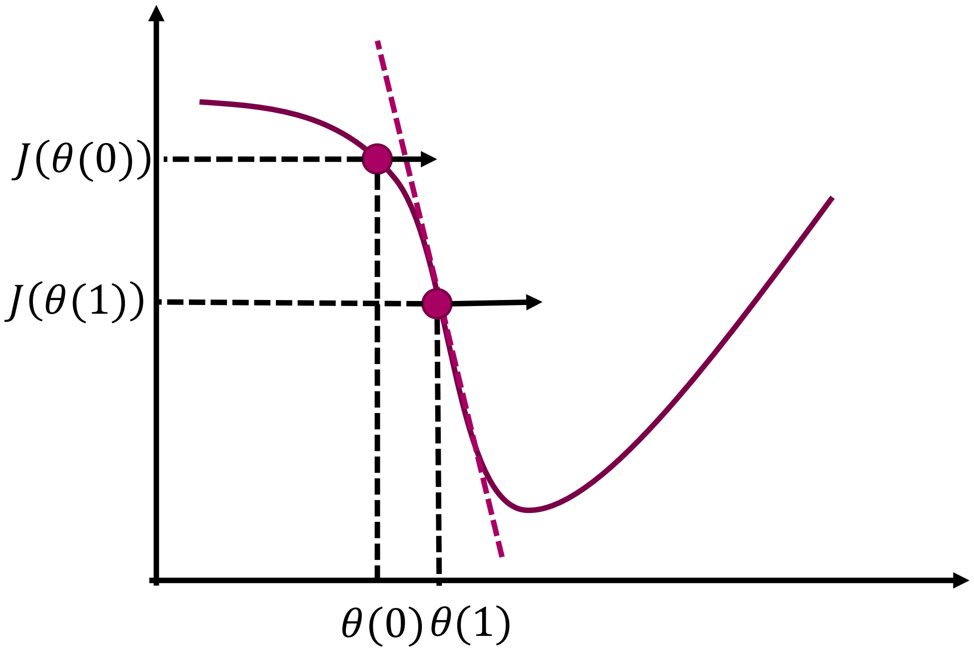

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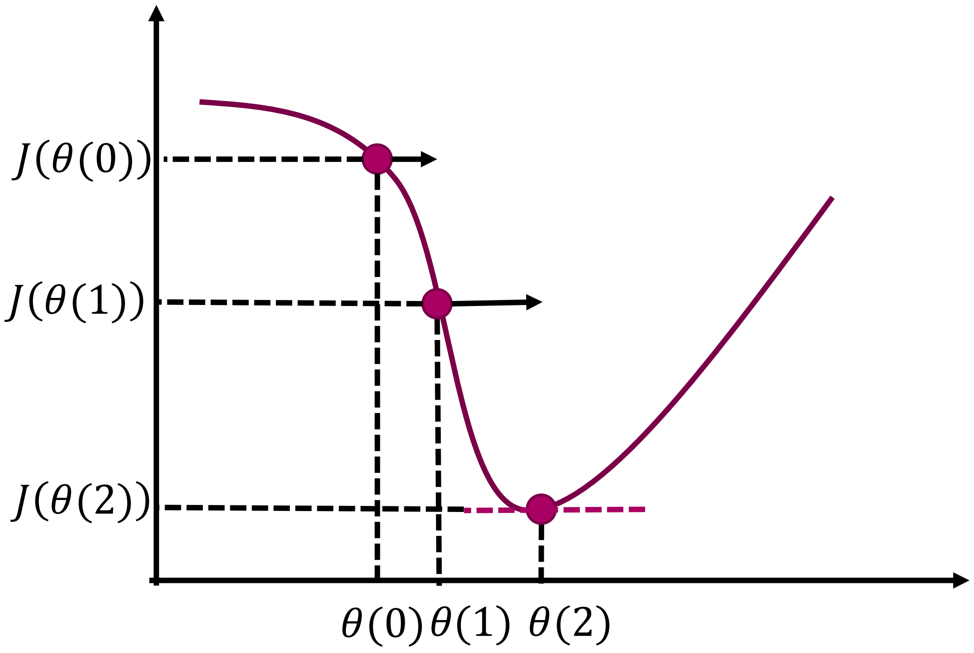

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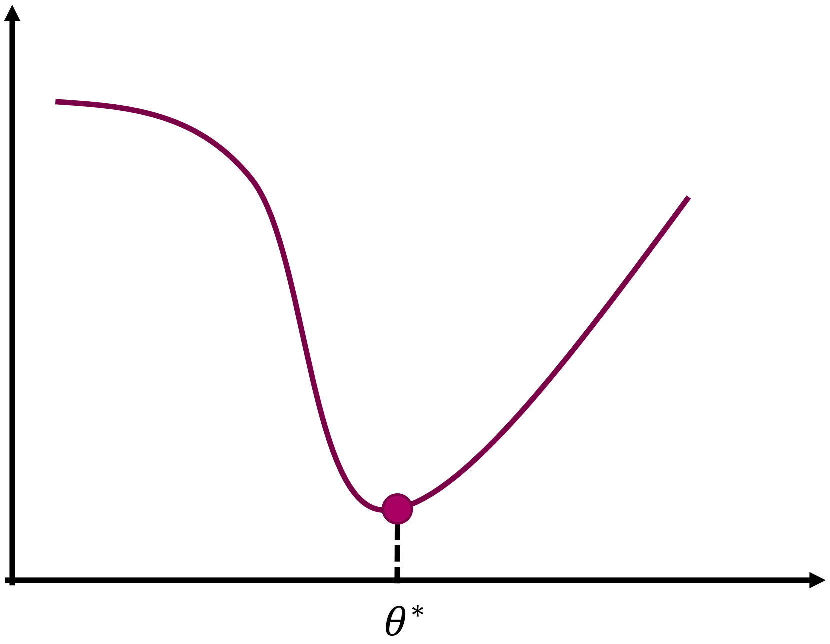

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- Use a 1st order Taylor expansion of J:

$$J(\boldsymbol{\theta}) \cong J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla J(\boldsymbol{\theta}_0)$$

- Move in the direction with negative slope

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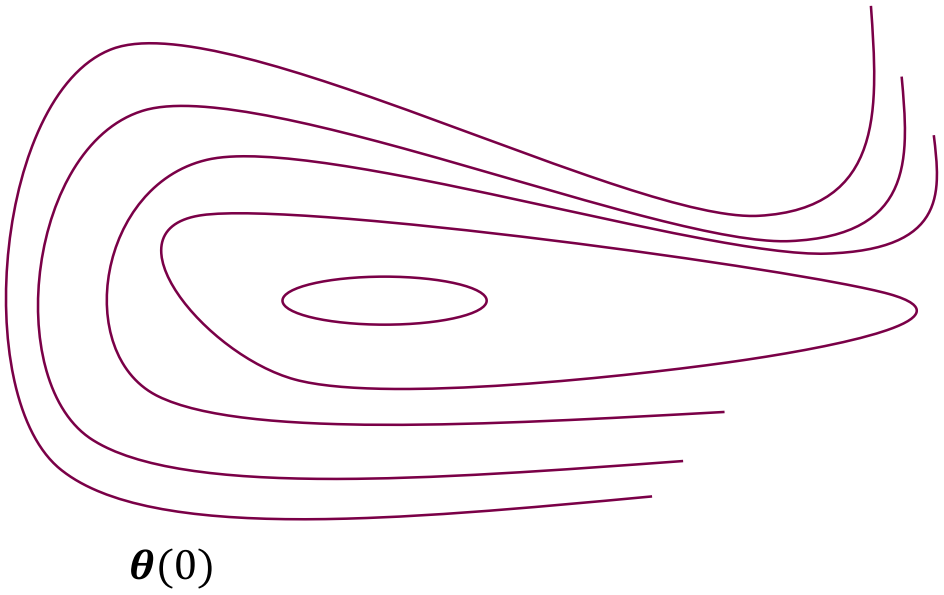

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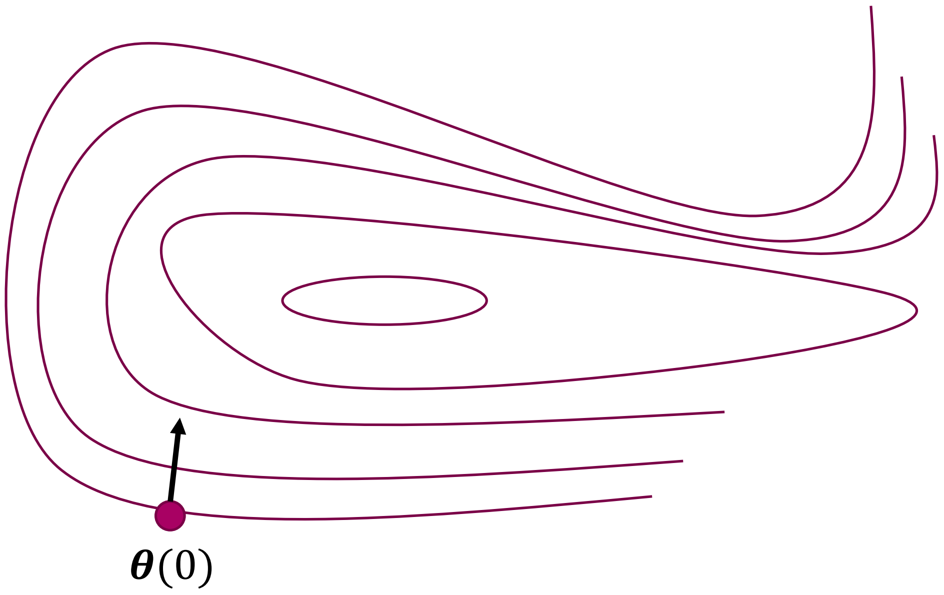

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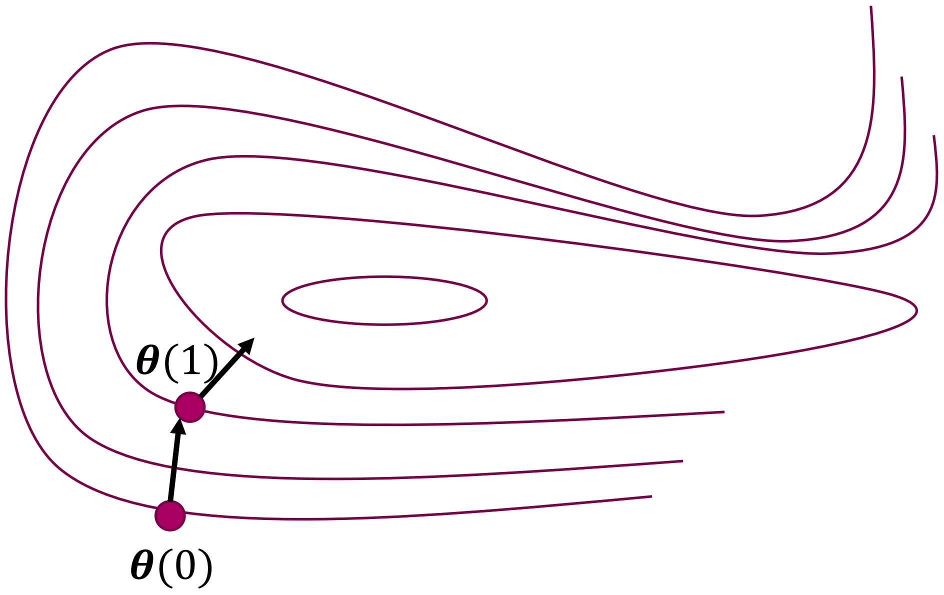

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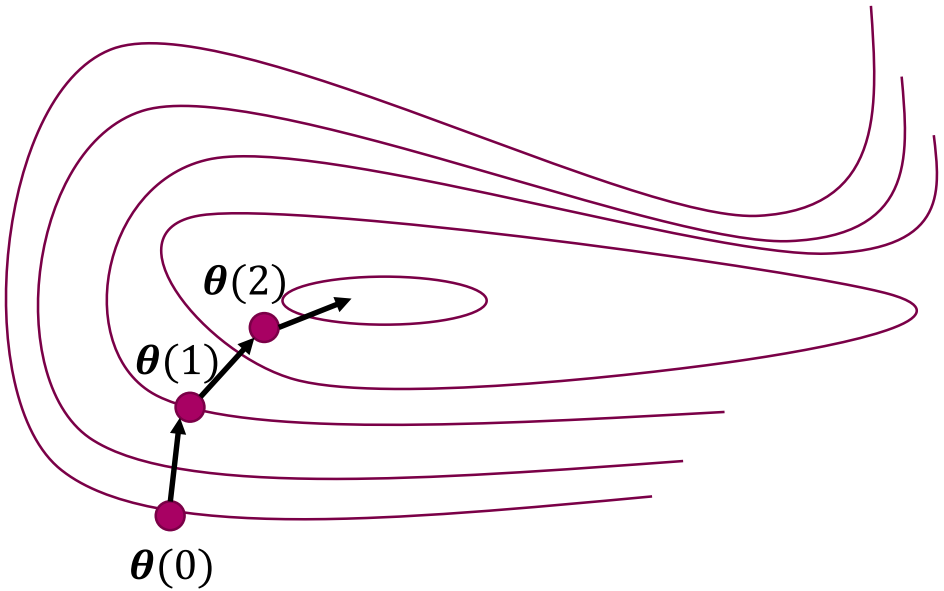

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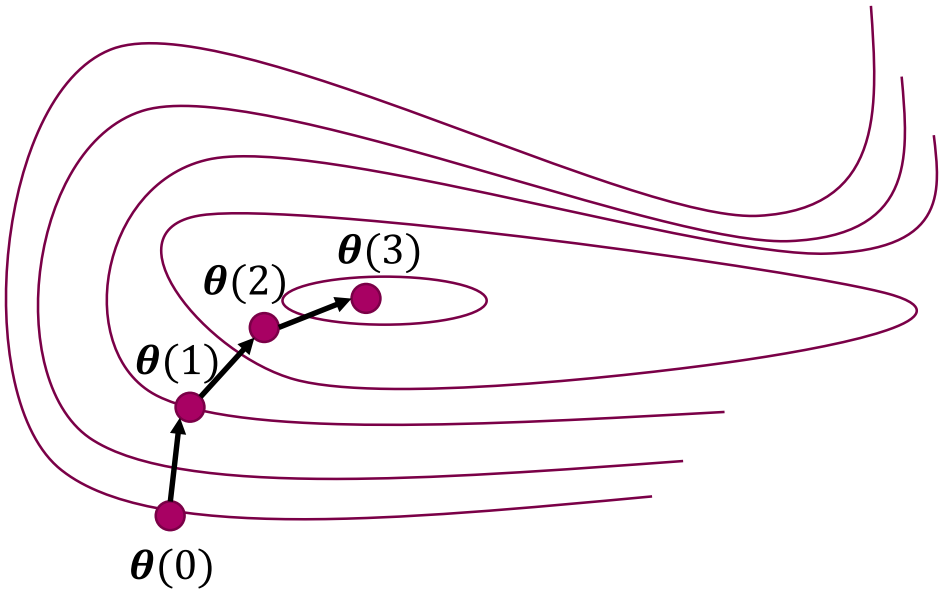
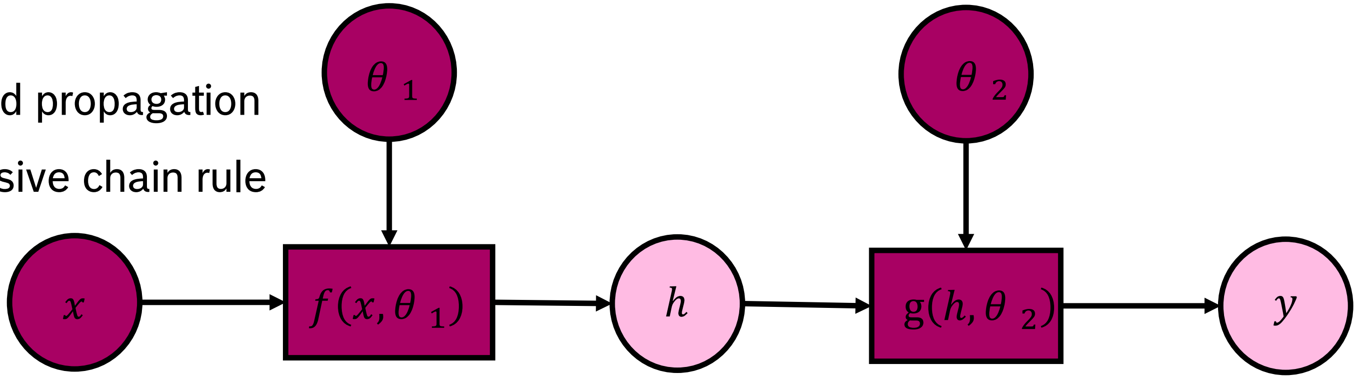


Optimization
Computing the Gradient: The Backpropagation Algorithm

- **Input:** function composition

- **Output:** gradient with respect to either:
  - parameter – gradient descent (typical)
  - input – adversarial training, deep dreaming, network analysis

- **Steps:**
  - Step 1: Compute y by forward propagation
  - Step 2: Compute $\frac{\partial y}{\partial \theta}$ by recursive chain rule applications



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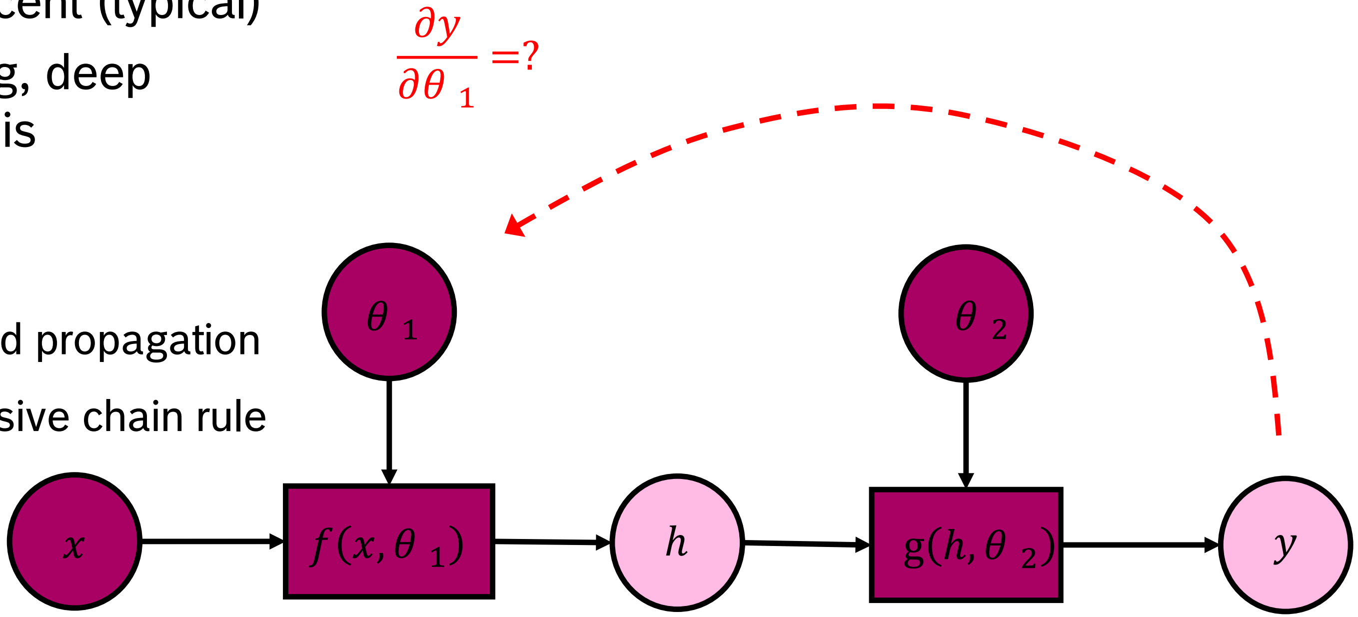

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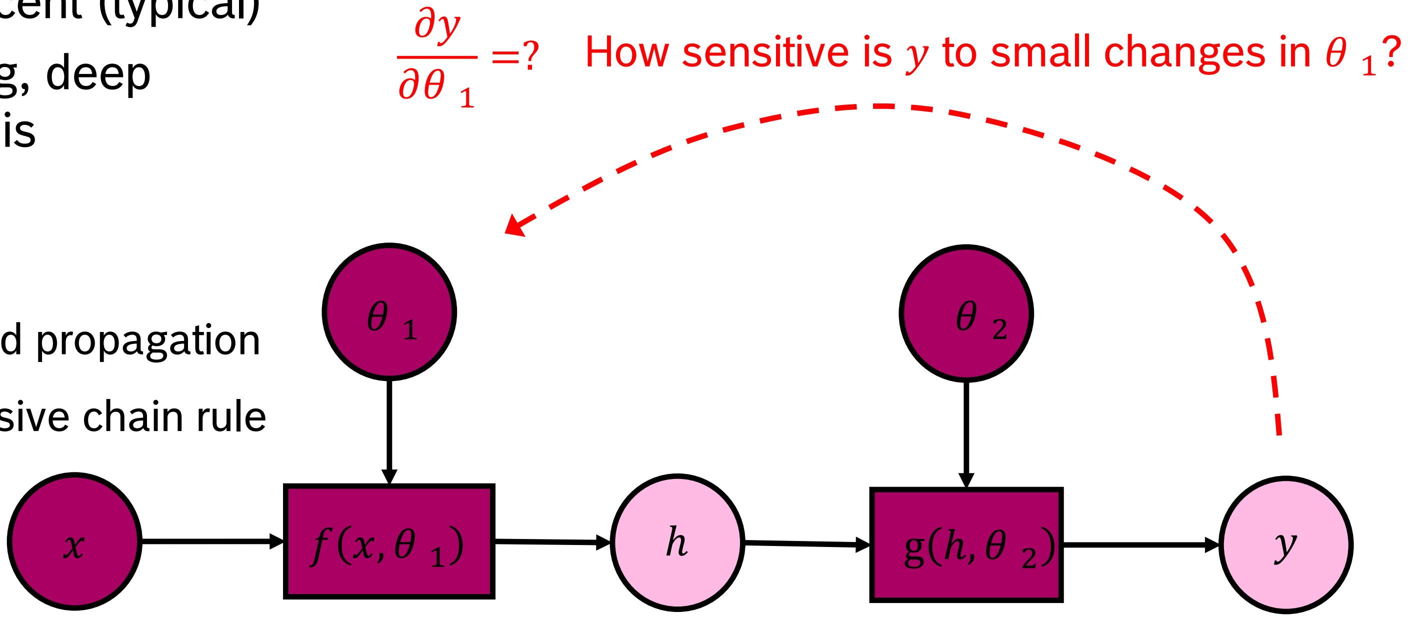

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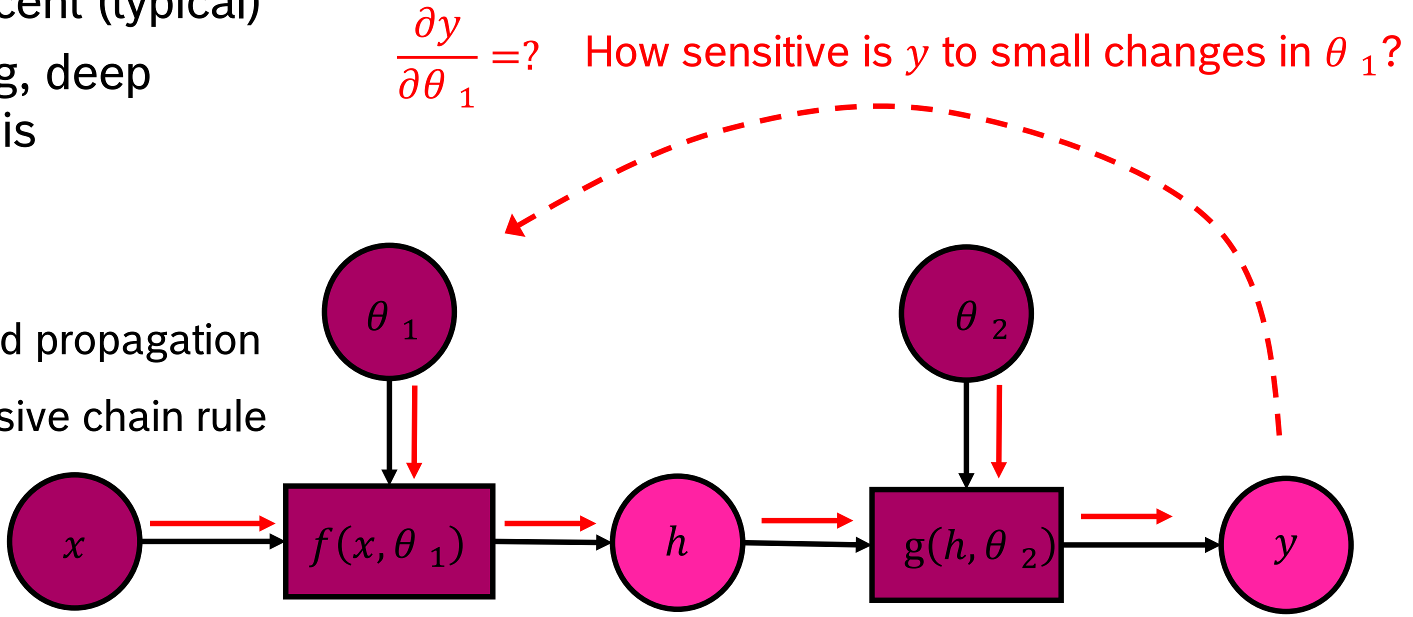

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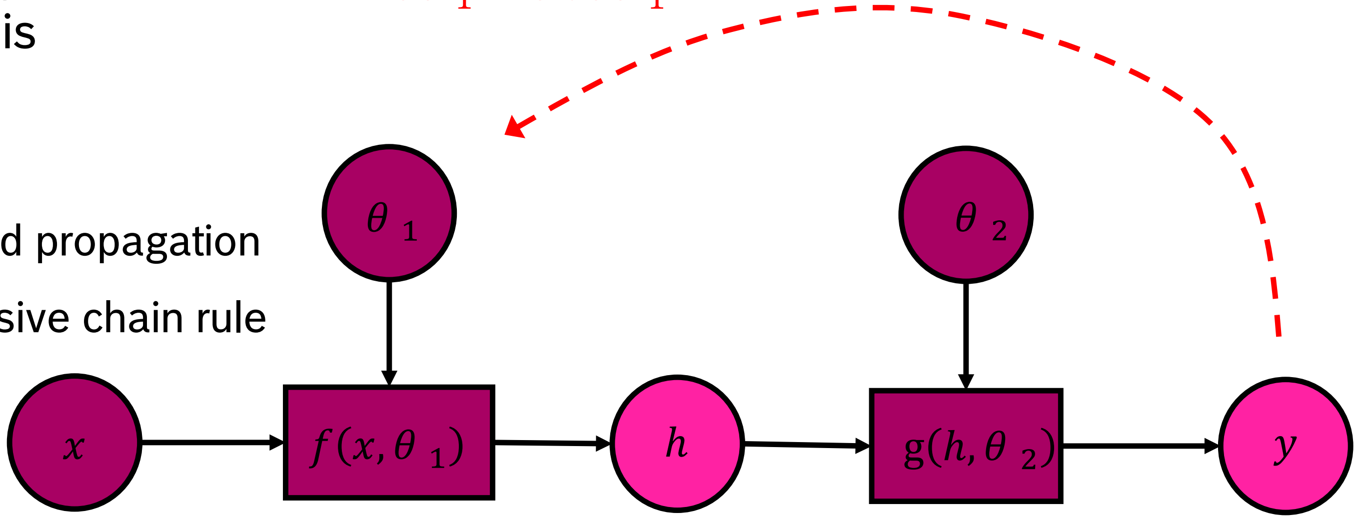
$$\frac{\partial y}{\partial \theta_1} = \frac{\partial y}{\partial h}\frac{\partial h}{\partial \theta_1}$$



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How sensitive is y to small changes in h?

