Introduction to Machine Learning: Lecture II

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The Plan

- Lecture 1
  - Introduction to Machine Learning fundamentals
  - Linear Models
- Lecture 2
  - Neural Networks
  - Deep Neural Networks
  - Convolutional, Recurrent, and Graph Neural Networks
- Lecture 3
  - Unsupervised Learning
  - Autoencoders
  - Generative Adversarial Networks and Normalizing Flows

Modern Neural Networks

People are now building a **new kind of software** by assembling networks of **parameterized functional blocks** and by **training them from examples using some form of gradient-based optimization**.

- Yann LeCun, 2018

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- Non-linear operations of data with parameters
- Layers (set of operations) designed to perform specific mathematical operations
- Chain together layers to perform desired computation
- Train system (with examples) for desired computation using gradient descent

Modern Neural Networks

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An increasingly large number of people are **defining the networks procedurally in a data-dependent way** (with loops and conditionals), allowing them **to change dynamically as a function of the input data** fed to them. It's really very much **like a regular program, except it's parameterized**

- Yann LeCun, 2018

The Plan

- Deep Learning is a HUGE field
  - O(10,000) papers submitted to conferences

- I'm will condense *some* parts of what you would find in *some lectures* of a Deep Learning course

- Highly recommend taking the time to go more slowly through lectures from a class. Online-available Recommendations:
  - Francois Fleuret course at University of Geneva
  - Gilles Louppe course at University of Liege
  - Yann LeCun & Alfredo Canziani course at NYU

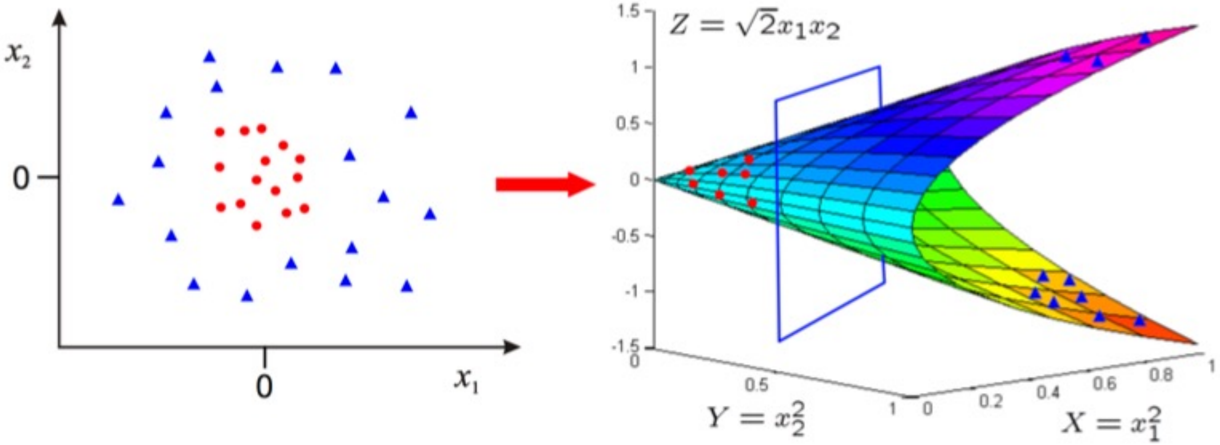
From Logistic Regression to Neural Networks

Adding non-linearity

- What if we want a non-linear decision boundary?
  - Choose basis functions, e.g: ϕ(x) ~ {x², sin(x), log(x), …}

$$p(y=1|\mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}^T\phi(\mathbf{x})}}$$

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$



Adding non-linearity

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- What if we don't know what basis functions we want?

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- Learn the basis functions directly from data

$$\phi(\mathbf{x};\mathbf{u}) \qquad \mathbb{R}^m \rightarrow \mathbb{R}^d$$

  - Where **u** is a set of parameters for the transformation

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  - Combines basis selection and learning
  - Several different approaches, focus here on neural networks
  - Complicates the optimization

Neural Networks

- Define the basis functions j = {1…d}

$$\phi_j(\mathbf{x};\,\mathbf{u}) = \sigma(\mathbf{u}_j{}^T\mathbf{x})$$

Neural Networks

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- Put all $\mathbf{u}_j \in \mathbb{R}^{1\text{xm}}$ vectors into matrix **U**

$$\phi(\mathbf{x}; \mathbf{U}) = \sigma(\mathbf{U}\mathbf{x}) = \begin{bmatrix} \sigma(\mathbf{u}_1{}^T\mathbf{x}) \\ \sigma(\mathbf{u}_2{}^T\mathbf{x}) \\ \dots \\ \sigma(\mathbf{u}_d{}^T\mathbf{x}) \end{bmatrix} \in \mathbb{R}^d$$

  - σ is a point-wise non-linearity acting on each vector element

Neural Networks

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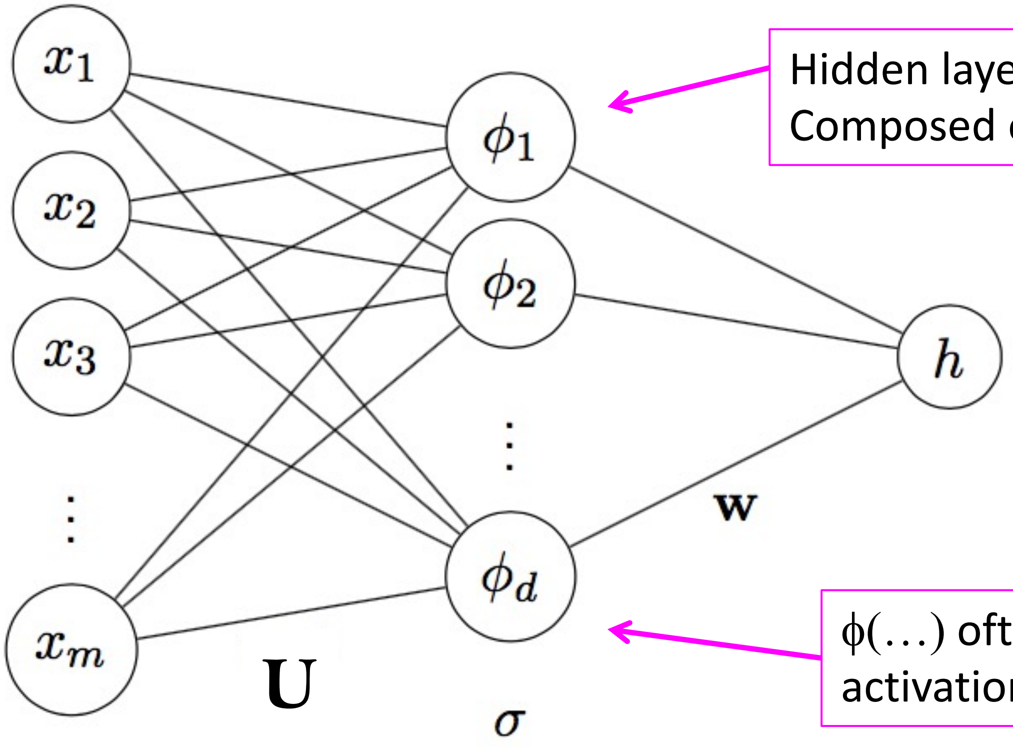
- Full model becomes

$$h(\mathbf{x};\, \mathbf{w}, \mathbf{U}) = \mathbf{w}^T \phi(\mathbf{x};\, \mathbf{U})$$

Feed Forward Neural Network



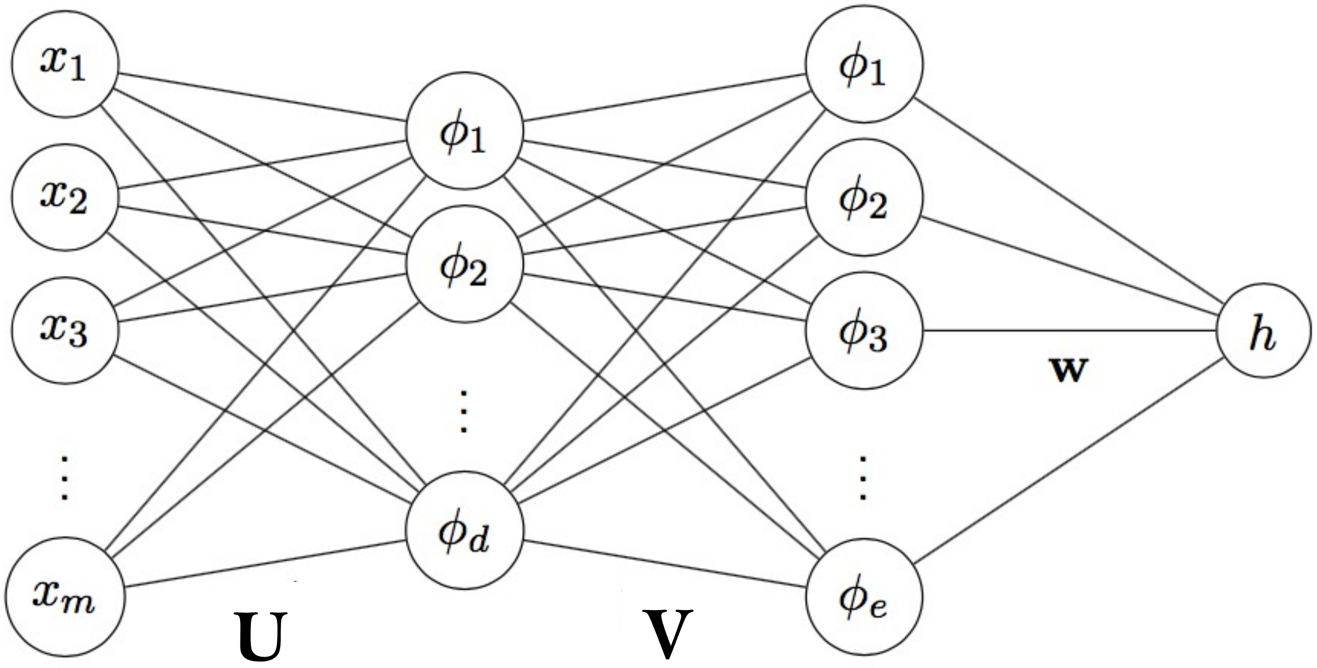
Hidden layer
Composed of *neurons*

ϕ(…) often called the activation function

$$\phi(\mathbf{x}) = \sigma(\mathbf{U}\mathbf{x})$$

$$h(\mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x})$$

Multi-layer Neural Network



- Multilayer NN
  - Each layer adapts basis functions based on previous layer

Neural Network Optimization Problem

- Neural Network Model: $h(\mathbf{x}) = \mathbf{w}^T \sigma(\mathbf{U}\mathbf{x})$

- **Classification**: Cross-entropy loss function

$$p_i = p(y_i = 1 | \mathbf{x}_i) = \sigma(h(\mathbf{x}_i))$$

$$L(\mathbf{w}, \mathbf{U}) = -\sum_i y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i)$$

Neural Network Optimization Problem

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- **Regression**: Square error loss function

$$L(\mathbf{w}, \mathbf{U}) = \frac{1}{2} \sum_i (y_i - h(\mathbf{x}_i))^2$$

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- **Regression**: Square error loss function

$$L(\mathbf{w}, \mathbf{U}) = \frac{1}{2}\sum_i (y_i - h(\mathbf{x}_i))^2$$

- Minimize loss with respect to weights **w, U**

Minimizing loss with gradient descent:

- Parameter update:

$$w \leftarrow w - \eta \frac{\partial L(w, U)}{\partial w}$$

$$U \leftarrow U - \eta \frac{\partial L(w, U)}{\partial U}$$

- How to compute gradients?

Chain Rule – Symbolic Differentiation Painful!

$$L(\mathbf{w}, \mathbf{U}) = -\sum_i y_i \ln(\sigma(h(\mathbf{x}_i))) + (1 - y_i) \ln(1 - \sigma(h(\mathbf{x}_i)))$$

- Derivative of sigmoid: $\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1 - \sigma(x))$
- Chain rule to compute gradient w.r.t. **w**

$$\frac{\partial L}{\partial \mathbf{w}} = \frac{\partial L}{\partial h} \frac{\partial h}{\partial \mathbf{w}} = \sum_i y_i (1 - \sigma(h(\mathbf{x}_i)))\sigma(\mathbf{U}\mathbf{x}) + (1 - y_i)\sigma(h(\mathbf{x}))\sigma(\mathbf{U}\mathbf{x}_i)$$

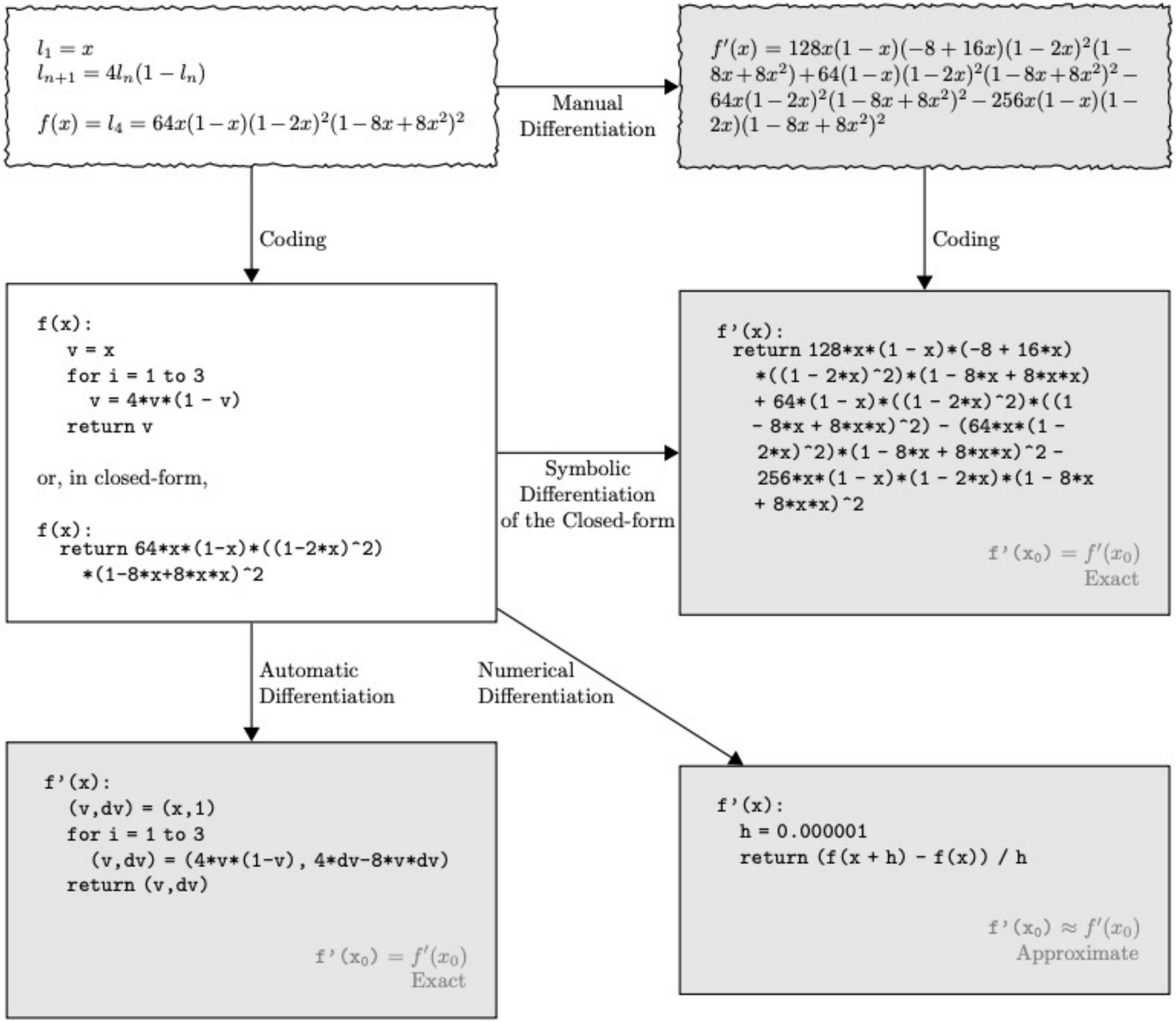
- Chain rule to compute gradient w.r.t. $\mathbf{u}_\mathrm{j}$

$$\frac{\partial L}{\partial \mathbf{u}_j} = \frac{\partial L}{\partial h} \frac{\partial h}{\partial \sigma} \frac{\partial \sigma}{\partial \mathbf{u}_j} =$$

$$= \sum_i y_i (1 - \sigma(h(\mathbf{x}_i))) w_j \sigma(\mathbf{u}_j \mathbf{x}_i)(1 - \sigma(\mathbf{u}_j \mathbf{x}_i))\mathbf{x}_i$$

$$+ (1 - y_i)\sigma(h(\mathbf{x}_i)) w_j \sigma(\mathbf{u}_j \mathbf{x}_i)(1 - \sigma(\mathbf{u}_j \mathbf{x}_i))\mathbf{x}_i$$

Differentiation in Code



$$l_1 = x$$
$$l_{n+1} = 4l_n(1-l_n)$$
$$f(x) = l_4 = 64x(1-x)(1-2x)^2(1-8x+8x^2)^2$$

$$f'(x) = 128x(1-x)(-8+16x)(1-2x)^2(1-8x+8x^2)+64(1-x)(1-2x)^2(1-8x+8x^2)^2-64x(1-2x)^2(1-8x+8x^2)^2-256x(1-x)(1-2x)(1-8x+8x^2)^2$$

```
f(x):
   v = x
   for i = 1 to 3
     v = 4*v*(1 - v)
   return v
```

or, in closed-form,

```
f(x):
  return 64*x*(1-x)*((1-2*x)^2)
    *(1-8*x+8*x*x)^2
```

```
f'(x):
 return 128*x*(1 - x)*(-8 + 16*x)
   *((1 - 2*x)^2)*(1 - 8*x + 8*x*x)
   + 64*(1 - x)*((1 - 2*x)^2)*((1
   - 8*x + 8*x*x)^2) - (64*x*(1 -
   2*x)^2)*(1 - 8*x + 8*x*x)^2 -
   256*x*(1 - x)*(1 - 2*x)*(1 - 8*x
   + 8*x*x)^2
```

$\texttt{f'}(\texttt{x}_0) = f'(x_0)$
Exact

```
f'(x):
  (v,dv) = (x,1)
  for i = 1 to 3
    (v,dv) = (4*v*(1-v), 4*dv-8*v*dv)
  return (v,dv)
```

$\texttt{f'}(\texttt{x}_0) = f'(x_0)$
Exact

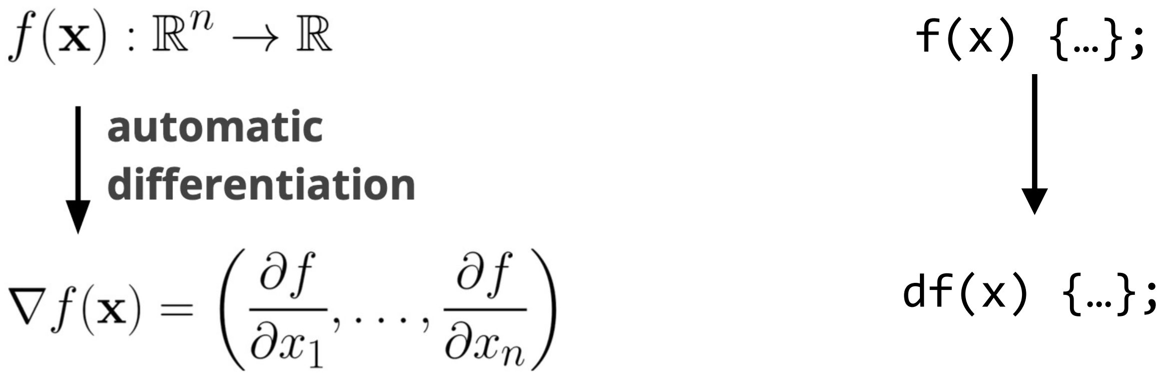
```
f'(x):
  h = 0.000001
  return (f(x + h) - f(x)) / h
```

$\texttt{f'}(\texttt{x}_0) \approx f'(x_0)$
Approximate

Baydin, Pearlmutter, Radul, Siskind. 2018. “Automatic Differentiation in Machine Learning: a Survey.” Journal of Machine Learning Research (**JMLR**)

Automatic Differentiation

- Exact derivatives for gradient-based optimization come from running **differentiable code** via **automatic differentiation**



$f(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$

automatic differentiation

$$\nabla f(\mathbf{x}) = \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_n} \right)$$

```
f(x) {…};
```

```
df(x) {…};
```

- Can compute derivatives not just of mathematical functions, but **derivatives of general purpose code** with control flow, loops, recursions, etc.

Forward and Reverse Mode

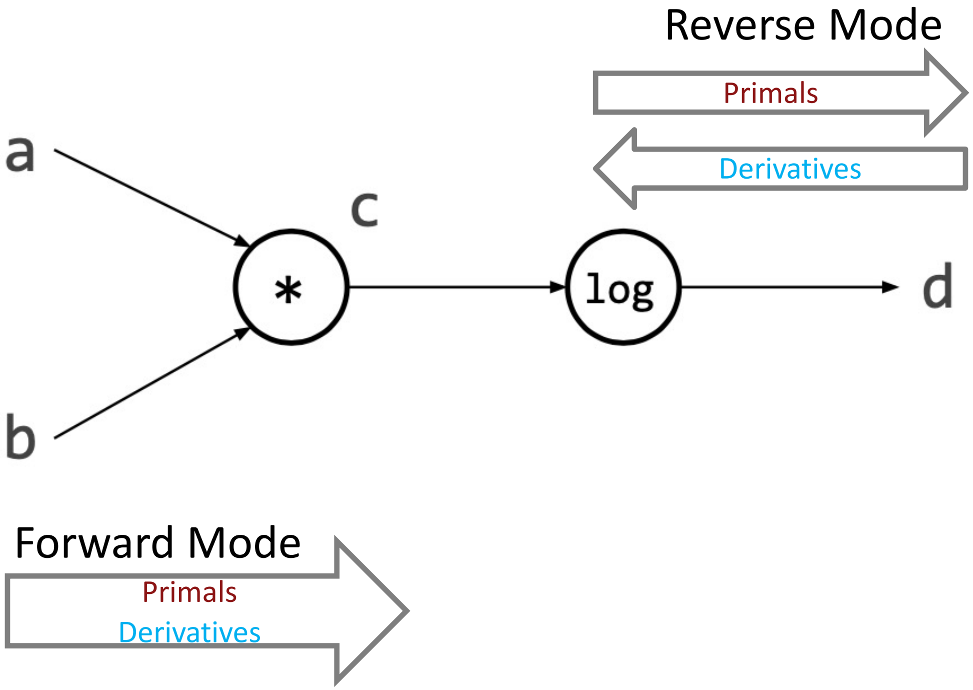
- Derivatives can be computed in **Forward Mode** and **Reverse Mode**

Forward Mode Single Evaluation: $\boldsymbol{f}(\boldsymbol{x})\colon\ \mathbb{R}^N \to \mathbb{R}^M$

$$\frac{d\boldsymbol{f}(\boldsymbol{x})}{d\boldsymbol{x}} = \begin{pmatrix} \frac{df_1}{dx_1} & \cdots & \frac{df_M}{dx_1} \\ \vdots & \ddots & \vdots \\ \frac{df_1}{dx_N} & \cdots & \frac{df_M}{dx_N} \end{pmatrix}$$

Reverse Mode Single Evaluation: $\boldsymbol{f}(\boldsymbol{x})\colon\ \mathbb{R}^N \to \mathbb{R}^M$

$$\frac{d\boldsymbol{f}(\boldsymbol{x})}{d\boldsymbol{x}} = \begin{pmatrix} \frac{df_1}{dx_1} & \cdots & \frac{df_M}{dx_1} \\ \vdots & \ddots & \vdots \\ \frac{df_1}{dx_N} & \cdots & \frac{df_M}{dx_N} \end{pmatrix}$$



Chain Rule: $\frac{\partial d}{\partial a} = \frac{\partial d}{\partial c}\frac{\partial c}{\partial a}$

Backpropagation

- Loss function composed of layers of nonlinearity

$$L\left(\phi^N\left(\ldots\phi^1(x)\right)\ \right)$$

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- Forward step (f-prop)
  - Compute and save intermediate computations

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- Backward step (b-prop) $\dfrac{\partial L}{\partial \phi^a} = \sum_j \dfrac{\partial \phi_j^{(a+1)}}{\partial \phi_j^a} \dfrac{\partial L}{\partial \phi_j^{(a+1)}}$

Backpropagation

- Loss function composed of layers of nonlinearity

$$L(\phi^{N}(\ldots\phi^{1}(x))\,)$$

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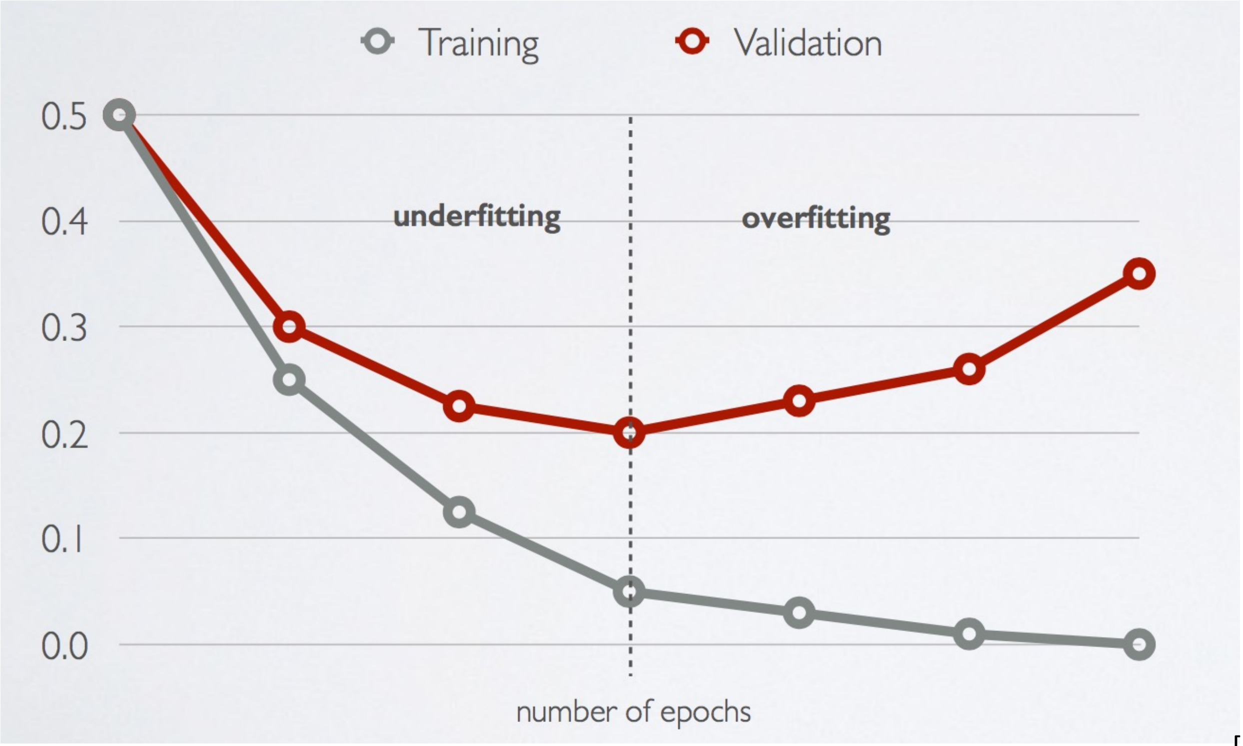
- Compute parameter gradients $$\frac{\partial L}{\partial \mathbf{w}^{a}} = \sum_{j} \frac{\partial \phi_{j}^{a}}{\partial \mathbf{w}^{a}} \frac{\partial L}{\partial \phi_{j}^{a}}$$

Training

- Repeat gradient update of weights to reduce loss
  - Each iteration through dataset is called an epoch

- Use validation set to examine for overtraining, and determine when to stop training

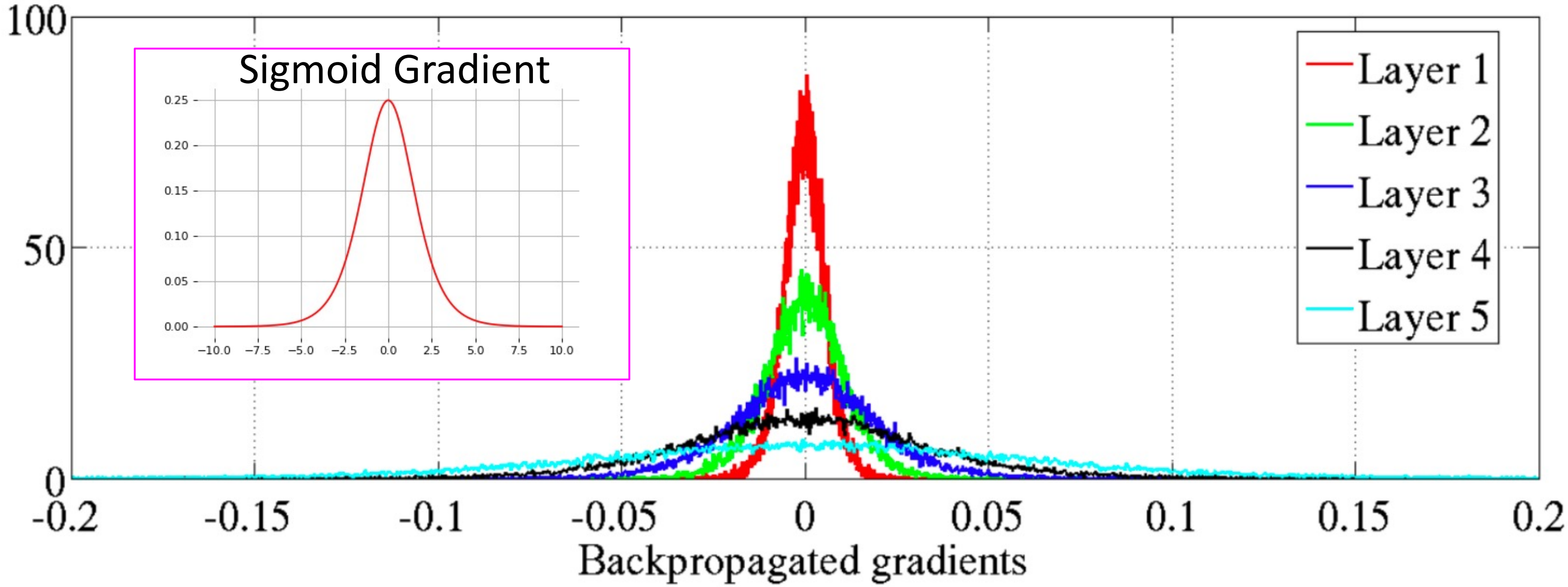


[graphic from H. Larochelle]

Vanishing Gradients

- Major challenge in DL: Vanishing Gradients

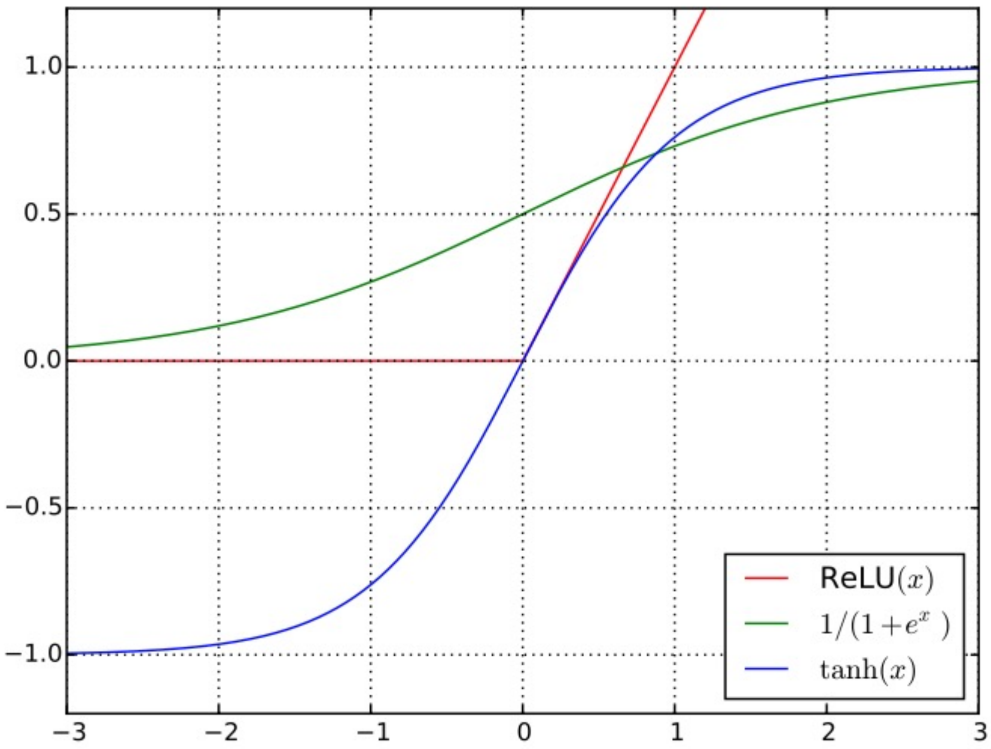
- Small gradients slow down / block, stochastic gradient descent → Limits ability to learn!



