Introduction to Information Theory

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Contents

References

- Following closely Chris Bishops' PRML book, Chapter 2
- Kevin Murphy's, Machine Learning: A probablistic perspective, Chapter 2
- Jaynes, E. T. (2003). Probability Theory: The Logic of Science. Cambridge University Press.
- Bertsekas, D. and J. Tsitsiklis (2008). Introduction to Probability. Athena Scientific. 2nd Edition
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Introduction to Information Theory

- ***Information theory*** is concerned

  - with representing data in a compact fashion (***data compression*** *or* ***source coding***), and
  - transmitting and storing it in a way that is robust to errors (***error correction or channel coding***).

- To compactly representing data requires *allocating short codewords to highly probable bit strings*, and reserving longer codewords to less probable bit strings.

  - e.g. in natural language, common words (“a”, “the”, “and”) are much shorter than rare words.

- D. MacKay, Information Theory, Inference and Learning Algorithms (Video Lectures)

Introduction to Information Theory

- Decoding messages sent over noisy channels requires having a good probability model of the kinds of messages that people tend to send.

- We need *models that can predict which kinds of data are likely and which unlikely*.

- David MacKay, Information Theory, Inference and Learning Algorithms , 2003 (available on line)
- Thomas M. Cover, Joy A. Thomas , Elements of Information Theory , Wiley, 2006.
- Viterbi, A. J. and J. K. Omura (1979). *Principles of Digital Communication and Coding*. McGraw-Hill.

Introduction to Information Theory

- Consider a discrete random variable x. We ask how much information ('degree of surprise') is received when we observe (learn) a specific value for this variable?

- Observing a highly probable event provides little additional information.

- If we have two events x and y that are unrelated, then the information gain from observing both of them should be $h(x, y) = h(x) + h(y)$.

- Two unrelated events will be statistically independent, so $p(x, y) = p(x)p(y)$.

Entropy

- From $h(x,y) = h(x) + h(y)$ and $p(x,y) = p(x)p(y)$, it is easily shown that $h(x)$ must be given by the logarithm of $p(x)$ and so we have

$$h(x) = -\log_2 p(x) \geq 0$$

the units of *h(x)* are bits ('binary digits')

- Low probability events correspond to high information content.

- When transmitting a random variable**, the average amount of transmitted information is:**

$$Entropy\ of\ X : \mathbb{H}[X] = -\sum_{k=1}^{K} p(X=k)\log_2 p(X=k)$$

Noiseless Coding Theorem (Shanon)

- **Example 1** (Coding theory): x discrete random variable with 8 possible states; how many bits to transmit the state of x?

All states equally likely $$\mathbb{H}[x] = -8 \times \frac{1}{8} \log_2 \frac{1}{8} = 3\, bits$$

- **Example 2**: consider a variable having 8 possible states $\{a, b, c, d, e, f, g, h\}$ for which the respective (non-uniform) probabilities are given by ($1/2$, $1/4$, $1/8$, $1/16$, $1/64$, $1/64$, $1/64$, $1/64$).

The entropy in this case is smaller than for the uniform distribution.

x	a	b	c	d	e	f	g	h
$p(x)$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{64}$	$\frac{1}{64}$	$\frac{1}{64}$	$\frac{1}{64}$
code	0	10	110	1110	111100	111101	111110	111111

Note: shorter codes for the more probable events vs longer codes for the less probable events.

$$\mathbb{H}[x] = -\frac{1}{2}\log_2\frac{1}{2} - \frac{1}{4}\log_2\frac{1}{4} - \frac{1}{8}\log_2\frac{1}{8} - \frac{1}{16}\log_2\frac{1}{16} - \frac{4}{64}\log_2\frac{1}{64} = 2\, bits$$

$$average\ code\ length = \frac{1}{2}\times 1 + \frac{1}{4}\times 2 + \frac{1}{8}\times 3 + \frac{1}{16}\times 4 + 4\times\frac{1}{64}\times 6 = 2\, bits$$

Shanon's Noiseless Coding Theorem (1948): The entropy is a lower bound on the number of bits needed to transmit the state of a random variable

Alternative Definition of Entropy

- Considering a set of N identical objects that are to be divided amongst a set of bins, such that there are n_i objects in the i^{th} bin. Consider the number of different ways of allocating the objects to the bins.

- In the i^{th} bin there are $n_i!$ ways of reordering the objects (microstates), and so the total number of ways of allocating the N objects to the bins is given by (multiplicity)

$$W = \frac{N!}{\prod_i n_i!}$$

- The entropy is defined as $\mathbb{H} = \frac{1}{N}\ln W = \frac{1}{N}\ln N! - \frac{1}{N}\sum_i \ln n_i!$

- We now consider the limit $N \to \infty$, $\ln N! \approx N\ln N - N, \ln n_i! \approx n_i \ln n_i - n_i$

$$\mathbb{H} = -\lim_{N\to\infty}\sum_i \frac{n_i}{N}\ln\frac{n_i}{N} = -\sum_i p_i \ln p_i$$