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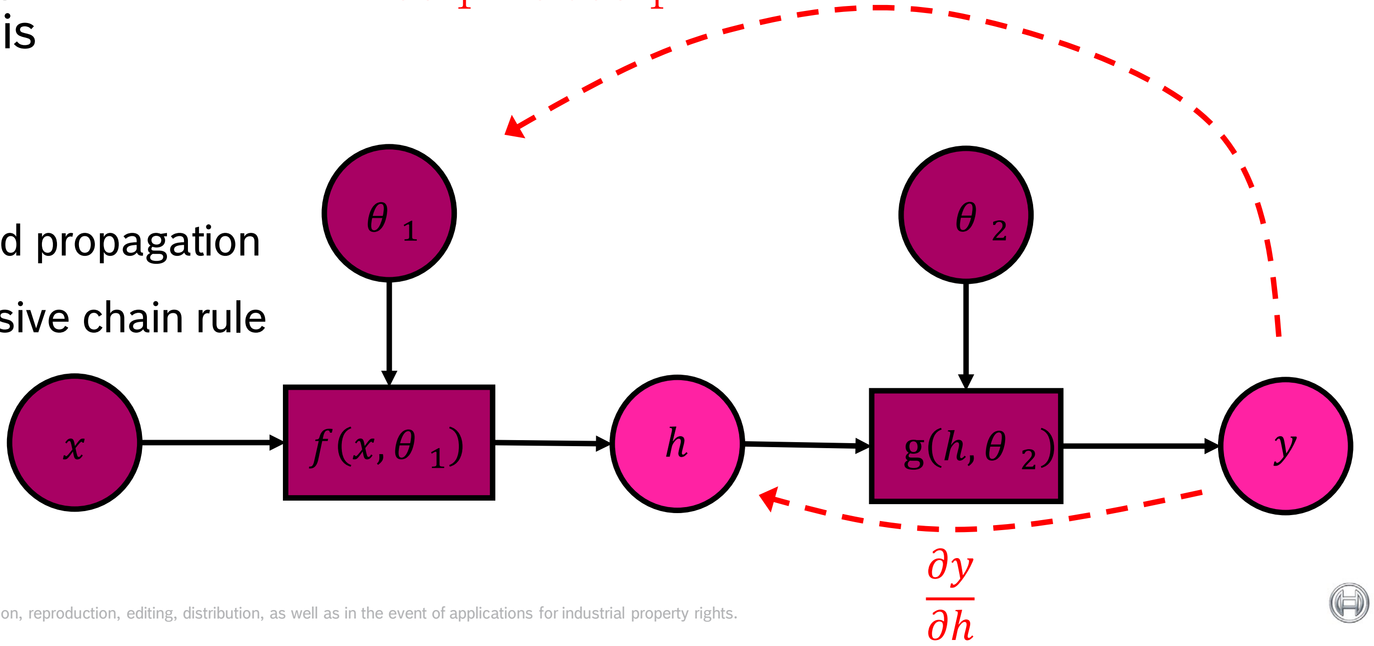

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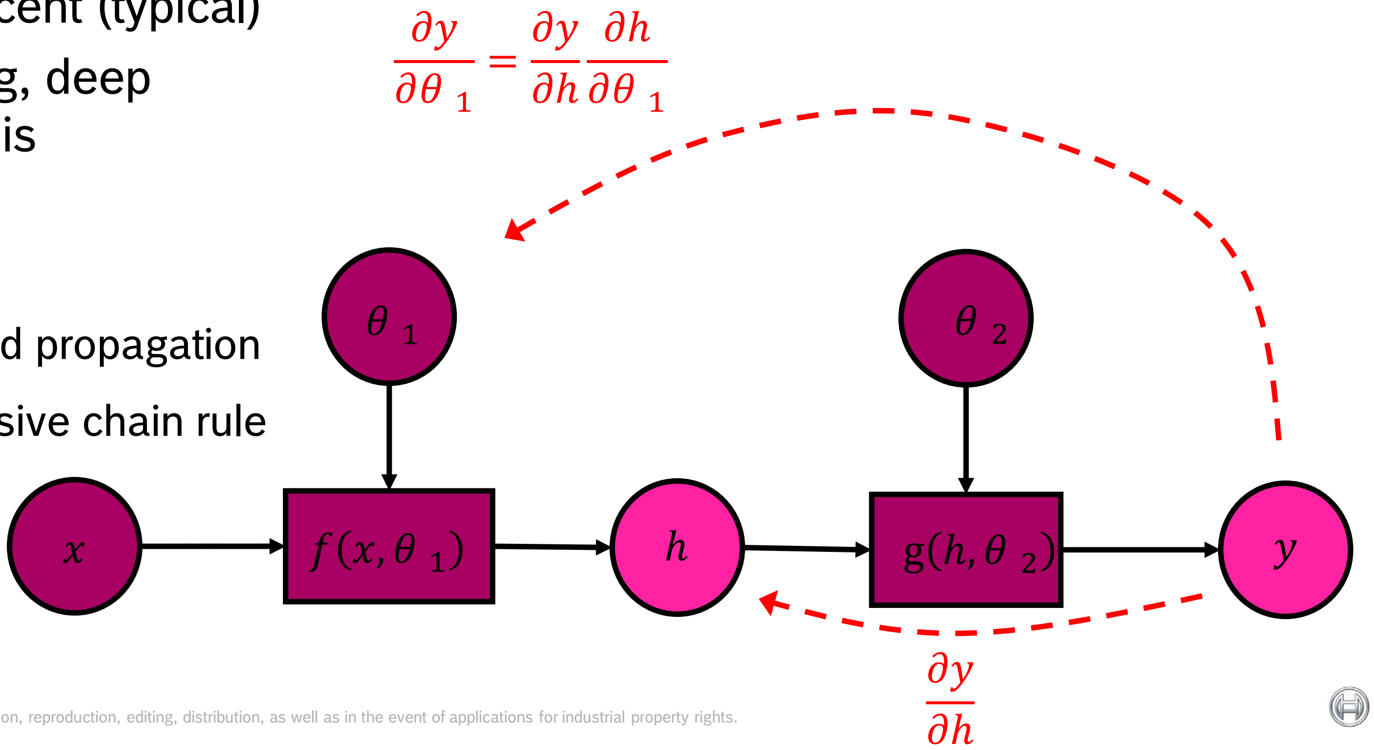

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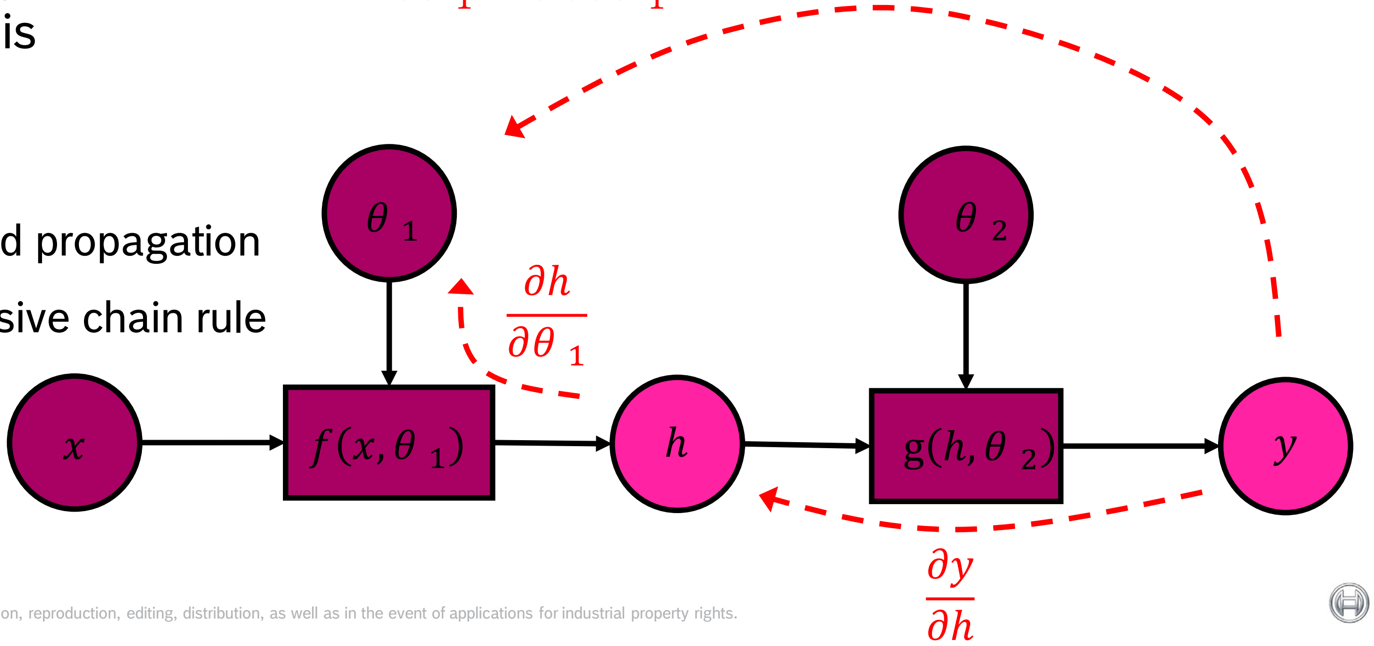
  - Step 2: Compute $\frac{\partial y}{\partial \theta}$ by recursive chain rule applications

$$\frac{\partial y}{\partial \theta_1} = \frac{\partial y}{\partial h}\frac{\partial h}{\partial \theta_1}$$



Optimization
Backpropagation: Extensions

- **Variants:**
  - **symbol-to-number**: nodes compute gradient numerically (Torch, Caffe, Pytorch)
  - **symbol-to-symbol**: augment the graph with nodes that compute the gradient (Theano, Tensorflow) – can simplify symbolic expressions!

- **Efficiency:**
  - Not optimal (special case of the **reverse mode differentiation algorithm**)
  - Finding the optimal formula is NP-complete *[Naumann, 2008]*

- **Implementation:**
  - **automatic differentiation** (transparent gradient computation)
  - new way of writing programs:

“Deep Learning est mort. Vive Differentiable Programming!” [Yann LeCun]

BOSCH

Optimization
Stochastic Gradient Descent

- **Problem:**
  - Empirical risk is too expensive (sums over **all** training samples):

$$\boldsymbol{\theta}^* = \operatorname{argmax}_{\boldsymbol{\theta}} \frac{1}{m} \sum_{\boldsymbol{i}=\mathbf{1}}^{\boldsymbol{n}} \log p_{\text{model}}(y_i | \boldsymbol{x}_i; \boldsymbol{\theta})$$

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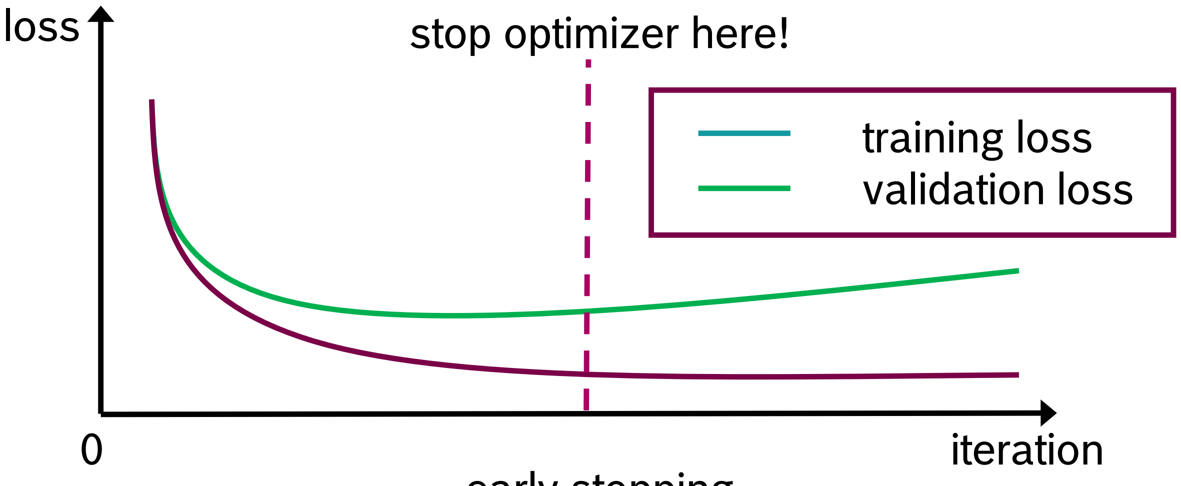
- **Solution:**
  - Compute gradient on a random set of samples, i.e. a **minibatch**
  - Use this as the approximation of the gradient for the full batch

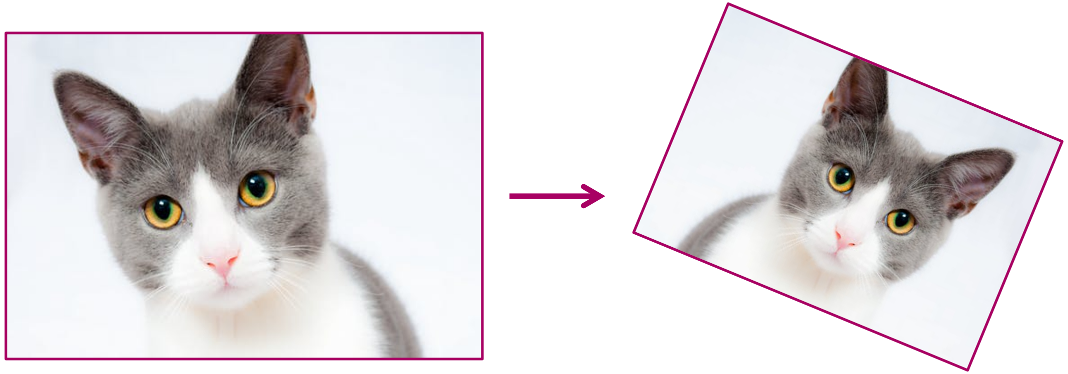
- **Minibatch size:**
  - Increases gradient accuracy (but less than linearly!)
  - Increases parallelism utilization
  - Increases memory utilization (assuming full parallelism)
  - Decreases regularization effect

Optimization
Regularization In Deep Learning (Revisited)

- **Optimizer:**
  - early stopping:
  - minibatch size
  - constrained optimization
- **Data augmentation:**
  - explicit input transformations
  - adversarial training

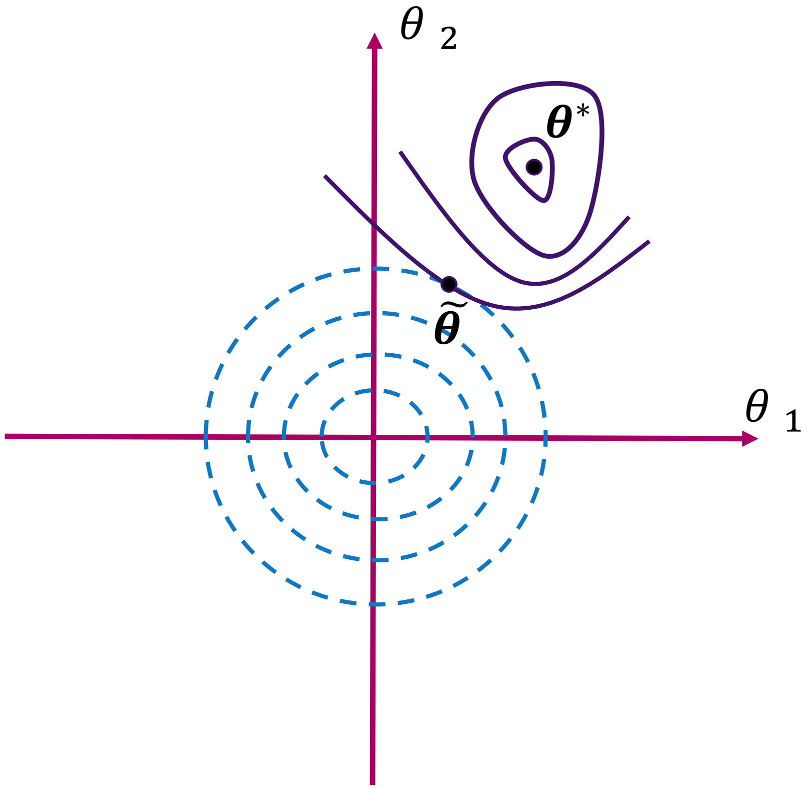


early stopping


explicit input transformation (mirroring, rotation, scaling)

Optimization
Regularization In Deep Learning (Revisited)

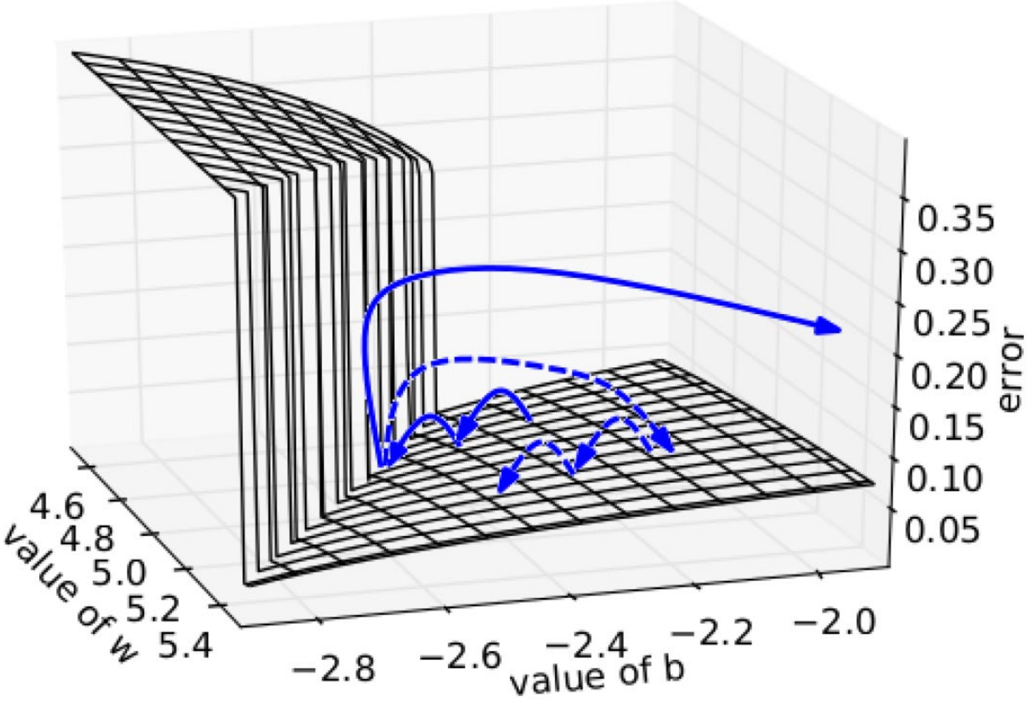
- **Model structure:**
  - sharing parameters
  - trimming parameters
  - multi-task learning
  - dropout
- **Objective function:**
  - weight decay
  - label smoothing



weight decay
(adapted from [1])

Optimization
Meta algorithms: Batch Normalization

- **Problem:**
  - sensitivity to one parameters often depends on others parameters
  - highly nonlinear behavior!
  - dangerous to update parameters at once
- **Solution:**
  - re-parameterize the network
  - add batch normalization layer:
    - computes mean and variance of each feature over the mini-batch
    - for each feature: subtracts mean and divides by variance
  - layer disappears at runtime (collapsed with the conv/fully connected layer)



(adapted from [1])

CONVOLUTIONAL **N**EURAL **N**ETWORKS

Convolutional Neural Networks
Deep Learning Recap

- **Machine Learning:**
  - Search for a program that maps features to correct answers
  - Feature design is hard!

