

Introduction to Entropy

Stochastic Processes Seminar

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Entropy and Mutual Information

Definition 1: Entropy

Definition

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space, \mathcal{X} a countable set, and $X : \Omega \rightarrow \mathcal{X}$ a discrete random variable.

Entropy wrt. base:
$$H_b(X) = \mathbb{E}(-\log_b p_X(X)) = - \sum_{x \in \text{supp}(X)} p_X(x) \log_b p_X(x)$$

Entropy conventionally:
$$H(X) = H_2(X)$$

Remark 1: Notation Conventions (1/2)

Remark

- 1 Let \mathcal{X}, \mathcal{Y} be countable sets and $X : \Omega \rightarrow \mathcal{X}$, $Y : \Omega \rightarrow \mathcal{Y}$ be discrete random variables on $(\Omega, \mathcal{A}, \mathbb{P})$. From now on, the random variables X, Y are always available for use.
- 2 We do **not** use the shorthand notations $p(x) = \mathbb{P}[X = x]$ and $p(y) = \mathbb{P}[Y = y]$, to keep the notation easily understandable.
- 3 We use the convention $\log = \log_2$, as the entropy H is defined wrt. base 2.

Remark 1: Notation Conventions (2/2)

Remark

- 4 We also use the following convention and justify it through a continuity argument:

$$0 \log 0 = \lim_{x \rightarrow 0^+} x \log x = \lim_{x \rightarrow 0^+} \frac{\log x}{\frac{1}{x}} = \lim_{x \rightarrow 0^+} \frac{\frac{1}{\ln(2)x}}{-\frac{1}{x^2}} = \lim_{x \rightarrow 0^+} \frac{-x}{\ln(2)} = 0$$

This choice is sensible, as $\log x$ is not defined for negative x .

- 5 The conventions, definitions and theorems are from Definitions, Theorems, Remarks and Exercises in *Elements of Information Theory*, second edition.

Remark 2: Existence of Entropy

Remark (Existence of Entropy)

Note that if $|\mathcal{X}|$ is finite, $(\forall p \in \mathbb{R}_+ : H_b(X) \text{ finite})$ and $H(X) \leq |\mathcal{X}|$ (see Theorem 5).

For $|\mathcal{X}|$ countably infinite, there are counterexamples where $H_b(X) = \infty$.

From now on, we will assume that entropy is finite.

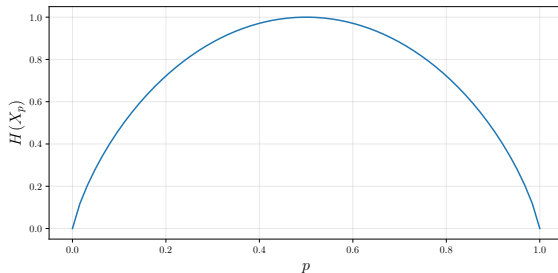
Example 1: Entropy of Bernoulli Variable

Example (Entropy of bernoulli variable)

Let $p \in (0, 1)$ and $X_p \sim B(1, p)$ be a weighted coin flip.

We can calculate the Entropy of X_p : $H(X_p) = -p \log p - (1 - p) \log(1 - p)$.

A visual inspection reveals that $H(X_p)$ seems to be maximised for $p = 0.5$ and minimised for $p \in \{0, 1\}$. An increase in uncertainty about the result of the coin flip seems to correspond with an increase in entropy.



Example 2: Entropy of Geometric Variable (1/3)

Example (Entropy of geometric variable)

Let $p \in (0, 1)$ and $X_p \sim G(p)$ be the number of times a weighted coin is flipped, until the first head occurs. We will calculate the Entropy of X_p . It will require the two well-known series:

$$\forall r \in (0, 1) : \sum_{n \in \mathbb{N}_0} r^n = \frac{1}{1 - r} \quad (1)$$

$$\forall r \in (0, 1) : \sum_{n \in \mathbb{N}_0} nr^n = \frac{r}{(1 - r)^2} \quad (2)$$

Example 2: Entropy of Geometric Variable (2/3)

