Introduction to Machine Learning (67577)
Lecture 10

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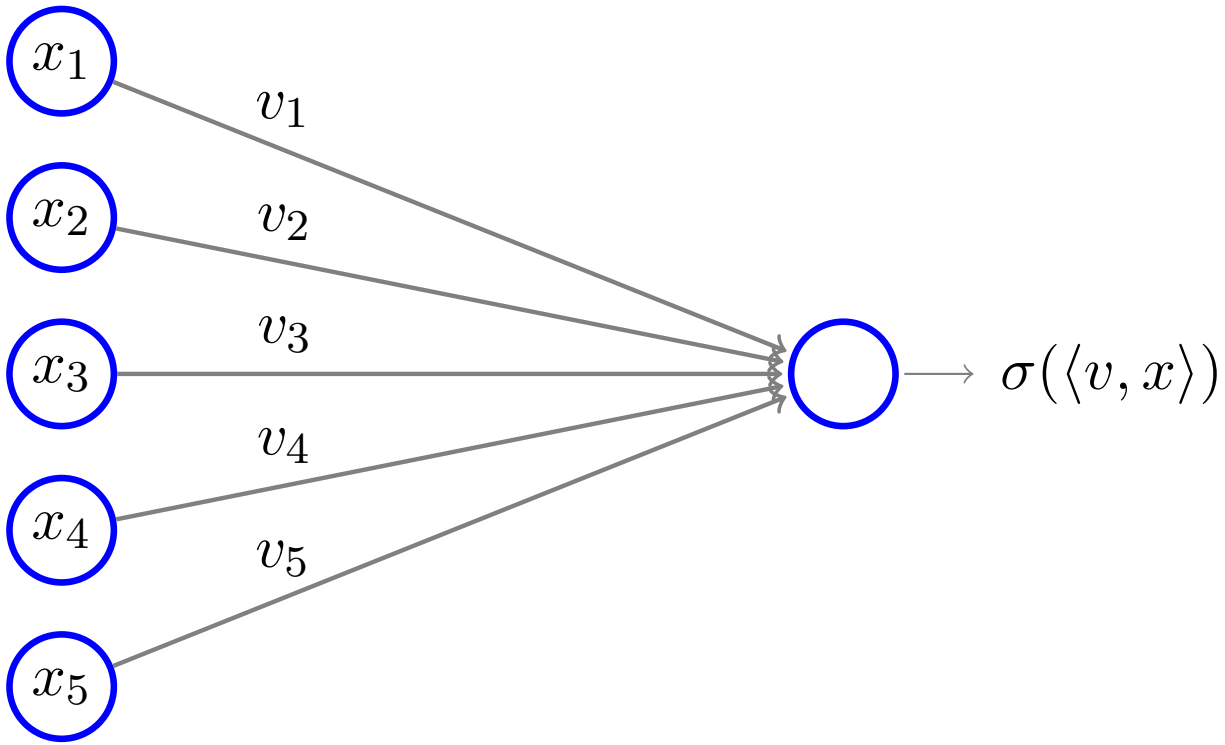
Neural Networks

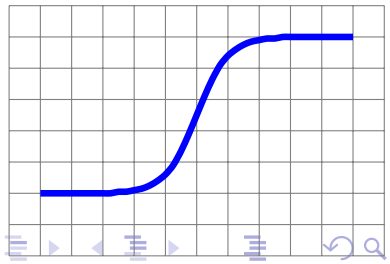
Outline

A Single Artificial Neuron

- A single neuron is a function of the form $\mathbf{x} \mapsto \sigma(\langle \mathbf{v}, \mathbf{x} \rangle)$, where $\sigma : \mathbb{R} \to \mathbb{R}$ is called the activation function of the neuron



- E.g., σ is a sigmoidal function



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- weights: $w : E \to \mathbb{R}$
- Calculation using breadth-first-search (BFS), where each neuron (node) receives as input:

