Deep Learning and Automatic Differentiation

from Theano to PyTorch

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Swiss National Supercomputing Centre
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UNIVERSITY OF
OXFORD

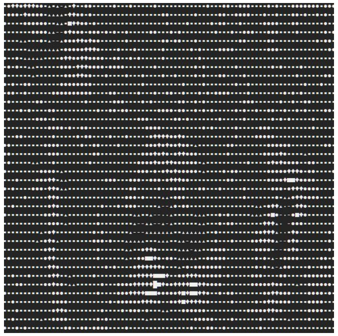
About me

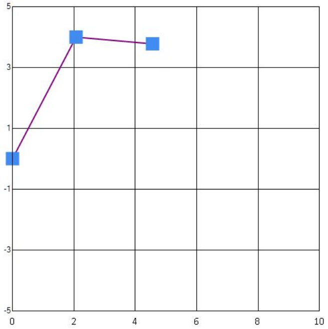
Postdoctoral researcher, University of Oxford

- Working with Frank Wood, Department of Engineering Science
- Working on probabilistic programming and its applications in science (high-energy physics and HPC)

Long-term interests:

- Automatic (algorithmic) differentiation (e.g. http://diffsharp.github.io)
- Evolutionary algorithms
- Computational physics





Deep learning

Deep learning

A reincarnation/rebranding of **artificial neural networks**, with roots in

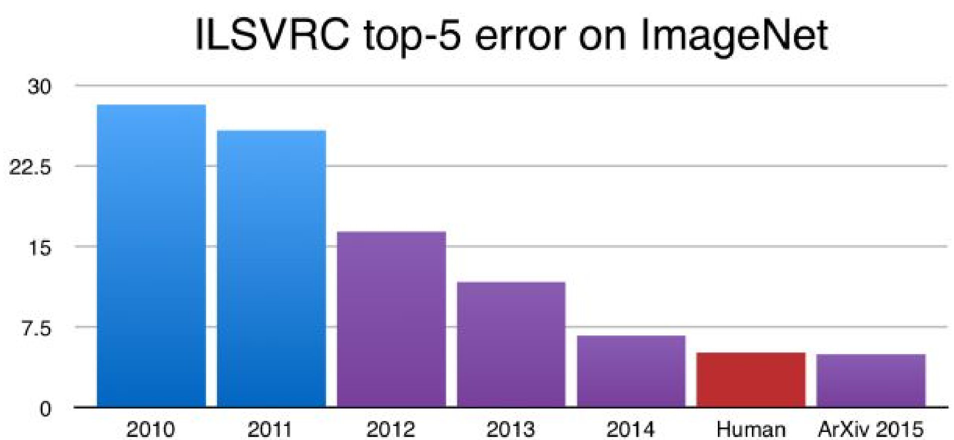
- Threshold logic (McCulloch & Pitts, 1943)
- Hebbian learning (Hebb, 1949)
- Perceptron (Rosenblatt, 1957)
- Backpropagation in NNs (Werbos, 1975; Rumelhart, Hinton, Williams, 1986)

Frank Rosenblatt with the Mark I Perceptron, holding a set of neural network weights

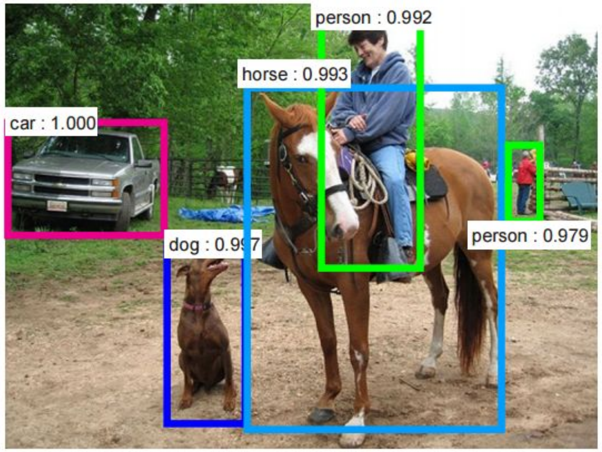
Deep learning

State of the art in **computer vision**

- ImageNet classification with deep convolutional neural networks (Krizhevsky et al., 2012)
  - Halved the error rate achieved with pre-deep-learning methods
- Replacing hand-engineered features
- Modern systems surpass human performance



Top-5 error rate for ImageNet
https://devblogs.nvidia.com/parallelforall/mocha-jl-deep-learning-julia/

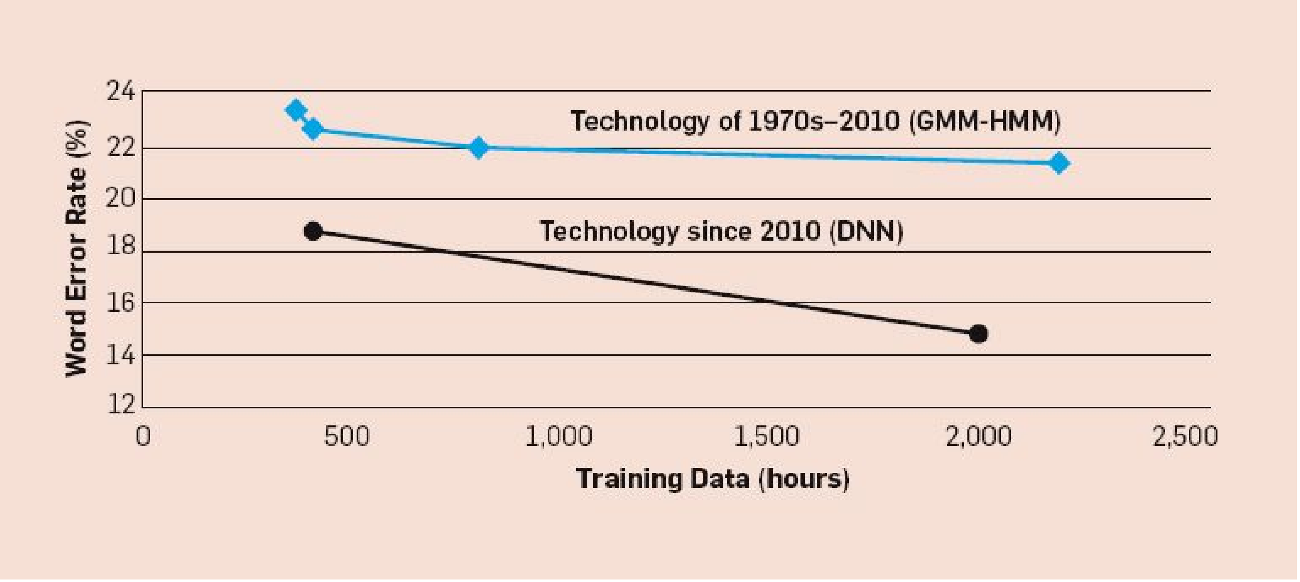


Faster R-CNN
(Ren et al., 2015)

Deep learning

State of the art in **speech recognition**

- Seminal work by Hinton et al. (2012)
  - First major industrial application of deep learning
- Replacing HMM-GMM-based models

