# TTIC 31230, Fundamentals of Deep Learning, Winter 2019

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# The Fundamental Equations of Deep Learning

## Early History

**1943**: McCullock and Pitts introduced the linear threshold "neuron".

**1962**: Rosenblatt applies a "Hebbian" learning rule. Novikoff proved the perceptron convergence theorem.

**1969**: Minsky and Papert publish the book *Perceptrons*.

The Perceptrons book greatly discourages work in artificial neural networks. Symbolic methods dominate AI research through the 1970s.

# 80s Renaissance

**1980**: Fukushima introduces the neocognitron (a form of CNN)

**1984**: Valiant defines PAC learnability and stimulates learning theory. Wins Turing Award in 2010.

**1985**: Hinton and Sejnowski introduce the Boltzman machine

**1986**: Rummelhart, Hinton and Williams demonstrate empirical success with backpropagation (itself dating back to 1961).

## 90s and 00s: Research In the Shadows

**1997**: Schmidhuber et al. introduce LSTMs

**1998**: LeCunn introduces convolutional neural networks (CNNs) (LeNet).

**2003**: Bengio introduces neural language modeling.

## Current Era

**2012**: Alexnet dominates the Imagenet computer vision challenge.

Google speech recognition converts to deep learning.

Both developments come out of Hinton's group in Toronto.

**2013**: Refinement of AlexNet continues to dramatically improve computer vision.

**2014**: Neural machine translation appears (Seq2Seq models).

Variational auto-encoders (VAEs) appear.

Graph networks for molecular property prediction appear.

Dramatic improvement in computer vision and speech recognition continues.

## Current Era

**2015**: Google converts to neural machine translation leading to dramatic improvements.

ResNet appears. This makes yet another dramatic improvement in computer vision.

Generative Adversarial Networks (GANs) appear.

**2016**: Alphago defeats Lee Sedol.

## Current Era

**2017**: AlphaZero learns both go and chess at super-human levels in a mater of hours entirely form self-play and advances computer go far beyond human abilities.

Unsupervised machine translation is demonstrated.

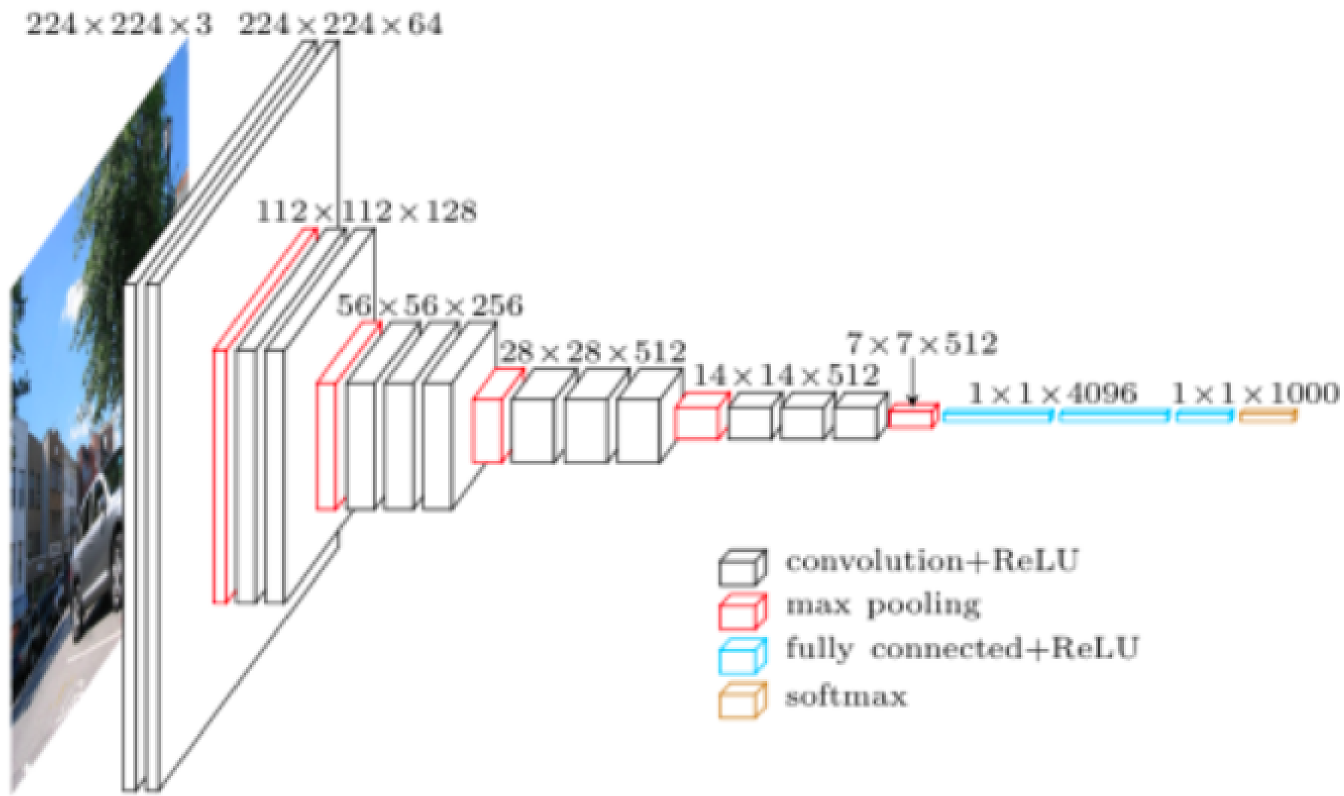
Progressive GANs.

