Lecture 12: Neural Network (Back-Propagation, Activation Functions, Advanced Architectures)

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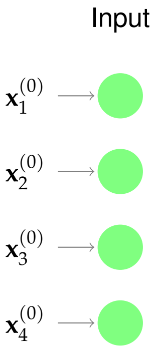
Step-by-Step: MLP Forward Pass



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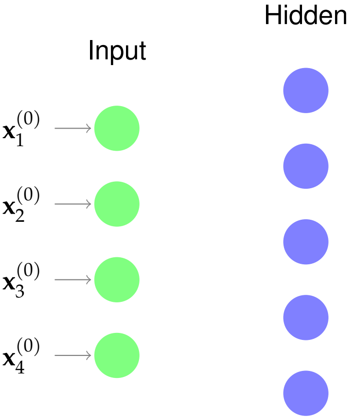

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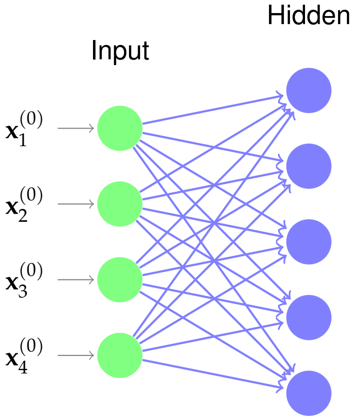

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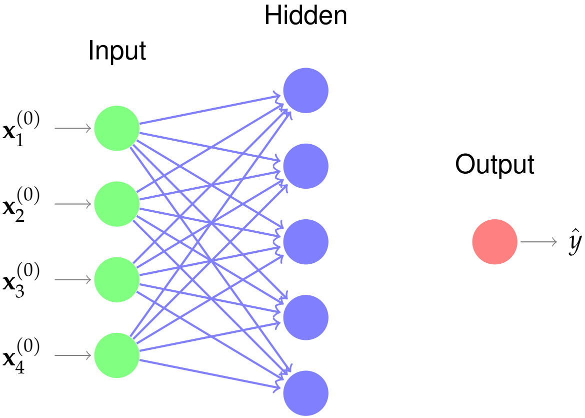

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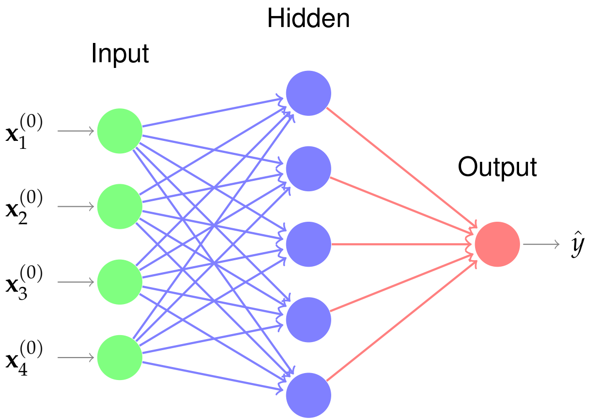

Final: $\hat{y} = \phi((\mathbf{W}^{(2)})^\top \mathbf{x}^{(1)} + b^{(2)})$

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- The last layer $\mathbb{R}^K \to \mathbb{R}$: It performs the desired ML task, either linear regression or classification.

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Training loss for a regression problem with $S_{\text{train}} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$:

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where

- f is the function represented by a NN.
- The overall function $y = f(\mathbf{x}^{(0)})$ can then be written as the composition:

$$f(\mathbf{x}^{(0)}) = f^{(L+1)} \circ \cdots \circ f^{(2)} \circ f^{(1)}(\mathbf{x}^{(0)}).$$

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- The function that is implemented by each layer in the form

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where $w_{i,j}^{(l)}$ is the edge weight that connects node i on layer $l-1$ to node j on layer l.

The back-propagation algorithm

Cost function:

$$\mathcal{L}_n = \left(y_n - f^{(L+1)} \circ \cdots \circ f^{(2)} \circ f^{(1)}(\mathbf{x}_n^{(0)}) \right)^2 ,$$

where $\mathbf{x}_n^{(l)} = f^{(l)}(\mathbf{x}_n^{(l-1)}) = \phi((\mathbf{W}^{(l)})^\top \mathbf{x}_n^{(l-1)} + \mathbf{b}^{(l)})$.

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Recall that we aim to compute:

$$\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}}, \qquad l = 1, \cdots, L+1,$$

$$\frac{\partial \mathcal{L}_n}{\partial b_j^{(l)}}, \qquad l = 1, \cdots, L+1.$$

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$$\begin{aligned}
\delta_j^{(l)} &= \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} && (5)\\
&= \sum_k \frac{\partial \mathcal{L}_n}{\partial z_k^{(l+1)}} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} && (6)\\
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  In vector form, we can write this as

$$\boldsymbol{\delta}^{(l)} = (\mathbf{W}^{(l+1)} \boldsymbol{\delta}^{(l+1)}) \odot \phi'(\mathbf{z}^{(l)}) \,, \tag{8}$$

  where $\odot$ denotes the Hadamard product (the point-wise multiplication of vectors).

Now that we have both $\mathbf{z}^{(l)}$ and $\boldsymbol{\delta}^{(l)}$ let us get back to our initial goal.

$$\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}} = \sum_k \frac{\partial \mathcal{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} = \underbrace{\frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}}}_{\delta_j^{(l)}} \underbrace{\frac{\partial z_j^{(l)}}{\partial w_{i,j}^{(l)}}}_{\mathbf{x}_i^{(l-1)}} = \delta_j^{(l)} \mathbf{x}_i^{(l-1)}$$

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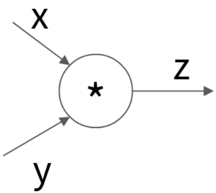
Modularized implementation: forward / backward API



(x,y,z are scalars)

Gate / Node / Function object: Actual PyTorch code

```
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z   # dz/dx * dL/dz
    grad_y = x * grad_z   # dz/dy * dL/dz
    return grad_x, grad_y
```

Need to cache some values for use in backward

Upstream gradient

Multiply upstream and local gradients

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The sigmoid

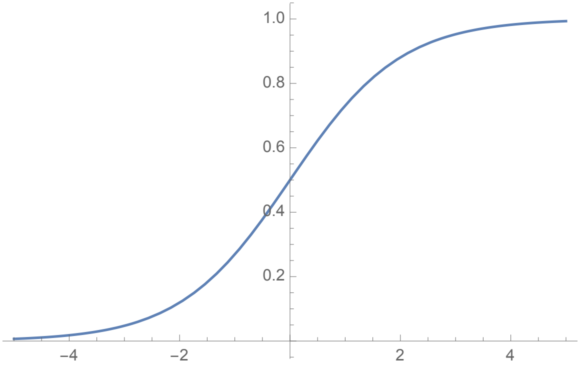

Figure: The sigmoid function $\phi(x)$.

$$\phi(x) = \frac{1}{1+e^{-x}} \tag{9}$$

- The sigmoid is always positive (not really an issue) and that it is bounded.
- For $|x|$ large, $\phi'(x) \sim 0$. This can cause the gradient to become very small ("vanishing gradient problem"), sometimes making learning slow.