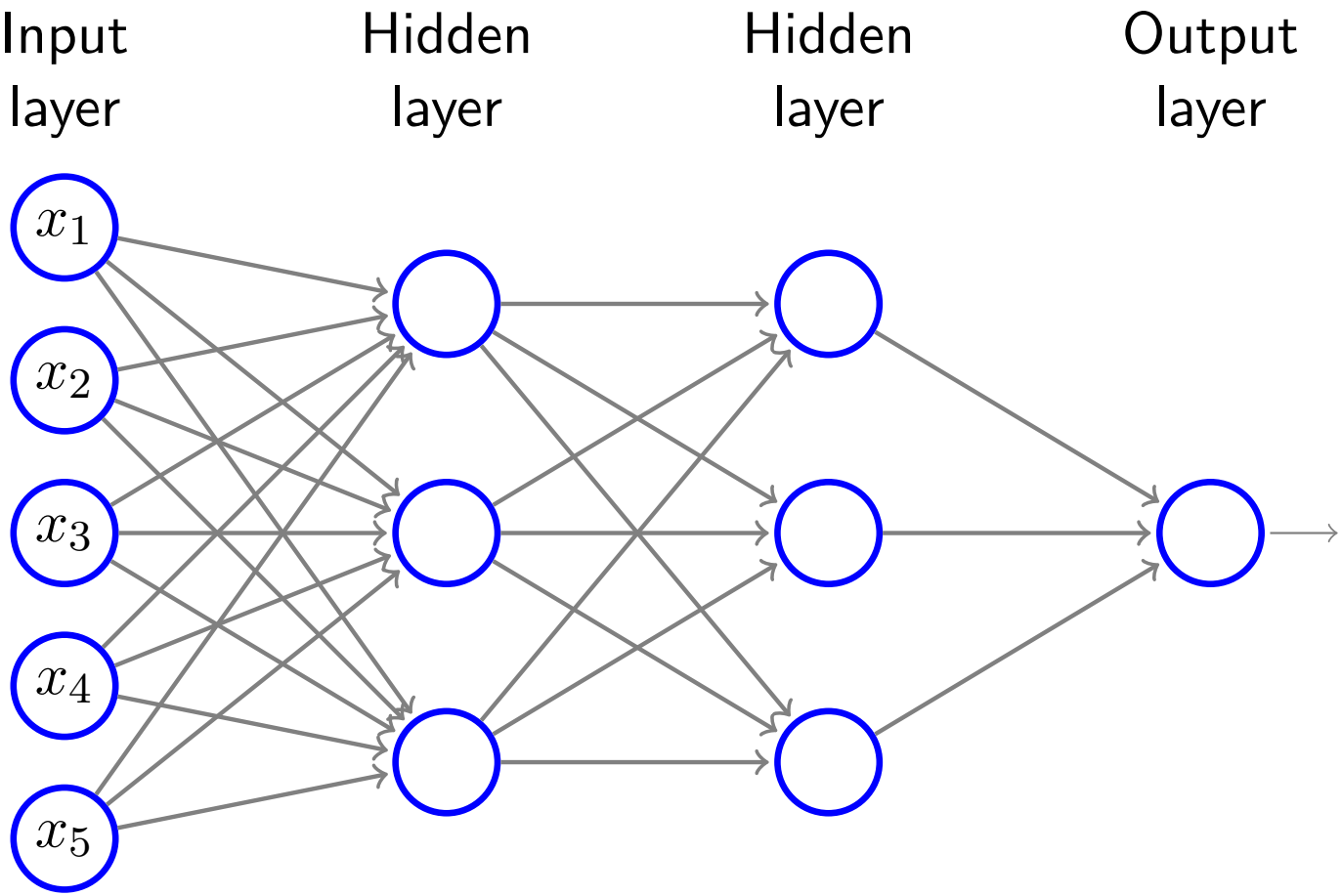
$$a[v] = \sum_{u \to v \in E} w[u \to v] o[u]$$

and output

$$o[v] = \sigma(a[v])$$

Multilayer Neural Networks

- Neurons are organized in layers: $V = \cup_{t=0}^{T} V_t$, and edges are only between adjacent layers
- Example of a multilayer neural network of depth 3 and size 6



Neural Networks as a Hypothesis Class

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- We can now study
  estimation error (sample complexity)
  approximation error (expressivenss)
  optimization error (computational complexity)

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- Representation trick: In practice, we only care about networks where each weight is represented using $O(1)$ bits, and therefore the VC dimension of such networks is $O(|E|)$, no matter what σ is
- We can further decrease the sample complexity by many kinds of regularization functions (this is left for an advanced course)

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- What type of functions can be implemented by networks of small size ?