**2018**: Unsupervised pre-training significantly improves a broad range of NLP tasks including question answering (but dialogue remains unsolved).

AlphaFold revolutionizes protein structure prediction.

## What is a Deep Network?

## VGG, Zisserman, 2014

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# What is a Deep Network?

We assume some set $\mathcal{X}$ of possible inputs, some set $\mathcal{Y}$ of possible outputs, and a parameter vector $\Phi \in \mathbb{R}^d$.

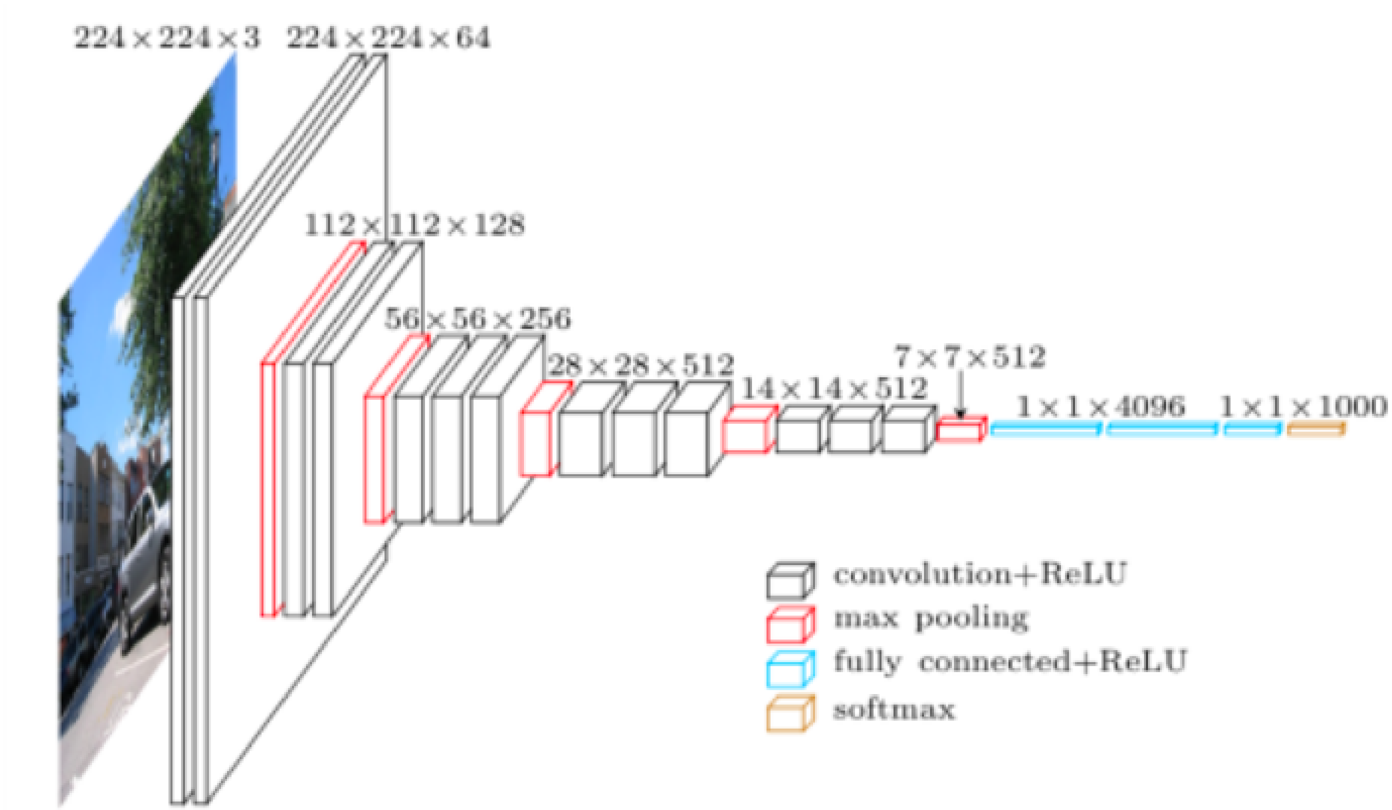
For a parameter vector $\Phi$, a given input $x \in \mathcal{X}$, and for each possible output $y \in \mathcal{Y}$ a deep network computes a probability distribution $P_\Phi(y|x)$ over the possible outputs $y \in \mathcal{Y}$.

# Softmax: Converting Scores to Probabilities

We start from a "score" function $s_\Phi(y|x) \in \mathbb{R}$.

$$
\begin{aligned}
P_\Phi(y|x) \; &= \; \frac{1}{Z}\, e^{s_\Phi(y|x)}; \quad Z = \sum_y e^{s_\Phi(y|x)} \\
&= \; \operatorname*{softmax}_y s_\Phi(y|x)