We can now directly calculate the Entropy of X_p :

$$H(X_p) = \sum_{x \in \mathbb{N}} -p(x) \log p(x) \quad (\text{Def. of Entropy})$$

$$= - \sum_{x \in \mathbb{N}} (1-p)^{x-1} p \log ((1-p)^{x-1} p) \quad (\text{Geometric mass func.})$$

$$= - \sum_{x \in \mathbb{N}} (1-p)^{x-1} p ((x-1) \log(1-p) + \log p) \quad (\text{Log rules})$$

$$= -p \log(1-p) \sum_{x \in \mathbb{N}_0} (1-p)^x x - p \log p \sum_{x \in \mathbb{N}_0} (1-p)^x \quad (\text{Factor out})$$

$$= -p \log(1-p) \frac{1-p}{p^2} - p \log p \frac{1}{p} \quad (\text{Use series 1, 2})$$

$$= \frac{-(1-p) \log(1-p) - p \log p}{p} \quad (\text{Simplify})$$

Example 2: Entropy of Geometric Variable (3/3)

For $p = 0.5$ we get $H(X_{0.5}) = \frac{-0.5 \log 0.5 - 0.5 \log 0.5}{0.5} = -2 \log 0.5 = 2$.

We can visually inspect $(0, 1) \rightarrow \mathbb{R}, p \mapsto H(X_p)$ to get a feeling for the entropy of X_p . An increase in p is linked to lower variance and more concentration of the distribution towards zero. Based on the plot, that increase looks to be linked to a lower entropy and vice-versa.

A simple strategy to determine X is to ask "Is $X = 1$ ", "Is $X = 2$ " and so on. The number of questions required is exactly X . Thus, the average number of questions is $\mathbb{E}(X_{0.5}) = \frac{1}{0.5} = 2$. This matches $H(X_{0.5}) = 2$.

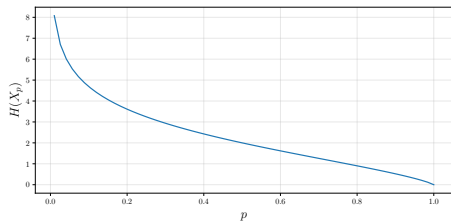


Figure 2: Geometric Entropy $H(X_p)$

Definition 2: Conditional, Joint, Relative Entropy, Mutual Information

Definition

Conditional Entropy: $H(X \mid Y) = -\mathbb{E} (\log p_{(X|Y)}(X \mid Y))$

$$= \sum_{(x,y) \in \mathcal{X} \times \mathcal{Y}} p_{(X,Y)}(x,y) \log p_{(X|Y)}(x \mid y)$$

Joint Entropy: $H(X, Y) = -\mathbb{E} (\log p_{(X,Y)}(X, Y))$ (dito)

Relative Entropy: $D(p \parallel q) = \mathbb{E}_{X \sim p} \left(\log \frac{p(X)}{q(X)} \right)$

$$= \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)} \quad (\text{also: KL-Divergence})$$

Mutual Information: $I(X; Y) = D(p_{(X,Y)} \parallel p_X p_Y)$

where p, q are probability mass functions on the same set \mathcal{X} , with conventions from Remark 3.

Remark 3: More Conventions

Remark

We have $D(p\|q) = \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)}$. To understand the conventions, we look at limit cases:

1 Case $p \in (0, 1], q = 0$: $\lim_{q \rightarrow 0^+} p \log \frac{p}{q} = \lim_{q \rightarrow 0^+} (p \log p - p \log q) = \infty$.

2 Case $p = 0, q \in (0, 1]$: $0 \log \frac{0}{q} = 0$.

3 Case $p = q = 0$: Case 1 logic yields ∞ and Case 2 logic yields 0.

As we want $\sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)}$ to sum over $x \in \mathcal{X}, p(x) > 0$, we choose $0 \log \frac{0}{0} = 0$.

If $p_Y(y) = 0$, we get $p_{(X,Y)}(x, y) = 0$. So $0 \log 0 = 0$ justifies that cond. entropy is well-defined.

