Foundations of Artificial Intelligence

14. Deep Learning

An Overview

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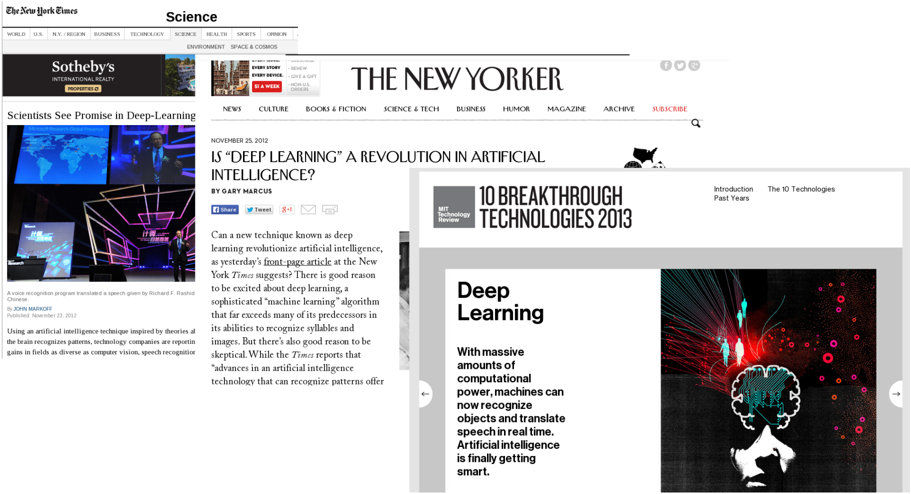
Albert-Ludwigs-Universität Freiburg

July 11, 2018

Motivation: Deep Learning in the News



The New York Times

Science

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ENVIRONMENT SPACE & COSMOS

Scientists See Promise in Deep-Learning

A voice recognition program translated a speech given by Richard F. Rashid Chinese.

By JOHN MARKOFF

Published: November 23, 2012

Using an artificial intelligence technique inspired by theories al the brain recognizes patterns, technology companies are reportin gains in fields as diverse as computer vision, speech recognitior

THE NEW YORKER

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NOVEMBER 25, 2012

IS "DEEP LEARNING" A REVOLUTION IN ARTIFICIAL INTELLIGENCE?

BY GARY MARCUS

Can a new technique known as deep learning revolutionize artificial intelligence, as yesterday's front-page article at the New York *Times* suggests? There is good reason to be excited about deep learning, a sophisticated "machine learning" algorithm that far exceeds many of its predecessors in its abilities to recognize syllables and images. But there's also good reason to be skeptical. While the *Times* reports that "advances in an artificial intelligence technology that can recognize patterns offer

MIT Technology Review

10 BREAKTHROUGH TECHNOLOGIES 2013

Introduction The 10 Technologies

Past Years

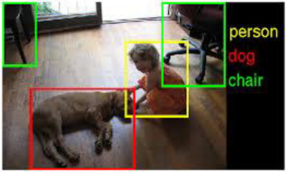
Deep Learning

With massive amounts of computational power, machines can now recognize objects and translate speech in real time. Artificial intelligence is finally getting smart.

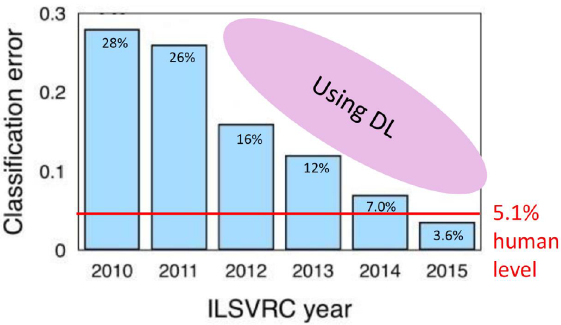
Motivation: Why is Deep Learning so Popular?

- Excellent empirical results, e.g., in computer vision

Object recognition



Self-driving cars



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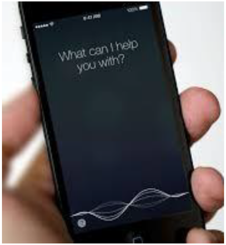
Speech recognition



skype™

Auto-Translator

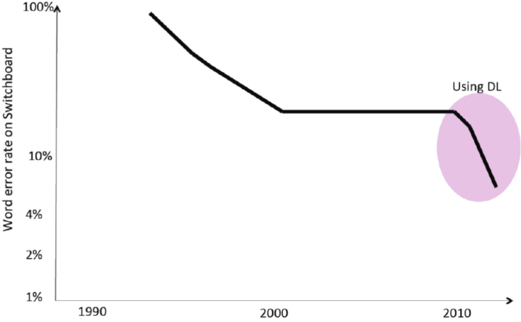


Image credit: Yoshua Bengio (data from Microsoft speech group)

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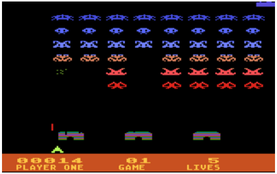
- Excellent empirical results, e.g., in reasoning in games

  - Superhuman performance in playing Atari games
    [Mnih et al, Nature 2015]



  - Beating the world's best Go player
    [Silver et al, Nature 2016]

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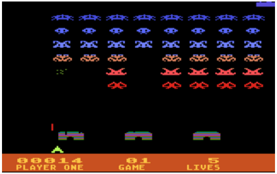

    - Beating the world's best Go player [Silver et al, Nature 2016]

- More reasons for the popularity of deep learning throughout

Lecture Overview

Lecture Overview

Some definitions

Representation learning

"a set of methods that allows a machine to be fed with raw data and to automatically discover the representations needed for detection or classification"