\end{aligned}
$$

# Note the Final Softmax Layer

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## The Fundamental Equation of Deep Learning

We assume a "population" probability distribution Pop on pairs $(x, y)$.

$$\begin{aligned}\Phi^* &= \operatorname*{argmin}_{\Phi}\ E_{(x,y)\sim\mathrm{Pop}}\ \mathcal{L}(x, y, \Phi) \\ &= \operatorname*{argmin}_{\Phi}\ E_{(x,y)\sim\mathrm{Pop}}\ -\ln\ P_\Phi(y|x)\end{aligned}$$

This loss function $\mathcal{L}(x, y, \Phi) = -\ln\ P_\Phi(y|x)$ is called **cross entropy loss**.

## Binary Classification

We have a population distribution over $(x, y)$ with $y \in \{-1, 1\}$.

We compute a single score $s_\Phi(x)$ where

for $s_\Phi(x) \geq 0$ predict $y = 1$

for $s_\Phi(x) < 0$ predict $y = -1$

## Softmax for Binary Classification

$$
\begin{aligned}
P_\Phi(y|x) &= \frac{1}{Z}\, e^{ys(x)} \\
&= \frac{e^{ys(x)}}{e^{ys(x)} + e^{-ys(x)}} \\
&= \frac{1}{1 + e^{-2ys(x)}} \\
&= \frac{1}{1 + e^{-m(y)}} \qquad m(y|x) = 2ys(x) \text{ is the margin}
\end{aligned}
$$