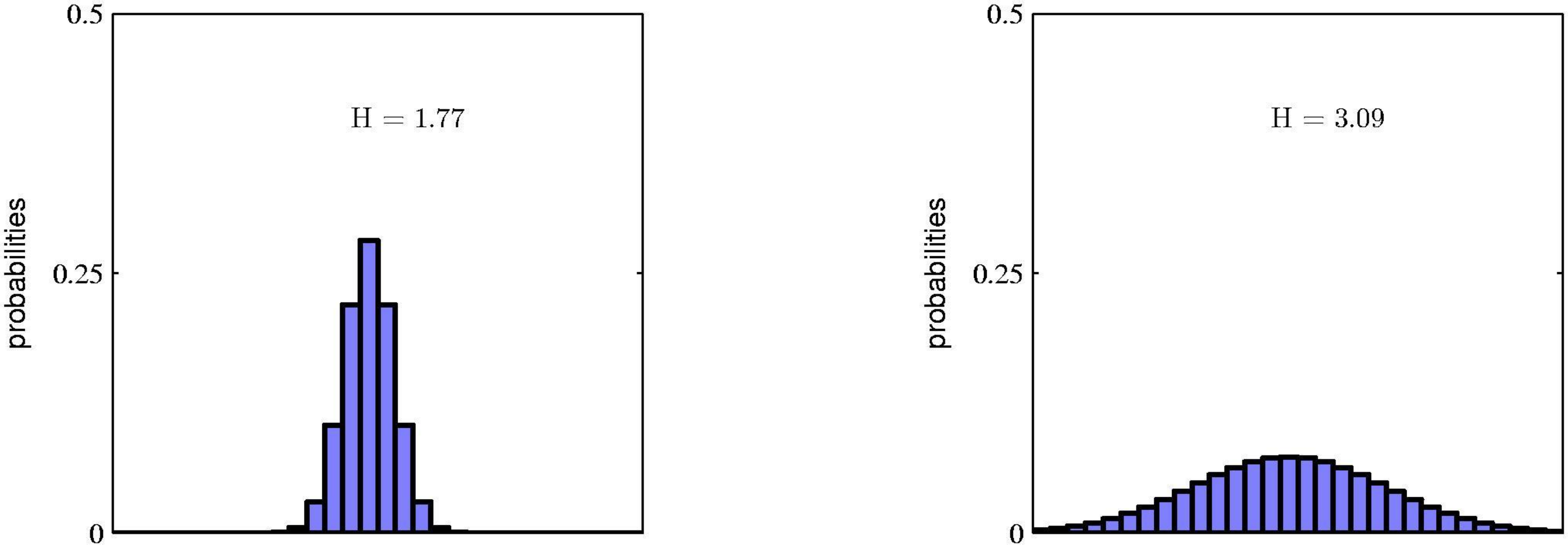
- p_i is the probability of an object assigned to the i^{th} bin.
- The occupation numbers p_i correspond to macrostates.

Alternative Definition of Entropy

- Interpret the bins as the states x_i of a discrete random variable X, where $p(X = x_i) = p_i$. The entropy of the random variable X is then

$$\mathbb{H}[p] = -\sum_i p(x_i) \ln p(x_i)$$

- *Distributions $p(x)$ that are sharply peaked around a few values will have a relatively low entropy, whereas those that are spread more evenly across many values will have higher entropy.*



Maximum Entropy: Uniform Distribution

- *The maximum entropy configuration* can be found by maximizing $\mathbb{H}$ using a Lagrange multiplier to enforce the normalization constraint on the probabilities. Thus we maximize

$$\overline{\mathbb{H}} = -\sum_i p(x_i)\ln p(x_i) + \lambda\left(\sum_i p(x_i) - 1\right)$$

- We find $p(x_i) = 1/M$, M is the number of possible states and $\mathbb{H} = \ln_2 M$.

- To verify that the stationary point is indeed a maximum, we can evaluate the 2nd derivative of the entropy, which gives

$$\frac{\partial^2 \overline{\mathbb{H}}}{\partial p(x_i)\partial p(x_j)} = -I_{ij}\frac{1}{p_i}$$

where I_{ij} are the elements of the identity matrix.

- ***For any discrete distribution with M states***, we have: $\mathbb{H}[x] \le \ln_2 M$

$$\mathbb{H} = -\sum_i p(x_i)\ln p(x_i) = \sum_i p(x_i)\ln\frac{1}{p(x_i)} \le \ln\sum_i p(x_i)\frac{1}{p(x_i)} = \ln M$$

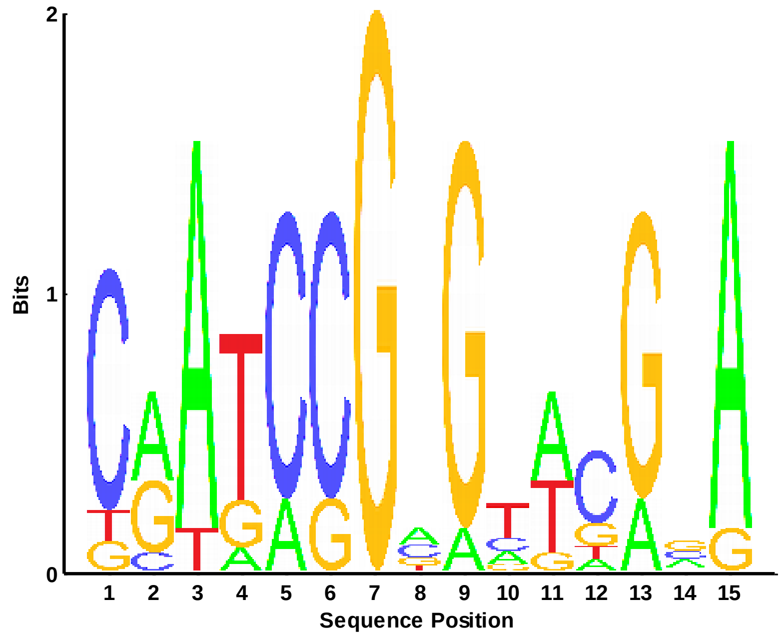
- Use Jensen's inequality (for the concave log)

For convex $f \Rightarrow f\left(\mathbb{E}[x]\right) \le \mathbb{E}[f(x)]$

$\mathbb{E}[\ln(x)] \le \ln\left(\mathbb{E}[x]\right)$, *Use* $x = \dfrac{1}{p(x)}$

Example: Biosequence Analysis

- Recall the DNA Sequence logo example earlier.
- The height of each bar is defined to be $2 - \mathbb{H}$, where $\mathbb{H}$ is the entropy of that distribution, and $2\ (= \ln_2 4)$ is the maximum possible entropy.
- Thus a bar of height 0 corresponds to a uniform distribution $(\ln_2 4)$, whereas a bar of height 2 corresponds to a deterministic distribution.