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"a set of methods that allows a machine to be fed with raw data and to automatically discover the representations needed for detection or classification"

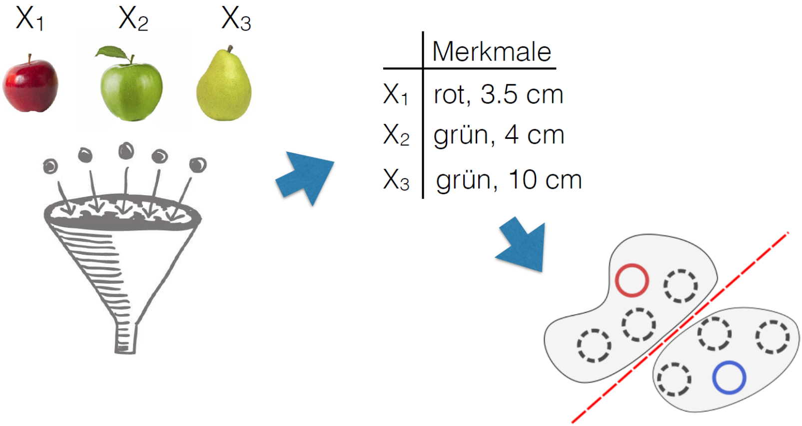
Deep learning

"representation learning methods with multiple levels of representation, obtained by composing simple but nonlinear modules that each transform the representation at one level into a [...] higher, slightly more abstract (one)"

(LeCun et al., 2015)

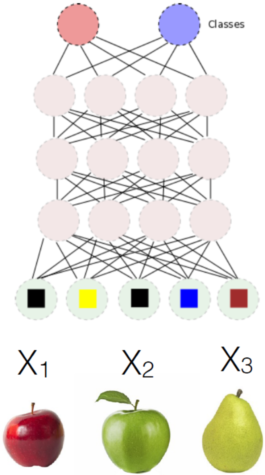
Standard Machine Learning Pipeline

- Standard machine learning algorithms are based on high-level attributes or features of the data
- E.g., the binary attributes we used for decisions trees
- This requires (often substantial) feature engineering

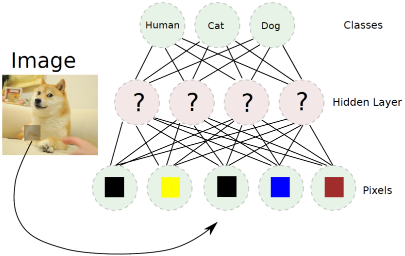


Representation Learning Pipeline

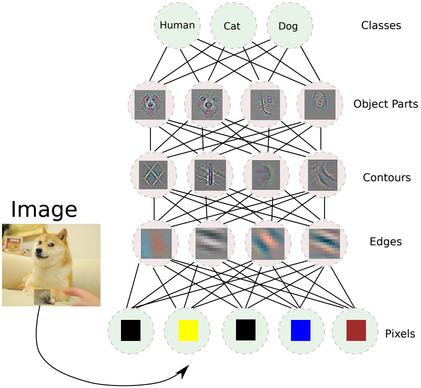
- Jointly learn features and classifier, directly from raw data
- This is also referrred to as end-to-end learning



Shallow vs. Deep Learning

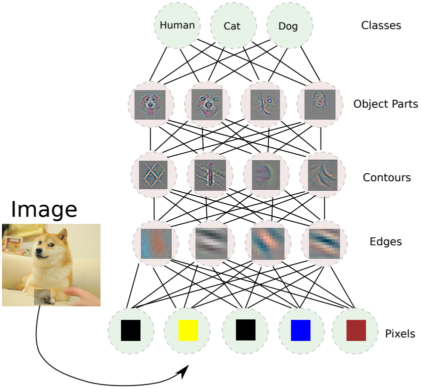


Shallow vs. Deep Learning



- Deep Learning: learning a hierarchy of representations that build on each other, from simple to complex

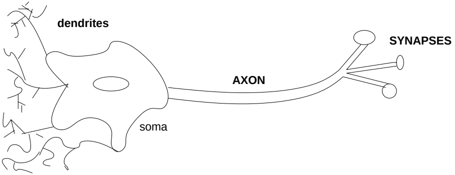
Shallow vs. Deep Learning



- Deep Learning: learning a hierarchy of representations that build on each other, from simple to complex
- Quintessential deep learning model: Multilayer Perceptrons

Biological Inspiration of Artificial Neural Networks

- Dendrites input information to the cell
- Neuron fires (has action potential) if a certain threshold for the voltage is exceeded
- Output of information by axon
- The axon is connected to dentrites of other cells via synapses
- Learning: adaptation of the synapse's efficiency, its synaptical weight



A Very Brief History of Neural Networks

- Neural networks have a long history
  - 1942: artificial neurons (McCulloch/Pitts)
  - 1958/1969: perceptron (Rosenblatt; Minsky/Papert)
  - 1986: multilayer perceptrons and backpropagation (Rumelhart)
  - 1989: convolutional neural networks (LeCun)

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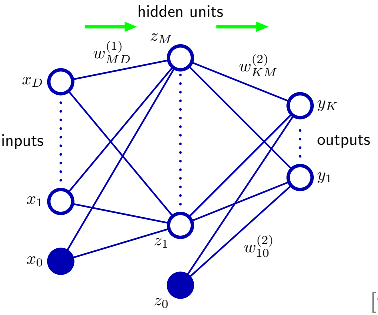
- Alternative theoretically motivated methods outperformed NNs
  - Exaggeraged expectations: "It works like the brain" (No, it does not!)
- Why the sudden success of neural networks in the last 5 years?
  - Data: Availability of massive amounts of labelled data
  - Compute power: Ability to train very large neural networks on GPUs
  - Methodological advances: many since first renewed popularization