What can we express with neural networks ?

- Theorem: Let $T : \mathbb{N} \to \mathbb{N}$ and for every n, let $\mathcal{F}_n$ be the set of functions that can be implemented using a Turing machine using runtime of at most $T(n)$. Then, there exist constants $b, c \in \mathbb{R}_+$ such that for every n, there is a graph (V_n, E_n) of size at most $c\,T(n)^2 + b$ such that $\mathcal{H}_{V_n,E_n,\text{sign}}$ contains $\mathcal{F}_n$.

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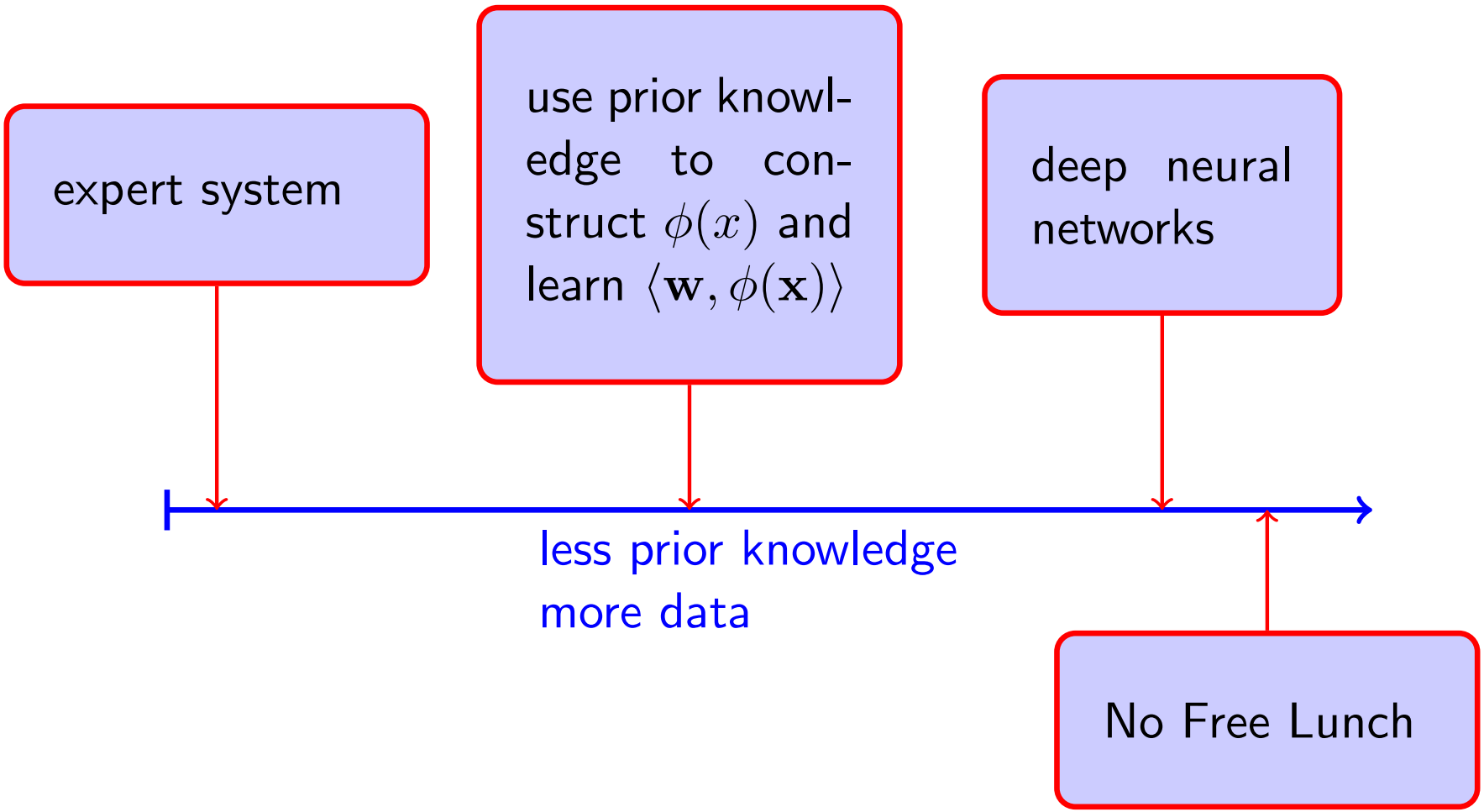
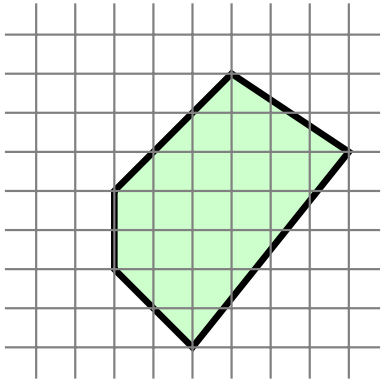
- Conclusion: A very weak notion of prior knowledge suffices — if we only care about functions that can be implemented in time $T(n)$, we can use neural networks of size $O(T(n)^2)$, and the sample complexity is also bounded by $O(T(n)^2)$!