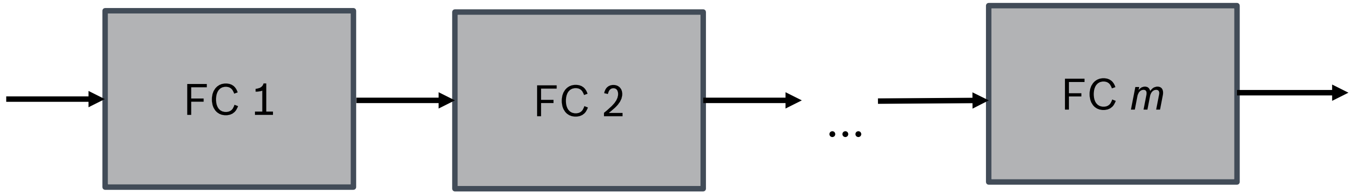
- **End-to-end Learning:**
  - Features are real-world observations
  - Learn several intermediate representation layers

- **Deep Learning:**
  - End-to-end learning with a lot of layers
  - How do we avoid the parameter space explosion? (overfitting)

Convolutional Neural Networks
A First Try: The Multi-Layer Perceptron

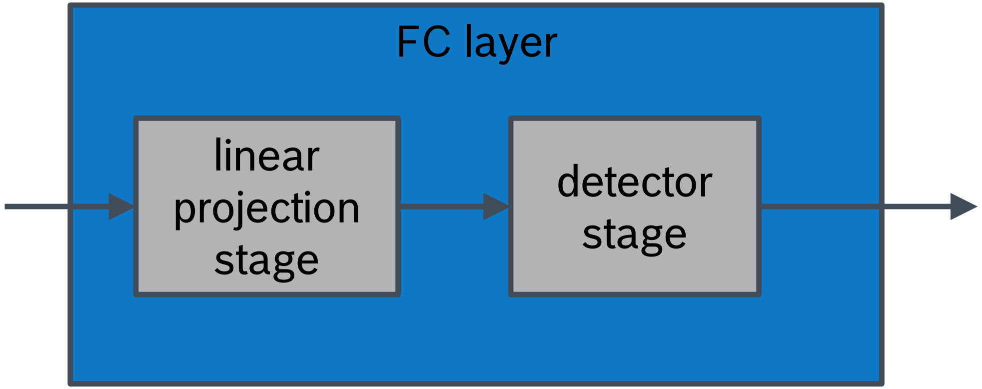
- **Idea:**
  - Level 1: match the input image to a set of patterns
  - Level 2: match the level 1 features to a set of patterns
  - …

- **Implementation:**
  - Fully Connected (FC) Layers



Convolutional Neural Networks
The Stages of an FC Layer

- **Stages:**
  - **Linear projection:** project feature vector $\mathbf{x}$ along a learned direction $\mathbf{w}$
  - **Detector:** is the projection y “strong enough” for a pattern match? (match strength z)



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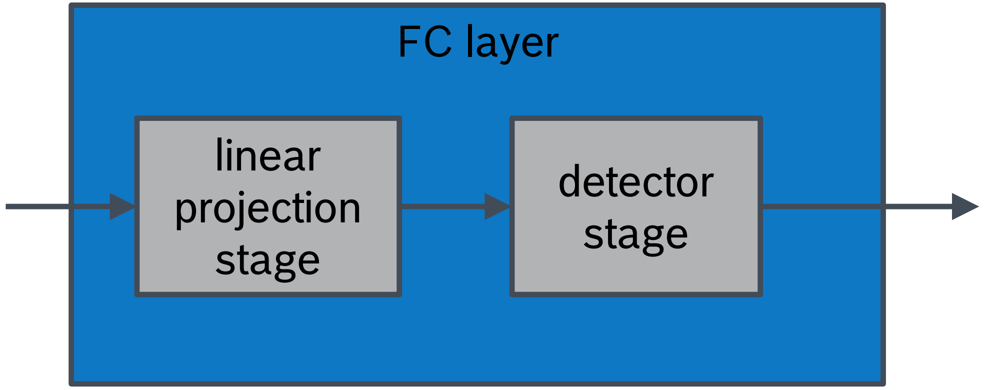

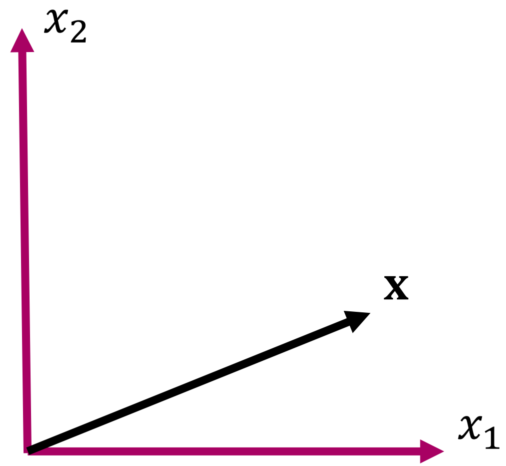

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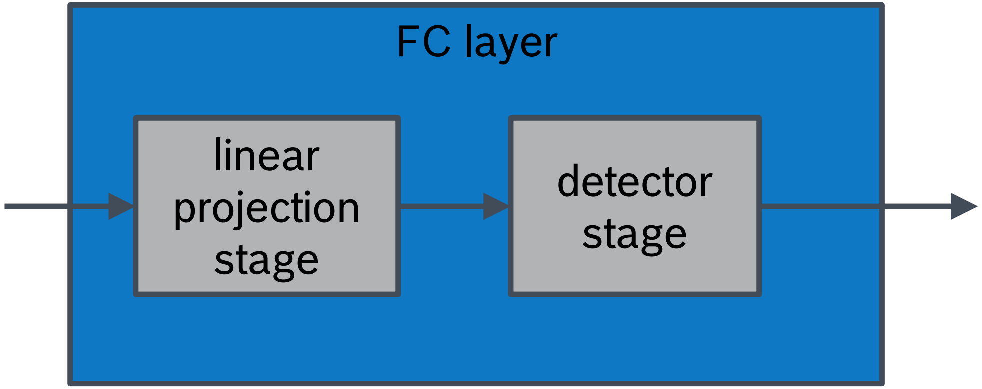

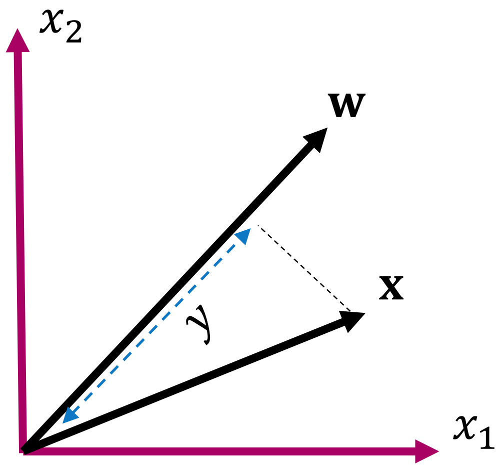

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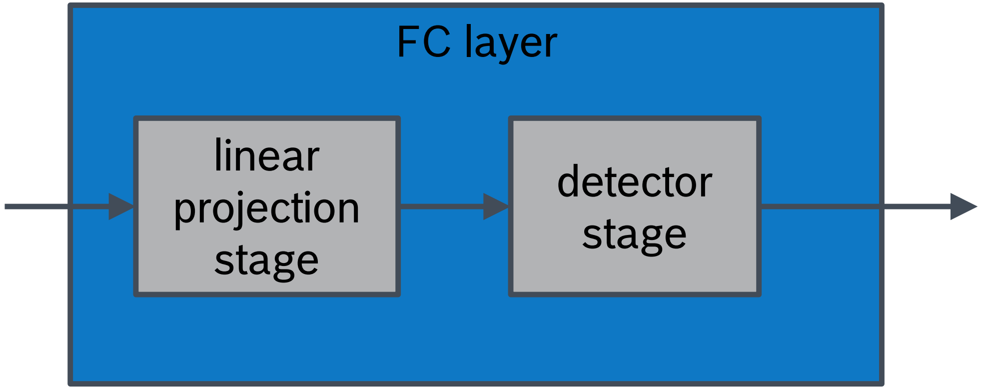
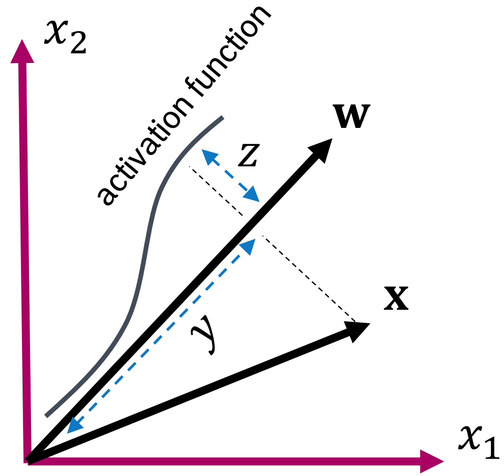
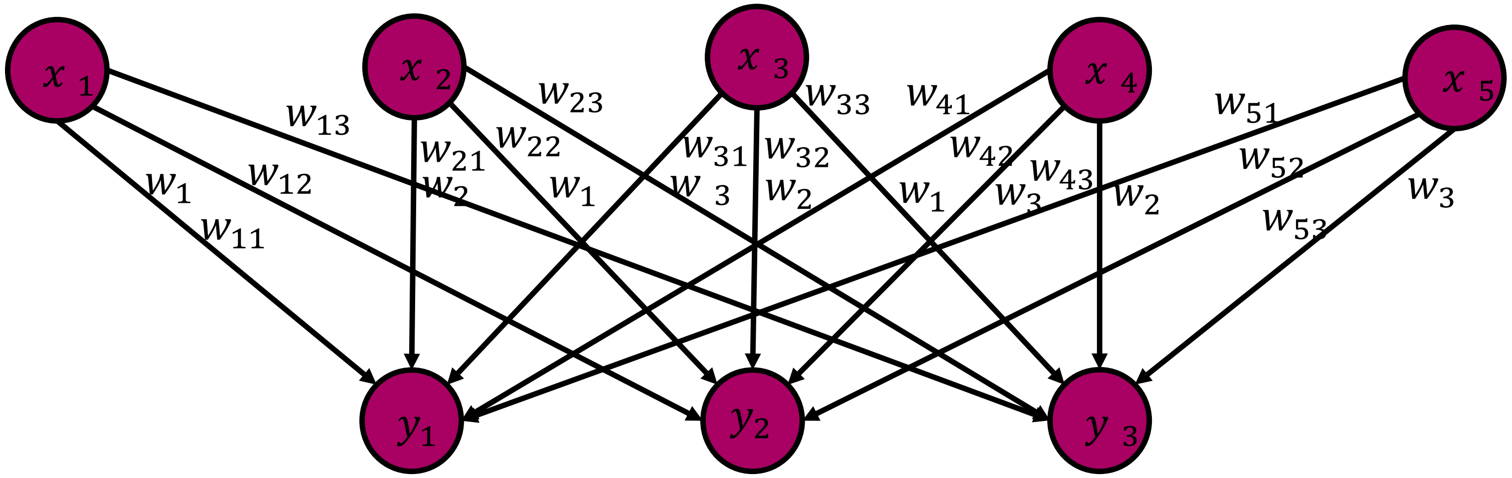


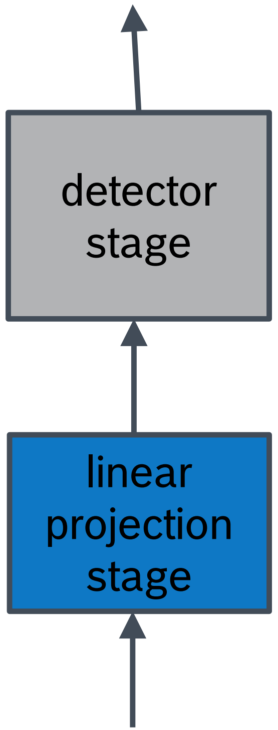


Convolutional Neural Networks
FC Layer: The Linear Projection Stage

- **Input:**
  - plain feature vector
  - do not exploit spatial/temporal structure

- **Output:**
  - each element a different linear combination of the input elements: $y_j = \sum_{i=1}^{N_{\text{in}}} w_{ij} \cdot x_i$

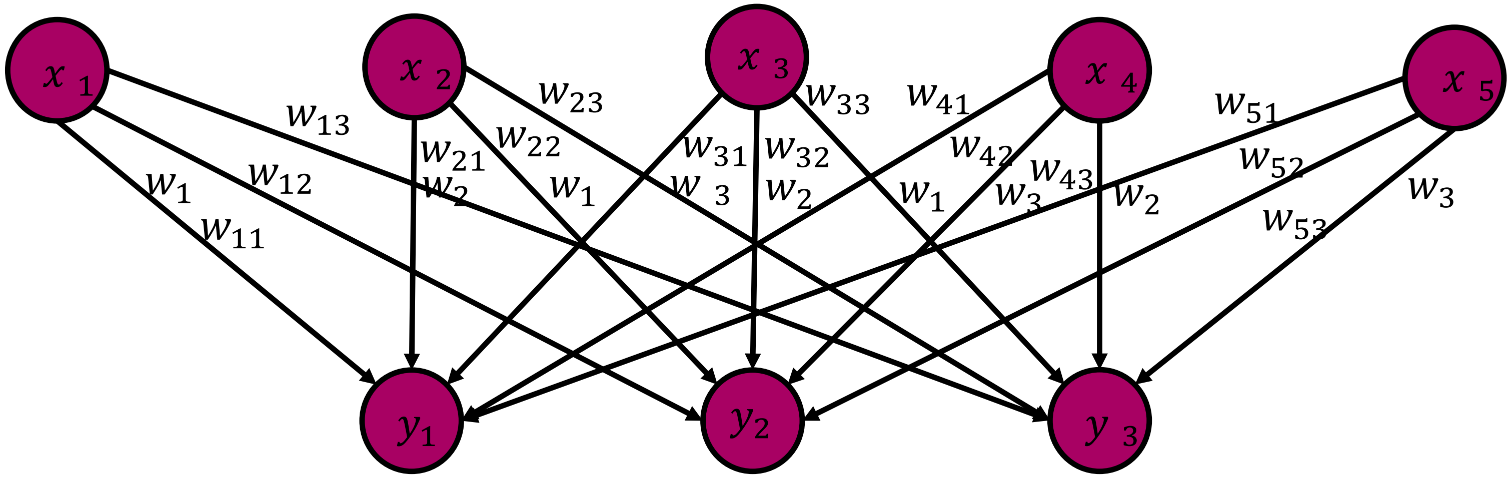


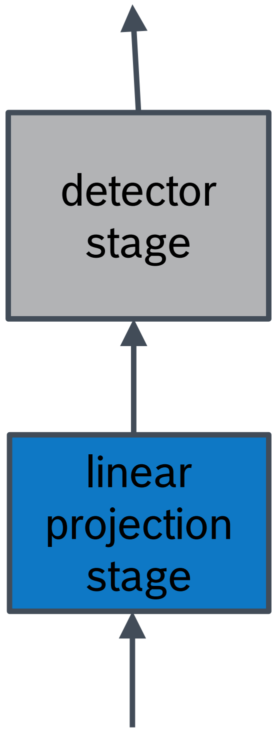


Convolutional Neural Networks
FC Layer: Complexity

- **Parameters:**
  - $N_{\text{in}} \cdot N_{\text{out}}$
  - *Example: 1 million parameters for a 256x256 input image!*

- **Time:**
  - Multiply-and-accumulates (MACs): $N_{\text{in}} \cdot N_{\text{out}}$





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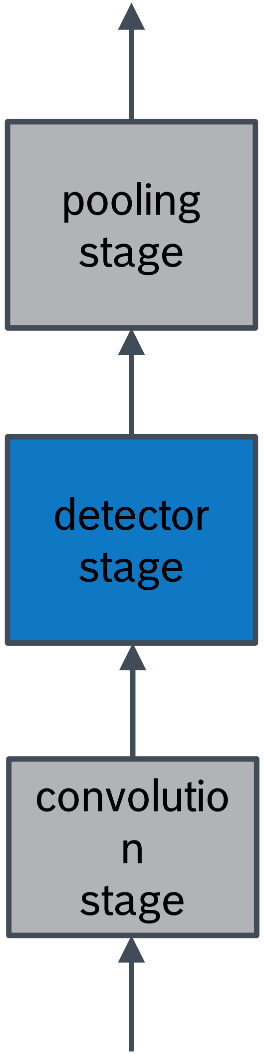
Convolutional Neural Networks
The Detector Stage

- **Requirements:**
  - Highly nonlinear behavior (soft thresholding)
  - Balance modeling power, efficiency, ease of optimization

- **State-of-the-art:**
  - Most obvious choices do not work well! (e.g. softplus)
  - Open research field



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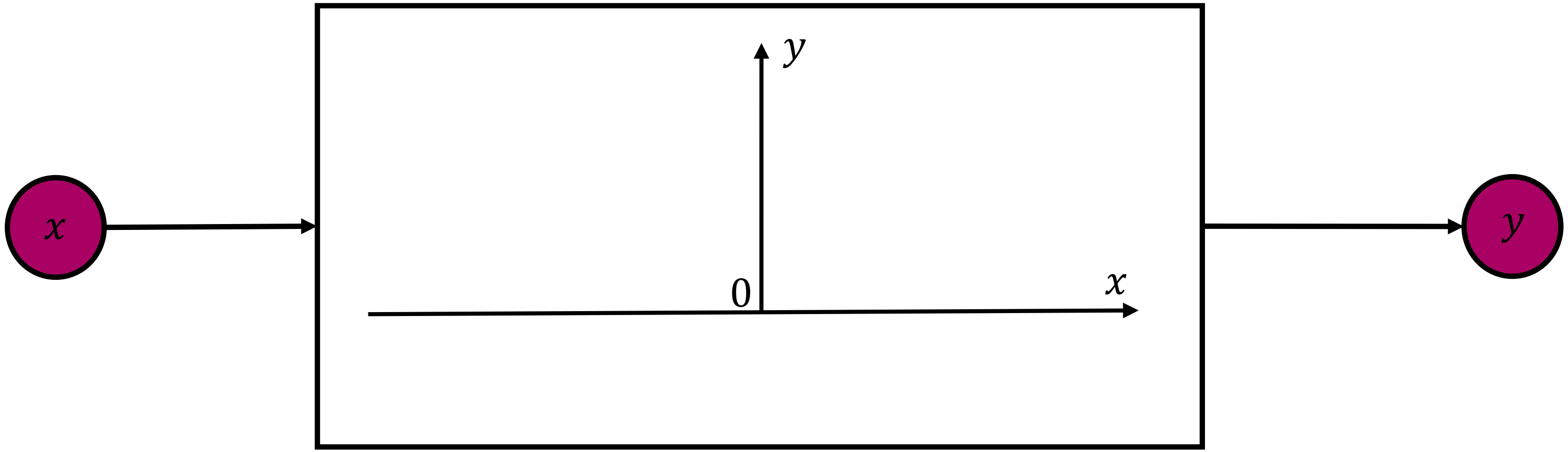

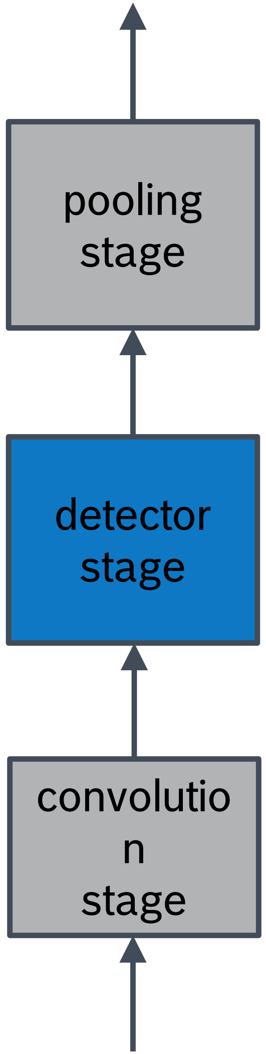

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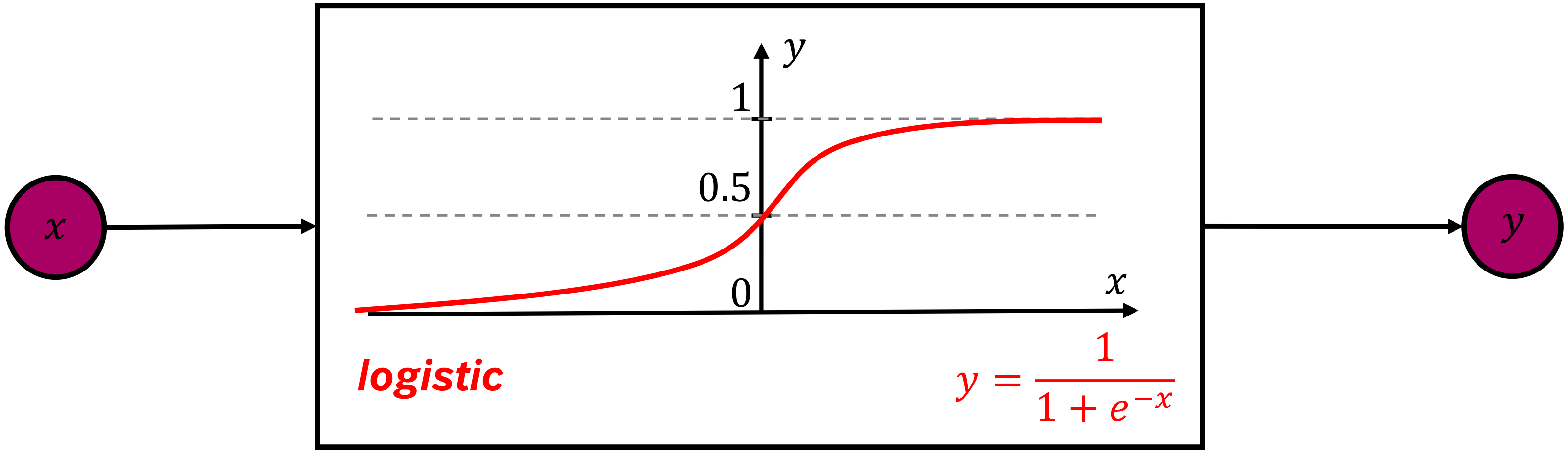

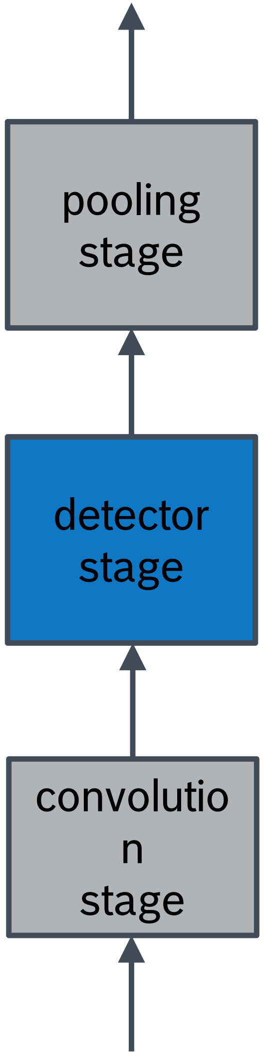

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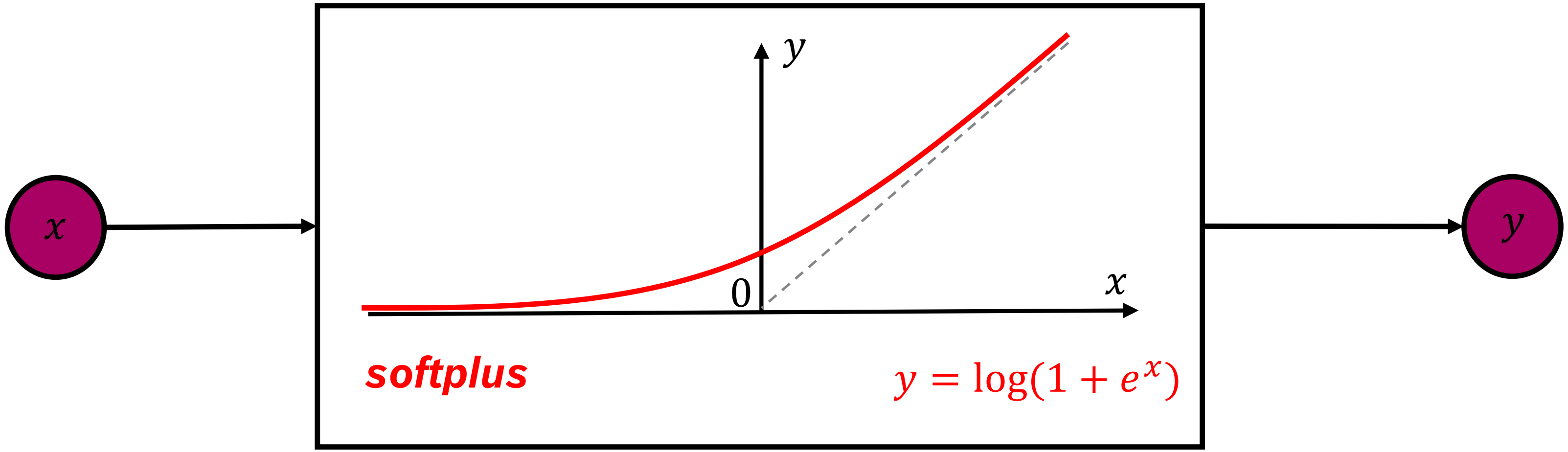

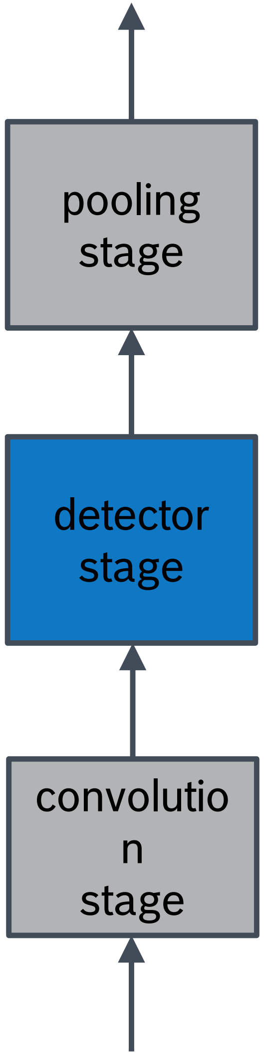

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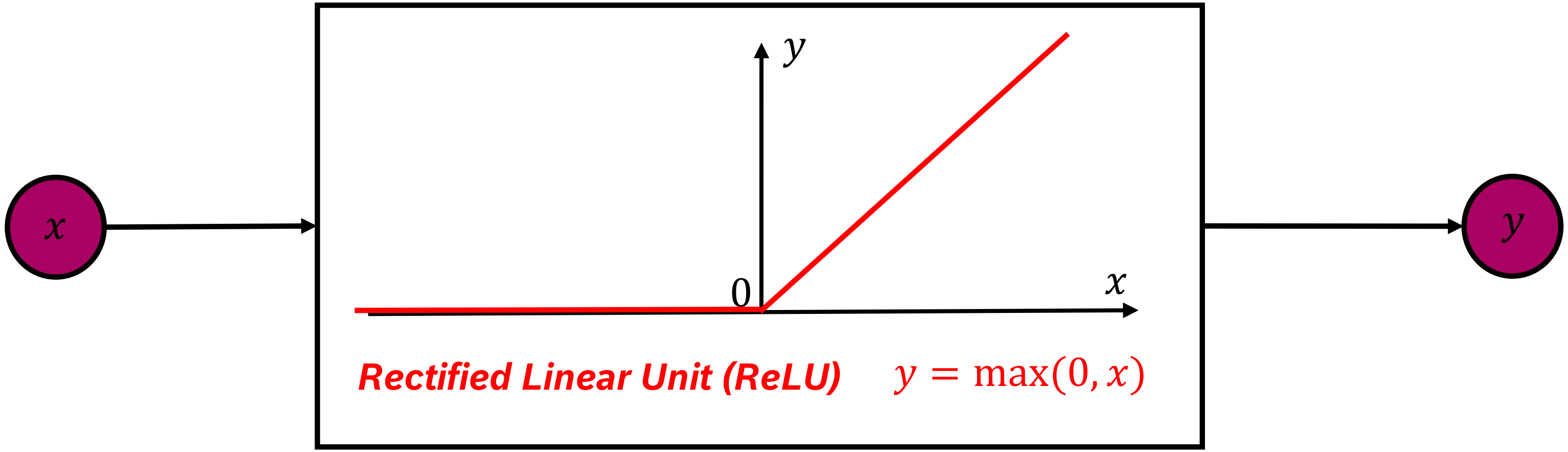
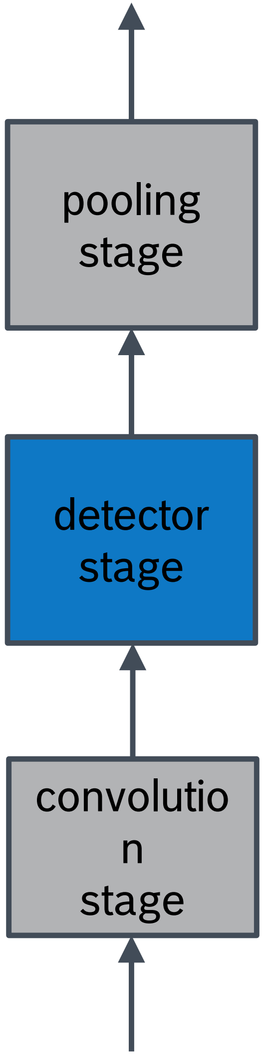
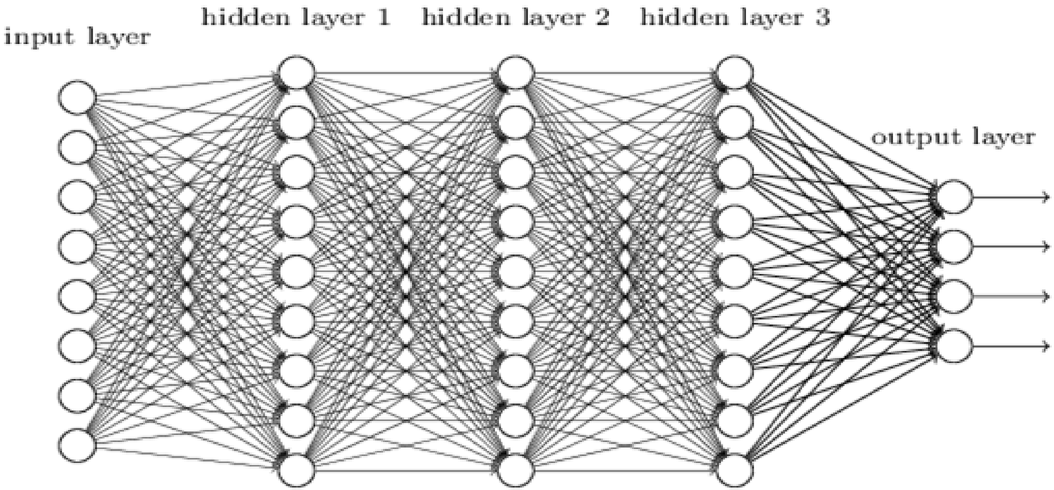




Convolutional Neural Networks
Does the Multi Layer Perceptron Work?

