TTIC 31230, Fundamentals of Deep Learning

David McAllester, Winter 2019

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 the 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.

Current Era

2014: Neural machine translation appears (Seq2Seq models).

Variational auto-encoders (VAEs) appear.

Generative Adversarial Networks (GANs) appear.

Graph neural networks appear (GNNs) revolutionizing the prediction of molecular properties.

Dramatic improvement in computer vision and speech recognition continues.

Current Era

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

ResNet (residual connections) appear. This makes yet another dramatic improvement in computer vision.

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 demonstrate high resolution realistic face generation.

Current Era

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

AlphaFold revolutionizes protein structure prediction.

2019: Vector quantized VAEs (VQ-VAE) demstrate that VAEs can be competative with GANs for high-resolution image generation.

Super-human performance is achieved on the GLUE natural langauge understanding benchmark.

2019: Natural Language Understanding

GLUE: General Language Understanding Evaluation

ArXiv 1804.07461

Corpus	|Train|	|Test|	Task	Metrics	Domain
			Single-Sentence Tasks		
CoLA	8.5k	**1k**	acceptability	Matthews corr.	misc.
SST-2	67k	1.8k	sentiment	acc.	movie reviews
			Similarity and Paraphrase Tasks		
MRPC	3.7k	1.7k	paraphrase	acc./F1	news
STS-B	7k	1.4k	sentence similarity	Pearson/Spearman corr.	misc.
QQP	364k	**391k**	paraphrase	acc./F1	social QA questions
			Inference Tasks		
MNLI	393k	**20k**	NLI	matched acc./mismatched acc.	misc.
QNLI	105k	5.4k	QA/NLI	acc.	Wikipedia
RTE	2.5k	3k	NLI	acc.	news, Wikipedia
WNLI	634	**146**	coreference/NLI	acc.	fiction books

Table 1: Task descriptions and statistics. All tasks are single sentence or sentence pair classification, except STS-B, which is a regression task. MNLI has three classes; all other classification tasks have two. Test sets shown in bold use labels that have never been made public in any form.

BERT and GLUE

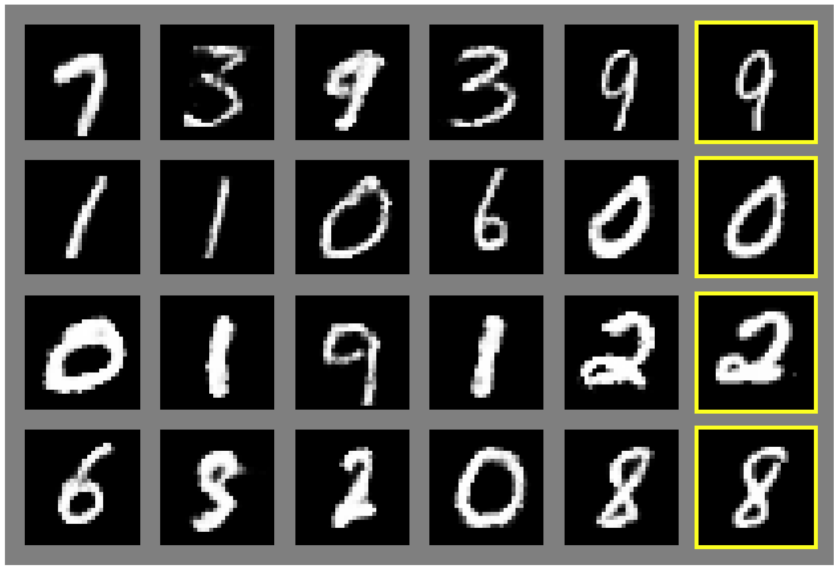
	Rank	Name	Model	URL	Score
	1	ERNIE Team - Baidu	ERNIE		90.1
	2	Microsoft D365 AI & MSR AI & GATECH	MT-DNN-SMART		89.9
	3	T5 Team - Google	T5		89.7
+	4	王玮	ALICE v2 large ensemble (Alibaba DAMO NLP)		89.5
	5	XLNet Team	XLNet (ensemble)		89.5
	6	ALBERT-Team Google Language	ALBERT (Ensemble)		89.4
	7	Microsoft D365 AI & UMD	FreeLB-RoBERTa (ensemble)		88.8
	8	Facebook AI	RoBERTa		88.5
	9	Junjie Yang	HIRE-RoBERTa		88.3
+	10	Microsoft D365 AI & MSR AI	MT-DNN-ensemble		87.6
	11	GLUE Human Baselines	GLUE Human Baselines		87.1