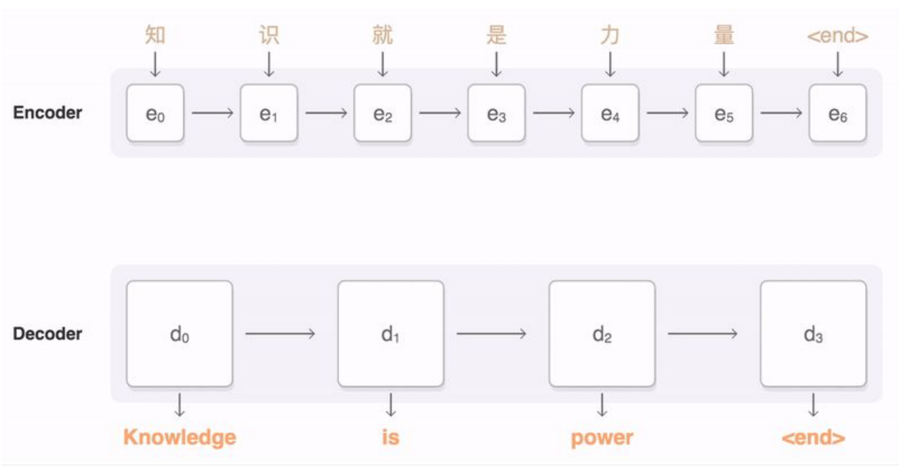


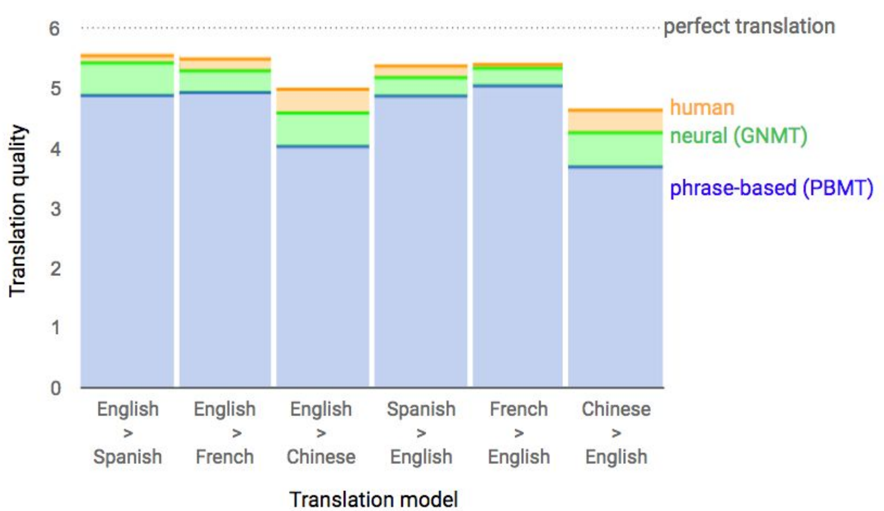
Recognition word error rates (Huang et al., 2014)

Deep learning

State of the art in **machine translation**

- Based on RNNs and CNNs (Bahdanu et al., 2015; Wu et al., 2016)
- Replacing statistical translation with engineered features
- Google (Sep 2016), Microsoft (Nov 2016), Facebook (Aug 2017) moved to neural machine translation
  https://techcrunch.com/2017/08/03/facebook-finishes-its-move-to-neural-machine-translation/





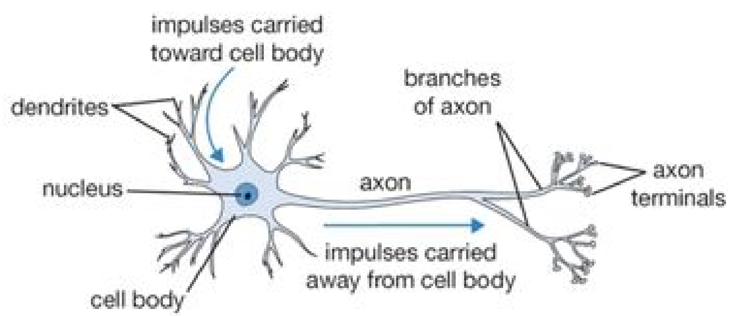
Google Neural Machine Translation System (GNMT)

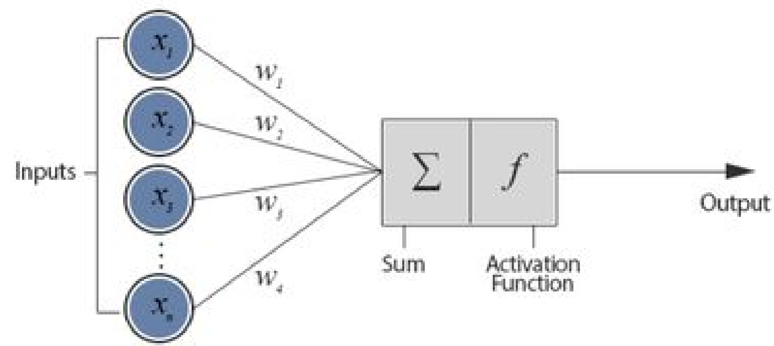
What makes deep learning tick?

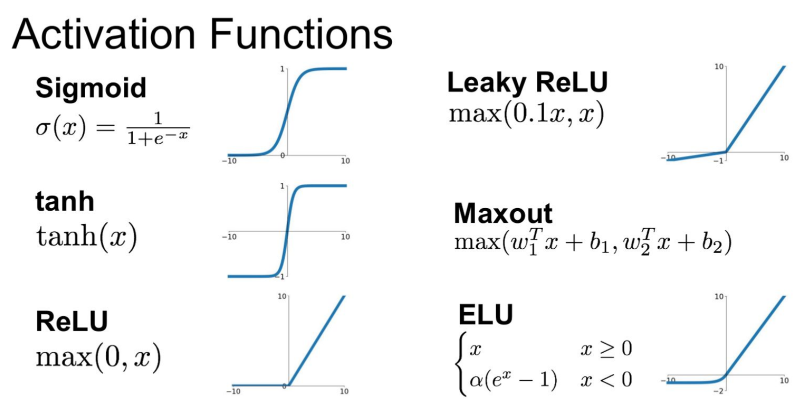
Deep neural networks

An artificial “neuron" is loosely based on the biological one

- Receive a set of weighted inputs (dendrites)
- Integrating and transforming (cell body)
- Passing the output further (axon)



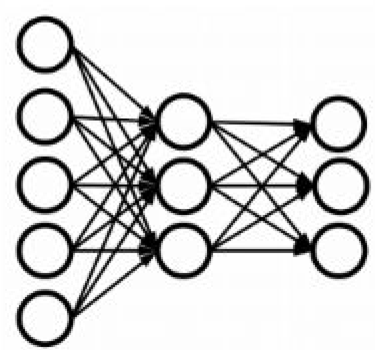


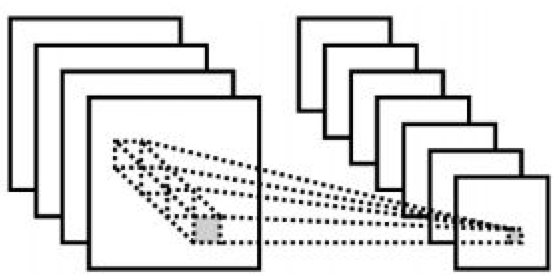


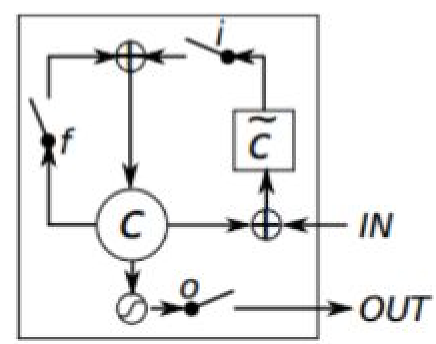
Deep neural networks

Three **main building blocks**

- Feedforward (Rosenblatt, 1957)
- Convolutional (LeCun et al., 1989)
- Recurrent (Hopfield, 1982; Hochreiter & Schmidhuber, 1997)