Backpropagated gradients normalized histograms (Glorot and Bengio, 2010).
Gradients for layers far from the output vanish to zero.

Slide credit: G. Louppe

Activation Functions



- **Vanishing gradient problem**
  - Derivative of sigmoid:

$$\frac{\partial\sigma(x)}{\partial x}=\sigma(x)(1-\sigma(x))$$

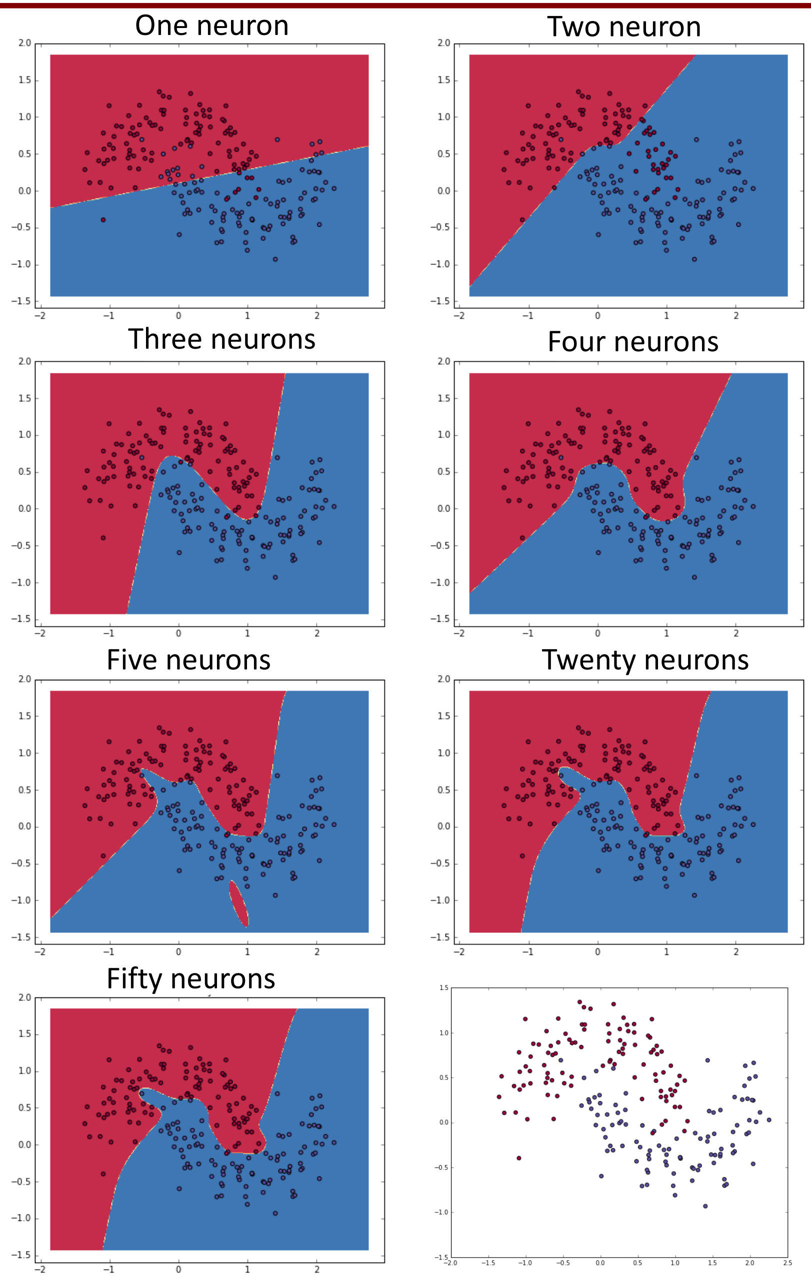
  - Nearly 0 when x is far from 0!
  - Can make gradient descent hard!

- **Rectified Linear Unit (ReLU)**
  - ReLU(x) = max{0, x}
  - Derivative is constant!

$$\frac{\partial ReLU(x)}{\partial x}=\begin{cases}1 & when\ x>0\\ 0 & otherwise\end{cases}$$

  - ReLU gradient doesn’t vanish

Neural Network Decision Boundaries


One neuron

Two neuron

Three neurons

Four neurons

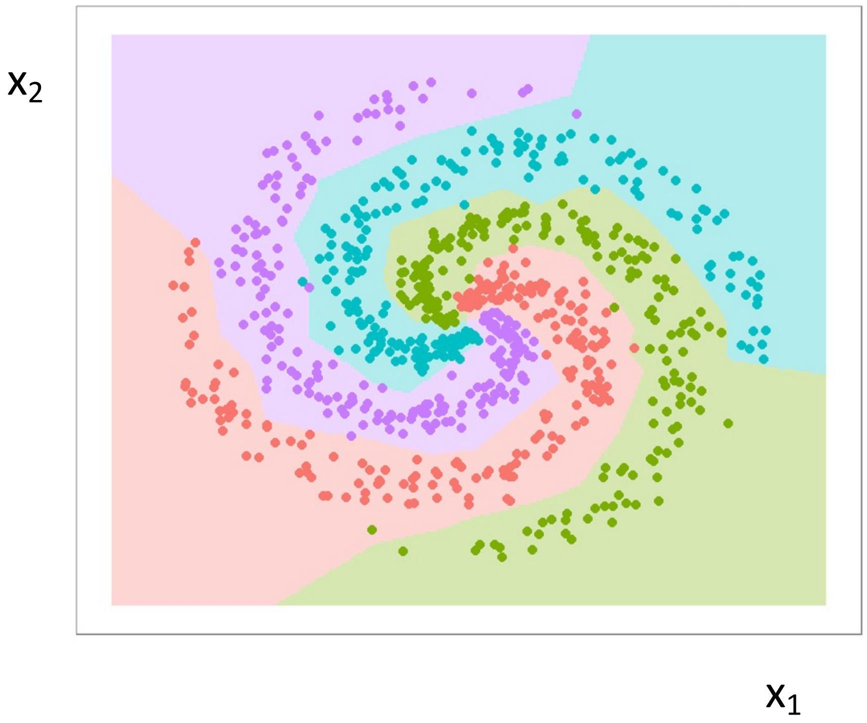
Five neurons

Twenty neurons

Fifty neurons

Image source

4-class classification
2-hidden layer NN
ReLU activations
L2 norm regularization



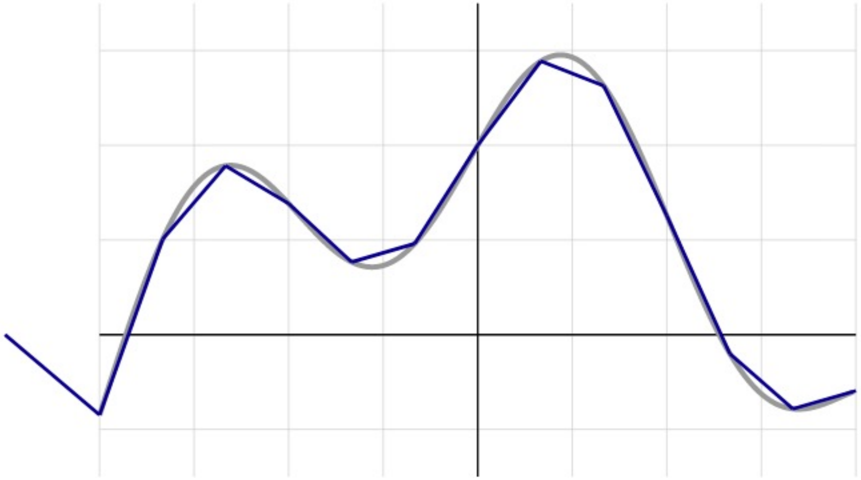
2-class classification
1-hidden layer NN
L2 norm regularization

Image source

Universal approximation theorem

- Feed-forward neural network with a single hidden layer containing a finite number of non-linear neurons (ReLU, Sigmoid, and others) can approximate continuous functions arbitrarily well on a compact space of $\mathbb{R}^n$

$$f(x) = \sigma(w_1 x + b_1) + \sigma(w_2 x + b_2) + \sigma(w_3 x + b_3) + \dots$$



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Universal approximation theorem

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- NOTE!
  - A better approximation requires a larger hidden layer and this theorem says nothing about the relation between the two.
  - We can make training error as low as we want by using a larger hidden layer. Result states nothing about test error
  - Doesn't say how to find the parameters for this approximation

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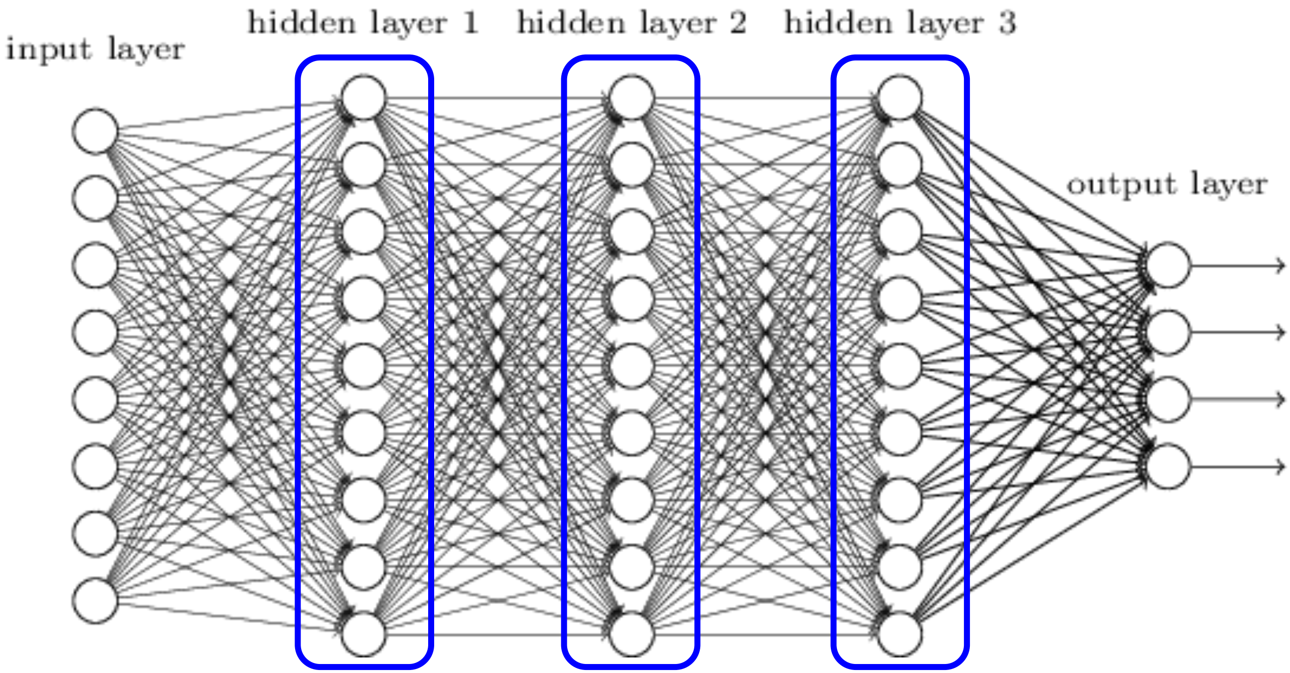
Deep Neural Networks



- As data complexity grows, need exponentially large number of neurons in a single-hidden-layer network to capture all structure in data

- Deep neural networks *factorize the learning* of structure in data across many layers

- Difficult to train, only recently possible with large datasets, fast computing (GPU / TPU) and new training procedures / network structures

Neural Network Zoo

- Structure of the networks, and the node connectivity can be adapted for problem at hand

- Moving inductive bias from feature engineering to model design

  - *Inductive bias*: Knowledge about the problem

  - *Feature engineering*: Hand crafted variables

  - *Model design*: The data representation and the structure of the machine learning model / network

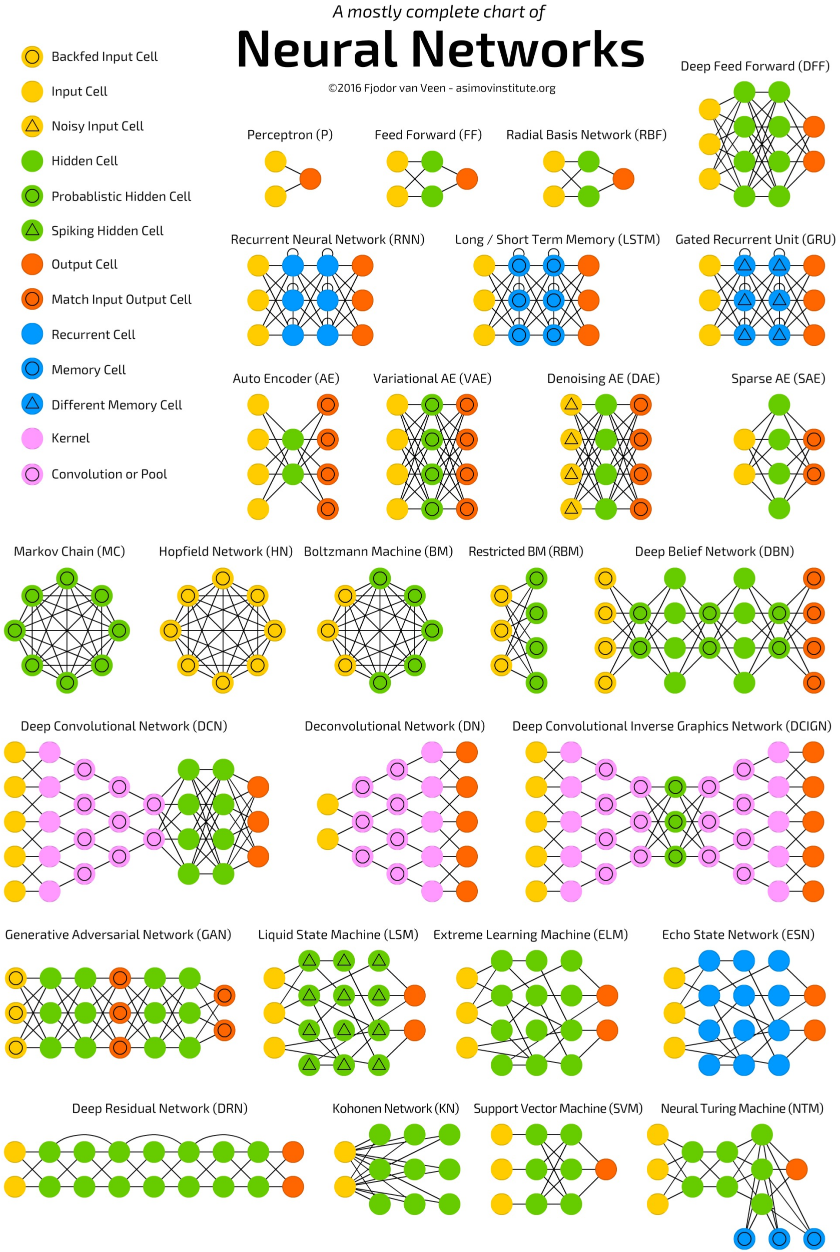

A mostly complete chart of
Neural Networks
©2016 Fjodor van Veen - asimovinstitute.org
Backfed Input Cell
Input Cell
Noisy Input Cell
Hidden Cell
Probablistic Hidden Cell
Spiking Hidden Cell
Output Cell
Match Input Output Cell
Recurrent Cell
Memory Cell
Different Memory Cell
Kernel
Convolution or Pool
Perceptron (P)
Feed Forward (FF)
Radial Basis Network (RBF)
Deep Feed Forward (DFF)
Recurrent Neural Network (RNN)
Long / Short Term Memory (LSTM)
Gated Recurrent Unit (GRU)
Auto Encoder (AE)
Variational AE (VAE)
Denoising AE (DAE)
Sparse AE (SAE)
Markov Chain (MC)
Hopfield Network (HN)
Boltzmann Machine (BM)
Restricted BM (RBM)
Deep Belief Network (DBN)
Deep Convolutional Network (DCN)
Deconvolutional Network (DN)
Deep Convolutional Inverse Graphics Network (DCIGN)
Generative Adversarial Network (GAN)
Liquid State Machine (LSM)
Extreme Learning Machine (ELM)
Echo State Network (ESN)
Deep Residual Network (DRN)
Kohonen Network (KN)
Support Vector Machine (SVM)
Neural Turing Machine (NTM)

Image credit: neural-network-zoo

Neural Network Zoo – "Optimization" Perspective

- A single layer network may need a width exponential in D to approximate a depth-D network's output
  - Simplified version of Telgarsky (2015, 2016)

Neural Network Zoo – "Optimization" Perspective

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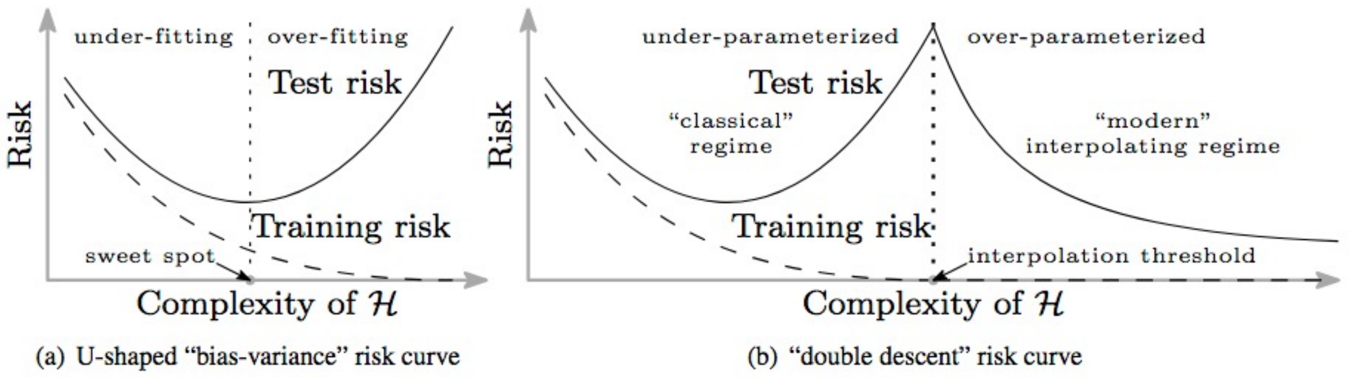
- Over-parametrizing a deep model often improves test performance, contrary to bias-variance tradeoff prediction

Belkin et. al. 2018



(a) U-shaped "bias-variance" risk curve

(b) "double descent" risk curve

Figure 1: Curves for training risk (dashed line) and test risk (solid line). (a) The classical *U-shaped risk curve* arising from the bias-variance trade-off. (b) The *double descent risk curve*, which incorporates the U-shaped risk curve (i.e., the "classical" regime) together with the observed behavior from using high complexity function classes (i.e., the "modern" interpolating regime), separated by the interpolation threshold. The predictors to the right of the interpolation threshold have zero training risk.

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Neural Network Zoo – "Optimization" Perspective

- A single layer network may need a width exponential in D to approximate a depth-D network's output
  - Simplified version of Telgarsky (2015, 2016)

- Over-parametrizing a deep model often improves test performance, contrary to bias-variance tradeoff prediction
  - But we must control that:
    - Gradients don't vanish
    - Gradient amplitude is homogeneous across network
    - Gradients are under control when weights change

Neural Network Zoo – “Optimization” Perspective

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  - Simplified version of Telgarsky (2015, 2016)

- Over-parametrizing a deep model often improves test performance, contrary to bias-variance tradeoff prediction

- Major part of deep learning is **trying to choose the right function…**

… instead of trying to improve training with regularization and new optimizers

- Need to **make gradient descent work**, even at the cost of a substantially engineering the model

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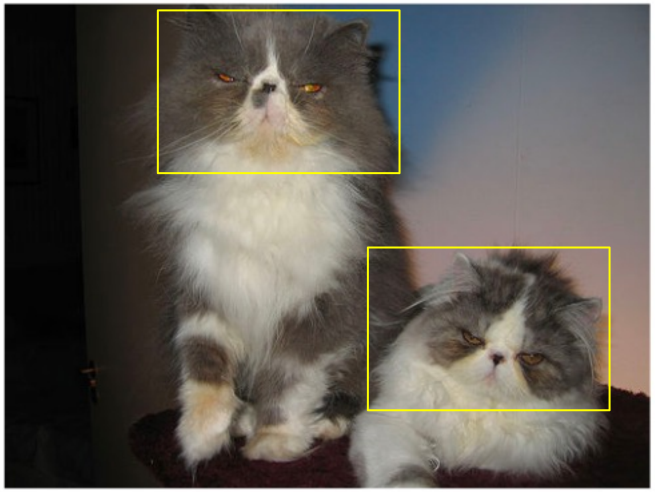
Convolutional Neural Networks

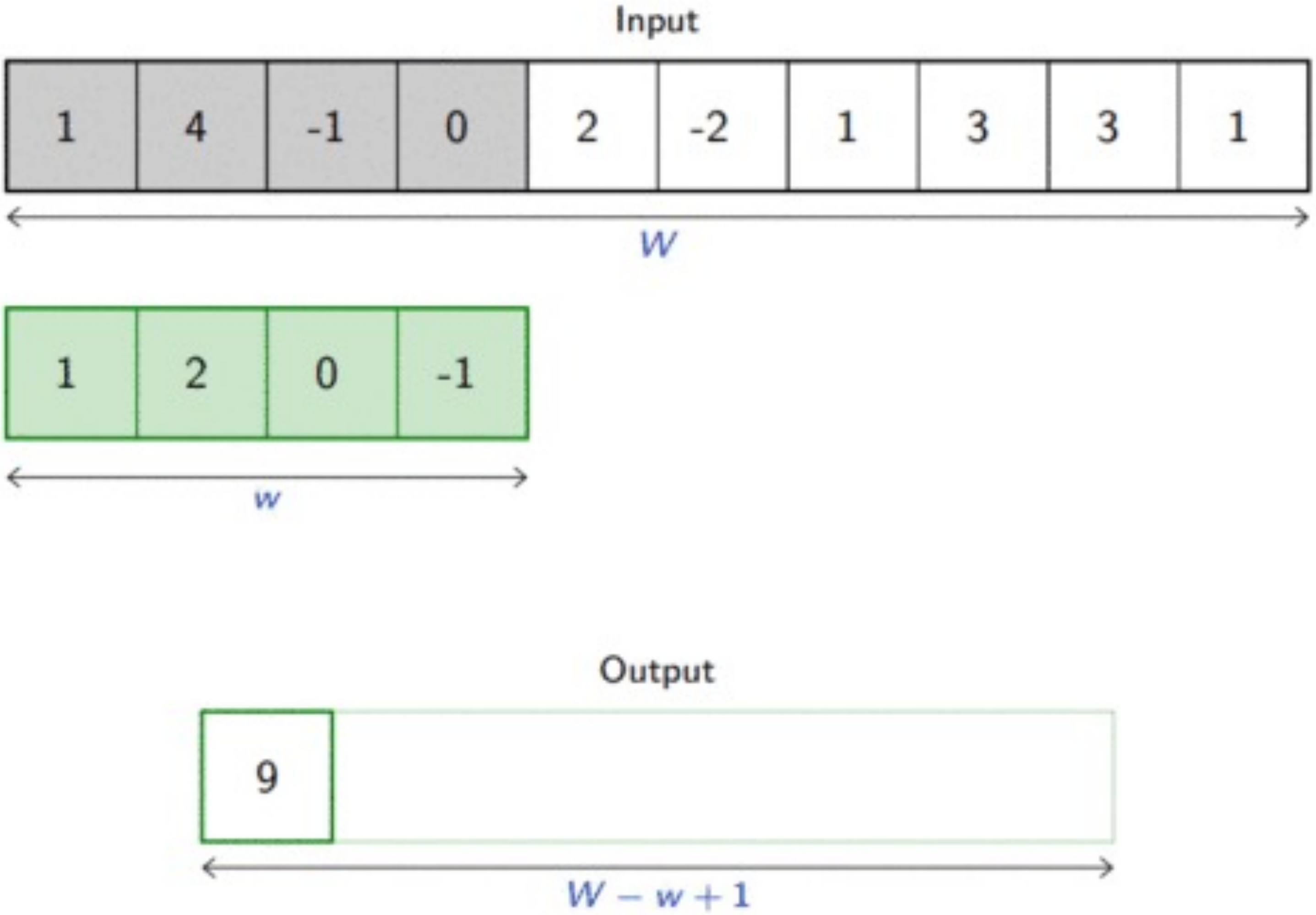
Convolutional Neural Networks

- When the structure of data includes “invariance to translation”, a representation meaningful at a certain location can / should be used everywhere



- Convolutional layers build on this idea, that the same “local” transformation is applied everywhere and preserves the signal structure

1D Convolutional Layer Example



Input

1	4	-1	0	2	-2	1	3	3	1

W

1	2	0	-1

w

Output

9

$W - w + 1$

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1D Convolutional Layers

- **Data:** $x \in \mathbb{R}^M$
- **Convolutional kernel of width k:** $u \in \mathbb{R}^k$