Example 3: Relative Entropy of Binomial Distributions (1/2)

Example

To understand the concept, we can now calculate the relative entropies for an example. Let $X \sim B(20, \alpha)$ and $Y \sim B(20, \beta)$ with $(\alpha, \beta) \in [0, 1]^2$.

$$D(p_X \| p_Y) = \sum_{x=0}^{20} p_X(x) \log \frac{p_X(x)}{p_Y(x)}$$

$$\alpha = 0, \beta = 1 : D(p_X \| p_Y) = 1 \log \frac{1}{0} + 0 \log \frac{0}{1} = \infty + 0 = \infty$$

$$\alpha = 0.1, \beta = 0.9 : D(p_X \| p_Y) \approx 50.7$$

$$\alpha = 0.3, \beta = 0.7 : D(p_X \| p_Y) \approx 9.8$$

$$\alpha = 0.5, \beta = 0.5 : D(p_X \| p_Y) = \sum_{x=0}^{20} p(x) \log 1 = 0$$

Example 3: Relative Entropy of Binomial Distributions (2/2)

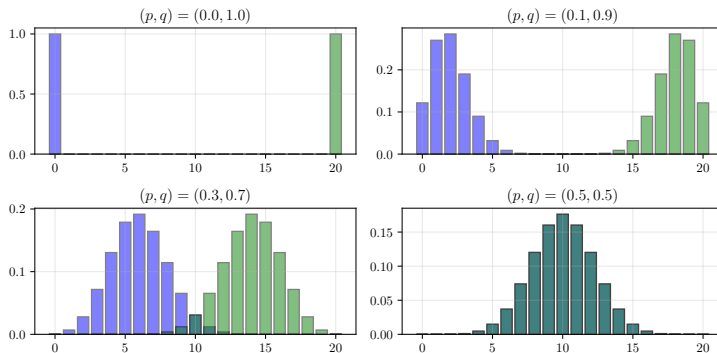


Figure 3: Relative Entropies of Binomial Distributions

Intuitively, the more overlap the distributions have, the closer to zero the relative entropy is.

Mutual Information and Chain Rules

Theorem 1: Chain Rule for Entropy

Theorem (Chain Rule for Entropy)

We have $H(X, Y) = H(X) + H(Y | X)$

Proof.

$$\begin{aligned} H(X, Y) &= -\mathbb{E}(\log p(X, Y)) = -\mathbb{E}(\log p(Y | X)p(X)) \\ &= -\mathbb{E}(\log p(Y | X)) - \mathbb{E}(\log p(X)) = H(X) + H(Y | X) \end{aligned}$$



Theorem 2: Mutual Information Equivalences

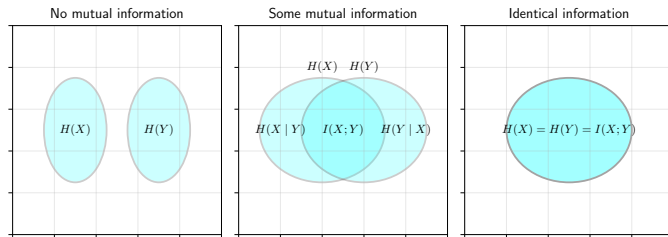


Figure 4: Relationship between Entropy, Conditional Entropy and Mutual Information

Theorem 2: Mutual Information Equivalences (Statement)

Theorem

There are multiple equivalent ways to express Mutual Information:

- 1 $I(X; Y) = H(Y) - H(Y|X)$
- 2 $I(X; Y) = I(Y; X)$
- 3 $I(Y; X) = H(X) - H(X|Y)$
- 4 $I(X; Y) = H(X) + H(Y) - H(X, Y)$
- 5 $I(X; X) = H(X)$

Theorem 2: Proof of (1)

Proof of (1).

We can use the definition of mutual information and relative entropy to obtain:

$$\begin{aligned} I(X; Y) &= D(p_{(X,Y)} \| p_X p_Y) && \text{(by def. of mutual info.)} \\ &= \mathbb{E}_{p_{(X,Y)}} \left(\log \frac{p_{(X,Y)}(X, Y)}{p_X(X) p_Y(Y)} \right) && \text{(by def. relative entropy)} \\ &= \mathbb{E}_{p_{(X,Y)}} \left(\log \frac{p_X(X) p_{(Y|X)}(Y | X)}{p_X(X) p_Y(Y)} \right) && \text{(using cond. probability)} \\ &= \mathbb{E}_{p_{(X,Y)}} \left(\log \frac{p_{(Y|X)}(Y | X)}{p_Y(Y)} \right) && \text{(simplify fraction)} \\ &= \mathbb{E}_{p_{(X,Y)}} (\log p_{(Y|X)}(Y | X)) - \mathbb{E}_{p_{(X,Y)}} (\log p_Y(Y)) && \text{(simplify logarithm)} \\ &= -H(Y | X) + H(Y) && \text{(by def. of entropy)} \end{aligned}$$



