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.

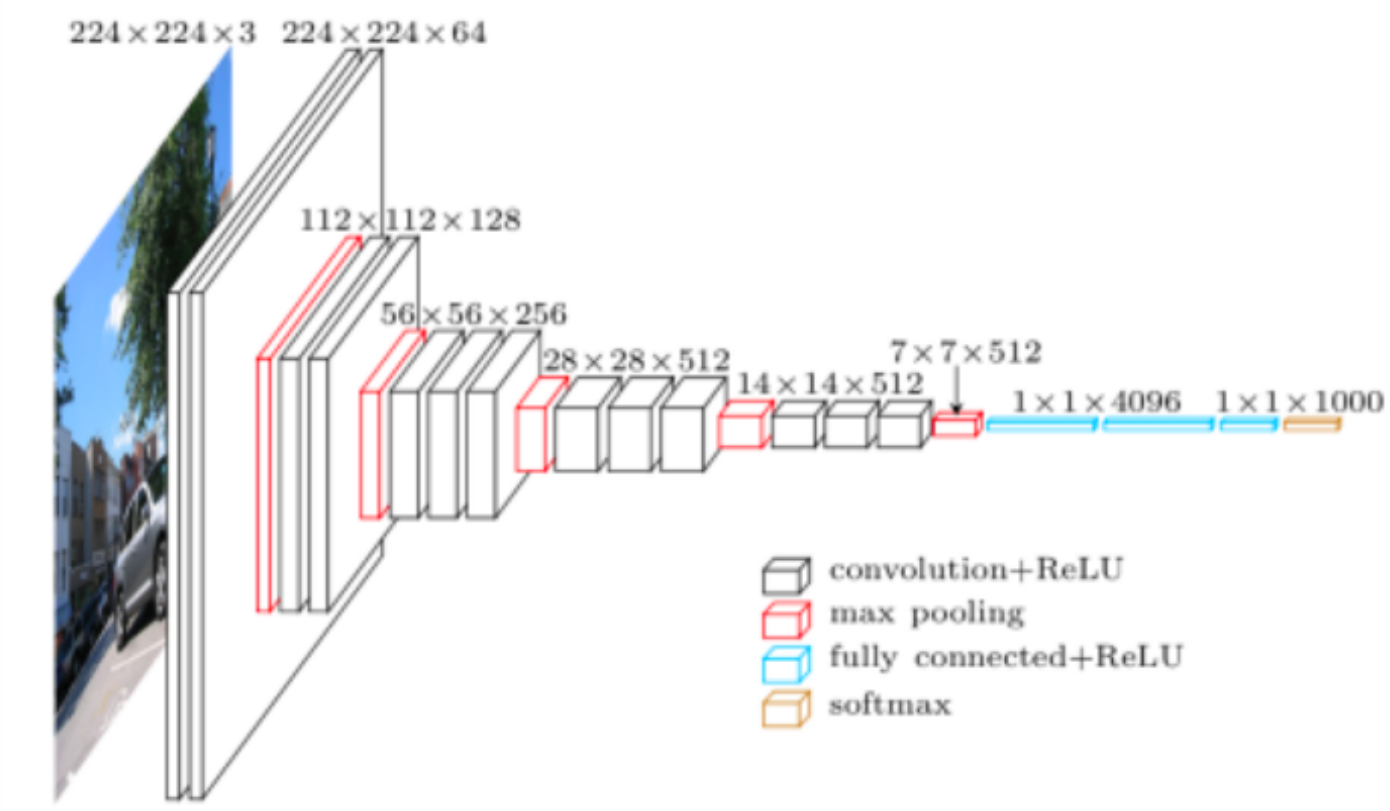
Progressive GANs.

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



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 $y \in \mathcal{Y}$.