- **Rarely!** ☹

- **Problems:**
  - Huge number of parameters
  - Low spatial invariance



Convolutional Neural Networks
Intuition

- **Solution:**
  - Scan for smaller local patterns and successively group them into larger ones
  - Introduce Convolutional (CONV) Layers

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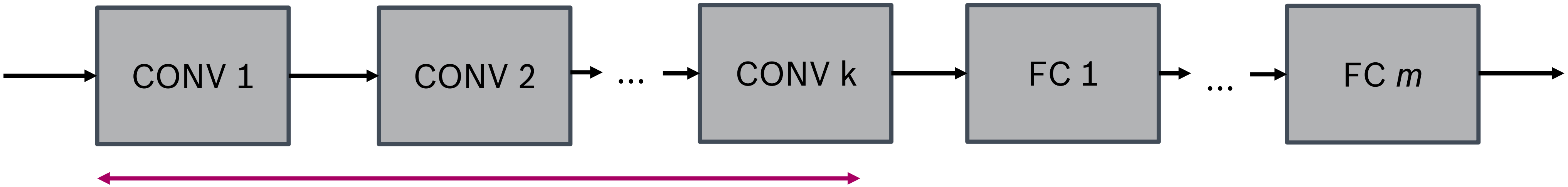

locate spatial/temporal patterns
(edges, circular patterns, nose, mouth, etc.)

many layers but few parameters per layer

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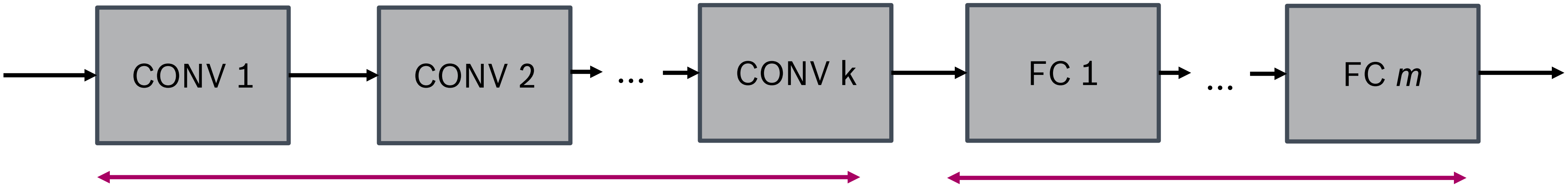


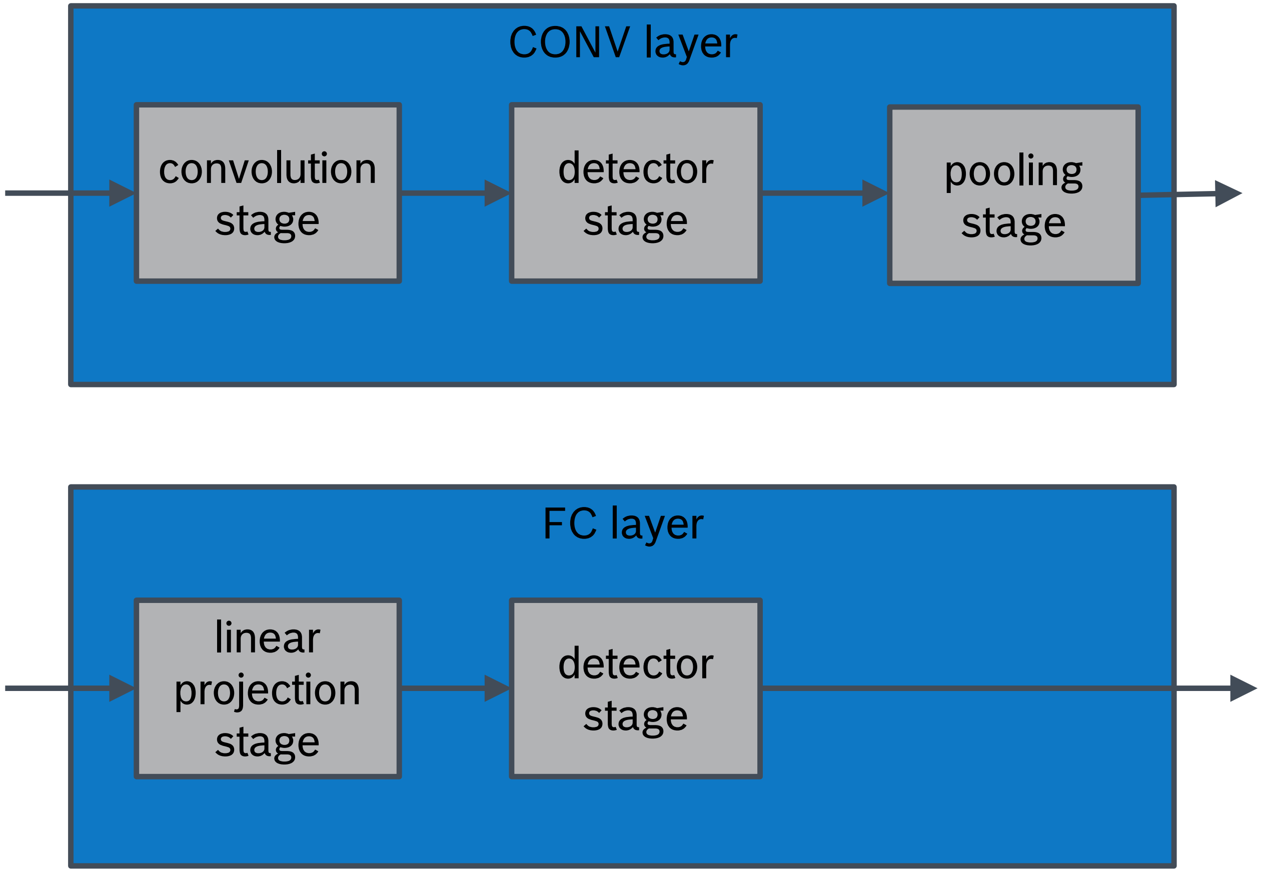
locate spatial/temporal patterns
(edges, circular patterns, nose, mouth, etc.)

many layers but few parameters per layer

recognize the presence of abstract patterns
(face-frontal, face-profile-left, face, etc.)

many parameters per layer but few layers

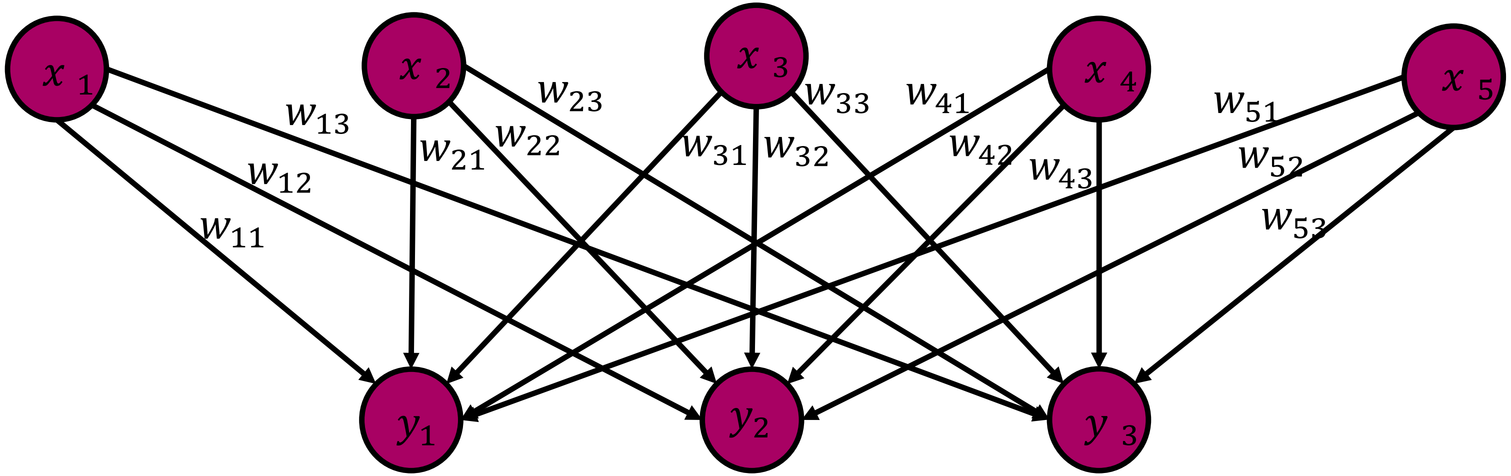
Convolutional Neural Networks
Layer Stages

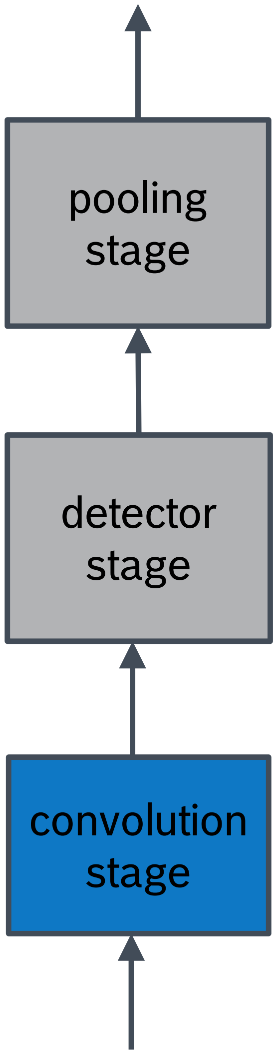


Convolutional Architectures
CONV Layer: The Convolution Stage (1D case)

- **Idea:**
  - Exploit grid-like topology in real data (time series, images)
  - Replace fully connected topology with convolution (or correlation):

$$y_j = \sum_{i=1}^{N_\mathrm{w}} w_i \cdot x_{i+j-1}$$





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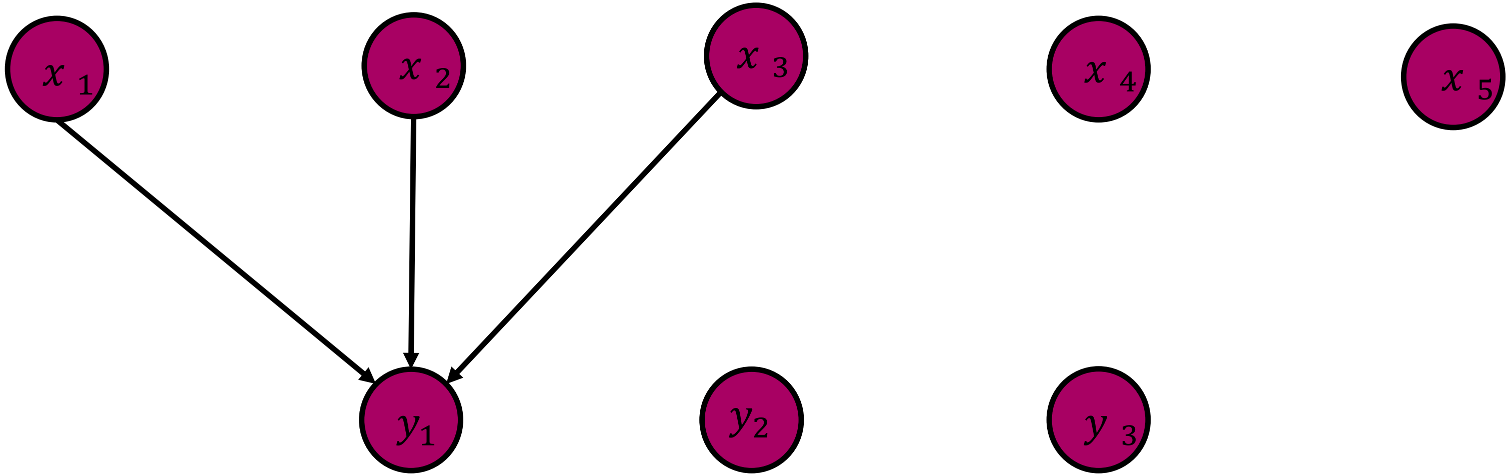

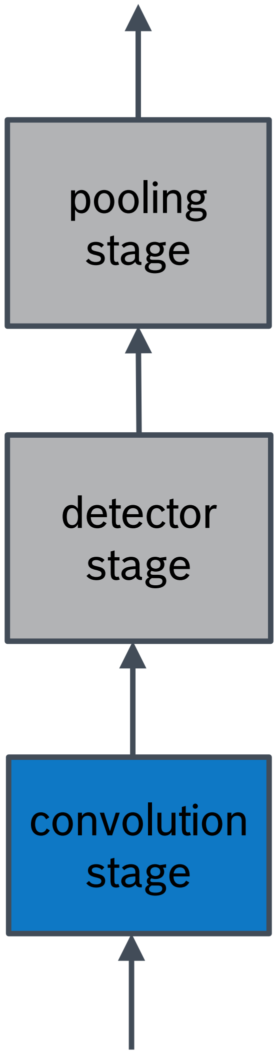

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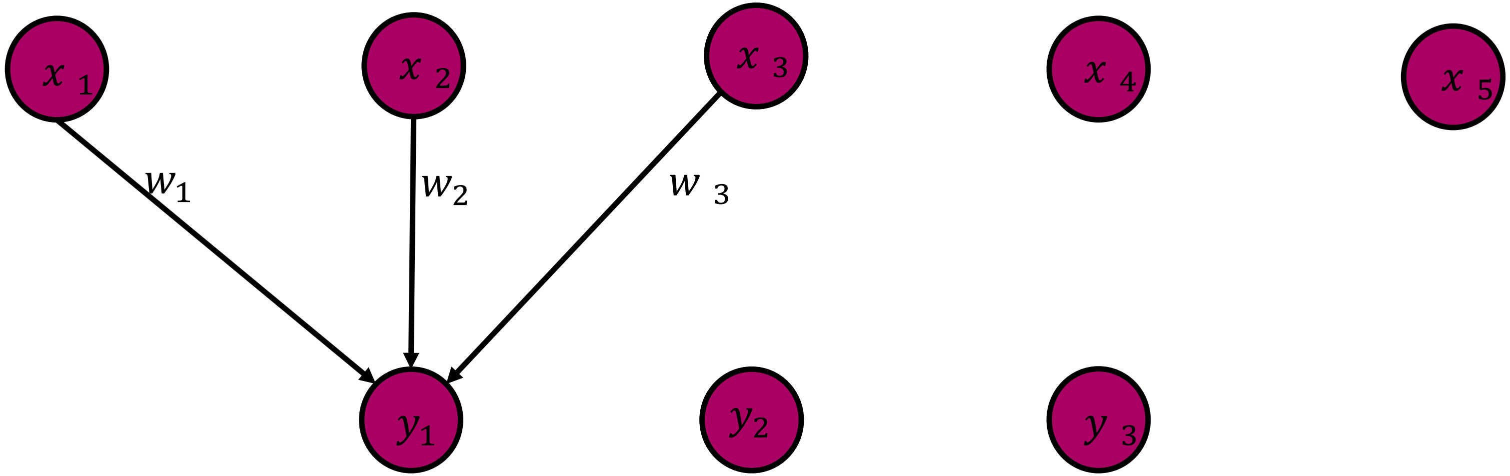

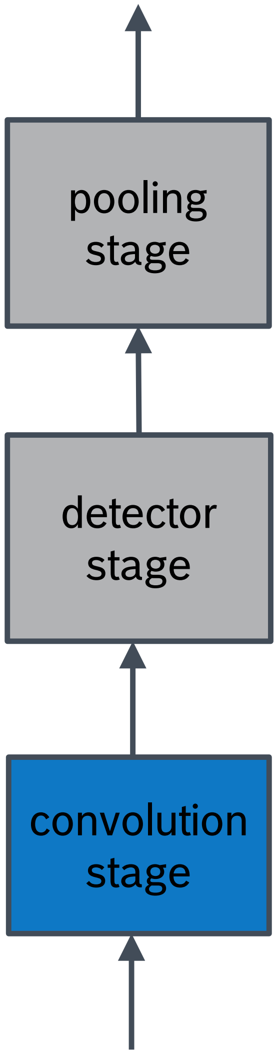

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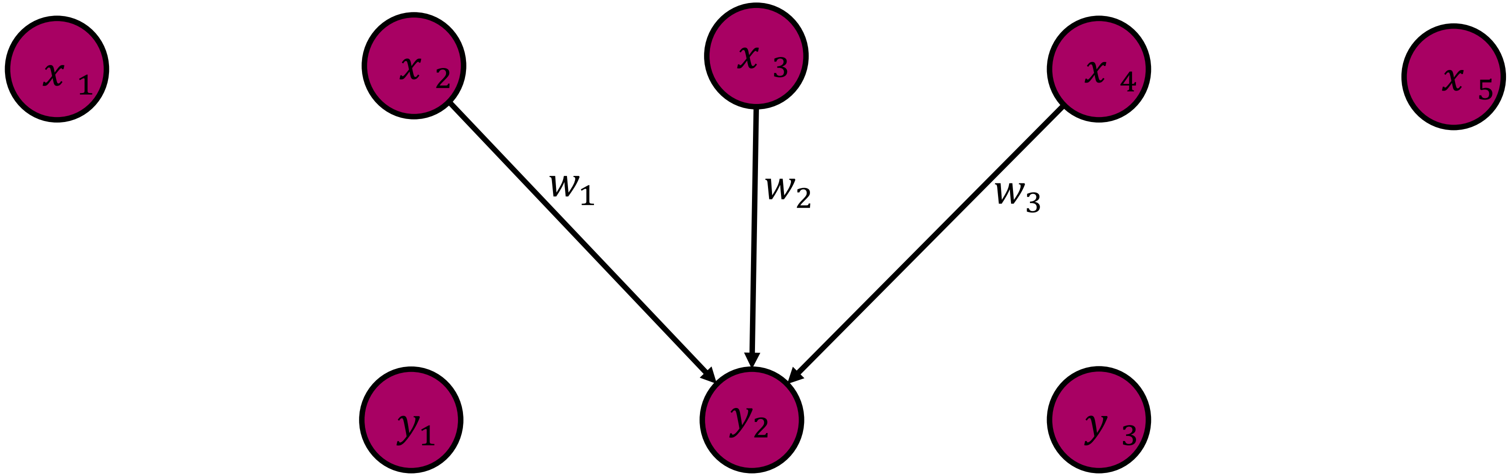

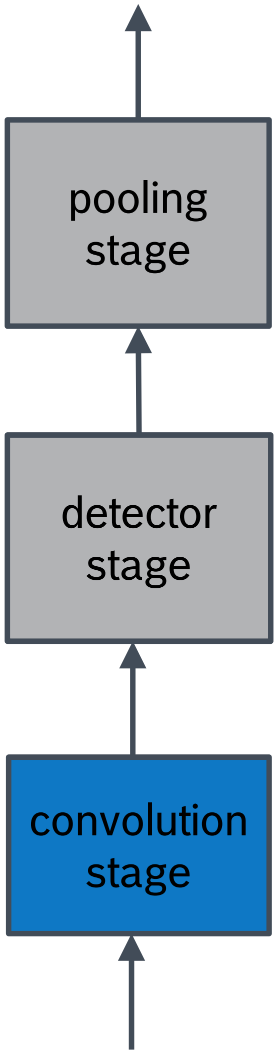

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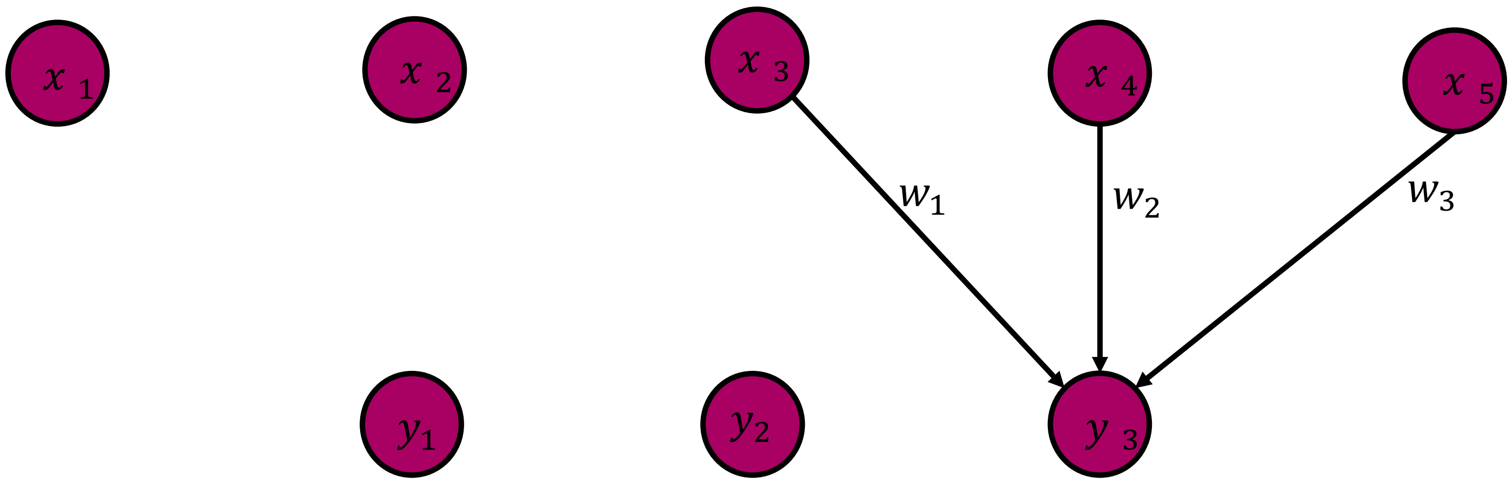