- Convolution $x \circledast u$ is vector of size M-k+1

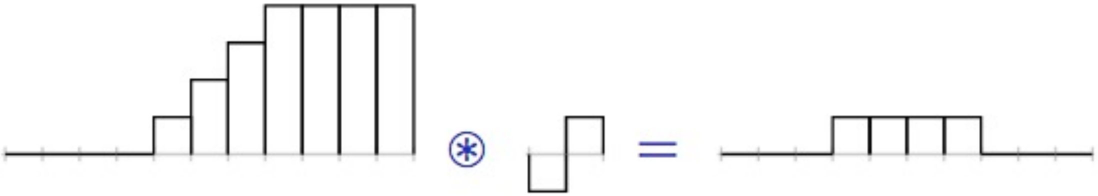
$$(x \circledast \mathrm{u})_i = \sum_{b=0}^{k-1} x_{i+b} u_b$$

- Scan across data and multiply by kernel elements

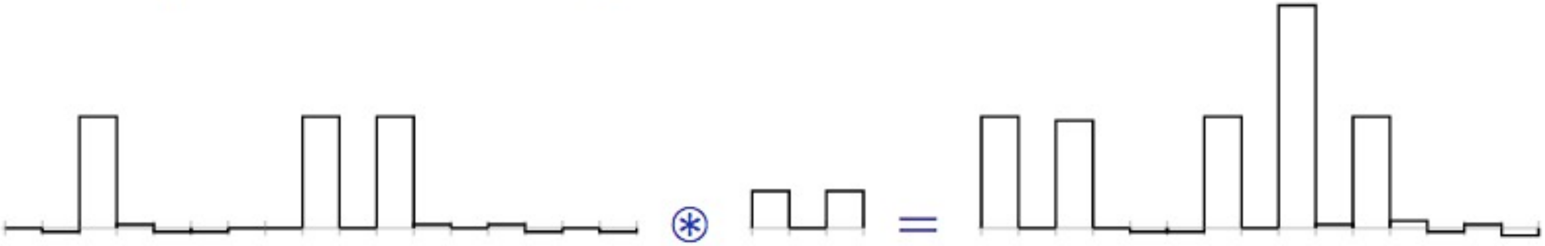
Convolutional Filters

Convolution can implement in particular differential operators, *e.g.*

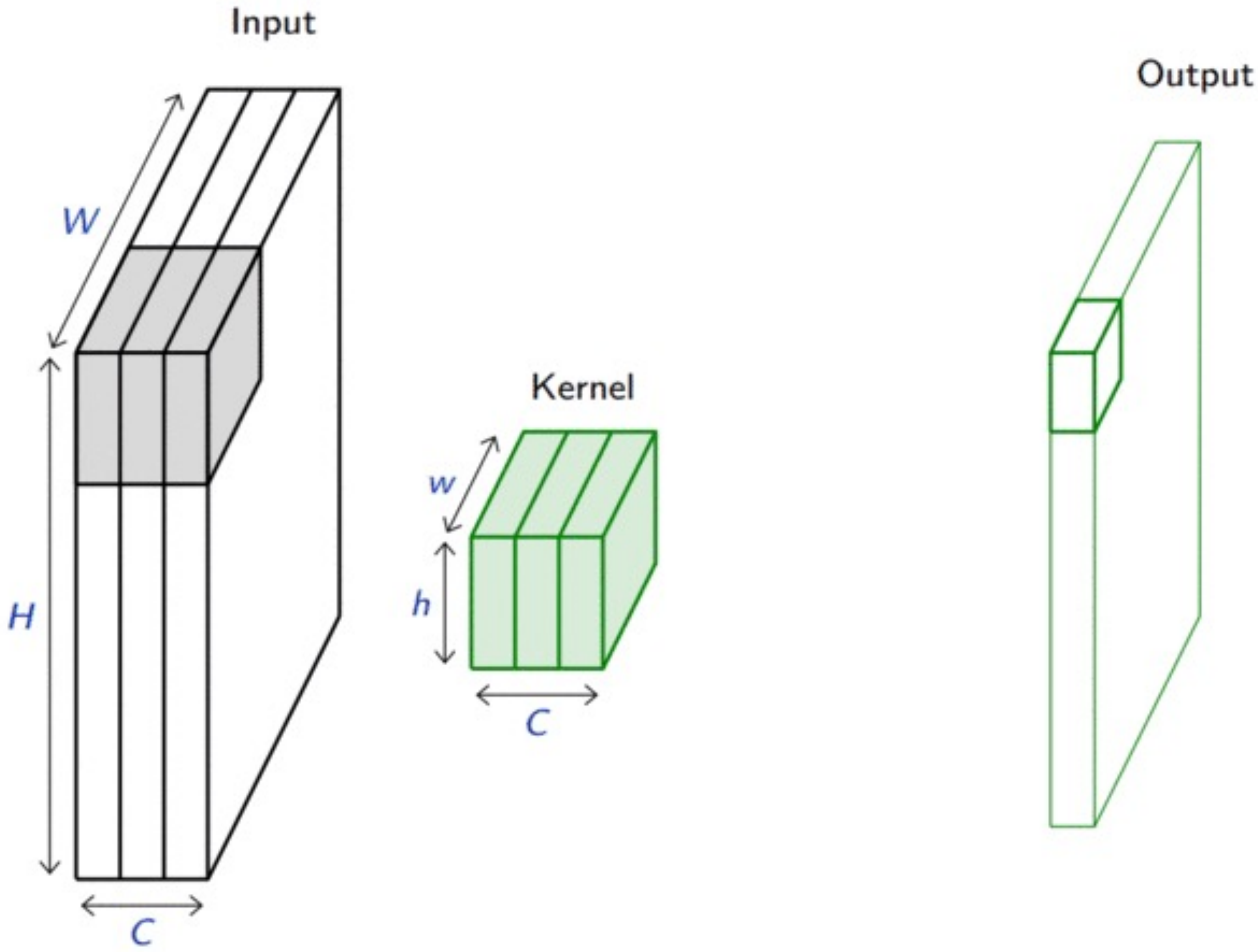
$$(0,0,0,0,1,2,3,4,4,4,4) \circledast (-1,1) = (0,0,0,1,1,1,1,0,0,0).$$



or crude “template matcher”, *e.g.*

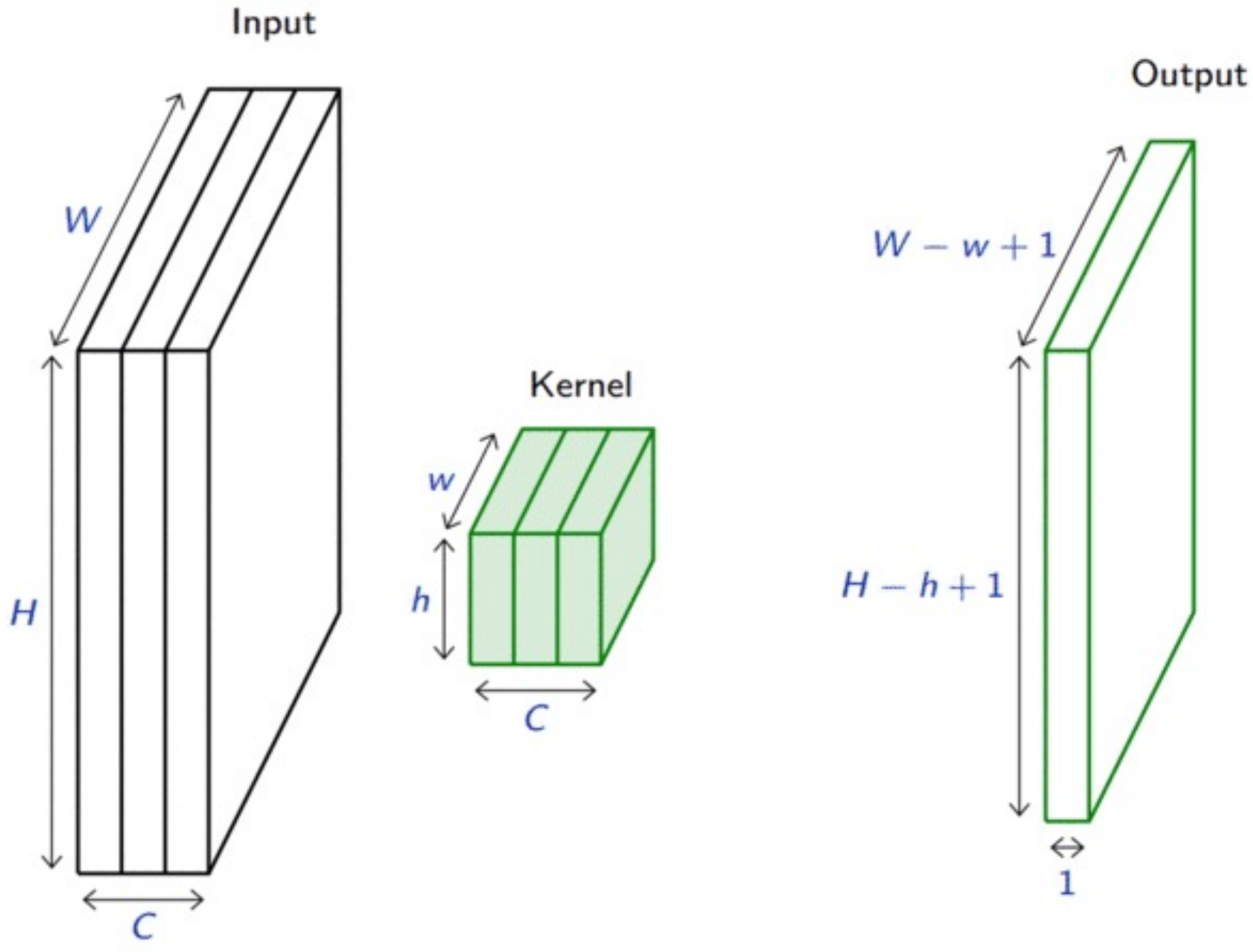


2D Convolution Over Multiple Channels



Fleuret, Deep Learning Course

2D Convolution Over Multiple Channels



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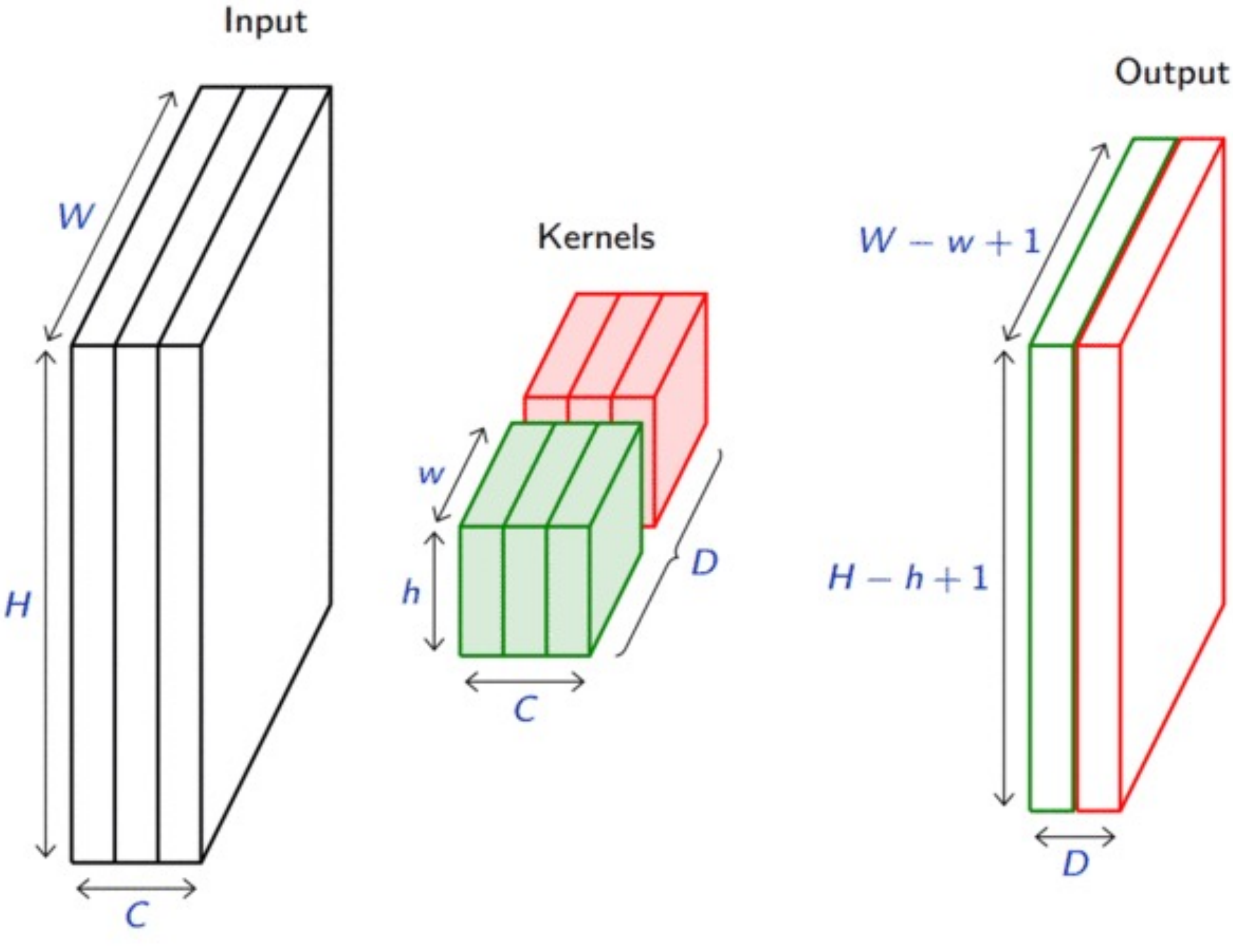
2D Convolution Over Multiple Channels



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2D Convolutional Layer

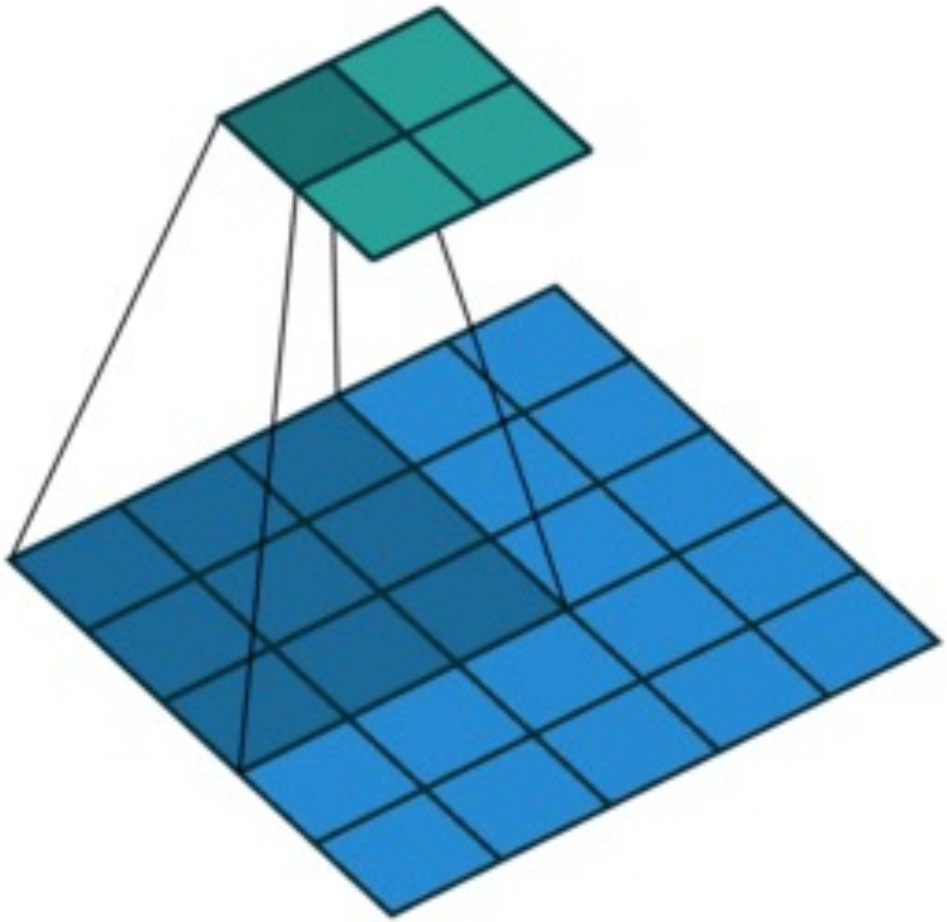
- Input data (tensor) **x** of size C×H×W
  - C channels (e.g. RGB in images)

- Learnable Kernel **u** of size C×h×w
  - The size h×w is the *receptive field*

$$(\boldsymbol{x} \circledast \boldsymbol{u})_{i,j} = \sum_{c=0}^{C-1} (\boldsymbol{x}_c \circledast \boldsymbol{u}_c)_{i,j} = \sum_{c=0}^{C-1} \sum_{n=0}^{h-1} \sum_{m=0}^{w-1} \boldsymbol{x}_{c,n+i,m+j} \boldsymbol{u}_{c,n,m}$$

- Output size $(H-h+1)\times(W-w+1)$ for each kernel
  - Often called *Activation Map* or *Output Feature Map*

Stride – Step Size When Moving Kernel Across Input



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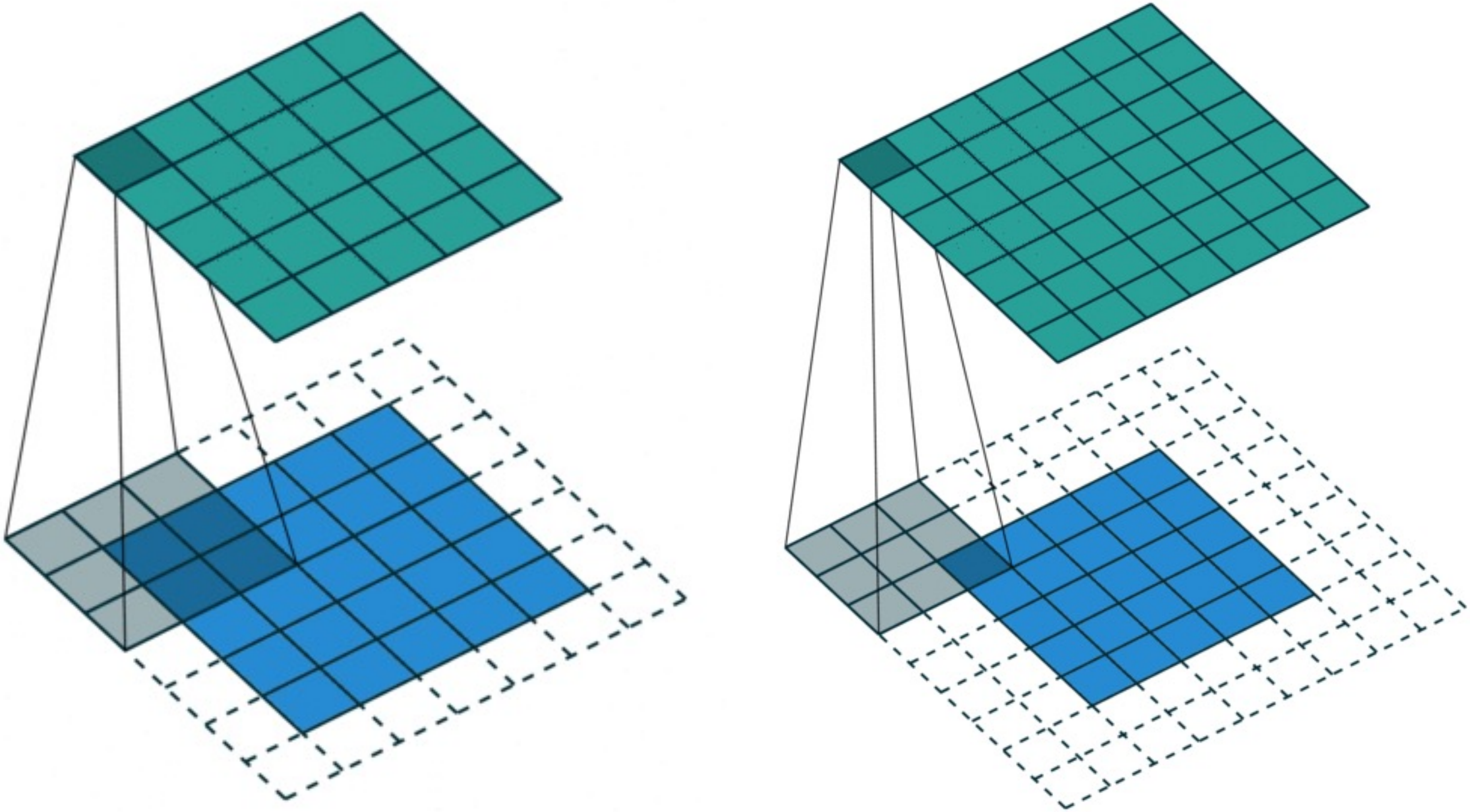
Padding – Size of Zero Frame Around Input



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Shared Weights: Economic and Equivariant

- Parameters are *shared* by each neuron producing an output in the activation map

- Dramatically reduces number of weights needed to produce an activation map
  - Data: 256×256×3 RGB image
  - Kernel: 3×3×3 → 27 weights
  - Fully connected layer:
    - 256×256×3 inputs → 256×256×3 outputs → $O(10^{10})$ weights

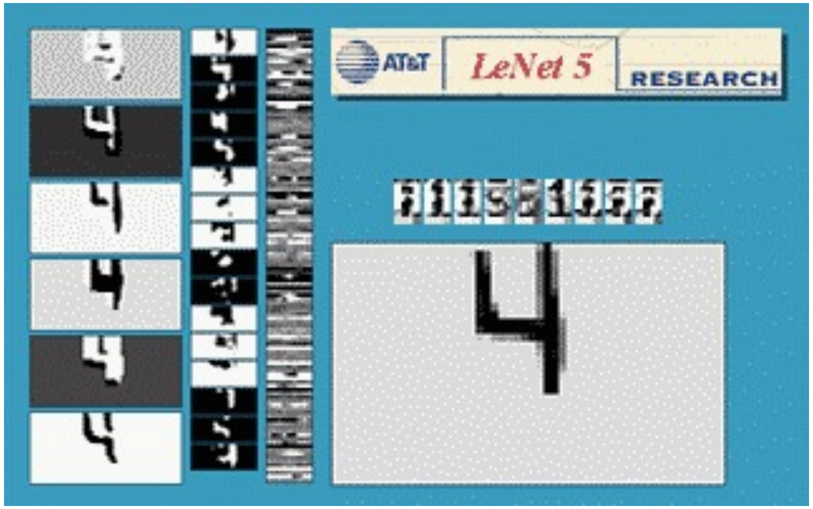
Y. LeCun et. al. 1998

Shared Weights: Economic and Equivariant

- Parameters are *shared* by each neuron producing an output in the activation map

- Dramatically reduces number of weights needed to produce an activation map

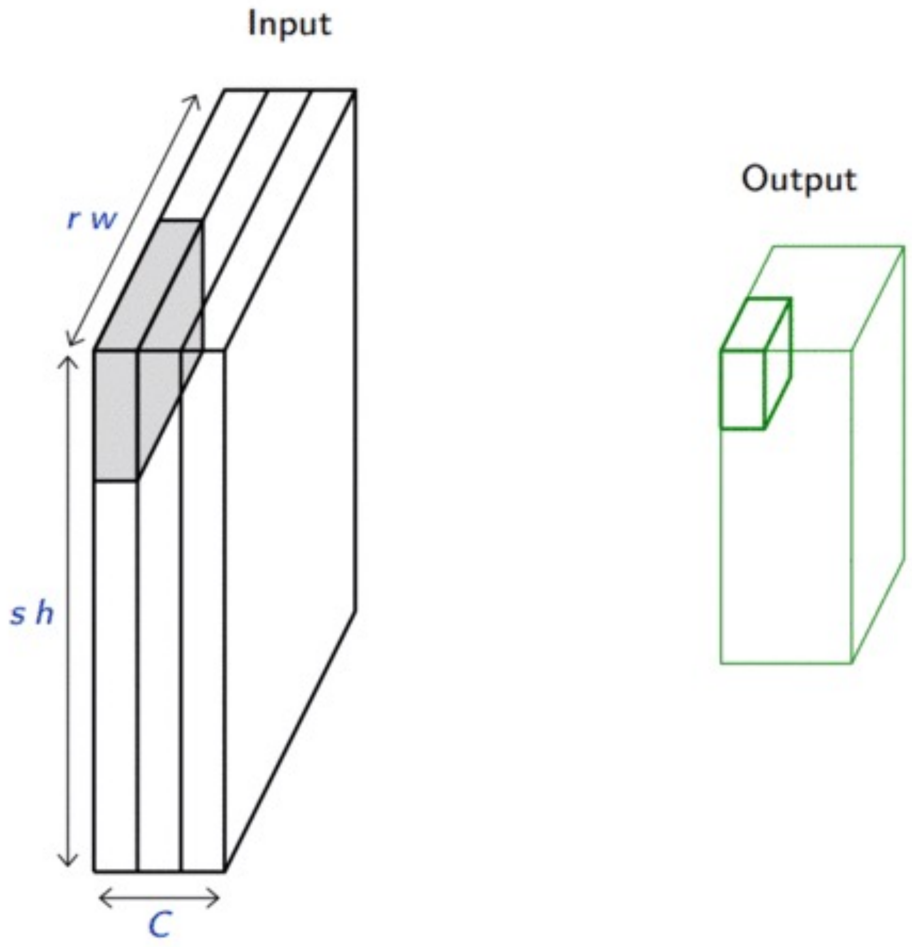
- Convolutional layer does pattern matching at any location → Equivariant to translation



Y. LeCun et. al. 1998

Pooling

- In each channel, find *max* or *average* value of pixels in a pooling area of size $h{\times}w$



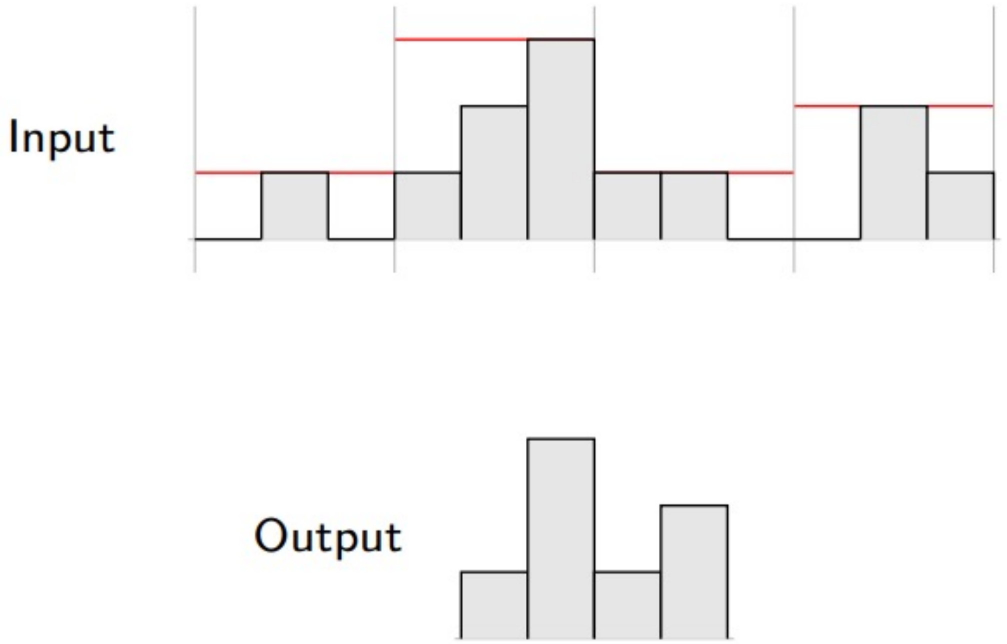
Fleuret, Deep Learning Course

Pooling

- In each channel, find *max* or *average* value of pixels in a pooling area of size $h \times w$

- Invariance to permutation within pooling area

- Invariance to local perturbations

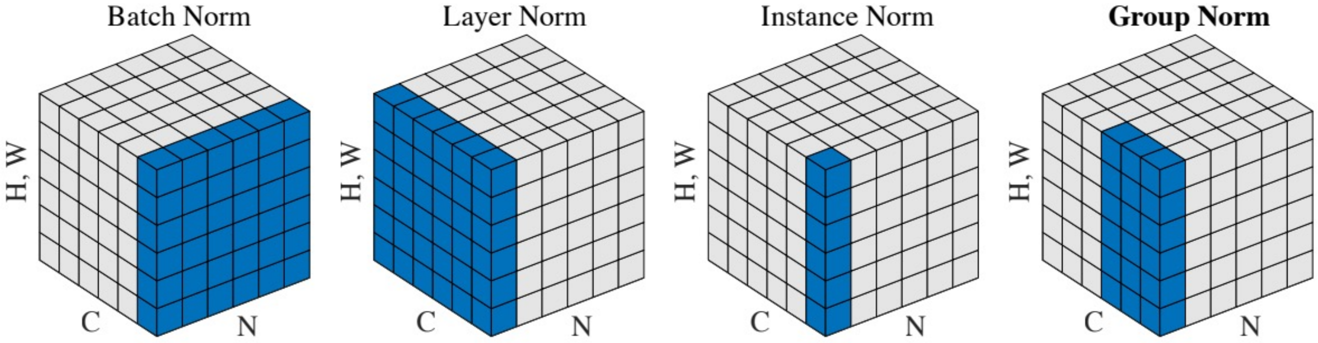


Normalization

- Maintaining proper statistics of the activations and derivatives is a critical issue to allow the training of deep architectures

“Training Deep Neural Networks is complicated by the fact that **the distribution of each layer’s inputs changes during training, as the parameters of the previous layers change**. This slows down the training by requiring lower learning rates and careful parameter initialization …”