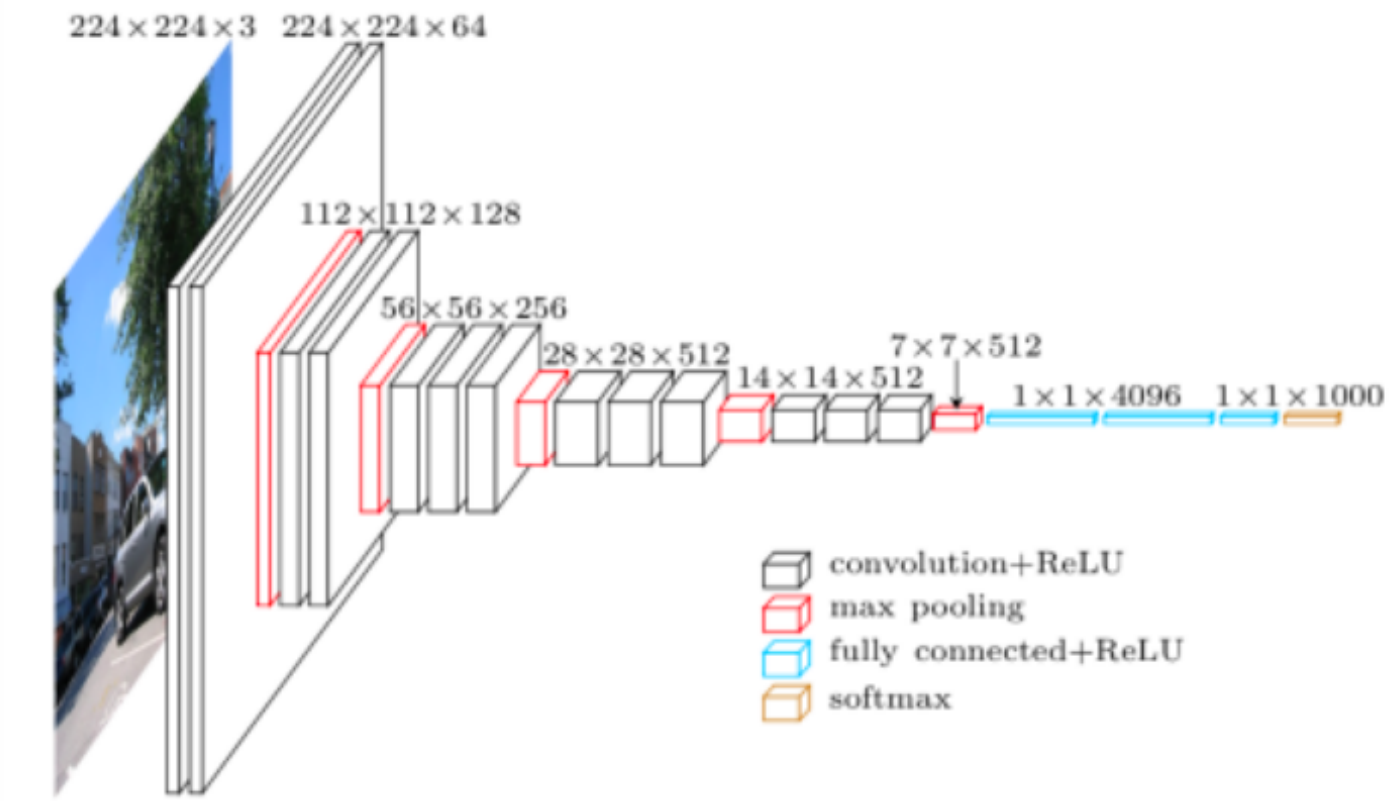
Softmax: Converting Scores to Probabilities

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

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

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

Note the Final Softmax Layer



Davi Frossard

The Fundamental Equation of Deep Learning

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

$$\Phi^* = \operatorname*{argmin}_{\Phi} E_{(x,y)\sim \text{Pop}}\, \mathcal{L}(x, y, \Phi)$$

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

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

$$
\begin{aligned}
\Phi^* &= \underset{\Phi}{\operatorname{argmin}}\ E_{(x,y)\sim \mathrm{Pop}}\ \mathcal{L}(x, y, \Phi) \\
&= \underset{\Phi}{\operatorname{argmin}}\ E_{(x,y)\sim \mathrm{Pop}}\ -\ln P_\Phi(y|x) \\
&= \underset{\Phi}{\operatorname{argmin}}\ E_{(x,y)\sim \mathrm{Pop}}\ \ln\left(1 + e^{-m(y|x)}\right) \\
\ln\left(1 + e^{-m(y|x)}\right) &\approx 0 \quad \text{for } m(y|x) >> 1 \\
\ln\left(1 + e^{-m(y|x)}\right) &\approx -m(y|x) \quad \text{for } -m(y|x) >> 1
\end{aligned}
$$

