

TTIC 31230, Fundamentals of Deep Learning, Winter 2019

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The Fundamental Equations of Deep Learning

Early History

1943: McCulloch 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: Rumelhart, 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: LeCun 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 matter of hours entirely from self-play and advances computer go far beyond human abilities.

Unsupervised machine translation is demonstrated.

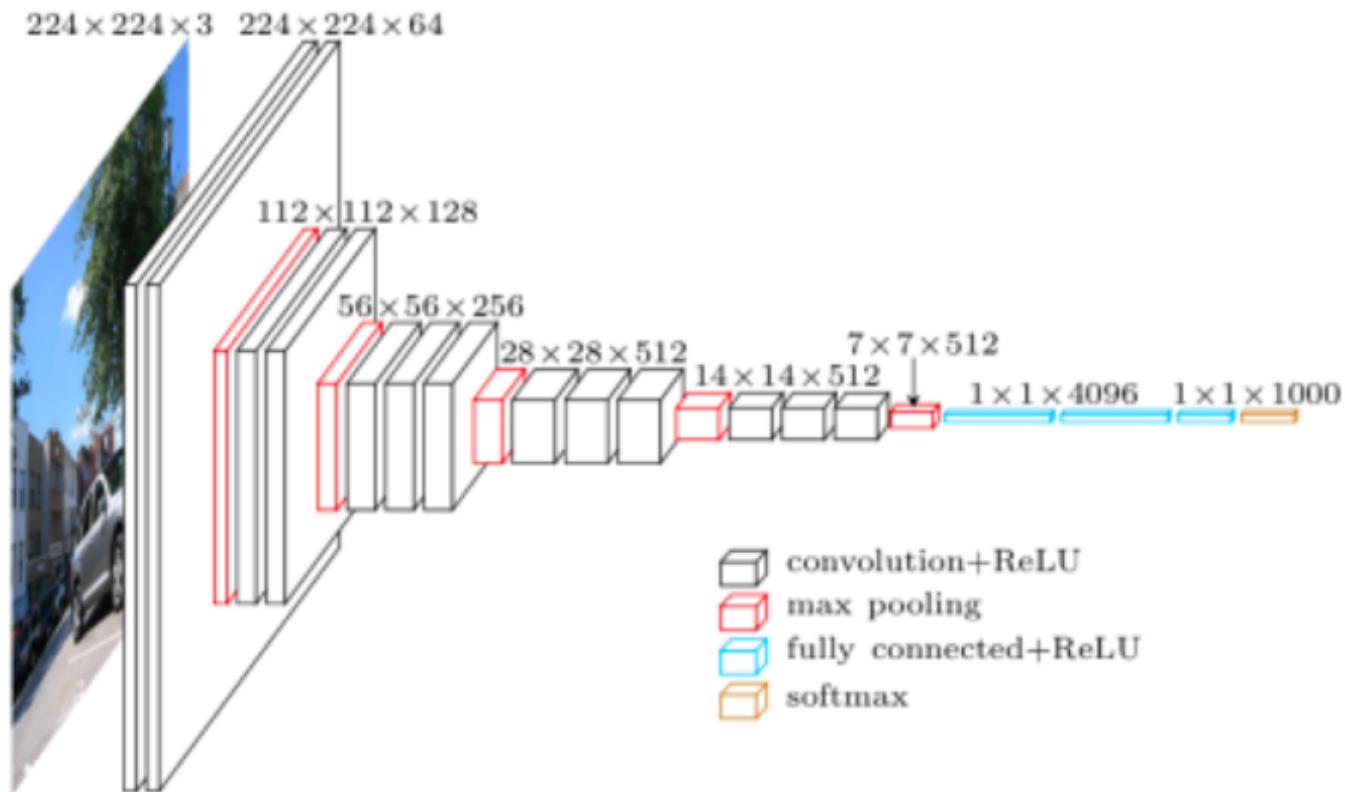
Progressive GANs.

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 $\Phi \in \mathbb{R}^d$.

