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.

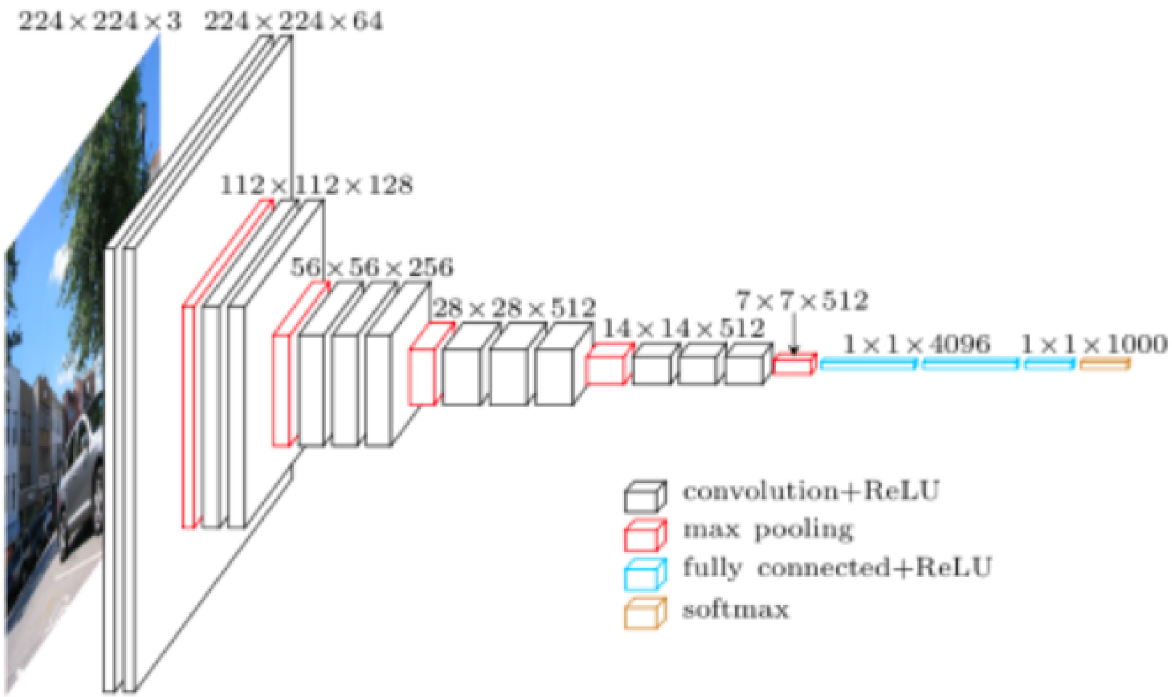
Progressive GANs.

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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138 Million Parameters

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 $\Phi \in \mathbb{R}^d$ and $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ a deep network computes a probability $P_\Phi(y|x)$.