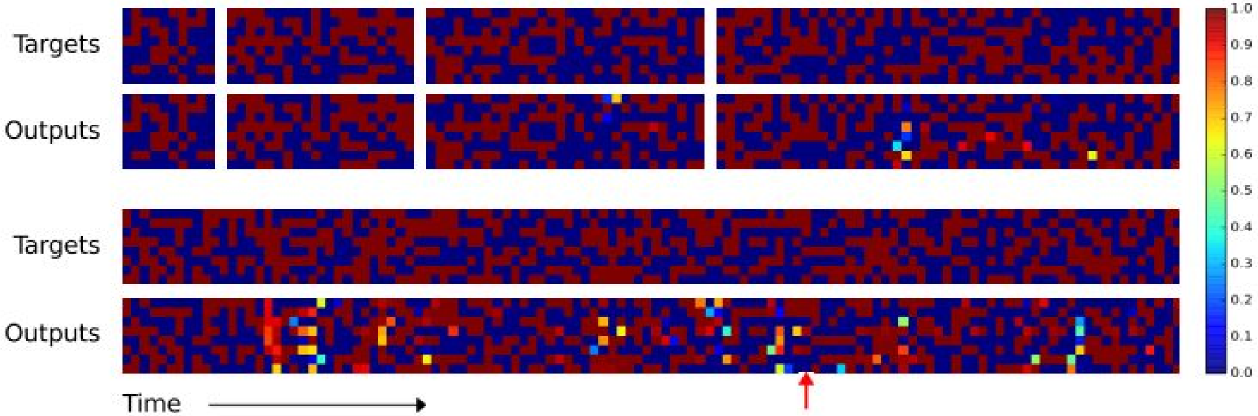




Deep neural networks

Newer additions introduce **(differentiable) algorithmic elements**

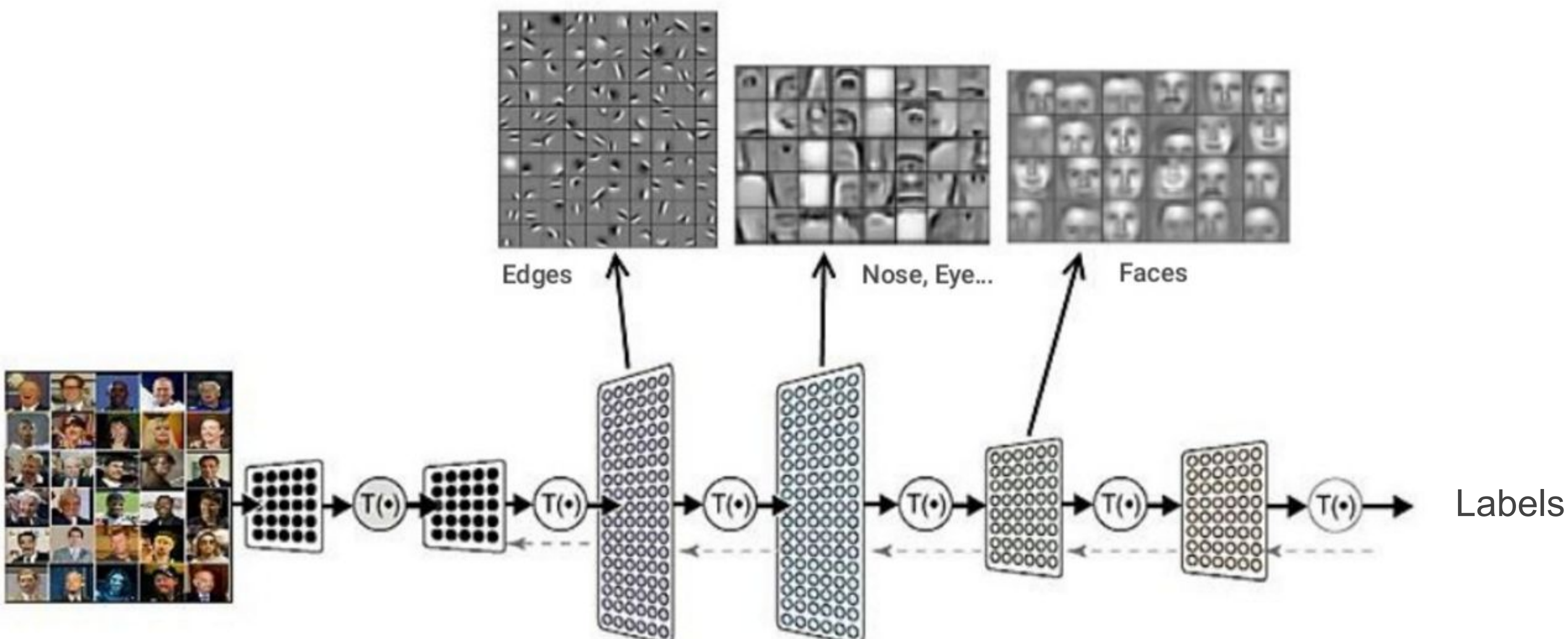
- Neural Turing Machine (Graves et al., 2014)
  - Can infer algorithms: copy, sort, recall
- Stack-augmented RNN (Joulin & Mikolov, 2015)
- End-to-end memory network (Sukhbaatar et al., 2015)
- Stack, queue, deque (Grefenstette et al., 2015)
- Discrete interfaces (Zaremba & Sutskever, 2015)



Neural Turing Machine on copy task (Graves et al., 2014)

Deep neural networks

- Deep, distributed representations learned end-to-end (also called "representation learning")
  - From **raw pixels** to **object labels**
  - From **raw waveforms of speech** to **text**

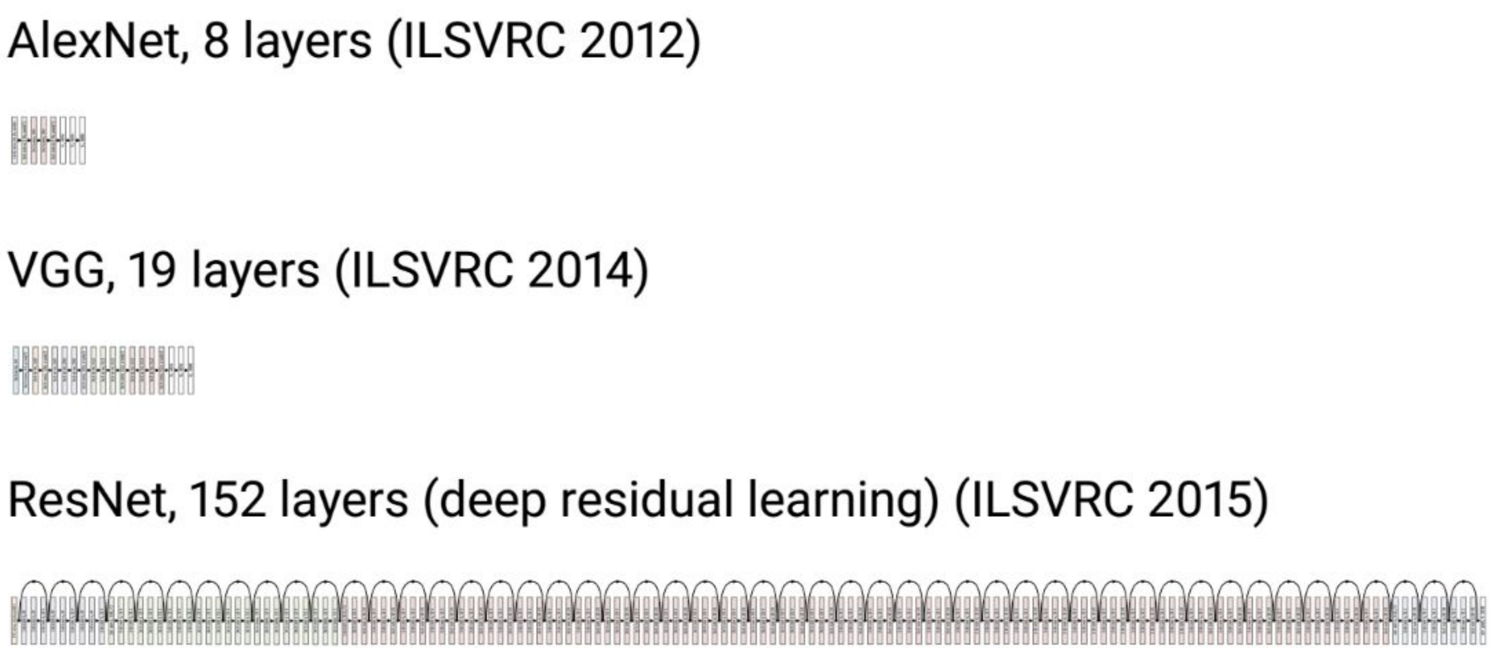


(Masuch, 2015)