seqlogoDemo from PMTK

Binary Variable

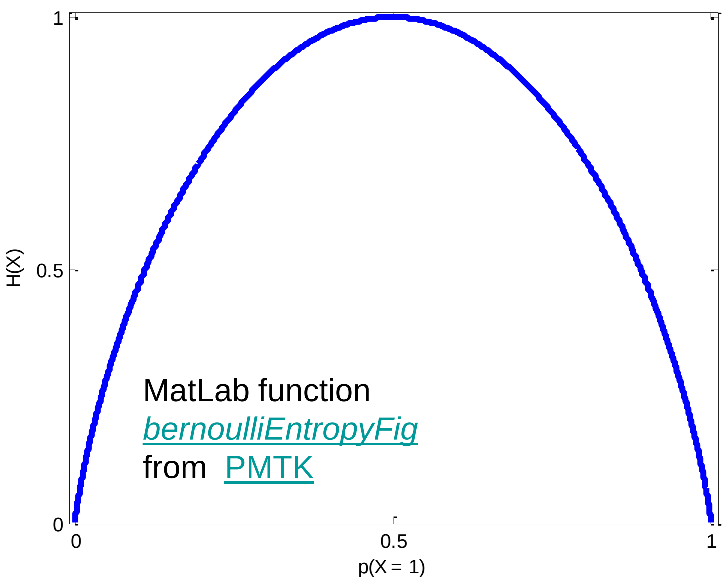
- Consider binary random variables, $X \in \{0, 1\}$, we can write $p(X = 1) = \theta$ and $p(X = 0) = 1 - \theta$.

$$X \in \{0,1\},\ p(X=1)=\theta,\ p(X=0)=1-\theta$$

- Hence the entropy becomes (binary entropy function)

$$\mathbb{H}[X] = -\left[\theta \log_2 \theta + (1-\theta)\log_2(1-\theta)\right]$$

- *The maximum value of 1 occurs when the distribution is uniform, $\theta = 0.5$.*



Differential Entropy

- Divide x into bins of width Δ. Assuming $p(x)$ is continuous, for each such bin, there must exist x_i such that

$$\int_{i\Delta}^{(i+1)\Delta} p(x)dx = p(x_i)\Delta = \textit{probability in falling in bin } \Delta$$

$$\mathbb{H}_\Delta = -\sum_i p(x_i)\Delta \ln\left(p(x_i)\Delta\right) = -\sum_i p(x_i)\Delta \ln\left(p(x_i)\right) - \ln\Delta$$

$$\lim_{\Delta\to 0}\left\{\sum_i p(x_i)\Delta \ln p(x_i)\right\} = -\int p(x)\ln p(x)dx \textit{ (can be negative)}$$

- *The $\ln\Delta$ term is omitted since it diverges as Δ→0 (indicating that infinite bits are needed to describe a continuous variable)*

Differential Entropy

- For a density defined over multiple continuous variables, denoted collectively by the vector $\boldsymbol{x}$, the differential entropy is given by

$$\mathbb{H}[\boldsymbol{x}] = -\int p(\boldsymbol{x}) \ln p(\boldsymbol{x}) d\boldsymbol{x}$$

- *Differential (unlike the discrete) entropy can be negative*

- When doing variable transformation $\boldsymbol{y}(\boldsymbol{x})$, use $p(\boldsymbol{x})d\boldsymbol{x} = p(\boldsymbol{y})d\boldsymbol{y}$, e.g. if $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ then:

$$\mathbb{H}[\boldsymbol{x}] = -\int p(\boldsymbol{y}) \ln\left(p(\boldsymbol{y}) |\boldsymbol{A}| \right) d\boldsymbol{y} = \mathbb{H}[\boldsymbol{y}] - \ln|\boldsymbol{A}| \Rightarrow \mathbb{H}[\boldsymbol{y}] = \mathbb{H}[\boldsymbol{x}] + \ln|\boldsymbol{A}|$$

Differential Entropy and the Gaussian Distribution

- The distribution that maximizes the differential entropy with constraints on the first two moments is a Gaussian:

$$\widetilde{\mathbb{H}} = -\int p(x)\ln p(x)dx + \lambda_1 \underbrace{\left(\int_{-\infty}^{+\infty} p(x)dx - 1\right)}_{Normalization} + \lambda_2 \underbrace{\left(\int_{-\infty}^{+\infty} xp(x)dx - \mu\right)}_{Given\ mean} + \lambda_3 \underbrace{\left(\int_{-\infty}^{+\infty} (x-\mu)^2 p(x)dx - \sigma^2\right)}_{Given\ std}$$

- Using calculus of variations ,

$$\delta\widetilde{\mathbb{H}} = -\int \delta p(x)\ln p(x)dx - \int \delta p(x)dx + \lambda_1 \int \delta p(x)dx + \lambda_2 \int x\delta p(x)dx + \lambda_3 \int (x-\mu)^2 \delta p(x)dx = 0$$

$$p(x) = e^{-1+\lambda_1+\lambda_2 x+\lambda_3 (x-\mu)^2} \underset{Use\ the\ constraints}{\Rightarrow} p(x) = \frac{1}{\left(2\pi\sigma^2\right)^{1/2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- Evaluating the differential entropy of the Gaussian, we obtain (an expression for a multivariate Gaussian is also given)

$$\mathbb{H}[x] = \frac{1}{2}\left(1+\ln\left(2\pi\sigma^2\right)\right) = \frac{1}{2}\ln\left(\left(2\pi e\right)^d \det\Sigma\right), d = 1, \det\Sigma = \sigma^2$$

Note $\mathbb{H}[x] < 0$ *for* $\sigma^2 < 1/(2\pi e)$

Kullback-Leibler Divergence and Cross Entropy

- Consider some unknown distribution $p(x)$, and suppose that we have modeled this using an approximating distribution $q(x)$.

- If we use $q(x)$ to construct a coding scheme for the purpose of transmitting values of x to a receiver, then the additional information to specify x is:

$$KL\left(p\,\|\,q\right) = \underbrace{-\int p(x)\ln q(x)dx}_{\substack{\text{I transmit q(x) but}\\ \text{I average it with the}\\ \text{exact probability p(x)}}} - \left(-\int p(x)\ln p(x)dx\right) = -\int p(x)\ln\left\{\frac{q(x)}{p(x)}\right\}dx$$

- The *cross entropy* is defined as:

$$\mathbb{H}\left(p,q\right) = -\int p(x)\ln q(x)dx$$

KL Divergence and Cross Entropy

- The cross entropy $\mathbb{H}(p,q) = -\int p(x)\ln q(x)dx$ is the average number of bits needed to encode data coming from a source with distribution *p* when we use model *q* to define our codebook.