Lecture Overview

Multilayer Perceptrons



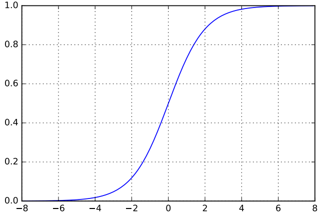
[figure from Bishop, Ch. 5]

- Network is organized in layers
  - Outputs of k-th layer serve as inputs of $k+1$th layer
- Each layer k only does quite simple computations:
  - Linear function of previous layer's outputs $\mathbf{z}_{k-1}$: $\mathbf{a}_k = \mathbf{W}_k\mathbf{z}_{k-1} + \mathbf{b}_k$
  - Nonlinear transformation $\mathbf{z}_k = h_k(\mathbf{a}_k)$ through activation function h_k

Activation Functions - Examples

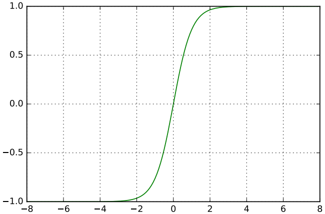
Logistic sigmoid activation function:

$$h_{logistic}(a) = \frac{1}{1 + \exp(-a)}$$



Logistic hyperbolic tangent activation function:

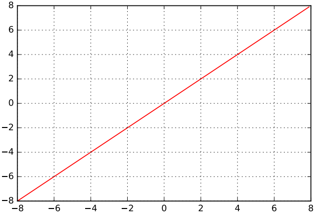
$$h_{tanh}(a) = \tanh(a)$$
$$= \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}\}$$



Activation Functions - Examples (cont.)

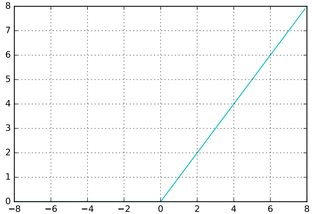
Linear activation function:

$$h_{linear}(a) = a$$



Rectified Linear (ReLU) activation function:

$$h_{relu}(a) = \max(0, a)$$



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Depending on the task, typically:

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- for multiclass classification: K output neurons and softmax activation

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$\rightarrow$ so for the complete output layer:

$$\hat{\mathbf{y}}(\mathbf{x}, \mathbf{w}) = \begin{bmatrix} p(y_1 = 1|\mathbf{x}) \\ p(y_2 = 1|\mathbf{x}) \\ \vdots \\ p(y_K = 1|\mathbf{x}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{K} \exp((\mathbf{a})_j)} \exp(\mathbf{a})$$

Loss function to be minimized

- Consider binary classification task using a single output unit with logistic sigmoid activation function:

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$$\begin{aligned} p(y_n = 1 \mid \mathbf{x}_n, \mathbf{w}) &= \hat{y}(\mathbf{x}_n, \mathbf{w}) \\ p(y_n = 0 \mid \mathbf{x}_n, \mathbf{w}) &= 1 - \hat{y}(\mathbf{x}_n, \mathbf{w}) \end{aligned}$$

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- Rewritten:

$$p(y_n \mid \mathbf{x}_n, \mathbf{w}) = \hat{y}(\mathbf{x}_n, \mathbf{w})^{y_n} \{1 - \hat{y}(\mathbf{x}_n, \mathbf{w})\}^{1-y_n}$$

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- Min. negative log likelihood of this distribution (aka cross entropy):

$$L(\mathbf{w}) = -\sum_{n=1}^{N} \{y_n \ln \hat{y}_n + (1 - y_n) \ln(1 - \hat{y}_n)\}$$

Loss function to be minimized

- For multiclass classification, use generalization of cross-entropy error:

$$L(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} y_{kn} \ln \hat{y}_k(\mathbf{x}_n, \mathbf{w})$$

- For regression, e.g., use squared error function:

$$L(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{\hat{y}(\mathbf{x}_n, \mathbf{w}) - y_n\}^2$$

Optimizing a loss / error function

- Given training data $\mathcal{D} = \langle(\mathbf{x}_i, y_i)\rangle_{i=1}^{N}$ and topology of an MLP
- Task: adapt weights w to minimize the loss:

$$\underset{\mathbf{w}}{minimize}\ L(\mathbf{w}; \mathcal{D})$$

- Interpret L just as a mathematical function depending on $\mathbf{w}$ and forget about its semantics, then we are faced with a problem of mathematical optimization

Lecture Overview

Optimization theory

- Discusses mathematical problems of the form:

$$\underset{\mathbf{u}}{minimize}\ f(\mathbf{u}),$$

where $\vec{u}$ is any vector of suitable size.

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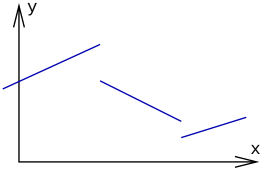
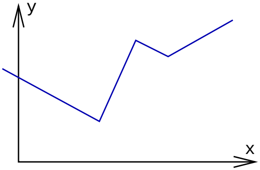
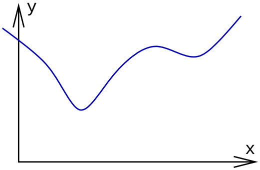
- Simplification: here, we only consider functions f which are continuous and differentiable



non continuous function
(disrupted)



continuous, non differentiable function (folded)



differentiable function
(smooth)

Optimization theory (cont.)

- A global minimum $\vec{u}^*$ is a point such that:

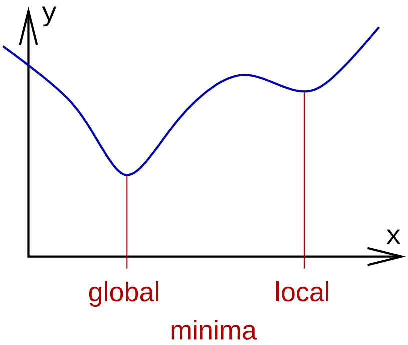
$$f(\mathbf{u}^*) \leq f(\mathbf{u})$$

  for all $\mathbf{u}$.