Tanh

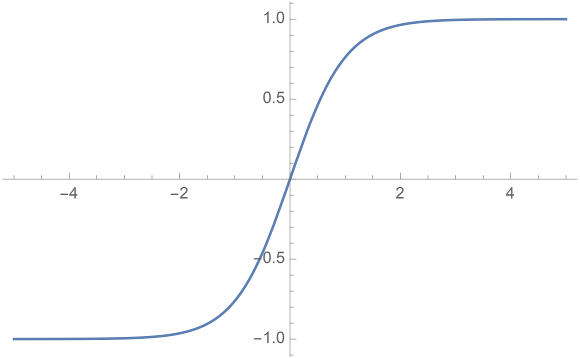

Figure: $\tanh(x)$.

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\phi(2x) - 1 \qquad (10)$$

- $\tanh(x)$ is "balanced" (positive and negative) and that it is bounded.
- It has the same problem as the sigmoid function, namely for $|x|$ large, $\tanh'(x) \sim 0$.

Rectified linear Unit – ReLU

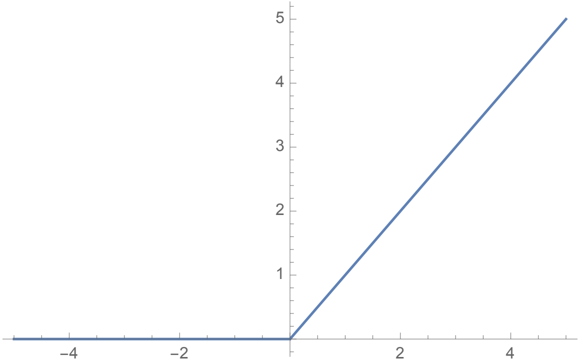

Figure: The ReLU $(x)_+$.

$$(x)_+ = \max\{0, x\}, \tag{11}$$

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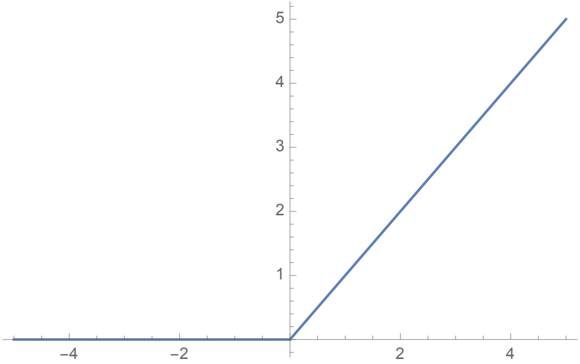

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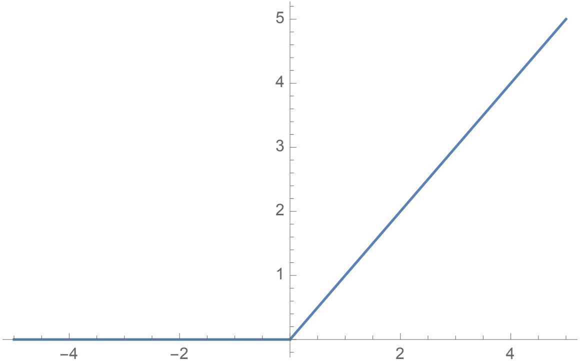

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- ReLU is always positive and is unbounded.
- Its derivative is 1 (and does not vanish) for positive values of x (it has 0 derivative for negative values of x though)

Leaky ReLU

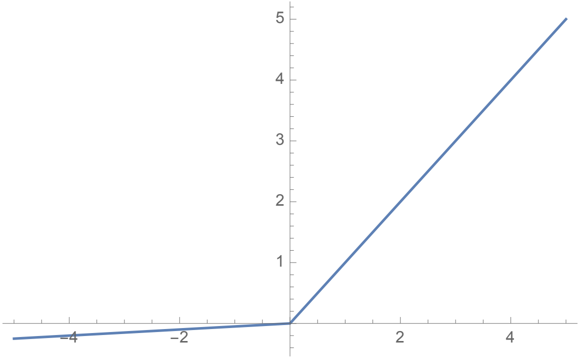

Figure: LReLU with $\alpha = 0.05$

In order to solve the 0-derivative problem of the ReLU (for negative values of x) one can add a very small slope α in the negative part.

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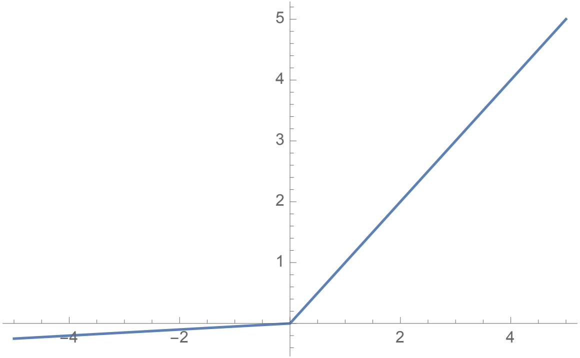

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- The constant α is of course a hyper-parameter that can be optimized.

Maxout

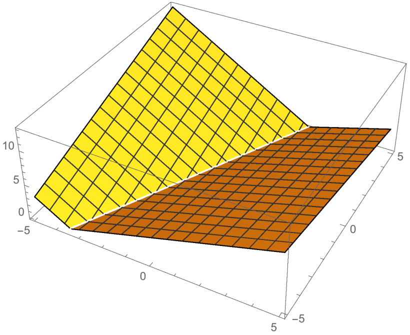

Figure: Maxout function with two terms, max$\{x_1 - 0.5x_2 + 1, -2x_1 + x_2 - 2\}$.

The maxout generalizes ReLU and LReLU.

$$f(\mathbf{x}) = \max\{\mathbf{x}^\top \mathbf{w}_1 + b_1, \cdots, \mathbf{x}^\top \mathbf{w}_k + b_k\} \tag{13}$$

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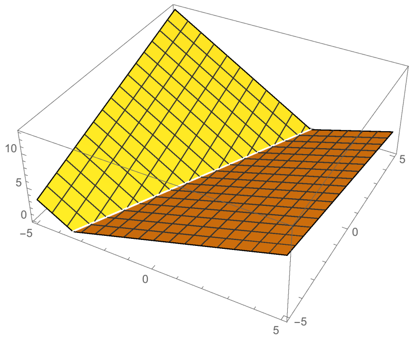

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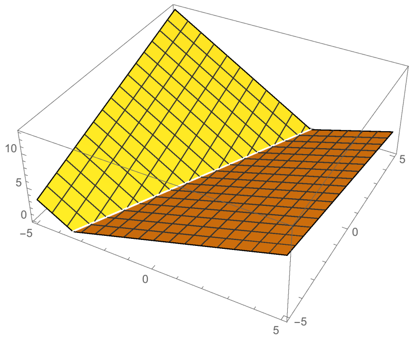

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- This activation function is quite different from the previous cases.
- In the previous cases we computed a weighted sum and then applied the activation function to it, whereas here we compute two or more different weighted sums and then choose the maximum.