Theorem 3: Chain Rules

Theorem (Chain Rules)

Let $n \in \mathbb{N}$, $n \geq 2$, $(X_1, \dots, X_n) \sim p(x_1, \dots, x_n)$ and Y a random variable. The following statements about Entropy and Mutual Information are called Chain Rules:

- 1 $H(X_1, \dots, X_n) = \sum_{i=1}^n H(X_i | X_{i-1}, \dots, X_1)$
- 2 $D(p(x) \| q(x)) = D(p(x | y) \| q(x | y)) + D(p(y) \| q(y))$
- 3 $I(X_1, \dots, X_n; Y) = \sum_{i=1}^n I(X_i; Y | X_{i-1}, \dots, X_1)$

Theorem 3: Proof of (1)

Proof of (1).

Prove this result using induction by n .

Base case $n = 2$: Chain rule for two variables.

Assume the theorem holds for $n - 1$. Induction case $n - 1$ to n :

$$\begin{aligned} H(X_1, \dots, X_n) &= H(X_n | X_1, \dots, X_{n-1}) + H(X_1, \dots, X_{n-1}) && \text{(apply base case)} \\ &= H(X_n | X_1, \dots, X_{n-1}) + \sum_{i=1}^{n-1} H(X_i | X_{i-1}, \dots, X_1) && \text{(induction hypothesis)} \end{aligned}$$



Inequalities for Entropy and Mutual Information

Remark 4: Convexity

Remark

We use the common definition of convex functions and concave functions from analysis.

Theorem 4: Jensen's Inequality

Theorem (Jensen's Inequality)

Let $\mathcal{X} \subset \mathbb{R}$ and $f : \mathcal{X} \rightarrow \mathbb{R}$ a function.

- 1 If f is convex, we have $\mathbb{E}f(X) \geq f(\mathbb{E}X)$.
- 2 If f is concave, we have $\mathbb{E}f(X) \leq f(\mathbb{E}X)$.
- 3 If the inequality is strict we have $\mathbb{E}(X) = X$ almost surely.

Corollary 1: Non-negativity (Statement)

Corollary

Entropy and Mutual Information are non-negative:

- 1 $0 \leq H(X)$
- 2 $0 \leq D(p\|q)$
- 3 $0 \leq I(X; Y)$

Corollary 1: Proof of (1)

Proof of (1).

Note that $\log(\frac{1}{[0,1]}) = \log([1, \infty]) = [0, \infty]$ and $p(X)(\mathcal{X}) \in [0, 1]$.

Using the monotonicity of the expected value, we obtain

$$0 \leq \mathbb{E} \left(\log \left(\frac{1}{p(X)} \right) \right) = -\mathbb{E} (\log (p(X))) = H(X)$$



Corollary 1: Proof of (2)

Proof of (2).

We can prove this using Jensens Inequality on a *concave* function:

$$\begin{aligned} -D(p(x)\|q(x)) &= -\mathbb{E}_p \left(\log \frac{p(X)}{q(X)} \right) = \mathbb{E}_p \left(\log \frac{q(X)}{p(X)} \right) && \text{(def. of relative entropy)} \\ &\leq \log \left(\mathbb{E}_p \frac{q(X)}{p(X)} \right) && \text{(Jensen's inequality)} \\ &= \log \left(\sum_{x \in \mathcal{X}} p(x) \frac{q(x)}{p(x)} \right) = \log \left(\sum_{x \in \mathcal{X}} q(x) \right) = \log(1) = 0 && \text{(def. of exp. value, since } \sum_{x \in \mathcal{X}} q(x) = 1 \text{)} \end{aligned}$$

So equivalently, we have $D(p(x)\|q(x)) \geq 0$. □

Corollary 1: Proof of (3)

Proof of (3).

Follows from part (2): $I(X; Y) = D(p(x, y) \| p(x)p(y)) \geq 0$. □

Advanced Properties of Entropy

Remark 5: Question 2 – What finite distributions extremize entropy?

Remark

Question 2: What finite distribution minimises and what distribution maximises the value of Entropy?

