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.

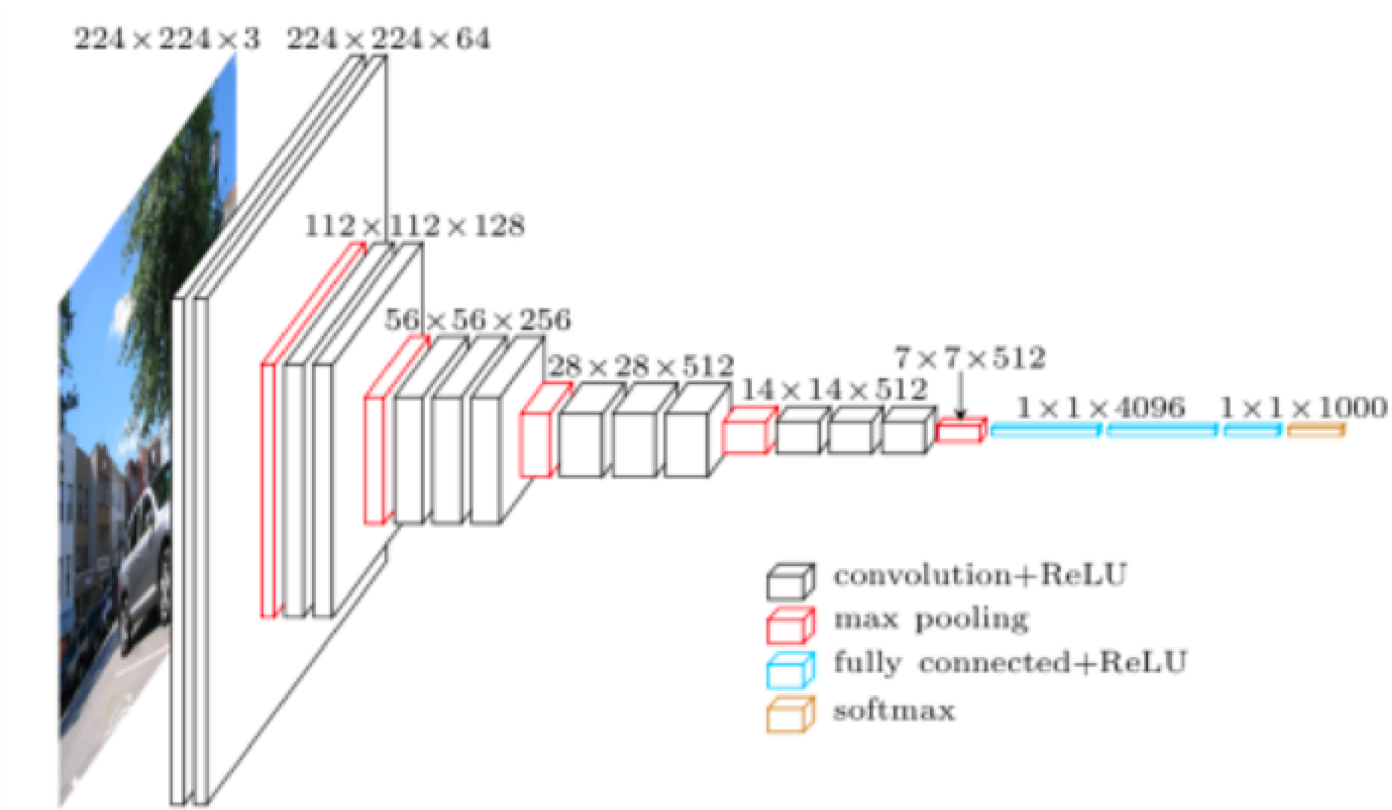
Progressive GANs.