The Fundamental Equation of Deep Learning

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

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

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

A Second Fundamental Equation

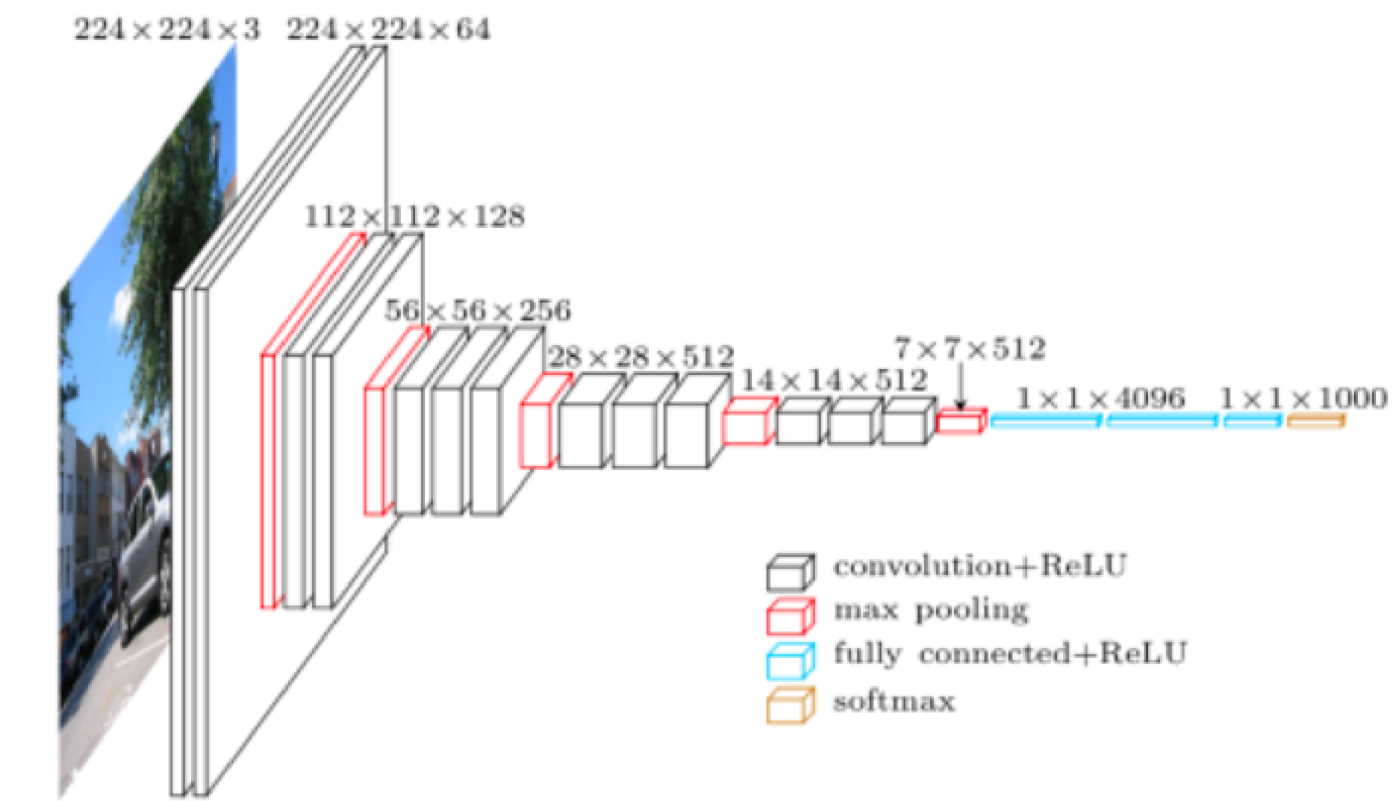
Softmax: Converting Scores to Probabilities

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

$$P_\Phi(y|x) = \frac{1}{Z}\, e^{s_\Phi(y|x)}; \quad Z = \sum_y e^{s_\Phi(y|x)}$$

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

Note the Final Softmax Layer



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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)

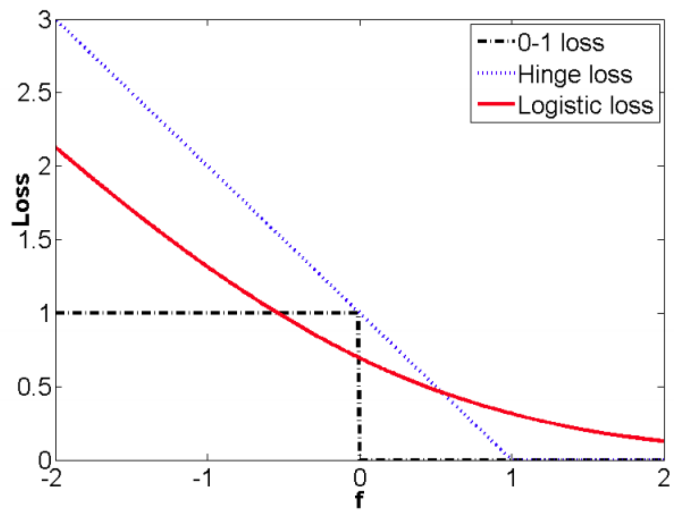


Image Classification (Multiclass Classification)

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.

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

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

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

Fuundamental Equation: Unconditional Form

$$\Phi^* = \operatorname*{argmin}_{\Phi} E_{y \sim \mathrm{Pop}} \; -\ln P_\Phi(y)$$

Entropy of a Distribution

The entropy of a distribution Pop is defined by

$$H(\text{Pop}) = E_{y \sim \text{Pop}} \; - \ln P(y) \;\; \text{in units of “nats”}$$

$$H_2(\text{Pop}) = E_{y \sim \text{Pop}} \; - \log_2 P(y) \; \text{in units of bits}$$

Example: Let Q be a uniform distribution on 256 values.

$$E_{y \sim Q} \; - \log_2 Q(y) = -\log_2 \frac{1}{256} = \log_2 256 = 8 \text{ bits} = 1 \text{ byte}$$

$$1 \text{ nat} = \frac{1}{\ln 2} \text{ bits} \approx 1.44 \text{ bits}$$

The Coding Interpretation of Entropy

We can interpret $H_2(Q)$ as the number of bits required an average to represent items drawn from distribution Q.