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  - Variable image sizes need different weight matrices $\mathbf{W}$.
  - Fixed-size images still lead to huge weight matrices ($(W \times H \times C) \times D$ parameters).

Introduction: Why Not MLPs for Images?

- MLPs map unstructured vectors $\mathbf{x} \in \mathbb{R}^D$ to outputs.
- Images have 2D spatial structure ($\mathbf{x} \in \mathbb{R}^{W \times H \times C}$).
- Applying MLPs directly to images is problematic:
  - Variable image sizes need different weight matrices $\mathbf{W}$.
  - Fixed-size images still lead to huge weight matrices ($(W \times H \times C) \times D$ parameters).
  - Lack of translation invariance: Pattern recognized in one location may not be recognized if shifted.

Lack of Translation Invariance in MLPs

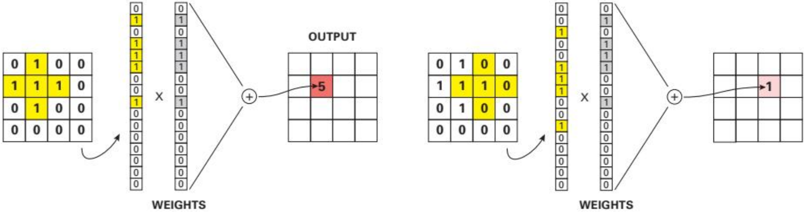

Figure: Detecting patterns with MLPs lacks translation invariance. A matched filter (weight vector) gives a strong response when the pattern aligns perfectly (left) but a weak response when shifted (right).

The CNN Solution: Convolution

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  - Translation invariance (filters applied across all locations).

Convolution as Template Matching

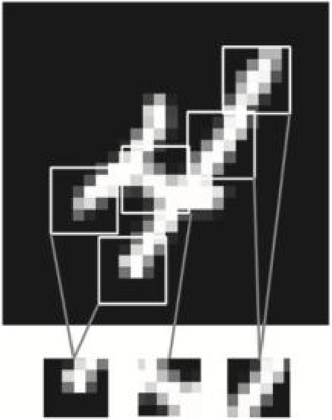

Figure: Classifying a digit by matching discriminative features (templates) in specific relative locations.

Common Layers: Convolution in 1D

- Continuous convolution: $[f \oplus g](z) = \int f(u)g(z-u)du$.

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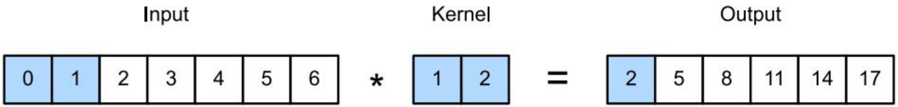
  - Compute element-wise product sum at each position.
- Example: $[\mathbf{w} \circledast \mathbf{x}](i) = \sum_{u=0}^{L-1} w_u x_{i+u}$ (often means cross-correlation in DL).

1D Convolution / Cross-Correlation Example



as

Figure: 1D cross-correlation: Sliding a filter (bottom) over an input sequence (top) to produce an output sequence (middle).

Note: Deep learning libraries often implement cross-correlation but call it convolution.

Convolution in 2D

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- Output at (i,j) is the weighted sum of the input patch centered at (i,j).

Step-by-Step: 2D Convolution Operation

Input $\mathbf{X}$

x_{03}	x_{13}	x_{23}	x_{33}
x_{02}	x_{12}	x_{22}	x_{32}
x_{01}	x_{11}	x_{21}	x_{31}
x_{00}	x_{10}	x_{20}	x_{30}

Filter $\mathbf{W}$

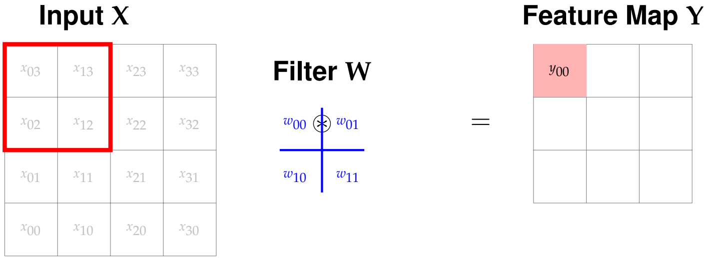
$\circledast$

w_{00}	w_{01}
w_{10}	w_{11}

$=$

Feature Map $\mathbf{Y}$

Step-by-Step: 2D Convolution Operation



Step 1: $$\mathbf{y}_{00} = \sum \mathbf{W} \odot \mathbf{X}_{0:2,0:2}$$

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w_{00}	w_{01}
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$=$

Feature Map $\mathbf{Y}$

	y_{01}	

Step 2: Slide stride=1. $\mathbf{y}_{01} = \sum \mathbf{W} \odot \mathbf{X}_{0:2,1:3}$

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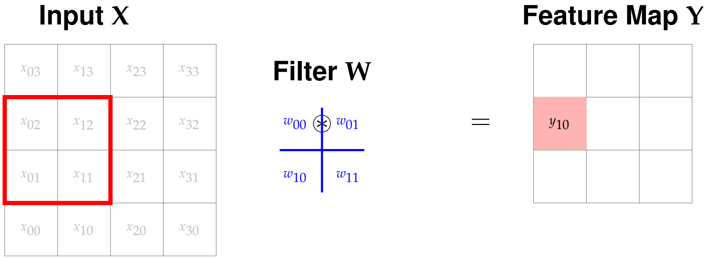

Step 3: Next row. $\mathbf{y}_{10} = \sum \mathbf{W} \odot \mathbf{X}_{1:3,0:2}$

Step-by-Step: 2D Convolution Operation

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Filter $\mathbf{W}$

$$\circledast \quad \begin{array}{c|c} w_{00} & w_{01} \\ \hline w_{10} & w_{11} \end{array} \quad =$$

Feature Map $\mathbf{Y}$

y	y	y
y	y	y
y	y	y

Process repeats for all spatial locations.

2D Convolution as Feature Detection

- Output $\mathbf{Y} = \mathbf{W} \circledast \mathbf{X}$ is called a **feature map**.
- Output is large where the image patch matches the filter $\mathbf{W}$.
- Example: Filter matching a diagonal line.