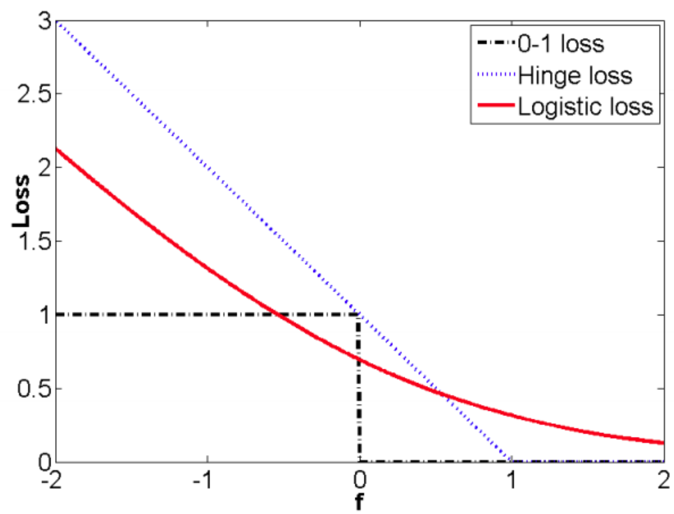
## Logistic Regression for Binary Classification

$$
\begin{aligned}
\Phi^* &= \operatorname*{argmin}_\Phi \; E_{(x,y)\sim\mathrm{Pop}}\, \mathcal{L}(x,y,\Phi) \\
&= \operatorname*{argmin}_\Phi \; E_{(x,y)\sim\mathrm{Pop}}\; -\ln P_\Phi(y|x) \\
&= \operatorname*{argmin}_\Phi \; E_{(x,y)\sim\mathrm{Pop}}\; \ln\left(1+e^{-m(y|x)}\right)
\end{aligned}
$$

$$\ln\left(1+e^{-m(y|x)}\right) \approx 0 \quad \text{for } m(y|x) >> 1$$

$$\ln\left(1+e^{-m(y|x)}\right) \approx -m(y|x) \quad \text{for } -m(y|x) >> 1$$

# Log Loss vs. Hinge Loss (SVM loss)



## Image Classification (Multiclass Classification)

We have a population distribution over $(x, y)$ with $y \in \{y_1, \ldots, y_k\}$.

$$P_\Phi(y|x) = \operatorname*{softmax}_y \; s_\Phi(y|x)$$

$$\begin{aligned} \Phi^* &= \operatorname*{argmin}_\Phi \; E_{(x,y)\sim \mathrm{Pop}} \, \mathcal{L}(x, y, \Phi) \\ &= \operatorname*{argmin}_\Phi \; E_{(x,y)\sim \mathrm{Pop}} \; -\ln P_\Phi(y|x) \end{aligned}$$

## Machine Translation (Structured Labeling)

We have a population of translation pairs $(x, y)$ with $x \in V_x^*$ and $y \in V_y^*$ where $V_x$ and $V_y$ are source and target vocabularies respectively.

$$P_\Phi(w_{t+1}|x, w_1, \ldots, w_t) \;=\; \operatorname*{softmax}_{w \in V_y \cup \text{<EOS>}} \; s_\Phi(w \mid x, w_1, \ldots, w_t)$$

$$P_\Phi(y|x) \;=\; \prod_{t=0}^{|y|} P_\Phi(y_{t+1} \mid x, y_1, \ldots, y_t)$$

$$\begin{aligned} \Phi^* \;&=\; \operatorname*{argmin}_\Phi \; E_{(x,y)\sim \text{Pop}} \, \mathcal{L}(x, y, \Phi) \\ &=\; \color{red}{\operatorname*{argmin}_\Phi \; E_{(x,y)\sim \text{Pop}} \; - \ln \; P_\Phi(y|x)} \end{aligned}$$