We want to use fewer bits for common items.

There exists a representation where, for all y, the number of bits used to represent y is no larger than $-\log_2 y + 1$ (Shannon's source coding theorem).

$$H(Q) = \frac{1}{\ln 2} H_2(Q) \approx 1.44\ H_2(Q)$$

Cross Entropy

Let P and Q be two distribution on the same set.

$$H(P,Q) = E_{y\sim P}\ -\ln\ Q(y)$$

$$\Phi^* = \operatorname*{argmin}_{\Phi}\ H(\mathrm{Pop}, P_\Phi)$$

H(P,Q) also has a data compression interpretation.

$H(P,Q)$ can be interpreted as 1.44 times the number of bits used to code draws from P when using the imperfect code defined by Q.

Entropy, Cross Entropy and KL Divergence

Let P and Q be two distribution on the same set.

$$\text{Entropy}: \quad H(P) = E_{y \sim P} \; -\ln\; P(y)$$

$$\text{CrossEntropy}: \quad H(P,Q) = E_{y \sim P} \; -\ln\; Q(y)$$

$$\text{KL Divergence}: \quad KL(P,Q) = H(P,Q) - H(P)$$

$$= E_{y \sim P} \quad \ln \frac{P(y)}{Q(y)}$$

We have $H(P,Q) \geq H(P)$ or equivalently $KL(P,Q) \geq 0$.

The Universality Assumption

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\ H(\mathrm{Pop}, P_\Phi) = \underset{\Phi}{\operatorname{argmin}}\ H(\mathrm{Pop}) + KL(\mathrm{Pop}, P_\Phi)$$

Universality assumption: P_Φ can represent any distribution and Φ can be fully optimized.

This is clearly false for deep networks. But it gives important insights like:

$$P_{\Phi^*} = \mathrm{Pop}$$

This is the motivatation for the fundamental equation.

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_Φ must cover all of the support of P.

For (2) Q_Φ concentrates all mass on the point maximizing P.

Asymmetry of KL Divergence

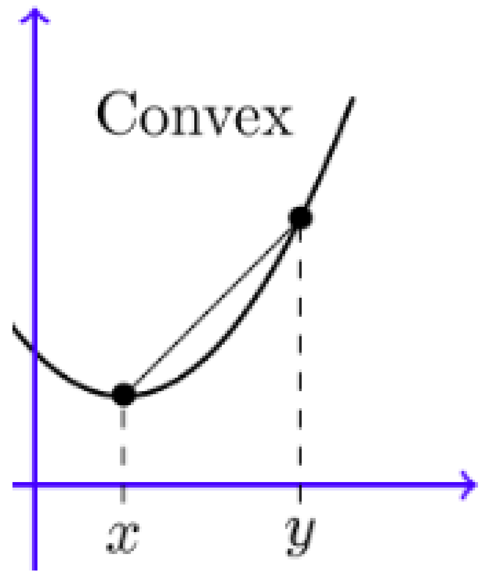
Consider

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

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

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

Proving $KL(P, Q) \geq 0$: Jensen's Inequality



For f convex (upward curving) we have

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

Proving $KL(P,q) \geq 0$

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

Summary

$$\Phi^* = \mathrm{argmin}_\Phi \;\; H(\mathrm{Pop}, P_\Phi) \text{ unconditional}$$

$$\Phi^* = \mathrm{argmin}_\Phi \;\; E_{x \sim \mathrm{Pop}} \; H(\mathrm{Pop}(y|x), P_\Phi(y|x)) \text{ conditional}$$

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

$$H(P,Q) \geq H(P), \quad KL(P,Q) \geq 0, \quad \mathrm{argmin}_Q \; H(P,Q) = P$$

Appendix: The Rearrangement Trick

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

$$KL(P, Q) \ = \ H(P, Q) - H(P)$$

The rearrangement trick applies to any expression of the form

$$E_{x \sim P} \ \ln \left(\prod_i A_i \right) = E_{x \sim P} \ \sum_i \ln A_i$$

END