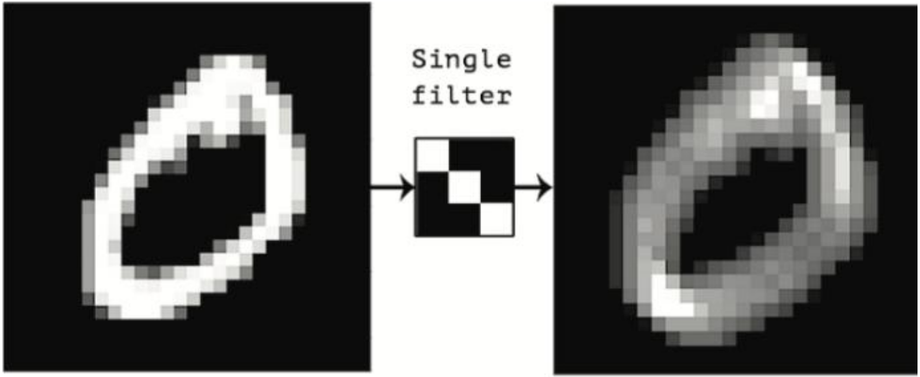

Figure: Convolving an image (left) with a 3x3 filter detecting diagonal lines (middle) produces a feature map (right) highlighting those features.

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- Shows CNNs are like MLPs with structured, sparse, weight-tied matrices.
- Achieves translation invariance and parameter reduction.

Boundary Conditions: Padding

- Problem: Convolution reduces output size. Convolving $f^h \times f^w$ filter on $x^h \times x^w$ image yields $(x^h - f^h + 1) \times (x^w - f^w + 1)$ output ('valid' convolution).

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  - Output size with padding p^h, p^w: $(x^h + 2p^h - f^h + 1) \times (x^w + 2p^w - f^w + 1)$.

Padding Example: Same Convolution

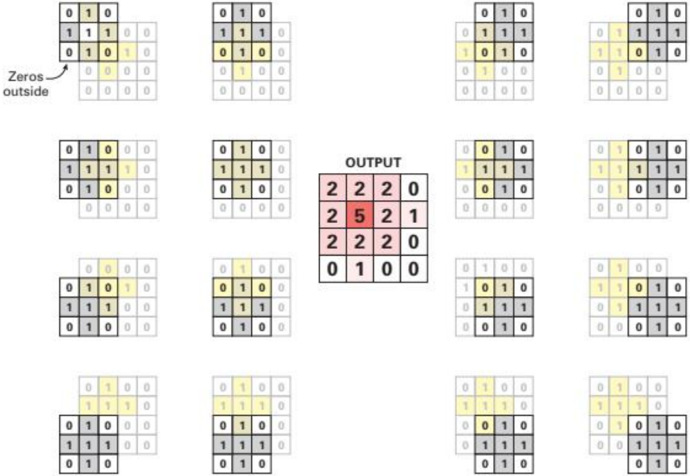

Figure: 'Same' convolution uses zero-padding to keep output size equal to input size.

Strided Convolution

- Problem: Neighboring outputs in feature maps are often redundant due to overlapping input patches.
- Solution: **Strided Convolution** skips inputs by a step size (stride) s.
- Reduces output size and computation.
- Output size with stride s^h, s^w and padding p^h, p^w:

$$\lfloor \frac{x^h + 2p^h - f^h + s^h}{s^h} \rfloor \times \lfloor \frac{x^w + 2p^w - f^w + s^w}{s^w} \rfloor$$

Padding and Stride Example

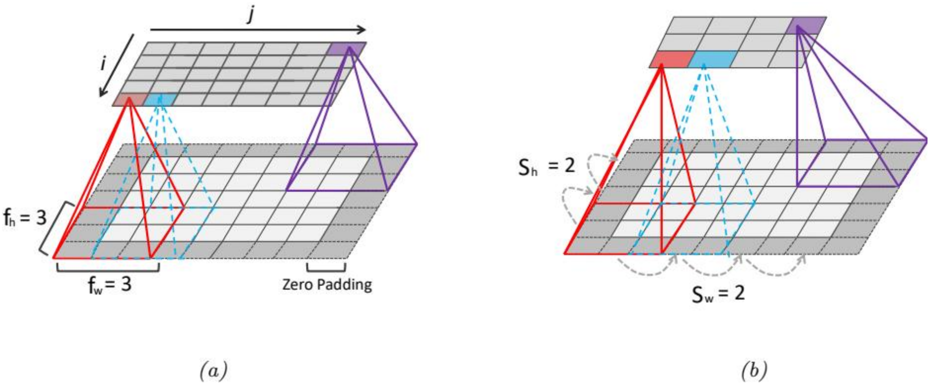

Figure: (a) 'Same' convolution (padding=1, stride=1) on 5x7 input with 3x3 filter gives 5x7 output. (b) Stride=2 gives 3x4 output.

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- Filter $\mathbf{W}$ becomes 3D: $H \times W \times C$.
- Each input channel c is convolved with its corresponding filter slice $\mathbf{W}_{:,:,c}$.
- Results are summed across channels (plus bias b) to produce a single output channel:

$$z_{i,j} = b + \sum_{u=0}^{H-1} \sum_{v=0}^{W-1} \sum_{c=0}^{C-1} x_{si+u,sj+v,c} w_{u,v,c}$$

Multiple Input Channels Visualization

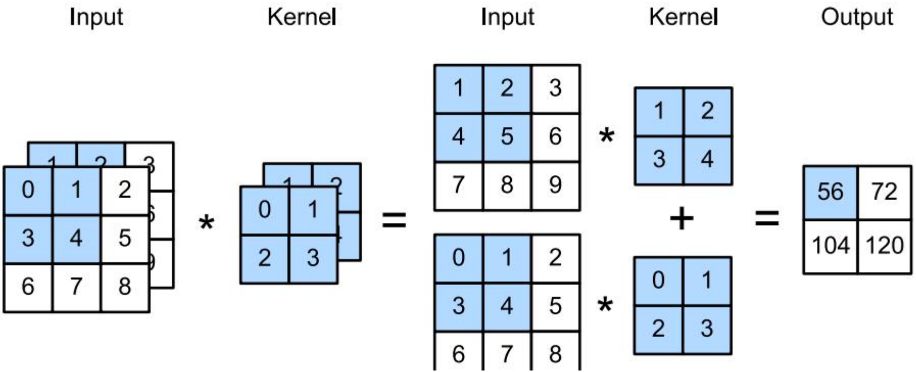

Figure: 2D convolution with a 2-channel input. Each input channel is convolved with a corresponding 2D filter slice, and the results are summed.