Ioffe, Szegedy,
Batch Normalization, ICML 2015



Wu, He, *Group Normalization*, CoRR 2018

Batch Normalization

- During training batch normalization shifts and rescales according to the mean and variance estimated on the batch.
  - During test, use empirical moments estimated during training

- Per-component mean and variance on the batch

$$m_{batch} = \frac{1}{B}\sum_{b=1}^{B} x_b$$

$$v_{batch} = \frac{1}{B}\sum_{1}^{B}(x_b - m_{batch})^2$$

- Normalize and compute output $\forall b = 1 \dots B$

$$z_b = \frac{x_b - m_{batch}}{\sqrt{v_{batch} + \epsilon}}$$

$$y_b = \gamma \odot z_b + \beta$$

  - γ and β are parameters to optimize

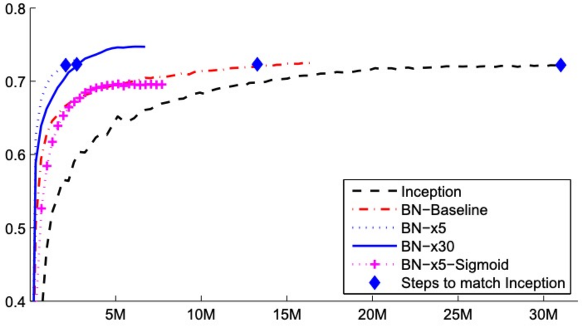
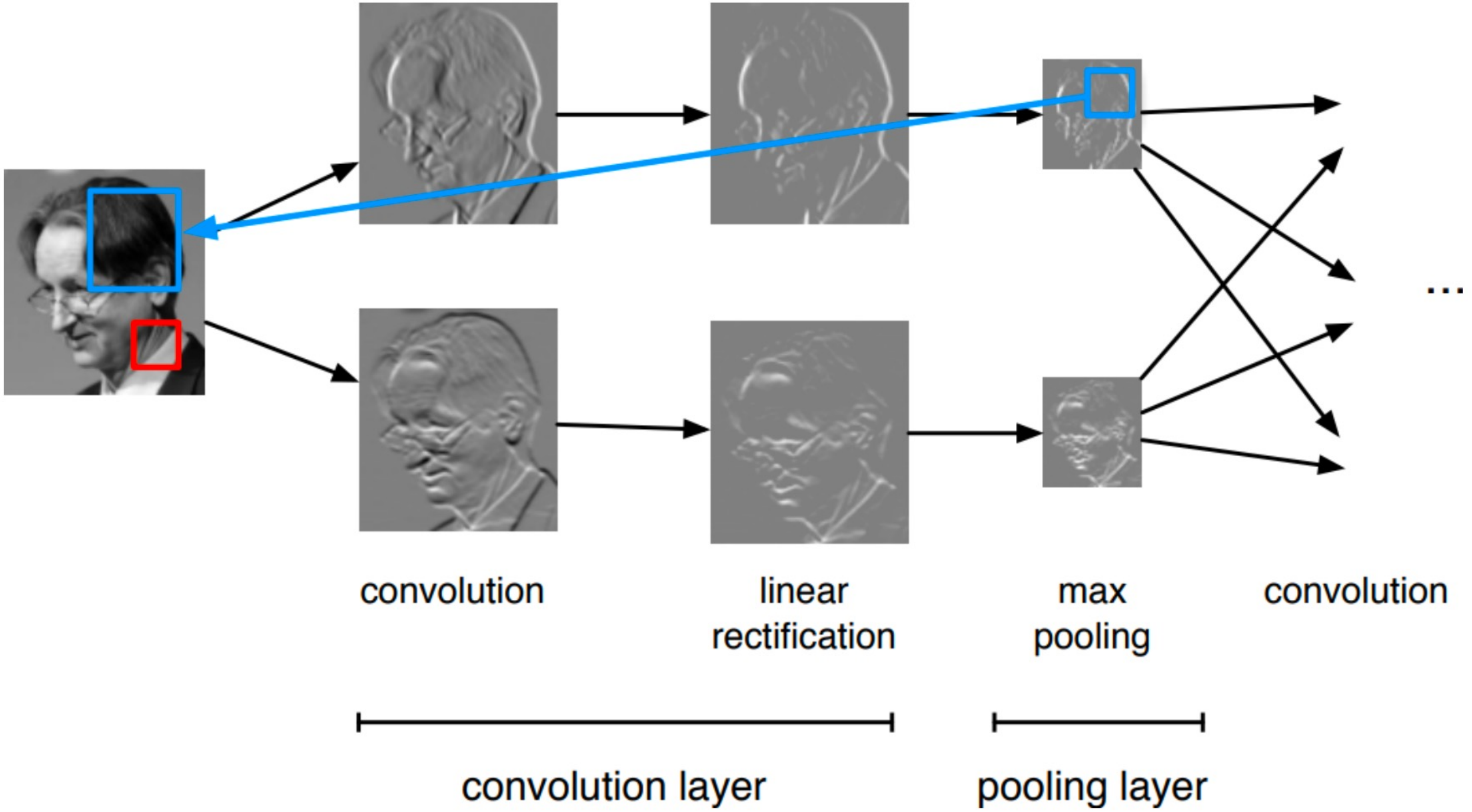


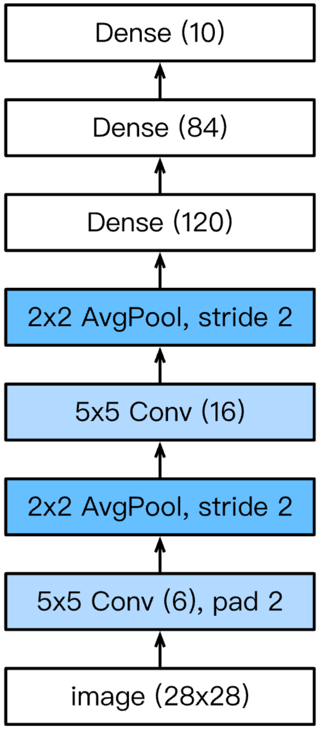
Figure 2: *Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.*

Convolutional Network

- A combination of convolution, pooling, ReLU, and fully connected layers



Convolutional Networks



Dense (10)

Dense (84)

Dense (120)

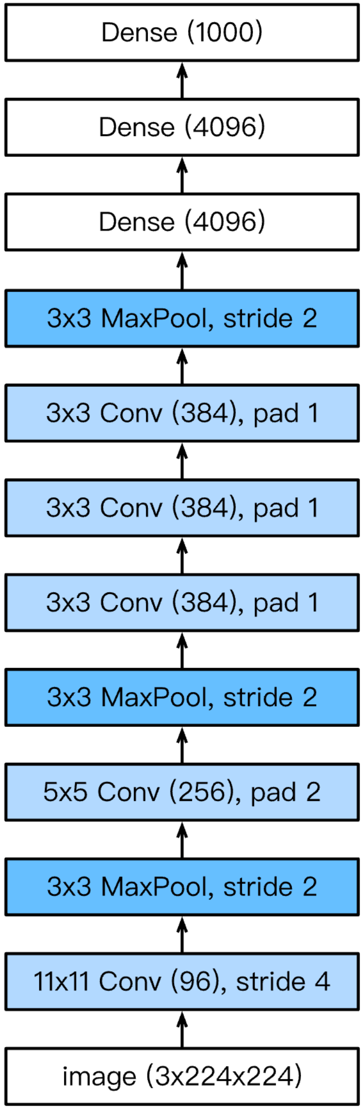
2x2 AvgPool, stride 2

5x5 Conv (16)

2x2 AvgPool, stride 2

5x5 Conv (6), pad 2

image (28x28)



Dense (1000)

Dense (4096)

Dense (4096)

3x3 MaxPool, stride 2

3x3 Conv (384), pad 1

3x3 Conv (384), pad 1

3x3 Conv (384), pad 1

3x3 MaxPool, stride 2

5x5 Conv (256), pad 2

3x3 MaxPool, stride 2

11x11 Conv (96), stride 4

image (3x224x224)

ImageNet Classification

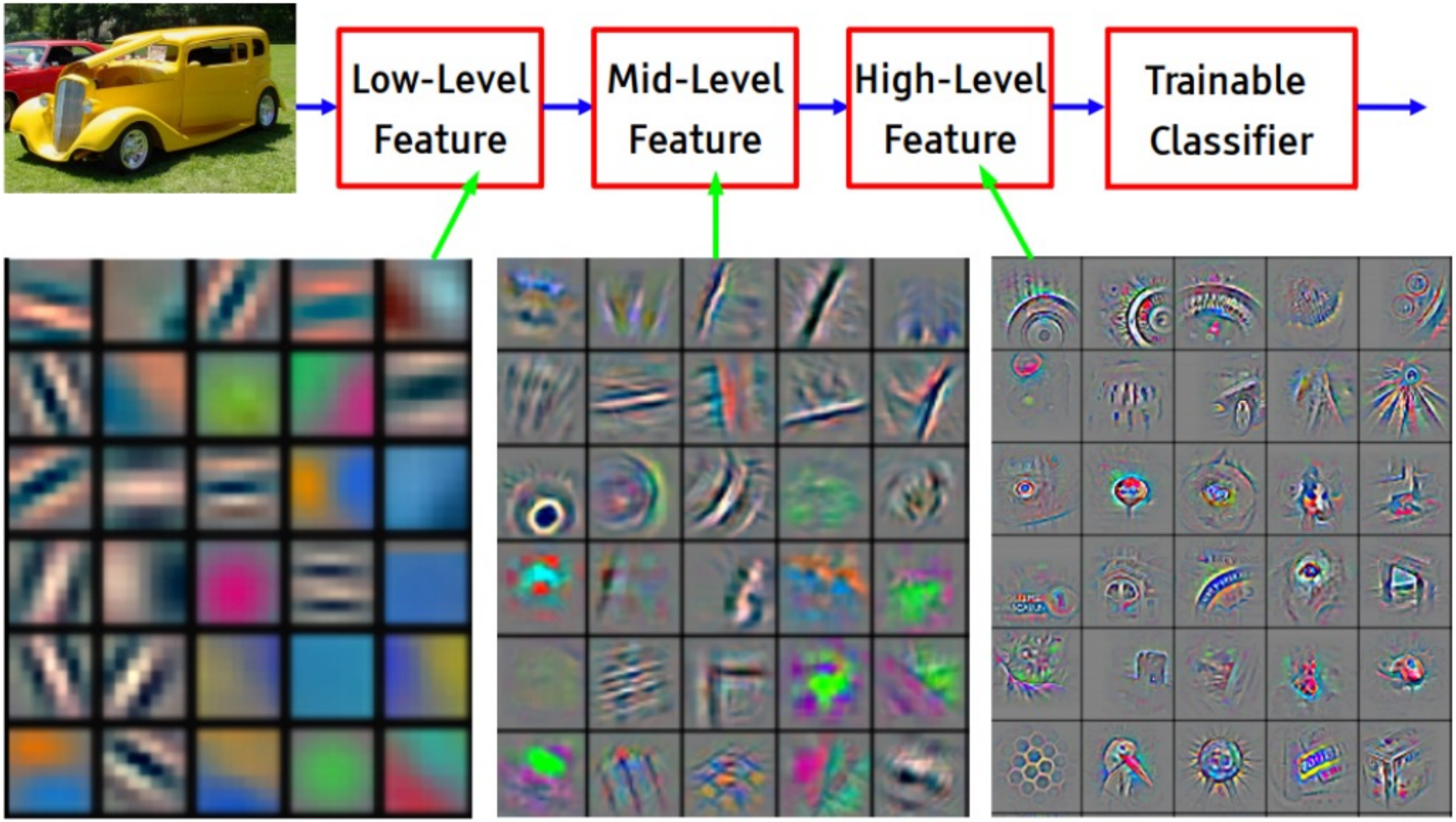
LeNet

(LeCun et al, 1998)

AlexNet

(Krizhevsky et al, 2012)

Hierarchical Composition of Features



Low-Level Feature

Mid-Level Feature

High-Level Feature

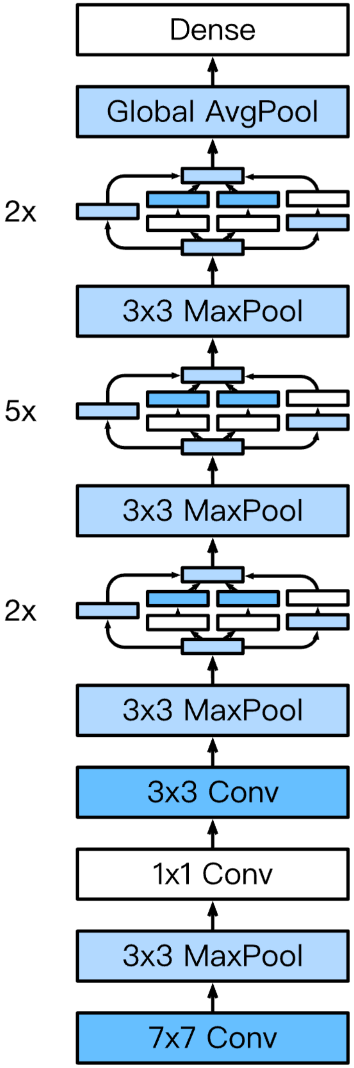
Trainable Classifier

Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

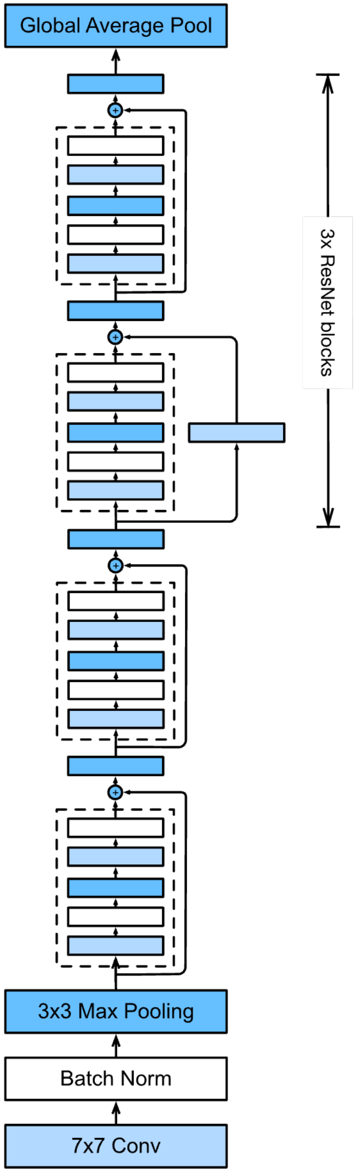
Deep CNNs

- To go deeper, architectures become much more complex
  - Multiple convolutions in parallel and recombined
  - Skip connections

- Recent ResNet-152 has 152 layers!



GoogLeNet
(Szegedy et al, 2014)

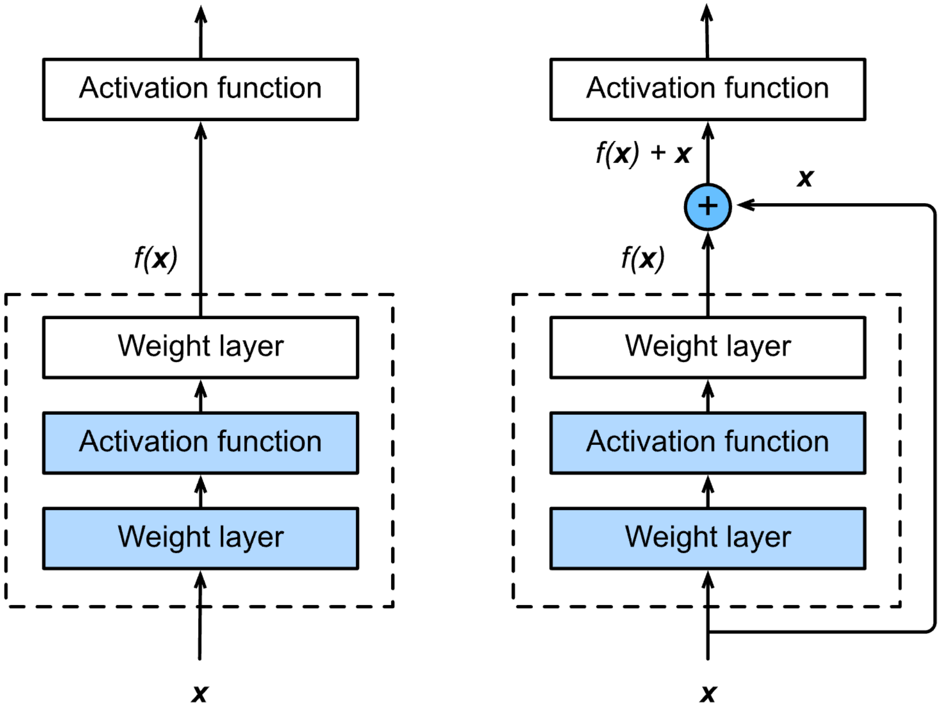


ResNet
(He et al, 2015)

Credits: Deep Dive in Deep Learning

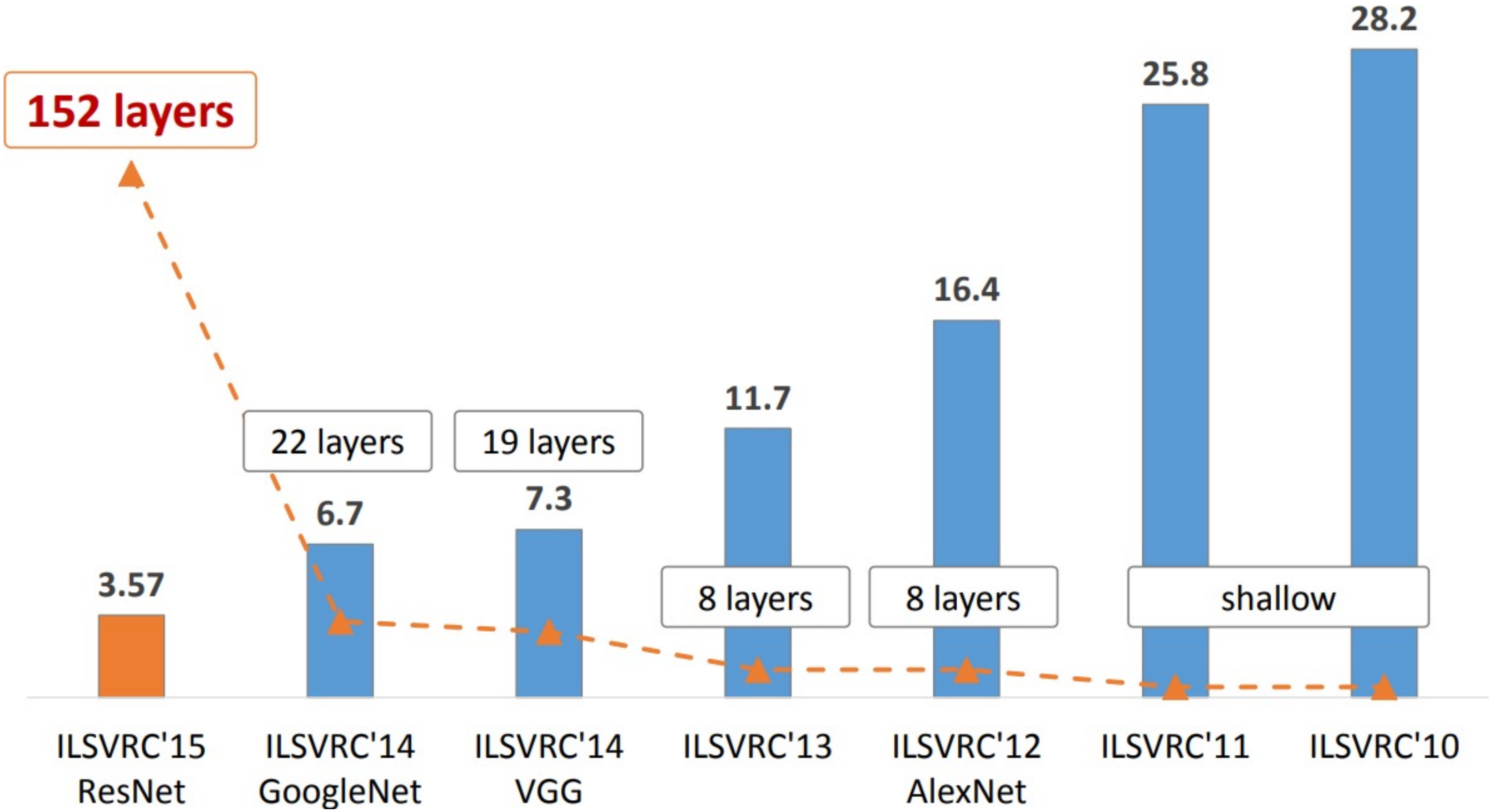
Residual Connections

- Training very deep networks is made possible because of the **skip connections** in the residual blocks. Gradients can shortcut the layers and pass through without vanishing.



Credits: Deep Dive in Deep Learning , and G. Louppe

Benefits of Depth



Recurrent Neural Networks

Sequential Data

- Many types of data are not fixed in size

- Many types of data have a temporal or sequence-like structure
  - Text
  - Video
  - Speech
  - DNA
  - …

- MLP expects fixed size data

- How to deal with sequences?

Sequential Data

- Given a set $\mathcal{X}$, let $S(\mathcal{X})$ be the set of sequences, where each element of the sequence $x_i \in \mathcal{X}$
  - $\mathcal{X}$ could reals $\mathbb{R}^M$, integers $\mathbb{Z}^M$, etc.
  - Sample sequence $x = \{x_1, x_2, \dots, x_T\}$

- Tasks related to sequences:
  - Classification $f\colon S(\mathcal{X}) \to \{\boldsymbol{p} \mid \sum_{c=1}^{N} p_i = 1\}$
  - Generation $f\colon \mathbb{R}^d \to S(\mathcal{X})$
  - Seq.-to-seq. translation $f\colon S(\mathcal{X}) \to S(\mathcal{Y})$

Credit: F. Fleuret

Recurrent States

- Input sequence $x \in S(\mathbb{R}^m)$ of *variable* length $T(x)$

- Standard approach: use recurrent model that maintains a **recurrent state** $\boldsymbol{h}_t \in \mathbb{R}^q$ updated at each time step t. For $t = 1, \dots, T(x)$:

$$\boldsymbol{h}_{t+1} = \phi(\boldsymbol{x}_t, \boldsymbol{h}_t; \theta)$$

  – Simplest model:

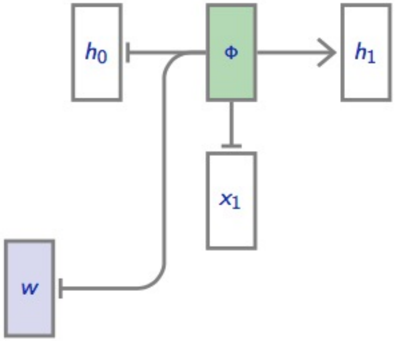
$$\phi(\boldsymbol{x}_t, \boldsymbol{h}_t; W, U) = \sigma(W\boldsymbol{x}_t + U\boldsymbol{h}_t)$$