- $\mathbb{H}(p)$=$\mathbb{H}(p,p)$ is the expected # of bits using the true model.

- *The KL divergence is the average number of extra bits needed to encode the data, because we used distribution q to encode the data instead of the true distribution p.*

- The "extra number of bits" interpretation makes it clear that

$$KL(p\|q) = -\int p(x)\ln q(x)dx - \left(-\int p(x)\ln p(x)dx\right) = -\int p(x)\ln\left\{\frac{q(x)}{p(x)}\right\}dx$$

- The KL distance is not a symmetrical quantity, that is

$$KL(p\|q) \neq KL(q\|p)$$

KL Divergence Between Two Gaussians

- Consider $p(x) = \mathcal{N}(x|\mu,\sigma^2)$ and $q(x) = \mathcal{N}(x|m,s^2)$.

$$KL(p\|q) = \underbrace{-\int p(x)\ln q(x)dx}_{\int \mathcal{N}(x|\mu,\sigma^2)\frac{1}{2}\left(\ln\left(2\pi s^2\right)+\frac{(x-m)^2}{s^2}\right)dx} \quad -\underbrace{\left(-\int p(x)\ln p(x)dx\right)}_{\frac{1}{2}\ln\left(2\pi e\sigma^2\right)}$$

- Note that the first term can be computed using the moments and normalization condition of a Gaussian and the second term from the differential entropy of a Gaussian.

- Finally we obtain:

$$\boxed{KL(p\|q) = \frac{1}{2}\left(\ln\left(\frac{s^2}{\sigma^2}\right) + \frac{\sigma^2+\mu^2-2\mu m+m^2}{s^2} - 1\right)}$$

KL Divergence Between Two Gaussians

- Consider now $p(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})$ and $q(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{m},\boldsymbol{L})$.

$$KL(p\,\|\,q) = \underbrace{-\int p(\boldsymbol{x})\ln q(\boldsymbol{x})d\boldsymbol{x}}_{\underbrace{\int \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma})\frac{1}{2}\left(D\ln(2\pi)+\ln|\boldsymbol{L}|+(\boldsymbol{x}-\boldsymbol{m})^T\boldsymbol{L}^{-1}(\boldsymbol{x}-\boldsymbol{m})\right)d\boldsymbol{x}}_{\frac{1}{2}\left(D\ln(2\pi)+\ln|\boldsymbol{L}|+Tr\left(\boldsymbol{L}^{-1}\left(\boldsymbol{\mu}\boldsymbol{\mu}^T+\boldsymbol{\Sigma}\right)\right)-\boldsymbol{\mu}^T\boldsymbol{L}^{-1}\boldsymbol{m}-\boldsymbol{m}^T\boldsymbol{L}^{-1}\boldsymbol{\mu}+\boldsymbol{m}^T\boldsymbol{L}^{-1}\boldsymbol{m}\right)}}$$

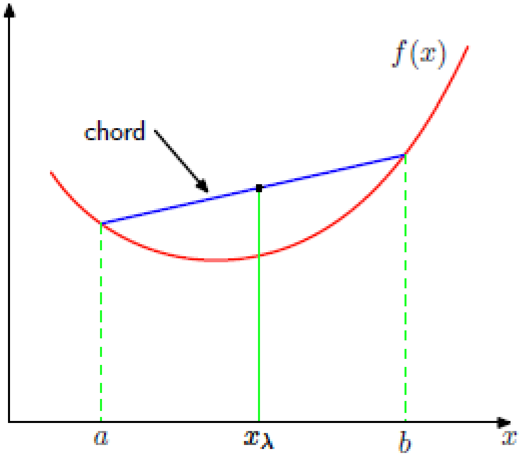
$$-\underbrace{\left(-\int p(\boldsymbol{x})\ln p(\boldsymbol{x})d\boldsymbol{x}\right)}_{\frac{1}{2}\ln|\boldsymbol{\Sigma}|+\frac{D}{2}\left(1+\ln(2\pi)\right)}$$

$$=\frac{1}{2}\left(-\frac{D}{2}+\ln\frac{|\boldsymbol{L}|}{|\boldsymbol{\Sigma}|}+Tr\left(\boldsymbol{L}^{-1}\left(\boldsymbol{\mu}\boldsymbol{\mu}^T+\boldsymbol{\Sigma}\right)\right)-\boldsymbol{\mu}^T\boldsymbol{L}^{-1}\boldsymbol{m}-\boldsymbol{m}^T\boldsymbol{L}^{-1}\boldsymbol{\mu}+\boldsymbol{m}^T\boldsymbol{L}^{-1}\boldsymbol{m}\right)$$

Jensen's Inequality

- *For a convex function f*, Jensen's inequality gives (can be proven easily by induction)

$$f\left(\sum_{i=1}^{M}\lambda_i x_i\right) \le \sum_{i=1}^{M}\lambda_i f(x_i),\ \lambda_i \ge 0 \ and \ \sum_i \lambda_i = 1$$



- This is equivalent (assume $M = 2$) to our requirement for convexity $f''(x) > 0$.