Multiple Output Channels

- Goal: Detect multiple types of features at each location.
- Use multiple filters, one for each desired output feature map d.
- Filter $\mathbf{W}$ becomes 4D: $H \times W \times C \times D$.
- $\mathbf{W}_{:,:,c,d}$ is the 2D filter for output channel d and input channel c.
- Output $z_{i,j,d}$ for feature map d is computed by summing convolutions across all input channels C:

$$z_{i,j,d} = b_d + \sum_{u=0}^{H-1} \sum_{v=0}^{W-1} \sum_{c=0}^{C-1} x_{si+u,sj+v,c} w_{u,v,c,d}$$

Multiple Input/Output Channels Visualization

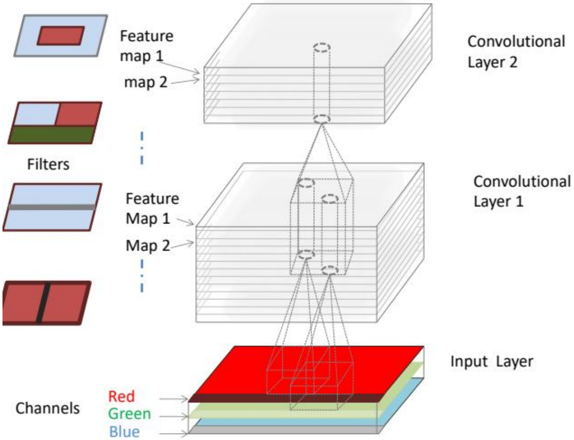

Figure: CNN with multiple channels. Input (3 channels) -> Conv Layer 1 (multiple channels) -> Conv Layer 2 (more channels). Cylinders represent feature vectors (hypercolumns) at specific locations.

1x1 Convolution (Pointwise Convolution)

- A special case with filter size 1×1.
- Computes a weighted combination of input channels *at the same location*.

$$z_{i,j,d} = b_d + \sum_{c=0}^{C-1} x_{i,j,c} w_{0,0,c,d}$$

- Changes the number of channels ($C \to D$) without changing spatial dimensions (H, W).
- Equivalent to applying a small MLP (Dense layer) independently to each spatial location's feature vector.
- Used in modern architectures (e.g., bottleneck layers, network-in-network).

1x1 Convolution Visualization

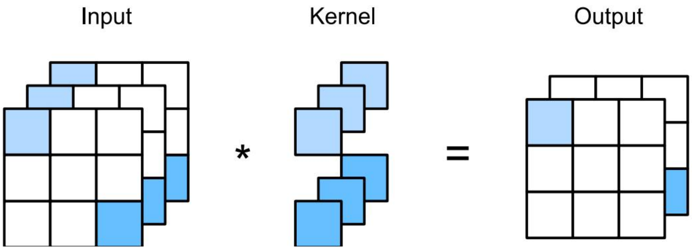

Figure: Mapping 3 input channels to 2 output channels using 1x1 convolution (filter size 1x1x3x2).

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- Pooling layers reduce spatial resolution and introduce local invariance.

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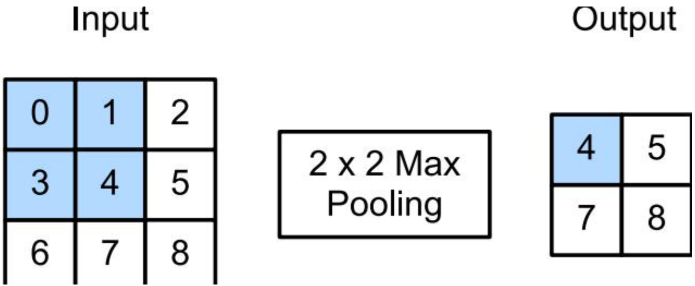

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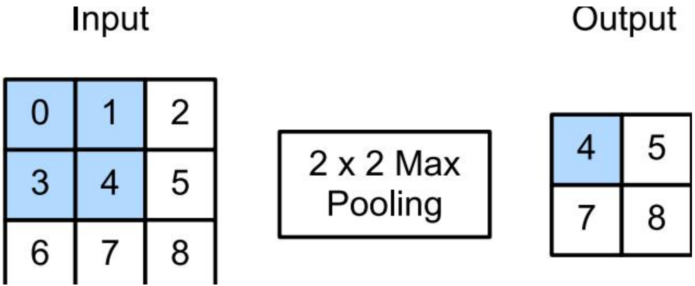

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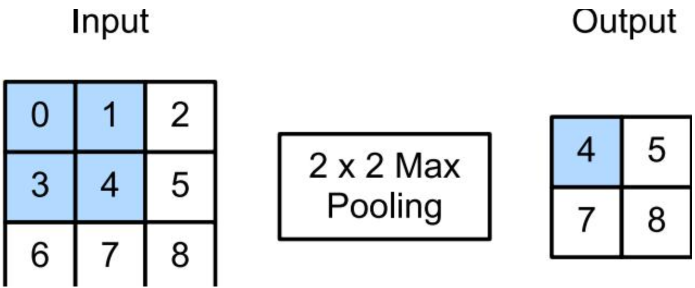

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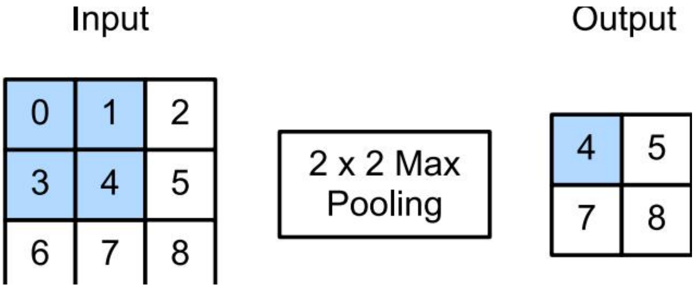

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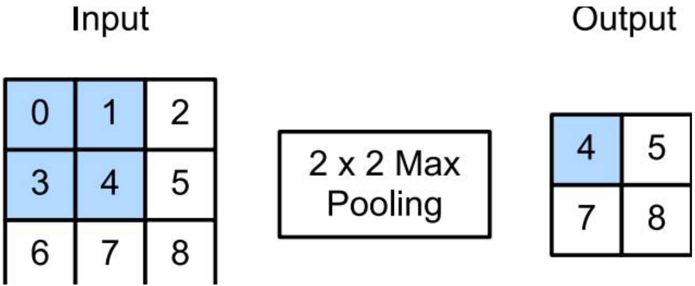
- Applied independently to each channel.