Deep neural networks

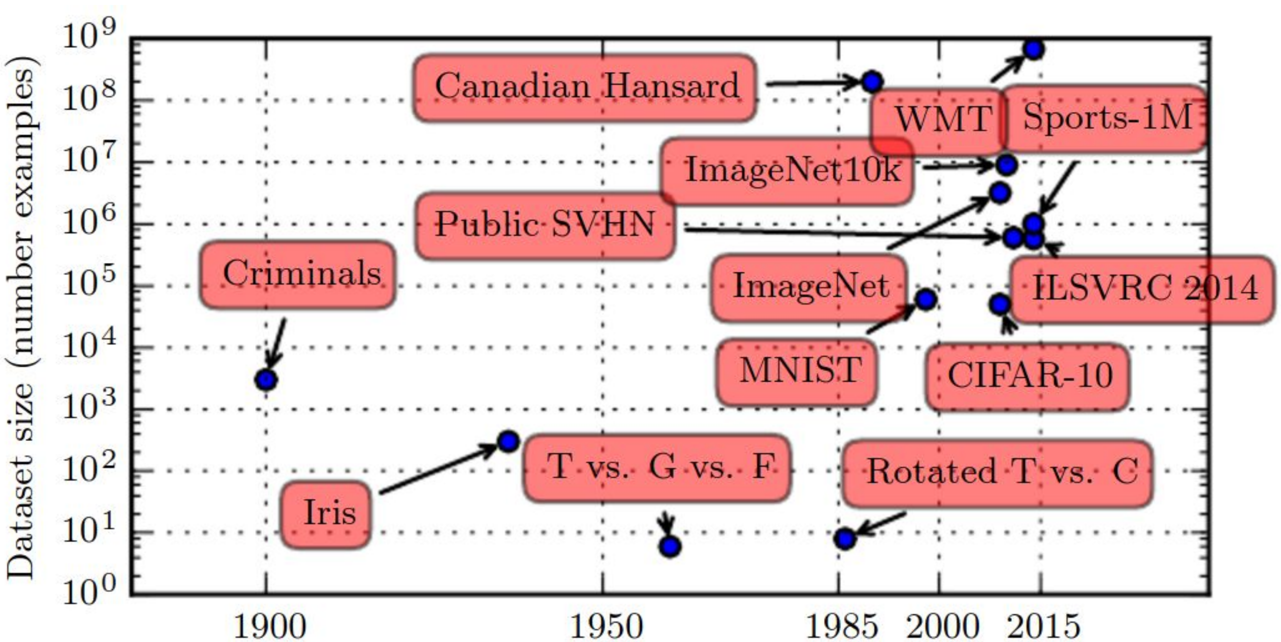
Deeper is better (Bengio, 2009)

- Deep architectures consistently beat shallow ones
- Shallow architectures exponentially inefficient for same performance
- Hierarchical, distributed representations achieve non-local generalization



Data

- Deep learning needs massive amounts of data
  - need to be labeled if performing supervised learning
- A rough rule of thumb: *"deep learning will generally match or exceed human performance with a dataset containing at least 10 million labeled examples."* (The Deep Learning book, Goodfellow et al., 2016)

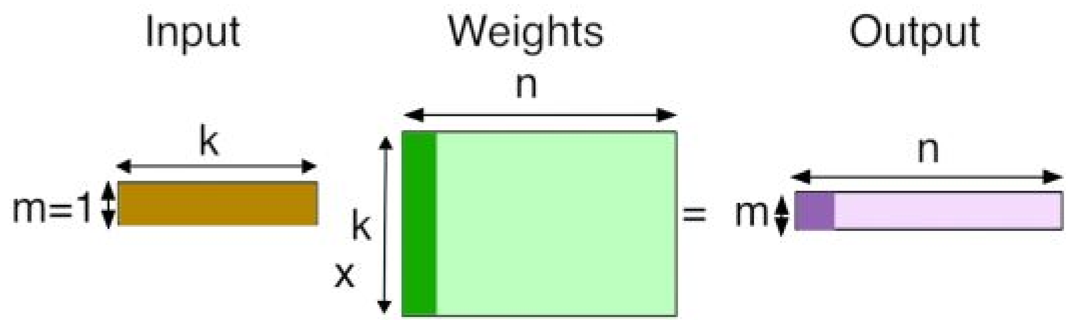


Dataset sizes (Goodfellow et al., 2016)

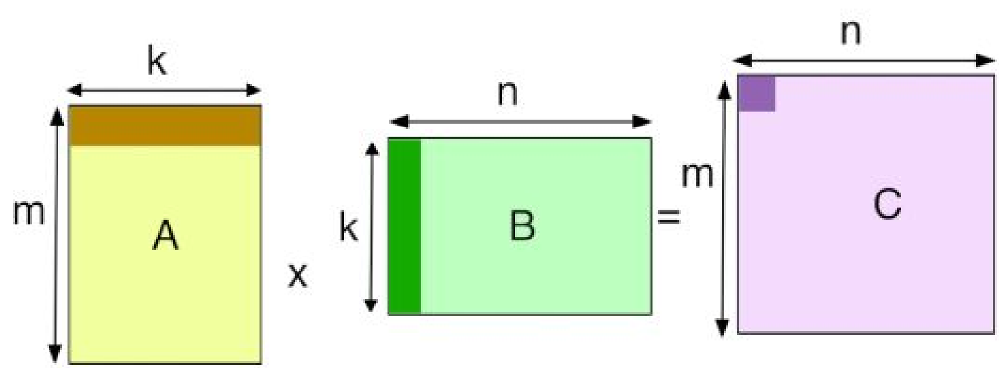
GPUs

Layers of NNs are conveniently expressed as series of **matrix multiplications**

One input vector,
n neurons of *k* inputs



A batch of *m* input vectors



GPUs

- BLAS (mainly GEMM) is at the hearth of mainstream deep learning, commonly running on off-the-shelf graphics processing units
- Rapid adoption after
  - Nvidia released CUDA (2007)
  - Raina et al. (2009) and Ciresan et al. (2010)
- ASICs such as tensor processing units (TPUs) are being introduced
  - As low as 8-bit floating point precision, better power efficiency

Nvidia Titan Xp (2017)

Google Cloud TPU server

Deep learning frameworks

- Modern tools make it **extremely easy to implement / reuse models**
- Off-the-shelf components
  - Simple: linear, convolution, recurrent layers
  - Complex: compositions of complex models (e.g., CNN + RNN)
- Base frameworks: Torch (2002), Theano (2011), Caffe (2014), TensorFlow (2015), PyTorch (2016)
- Higher-level model-building libraries: Keras (Theano & TensorFlow), Lasagne (Theano)
- High-performance low-level bindings: BLAS, Intel MKL, CUDA, Magma