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

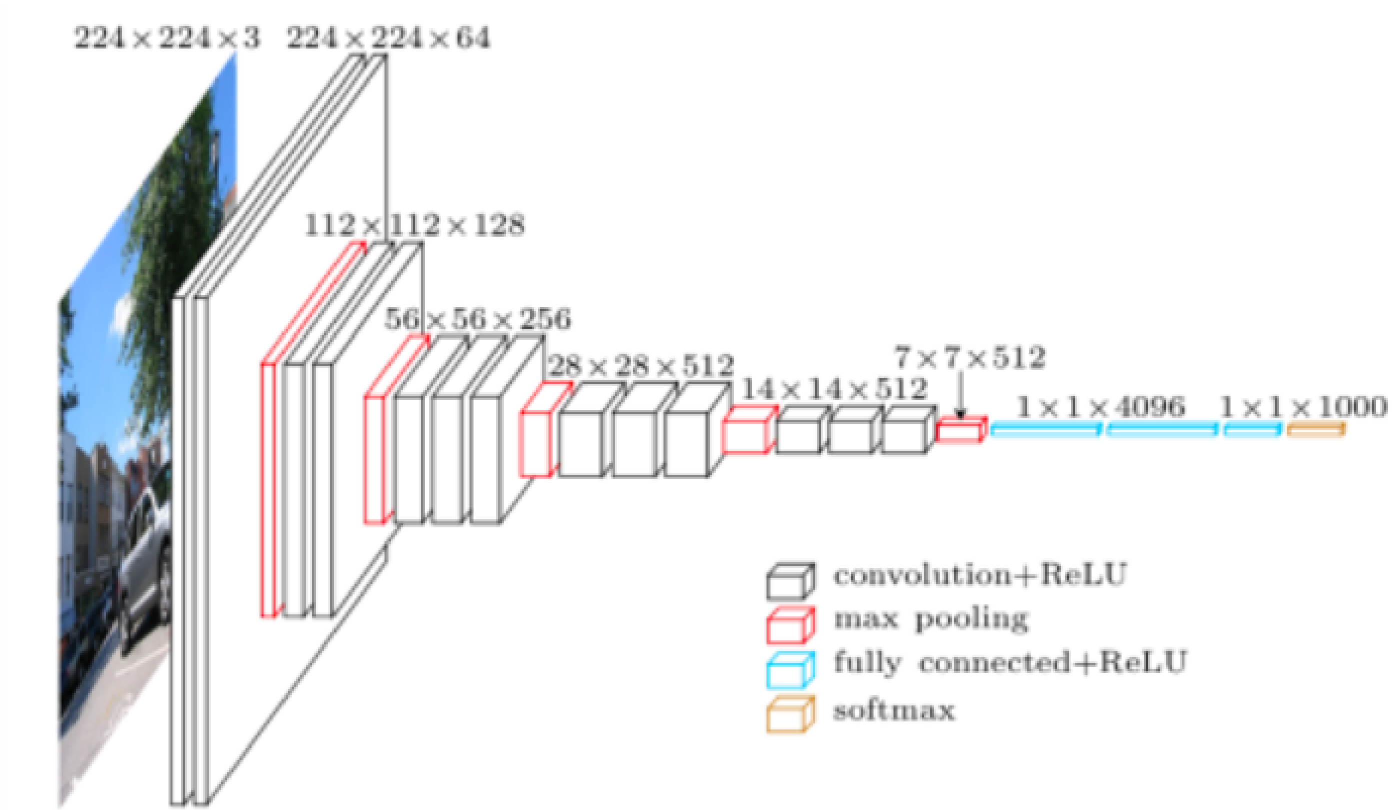
For a parameter vector Φ, a given input $x \in \mathcal{X}$, and for each possible output $y \in \mathcal{Y}$ a deep network computes a probability distribution $P_\Phi(y|x)$ over the possible outputs $y \in \mathcal{Y}$.

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).