The ultimate hypothesis class



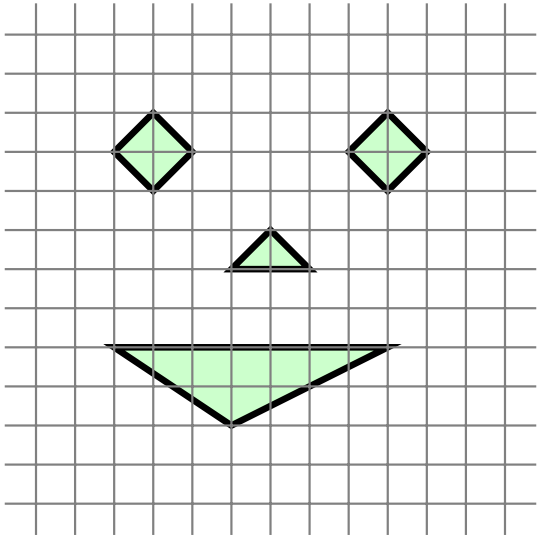
Geometric Intuition

- 2 layer networks can express intersection of halfspaces



Geometric Intuition

- 3 layer networks can express unions of intersection of halfspaces



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Runtime of learning neural networks

ERM problem:

$$\mathrm{ERM}(S) = \operatorname*{argmin}_{h \in \mathcal{H}_{V,E,\sigma}} L_S(h) = \operatorname*{argmin}_{w} L_S(h_{V,E,\sigma,w})$$

- Theorem: It is NP hard to implement the ERM rule with respect to $\mathcal{H}_{V,E,\mathrm{sign}}$ even for networks with a single hidden layer that contain just 4 neurons in the hidden layer.

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- But, maybe ERM is hard but some improper algorithm works ?
- Theorem: Under some average case complexity assumption, it is hard to learn neural networks of depth 2 and size $\omega(\log(d))$ even improperly

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- Not convex, no guarantees, can take a long time, but:
  - Often still works fine, finds a good solution
  - Easier than optimizing over Python programs ...