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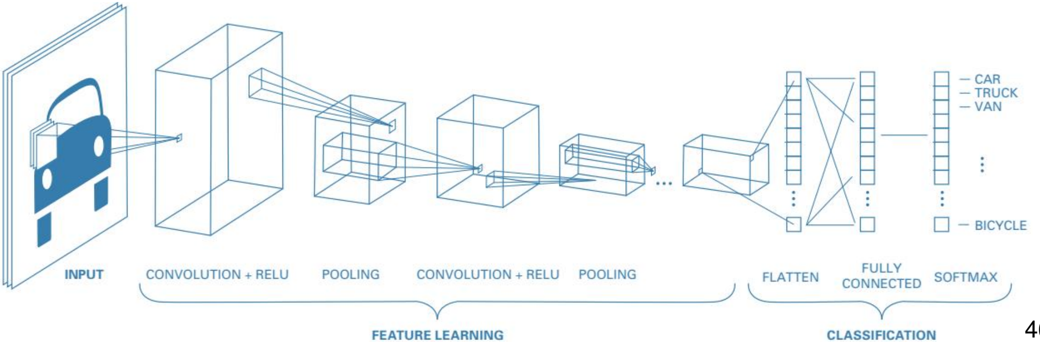
Pooling Layers: Average Pooling & Global Average Pooling

- **Average Pooling:** Computes the *average* value within the window instead of the max.
- **Global Average Pooling (GAP):** Averages over the *entire* spatial dimension of a feature map.
  - Converts an $H \times W \times D$ feature map to a $1 \times 1 \times D$ (or D-dimensional) vector.
  - Often used before the final classification layer.
  - Allows the network to handle variable input image sizes.

Putting It Together: Simple CNN Architecture

- Common pattern: [CONV -> ReLU -> POOL] x N -> FLATTEN -> DENSE -> SOFTMAX
- Convolutional layers extract features.
- Pooling layers reduce dimensionality and add invariance.
- Final dense layers perform classification based on high-level features.



Historical Context: LeNet

- Early successful CNN architecture by Yann LeCun et al. (1998) [LeC+98].
- Designed for digit recognition (MNIST).
- Similar pattern: CONV -> POOL -> CONV -> POOL -> DENSE -> DENSE -> OUTPUT.
- Used backpropagation and SGD for training.
- Inspired by earlier Neocognitron [Fuk75] and biological vision models [HW62].

Normalization Layers: Why?

- Training deep networks is hard (Vanishing/Exploding Gradients - Ch 13).
- Normalization layers help stabilize training.
- Idea: Standardize the statistics (mean, variance) of activations within layers.
- Analogy: Standardizing input features.

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  3. Scale and Shift: $\tilde{z}_n = \gamma \odot \hat{z}_n + \beta$ (γ, β are learnable parameters).
- Applied after CONV/DENSE layers, often before activation function.

Batch Normalization: Training vs. Test Time

- **Training:** Use mini-batch statistics ($\mu_{\mathcal{B}}, \sigma^2_{\mathcal{B}}$). Learn γ, β.
- **Testing:** Mini-batch statistics are unreliable (batch size might be 1).
  - Use population statistics (mean μ, variance σ^2) estimated from the entire training set (often using moving averages during training).
  - Freeze $\mu, \sigma^2, \gamma, \beta$.
  - The BN layer becomes a simple linear transform.
- BN layer behaves differently during training and inference.

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- Mechanism still debated ("Internal Covariate Shift" is likely not the full story).

Conclusion & Next Steps (CNNs)

- CNNs are essential for image data due to convolution's properties (parameter sharing, translation invariance).
- Key Layers: Convolution, Pooling, Normalization (esp. Batch Norm).
- Standard architectures combine these layers effectively.
- Modern CNNs (ResNet, EfficientNet) use advanced techniques but follow these core principles.

Table of Contents

Introduction to Sequence Modeling

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  - Long-term dependencies (e.g., "The **boy** who wore a red hat ... **was** happy").
- **Standard MLPs fail** because they expect fixed-size input and treat features as independent.

Recurrent Neural Networks (RNNs): The Core Idea

- **Core Concept:** Process the sequence one step at a time, maintaining an internal "memory" or **Hidden State** $(\mathbf{h}_t)$.

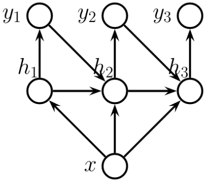

Figure: The hidden state $\mathbf{h}$ passes information forward through time.

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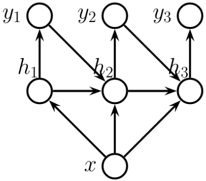

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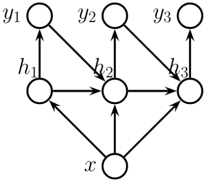
- **Step-by-Step Update:**
  1. **Input:** Current token $\mathbf{x}_t$.
  2. **Context:** Previous state $\mathbf{h}_{t-1}$ (summary of the past).
  3. **Update:** Compute new state $\mathbf{h}_t$ using shared weights $\mathbf{W}$.
  4. **Output:** Compute prediction $\mathbf{y}_t$ from $\mathbf{h}_t$.



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RNN: Mathematical Formulation

- A vanilla RNN typically uses the $\tanh$ activation function:

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\begin{aligned}
\mathbf{h}_t &= \tanh(\mathbf{W}_{hh}\mathbf{h}_{t-1} + \mathbf{W}_{xh}\mathbf{x}_t + \mathbf{b}_h) \\
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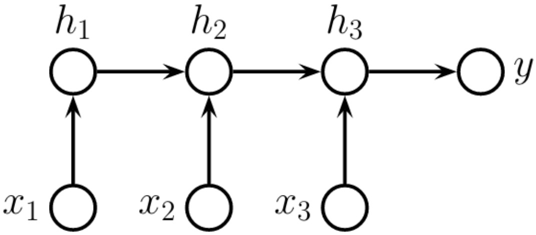
- **Parameters (Shared across all time steps):**
  - $\mathbf{W}_{xh}$: Weights mapping input to hidden.
  - $\mathbf{W}_{hh}$: Weights mapping hidden to hidden (recurrence).
  - $\mathbf{W}_{hy}$: Weights mapping hidden to output.

Architecture 1: Many-to-One (Sequence Classification)

- **Task:** Sentiment Analysis, Intent Classification.



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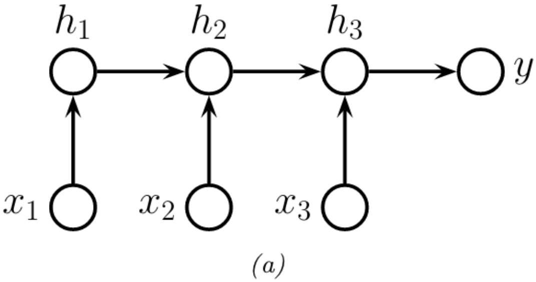

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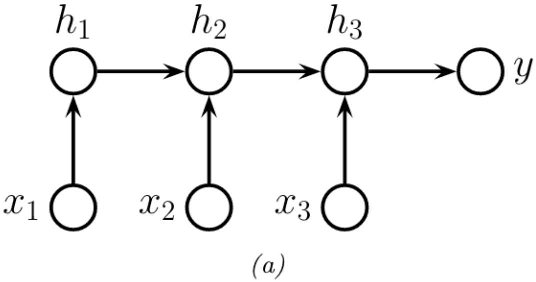
- **Intuition:** $\mathbf{h}_T$ is a vector summary of the whole sentence.