Learning: gradient-based optimization

Loss function

$$Q(\boldsymbol{w}) = \sum_{i=1}^{N} Q_i(\boldsymbol{w})$$

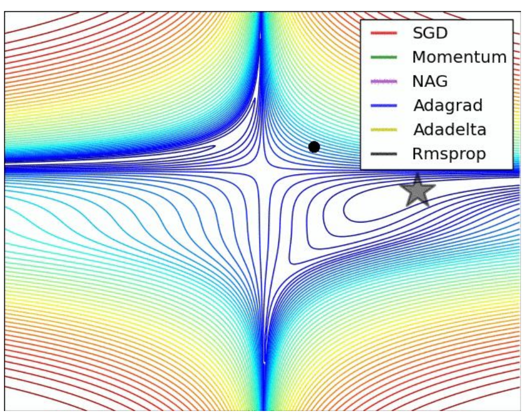
Parameter update

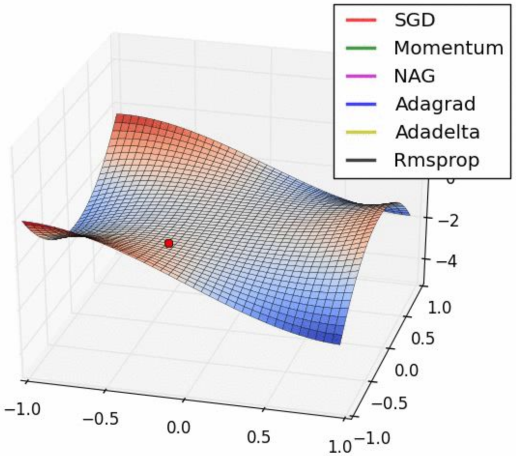
$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \eta \nabla_w Q(\boldsymbol{w})$$

Stochastic gradient descent (SGD)

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \eta \sum_{i=1}^{d} \nabla_w Q_i(\boldsymbol{w})$$

In practice we use SGD or adaptive-learning-rate varieties such as Adam, RMSProp





(Ruder, 2017)

http://ruder.io/optimizing-gradient-descent/

Deep learning

Neural networks

\+ Data

\+ Gradient-based optimization

Deep learning

Neural networks

\+ Data

\+ Gradient-based optimization

We need derivatives

How do we compute derivatives?

Manual

- Calculus 101, rules of differentiation

General Formulas

1. $$\frac{d}{dx}c = 0$$

2. $$\frac{d}{dx}[f(x) \mp g(x)] = f'(x) \mp g'(x)$$

3. $$\frac{d}{dx}[f(x)g(x)] = f'(x)g(x) + g'(x) + f(x)$$

4. $$\frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] = \frac{g(x)f'(x) - g'(x)f(x)}{(g(x))^2}$$

5. $$\frac{d}{dx}f(g(x)) = f'(g(x))g'(x)$$

6. $$\frac{d}{dx}x^n = nx^{n-1}$$

Exponential and Logarithmic Functions

7. $$\frac{d}{dx}e^{f(x)} = f'(x)e^{f(x)}$$

8. $$\frac{d}{dx}a^x = a^x\ln(a)$$

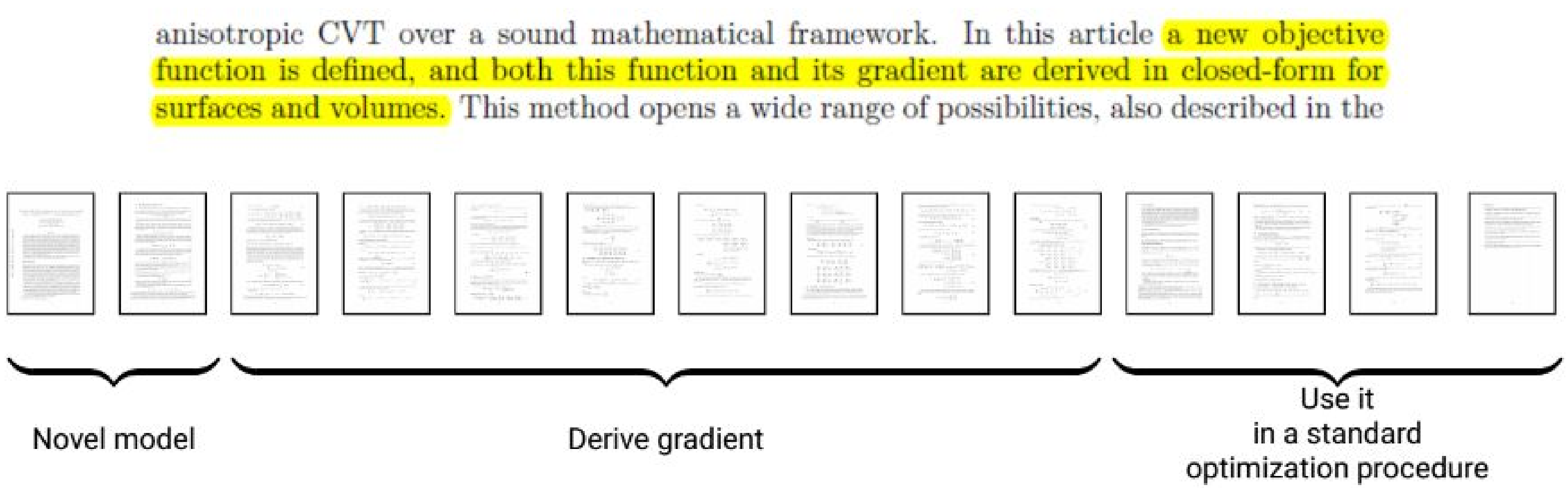
9. $$\frac{d}{dx}\ln(C|f(x)|) = \frac{d}{dx}[\ln(C) + \ln(f(x))] = \frac{f'(x)}{f(x)}$$

10. $$\frac{d}{dx}log_a(f(x)) = \frac{f'(x)}{xln(a)}$$

...

Manual

- Analytical derivatives are needed for theoretical insight
  - analytic solutions, proofs
  - mathematical analysis, e.g., stability of fixed points
- They are **unnecessary when we just need numerical derivatives** for optimization
- Until very recently, machine learning looked like this:

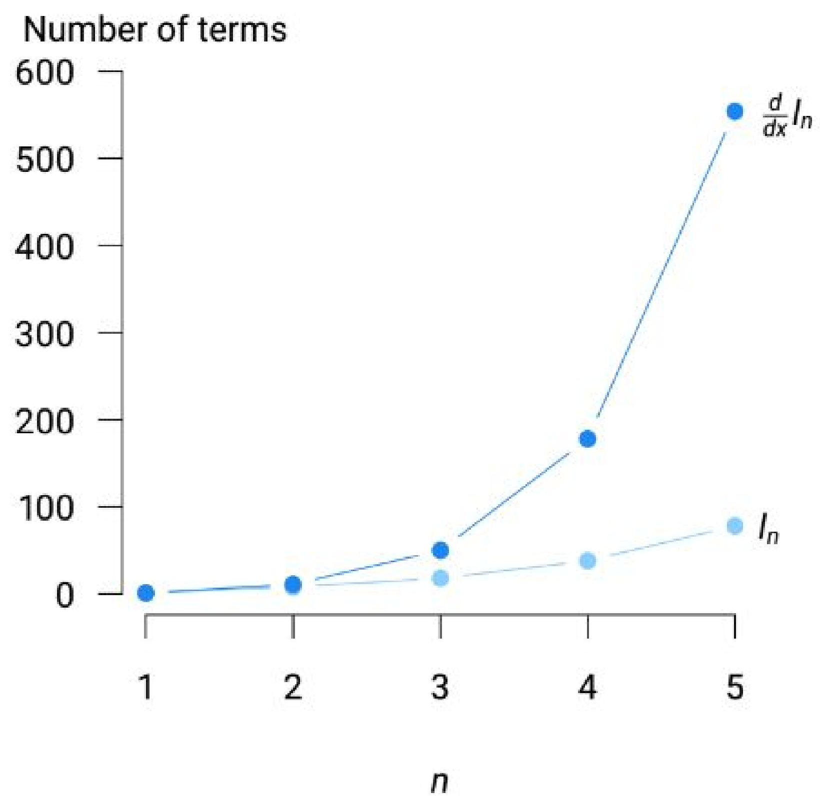


Symbolic derivatives

- Symbolic computation with Mathematica, Maple, Maxima, also deep learning frameworks such as Theano
- Main issue: **expression swell**