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where:
μ_t is momentum parameter (e.g. $\mu_t = 0.9$ for all t)
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- It is left to show how to calculate the gradient

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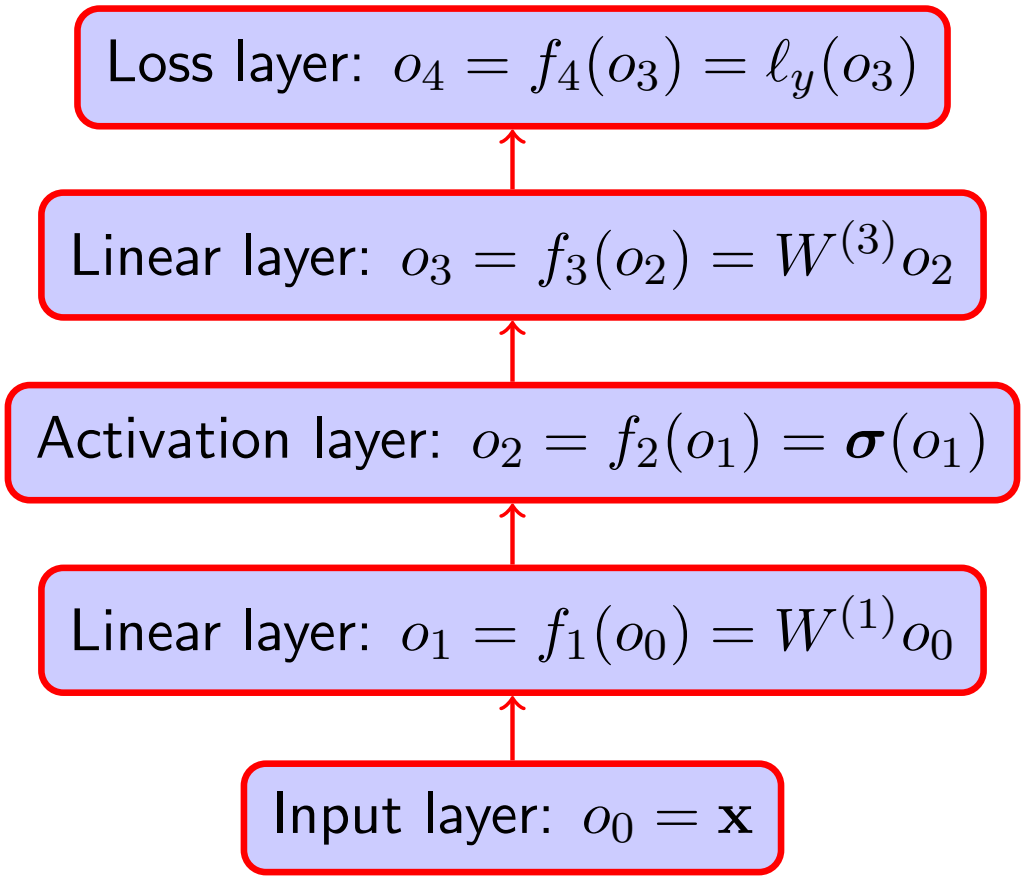
- Let $\ell_y : \mathbb{R}^k \to \mathbb{R}$ be the loss function given predictions $\boldsymbol{\theta} \in \mathbb{R}^k$ and label y.

Back-Propagation

It's convenient to describe the network as a sequence of simple layer functions:



Back-Propagation

- Can write $\ell(h_{\mathbf{w}}, (\mathbf{x}, y)) = (f_{T+1} \circ \ldots \circ f_3 \circ f_2 \circ f_1)(\mathbf{x})$
- Denote $F_t = f_{T+1} \circ \ldots \circ f_{t+1}$ and $\delta_t = J_{o_t}(F_t)$, then

$$\begin{aligned}\delta_t &= J_{o_t}(F_t) = J_{o_t}(F_{t-1} \circ f_{t+1}) \\ &= J_{f_{t+1}(o_t)}(F_{t-1}) J_{o_t}(f_{t+1}) = J_{o_{t+1}}(F_{t-1}) J_{o_t}(f_{t+1}) \\ &= \delta_{t+1} J_{o_t}(f_{t+1})\end{aligned}$$