  - *Assume $f''(x) > 0$ (strict convexity) for any x.*

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x^*)(x - x_0)^2 > f(x_0) + f'(x_0)(x - x_0)$$

$$For\ x = a,b: \left.\begin{array}{l} f(a) > f(x_0) + f'(x_0)(a - x_0) \\ f(b) > f(x_0) + f'(x_0)(b - x_0) \end{array}\right\} \Rightarrow \lambda f(a) + (1-\lambda) f(b) > f(x_0) + f'(x_0)(\underbrace{\lambda a + (1-\lambda) b}_{Set:\, x_0} - x_0)$$

Jensen's inequality is thus shown: $\lambda f(a) + (1-\lambda) f(b) > f\left(\lambda a + (1-\lambda) b\right)$

Jensen's Inequality

- Assume Jensen's inequality. We should show that $f''(x) > 0$ (strict convexity) for any x.
- Set the following: $a = b - 2\varepsilon, b = a + 2\varepsilon > a, \varepsilon > 0$. Using Jensen's inequality, we can easily derive the above equation as:

$$\frac{1}{2}f(a)+\frac{1}{2}f(b) > f\left(0.5a+0.5b\right)$$

$$=\frac{1}{2}f\left(0.5(b-2\varepsilon)+0.5b\right)+\frac{1}{2}f\left(0.5a+0.5(a+2\varepsilon)\right)$$

$$=\frac{1}{2}f(b-\varepsilon)+\frac{1}{2}f(a+\varepsilon) \Rightarrow f(b)-f(b-\varepsilon) > f(a+\varepsilon)-f(a)$$

- For ε small, we thus have:

$$\frac{f(b)-f(b-\varepsilon)}{\varepsilon} > \frac{f(a+\varepsilon)-f(a)}{\varepsilon} \; or \; f'(b) > f'(a) \Rightarrow f(.) \; is \; convex$$

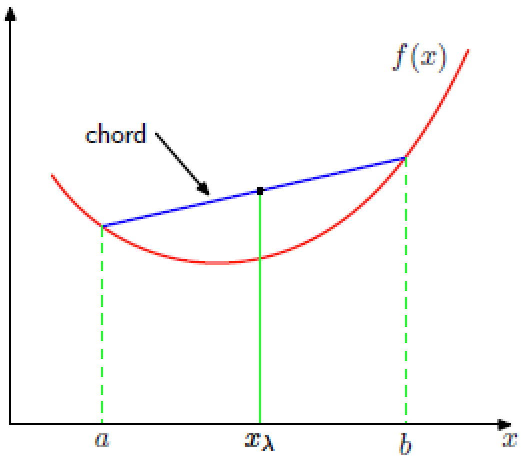
Jensen's Inequality

- Using Jensen's inequality $f\left(\sum_{i=1}^{M}\lambda_i x_i\right) \leq \sum_{i=1}^{M}\lambda_i f(x_i),\ \lambda_i \geq 0\ and\ \sum_i \lambda_i = 1$ for a discrete random variable results in:

$$Set:\ \lambda_i = p_i \Rightarrow f\left(\mathbb{E}[x]\right) \leq \mathbb{E}[f(x)]$$

- We can generalize this result to continuous random variables:

$$(for\ continuous\ rv)\ f\left(\int xp(x)dx\right) \leq \int f(x)p(x)dx$$



- We will use this shortly in the context of the KL distance.
- *We often use Jensen's inequality for concave functions (e.g. $\log x$). In that case, be sure you reverse the inequality!*

$$-\log\left(\mathbb{E}[x]\right) \leq \mathbb{E}[-\log(x)] \Rightarrow$$
$$\mathbb{E}[\log(x)] \leq \log\left(\mathbb{E}[x]\right)$$

Jensen's Inequality: Example

- As another example of Jensen's inequality, consider the arithmetic and geometric means of a set of real variables:

$$\bar{x}_A = \frac{1}{M}\sum_{i=1}^{M} x_i \,,\; \bar{x}_G = \left(\prod_{i=1}^{M} x_i\right)^{1/M}$$

- Using Jensen's inequality for $f(x) = \log(x)$ (concave), i.e.

$\mathbb{E}[\ln(x)] \le \ln(\mathbb{E}[x])$, we can show:

Uniform distribution $p(x_i) = \frac{1}{M}$

$$\ln\bar{x}_G = \frac{1}{M}\ln\left(\prod_{i=1}^{M} x_i\right) = \sum_{i=1}^{M}\frac{1}{M}\ln x_i \le \ln\left(\sum_{i=1}^{M}\frac{1}{M}x_i\right) = \ln\bar{x}_A \Rightarrow \bar{x}_G \le \bar{x}_A$$

The Kullback-Leibler Divergence

$$\mathbb{E}\left[\log(x)\right] \leq \log\left(\mathbb{E}\left[x\right]\right)$$

- Using Jensen's inequality, we can show *($-\log$ is a convex function)* that:

$$KL\left(p \,\|\, q\right) = -\int p(x) \ln\left\{\frac{q(x)}{p(x)}\right\} dx \geq -\ln \int p(x) \frac{q(x)}{p(x)} dx = -\ln \int q(x) dx = 0$$

- Thus we derive the following Information Inequality:

$$KL\left(p \,\|\, q\right) \geq 0, \, with \; KL\left(p \,\|\, q\right) \geq 0 \; if \;\; and \; only \; if \;\; p(x) = q(x)$$

Principle of Insufficient Reason

- An important consequence of the information inequality is that *the discrete distribution with the maximum entropy is the uniform distribution*.

- More precisely, $\mathbb{H}(X) \leq \log|\mathcal{X}|$, where $|\mathcal{X}|$ is the number of states for X, with equality iff $p(x)$ is uniform. To see this, let $u(x) = 1/|\mathcal{X}|$. Then

$$KL\left(p \| u\right) = -\sum_x p(x)\log u(x) + \sum_x p(x)\log p(x) = \log|\mathcal{X}| - \mathbb{H}(x) \geq 0$$

- This ***principle of insufficient reason***, argues in favor of using uniform distributions when there are no other reasons to favor one distribution over another.

The Kullback-Leibler Divergence

- Data compression is in some way related to density estimation.

- The Kullback-Leibler divergence is measuring the distance between two distributions and it is zero when the two densities are identical.