## Entropy, Cross Entropy and KL Divergence

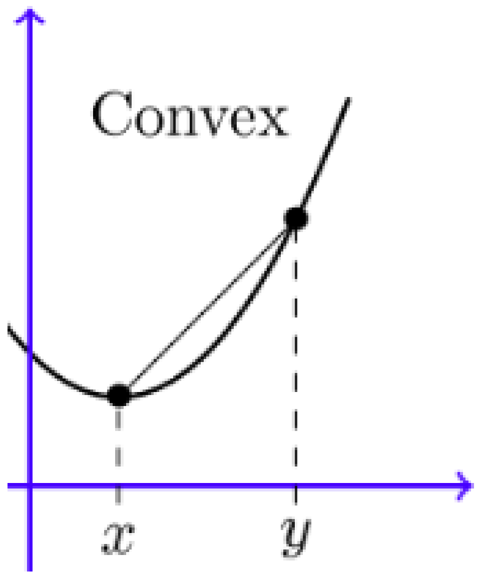
Let $P$ and $Q$ be two probability distributions on the same set $\mathcal{Y}$.

$$\begin{array}{lrcl}
\text{Entropy :} & H(P) & = & E_{y\sim P}\;\; -\ln\; P(y) \\
\text{CrossEntropy :} & H(P,Q) & = & E_{y\sim P}\;\; -\ln\; Q(y) \\
\text{KL Divergence :} & KL(P,Q) & = & E_{y\sim P}\;\;\; \ln\; \frac{P(y)}{Q(y)}
\end{array}$$

Cross Entropy Loss:

$$E_{(x,y)\sim \mathrm{Pop}}\; -\ln P_\Phi(y|x) \;\;=\;\; E_{x\sim \mathrm{Pop}}\, H(\mathrm{Pop}(y|x), P_\Phi(y|x))$$

## Jensen's Inequality




For $f$ convex (upward curving) we have

$$E[f(x)] \geq f(E[x])$$

## KL Divergence

$$KL(P,Q) \geq 0$$

Proof:

$$\begin{aligned}
KL(P,Q) &= E_{y\sim P} \ -\log \frac{Q(y)}{P(y)} \\
&\geq -\log E_{x\sim P} \ \frac{Q(y)}{P(y)} \\
&= -\log \sum_y \ P(y)\frac{Q(y)}{P(y)} \\
&= -\log \sum_y Q(y) \\
&= 0
\end{aligned}$$

## Fundamental Equations

$$KL(P,Q) \geq 0$$

$$H(P,Q) = H(P) + KL(P,Q)$$

$$\operatorname*{argmin}_Q H(P,Q) = P$$

$$\begin{aligned} \operatorname*{argmin}_{Q(y|x)} \; E_{(x,y)\sim\mathrm{Pop}} \; -\ln Q(y|x) &= \operatorname*{argmin}_{Q(y|x)} \; E_{x\sim\mathrm{Pop}} \; H(\mathrm{Pop(y|x)}, Q(y|x)) \\ &= \mathrm{Pop}(y|x) \end{aligned}$$

## Asymmetry of Cross Entropy

Consider

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\; H(P, Q_\Phi) \qquad (1)$$

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\; H(Q_\Phi, P) \qquad (2)$$

For (1) $Q_\Phi$ must cover all of the support of $P$.

For (2) $Q_\Phi$ concentrates all mass on the point maximizing $P$.

## Asymmetry of KL Divergence

Consider

$$\begin{aligned}\Phi^* &= \underset{\Phi}{\operatorname{argmin}}\; KL(P, Q_\Phi) \\ &= \underset{\Phi}{\operatorname{argmin}}\; H(P, Q_\Phi) \qquad (1)\end{aligned}$$

$$\begin{aligned}\Phi^* &= \underset{\Phi}{\operatorname{argmin}}\; KL(Q_\Phi, P) \\ &= \underset{\Phi}{\operatorname{argmin}}\, H(Q_\Phi, P) - H(Q_\Phi) \qquad (2)\end{aligned}$$

If $Q_\Phi$ is not universally expressive we have that (1) still forces $Q_\Phi$ to cover all of $P$ (or else the KL divergence is infinite) while (2) allows $Q_\Phi$ to be restricted to a single mode of $P$ (a common outcome).

**END**