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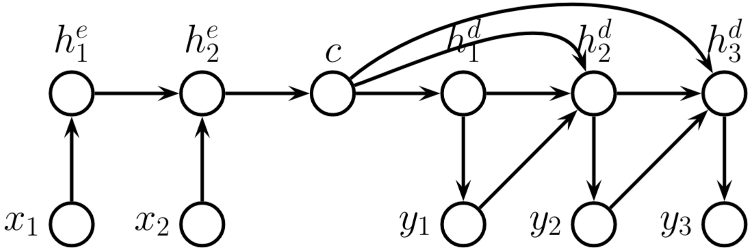

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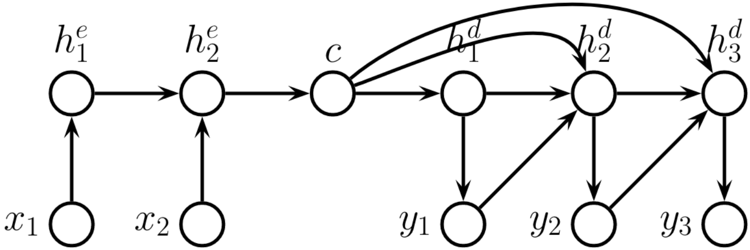
Architecture 2: Many-to-Many (Seq2Seq)

- **Task:** Machine Translation, Summarization.
- **Encoder-Decoder Architecture:**
  1. **Encoder:** Process input $\mathbf{x}$ into context vector $\mathbf{c}$ (usually final state $\mathbf{h}_T$).
  2. **Decoder:** Generate output $\mathbf{y}$ one word at a time, conditioned on $\mathbf{c}$.



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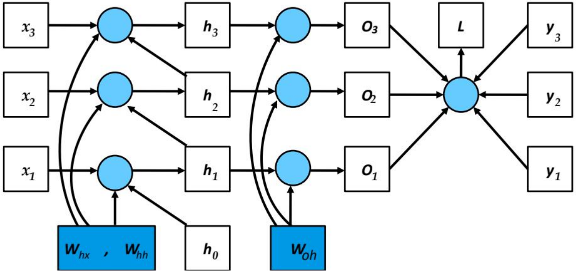
Training: Backpropagation Through Time (BPTT)

- To train an RNN, we "unroll" it over time and treat it like a very deep MLP.



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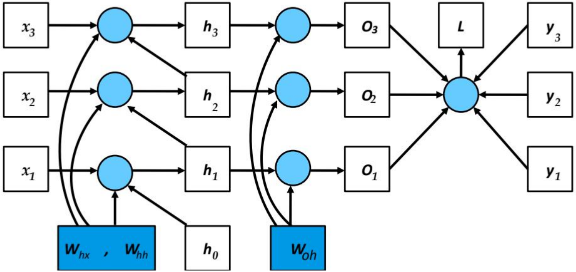

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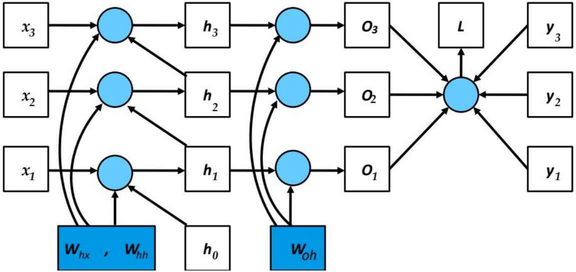
- Since $\mathbf{h}_t = \tanh(\mathbf{W}\mathbf{h}_{t-1} + \dots)$, the term $\frac{\partial \mathbf{h}_t}{\partial \mathbf{h}_{t-1}}$ depends on $\mathbf{W}$.



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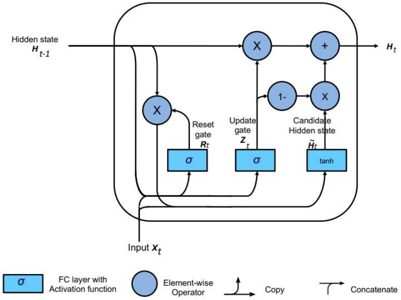
- **Solution:** Gated Architectures (LSTM, GRU).

Gated Recurrent Units (GRU): Intuition

- Standard RNN overwrites $\mathbf{h}_t$ at every step. GRUs typically decide *how much* to update.



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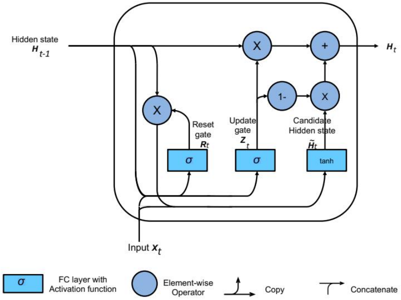

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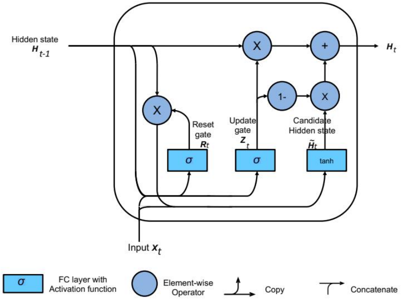

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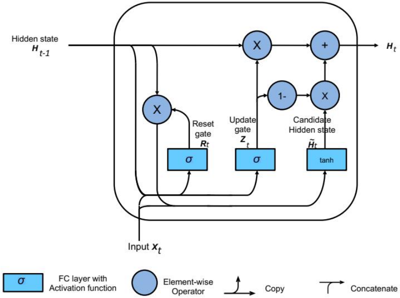
- This creates a "gradient superhighway" back through time, solving vanishing gradients.



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The Attention Mechanism: Step-by-Step

Problem: Encoding a long sentence into a single vector $\mathbf{c}$ loses information. **Solution:** Let the decoder "look" at all encoder states $\mathbf{h}_1, \ldots, \mathbf{h}_T$ dynamically.

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- **Step 3 (Context):** Compute weighted average of encoder states.

$$\mathbf{c}_t = \sum_i \alpha_{t,i} \mathbf{h}_i$$

Visualizing Attention

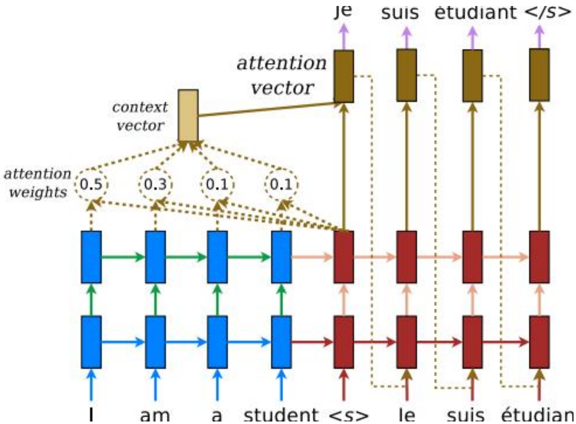

Figure: The decoder (blue) attends to relevant encoder states (red) to generate the next word.