- A local minimum $\mathbf{u}^+$ is a point such that exist $r > 0$ with

$$f(\mathbf{u}^+) \leq f(\mathbf{u})$$

  for all points $\vec{u}$ with $||\vec{u} - \vec{u}^+|| < r$



Optimization theory (cont.)

- Analytical way to find a minimum:
  For a local minimum $\mathbf{u}^+$, the gradient of f becomes zero:

$$\frac{\partial f}{\partial u_i}(\mathbf{u}^+) = 0 \quad \text{for all } i$$

  Hence, calculating all partial derivatives and looking for zeros is a good idea

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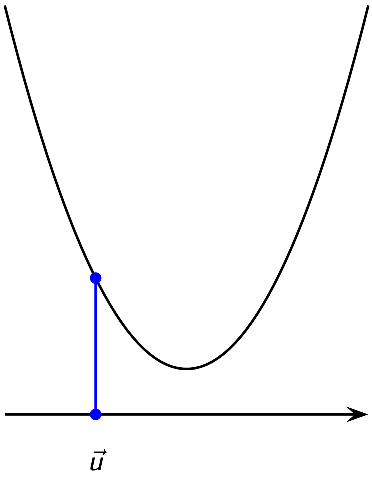
- But: for neural networks, we can't write down a solution for the minimization problem in closed form
  - even though $\frac{\partial f}{\partial u_i} = 0$ holds at (local) solution points

  $\rightarrow$ need to resort to iterative methods

Optimization theory (cont.)

- Numerical way to find a minimum, searching:
  assume we start at point $\mathbf{u}$.

  Which is the best direction to search for a point $\mathbf{v}$ with $f(\mathbf{v}) < f(\mathbf{u})$?



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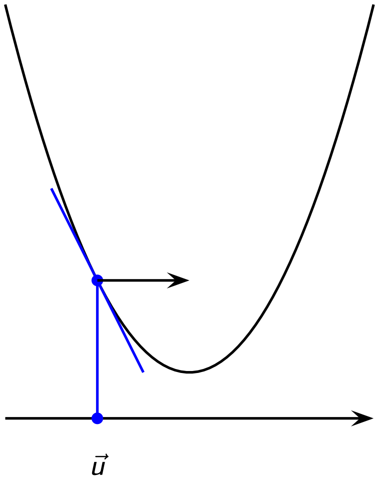

slope is negative (descending), go right!

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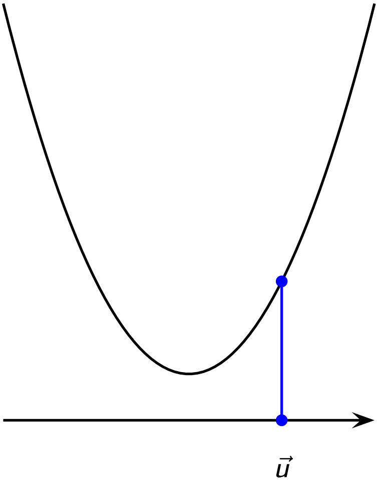

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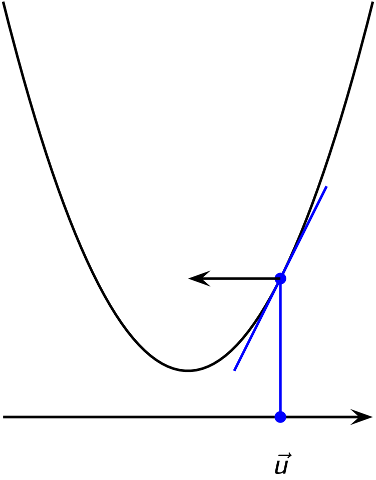

slope is positive (ascending), go left!

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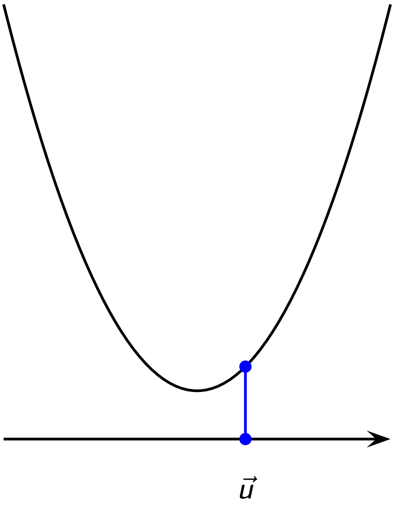

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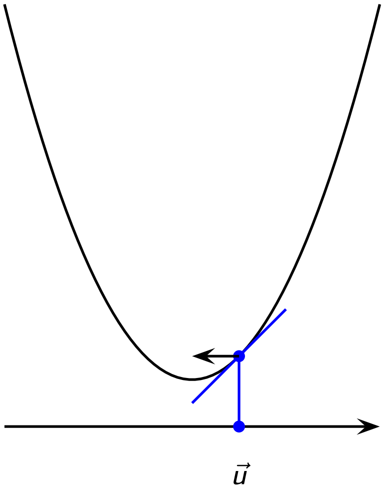

slope is small, small step!