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

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)

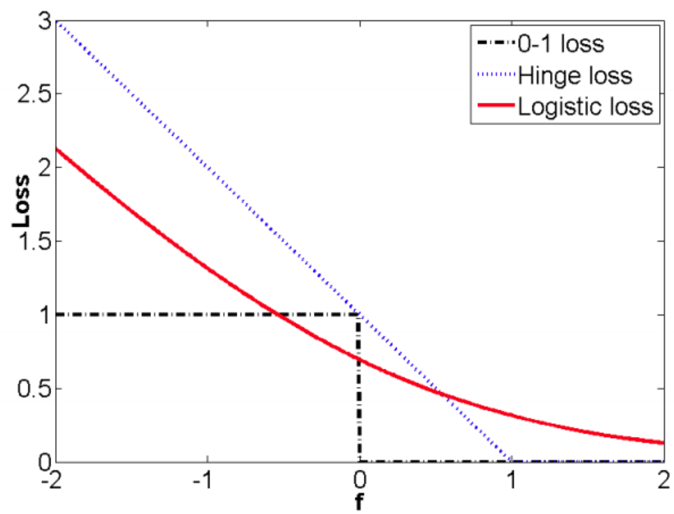


Image Classification (Multiclass Classification)

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.

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

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

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

Shannon's Source Coding Theorem

Consider a population probability distribution Pop on a discrete variable y.

Define

$$H_2(y) = E_y \; -\log_2 P(y) = H(y)/(\ln 2)$$

For any bit string c let $|c|$ be the number of bits in (the length of) c.

Theorem: There exists a coding function $c(y)$ such that for all y

$$|c(y)| \leq (-\log_2 \; P(y)) + 1$$

and therefore

$$E_y \; |c(y)| \leq H_2(y) + 1$$

Theorem: For any coding scheme c

$$E_y|c(y)| \geq H_2(y)$$

Cross Entropy Coding Theorem

Consider

$$H_2(P,Q) = E_y \; -\log_2 \, Q(y) = H(P,Q)/(\ln 2)$$

This can be interpreted as the number of bits used to code draws from P when using the optimal for distribution Q.

Entropy, Cross Entropy and KL Divergence

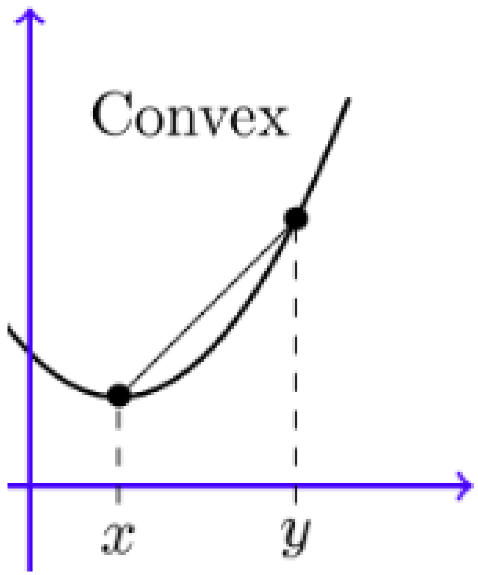
Let P and Q be two probability distributions on the same set $\mathcal{Y}$.

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

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:

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

The Rearrangement Trick

$$
\begin{aligned}
H(P,Q) &\doteq E_{x\sim P}\ -\ln Q(x) \\
&= E_{x\sim P}\ -\ln\ \left(P(x)\,\frac{Q(x)}{P(x)}\right) \\
&= E_{x\sim P}\ \left(-\ln P(x) + \ln\frac{P(x)}{Q(x)}\right) \\
&= (E_{x\sim P}\ -\ln P(x)) + \left(E_{x\sim P(x)}\ln\frac{P(x)}{Q(x)}\right) \\
&= H(P) + KL(P,Q) \\
&\geq H(P)
\end{aligned}
$$

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

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

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_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).