- Suppose the data is generated from an unknown $p(\boldsymbol{x})$ that we try to approximate with a parametric model $q(\boldsymbol{x}|\theta)$. Suppose we have observed training points $\boldsymbol{x}_n \sim p(\boldsymbol{x}), n = 1, \ldots, N$. Then:

$$KL\left(p \| q\right) = -\int p(x) \ln\left\{\frac{q(x)}{p(x)}\right\} dx \underset{\substack{\text{Sample average} \\ \text{approximation} \\ \text{of the mean}}}{\approx} \frac{1}{N}\sum_{n=1}^{N}\left\{-\ln q\left(\boldsymbol{x}_n \mid \theta\right) + \ln p(\boldsymbol{x}_n)\right\}$$

The KL Divergence Vs. MLE

- Note that only the first term is a function of q.

- Thus minimizing $KL(p \| q)$ is equivalent to maximizing the likelihood function for θ under the distribution q.

$$KL(p \| q) = -\int p(\boldsymbol{x}) \ln \left\{ \frac{q(\boldsymbol{x})}{p(\boldsymbol{x})} \right\} dx \approx \frac{1}{N} \sum_{n=1}^{N} \left\{ -\ln q(\boldsymbol{x}_n \mid \theta) + \ln p(\boldsymbol{x}_n) \right\}$$

- So the MLE estimate minimizes the KL divergence to the empirical distribution

$$p_{emp}(\boldsymbol{x}) = \frac{1}{N} \sum_{n=1}^{N} \delta_{\boldsymbol{x}_n}(\boldsymbol{x})$$

$$\arg\min_{q} KL\left(p_{emp}(\boldsymbol{x}) \| q\right) = -\int p_{emp}(\boldsymbol{x}) \ln \left\{ \frac{q(\boldsymbol{x})}{p_{emp}(\boldsymbol{x})} \right\} d\boldsymbol{x} = const - \frac{1}{N} \sum_{n=1}^{N} \ln q(\boldsymbol{x}_n \mid \theta)$$

Conditional Entropy

- For a joint distribution, *the conditional entropy* is

$$\mathbb{H}[y \mid x] = -\iint p(y,x) \ln p(y \mid x) dy dx$$

- This represents the average information to specify y if we already know the value of x

- It is easily seen, using $p(y,x) = p(y \mid x) p(x)$, and substituting inside the log in $\mathbb{H}[x,y] = -\iint p(x,y) \ln p(x,y) dy dx$ that the conditional entropy satisfies the relation

$$\mathbb{H}[x,y] = \mathbb{H}[y \mid x] + \mathbb{H}[x]$$

where $\mathbb{H}[x,y]$ is the differential entropy of $p(x,y)$ and $\mathbb{H}[x]$ is the differential entropy of $p(x)$.

Conditional Entropy for Discrete Variables

- Consider *the conditional entropy* for discrete variables

$$\mathbb{H}[y\,|\,x] = -\sum_i \sum_j p(y_i, x_j) \ln p(y_i\,|\,x_j)$$

- To understand further the meaning of conditional entropy, *let us consider the implications of* $\mathbb{H}[y|x] = 0$.

- We have:

$$\mathbb{H}[y\,|\,x] = \sum_i \sum_j \underbrace{\left(-p(y_i\,|\,x_j) \ln p(y_i\,|\,x_j)\right)}_{\geq 0} p(x_j) = 0$$

- From this we can conclude that $\textit{For each } x_j \textit{ s.t. } p(x_j) \neq 0$

$$\textit{the following must hold}: p(y_i\,|\,x_j) \ln p(y_i\,|\,x_j) = 0$$

- Since $plogp = 0 \leftrightarrow p = 0$ or $p = 1$ and since $p(y_i|x_j)$ is normalized, there is only one y_i s.t. $p(y_i\,|\,x_j) = 1$ with all other $p(.\,|\,x_j) = 0$. Thus y is a function of x.

Mutual Information

- If the variables are not independent, we can gain some idea of whether they are 'close' to being independent by considering the KL divergence between the joint distribution and the product of the marginals:

$$Mutual\ Information : \mathbb{I}[x,y] = KL\big(p(x,y)\,||\,p(x)p(y)\big) =$$

$$= -\iint p(x,y)\ln\frac{p(x)p(y)}{p(x,y)}dxdy \geq 0$$

$$\mathbb{I}[x,y] = 0 \ iff \ \ x,y \ independent$$

- The mutual information is related to the conditional entropy through

$$\mathbb{I}[x,y] = -\iint p(x,y)\ln\frac{p(y)}{p(y|x)}dxdy = \mathbb{H}[y] - \mathbb{H}[y|x] \Rightarrow$$

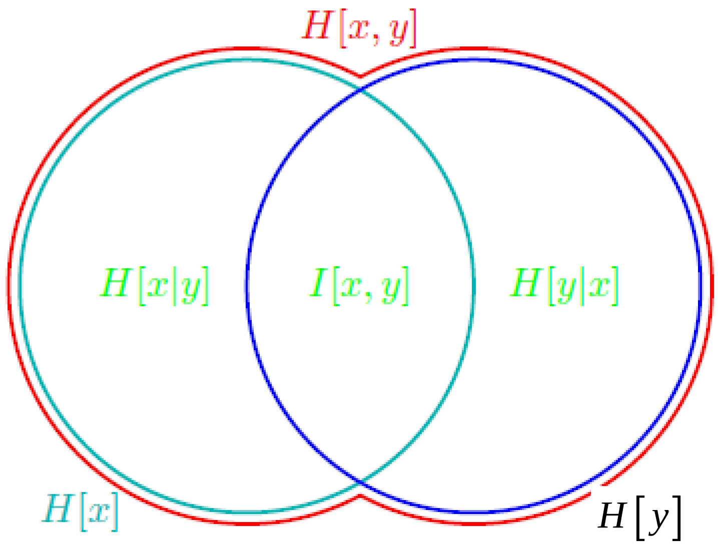
$$\mathbb{I}[x,y] = \mathbb{H}[x] - \mathbb{H}[x|y] = \mathbb{H}[y] - \mathbb{H}[y|x]$$

Mutual Information

- The mutual information represents the reduction in the uncertainty about x once we learn the value of y (and reversely).

$$\mathbb{I}[x,y]=\mathbb{H}[x]-\mathbb{H}[x\,|\,y]=\mathbb{H}[y]-\mathbb{H}[y\,|\,x]$$

$$\mathbb{H}[x]\geq\mathbb{H}[x\,|\,y]$$
$$\mathbb{H}[y]\geq\mathbb{H}[y\,|\,x]$$



- In a Bayesian setting, $p(x)$ =prior, $p(x|y)$ posterior, and $\mathbb{I}[x,y]$ represents the reduction in uncertainty in x once we observe y.