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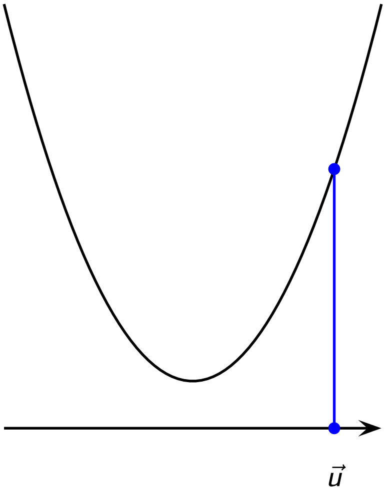

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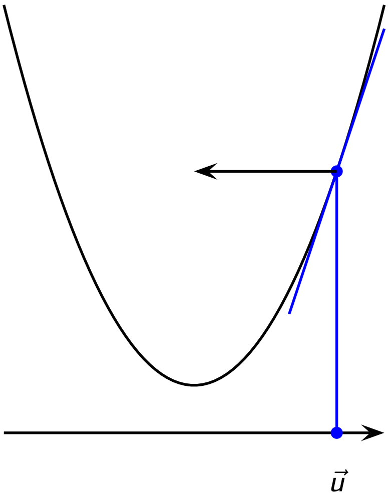

slope is large, large step!

Optimization theory (cont.)

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  Which is the best direction to search for a point $\mathbf{v}$ with $f(\mathbf{v}) < f(\mathbf{u})$?

  Which is the best stepwidth?
- general principle:

$$v_i \leftarrow u_i - \epsilon \frac{\partial f}{\partial u_i}$$

$\epsilon > 0$ is called learning rate

Gradient descent

- Gradient descent approach:

Require: mathematical function f, learning rate $\epsilon > 0$
Ensure: returned vector is close to a local minimum of f

1: choose an initial point $\mathbf{u}$
2: **while** $||\nabla_{\mathbf{u}} f(\mathbf{u})||$ not close to 0 **do**
3: $\quad \mathbf{u} \leftarrow \mathbf{u} - \epsilon \cdot \nabla_{\mathbf{u}} f(\mathbf{u})$
4: **end while**
5: **return** $\mathbf{u}$

- Note: $\nabla_{\mathbf{u}} f := [\frac{\partial f}{\partial u_1}, \ldots, \frac{\partial f}{\partial u_K}]$ for K-dimensionsal $\mathbf{u}$

Calculating partial derivatives

- Our typical loss functions are defined across data points:

$$L(\mathbf{w}) = \sum_{n=1}^{N} L_n(\mathbf{w}) = L(f(\mathbf{x_n};\mathbf{w}), y_n)$$

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- We can compute their partial derivatives as a sum over data points:

$$\frac{\partial L}{\partial w_j} = \sum_{n=1}^{N} \frac{\partial L_n}{\partial w_j}$$

- The method of backpropagation makes consistent use of the chain rule of calculus to compute the partial derivatives $\frac{\partial L_n}{\partial w_j}$ w.r.t. each network weight w_j, re-using previously computed results
  - Backpropagation is not covered here, but, e.g., in ML lecture

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  - But using more data has diminishing returns w.r.t reduction in error
  - Usually faster progress by updating more often based on cheaper, less accurate estimates of the gradient
- Common approach in practice: compute gradients over mini-batches
  - Mini-batch: small subset of the training data
  - Today, this is commonly called stochastic gradient descent (SGD)

Stochastic gradient descent

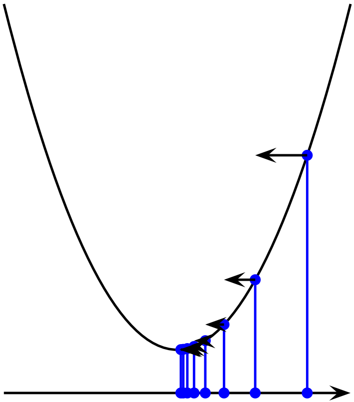
- Stochastic gradient descent (SGD)

Require: mathematical function f, learning rate $\epsilon > 0$
Ensure: returned vector is close to a local minimum of f

choose an initial point $\mathbf{w}$
while stopping criterion not met **do**
    Sample a minibatch of m examples $\mathbf{x^{(1)}}, \ldots, \mathbf{x^{(m)}}$ with corresponding targets $\mathbf{y}^{(i)}$ from the training set
    Compute gradient $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\mathbf{w}} \sum_{i=1}^{m} L(f(\mathbf{x^{(i)}}; \mathbf{w}), \mathbf{y^{(i)}})$
    Update parameter: $\mathbf{w} \leftarrow \mathbf{w} - \epsilon \cdot \mathbf{g}$
end while
return $\mathbf{w}$

Problems with suboptimal choices for learning rate

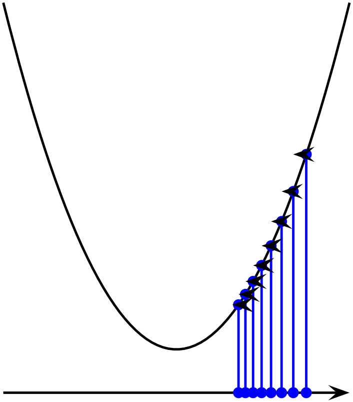
- choice of ϵ
  1. case small ϵ: convergence



Problems with suboptimal choices for learning rate

- choice of ϵ

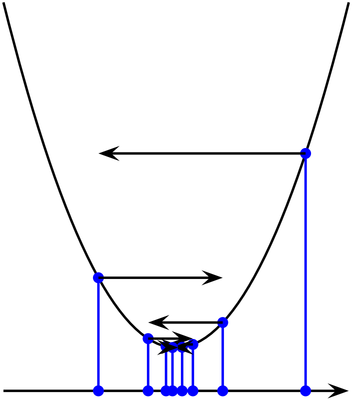
  2. case very small ϵ: convergence, but it may take very long