- Note that

$$J_{o_t}(f_{t+1}) = \begin{cases} W^{(t+1)} & \text{for linear layer} \\ \mathrm{diag}(\boldsymbol{\sigma}'(o_t)) & \text{for activation layer} \end{cases}$$

- Using the chain rule again we obtain

$$J_{W^{(t)}}(\ell(h_{\mathbf{w}}, (\mathbf{x}, y))) = \delta_t o_{t-1}^\top$$

Back-Propagation: Pseudo-code

Forward:

- set $o_0 = \mathbf{x}$ and for $t = 1, 2, \ldots, T$ set

$$o_t = f_t(o_{t-1}) = \begin{cases} W^{(t)} o_{t-1} & \text{for linear layer} \\ \boldsymbol{\sigma}(o_{t-1}) & \text{for activation layer} \end{cases}$$

Backward:

- set $\delta_{T+1} = \nabla \ell_y(o_T)$ and for $t = T, T-1, \ldots, 1$ set

$$\delta_t = \delta_{t+1} J_{o_t}(f_{t+1}) = \delta_{t+1} \cdot \begin{cases} W^{(t+1)} & \text{for linear layer} \\ \mathrm{diag}(\boldsymbol{\sigma}'(o_t)) & \text{for activation layer} \end{cases}$$

- For linear layers, set the gradient w.r.t. the weights in $W^{(t)}$ to be the elements of the matrix $\delta_t o_{t-1}^\top$

Outline

Convolutional Networks

- Designed for computer vision problems
- Three main ideas:
  - Convolutional layers: use the same weights on all patches of the image
  - Pooling layers: decrease image resolution (good for translation invariance, for higher level features, and for runtime)
  - Contrast normalization layers: let neurons "compete" with adjacent neurons

Convolutional and Pooling

- Layers are organized with three dimensional arrays, corresponding to width, height, and channel. E.g., in the first layer, if we have an RGB image of width 40 and heigh 80 than we have three channels, each of which is a 40x80 image

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- Weight sharing: Each "neuron" maps the previous layer into a new image by convolving the previous layer with a "kernel"

$$o^+(h,w,c) = \sum_{c'} \sum_{i=1}^{k_h} \sum_{j=1}^{k_w} W(c,i,j,c') o(h+i, w+j, c') + b(c)$$