Note that $\mathbb{H}[x,y] \leq \mathbb{H}[x] + \mathbb{H}[y]$

- This is easy to prove noticing that

$$\mathbb{I}[x,y] = \mathbb{H}[y] - \mathbb{H}[y \mid x] \geq 0 \; (KL\ \textit{divergence})$$

and

$$\mathbb{H}[x,y] = \mathbb{H}[y \mid x] + \mathbb{H}[x]$$

from which

$$\mathbb{H}[x,y] = \mathbb{H}[x] + \mathbb{H}[y] - \mathbb{I}[x,y] \leq \mathbb{H}[x] + \mathbb{H}[y]$$

- *The equality here is true only if x, y are independent:*

$$\mathbb{H}[x,y] = -\iint p(x,y) \ln p(x,y) dy dx = -\iint p(x,y) \left(\ln p(x) + \ln p(y) \right) dy dx = \mathbb{H}[x] + \mathbb{H}[y]$$

(sufficiency condition)

$\mathbb{H}[y \mid x] = \mathbb{H}[y] \Rightarrow \mathbb{I}[x,y] = 0 \Rightarrow p(x,y) = p(x)p(y)$ (necessary condition)

Mutual Information for Correlated Gaussians

- Consider two correlated Gaussians as follows:

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} X \\ Y \end{pmatrix} \middle| \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{bmatrix} \sigma^2 & \rho\sigma^2 \\ \rho\sigma^2 & \sigma^2 \end{bmatrix} \right)$$

- For each of these variables we can write:

$$\mathbb{H}[X] = \mathbb{H}[Y] = \frac{1}{2}\ln\left(2\pi e\sigma^2\right)$$

- The joint entropy is also given similarly as

$$\mathbb{H}[X,Y] = \frac{1}{2}\ln\left((2\pi e)^2 \underbrace{\sigma^4(1-\rho^2)}_{\det\Sigma} \right)$$

- *Thus:*

$$\mathbb{I}[x,y] = \mathbb{H}[x] + \mathbb{H}[y] - \mathbb{H}[x,y] = \frac{1}{2}\log\frac{1}{1-\rho^2}$$

- *Note:*

$$\rho = 0 \; (independent \; X,Y) \Rightarrow \mathbb{I}[x,y] = 0$$

$$\rho = \pm 1 \; (linear \; correlated \; X = \pm Y) \Rightarrow \mathbb{I}[x,y] = \infty$$

Pointwise Mutual Information

- A quantity which is closely related to MI is the ***pointwise mutual information*** *or PMI*. For two events (not random variables) x and y, this is defined as

$$PMI(x,y) =: -\log \frac{p(x)p(y)}{p(x,y)} = \log \frac{p(x|y)}{p(x)} = \log \frac{p(y|x)}{p(y)}$$

- This measures the discrepancy between these events occurring together compared to what would be expected by chance. *Clearly the MI, $\mathbb{I}[x,y]$, of X and Y is just the expected value of the PMI.*

- *This is the amount we learn from updating the prior $p(x)$ into the posterior $p(x|y)$,* or equivalently, updating the prior $p(y)$ into the posterior $p(y|x)$.

Mutual Information

- For continuous random variables, it is common to first ***discretize*** *or* ***quantize*** *them into bins*, and computing how many values fall in each histogram bin (Scott 1979).

- The number of bins used, and the location of the bin boundaries, can have a significant effect on the results.

- One can estimate the MI directly, *without performing density estimation* (Learned-Miller, 2004). Another approach is to *try many different bin sizes and locations, and to compute the maximum MI achieved*.

- Scott, D. (1979). On optimal and data-based histograms, *Biometrika 66*(3), 605–610.
- Learned-Miller, E. (2004). Hyperspacings and the estimation of information theoretic quantities. Technical Report 04-104, U. Mass. Amherst Comp. Sci. Dept.
- Reshef, D., Y. Reshef, H. Finucane, S. Grossman, G. McVean, P. Turnbaugh, E. Lander, M. Mitzenmacher, and P. Sabeti (2011, December). Detecting novel associations n large data sets. *Science 334*, 1518–1524.
- Speed, T. (2011, December). A correlation for the 21st century. *Science 334*, 152–1503.

*Use MatLab function *miMixedDemo* from Kevin Murphys' PMTK

Maximal Information Coefficient

- This statistic appropriately normalized is known as the **maximal information coefficient** (MIC).

- We first define: $m(x,y)=\dfrac{\max_{G\in\mathcal{G}(x,y)}\mathbb{I}\big(X(G);Y(G)\big)}{\log\min(x,y)}$

- *Here* $\mathcal{G}(x,y)$ is the set of $2d$ *grids of size* $x\times y$, and $X(G), Y(G)$ *represents a discretization of the variables onto this grid* (The maximization over bin locations is performed efficiently using *dynamic programming*)

- Now define the MIC as

$$MIC=\max_{x,y:\,xy<B} m(x,y)$$

- Reshef, D., Y. Reshef, H. Finucane, S. Grossman, G. McVean, P. Turnbaugh, E. Lander, M. Mitzenmacher, and P. Sabeti (2011, December). Detecting novel associations n large data sets. *Science 334*, 1518–1524.