Problems with suboptimal choices for learning rate

- choice of ϵ

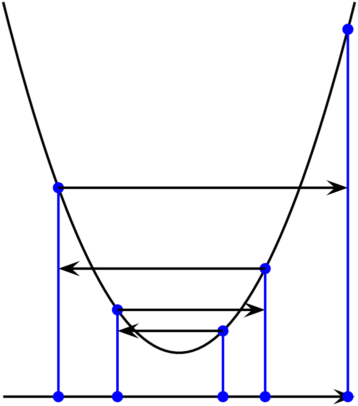
  3. case medium size ϵ: convergence



Problems with suboptimal choices for learning rate

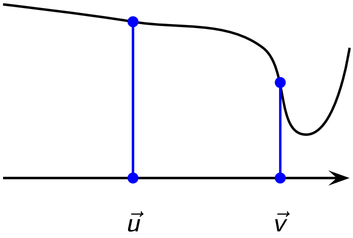
- choice of ϵ

  4. case large ϵ: divergence



Other reasons for problems with gradient descent

- flat spots and steep valleys:
  need larger ϵ in $\vec{u}$ to jump over the uninteresting flat area but need smaller ϵ in $\vec{v}$ to meet the minimum



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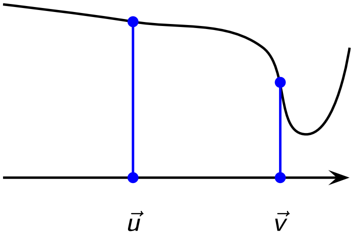
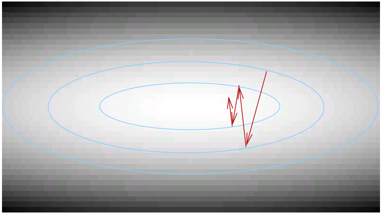
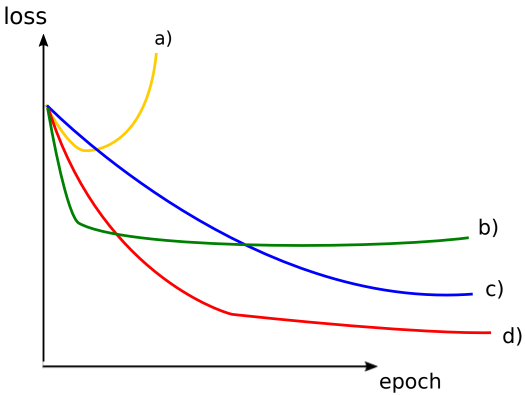


- zig-zagging:
  in higher dimensions: ϵ is not appropriate for all dimensions



Learning rate quizz

Which curve denotes low, high, very high, and good learning rate?



Gradient descent – Conclusion

- Pure gradient descent is a nice framework
- In practice, stochastic gradient descent is used
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Heuristics to overcome problems of gradient descent:

- Gradient descent with momentum
- Individual learning rates for each dimension
- Adaptive learning rates
- Decoupling steplength from partial derivates

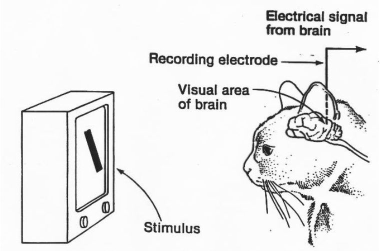
Lecture Overview

Lecture Overview

Historical context and inspiration from Neuroscience

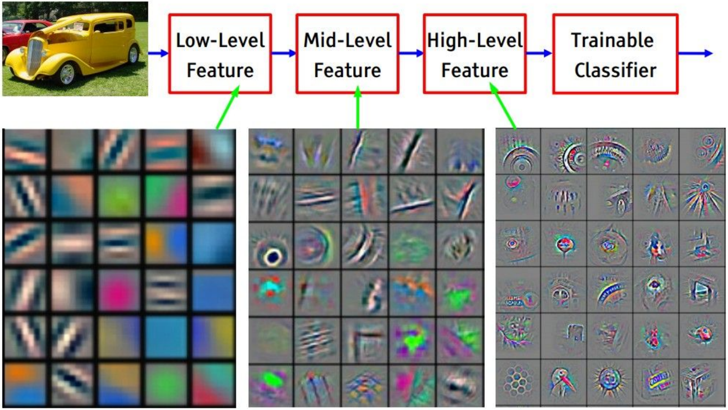
Hubel & Wiesel (Nobel prize 1981) found in several studies in the 1950s and 1960s:

- Visual cortex has feature detectors (e.g., cells with preference for edges with specific orientation)
  - edge location did not matter
- Simple cells as local feature detectors
- Complex cells pool responses of simple cells
- There is a feature hierarchy



Learned feature hierarchy

[From recent Yann LeCun slides]



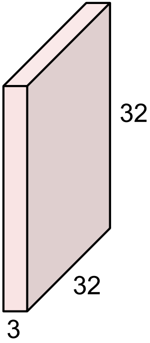
Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

[slide credit: Andrej Karpathy]

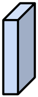
Convolutions illustrated

Filters always extend the full depth of the input volume

32x32x3 image



5x5x3 filter



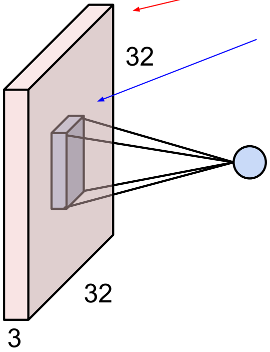
Convolve the filter with the image i.e. "slide over the image spatially, computing dot products"

[slide credit: Andrej Karpathy]

Convolutions illustrated (cont.)