- The model learns alignment automatically (e.g., aligning "European" with "Européenne").

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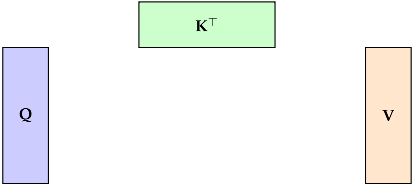
  - **Value ($\mathbf{V}$):** What is the content of this item?
- In Self-Attention, every word generates its own $\mathbf{Q}, \mathbf{K}$, and $\mathbf{V}$ vectors.

Step-by-Step: Self-Attention Mechanism



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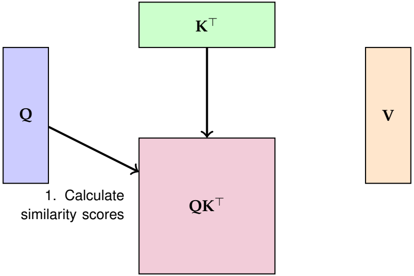

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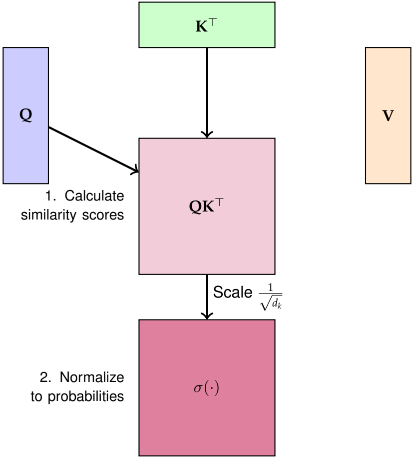

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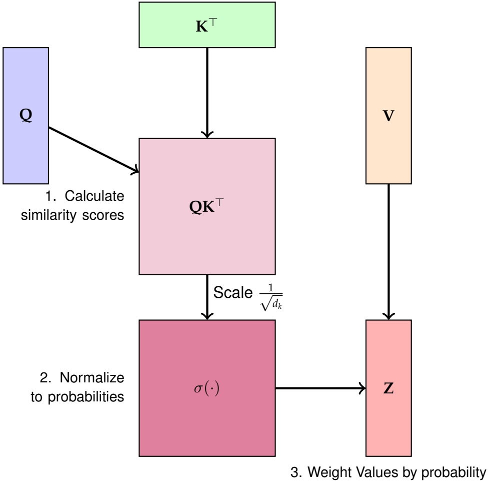
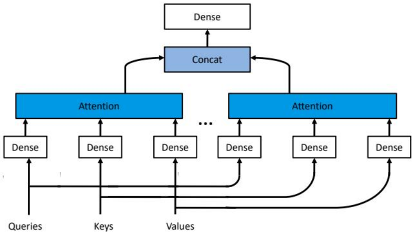


$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{QK}^\top}{\sqrt{d_k}}\right)\mathbf{V}$$

Multi-Head Attention

- A single attention layer might focus only on syntax.



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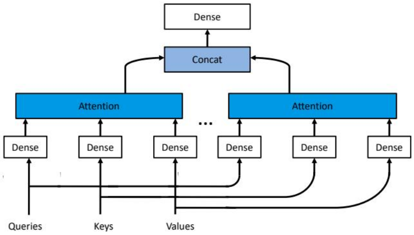

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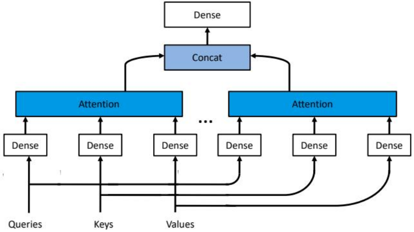

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- Concatenate the results:

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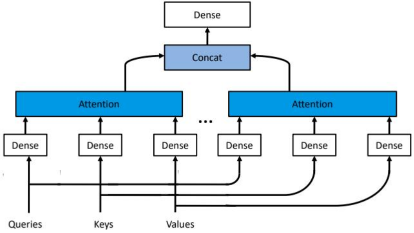

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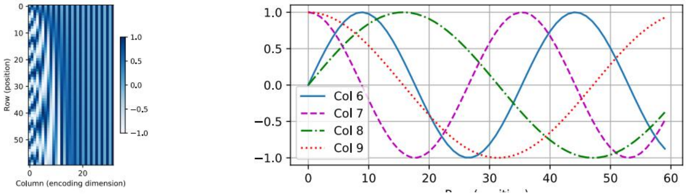

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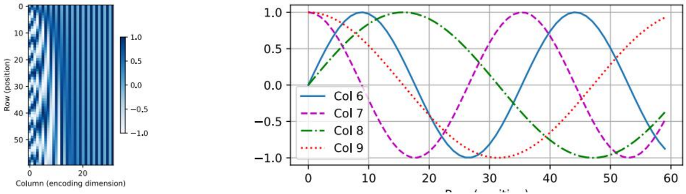

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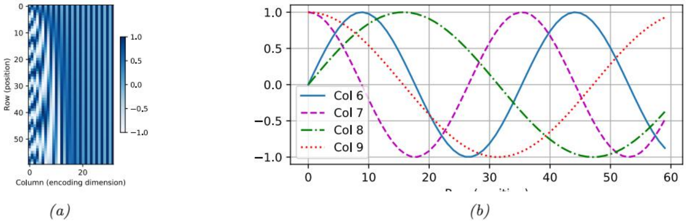

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$$\mathbf{x}_{\text{input}} = \mathbf{x}_{\text{word\_embedding}} + PE_{\text{position}}$$

- Transformer uses fixed Sinusoidal functions so the model can learn relative positions easily.

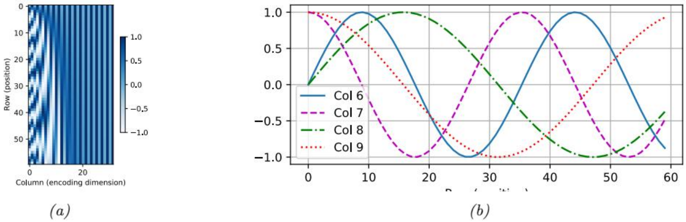

Figure: Sinusoidal Positional Encodings.

Summary: RNN vs Transformer

Feature	**RNN / LSTM**	**Transformer**
Processing	Sequential ($O(N)$)	Parallel ($O(1)$)
Long Distance	Hard (Vanishing Grad)	Easy (Direct Attention)
Complexity	$O(N)$	$O(N^2)$ (Heavy for long seq)
Inductive Bias	Recency	Global Interaction

- Transformers are now the state-of-the-art for NLP (BERT, GPT) and increasingly for Computer Vision (ViT).