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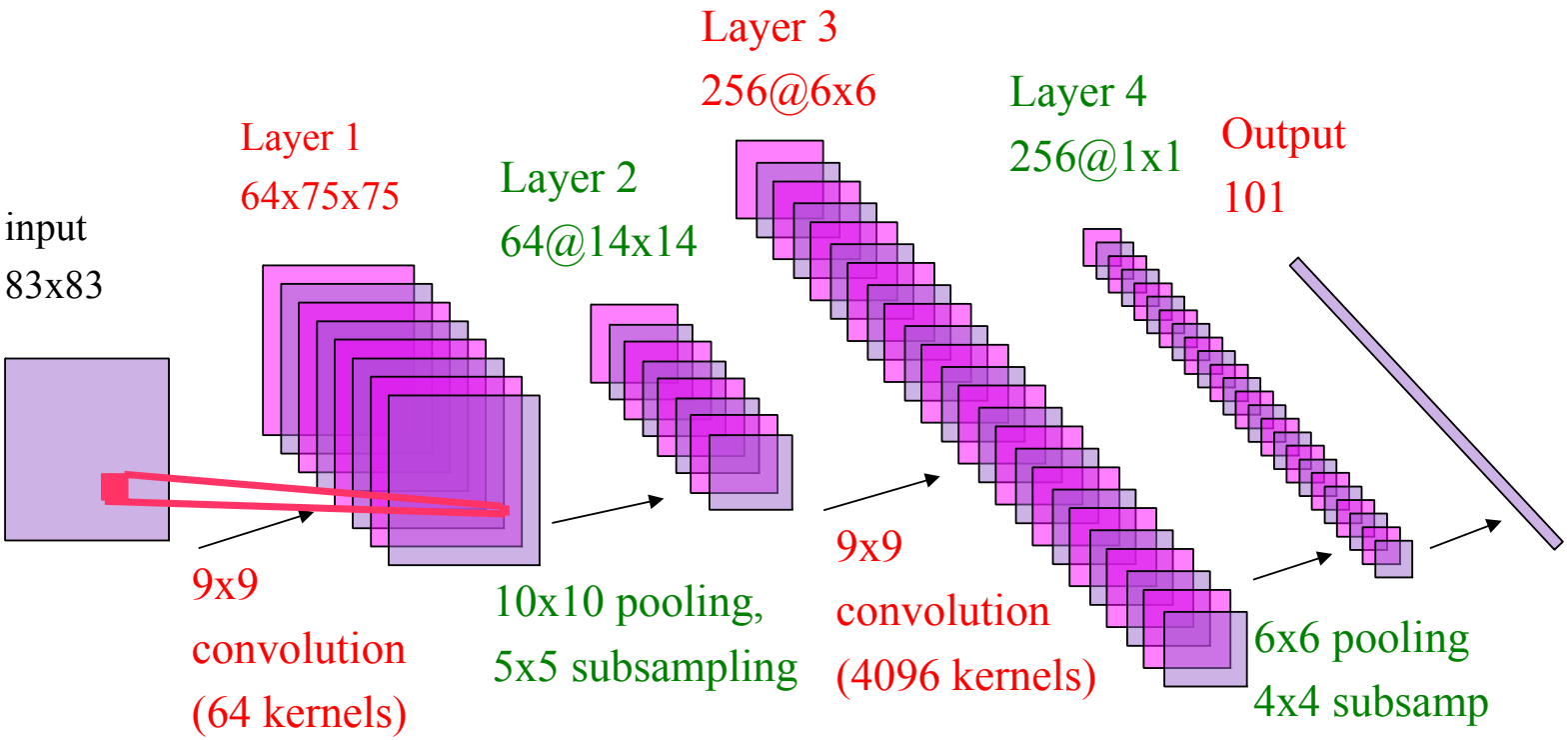
- A pooling layer reduces the resolution of each image in the previous layer

Convolutional Network (ConvNet)

Y LeCun
MA Ranzato



Neural Networks as Feature Learning

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- Shallow neurons corresponds to low level features while deep neurons correspond to high level features