Density Estimation

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

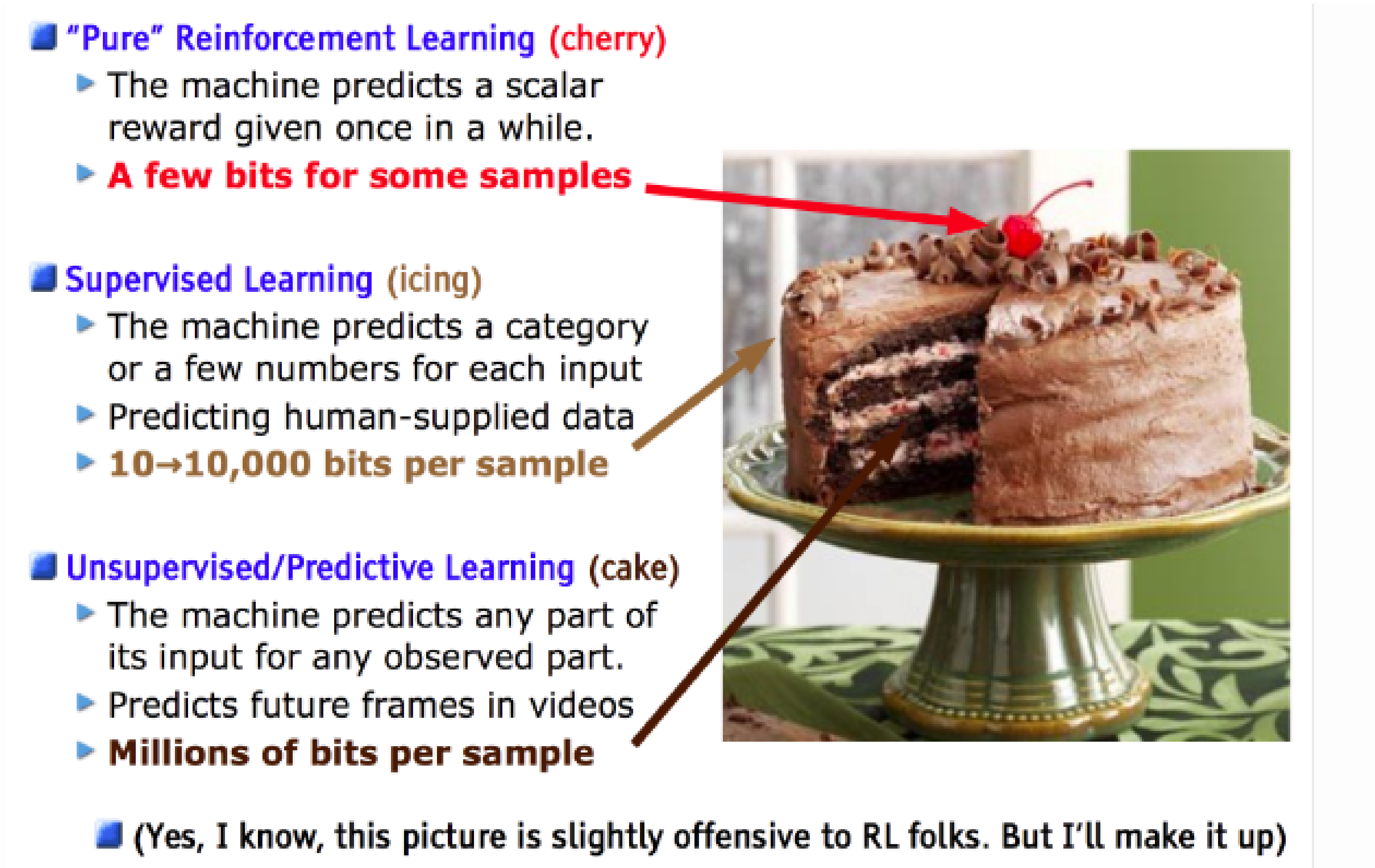
We have unconditional cross-entropy training.

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

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

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

Unsupervised Learning



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