BERT and SuperGLUE

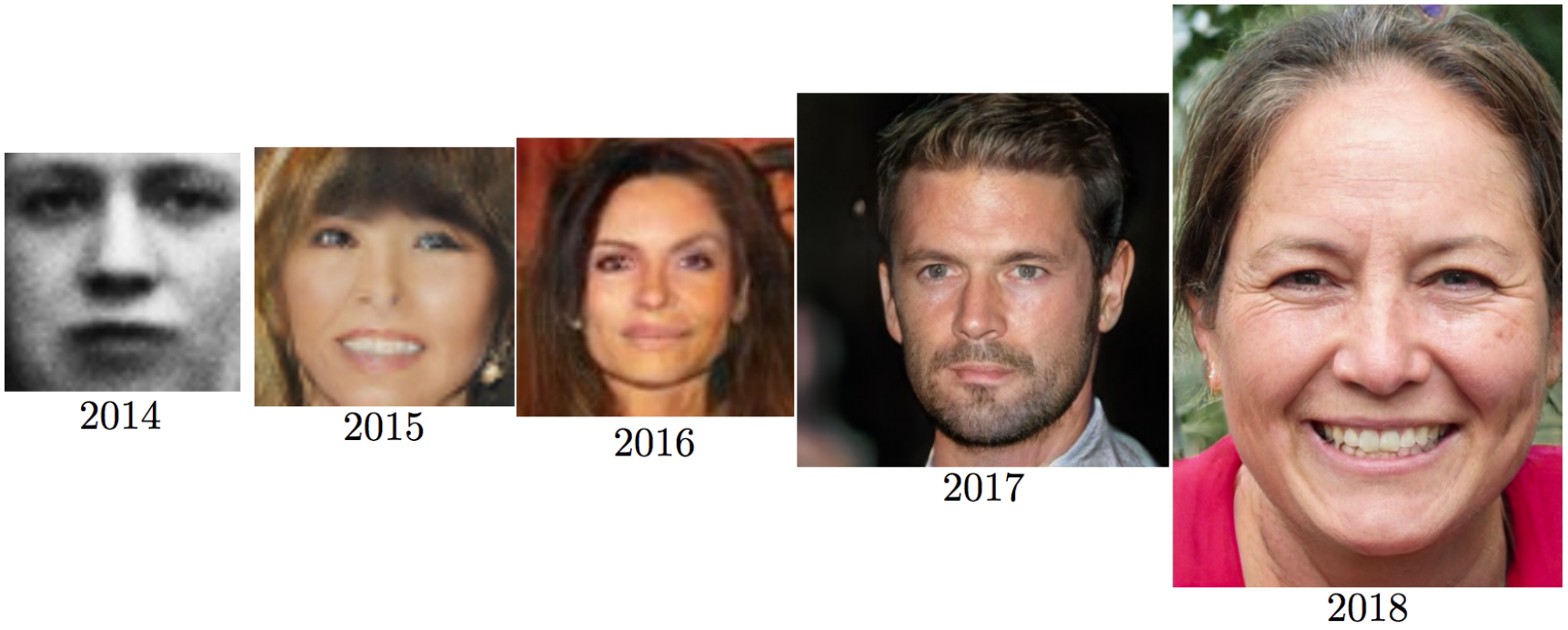
Rank	Name	Model	URL	Score
1	SuperGLUE Human Baselines	SuperGLUE Human Baselines		89.8
2	T5 Team - Google	T5		88.9
3	Facebook AI	RoBERTa		84.6
4	IBM Research AI	BERT-mtl		73.5
5	SuperGLUE Baselines	BERT++		71.5
		BERT		69.0