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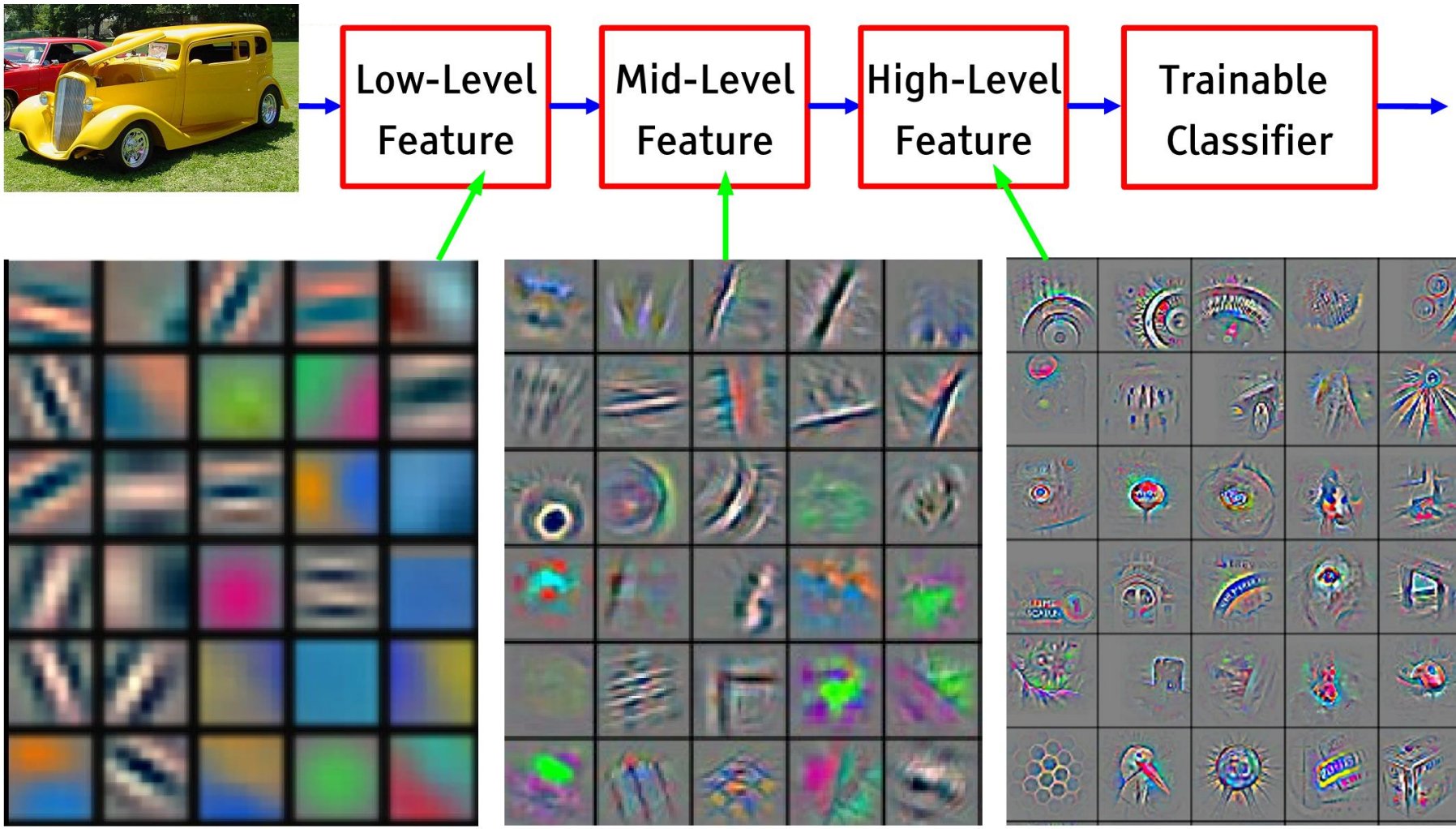

Taken from Yan LeCun's deep learning tutorial

Multiclass/Multitask/Feature Sharing/Representation learning

- Neurons in intermediate layers are shared by different tasks/classes
- Only last layer is specific to task/class
- Sometimes, network is optimized for certain classes, but the intermediate neurons are used as features for a new problem. This is called transfer learning. The last hidden layer can be thought of as a representation of the instance.

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- Very large networks: often, the number of parameters is very large, even much larger than the number of examples. This might lead to overfitting, which is (partially) avoided by many types of regularization

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- Training on GPU

Historical Remarks

- 1940s-70s:
  - Inspired by learning/modeling the brain (Pitts, Hebb, and others)
  - Perceptron Rule (Rosenblatt), Multilayer perceptron (Minksy and Papert)
  - Backpropagation (Werbos 1975)
- 1980s – early 1990s:
  - Practical Back-prop (Rumelhart, Hinton et al 1986) and SGD (Bottou)
  - Initial empirical success
- 1990s-2000s:
  - Lost favor to implicit linear methods: SVM, Boosting
- 2006 –:
  - Regain popularity because of unsupervised pre-training (Hinton, Bengio, LeCun, Ng, and others)
  - Computational advances and several new tricks allow training HUGE networks. Empirical success leads to renewed interest
  - 2012: Krizhevsky, Sustkever, Hinton: significant improvement of state-of-the-art on imagenet dataset (object recognition of 1000 classes), without unsupervised pre-training

Summary

- Neural networks can be used to construct the ultimate hypothesis class
- Computationally, it's impossible to train neural networks
- . . . but, empirically, it works reasonably well
- Leads to state-of-the-art on many real world problems
- Biggest theoretical question: When does it work and why ?