- Predictions can be made at any time t from the recurrent state

$$\boldsymbol{y}_t = \psi(\boldsymbol{h}_t; \theta)$$

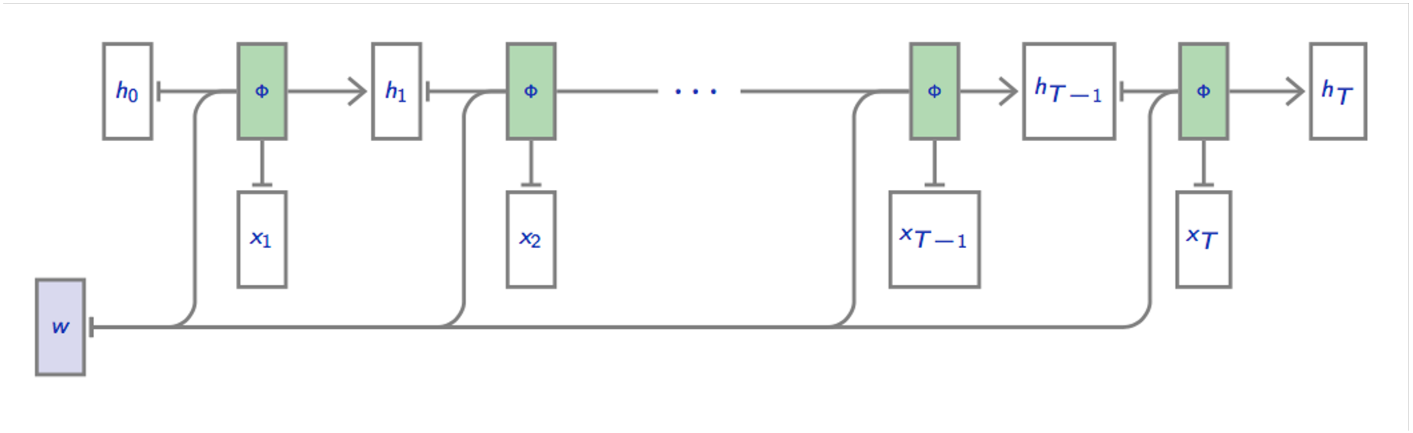
Credit: F. Fleuret

Recurrent Neural Networks



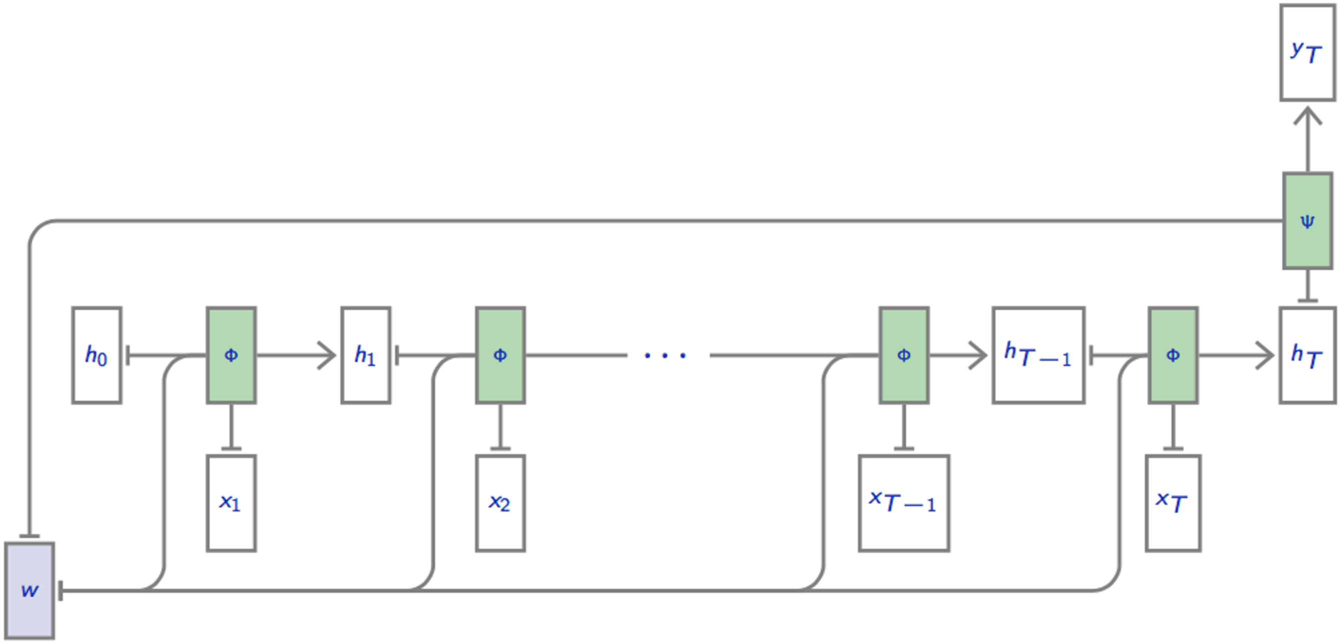
Credit: F. Fleuret

Recurrent Neural Networks



Credit: F. Fleuret

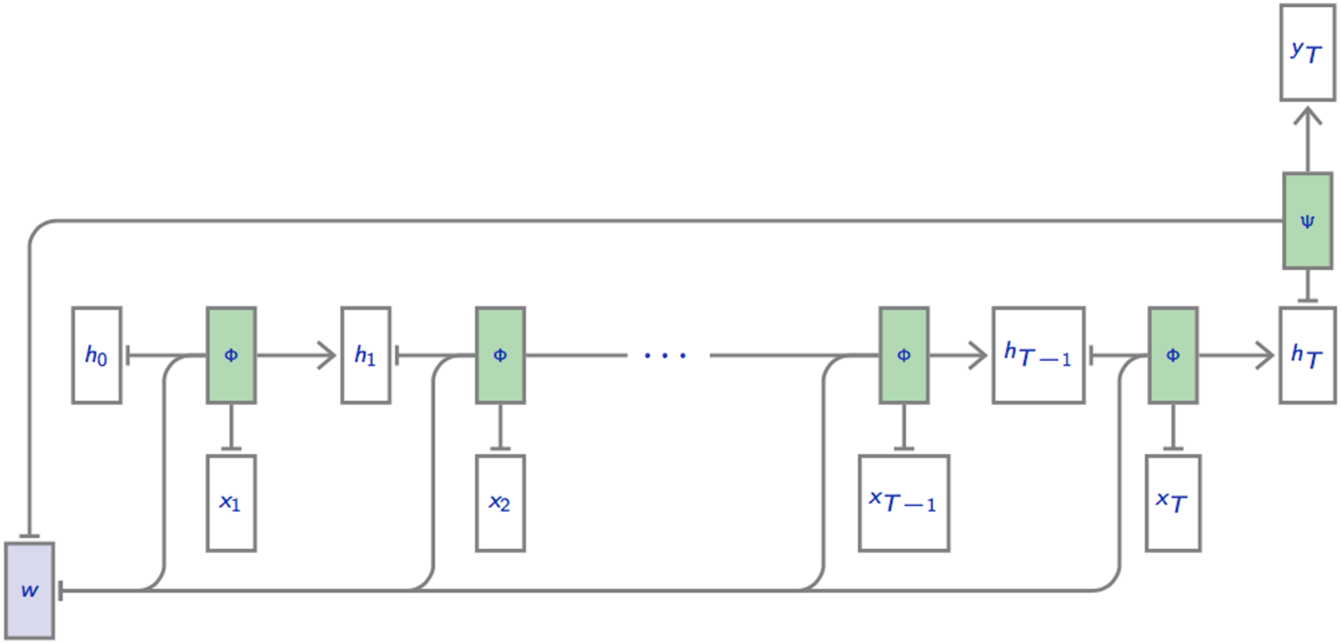
Recurrent Neural Networks



Credit: F. Fleuret

Recurrent Neural Networks

[0.98] → Positive Sentiment



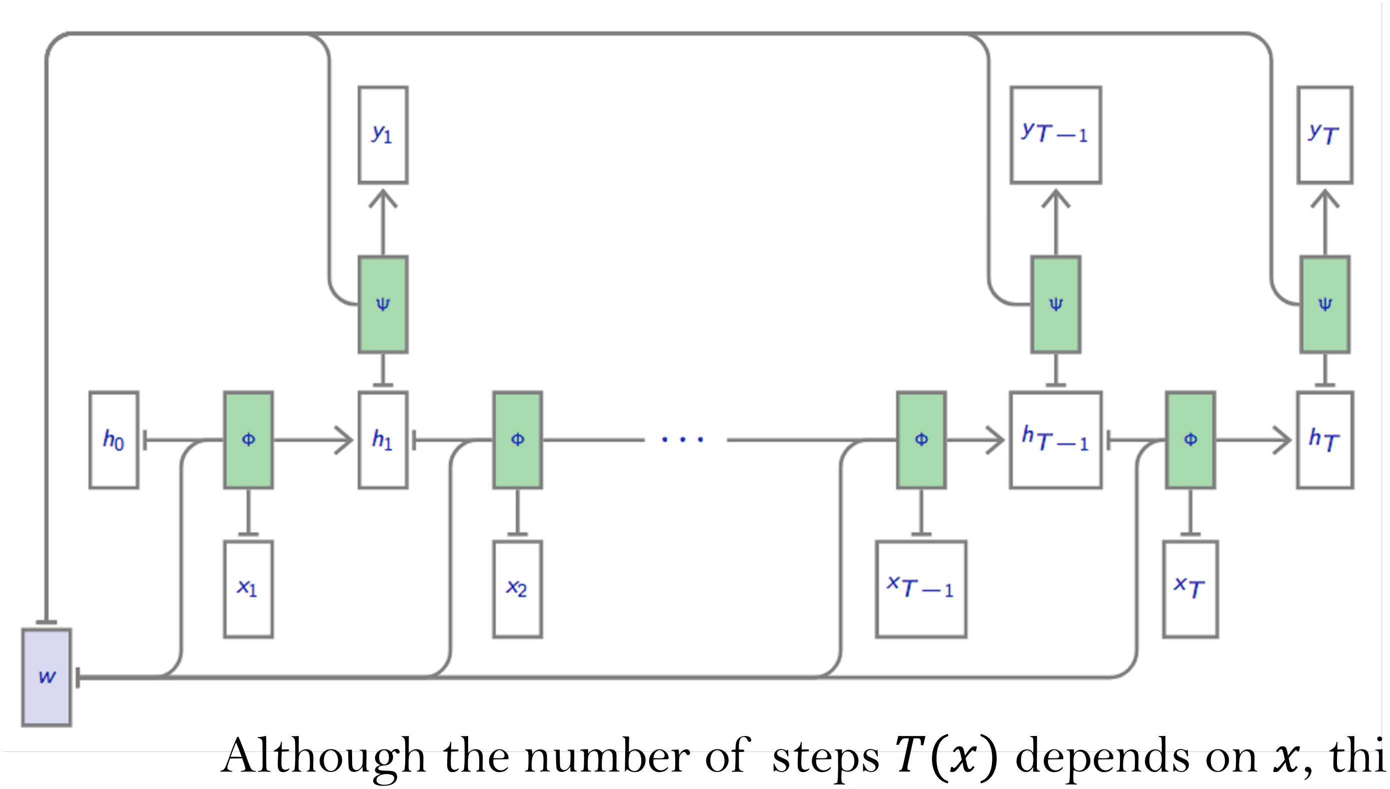
Sentiment Analysis

The movie was great

Credit: F. Fleuret

Recurrent Neural Networks

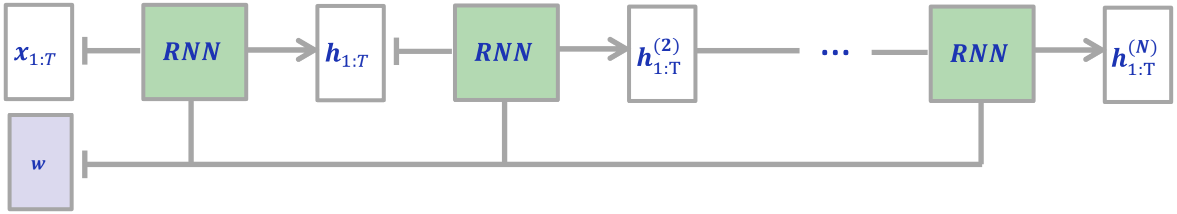
Prediction per sequence element



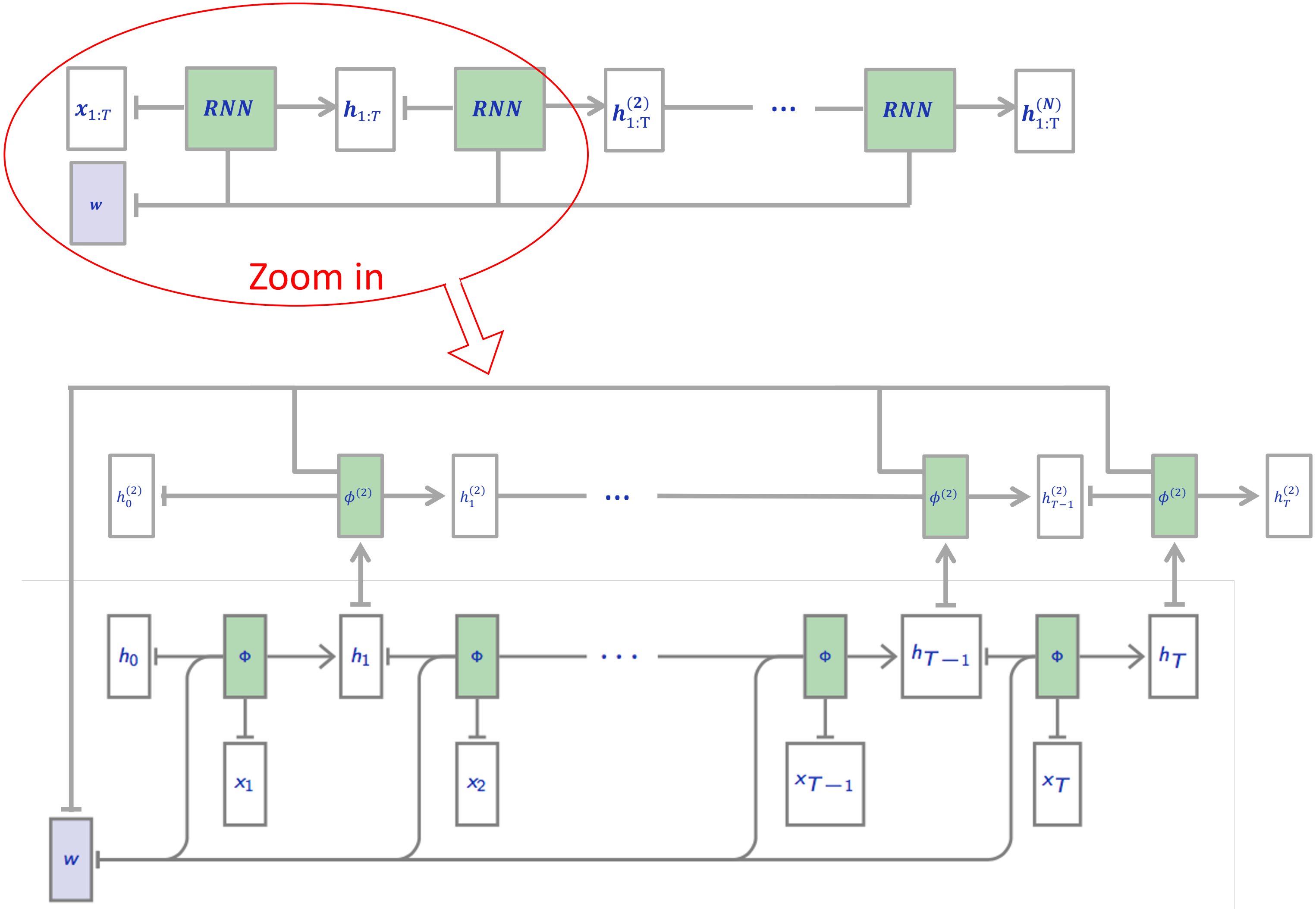
Although the number of steps $T(x)$ depends on x, this is a standard computational graph and automatic differentiation can deal with it as usual. This is known as "backpropagation through time" (Werbos, 1988)

Credit: F. Fleuret

Stacked RNN



Stacked RNN



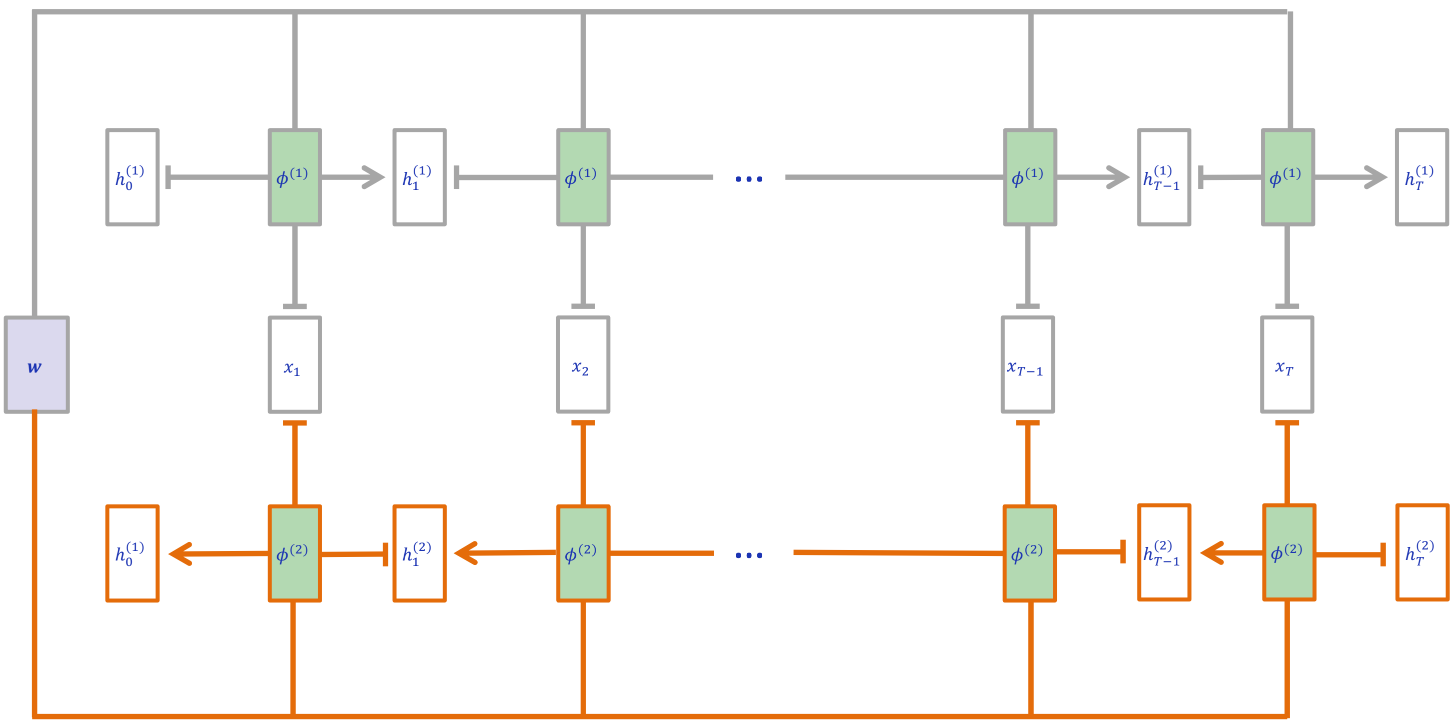
2nd RNN Layer

1st RNN Layer

Two Stacked LSTM Layers

Bi-Directional RNN

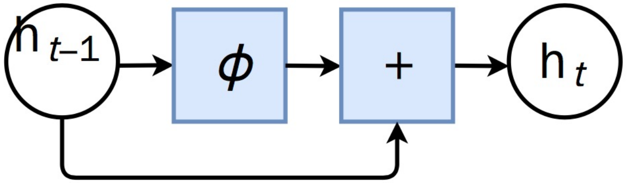
Forward in time RNN Layer



Backward in time RNN Layer

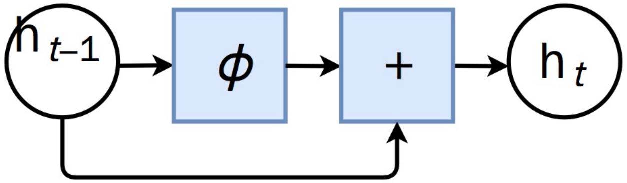
Gating

- Gating:
  - network can grow very deep, in time → vanishing gradients.
  - *Critical component*: add pass-through (additive paths) so recurrent state does not go repeatedly through squashing non-linearity.



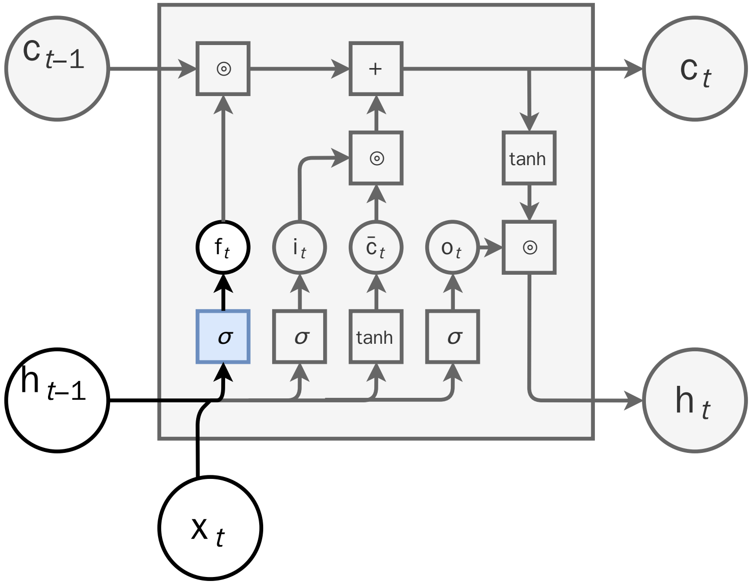
Credit: Gilles Louppe

Long Short Term Memory (LSTM)



- Gating:
  - network can grow very deep, in time → vanishing gradients.
  - *Critical component*: add pass-through (additive paths) so recurrent state does not go repeatedly through squashing non-linearity.

- LSTM:
  - Add internal state separate from output state
  - Add input, output, and forget gating

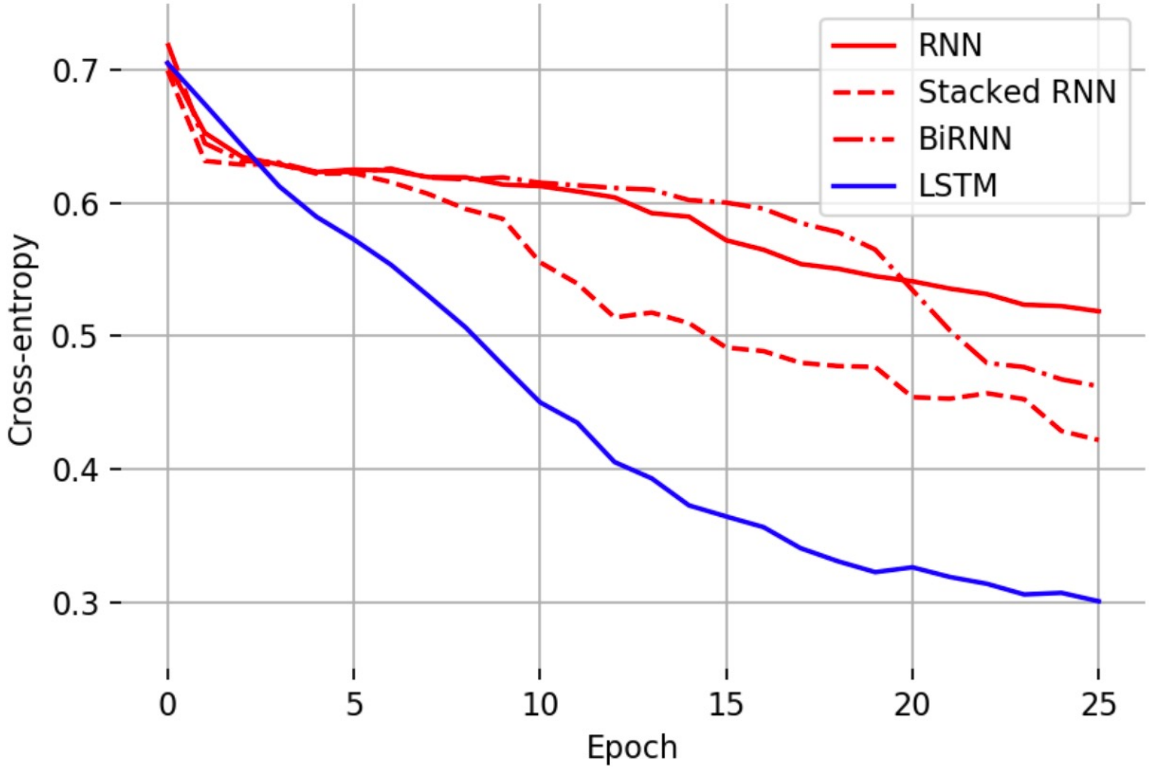


Credit: Gilles Louppe

Comparison on Toy Problem

Learn to recognize palindrome
Sequence size between 1 to 10

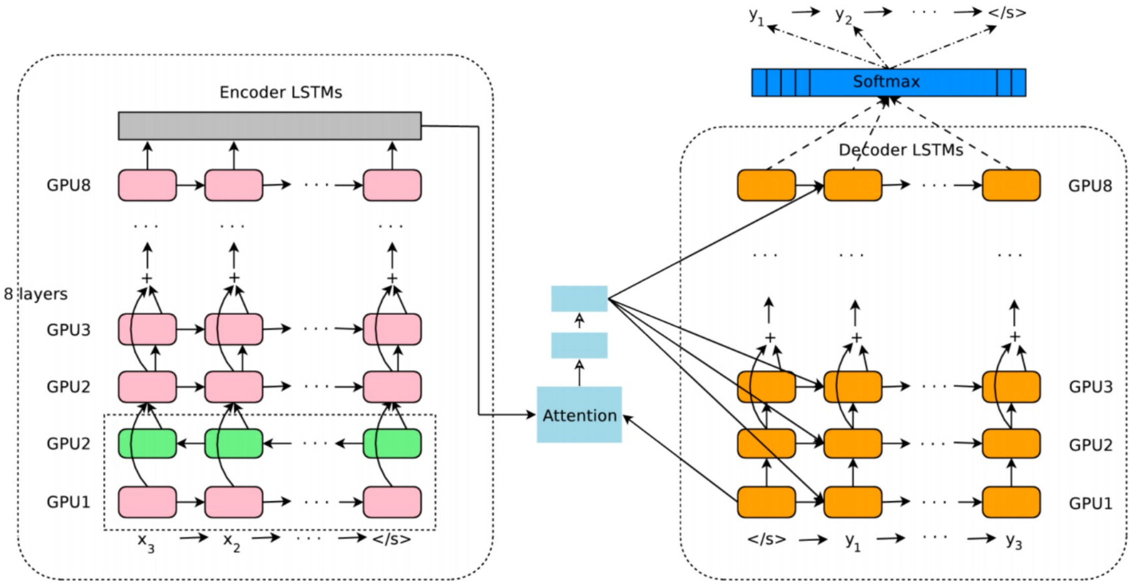
$\mathbf{x}$	y
$(1, 2, 3, 2, 1)$	1
$(2, 1, 2)$	1
$(3, 4, 1, 2)$	0
(0)	1
$(1, 4)$	0

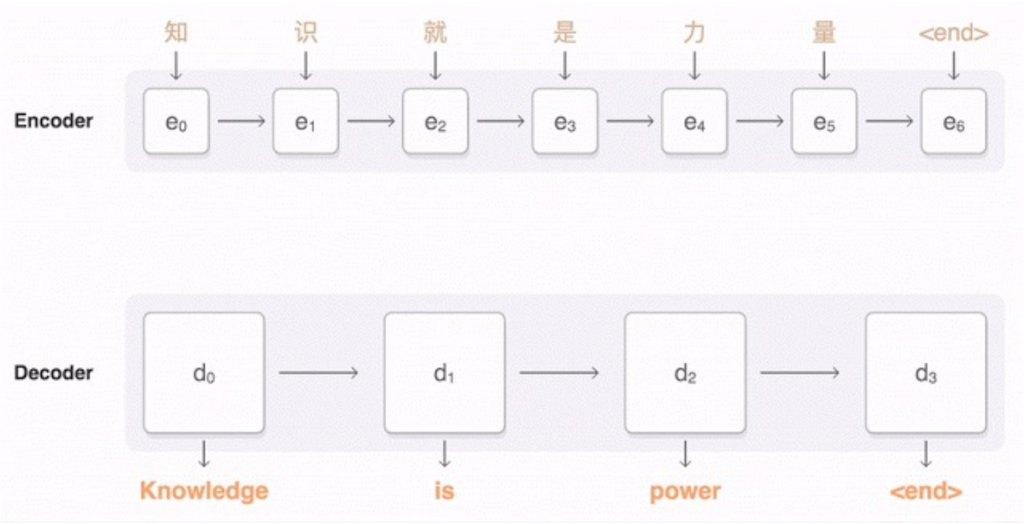


Slide credit: G. Louppe

Examples

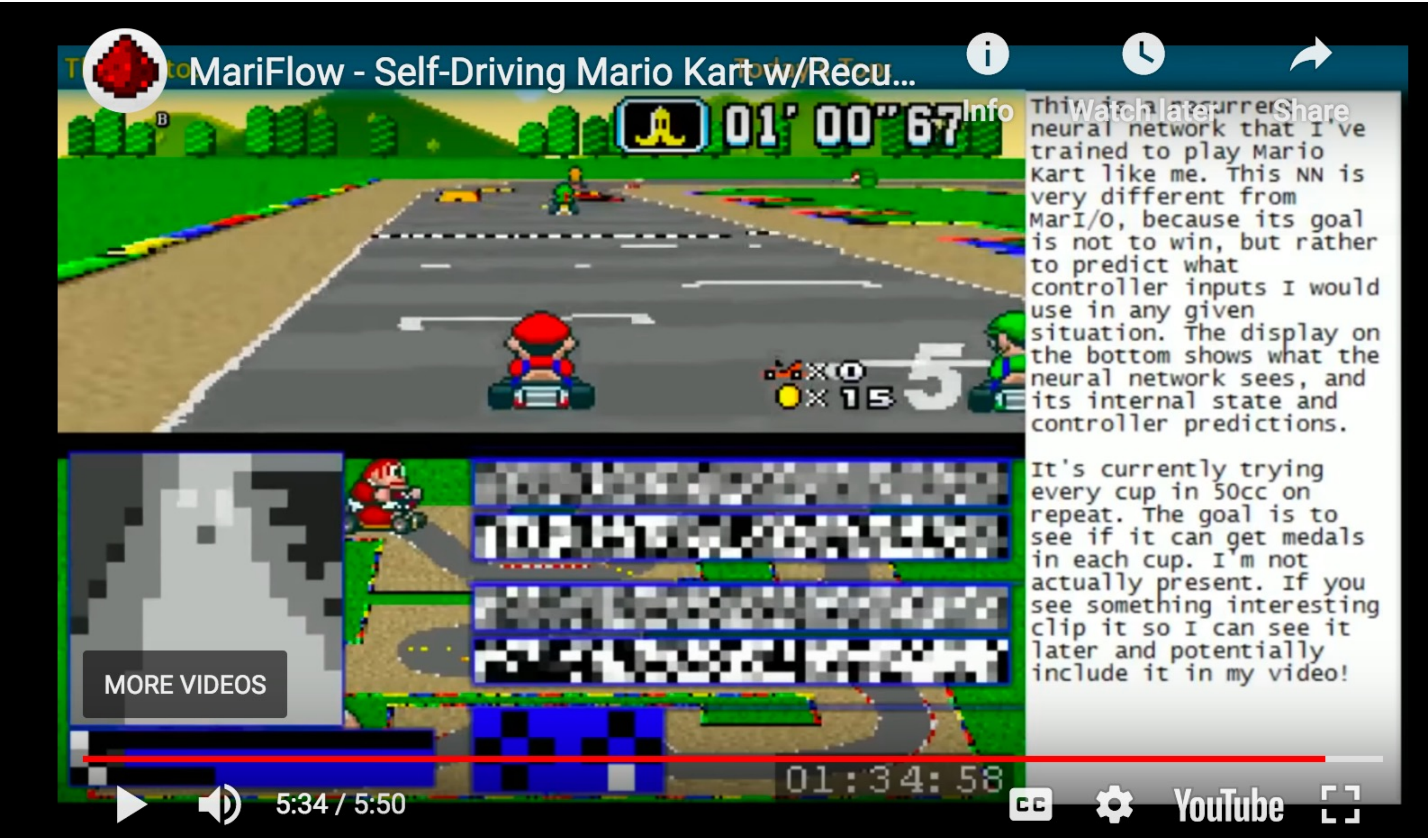
Neural machine translation





Y. Wu et al, 2016

Examples



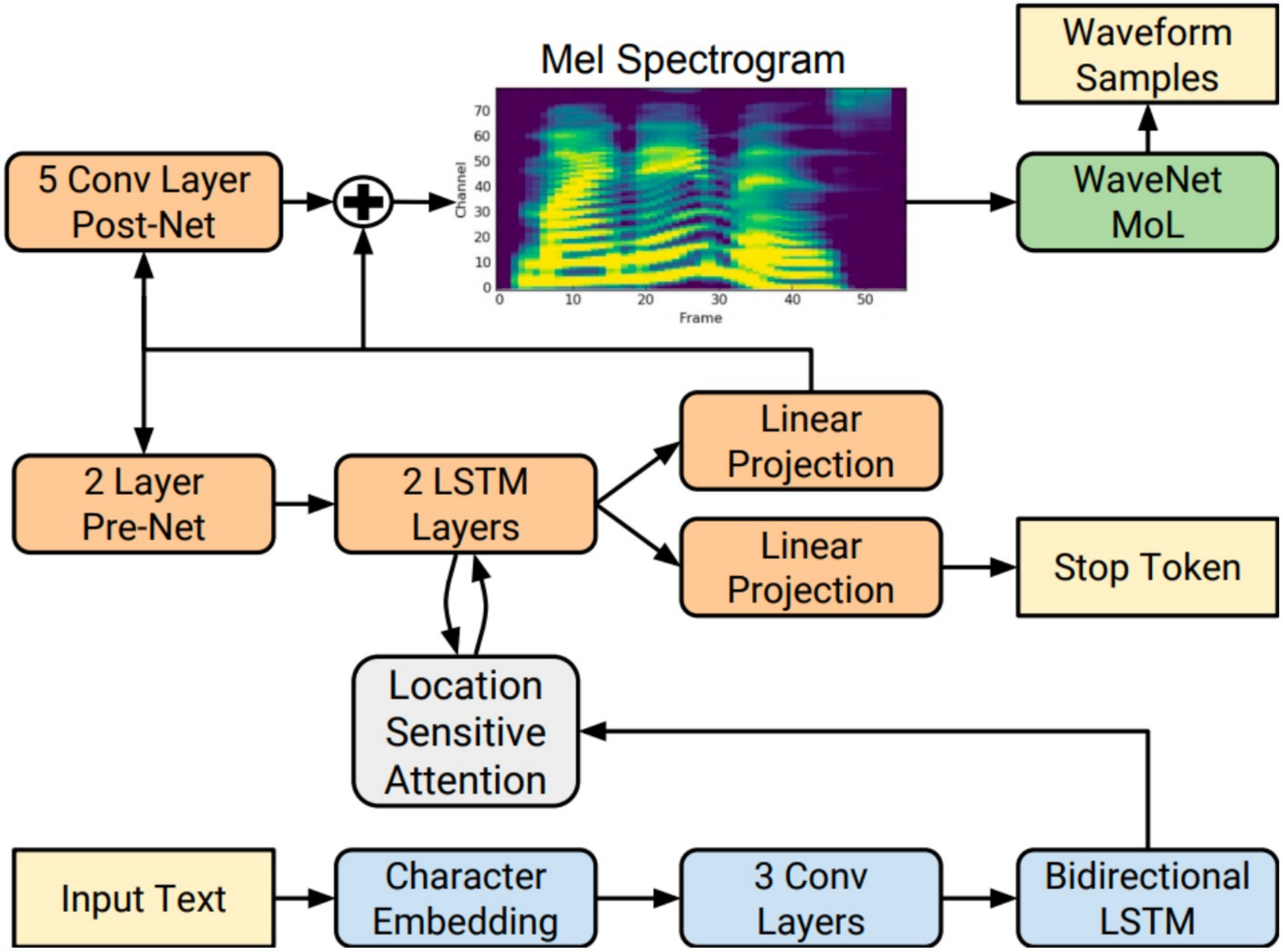
This is a recurrent neural network that I've trained to play Mario Kart like me. This NN is very different from MarI/O, because its goal is not to win, but rather to predict what controller inputs I would use in any given situation. The display on the bottom shows what the neural network sees, and its internal state and controller predictions.