Logistic map $l_{n+1} = 4l_n(1 - l_n)$, $l_1 = x$

n	l_n	$\frac{d}{dx} l_n$
1	x	1
2	$4x(1-x)$	$4(1-x) - 4x$
3	$16x(1-x)(1-2x)^2$	$16(1-x)(1-2x)^2 - 16x(1-2x)^2 - 64x(1-x)(1-2x)$
4	$64x(1-x)(1-2x)^2(1-8x+8x^2)^2$	$128x(1-x)(-8+16x)(1-2x)^2(1-8x+8x^2) + 64(1-x)(1-2x)^2(1-8x+8x^2)^2 - 64x(1-2x)^2(1-8x+8x^2)^2 - 256x(1-x)(1-2x)(1-8x+8x^2)^2$



Symbolic derivatives

- Symbolic computation with, e.g., Mathematica, Maple, Maxima
- Main limitation: **only applicable to closed-form expressions**

You can find the derivative of:

```
In [1]: def f(x):
            return 64 *(1-x) *(1-2*x)^2 *(1-8*x+8*x*x)^2
```

But not of:

```
In [2]: def f(x,n):
            if n == 1:
                return x
            else:
                v = x
                for i in range(1,n):
                    v = 4*v*(1-v)
                return v
```

In deep learning, symbolic graph builders such as Theano and TensorFlow face issues with control flow, loops, recursion

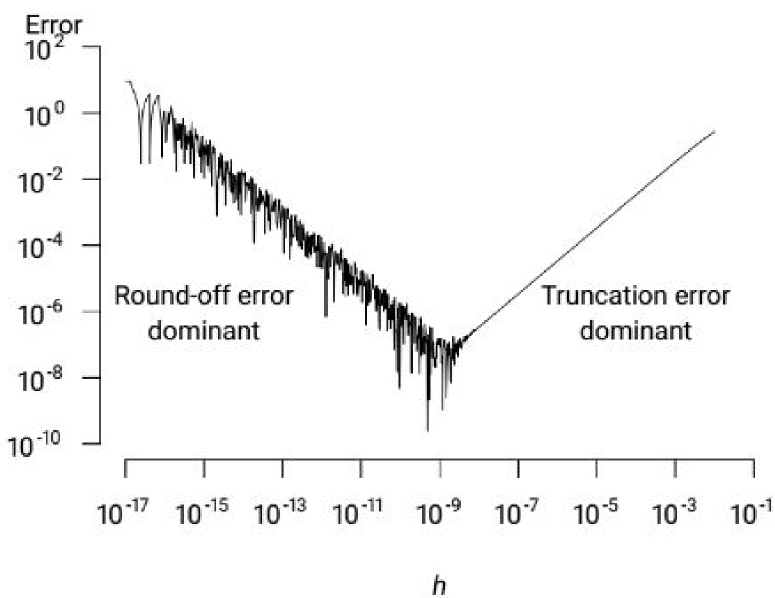
Numerical differentiation

Finite differences, for example:

$f : \mathbb{R}^n \to \mathbb{R}$, approximate the gradient $\nabla f = \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_n}\right)$ using

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \frac{f(\mathbf{x} + h\mathbf{e}_i) - f(\mathbf{x})}{h}, \; 0 < h \ll 1$$

But we have to select h and we face **approximation errors**



Computed using

$$E(h, x^*) = \left| \frac{f(x^* + h) - f(x^*)}{h} - \frac{d}{dx} f(x)\Big|_{x^*} \right|$$

$$f(x) = 64x(1-x)(1-2x)^2(1-8x+8x^2)^2$$

$$x^* = 0.2$$

Numerical differentiation

Better approximations exist

- Higher-order finite differences
  E.g.
  $$\frac{\partial f(\mathbf{x})}{\partial x_i} = \frac{f(\mathbf{x} + h\mathbf{e}_i) - f(\mathbf{x} - h\mathbf{e}_i)}{2h} + O(h^2) \ ,$$
- Richardson extrapolation
- Differential quadrature

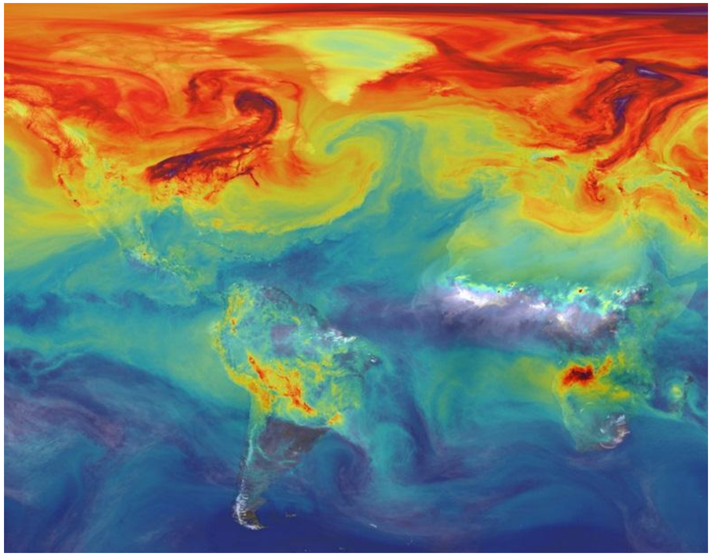
but they increase rapidly in complexity and never completely eliminate the error

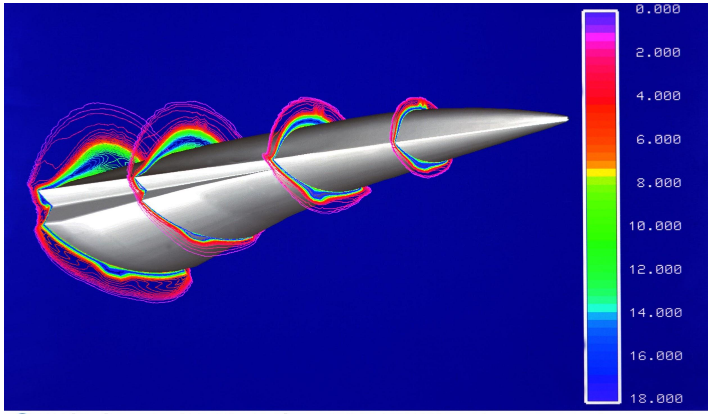
Automatic differentiation

- Small but established subfield of scientific computing
  http://www.autodiff.org/

- Traditional application domains:
  - Computational fluid dynamics
  - Atmospheric sciences
  - Engineering design optimization
  - Computational finance

AD has shared roots with the backpropagation algorithm for neural networks, but it is more general





NASP–Computer Aided Design Computational Fluid Dynamics
NASA Langley Research Center 6/6/1988 Image # EL–1996–00191

Automatic differentiation

Given an algorithm **A**,

- build an augmented algorithm **A'**
- for each value, keep a primal and a derivative component (dual numbers)
- compute the derivatives along with the original values

All algorithms are compositions of a finite set of elementary operations (with known derivatives)

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

```
f'(a, a', b, b'):
    (c, c') = (a*b, a'*b + a*b')
    (d, d') = (sin c, c' * cos c)
    return (d, d')
```

Automatic differentiation

Given an algorithm **A**,

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```
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→

```
f’(a, a’, b, b’):
   (c, c’) = (a*b, a’*b + a*b’)
   (d, d’) = (sin c, c’ * cos c)
   return (d, d’)
```

Exact derivatives, not an approximation

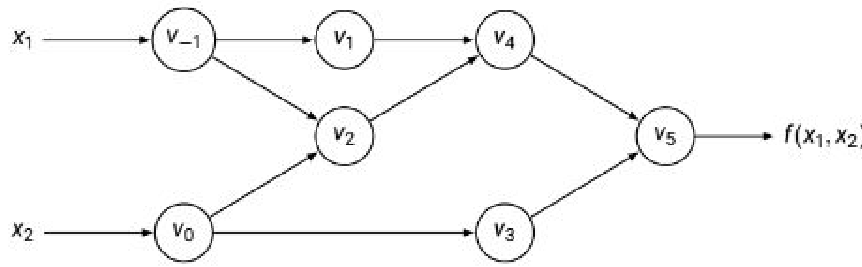
Automatic differentiation

AD has two main modes:

- **Forward mode:** straightforward
- **Reverse mode**: slightly more difficult, when you see it for the first time

Forward mode

Let's take $y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$

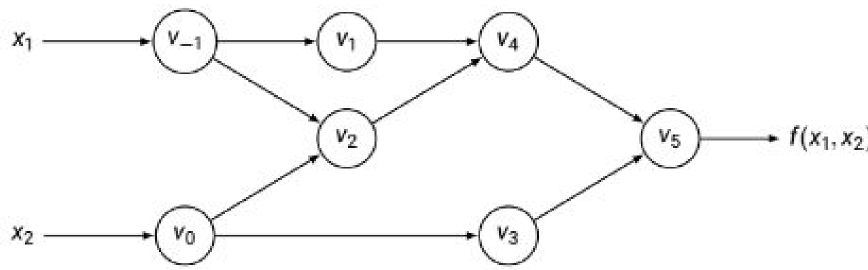


Derivatives propagate: independent $\rightarrow$ dependent

- select a var. of differentiation x_i
- augment each intermediate value v_j with $\dot{v}_j = \frac{\partial v_j}{\partial x_i}$
- set $\dot{x}_i = 1$
- run the algorithm forward

Forward mode

Let's take $y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$



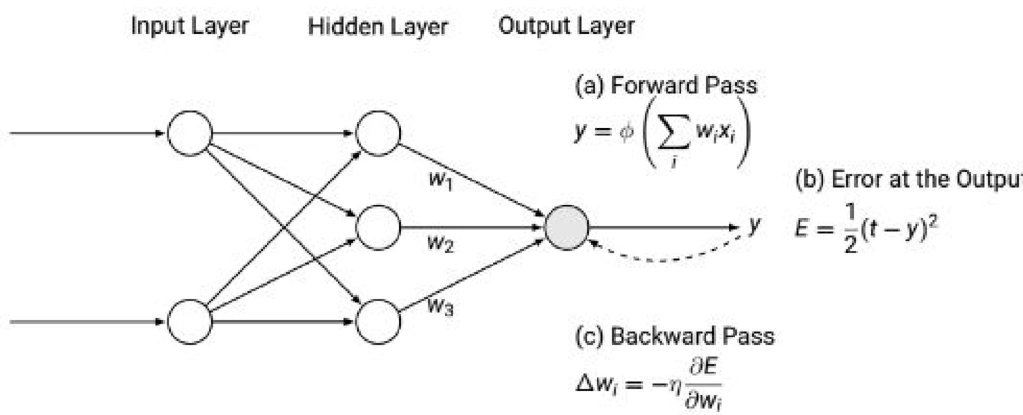
Forward Evaluation Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Forward Derivative Trace		
$\dot{v}_{-1}$	$= \dot{x}_1$	$= 1$
$\dot{v}_0$	$= \dot{x}_2$	$= 0$
$\dot{v}_1$	$= \dot{v}_{-1} / v_{-1}$	$= 1/2$
$\dot{v}_2$	$= \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$\dot{v}_3$	$= \dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$
$\dot{v}_4$	$= \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$\dot{v}_5$	$= \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$
$\boldsymbol{\dot{y}}$	$\boldsymbol{= \dot{v}_5}$	$\mathbf{= 5.5}$

Reverse mode

If you know the maths behind backpropagation,
you know reverse mode AD

Backpropagation **is just a special case** of reverse mode AD



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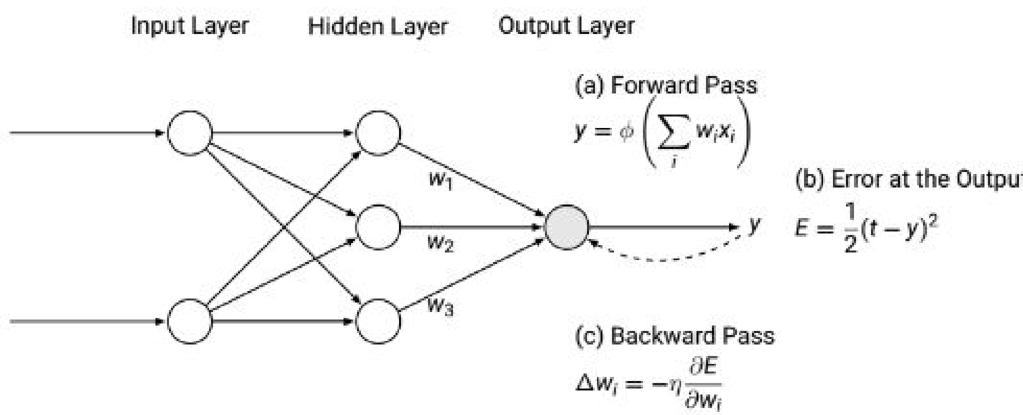
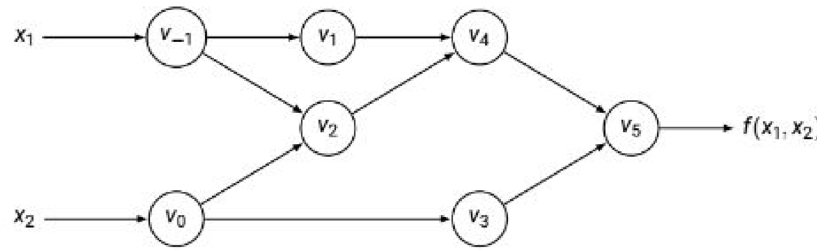


Origins in the same papers (Bryson and Ho, 1969; Werbos, 1974)
Backprop. brought to fame by Rumelhart et al. (1986)

AD and machine learning communities somehow managed to stay disconnected

Reverse mode

Again take $y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$



Derivatives propagate: dependent $\rightarrow$ independent
1st stage:

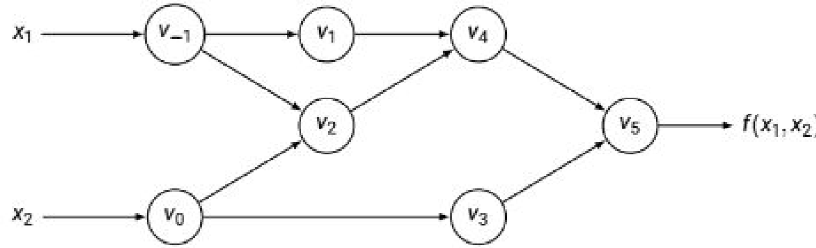
- run your original code forward

2nd stage:

- select a dependent var. y_j
- augment each intermediate value v_i with $\bar{v}_i = \frac{\partial y_j}{\partial v_i}$ (adjoint)
- set $\bar{y}_j = 1$
- run the algorithm backward

Reverse mode

Again take $y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$



Forward Evaluation Trace

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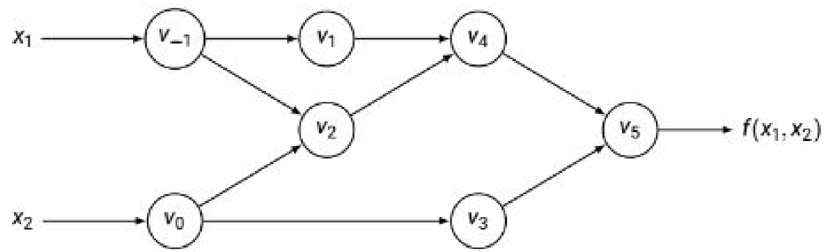
y	$= v_5$	$= 11.652$