Let $X_p \sim B(p_1, \dots, p_n)$ be a categorical distribution. We can write the question as an optimisation problem: $\min_{p \in \mathbb{R}^n, \|p\|_1=1, p \geq 0} H(X_p)$.

From the figures, it seems plausible that the uniform distribution maximises entropy and a peaked distribution minimises entropy.

Theorem

- A peaked distribution minimises entropy: $H(X) = 0 \iff \exists x \in \mathcal{X} : p_X(x) = 1$.
- The uniform distribution maximizes entropy: $H(X) = \log |\mathcal{X}| \iff X \sim U(\mathcal{X})$.

Remark 5: Natural Questions about Entropy

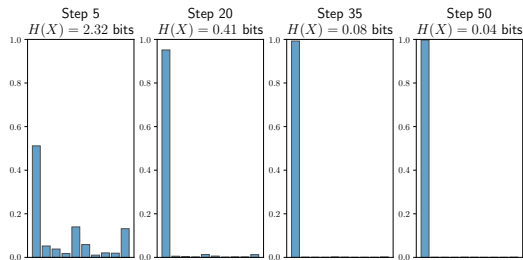


Figure 5: Peak Distribution minimises Entropy

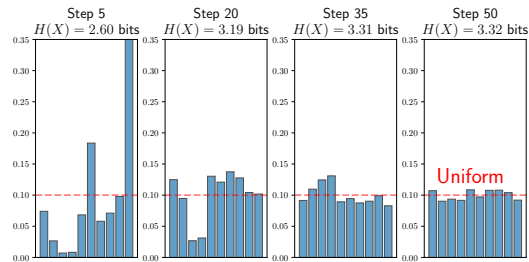


Figure 6: Uniform Distribution maximises Entropy

Theorem 5: Proof – Peaked distribution minimises entropy

Proof.

Let X be a discrete random variable with an entropy. Then we have

$$\begin{aligned} H(X) = 0 &\iff \forall x \in \mathcal{X} : p_X(x) \log p_X(x) = 0 \\ &\iff \forall x \in \mathcal{X} : p_X(x) = 0 \oplus p_X(x) = 1 \end{aligned}$$



Theorem 5: Proof – Uniform distribution maximises entropy

Proof.

Let $Y \sim U(\mathcal{X})$ st. $\forall x \in \mathcal{X} : q(x) = \frac{1}{|\mathcal{X}|}$.

$$\begin{aligned} 0 \leq D(p\|q) &= \mathbb{E}_p \left(\log \frac{p(X)}{q(X)} \right) = \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)} \\ &= \sum_{x \in \mathcal{X}} p(x) \log (p(x)|\mathcal{X}|) = \sum_{x \in \mathcal{X}} p(x) \log p(x) + \log |\mathcal{X}| \sum_{x \in \mathcal{X}} p(x) \\ &= -H(X) + \log |\mathcal{X}| = \log |\mathcal{X}| - H(X) \end{aligned}$$

This is equivalent to $H(X) \leq \log |\mathcal{X}|$. Lastly, Jensen's Inequality (3) yields the equivalence. \square

The Log-Sum Inequality and Convexity

Theorem 6: Log-Sum Inequality

Theorem (Log-Sum Inequality)

Let $n \in \mathbb{N}$, $a_1, \dots, a_n, b_1, \dots, b_n \geq 0$. Then we have

$$\sum_{i=1}^n a_i \log \frac{a_i}{b_i} \geq \left(\sum_{i=1}^n a_i \right) \log \frac{\sum_{i=1}^n a_i}{\sum_{i=1}^n b_i}$$

Theorem 7: Convexity of Relative Entropy

Theorem (Convexity of Relative Entropy)

$D(\cdot\|\cdot)$ is a convex function. This means that

$$\begin{aligned}\forall p_1, q_1, p_2, q_2, \forall \lambda \in [0, 1] : \quad & D(\lambda p_1 + (1 - \lambda)p_2 \| \lambda q_1 + (1 - \lambda)q_2) \\ & \leq \lambda D(p_1 \| q_1) + (1 - \lambda)D(p_2 \| q_2)\end{aligned}$$

Theorem 7: Proof

Proof.

Let p_1, q_1, p_2, q_2 be probability mass functions on \mathcal{X} . Let $\lambda \in (0, 1)$.

First of all, the set of probability densities is convex. So the above statement is well-defined.