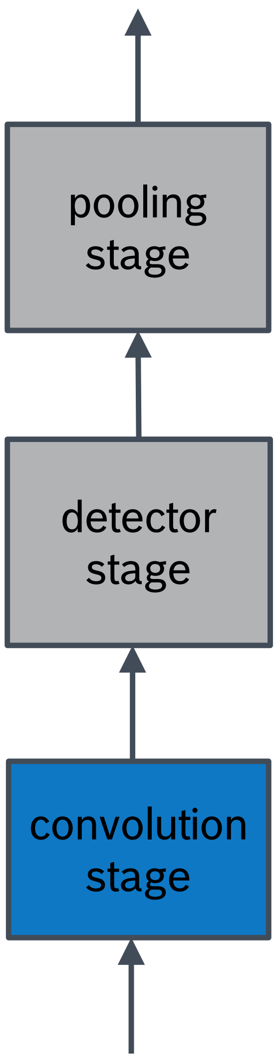

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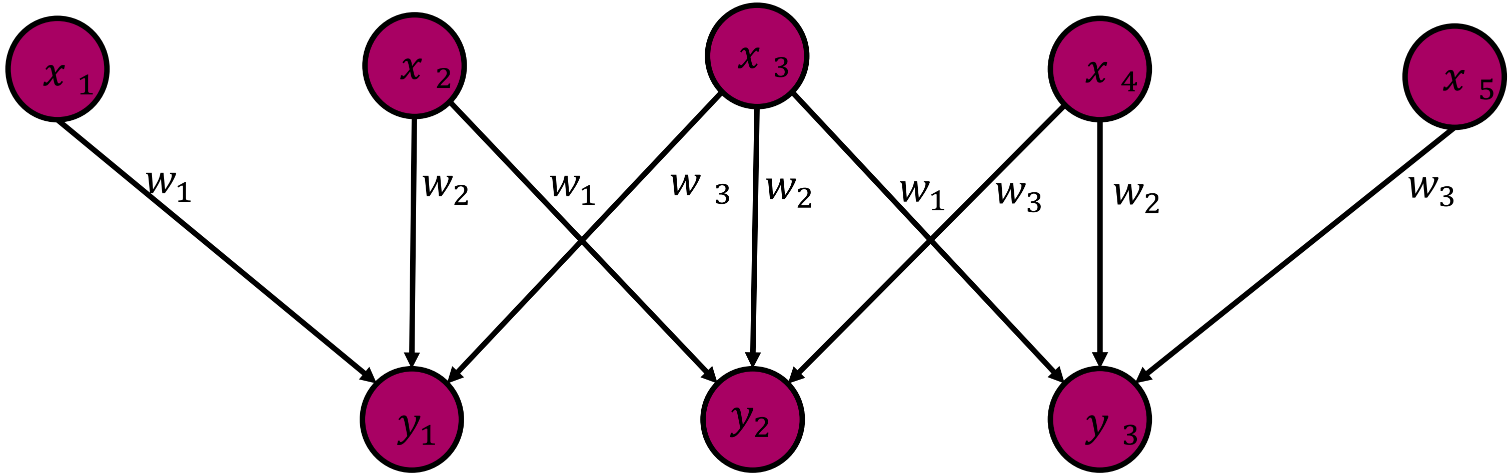
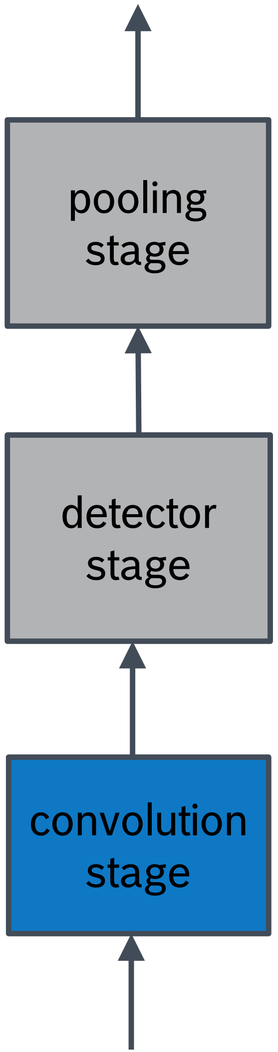
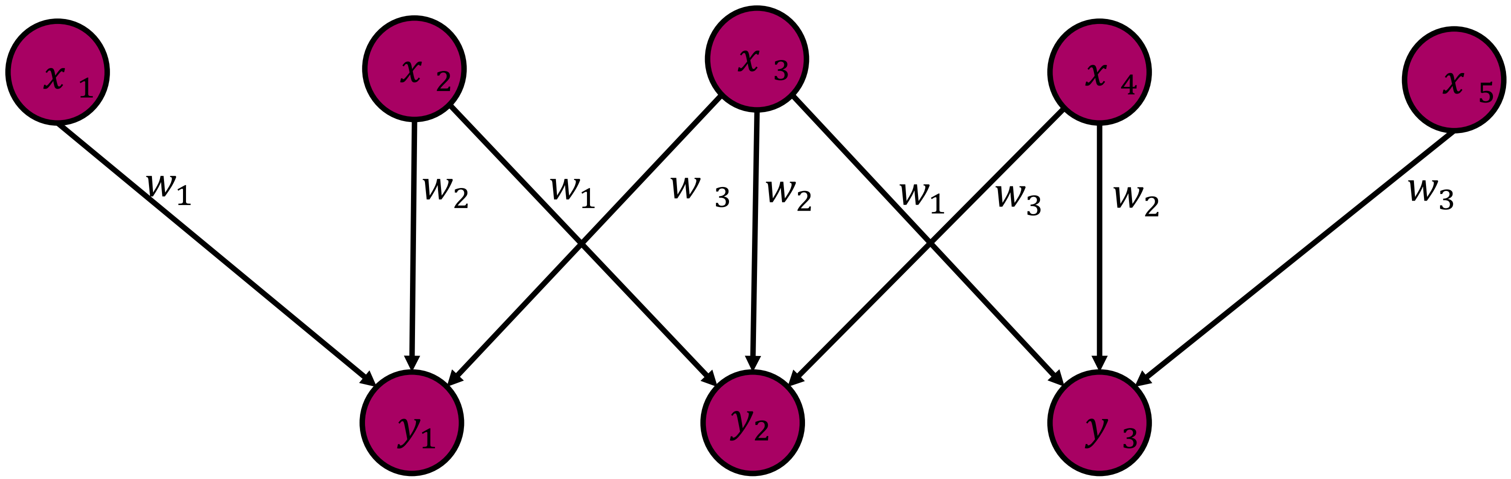
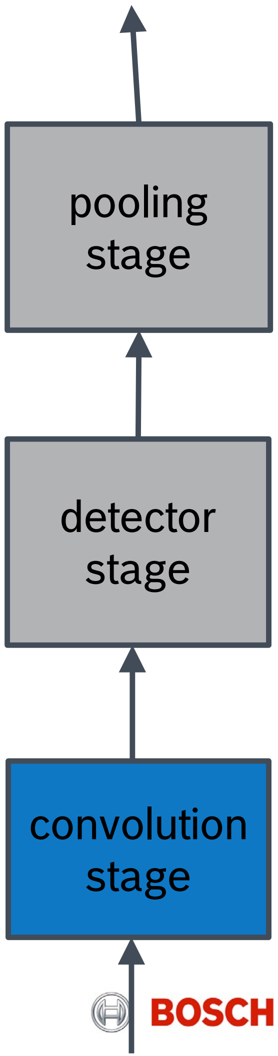




Convolutional Neural Networks
CONV Layer: The Convolution Stage (1D case)

- **Number of Parameters:** K_w (does not depend on the input size!)
  - We have actually regularized the FC layer!
  - Parameter trimming: $w_{ij} = 0, \text{for } 0 \leq i - j < N_\mathrm{w}$
  - Parameter tying: $w_{ij} = w_{kl}, \text{for } (k - i) = (l - j)$





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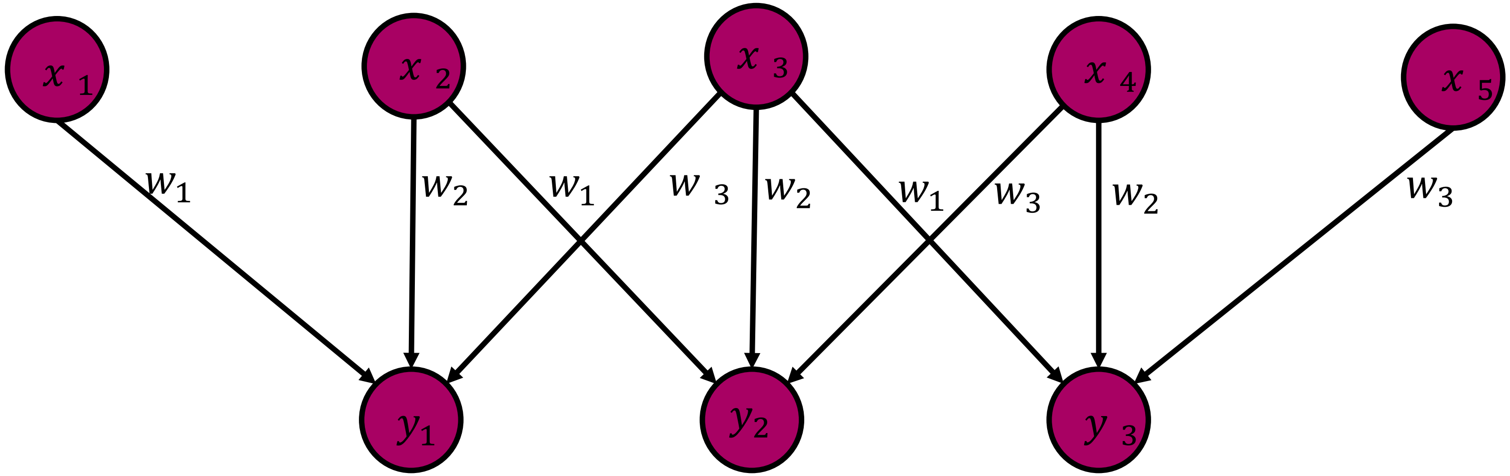
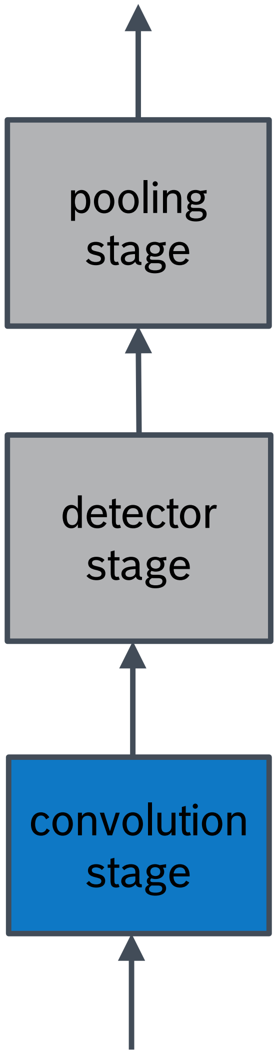
Convolutional Neural Networks
CONV Layer: The Convolution Stage (1D case)

- **Time Complexity:** $N_{\mathrm{w}} \cdot N_{\mathrm{out}}$ MACs

What is the speedup over a 1D Fully connected layer with the same number of inputs?





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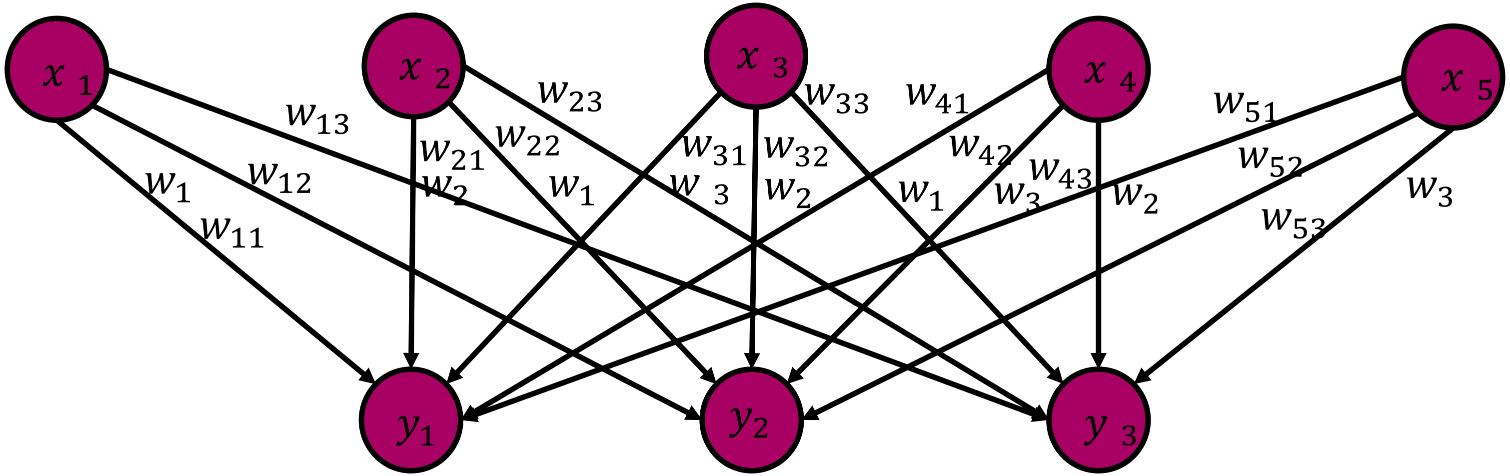

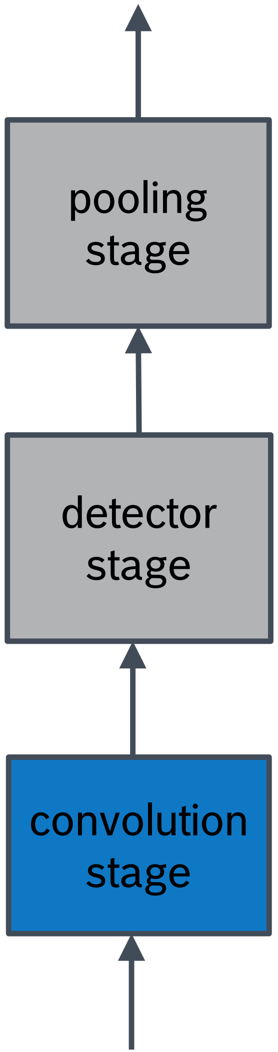

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Convolutional Neural Networks
CONV Layer: The Convolution Stage (1D case)

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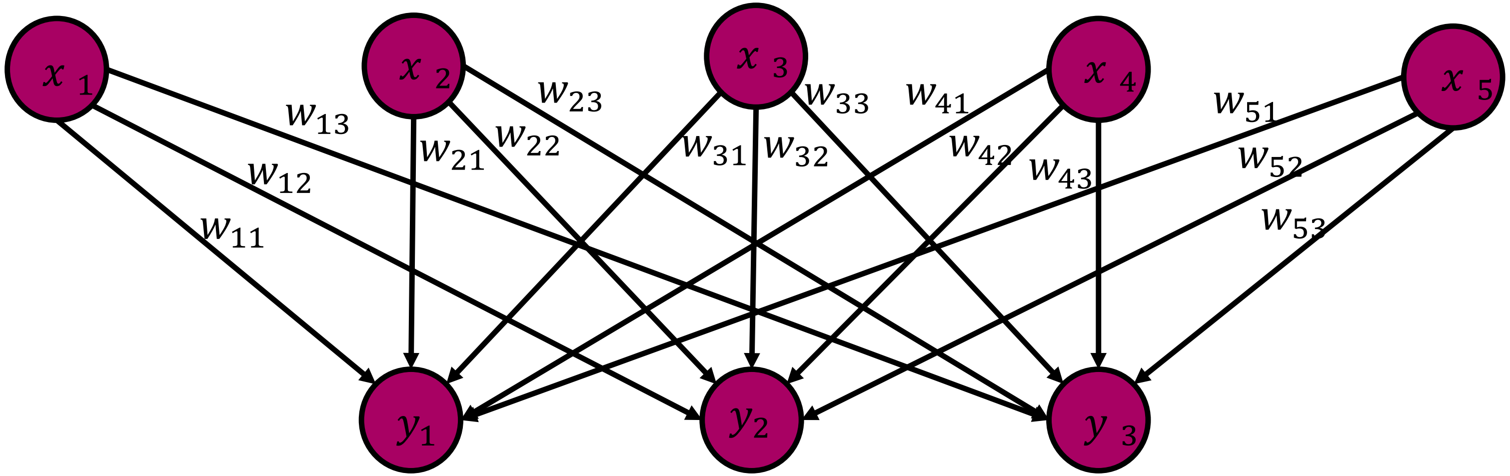

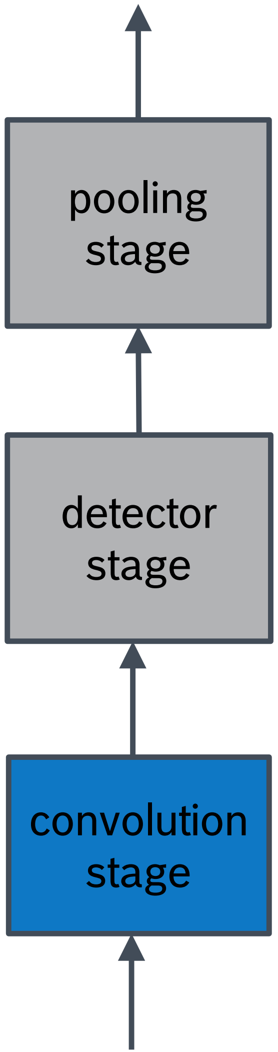

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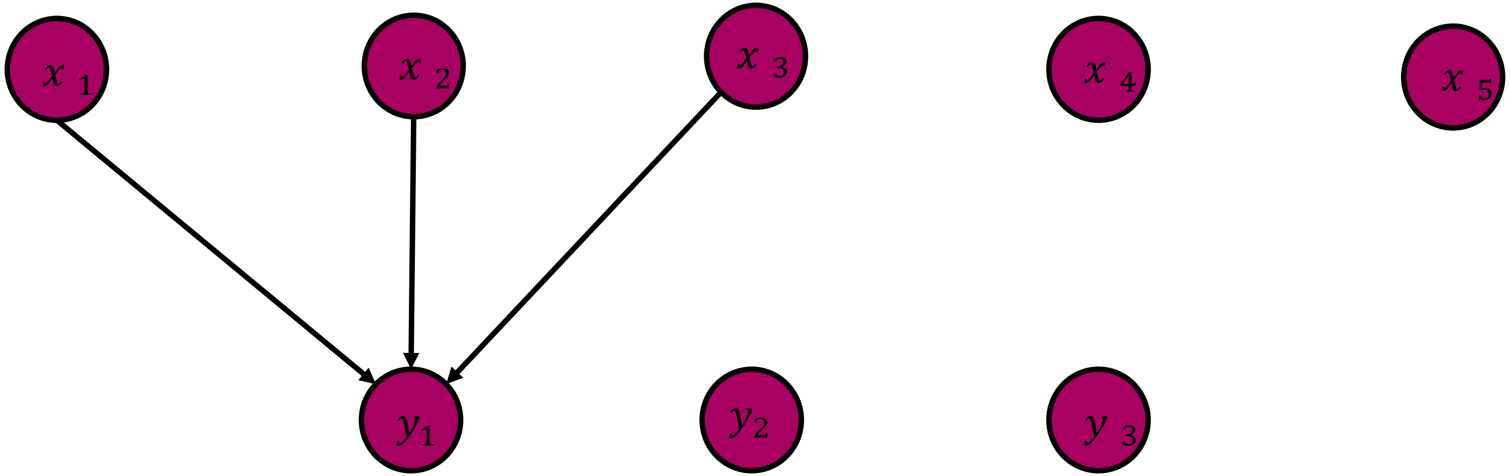

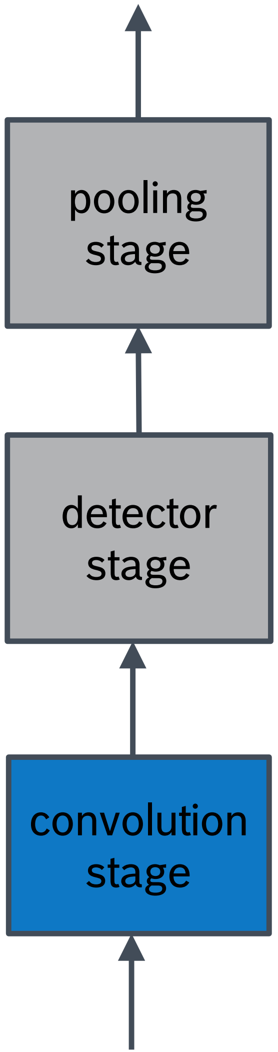

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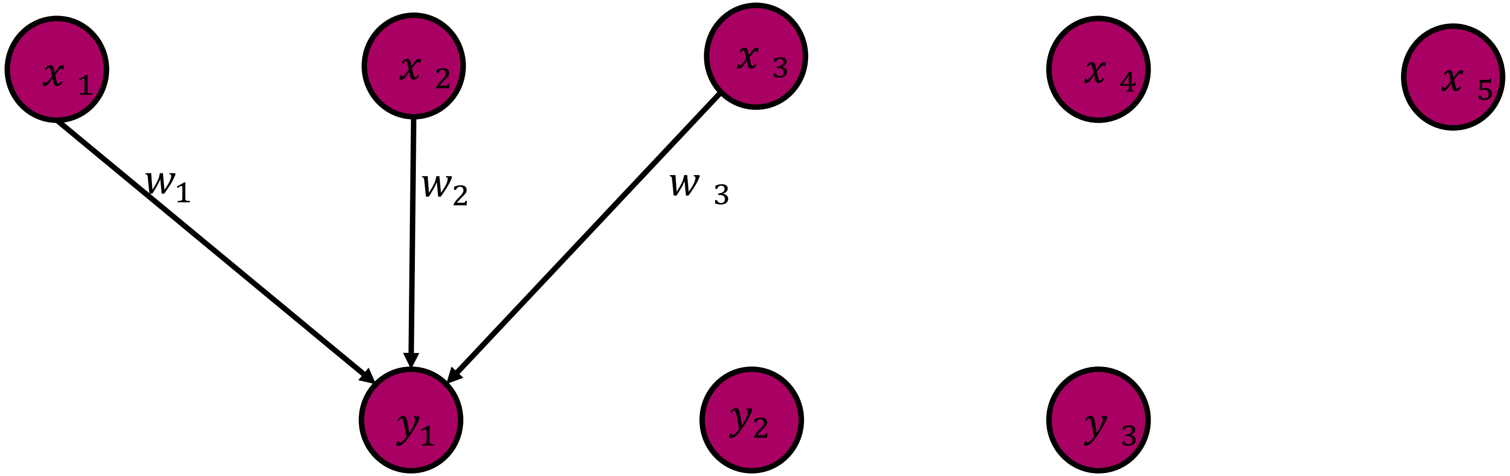

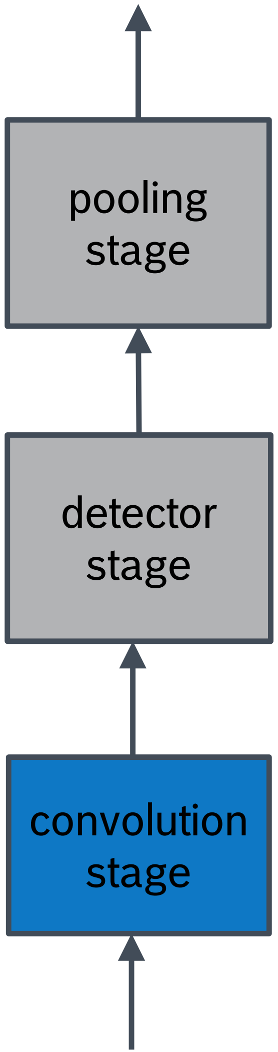

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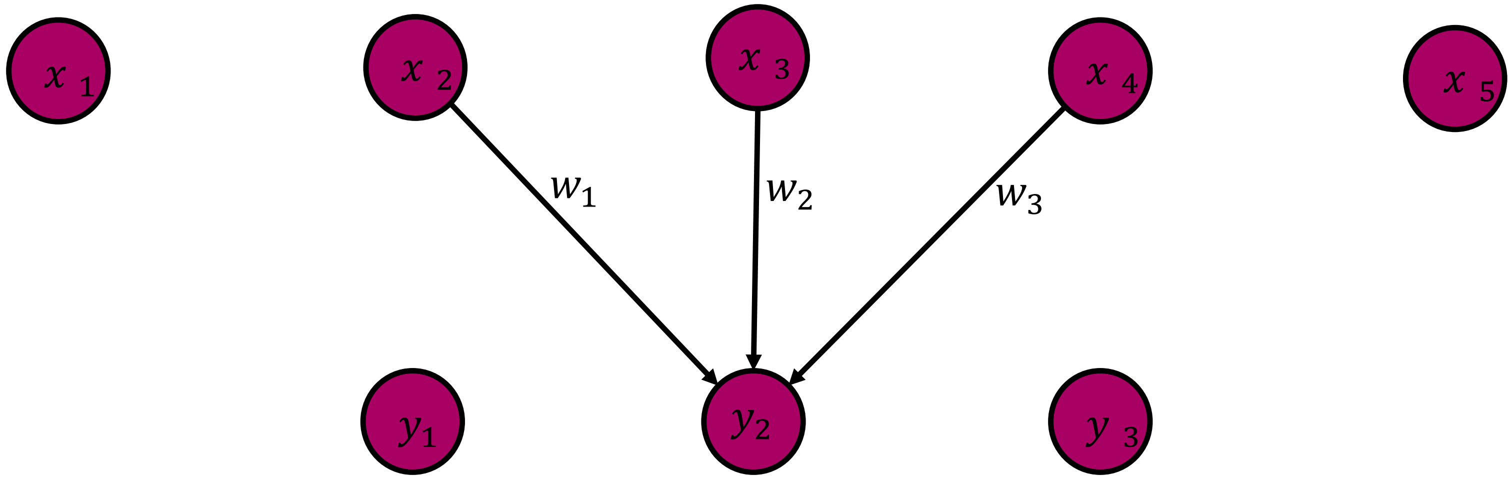