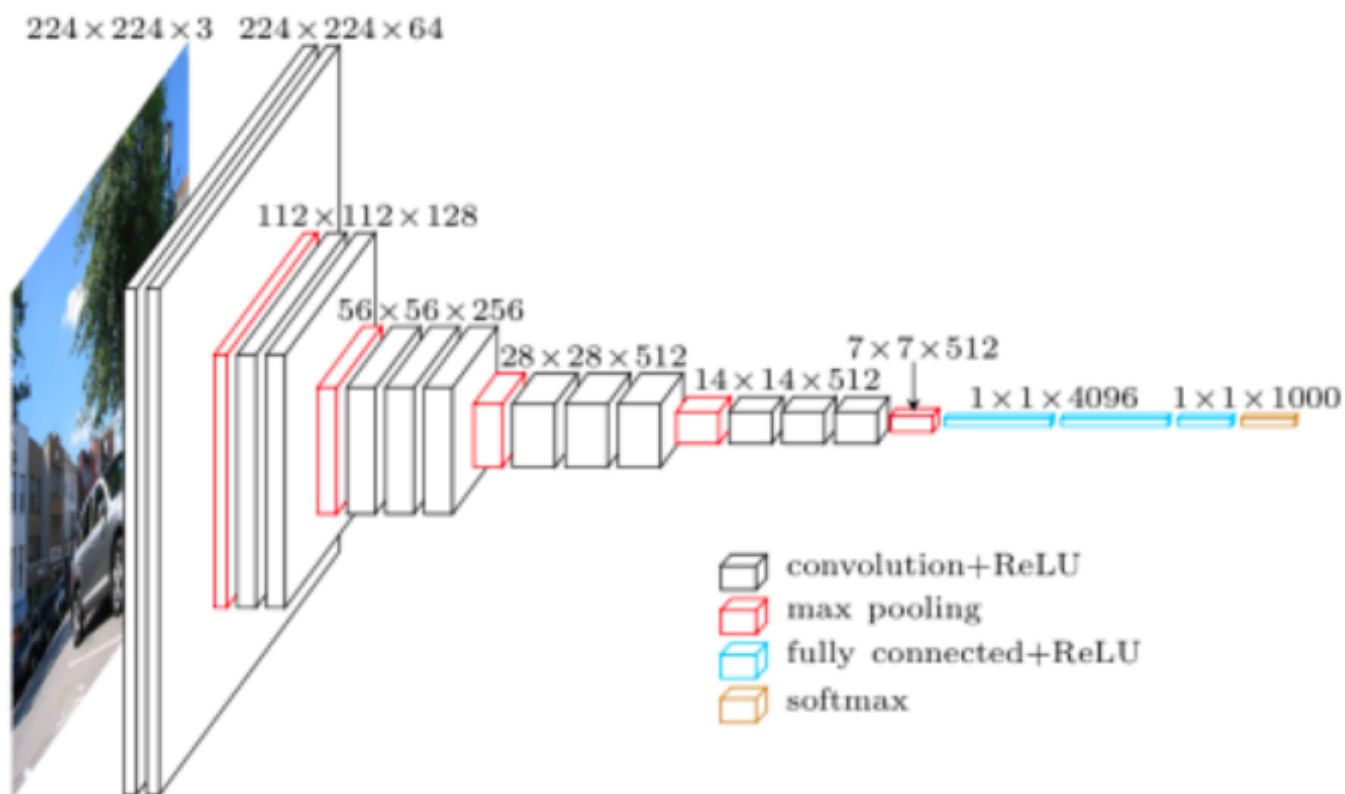
For a parameter vector Φ , a given input $x \in \mathcal{X}$, and for each possible output $y \in \mathcal{Y}$ a deep network computes a probability distribution $P_\Phi(y|x)$ over the possible outputs $y \in \mathcal{Y}$.

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) .

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

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

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

Logistic Regression for Binary Classification

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

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

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

Log Loss vs. Hinge Loss (SVM loss)

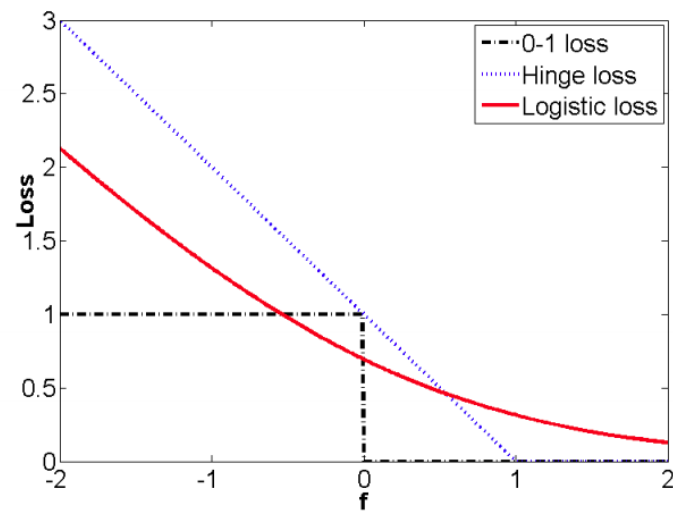


Image Classification (Multiclass Classification)

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

$$P_{\Phi}(y|x) = \underset{y}{\text{softmax}} \ s_{\Phi}(y|x)$$

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

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.

$$P_{\Phi}(w_{t+1}|x, w_1, \dots, w_t) = \operatorname{softmax}_{w \in V_y \cup \langle \text{EOS} \rangle} s_{\Phi}(w \mid x, w_1, \dots, w_t)$$

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

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

Entropy, Cross Entropy and KL Divergence

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

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

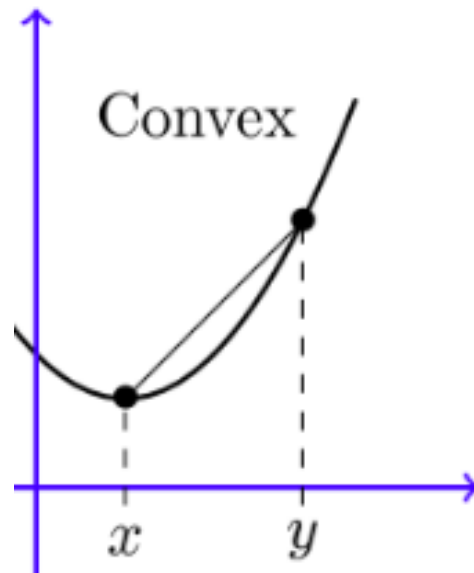
$$\text{CrossEntropy :} \quad H(P, Q) = E_{y \sim P} - \ln Q(y)$$

$$\text{KL Divergence :} \quad KL(P, Q) = E_{y \sim P} \ln \frac{P(y)}{Q(y)}$$

Cross Entropy Loss:

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

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

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

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

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

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

Asymmetry of Cross Entropy

Consider

$$\Phi^* = \operatorname{argmin}_{\Phi} H(P, Q_{\Phi}) \quad (1)$$

$$\Phi^* = \operatorname{argmin}_{\Phi} H(Q_{\Phi}, P) \quad (2)$$

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

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

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

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).

END