It's currently trying every cup in 50cc on repeat. The goal is to see if it can get medals in each cup. I'm not actually present. If you see something interesting clip it so I can see it later and potentially include it in my video!

Self-driving Mario Kart with RNN: YouTube video

Examples

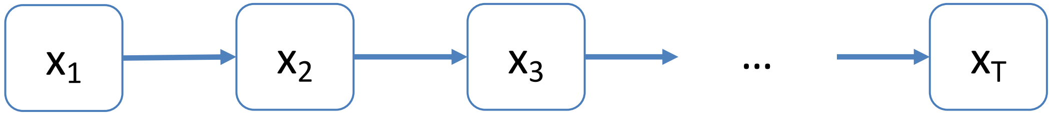
Text-to-speech synthesis



Shen et al., 2017

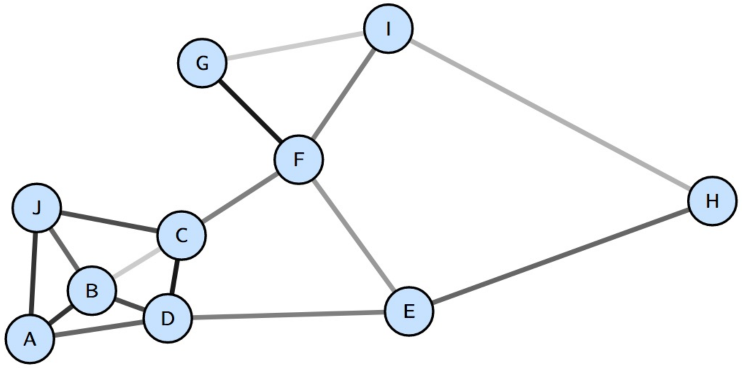
Graph Data

Graph Data



- Sequential data has single (directed) connections from data at current time to data at next time

- What about data with more complex dependencies



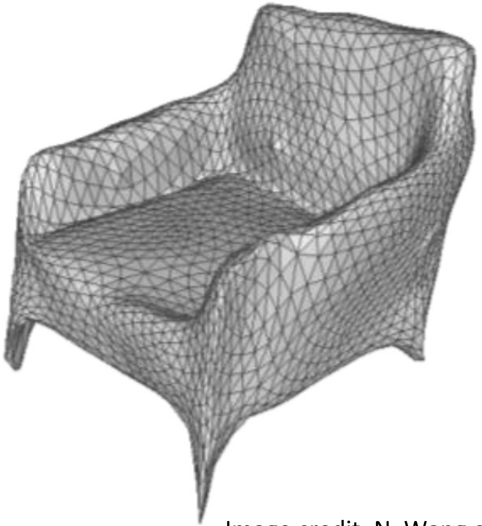
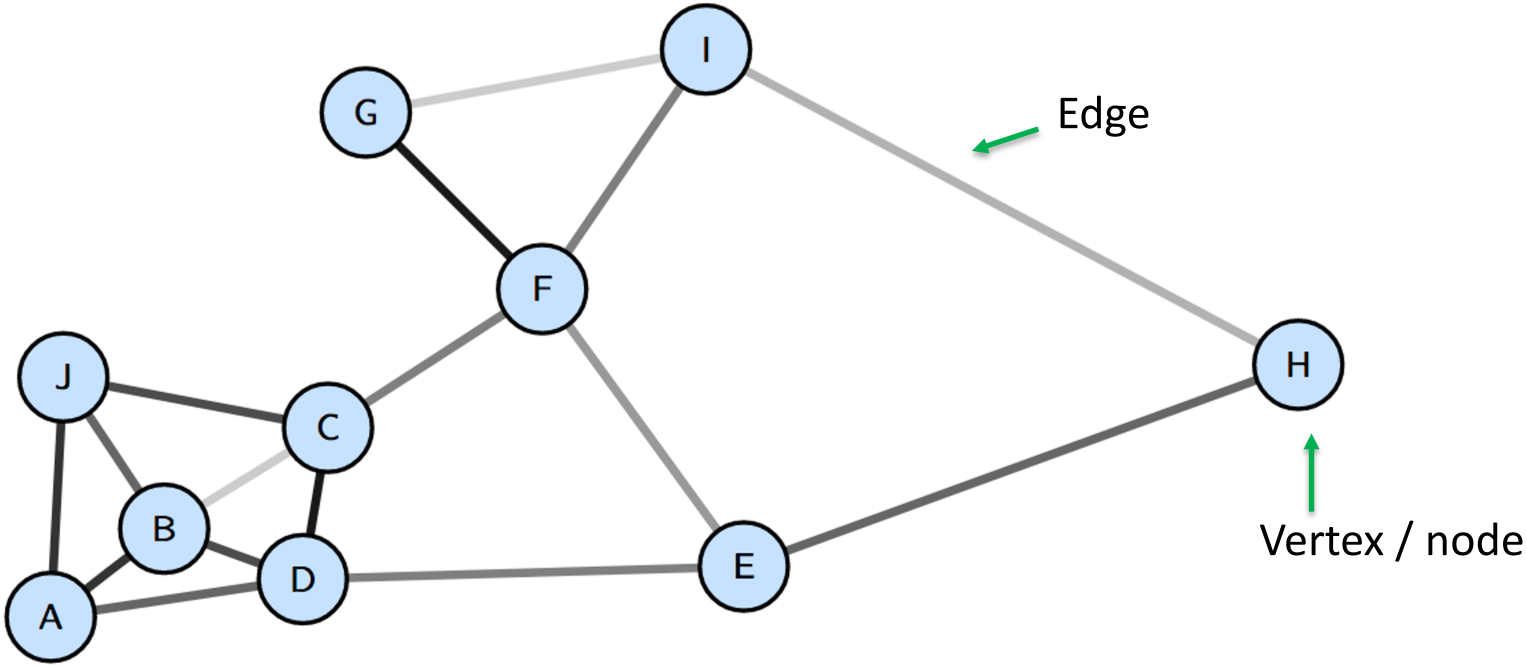


Image Credit: I. Henrion

Image credit: N. Wang et al., 2018

Graphs



- Adjacency matrix: $A_{ij} = \delta(edge\ between\ vertex\ i\ and\ j)$

- Each node can have features

- Each edge can have features, e.g. distance between nodes

Image Credit: I. Henrion

Neural Message Passing

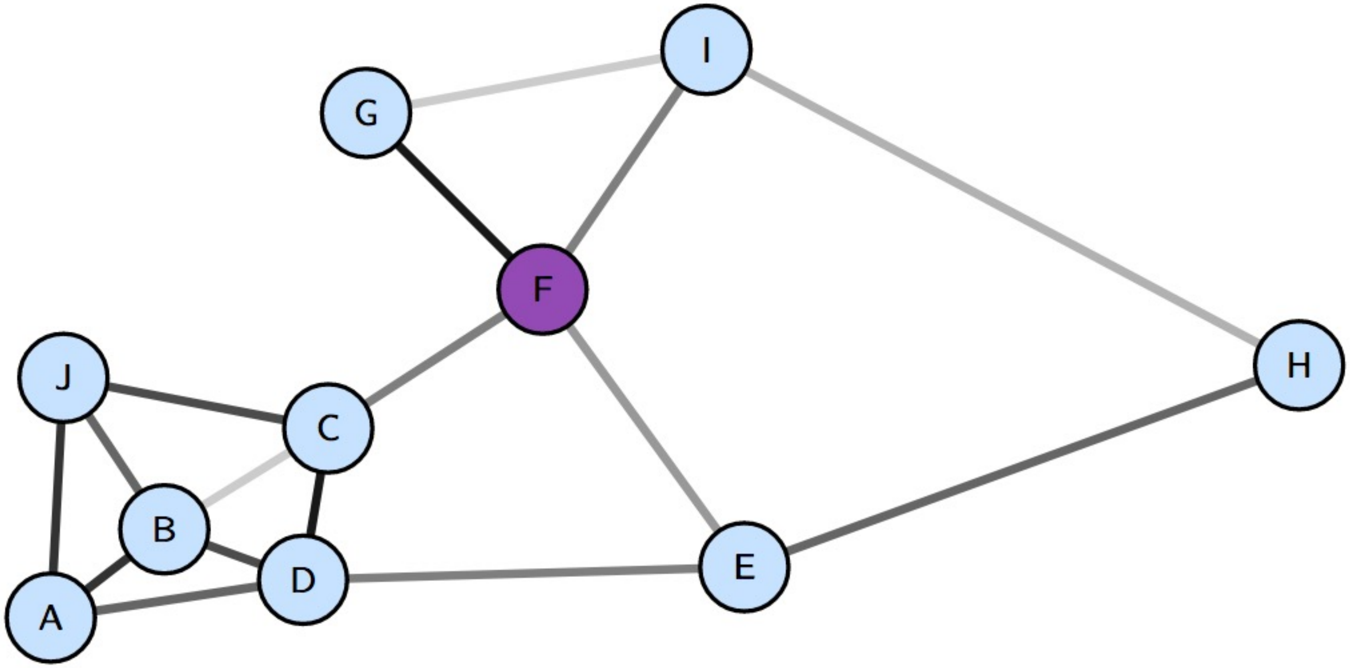
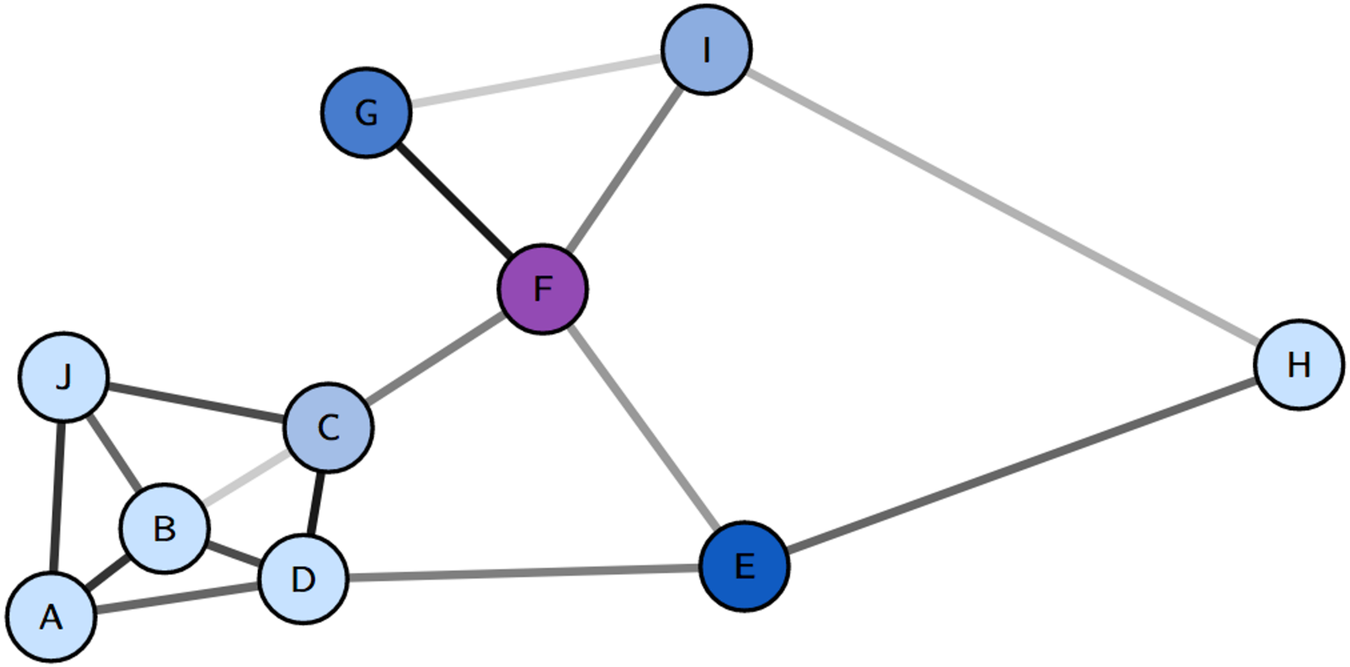


Image Credit: I. Henrion

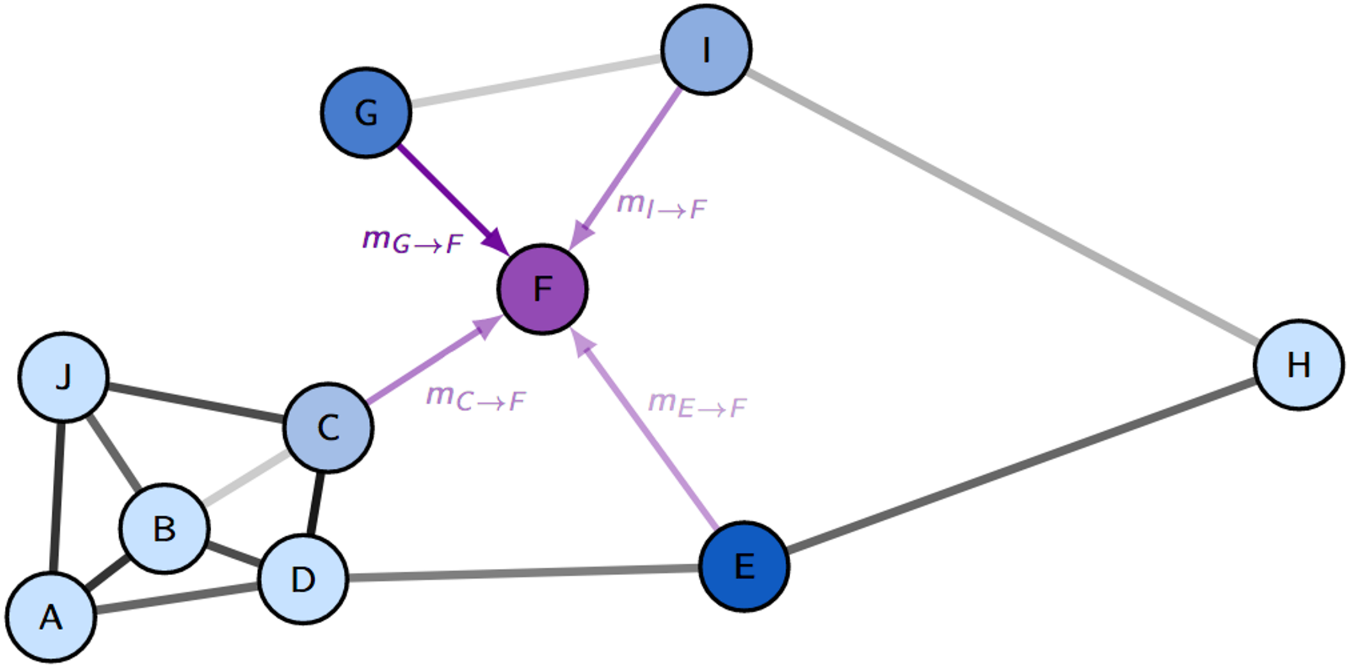
Neural Message Passing



$$\tilde{m}_j^t = f(h_j^{t-1})$$

Image Credit: I. Henrion

Neural Message Passing

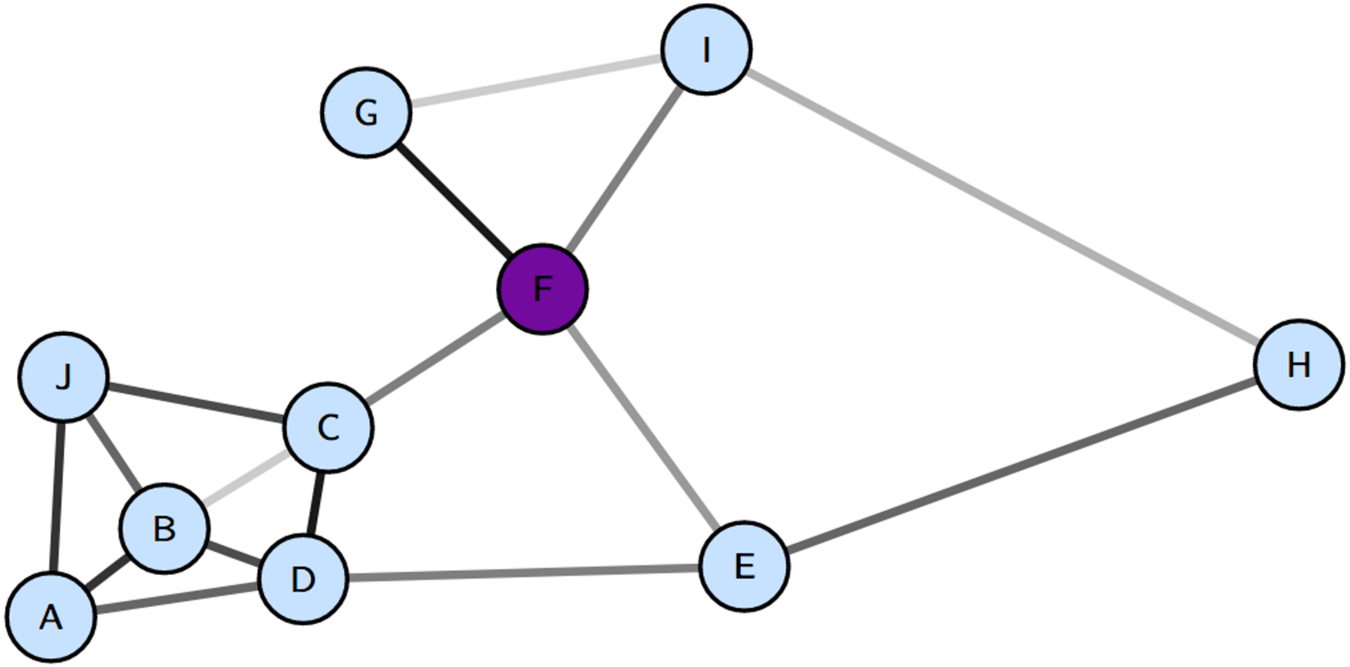


$$\tilde{m}_j^t = f(h_j^{t-1})$$

$$m_{j \to i}^t = \sigma(A_{ij} \tilde{m}_j^t)$$

Image Credit: I. Henrion

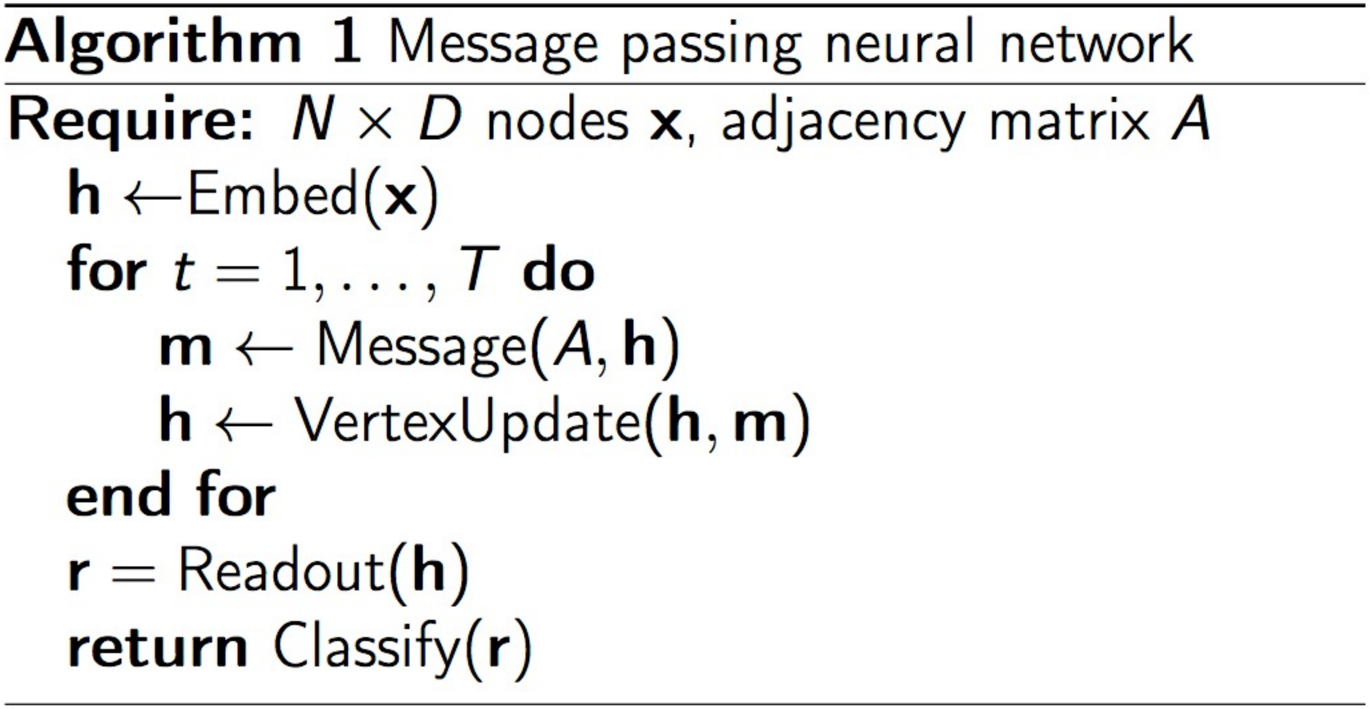
Neural Message Passing



$$\tilde{m}_j^t = f(h_j^{t-1})$$
$$m_{j\to i}^t = \sigma(A_{ij}\tilde{m}_j^t)$$
$$h_i^t = \mathrm{GRU}(h_i^{t-1}, \Sigma_j m_{j\to i}^t)$$

Image Credit: I. Henrion

Neural Message Passing



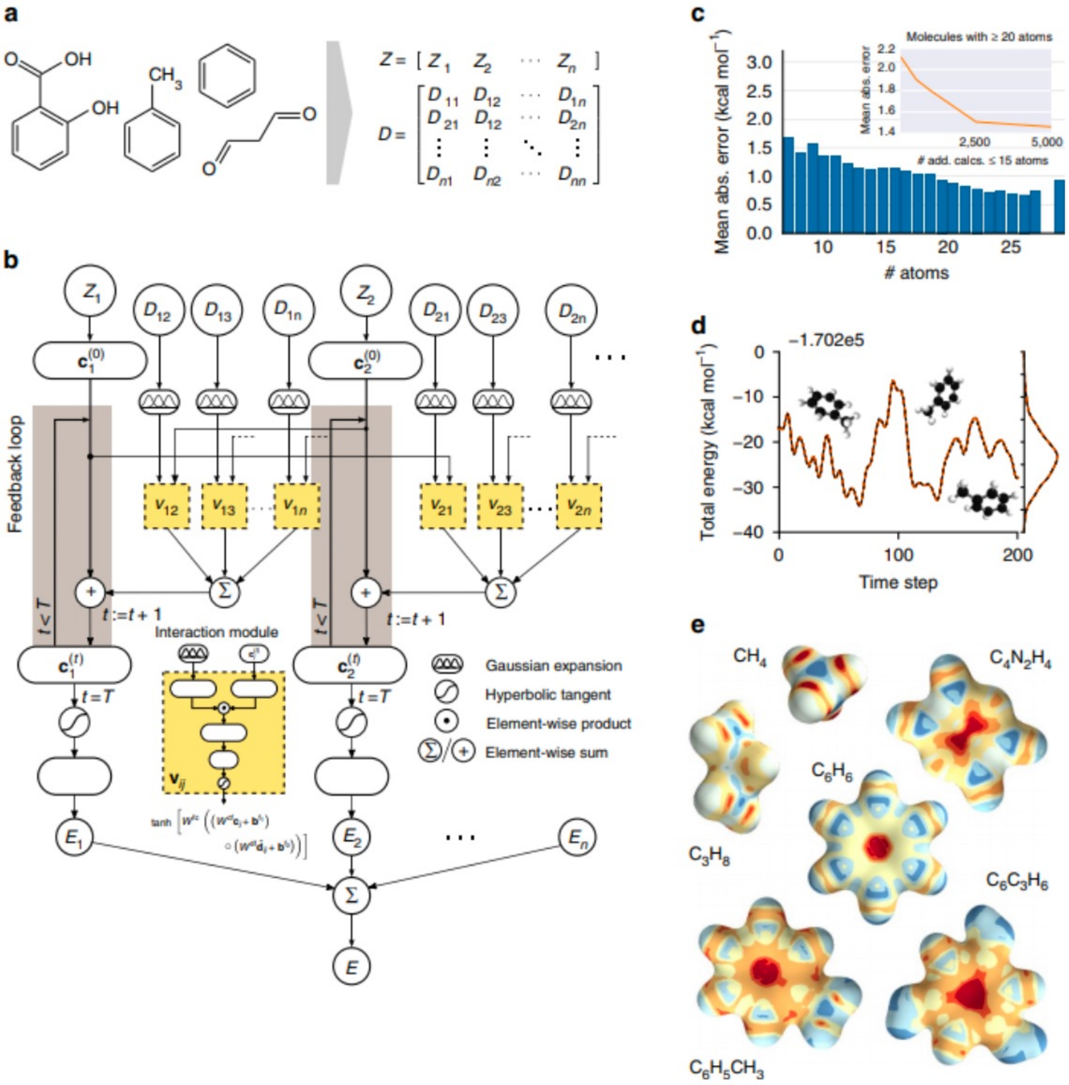
Algorithm 1 Message passing neural network

```
Require: $N \times D$ nodes $\mathbf{x}$, adjacency matrix $A$
  $\mathbf{h} \leftarrow \text{Embed}(\mathbf{x})$
  for $t = 1, \ldots, T$ do
      $\mathbf{m} \leftarrow \text{Message}(A, \mathbf{h})$
      $\mathbf{h} \leftarrow \text{VertexUpdate}(\mathbf{h}, \mathbf{m})$
  end for
  $\mathbf{r} = \text{Readout}(\mathbf{h})$
  return Classify($\mathbf{r}$)
```

Image Credit: I. Henrion

Examples

Quantum chemistry with graph networks



Schutt et al. 2017

Examples

Learning to simulate physics with graph networks

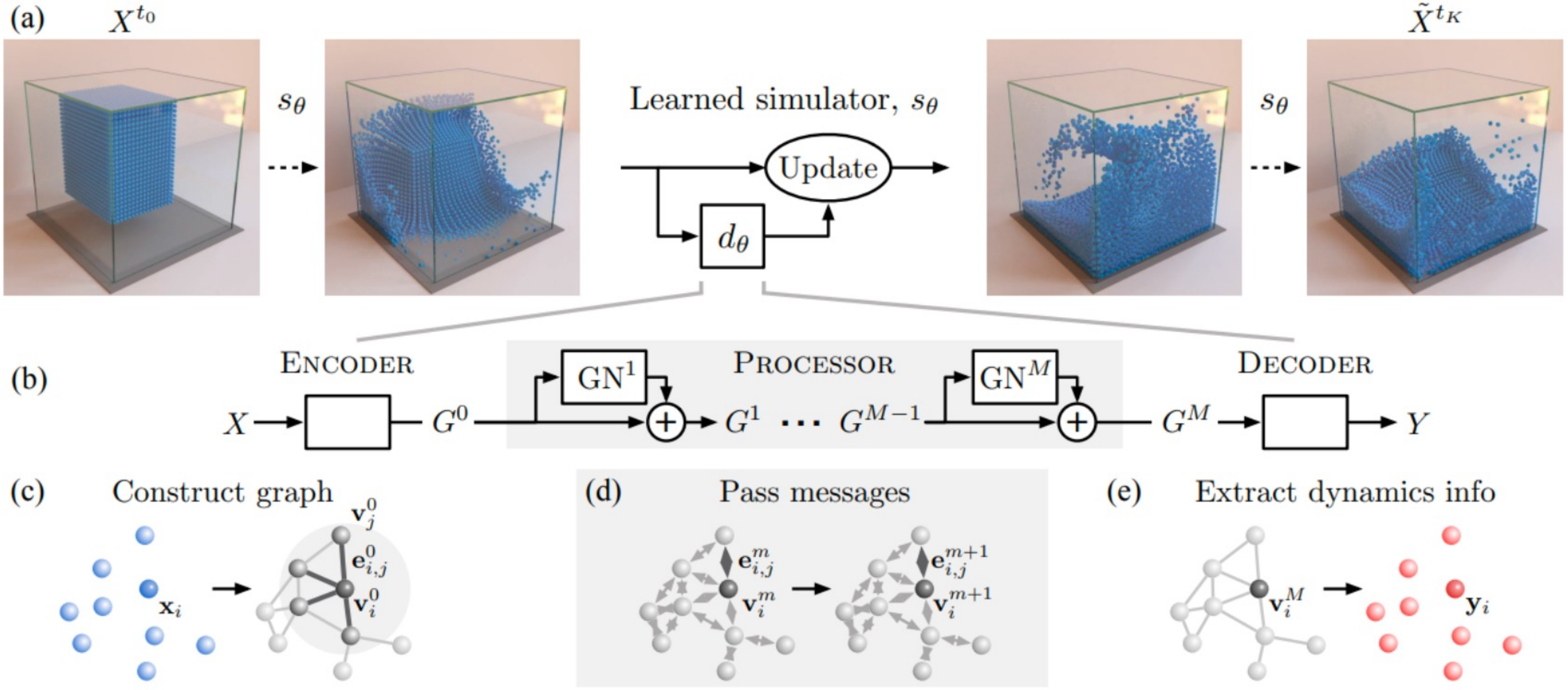


Figure 2. **(a)** Our GNS predicts future states represented as particles using its learned dynamics model, d_θ, and a fixed update procedure. **(b)** The d_θ uses an "encode-process-decode" scheme, which computes dynamics information, Y, from input state, X. **(c)** The ENCODER constructs latent graph, G^0, from the input state, X. **(d)** The PROCESSOR performs M rounds of learned message-passing over the latent graphs, $G^0, \ldots, G^M$. **(e)** The DECODER extracts dynamics information, Y, from the final latent graph, G^M.