Log Loss vs. Hinge Loss (SVM loss)

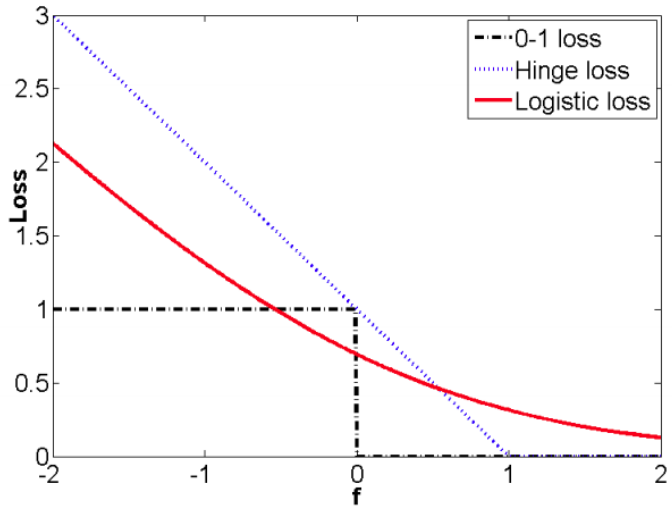


Image Classification (Multiclass Classification)

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

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

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

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.

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

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

$$\Phi^* = \underset{\Phi}{\text{argmin}} \; E_{(x,y)\sim \text{Pop}} \, \mathcal{L}(x, y, \Phi)$$

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

Entropy, Cross Entropy and KL Divergence

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

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

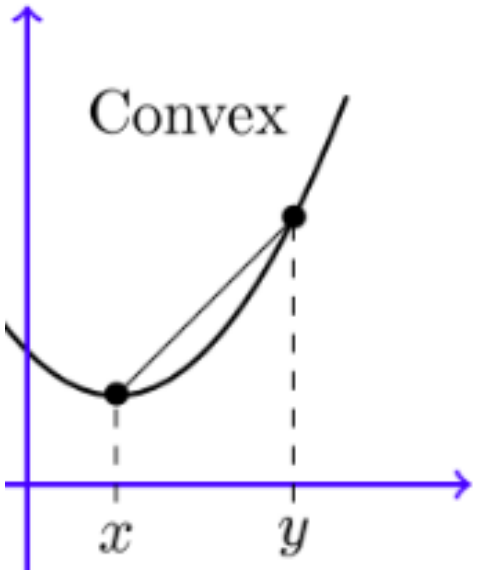
$$\text{CrossEntropy}: \quad H(P,Q) = E_{y\sim P} - \ln Q(y)$$

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

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

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

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

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

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

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

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

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

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).

Density Estimation

Anything that can be done conditionally $P_\Phi(y|x)$ can also be done unconditionally $P_\Phi(y)$.

We have unconditional cross-entropy training.

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

This is **distribution modeling** or **density estimation**.

Density estimation is sometimes equated with **unsupervised learning**.
A primary example is **language modeling**.

Unsupervised Learning

- "Pure" Reinforcement Learning (cherry)
  - The machine predicts a scalar reward given once in a while.
  - **A few bits for some samples**
- Supervised Learning (icing)
  - The machine predicts a category or a few numbers for each input
  - Predicting human-supplied data
  - **10→10,000 bits per sample**
- Unsupervised/Predictive Learning (cake)
  - The machine predicts any part of its input for any observed part.
  - Predicts future frames in videos
  - **Millions of bits per sample**

- (Yes, I know, this picture is slightly offensive to RL folks. But I'll make it up)

Unsupervised Learning

By "unsupervised learning" we will mean learning from **massively available** data. This is not a mathematical definition.

Massive: images, audio, text, video, click-through data.

Less Massive: car control data, stereo image pairs, closed captioned video, captioned images.

Big: Manually annotated images or audio.

Small: manually annotated text — parse trees, named entities, semantic roles, coreference, entailment.

Smallest: Manually annotated text in an obscure language.

Colorization

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

We have massive data for colorization.

Colorization is unsupervised structured labeling.

END