32x32x3 image

5x5x3 filter w

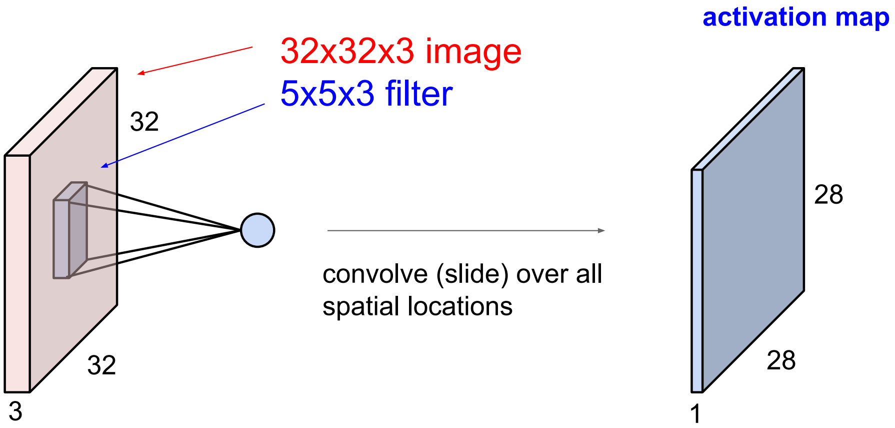


1 number:
the result of taking a dot product between the filter and a small 5x5x3 chunk of the image (i.e. 5*5*3 = 75-dimensional dot product + bias)

$$w^T x + b$$

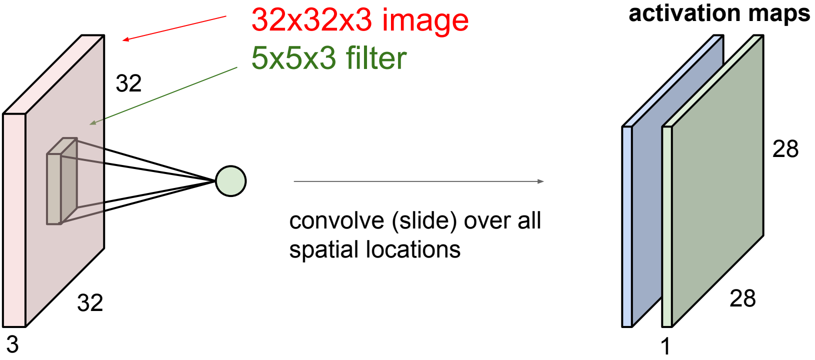
[slide credit: Andrej Karpathy]

Convolutions illustrated (cont.)



[slide credit: Andrej Karpathy]

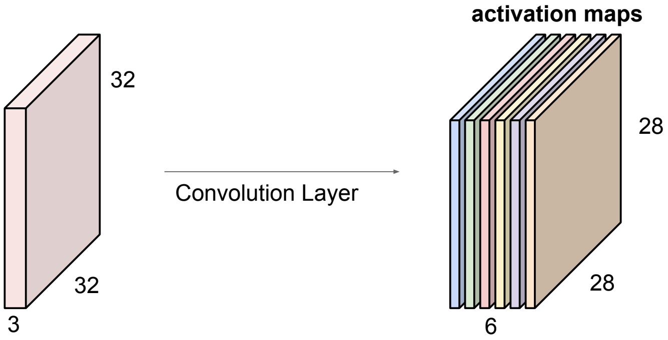
consider a second, green filter



[slide credit: Andrej Karpathy]

Convolutions – several filters

For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:

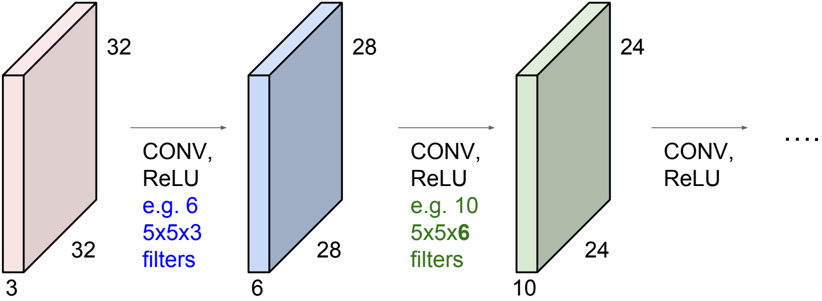


We stack these up to get a "new image" of size 28x28x6!

[slide credit: Andrej Karpathy]

Stacking several convolutional layers

Convolutional layers stacked in a ConvNet



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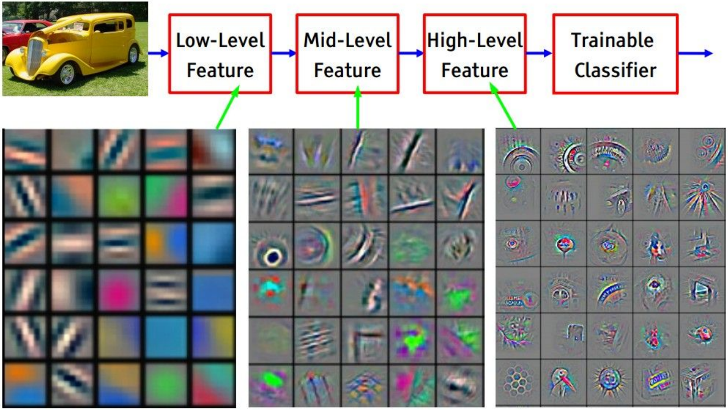

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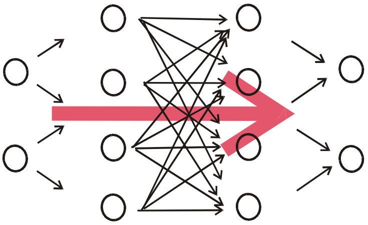
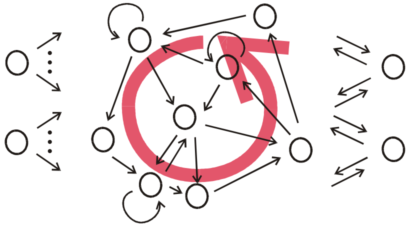
Lecture Overview