Sanchez-Gonzalez et al. 2020

Summary

- Neural Networks allow us to combine non-linear basis selection with feature learning
  - Care needed to train them and ensure they don't overfit

- Deep neural networks allow us to learn complex function by hierarchically structuring the feature learning

- We can use our inductive bias (knowledge) to define models that are well adapted to our problem

- Many neural networks structures are available for training models on a wide array of data types.

End of Lecture II

Backup

Automatic Differentiation

Automatic Differentiation Example

- All numerical algorithms, when executed, evaluate to compositions of a finite set of elementary operations with known derivatives
  - Represent as a **computational graph** showing dependencies

$$f(a,b) = \log(ab)$$

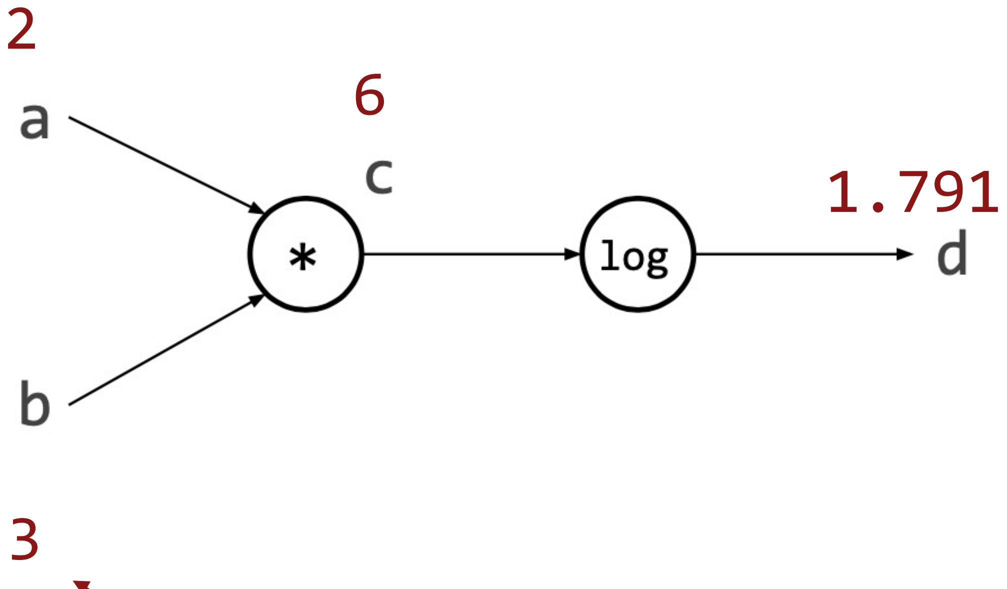
$$\nabla f(a,b) = \left(\frac{1}{a}, \frac{1}{b}\right)$$

Automatic Differentiation Example

- All numerical algorithms, when executed, evaluate to compositions of a finite set of elementary operations with known derivatives
  - Represent as a **computational graph** showing dependencies

```
f(a, b):
    c = a * b
    d = log(c)
    return d
```

```
f(2, 3) = 1.791
```



Primals

Automatic Differentiation Example

- All numerical algorithms, when executed, evaluate to compositions of a finite set of elementary operations with known derivatives
  - Represent as a **computational graph** showing dependencies

```
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    c = a * b
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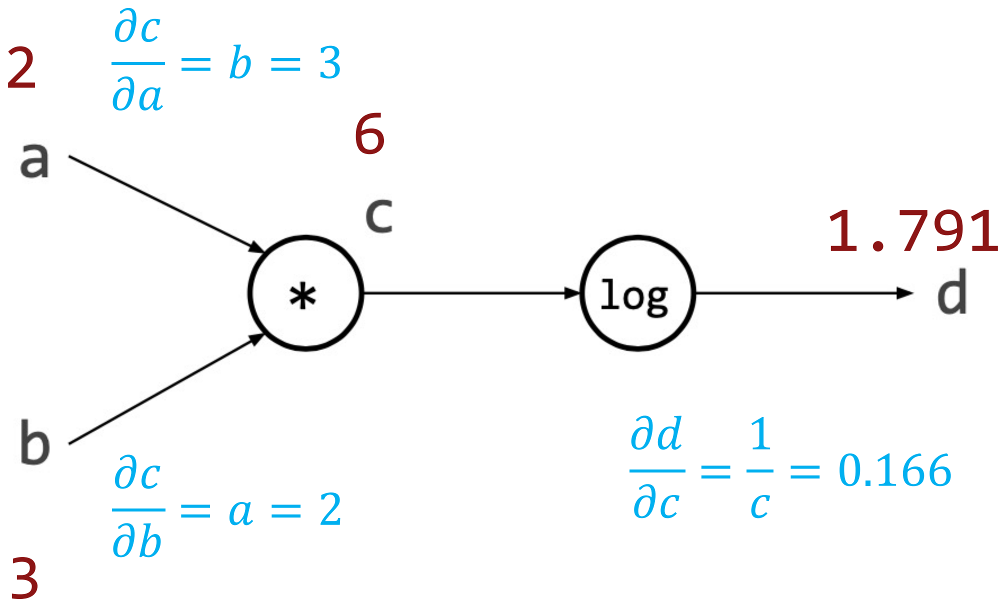


$$\frac{\partial c}{\partial a} = b = 3$$

$$\frac{\partial c}{\partial b} = a = 2$$

$$\frac{\partial d}{\partial c} = \frac{1}{c} = 0.166$$