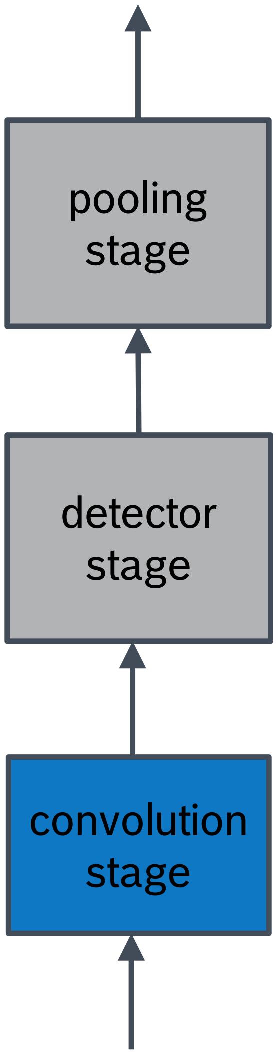

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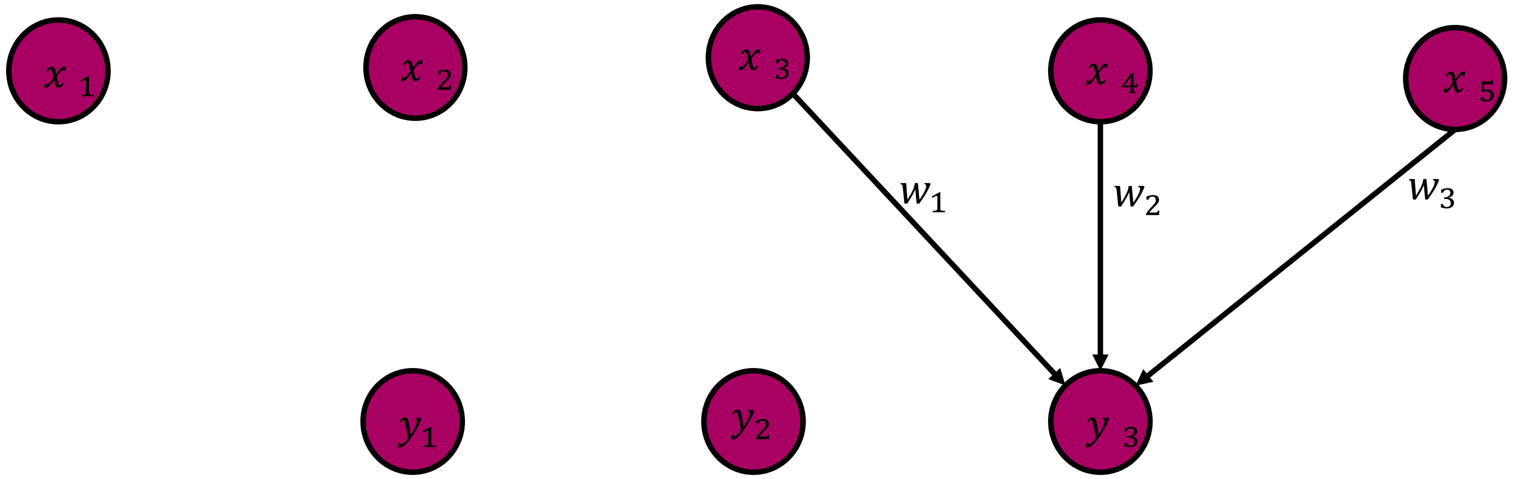

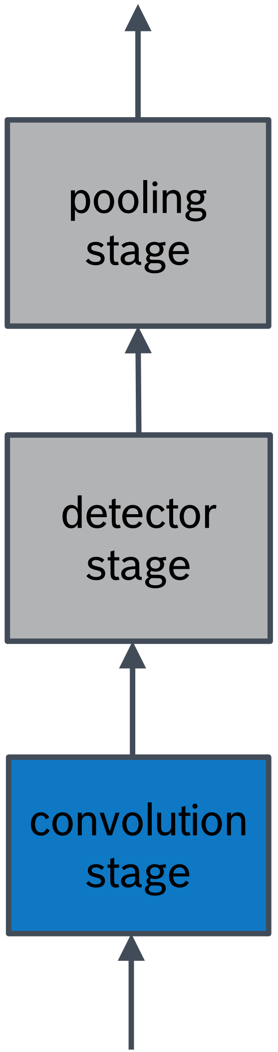

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Convolutional Neural Networks

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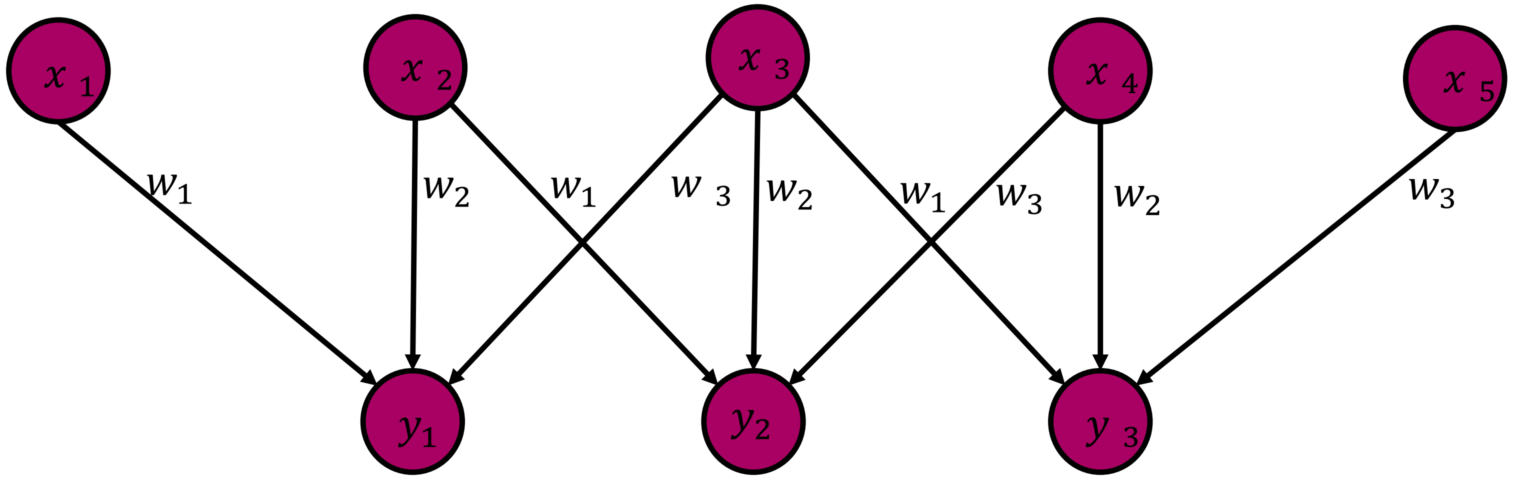

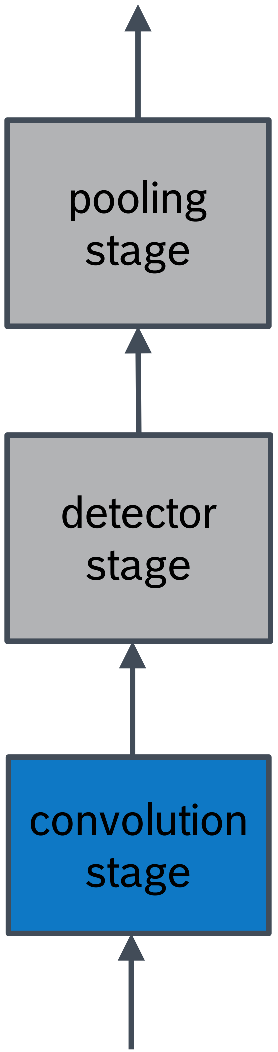

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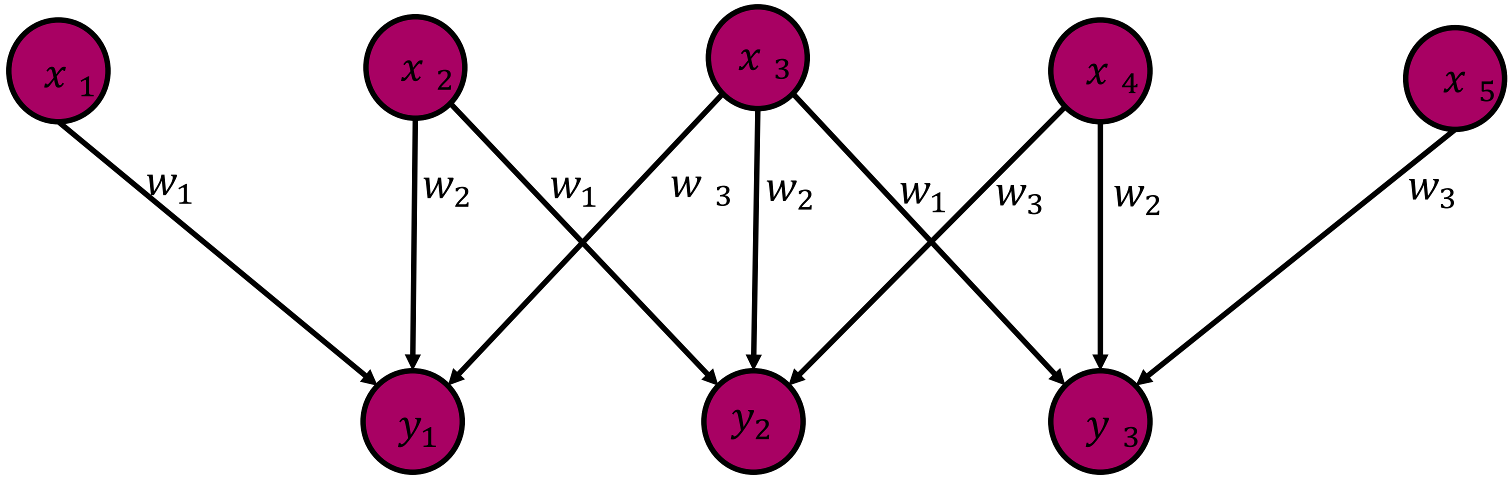

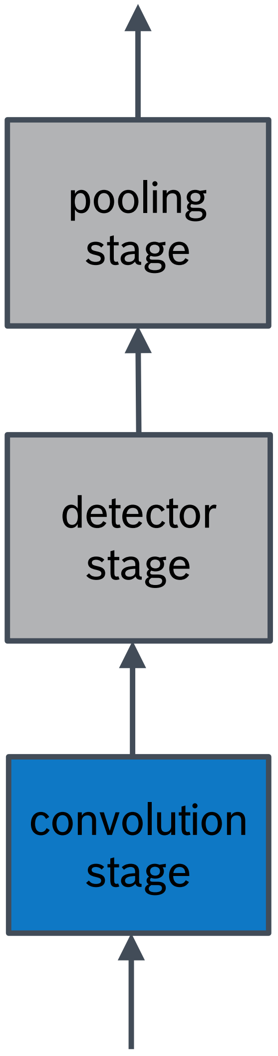

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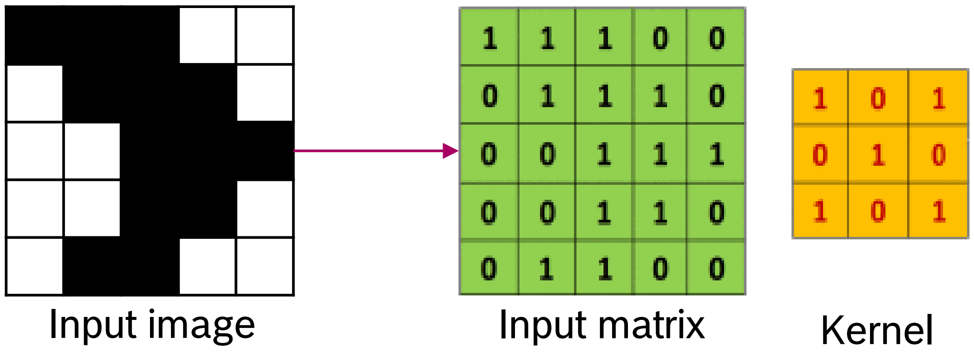
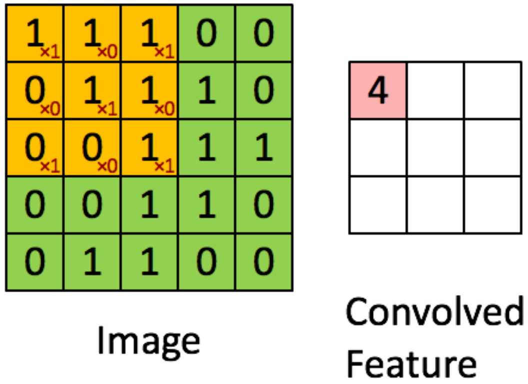
Convolutional Neural Networks
CONV Layer: The Convolution Stage (2D case)

- **Input:** $W_{\mathrm{in}} \times H_{\mathrm{in}}$ matrix (*e.g.* binary image)
- **Parameters:** $W_{\mathrm{k}} \times H_{\mathrm{k}}$ matrix (filter)
- **Operation:**
  - Slide the kernel over the input matrix
  - At each position calculate element wise multiplication
  - Calculate the sum of products
- **Output:**
  - $W_{\mathrm{out}} \times H_{\mathrm{out}}$ matrix (activation map)

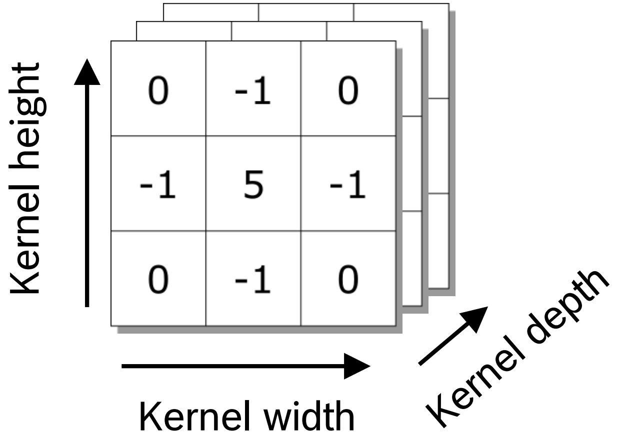


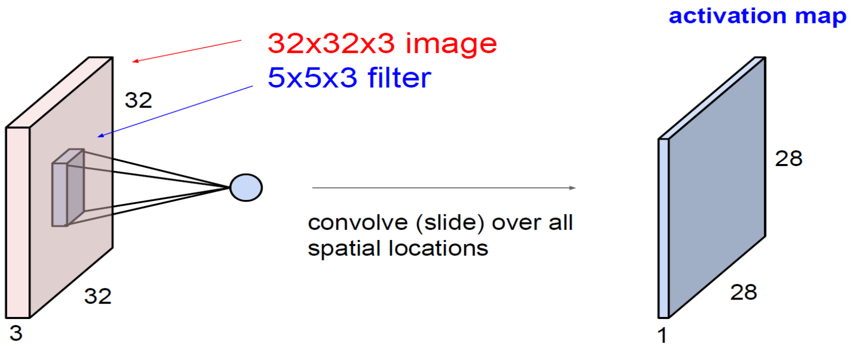


Source: http://deeplearning.stanford.edu/wiki/index.php/Feature_extraction_using_convolution

Convolutional Neural Networks
CONV Layer: The Convolution Stage (3D input)

- **Input:** $D_{\text{in}} \times W_{\text{in}} \times H_{\text{in}}$ tensor (D_{in} stacked matrices)
  - D_{in} is the depth of the input (*e.g.* 3 for an RGB image)
- **Parameters:** $D_{\text{in}} \times W_{\text{k}} \times H_{\text{k}}$ matrix (kernel)
  - Must have the same depth as the input
- **Operation:**
  - Slide the kernel over the width and height of the input
  - At each position calculate element wise multiplication
  - Calculate the sum of products
  - This is still 2D convolution (we do **not** slide along depth!)
- **Output:** $W_{\text{out}} \times H_{\text{out}}$ matrix (depth 1)





Source: https://leonardoaraujosantos.gitbooks.io/artificial-inteligence/content/convolutional_neural_networks.html

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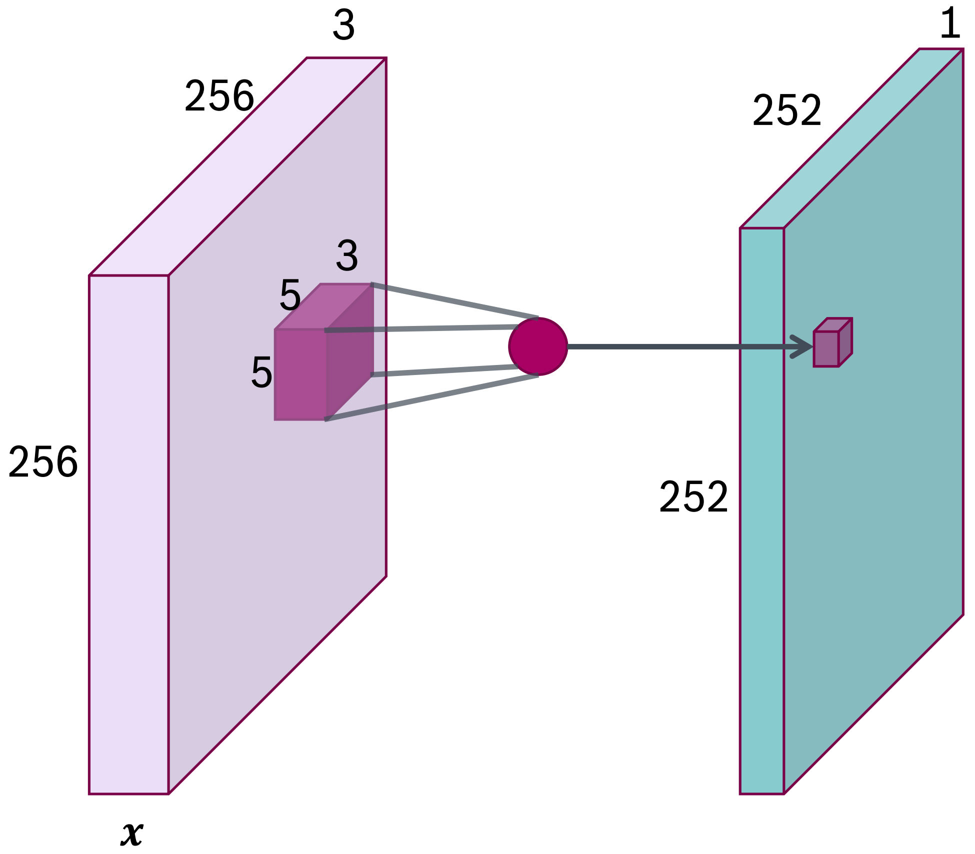
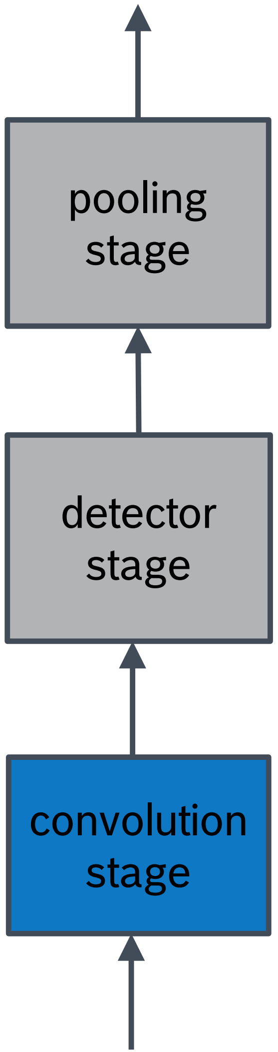
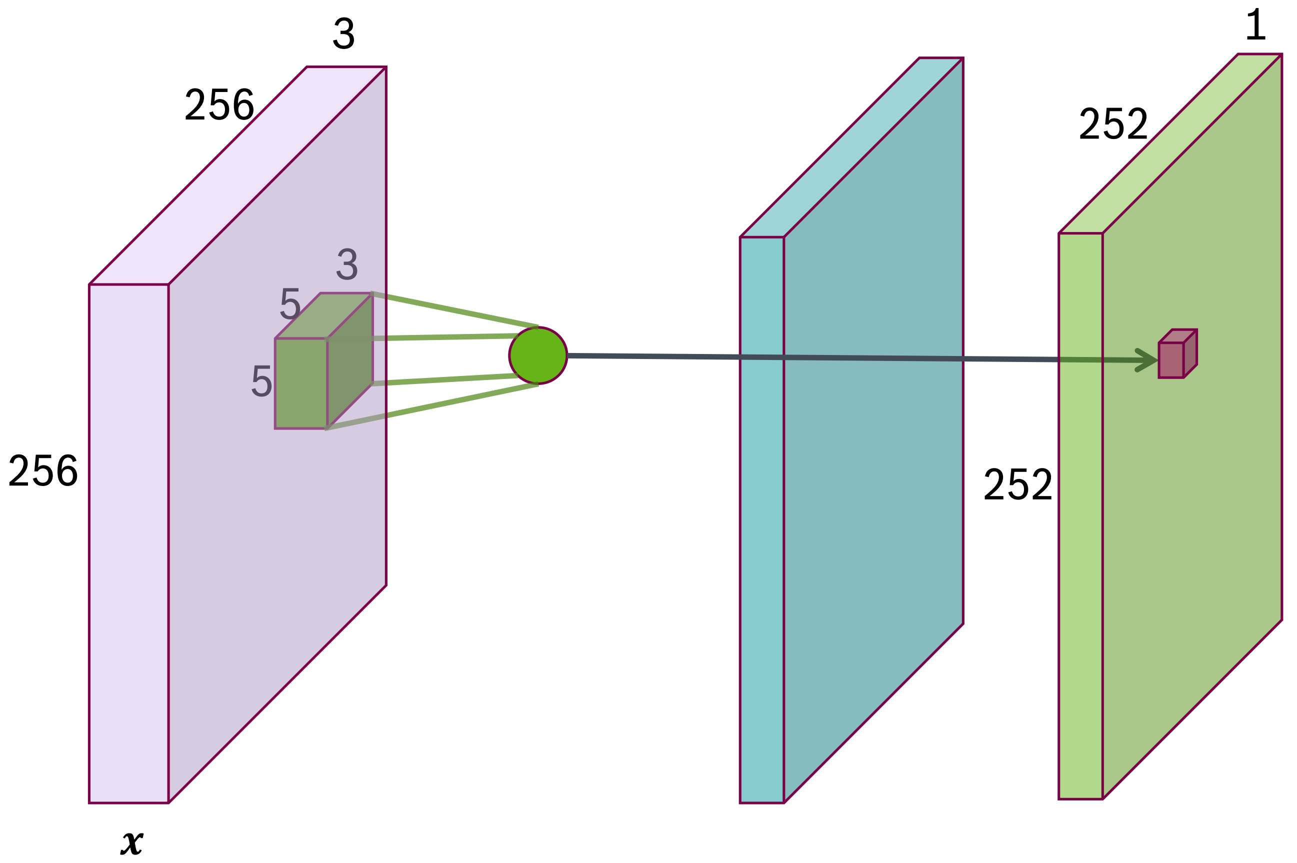
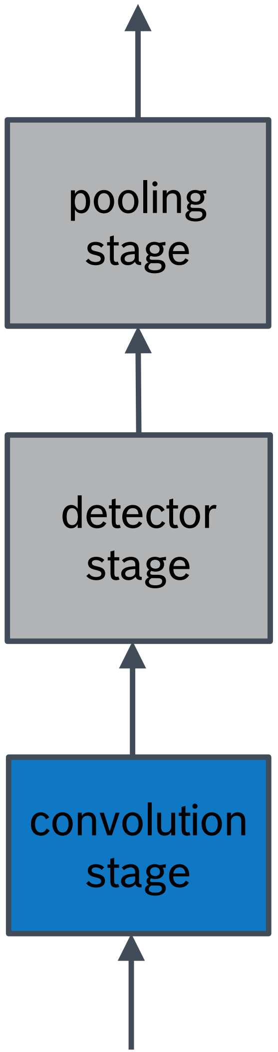
Convolutional Neural Networks
CONV Layer: The Convolution Stage (several kernels)





Convolutional Neural Networks
CONV Layer: The Convolution Stage (several kernels)