Feedforward vs Recurrent Neural Networks





[Source: Jaeger, 2001]

Recurrent Neural Networks (RNNs)

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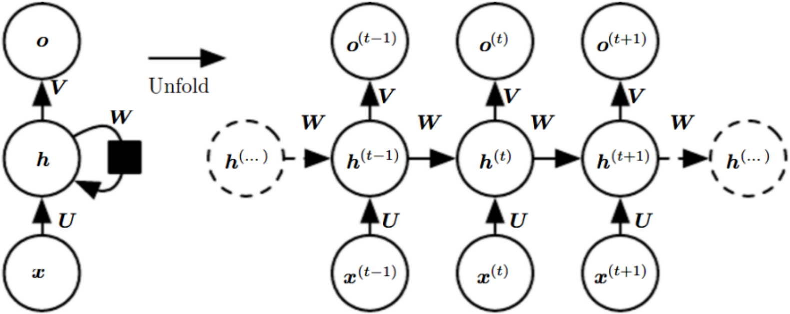
- Implement dynamical systems rather than function mappings, and can approximate any dynamical system with arbitrary precision
- They are Turing-complete [Siegelmann and Sontag, 1991]

Abstract schematic

With fully connected hidden layer:



[Goodfellow et al'2016]

one to many

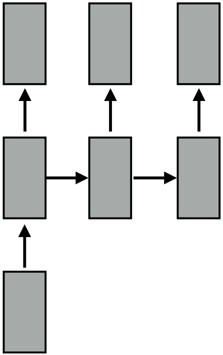
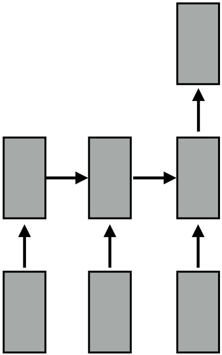


image caption generation

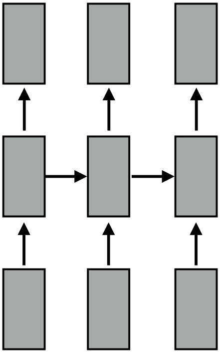
many to one



temporal classification

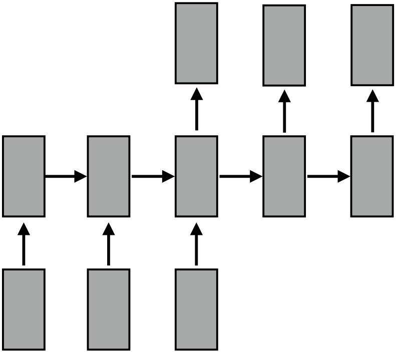
Sequence to sequence mapping (cont.)

many to many



video
frame labeling

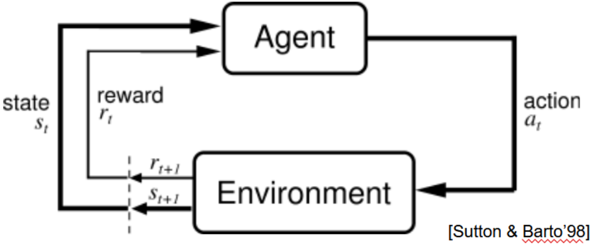
many to many



automatic
translation

Lecture Overview

Reinforcement Learning



- Finding optimal policies for MDPs
- Reminder: states $s \in S$, actions $a \in A$, transition model T, rewards r
- Policy: complete mapping $\pi : S \rightarrow A$ that specifies for each state s which action $\pi(s)$ to take

Deep Reinforcement Learning

- Policy-based deep RL
  - Represent policy $\pi : S \rightarrow A$ as a deep neural network with weights w
  - Evaluate w by "rolling out" the policy defined by w
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  - Examples: AlphaGo & modern Atari agents

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→ Use deep neural networks to represent policy / value function / model

Lecture Overview

An Exciting Approach to AI: Learning as an Alternative to Traditional Programming

- We don't understand how the human brain solves certain problems
  - Face recognition
  - Speech recognition
  - Playing Atari games
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- We can nevertheless learn these tasks from data/experience
- If the task changes, we simply re-train
- We can construct computer systems that are too complex for us to understand anymore ourselves...
  - E.g., deep neural networks have millions of weights.
  - E.g., AlphaGo, the system that beat world champion Lee Sedol
    - + David Silver, lead author of AlphaGo cannot say why a move is good
    - + Paraphrased: "You would have to ask a Go expert."

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- Allows end-to-end learning
  - no more need for many complicated subsystems
  - e.g., dramatically simplified Google's translation
- Very versatile/flexible
  - easy to combine building blocks
  - allows supervised, unsupervised, and reinforcement learning

Lots of Work on Deep Learning in Freiburg

- Computer Vision (Thomas Brox)
  - Images, video
- Robotics (Wolfram Burgard)
  - Navigation, grasping, object recognition
- Neurorobotics (Joschka Boedecker)
  - Robotic control
- Machine Learning (Frank Hutter)
  - Optimization of deep nets, learning to learn
- Neuroscience (Tonio Ball, Michael Tangermann, and others)
  - EEG data and other applications from BrainLinks-BrainTools

→ Details when the individual groups present their research

Summary by learning goals

Having heard this lecture, you can now . . .

- Explain the terms representation learning and deep learning
- Describe the main principles behind MLPs
- Describe how neural networks are optimized in practice
- On a high level, describe
  - Convolutional Neural Networks
  - Recurrent Neural Networks
  - Deep Reinforcement Learning