Generative Adversarial Nets (GANs)

Goodfellow et al., 2014



Moore's Law of AI
4.5 years of progress on faces



(Goodfellow 2019)

ArXiv 1406.2661, 1511.06434, 1607.07536, 1710.10196, 1812.04948
Goodfellow, ICLR 2019 Invited Talk

GANs for Imagenet

(Odena 2018)

BigGANs, Brock et al., 2018

Figure 1: Class-conditional samples generated by our model.

Variational Auto Encoders (VAEs, 2015)

[Alec Radford, 2015]

VAEs in 2019

VQ-VAE-2, Razavi et al. June, 2019

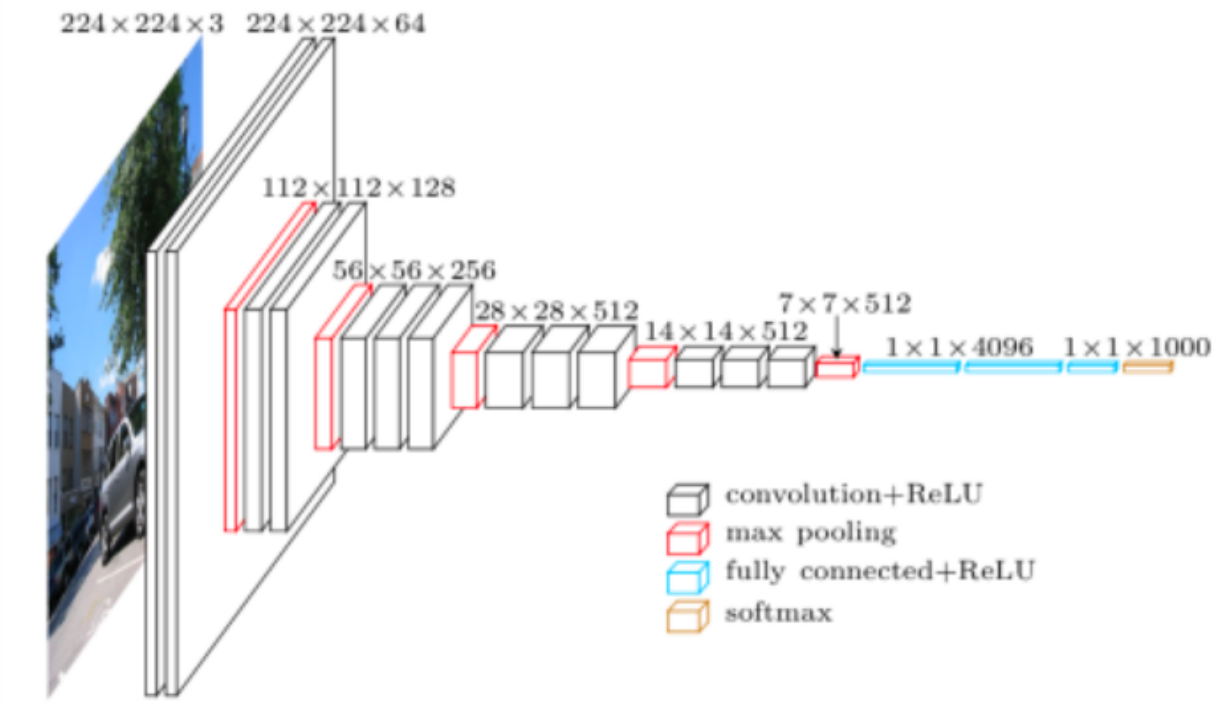
VAEs in 2019

Figure 1: Class-conditional 256x256 image samples from a two-level model trained on ImageNet.

VQ-VAE-2, Razavi et al. June, 2019

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).