Reverse Adjoint Trace

$\boldsymbol{\bar{x}_1}$	$\boldsymbol{= \bar{v}_{-1}}$		$\mathbf{= 5.5}$
$\boldsymbol{\bar{x}_2}$	$\boldsymbol{= \bar{v}_0}$		$\mathbf{= 1.716}$
$\bar{v}_{-1}$	$= \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}}$	$= \bar{v}_{-1} + \bar{v}_1 / v_{-1}$	$= 5.5$
$\bar{v}_0$	$= \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$	$= \bar{v}_0 + \bar{v}_2 \times v_{-1}$	$= 1.716$
$\bar{v}_{-1}$	$= \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0$	$= \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

Reverse mode

Again take $y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$



In [1]:
```
import torch
from torch import Tensor
from torch.autograd import Variable
```

In [2]:
```
x1 = Variable(Tensor([2]),requires_grad=True)
x2 = Variable(Tensor([5]),requires_grad=True)
```

In [3]:
```
v1 = torch.log(x1)
v2 = x1 * x2
v3 = torch.sin(x2)
v4 = v1 + v2
y = v4 - v3
```

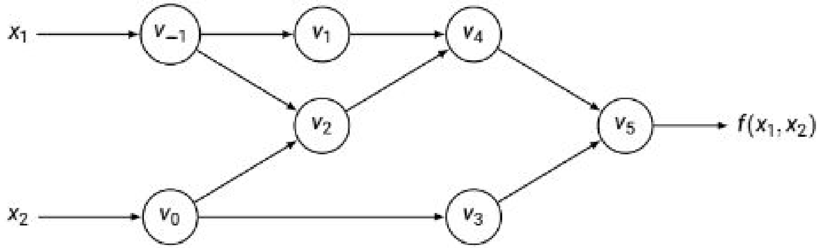
In [4]:
```
y.backward()
print(x1.grad.data)
print(x2.grad.data)
```

```
 5.5000
[torch.FloatTensor of size 1]


 1.7163
[torch.FloatTensor of size 1]
```

Reverse mode

Again take $y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$



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More on this in the afternoon exercise session

Forward vs reverse

In the extreme cases,

for $F : \mathbb{R} \to \mathbb{R}^m$, forward AD can compute all $\left(\frac{\partial F_1}{\partial x}, \ldots, \frac{\partial F_m}{\partial x} \right)$

for $f : \mathbb{R}^n \to \mathbb{R}$, reverse AD can compute $\nabla f = \left(\frac{\partial f}{\partial x_i}, \ldots, \frac{\partial f}{\partial x_n} \right)$

in **just one application**

Forward vs reverse

In the extreme cases,
for $F : \mathbb{R} \to \mathbb{R}^m$, forward AD can compute all $\left(\frac{\partial F_1}{\partial x}, \ldots, \frac{\partial F_m}{\partial x}\right)$
for $f : \mathbb{R}^n \to \mathbb{R}$, reverse AD can compute $\nabla f = \left(\frac{\partial f}{\partial x_i}, \ldots, \frac{\partial f}{\partial x_n}\right)$
in **just one application**

In general, for $f : \mathbb{R}^n \to \mathbb{R}^m$, the Jacobian $\mathbf{J} \in \mathbb{R}^{m \times n}$ takes

- $O(n \times \text{time}(f))$ with forward AD
- $O(m \times \text{time}(f))$ with reverse AD

Reverse mode performs better when $n \gg m$

Derivatives and deep learning frameworks

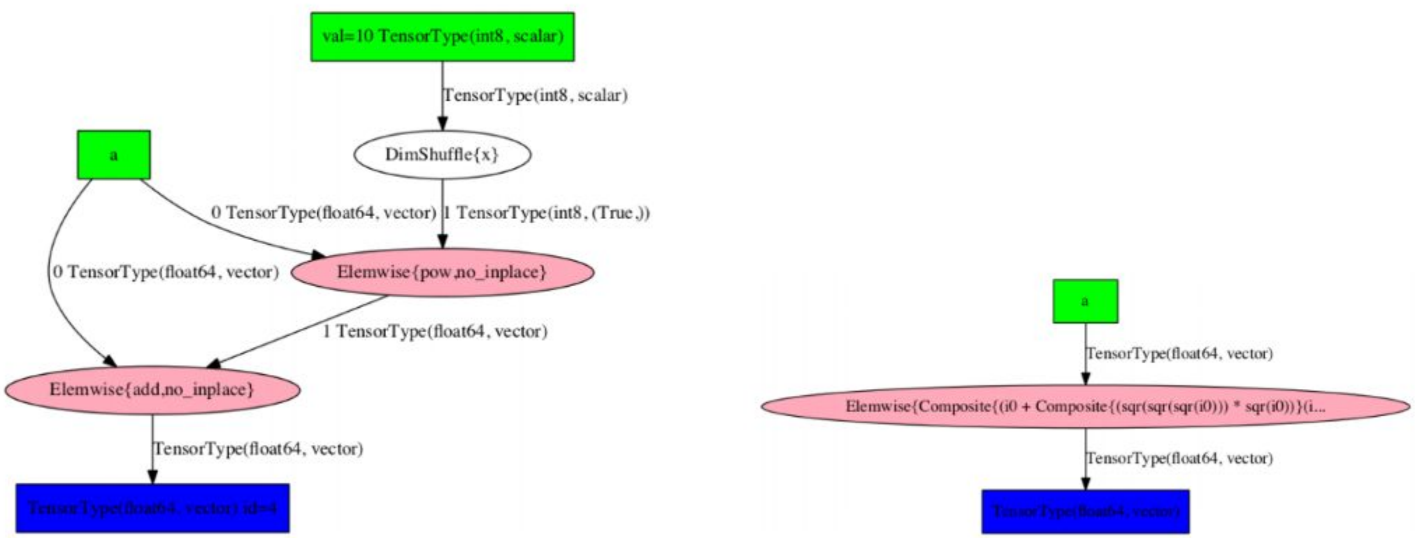
Deep learning frameworks

Two main families:

- Symbolic graph builders
- Dynamic graph builders (general-purpose AD)

Symbolic graph builders

- Implement models using symbolic placeholders, using a mini-language
- Severely limited (and unintuitive) control flow and expressivity
- The graph gets “compiled” to take care of expression swell



Graph compilation in Theano

Symbolic graph builders

Theano, TensorFlow, CNTK

You are limited to symbolic graph building, with the mini-language

For example, instead of this in pure Python (for A^k):

```
result = 1
for i in xrange(k):
  result = result * A
```

You build this symbolic graph:

```
import theano
import theano.tensor as T

k = T.iscalar("k")
A = T.vector("A")

# Symbolic description of a loop
result, updates = theano.scan(fn=lambda prior_result, A: prior_result * A,
                              outputs_info=T.ones_like(A),
                              non_sequences=A,
                              n_steps=k)
final_result = result[-1]

# compiled function that returns A**k
power = theano.function(inputs=[A,k], outputs=final_result, updates=updates)
```

Dynamic graph builders (general-purpose AD)

- Use general-purpose **automatic differentiation** operator overloading
- Implement models as regular programs, with full support for control flow, branching, loops, recursion, procedure calls

Dynamic graph builders (general-purpose AD)

autograd (Python) by Harvard Intelligent Probabilistic Systems Group
https://github.com/HIPS/autograd

- torch-autograd by Twitter Cortex
https://github.com/twitter/torch-autograd

- PyTorch
http://pytorch.org/

a general-purpose AD system that allows you to **implement models as regular Python programs** (more on this in the exercise session)

```
result = Variable(Tensor([1]))
for i in range(k):
    result = result * A
```

```
result.backward()
print(A.grad.data)
```

Summary

Summary

- Neural networks + data + gradient descent = deep learning
- General-purpose AD is the future of deep learning
- More distance to cover:
  - Implementations better than operator overloading exist in AD literature (source transformation) but not in machine learning
  - Forward AD is not currently present in any mainstream machine learning framework
  - Nesting of forward and reverse AD enables efficient higher-order derivatives such as Hessian-vector products

Thank you!

CSCS-ICS-DADSi Summer School
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UNIVERSITY OF
OXFORD

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