```
f(2, 3) = 1.791
df(2,3) = [0.5, 0.333]
```

Chain Rule: $\frac{\partial d}{\partial a} = \frac{\partial d}{\partial c}\frac{\partial c}{\partial a} = 0.166 * 3 = 0.5$

Automatic Differentiation

Problem: Compute gradients of z with respect to inputs $\{x_1, x_2\}$

$$z = \sin(x_1) + x_1 x_2$$

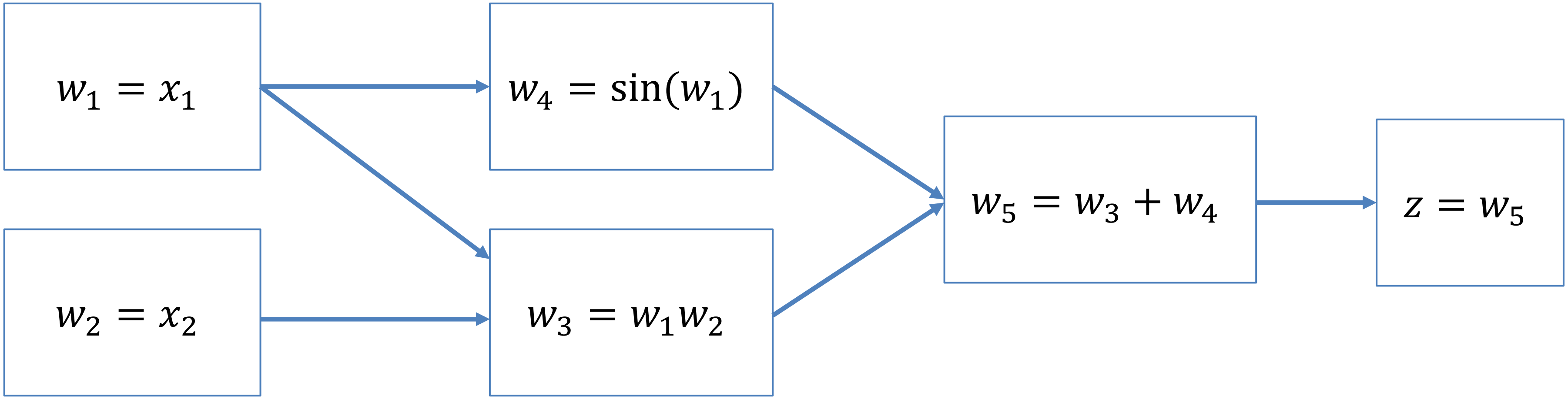
Automatic Differentiation

$$
\begin{aligned}
w_1 &= x_1 \\
w_2 &= x_2 \\
w_3 &= w_1 w_2 \\
w_4 &= \sin(w_1) \\
w_5 &= w_3 + w_4 \\
z &= w_5
\end{aligned}
$$

Problem: Compute gradients of z with respect to inputs $\{x_1, x_2\}$

$$z = \sin(x_1) + x_1 x_2$$

Organize as a computational Graph



Automatic Differentiation

$$\begin{aligned} w_1 &= x_1 \\ w_2 &= x_2 \\ w_3 &= w_1 w_2 \\ w_4 &= \sin(w_1) \\ w_5 &= w_3 + w_4 \\ z &= w_5 \end{aligned}$$

Problem: Compute gradients of z with respect to inputs $\{x_1, x_2\}$

We know the gradients of simple functions: $\sin(x)$, $x * y, x + y$ …

Chain rule:

$$\frac{dz}{dw_1} = \sum_{p \in parents} \frac{dz}{dw_p} \frac{dw_p}{dw_i}$$

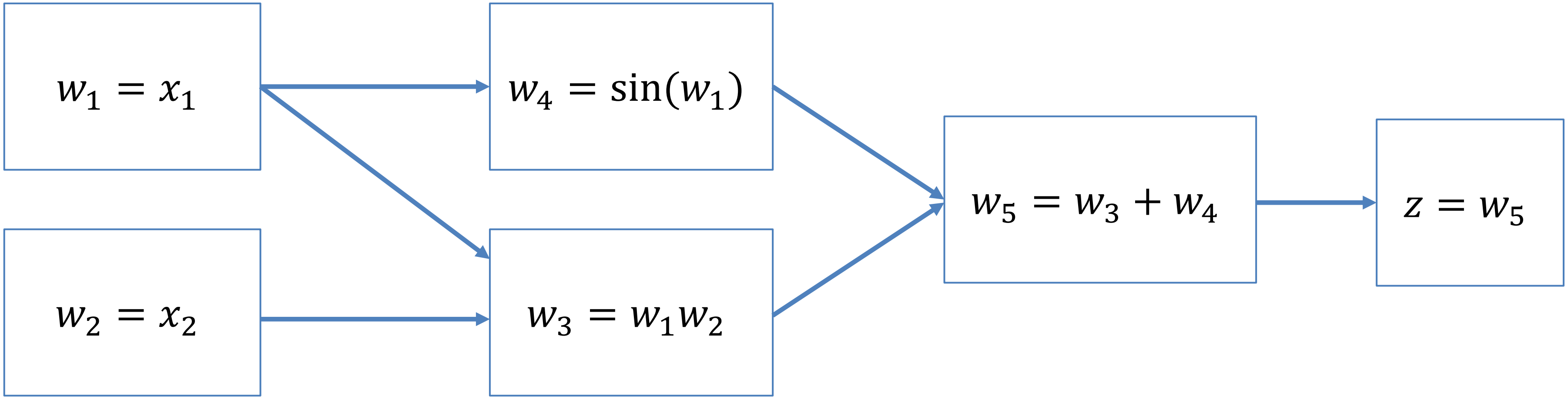
$$\frac{dw_1}{dx_1} = 1$$

$$\frac{dw_2}{dx_2} = 1$$

$$\frac{dw_3}{dw_1} = w_2 \quad \frac{dw_3}{dw_2} = w_1$$

$$\frac{dw_4}{dw_1} = \cos(w_1)$$

$$\frac{dw_5}{dw_3} = 1 \quad \frac{dw_5}{dw_4} = 1$$



$w_1 = x_1$

$w_2 = x_2$

$w_4 = \sin(w_1)$

$w_3 = w_1 w_2$

$w_5 = w_3 + w_4$

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Automatic Differentiation

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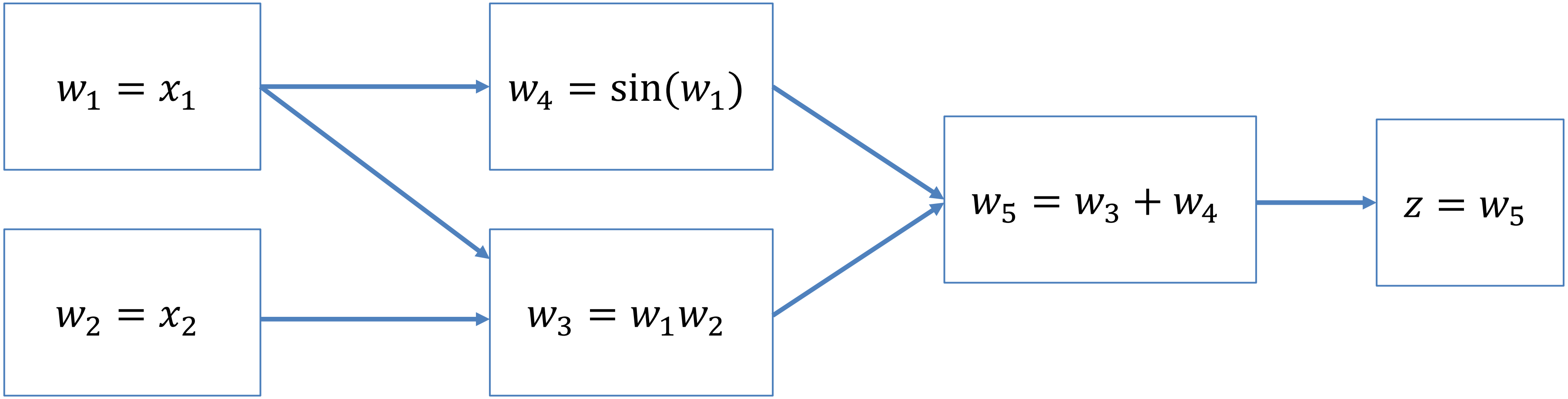
$$

Problem: Compute gradients of z with respect to inputs $\{x_1, x_2\}$

NOT going to find analytic derivative

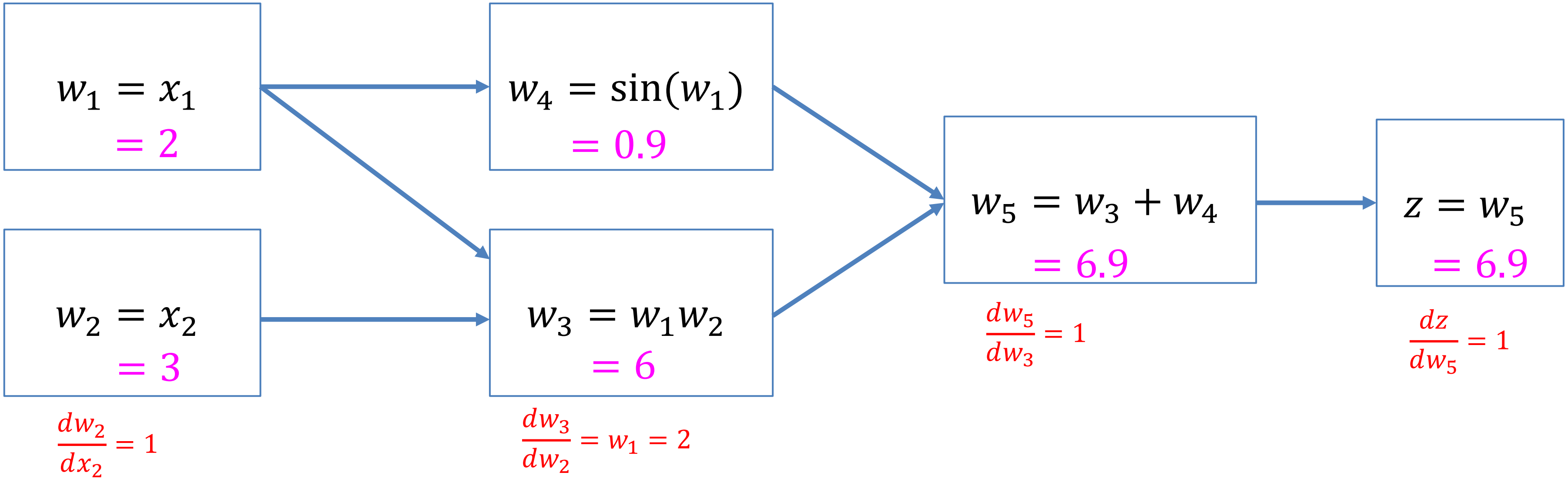
WILL find a way to compute value of gradient for a given input point



Forward Mode Automatic Differentiation

$w_1 = x_1 = 2$
$w_2 = x_2 = 3$
$w_3 = w_1 w_2 = 6$
$w_4 = \sin(w_1) = 0.9$
$w_5 = w_3 + w_4 = 6.9$
$z = w_5$

For each input, from input to output sequentially, evaluate graph and gradients and store values



Forward Mode Automatic Differentiation

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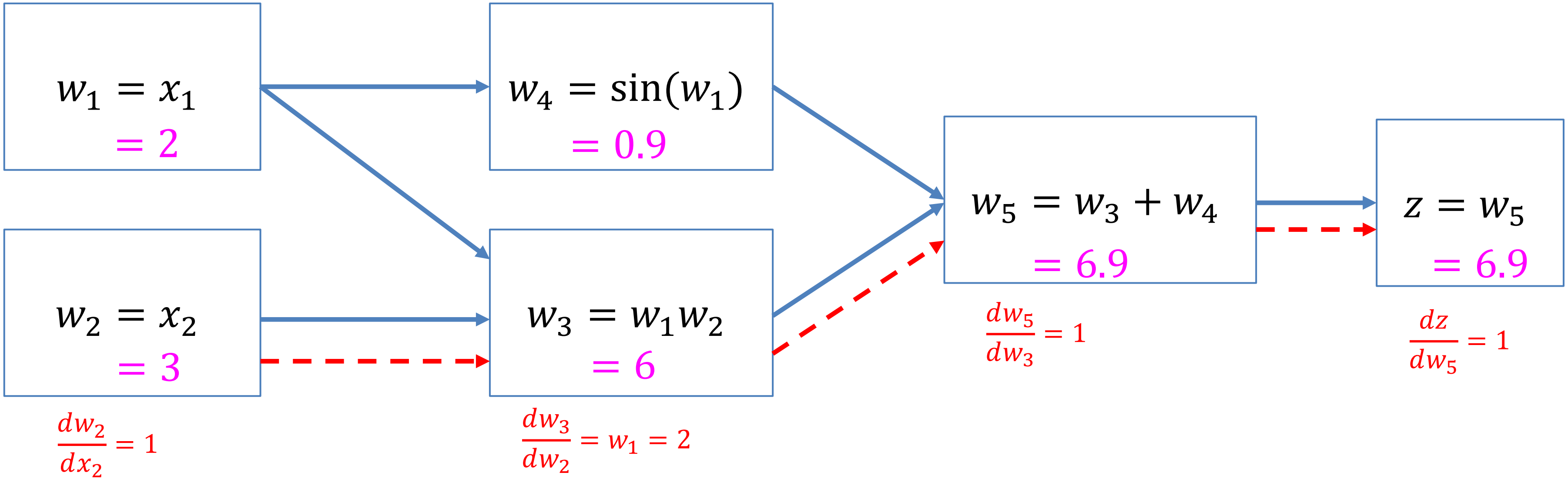
For each input, from input to output sequentially, evaluate graph and gradients and store values

Apply chain rule with multiplication

$$\frac{dz}{dx_2} = \frac{dw_2}{dx_2}\frac{dw_3}{dw_2}\frac{dw_5}{dw_3}\frac{dz}{dw_5} = 1 * 2 * 1 * 1 = 2$$



Forward Mode Automatic Differentiation

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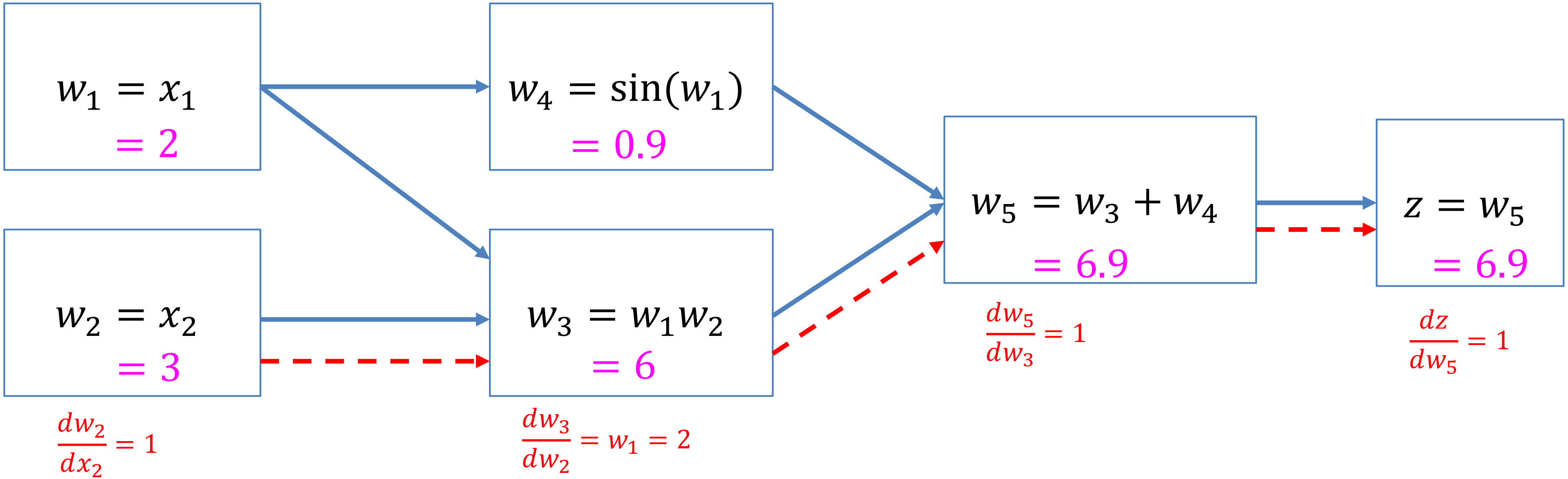
Forward Mode allows us to compute the gradient of one input with respect to all the output

Jacobian $$\frac{d\boldsymbol{z}}{d\boldsymbol{x}} = \begin{pmatrix} \frac{dz_1}{dx_1} & \cdots & \frac{dz_M}{dx_1} \\ \vdots & \ddots & \vdots \\ \frac{dz_1}{dx_N} & \cdots & \frac{dz_M}{dx_N} \end{pmatrix}$$

If we have 1 output (Loss) and many inputs → SLOW!



$w_1 = x_1$ $= 2$

$w_2 = x_2$ $= 3$

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$w_3 = w_1 w_2$ $= 6$

$w_5 = w_3 + w_4$ $= 6.9$

$z = w_5$ $= 6.9$

$\frac{dw_2}{dx_2} = 1$

$\frac{dw_3}{dw_2} = w_1 = 2$

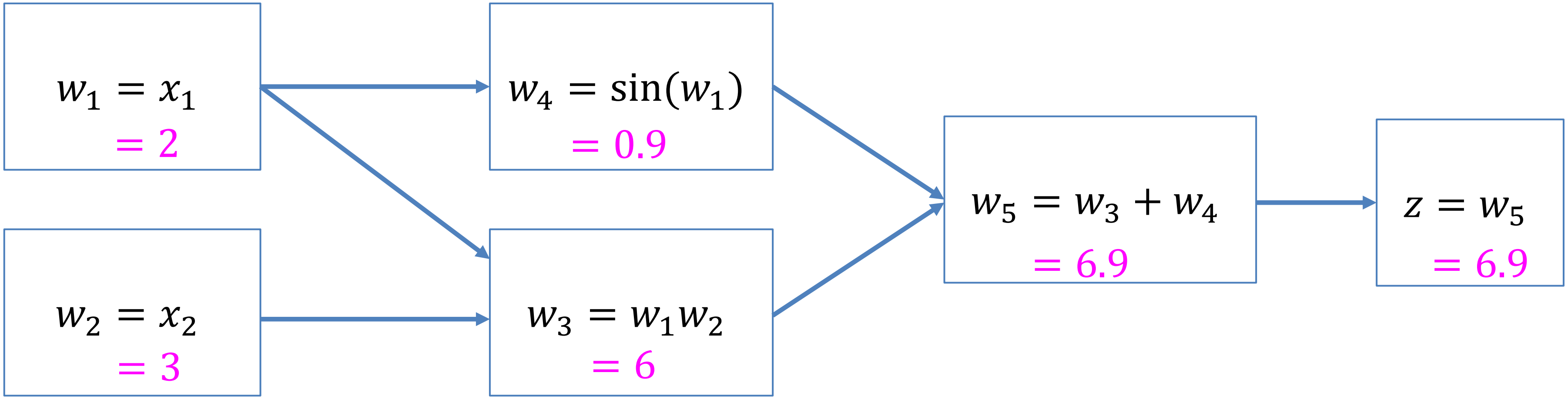
$\frac{dw_5}{dw_3} = 1$

$\frac{dz}{dw_5} = 1$

Reverse Mode Automatic Differentiation

$$\begin{aligned} w_1 &= x_1 = 2 \\ w_2 &= x_2 = 3 \\ w_3 &= w_1 w_2 = 6 \\ w_4 &= \sin(w_1) = 0.9 \\ w_5 &= w_3 + w_4 = 6.9 \\ z &= w_5 \end{aligned}$$

Evaluate graph and store values



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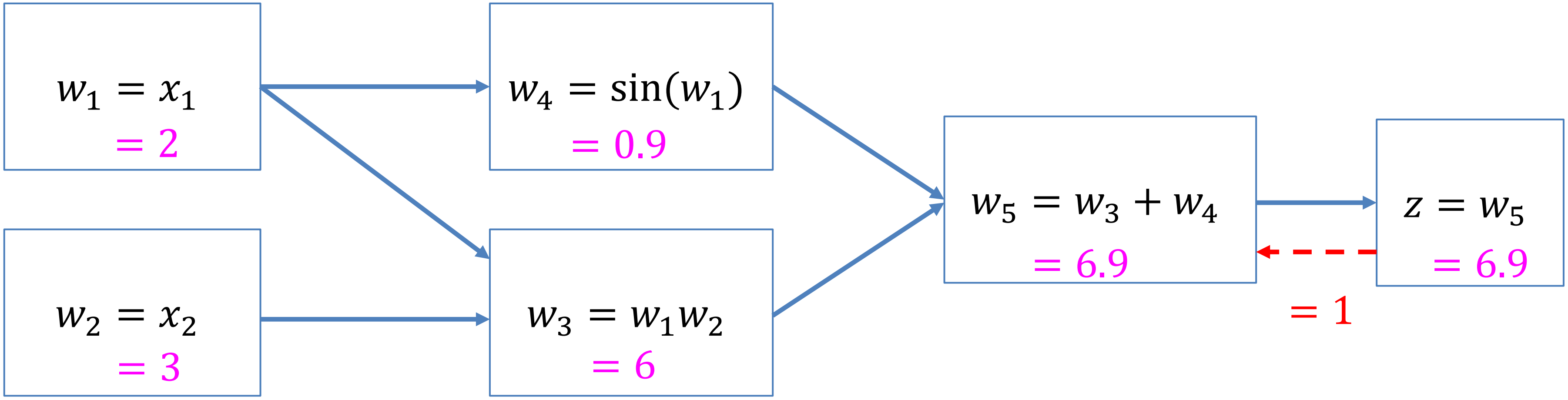
Compute derivatives with chain rule from end to beginning:

$$\frac{dz}{dw_5} = 1$$



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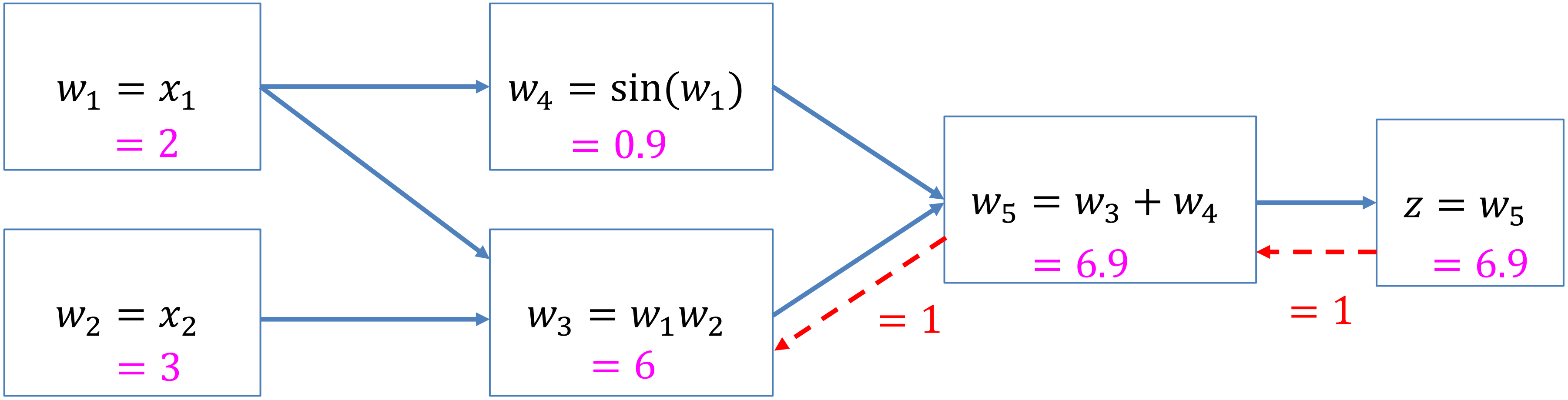

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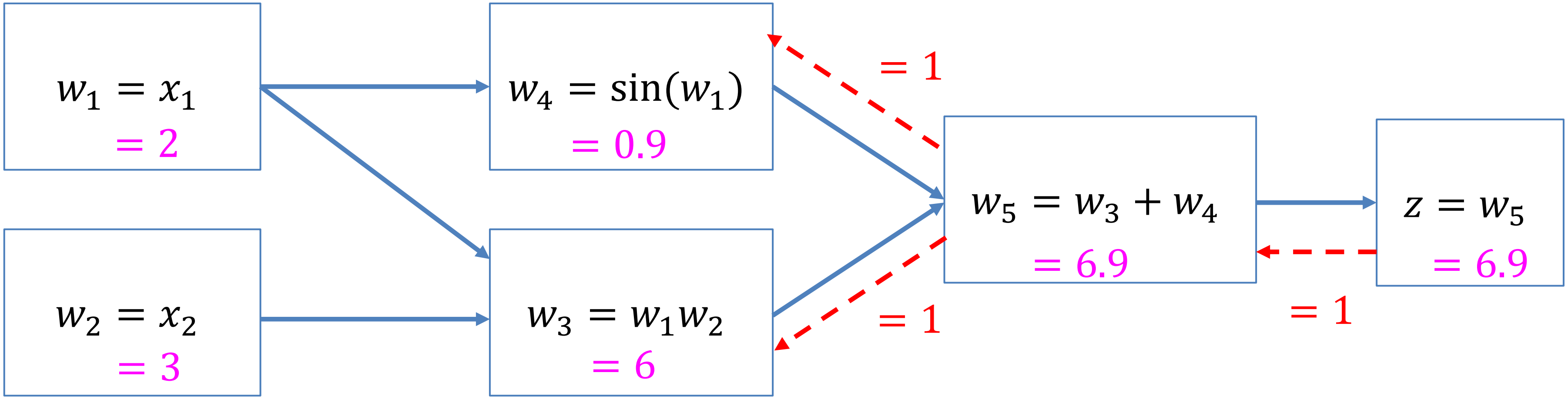

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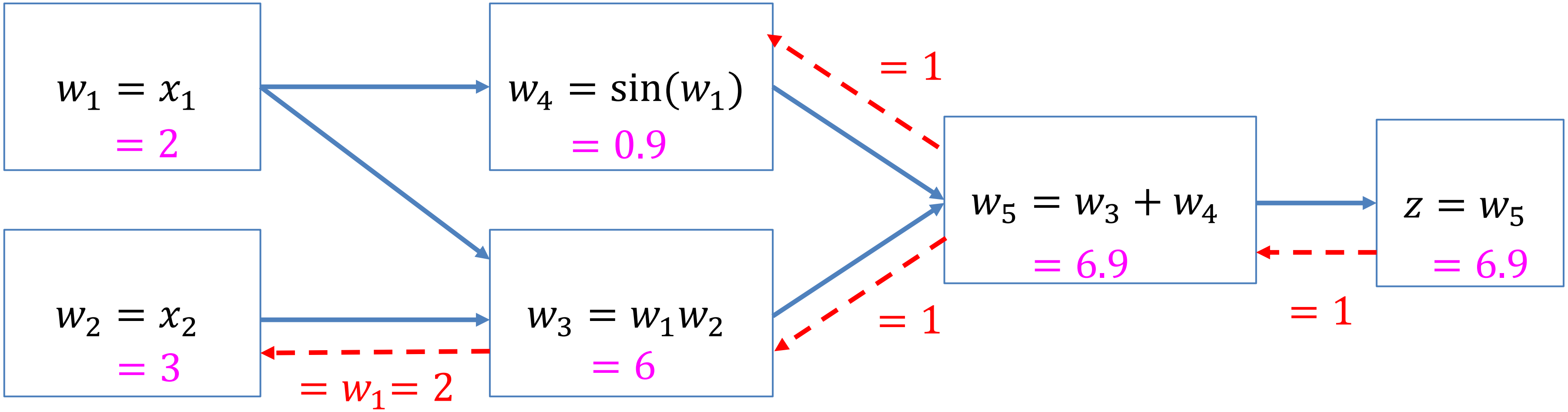
$$\frac{dz}{dw_2} = \frac{dz}{dw_3}\frac{dw_3}{dw_2} = 1\times w_1 = w_1 = 2$$



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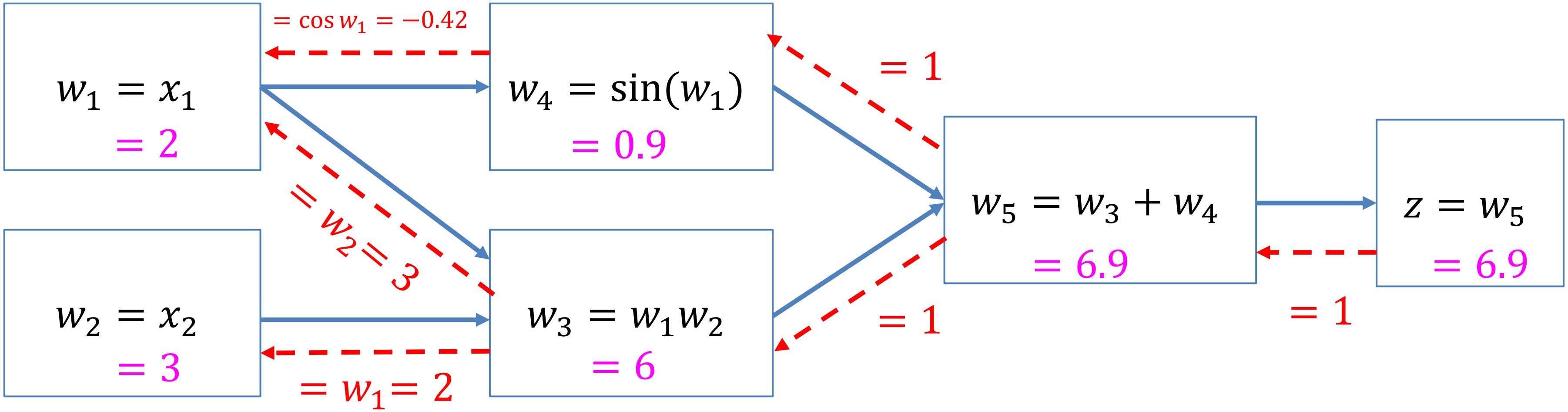
$$\frac{dz}{dw_2} = \frac{dz}{dw_3}\frac{dw_3}{dw_2} = 1\times w_1 = w_1 = 2$$

$$\frac{dz}{dw_1} = \frac{dz}{dw_4}\frac{dw_4}{dw_1} + \frac{dz}{dw_3}\frac{dw_3}{dw_1}$$
$$= \cos(w_1) + w_2 = \cos(2) + 3$$
$$= 2.58$$



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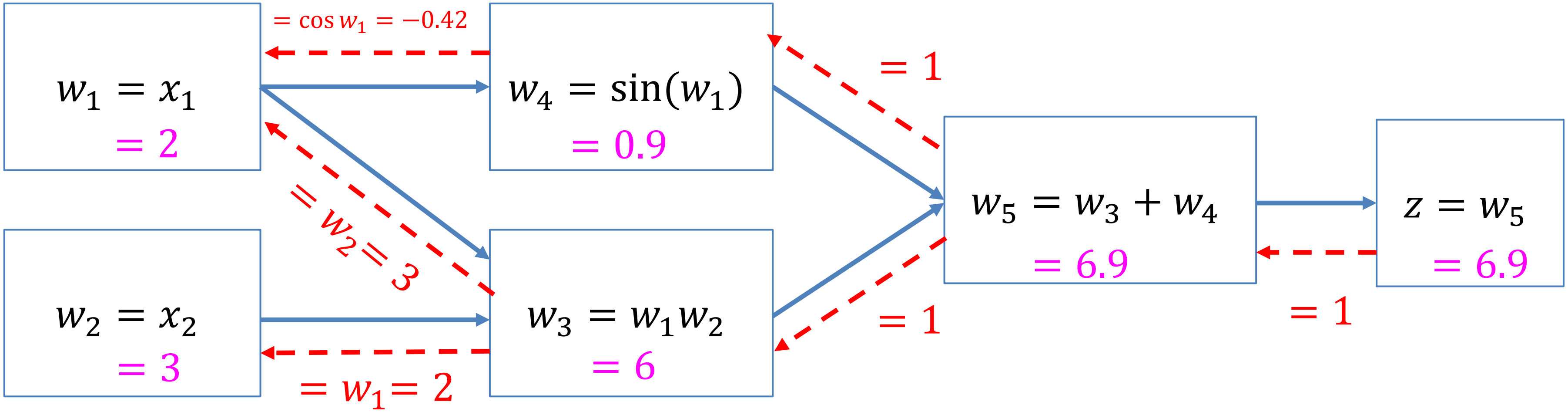
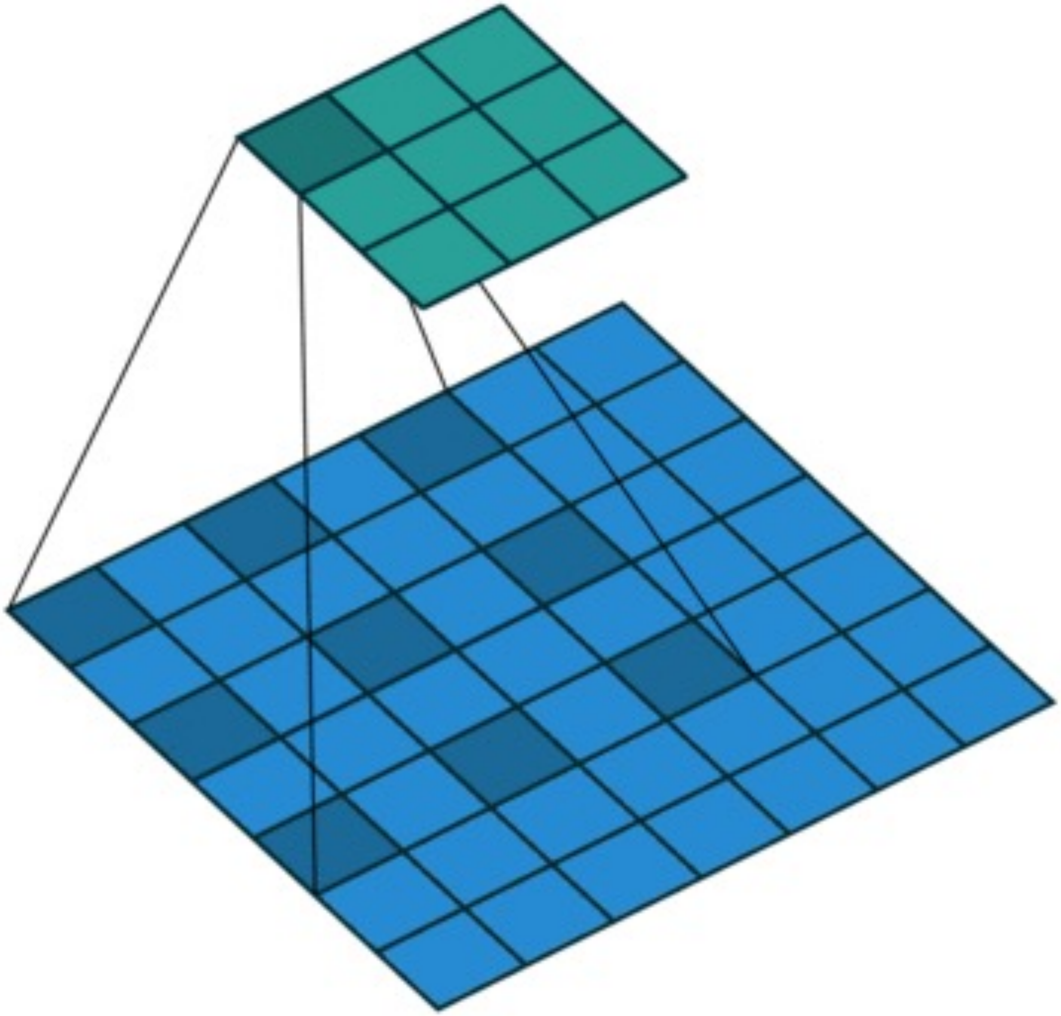
For each output, can compute the gradient w.r.t. all inputs in one pass!

Jacobian $$\frac{d\boldsymbol{z}}{d\boldsymbol{x}} = \begin{pmatrix} \frac{dz_1}{dx_1} & \cdots & \frac{dz_M}{dx_1} \\ \vdots & \ddots & \vdots \\ \frac{dz_1}{dx_N} & \cdots & \frac{dz_M}{dx_N} \end{pmatrix}$$



CNN

Dilation



Deep Sets

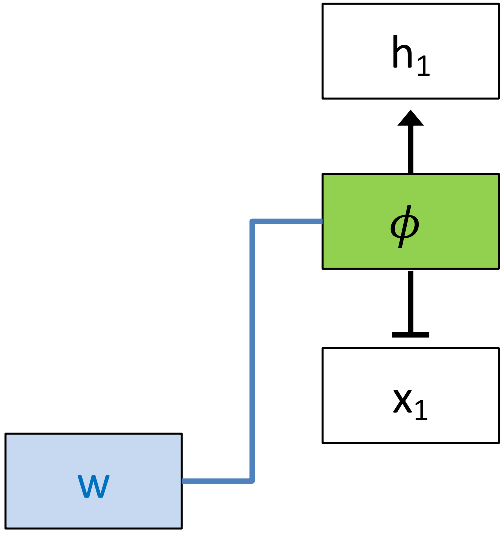
What if our data has no time structure?

- Data may be variable in length but have no temporal structure → *Data are sets of values*

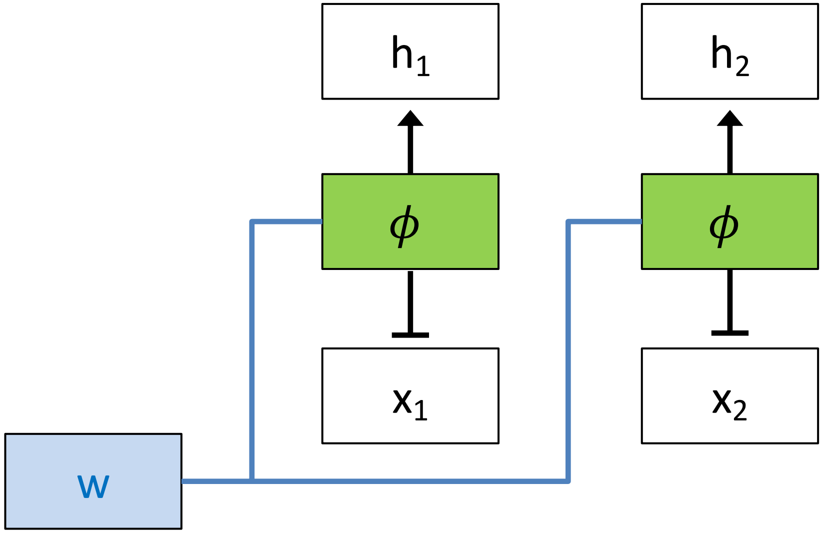
- *One option*: If we know about the data domain, could try to impose an ordering, then use RNN

- *Better option*: use system that can operate on variable length sets in permutation invariant way
  - Why permutation invariant → so order doesn't matter

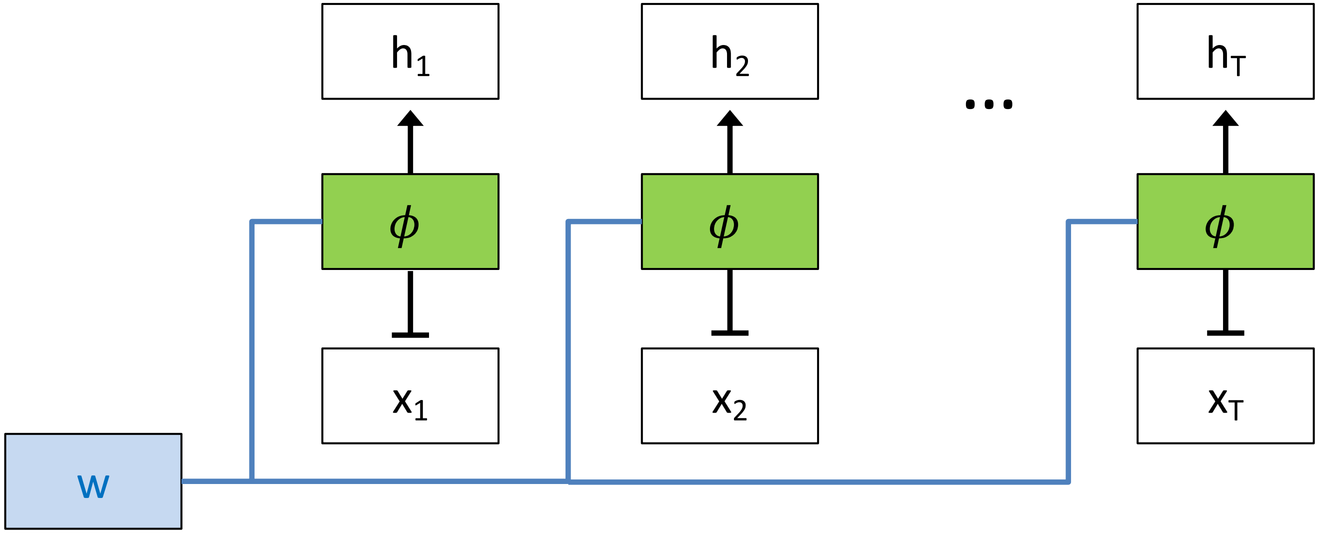
Deep Sets



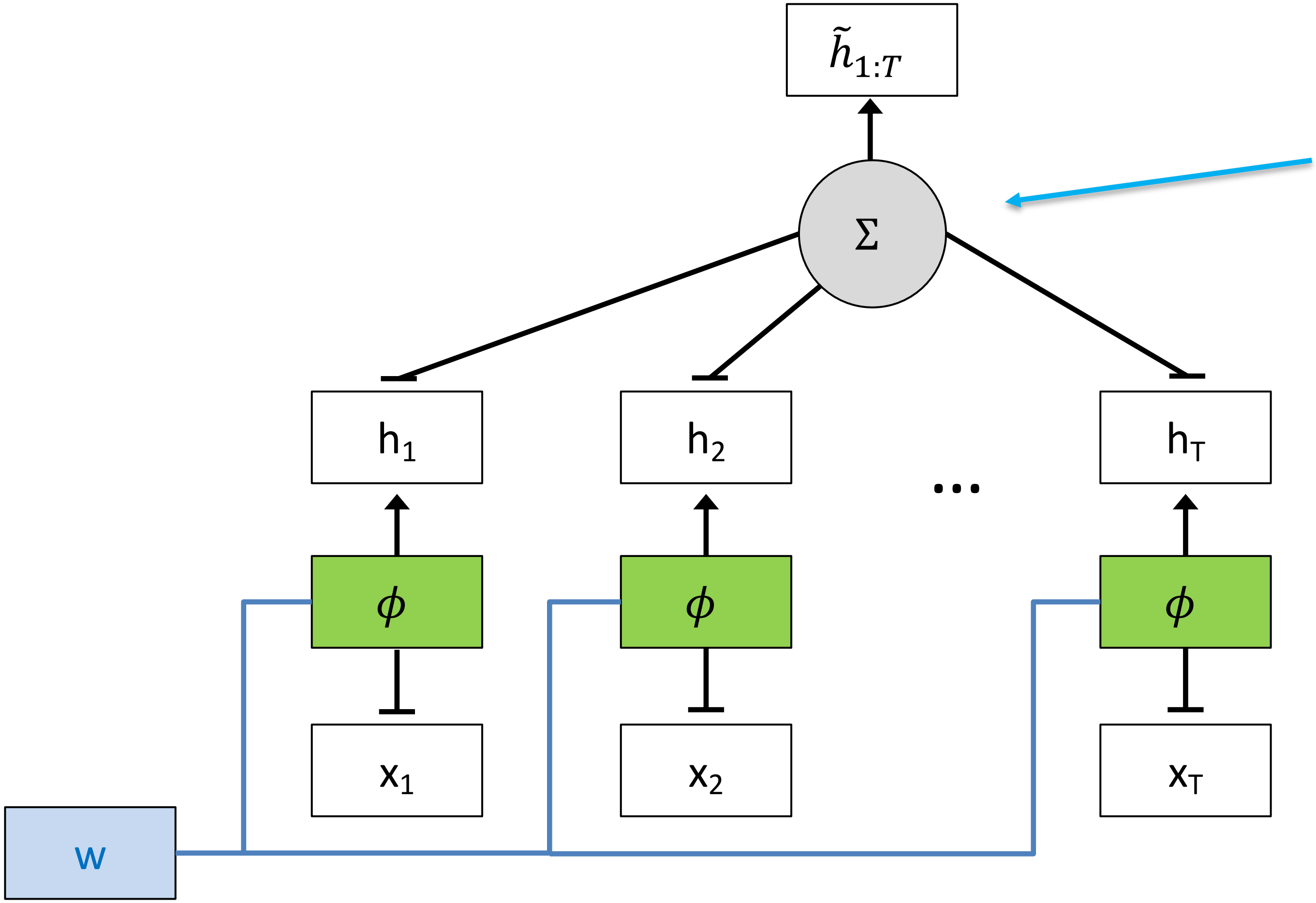
Deep Sets



Deep Sets

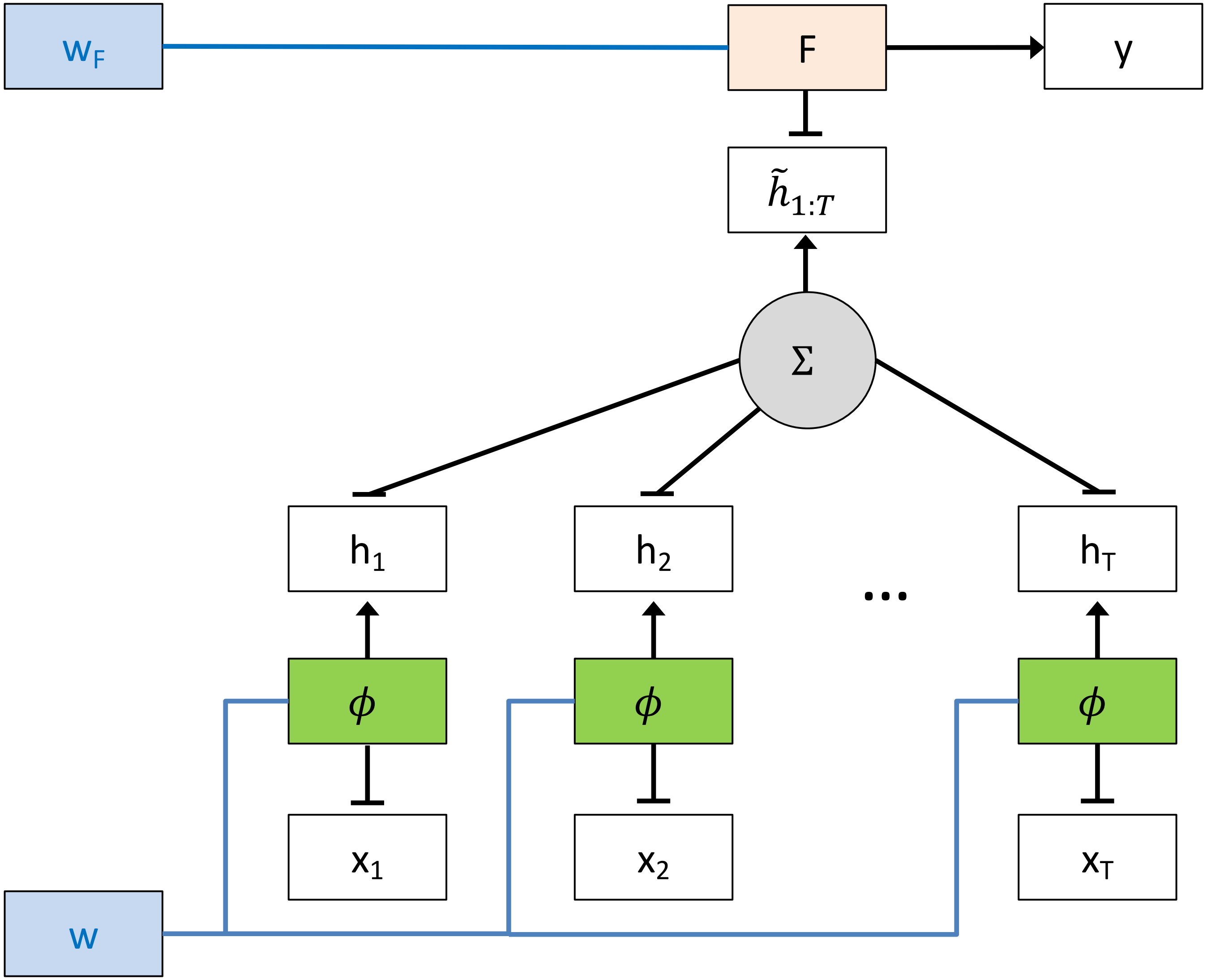


Deep Sets



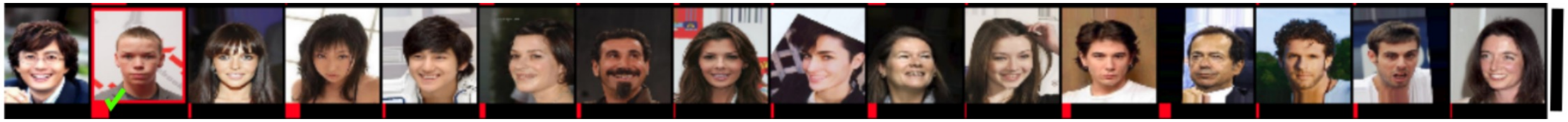
Permutation invariant operation: Sum, Max, …

Deep Sets



Examples

Outlier detection



M. Zaheer et. al 2017

Medical Imaging

With more complex architecture

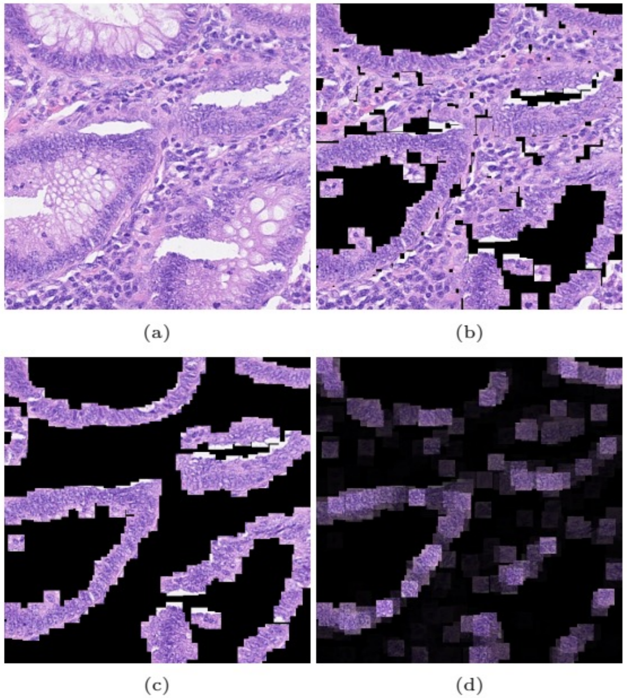


Figure 5. (a) H&E stained histology image. (b) 27×27 patches centered around all marked nuclei. (c) Ground truth: Patches that belong to the class epithelial. (d) Heatmap: Every patch from (b) multiplied by its corresponding attention weight, we rescaled the attention weights using $a'_k = (a_k - \min(\mathbf{a}))/(\max(\mathbf{a}) - \min(\mathbf{a}))$.

M. Ilse et al., 2018