Secondly, the inequality needs to be verified:

$$\begin{aligned} & D(\lambda p_1 + (1 - \lambda)p_2 \| \lambda q_1 + (1 - \lambda)q_2) \\ &= \sum_{x \in \mathcal{X}} (\lambda p_1(x) + (1 - \lambda)p_2(x)) \log \frac{\lambda p_1(x) + (1 - \lambda)p_2(x)}{\lambda q_1(x) + (1 - \lambda)q_2(x)} && \text{(by definition)} \\ &\leq \sum_{x \in \mathcal{X}} \lambda p_1(x) \log \frac{p_1(x)}{q_1(x)} + (1 - \lambda)p_2(x) \log \frac{p_2(x)}{q_2(x)} && \text{(log-sum inequality)} \\ &= \lambda D(p_1 \| q_1) + (1 - \lambda)D(p_2 \| q_2) && \text{(by definition)} \end{aligned}$$



Application to Optimisation

Example 5: MNIST Digit Classification

Example (MNIST Digit Classification)

We can now apply the concept of Relative Entropy to solve a common classification problem from machine learning. Let Ω be the set of 28x28 pixel images that contain exactly one handwritten digit from 0 to 9. The task is to predict the digit 0 to 9, based on the input image $\omega \in \Omega$.

In order to accomplish this task, we define a model $f : \mathbb{R}^n \rightarrow \mathbb{R}_+^{10}$ with $n \in \mathbb{N}$. This function f takes parameters as inputs that allow it to output a probability mass function that indicates the digit in the image. So $\forall \omega \in \Omega : f(\omega) \geq 0 \wedge \sum_{i=1}^{10} f(\omega)_i = 1$.

Example 5: MNIST Digit Classification (1/2)

The optimisation objective is

$$\Phi = \operatorname{argmin}_{\phi \in \mathbb{R}^n} D(d \| f_{\phi})$$

As we have shown in Theorem 7, the Relative Entropy is a convex function.

For f , we can use a two-layer convolutional neural network with dropout. In this case, the model f is not a convex function itself. So the optimisation objective is not convex either. But at least the loss function $D(d \| \cdot)$ is convex. We can now use Stochastic Gradient Descent to optimise for 60 steps with step size $5e-3$ and batch size 512.

Example 5: MNIST Digit Classification (2/2)

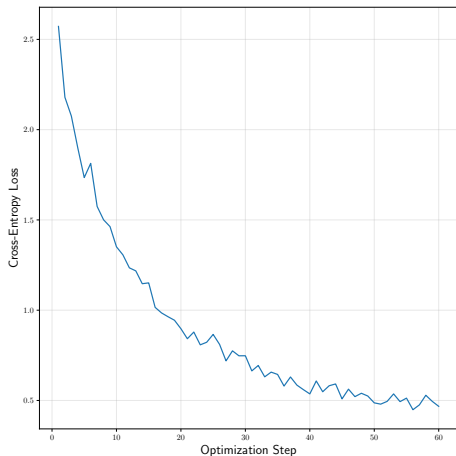


Figure 7: MNIST objective function

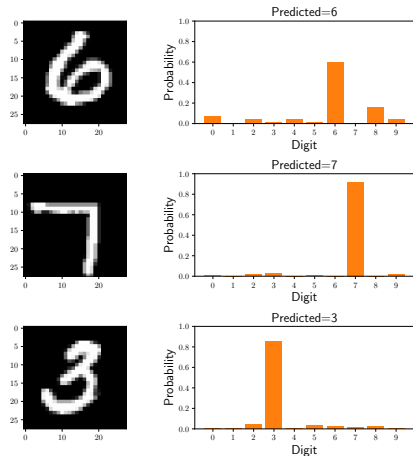


Figure 8: MNIST images and pred. digit distr.

Conclusion

- Defined **Entropy**, **Mutual Information**, and **Relative Entropy**
- Established **Chain Rules** for entropy and mutual information
- Proved **Jensen's Inequality** and non-negativity of entropy measures
- Showed which distributions **extremize entropy**
- Proved the **Log-Sum Inequality** and convexity of relative entropy
- Connected theory to practice via **Relative Entropy** loss in neural networks

 T. Cover and J. Thomas, *Elements of Information Theory*, Wiley, 2006.

Thank you!

Questions?