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

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

A Second Fundamental Equation

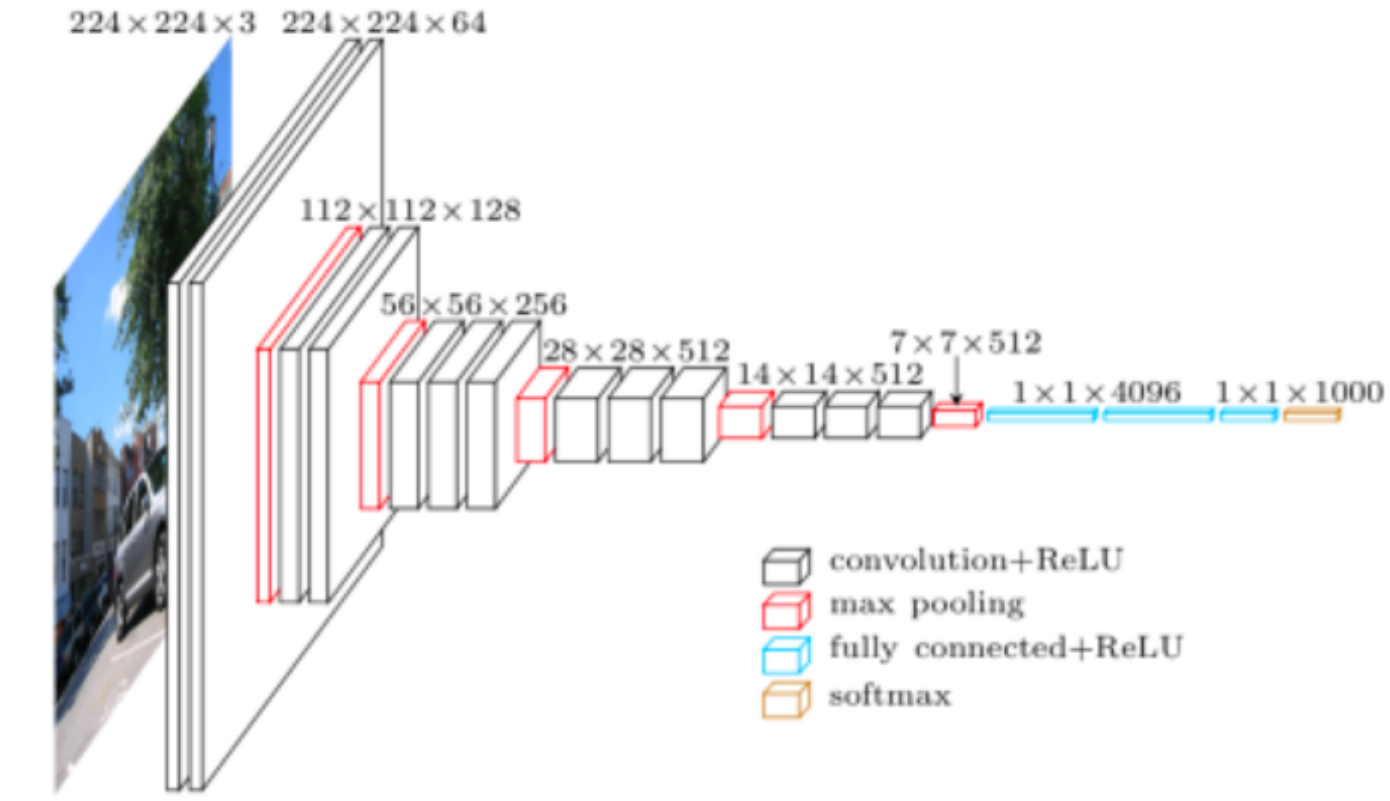
Softmax: Converting Scores to Probabilities

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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How Many Possibilities

We have $y \in \mathcal{Y}$ where $\mathcal{Y}$ is some set of "possibilities".