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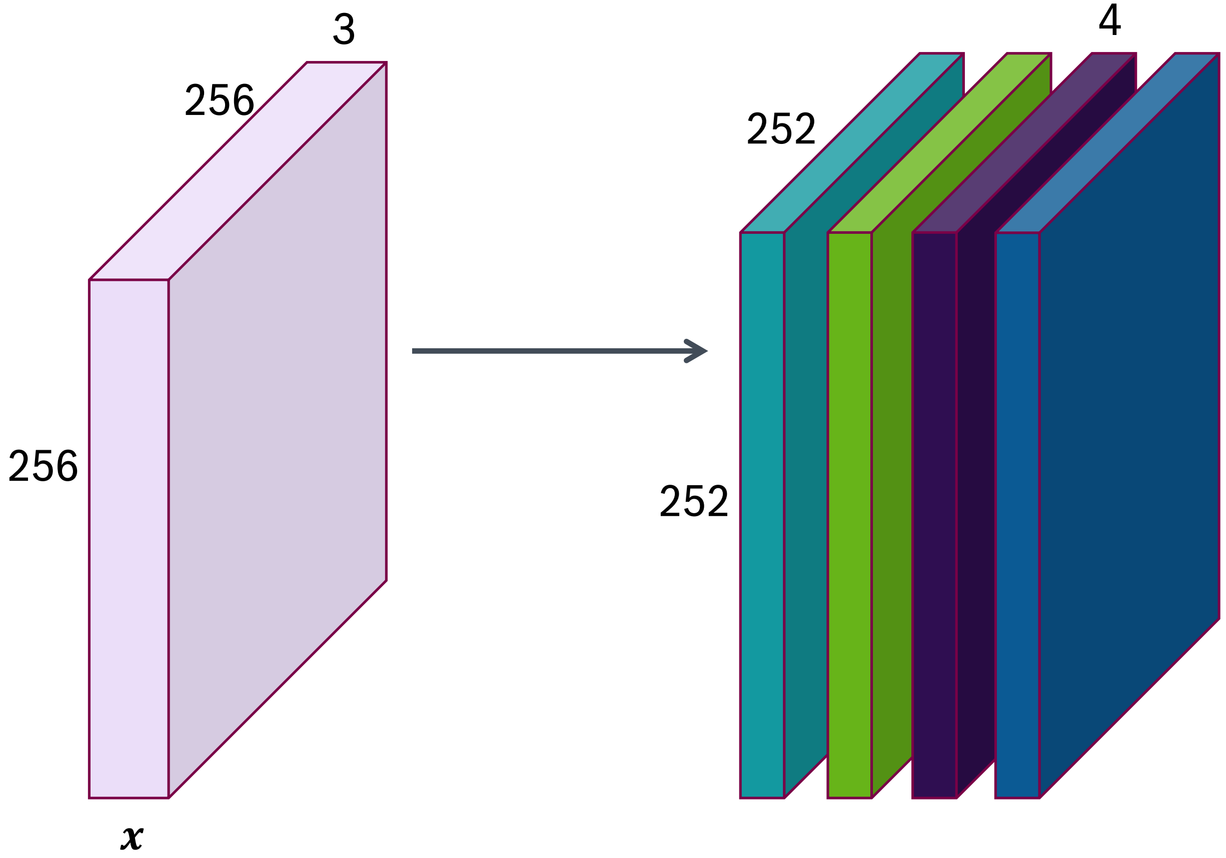
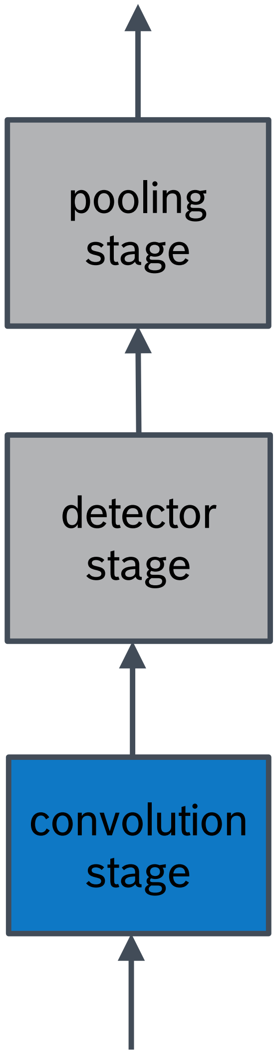
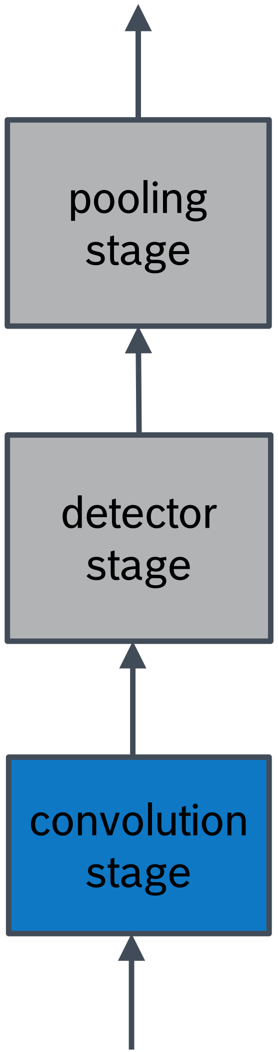




Convolutional Neural Networks
CONV Layer: The Convolution Stage (general case)

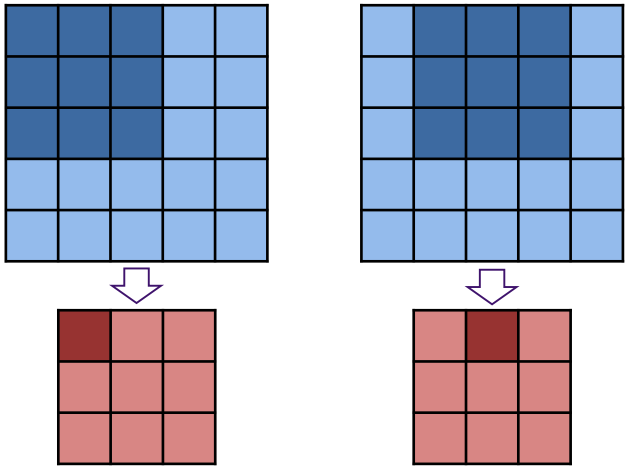
- **Input**: 3D tensor X of size $D_{\mathrm{in}} \times W_{\mathrm{in}} \times H_{\mathrm{in}}$ (D_{in} stacked matrices)
- **Parameters:** 4D tensor W of size $D_{\mathrm{out}} \times D_{\mathrm{in}} \times W_{\mathrm{k}} \times H_{\mathrm{k}}$ - **kernel bank**
  - D_{out} 3D tensors (**kernels**)
  - Each kernel consist of D_{in} 2D matrices (filters)
- **Output:** 3D tensor Y of size $D_{\mathrm{out}} \times (W_{\mathrm{in}} - W_{\mathrm{k}}) \times (H_{\mathrm{in}} - H_{\mathrm{k}})$ (D_{out} stacked matrices)
- **Operation:**
  - Slide each 3D kernel over the input tensor
  - At each position calculate element wise multiplication and sum up the products

$$y_{j,x,y} = \sum_{i=1}^{D_{\mathrm{in}}} \sum_{\Delta y=1}^{H_K} \sum_{\Delta x=1}^{W_K} w_{j,i,\Delta x,\Delta y} \cdot x_{i,x+\Delta x-1,y+\Delta y-1}$$

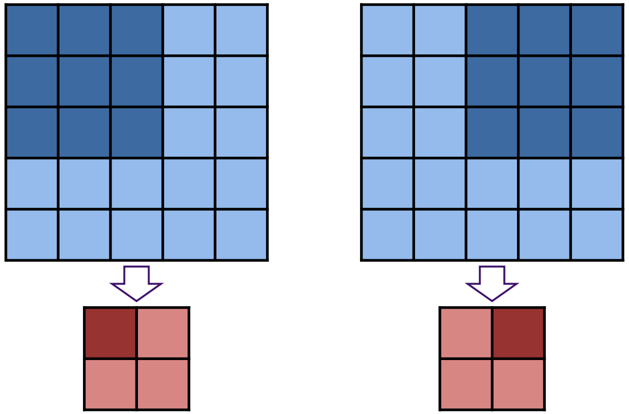


Convolutional Neural Networks
Conv Layer: The Stride Meta-Parameter

- **Motivation:**
  - Reduce the output size
  - Reduce computational complexity
- **Approach:**
  - control the step along each axis when sliding the kernel
- **Meta-parameters:**
  - **horizontal stride**: number of entries we move along the X axis at each step
  - **vertical stride**: number of entries we move along the Y axis at each step



Horizontal stride = 1



Horizontal stride = 2

Convolutional Neural Networks
CONV Layer: The Padding Meta-Parameter

- **Motivation:**
  - Avoid losing a few entries at the border
  - Keep input/output size ratio independent of the input size (1/stride)

- **Approach:**
  - Add zeros along the border of the input

- **Meta-parameters:**
  - **padding**: number of zeros to add along the border in each slice
  - Common values (assume square kernels of odd size):
    - $\frac{W_{\mathrm{k}}-1}{2}$: **same padding** scheme (preserve input size when stride=1)
    - 0: **valid padding** scheme (only "valid" kernel positions that fit inside the input generate output)

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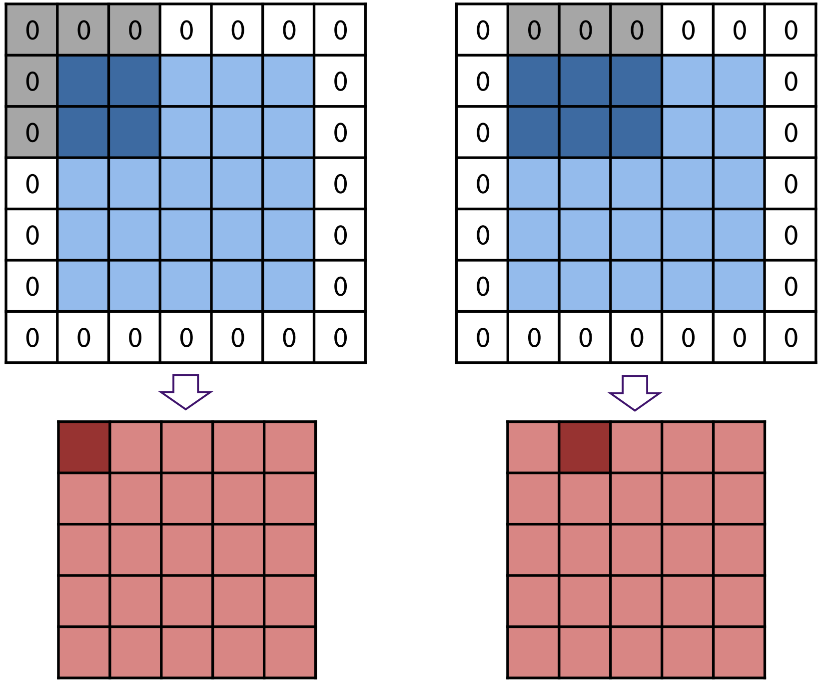
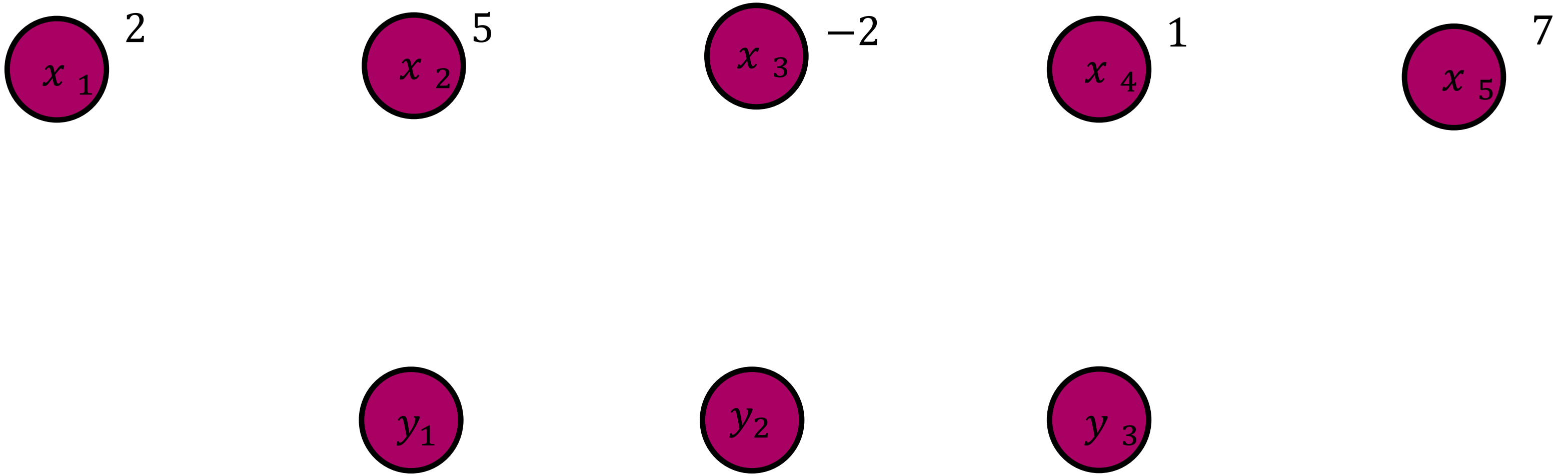
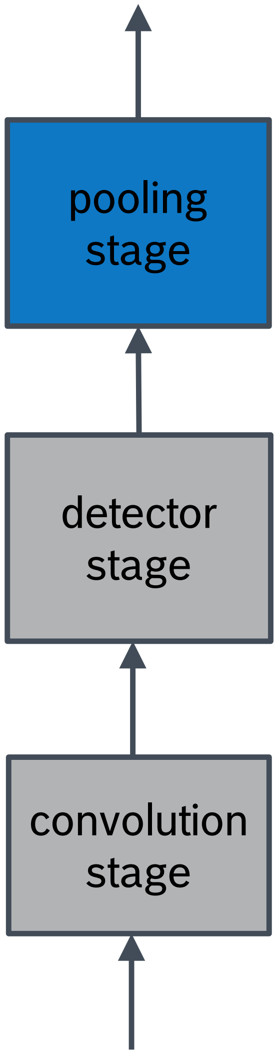


padding = 1

Convolutional Neural Networks
The Pooling Stage (1D case)

- **Idea:**
  - Add invariance to small translations
  - Collect statistics (max, average, etc.) over neighboring features
  - Downsample signal (optionally)
  - Handling inputs of variable size (dynamic pooling regions)





RBRO/ESA2 | 2018-11-08

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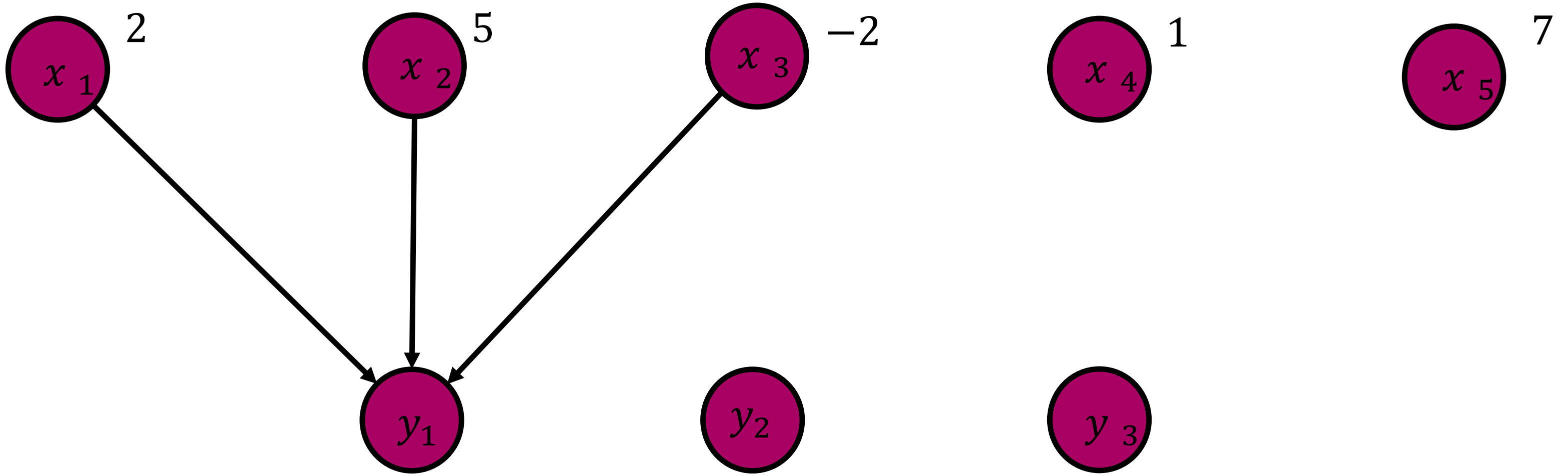

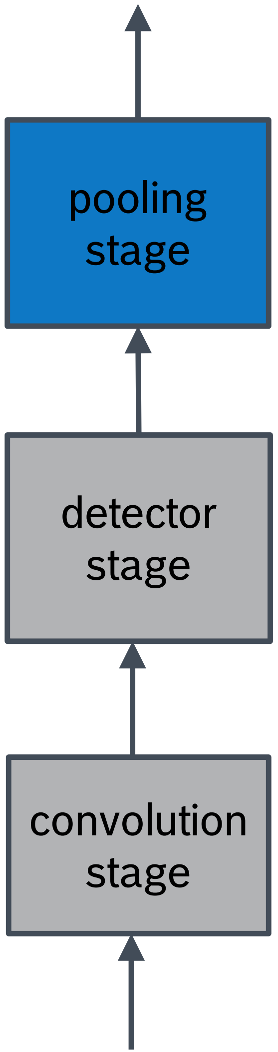

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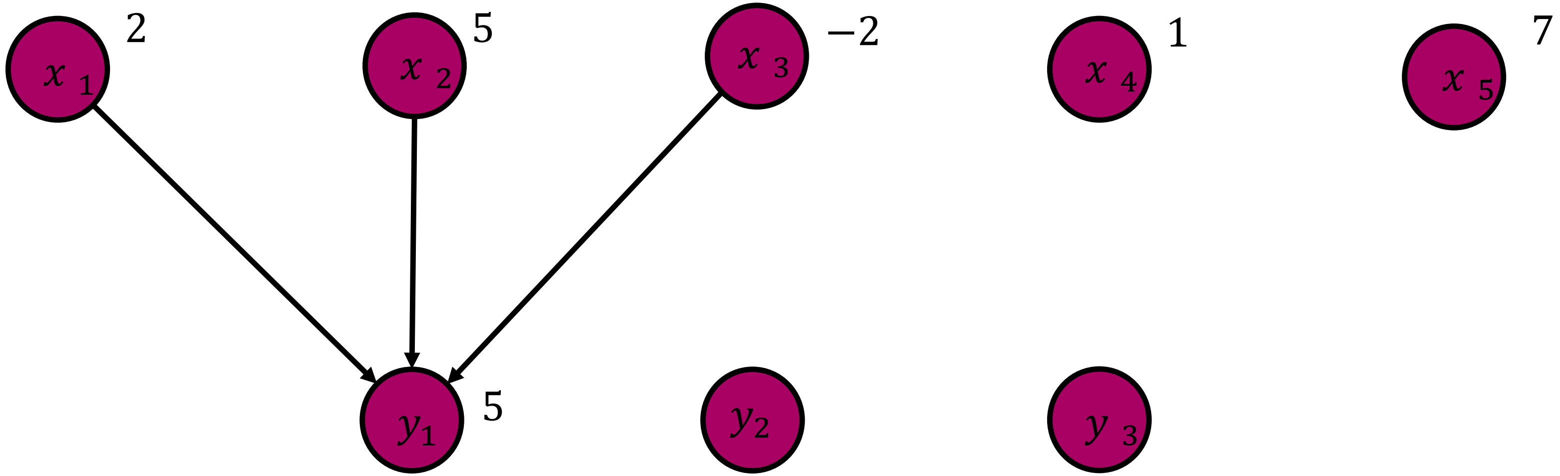

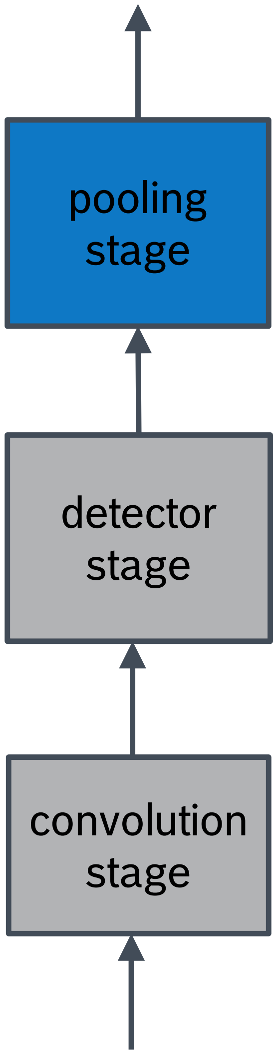

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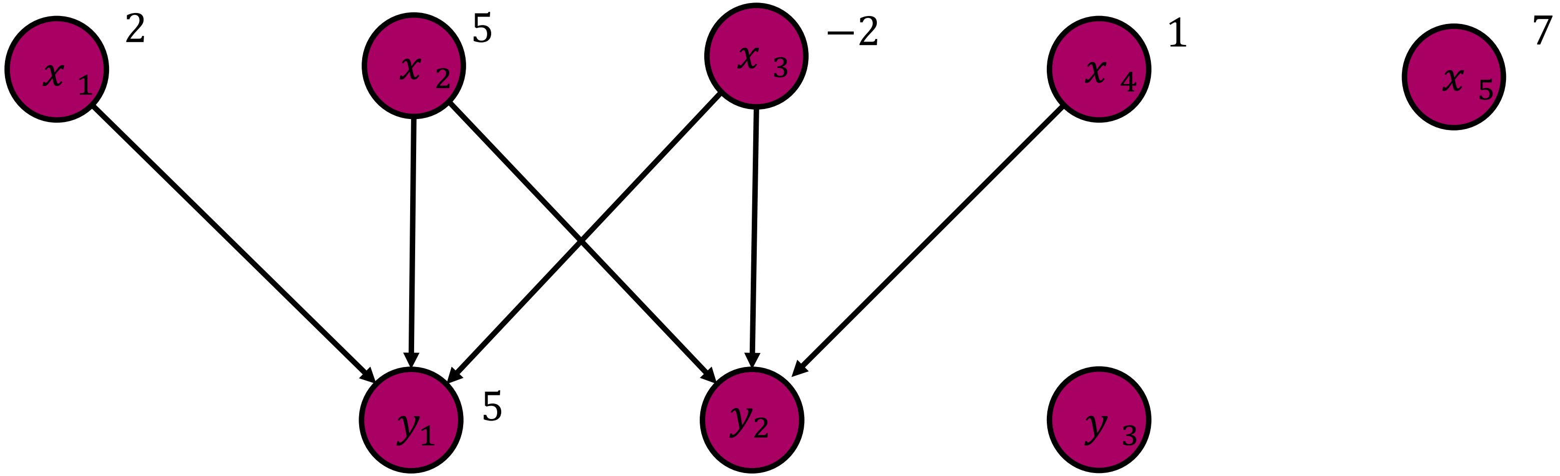

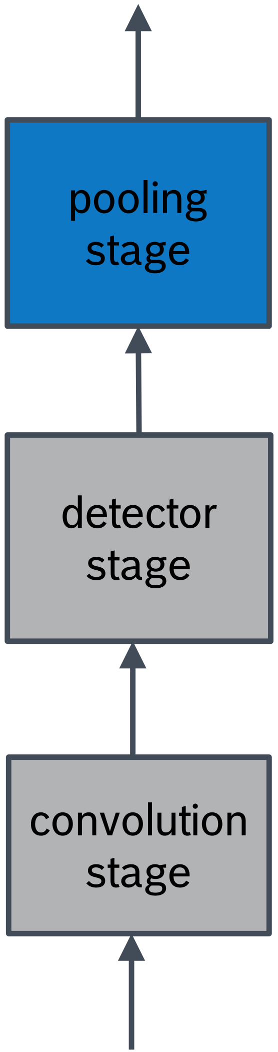

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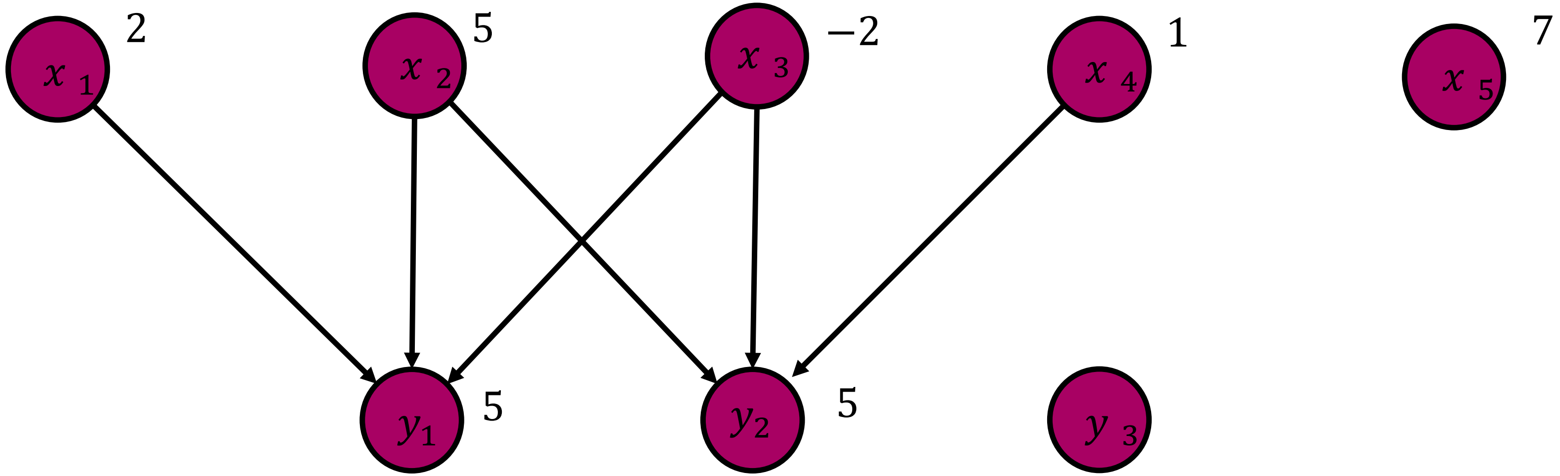