Binary: $Y = \{-1, 1\}$

Multiclass: $Y = \{y_1, \ldots y_k\}$ k manageable.

Structured: y is a "structured object" like a sentence. Here $|Y|$ is unmanageable.

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

$$P_\Phi(y|x) = \frac{1}{Z}\, e^{ys(x)}$$

$$= \frac{e^{ys(x)}}{e^{ys(x)} + e^{-ys(x)}}$$

$$= \frac{1}{1 + e^{-2ys(x)}}$$

$$= \frac{1}{1 + e^{-m(y)}} \qquad m(y|x) = 2ys(x) \text{ is the margin}$$

Logistic Regression for Binary Classification

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

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

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

Log Loss vs. Hinge Loss (SVM loss)

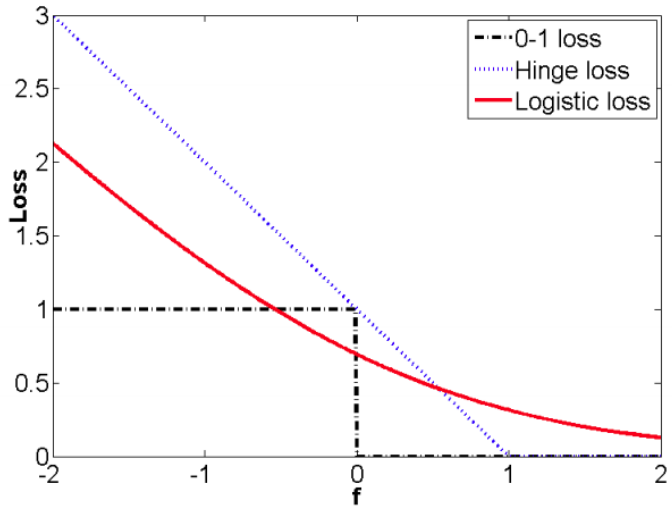


Image Classification (Multiclass Classification)

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

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

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

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.

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

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

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

Fuundamental Equation: Unconditional Form

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

Entropy of a Distribution

The entropy of a distribution P is defined by

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

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

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.

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

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

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.

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

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

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

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

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

The Universality Assumption

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

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:

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

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

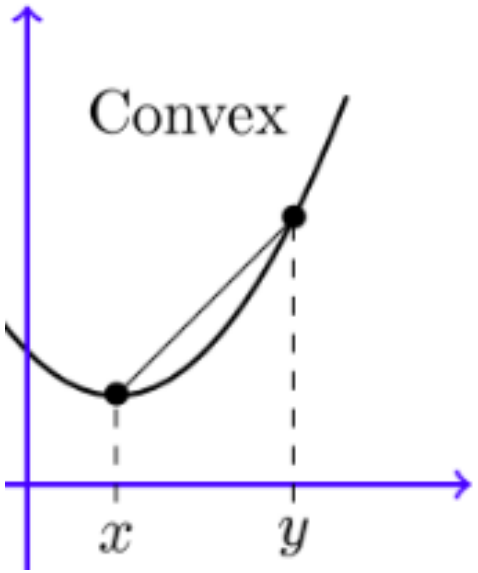
Consider

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

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

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

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

Summary

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

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

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

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

KL Divergence : $KL(P, Q) = H(P, Q) - H(P)$

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

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

Appendix: The Rearrangement Trick

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

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

Appendix: The Rearrangement Trick

$$\begin{aligned}
\text{ELBO} &= E_{z\sim P_\Psi(z|y)} \ln \frac{P_\Phi(z,y)}{P_\Psi(z|y)} \\
&= E_{z\sim P_\Psi(z|y)} \ln \frac{P_\Phi(z)P_\Phi(y|z)}{P_\Psi(z|y)} \\
&= E_{z\sim P_\Psi(z|y)} \ln \frac{P_\Phi(y)P_\Phi(z|y)}{P_\Psi(z|y)}
\end{aligned}$$

Each of the last two expressions can be grouped three different ways leading to six ways of writing the ELBO.

END