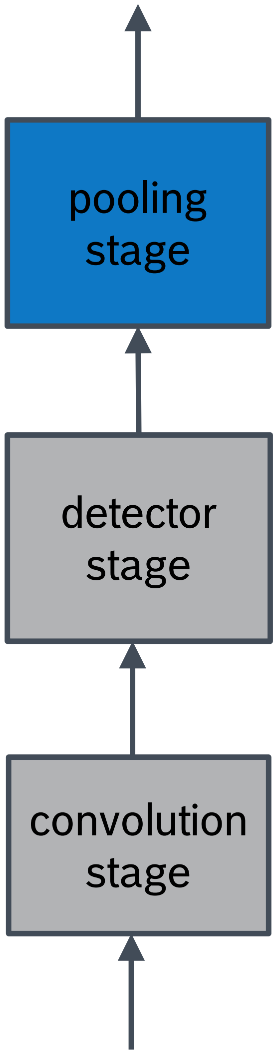

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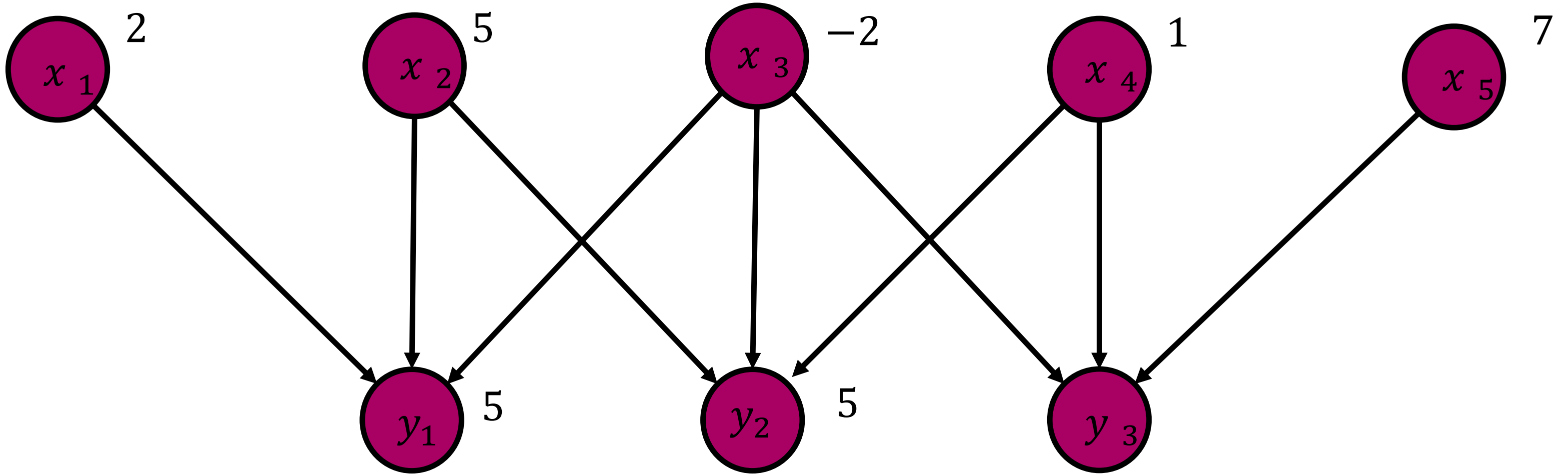

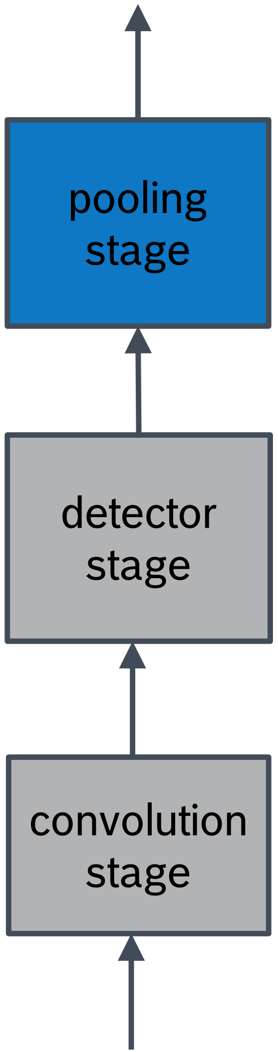

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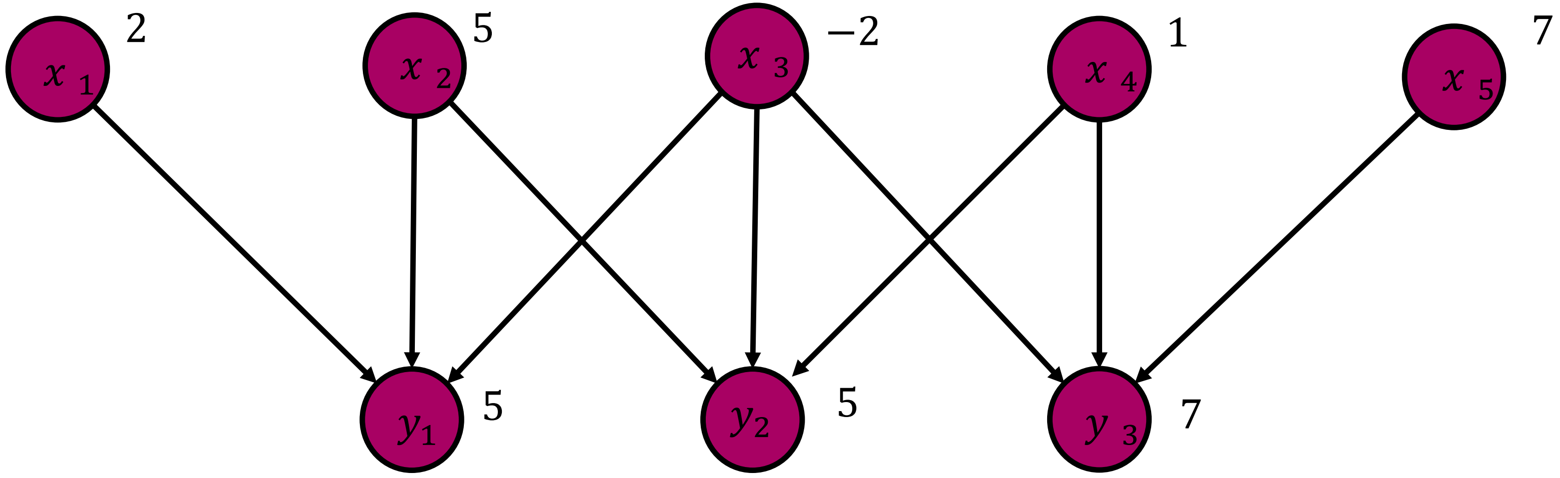

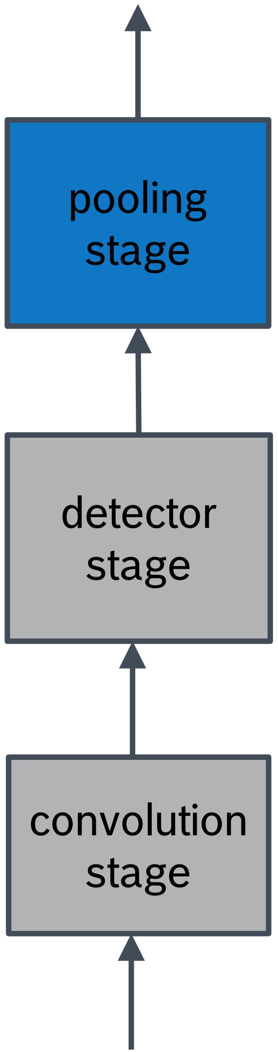

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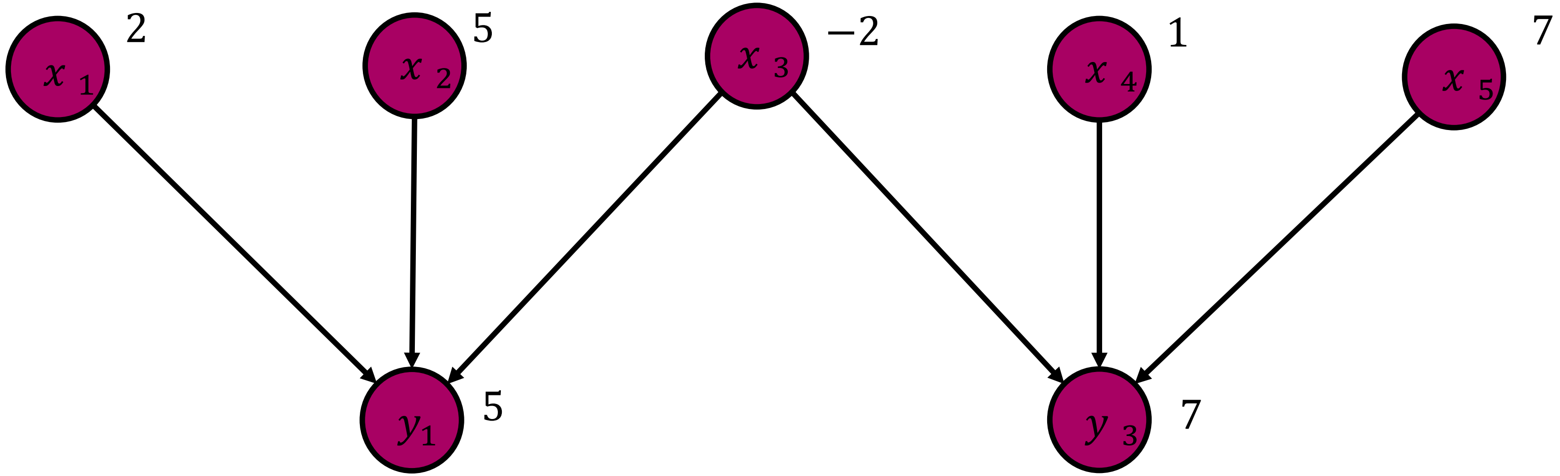
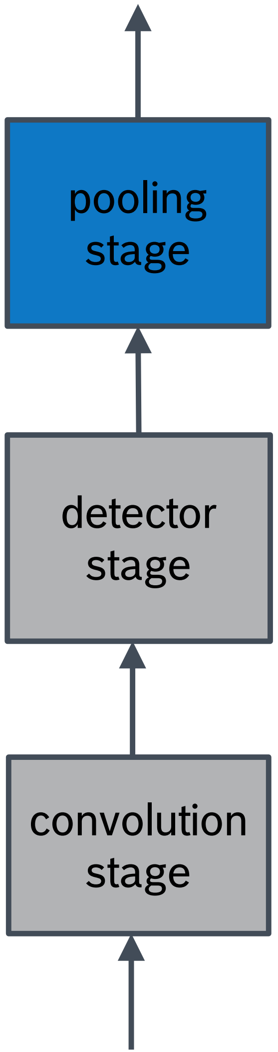
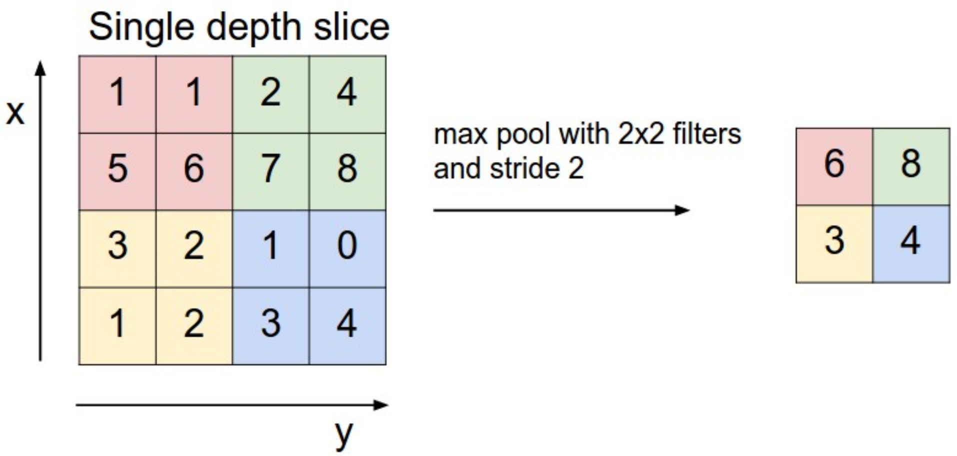


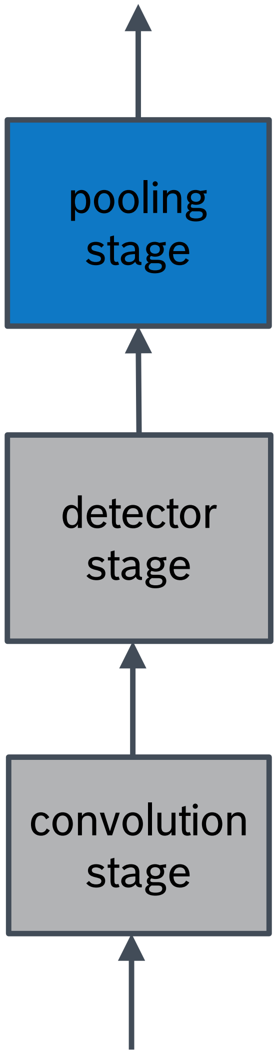


Convolutional Neural Networks
The Pooling Stage (2D case)

- **Operation:**
  - Slide window along width and height (with a given stride)
  - Compute statistics inside the window

- **Meta-Parameters:**
  - **Statistics:**
    - **max**: the winner detection takes all (most common in practice)
    - **average**: smooth out detection noise
  - **window size:** controls spatial invariance
  - **stride:** controls downsampling strength

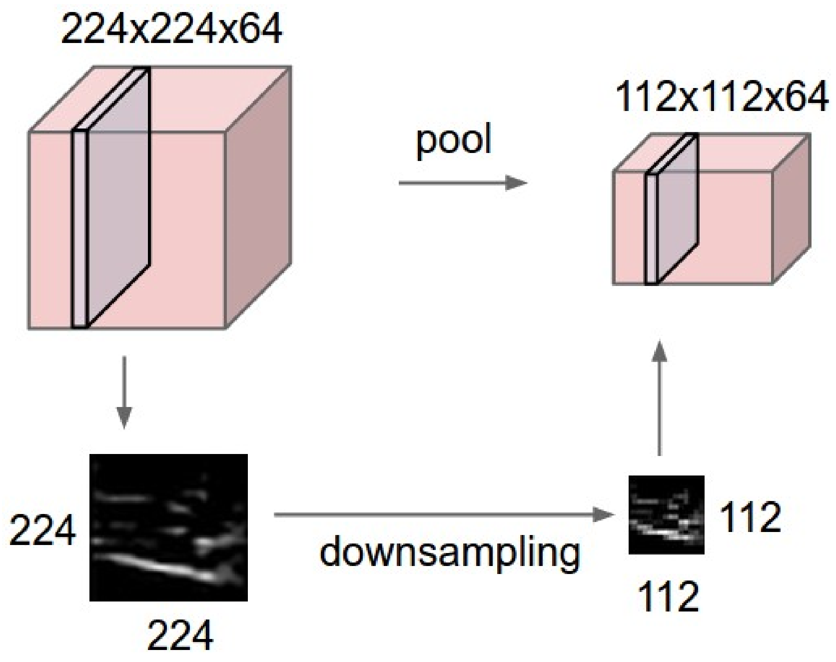




Source: http://cs231n.github.io/convolutional-networks/

Convolutional Neural Networks
The Pooling Stage (general case)

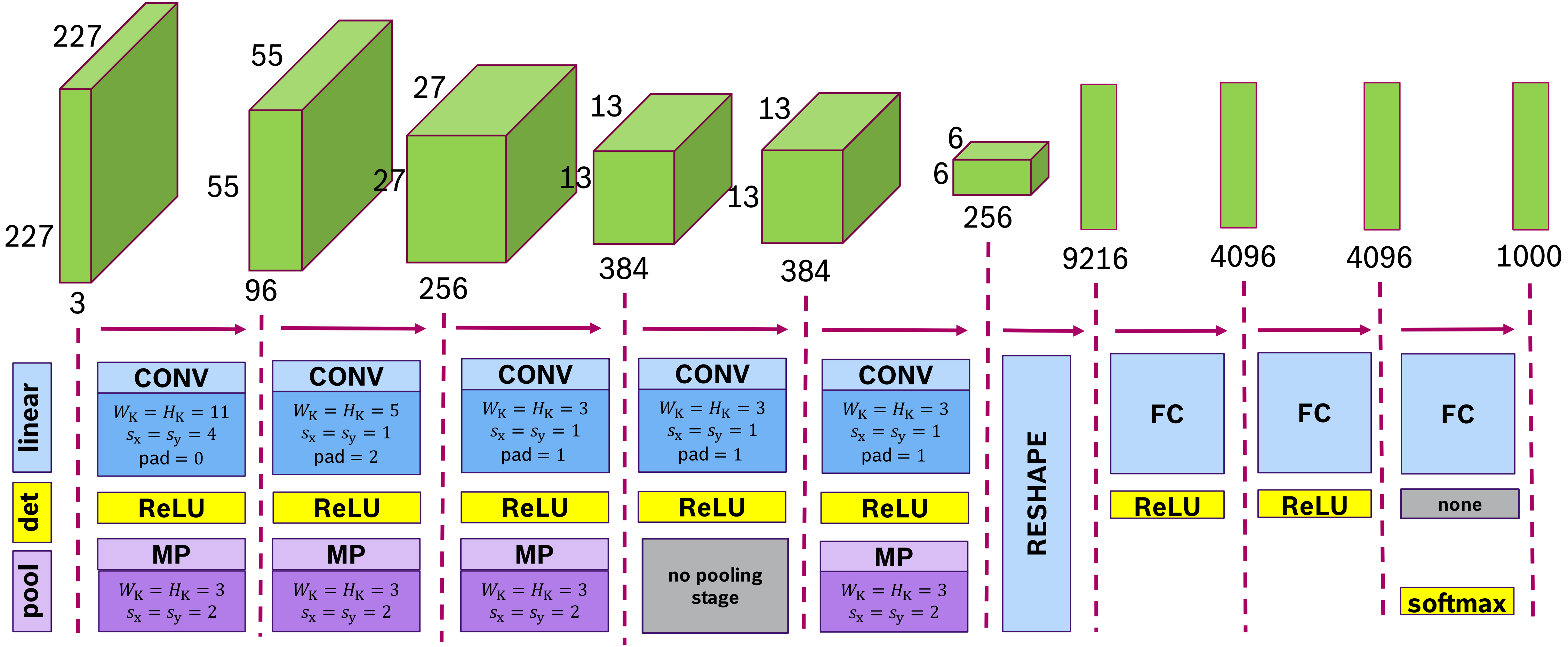
- **Input**: 3D tensor X of size $D_{\text{in}} \times W_{\text{in}} \times H_{\text{in}}$
- **Parameters:** none
- **Meta-parameters:**
  - statistic (max, avg)
  - kernel width/height $(W_{\text{K}}, H_{\text{K}})$
  - horizontal/vertical stride $(s_{\text{x}}, s_{\text{y}})$
- **Output:** 3D tensor Y of size $D_{\text{in}} \times W_{\text{in}} \times H_{\text{in}}$
- **Operation:** perform 2D pooling in each input slice <u>independently</u>



$$y_{j,x,y} = \max_{\substack{0 \le \Delta x < W_{\text{K}} \\ 0 \le \Delta y < H_{\text{K}}}} y_{j, s_{\text{x}} \cdot x + \Delta x, s_{\text{y}} \cdot y + \Delta y}$$

Source: http://cs231n.github.io/convolutional-networks/

Convolutional Neural Networks
Case Study: Image Classification (AlexNet)



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Convolutional Neural Networks
The Softmax Layer: Outputting Probability Distributions

- **Issue:**
  - How do we convert the output into a Multinoulli distribution?
  - Condition 1: Entries must be between 0 and 1
  - Condition 2: Must sum up to 1

- **Solutions:**
  - For binary classification: sigmoid for one class (condition 1), implicitly represent the other
  - General case: enforce competition using a **softmax layer**:

$$y_j = \frac{e^{x_j}}{\sum_{i=1}^{N_{\text{in}}} e^{x_i}}$$

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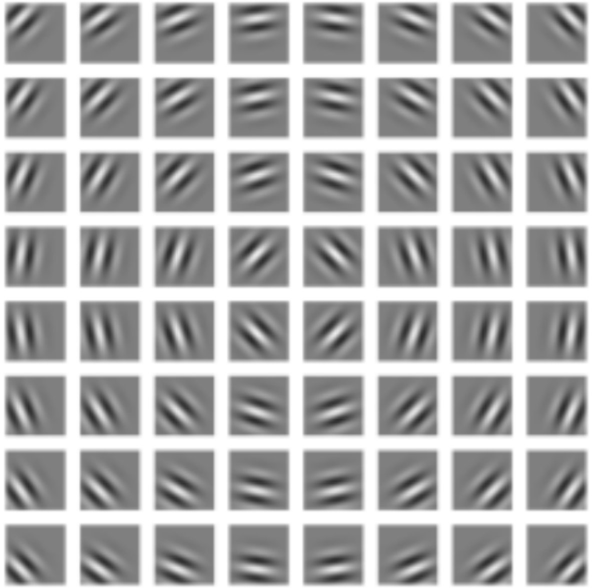
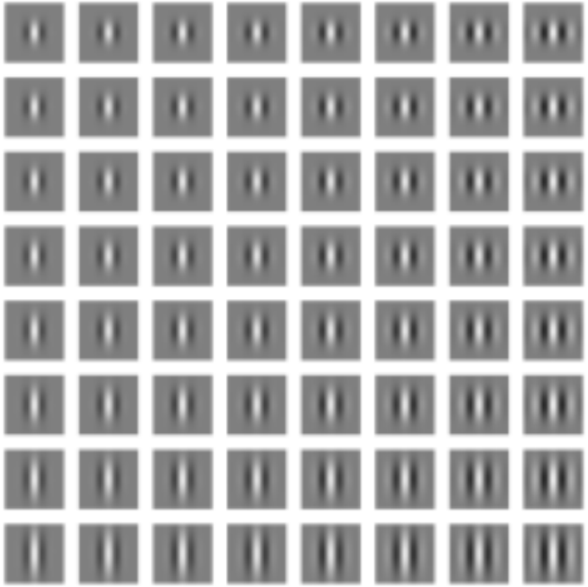
The Path to Deep Learning

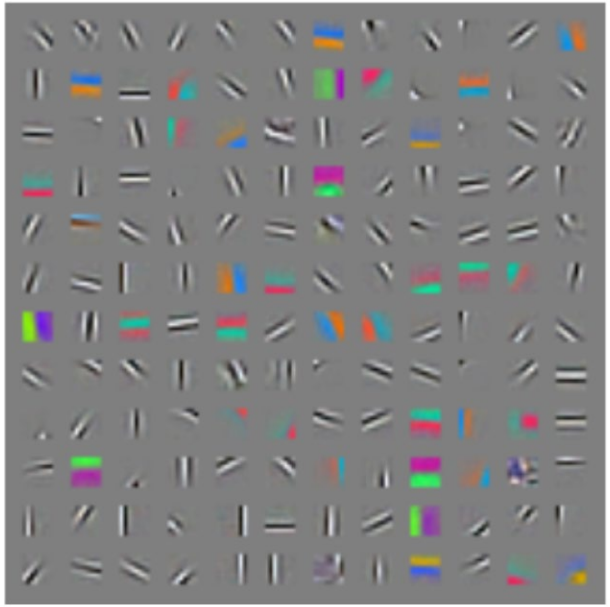
Learned Representations

- Kernels look similar to stimuli for early activation patterns for layers in the brain (V1 area)





Gabor Filters (similar to V1 activators)



Learned kernels in the first convolutional layer

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Convolutional Neural Network
Recap

- **Convolution:**
  - Hierarchical local pattern composition (biologically inspired)
  - Uniform equivariant processing across space (and/or time)
  - Can be seen as a strongly regularized fully connected layer
  - Huge reduction in the number of parameters!

- **Spatial pooling:**
  - Add spatial invariance by inserting pooling layers
  - Reduce feature map sizes (computational advantage)

- **Few additional layers (Connectivist Approach):**
  - FC: may be missing altogether, see Fully Convolutional Neural Networks (FCNs)
  - Softmax: convert outputs into probability distributions

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PERSPECTIVES

Perspectives
Active Research Areas

- The **statistical** challenge: labeled data is expensive
  - Supervised transfer learning: fueled the breakthrough (ImageNet)
  - Unsupervised pre-training: not that successful! Why?
  - Unsupervised/weakly supervised learning
  - Active learning

- The **computational** challenge: inference is expensive
  - Model compression/speedup (weight/response quantization)
  - Implicit generative models (*e.g.* GANs)

- The **optimization** challenge: slow/lack of convergence needs tuning
  - More or less the same algorithms as 3 decades ago! (SGD family)
  - Second order optimization (*e.g.* Hessian-Free optimization)

REFERENCES

Deep Learning for Computer Vision
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