Maximal Information Coefficient

- The MIC is defined as:

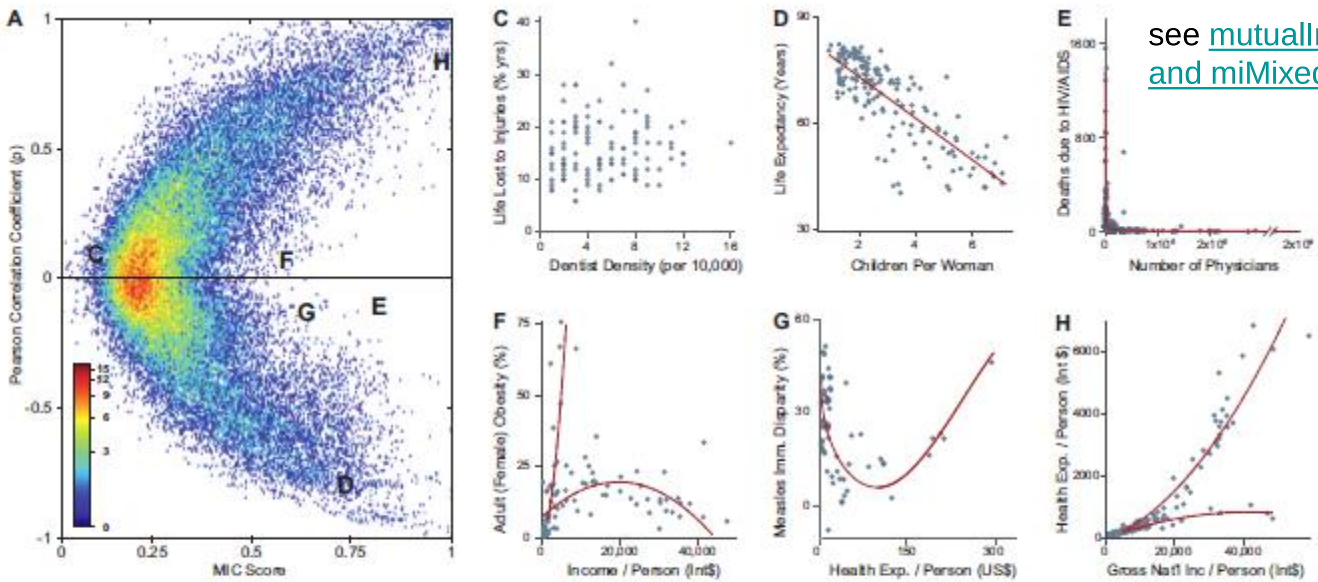
$$m(x,y) = \frac{\max_{G \in \mathcal{G}(x,y)} \mathbb{I}\big(X(G);Y(G)\big)}{\log \min(x,y)} \qquad MIC \equiv \max_{x,y:xy<B} m(x,y)$$

- B is some sample-size dependent bound on the number of bins we can use and still reliably estimate the distribution (Reshef et al. suggest $B \sim N^{0.6}$).

- MIC lies in the range $[0,1]$, where 0 represents no relationship between the variables, and 1 represents a noise-free relationship of any form, not just linear.

- Reshef, D., Y. Reshef, H. Finucane, S. Grossman, G. McVean, P. Turnbaugh, E. Lander, M. Mitzenmacher, and P. Sabeti (2011, December). Detecting novel associations n large data sets. *Science 334*, 1518–1524.

Correlation Coefficient Vs MIC

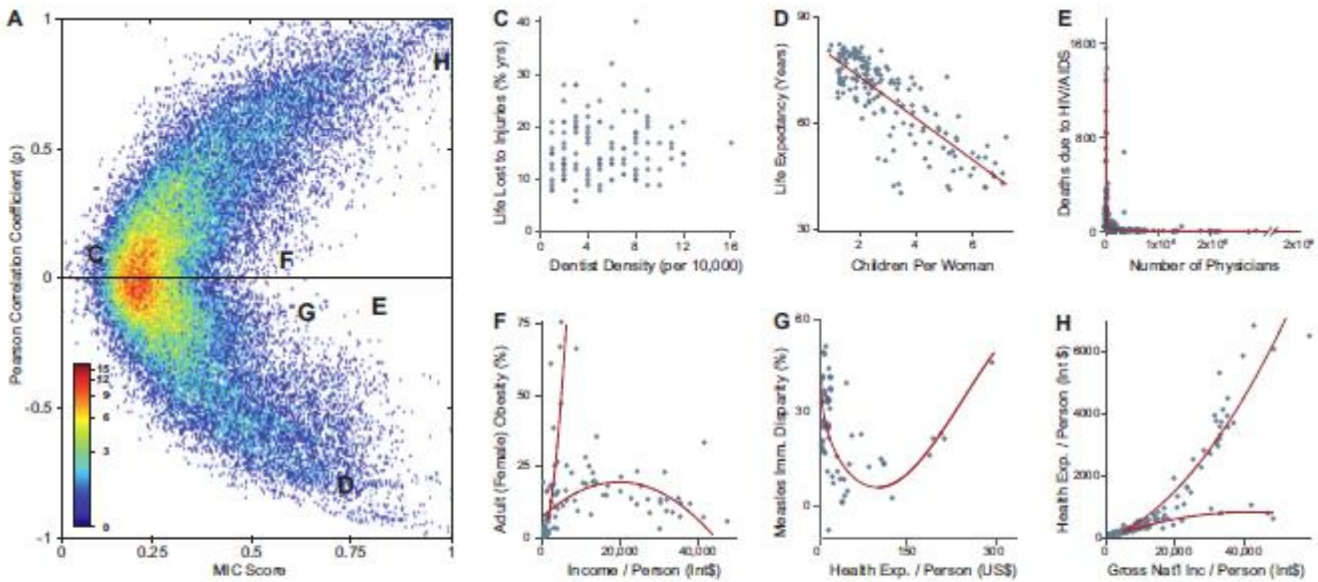


see [mutualInfoAllPairsMixed]() for [and miMixedDemo]()from [PMTK3]()

- [Reshef, D.,]()Y. Reshef, H. Finucane, S. Grossman, G. McVean, P. Turnbaugh, E. Lander, M. Mitzenmacher, and P. Sabeti (2011, December). [Detecting novel associations n large data sets](). *Science 334*, 1518–1524.

- The data consists of 357 variables measuring a variety of social, economic, etc. indicators, collected by WHO.
- On the left, we see the *correlation coefficient (CC) plotted against the MIC for all 63,566 variable pairs.*
- On the right, we see scatter plots for particular pairs of variables.

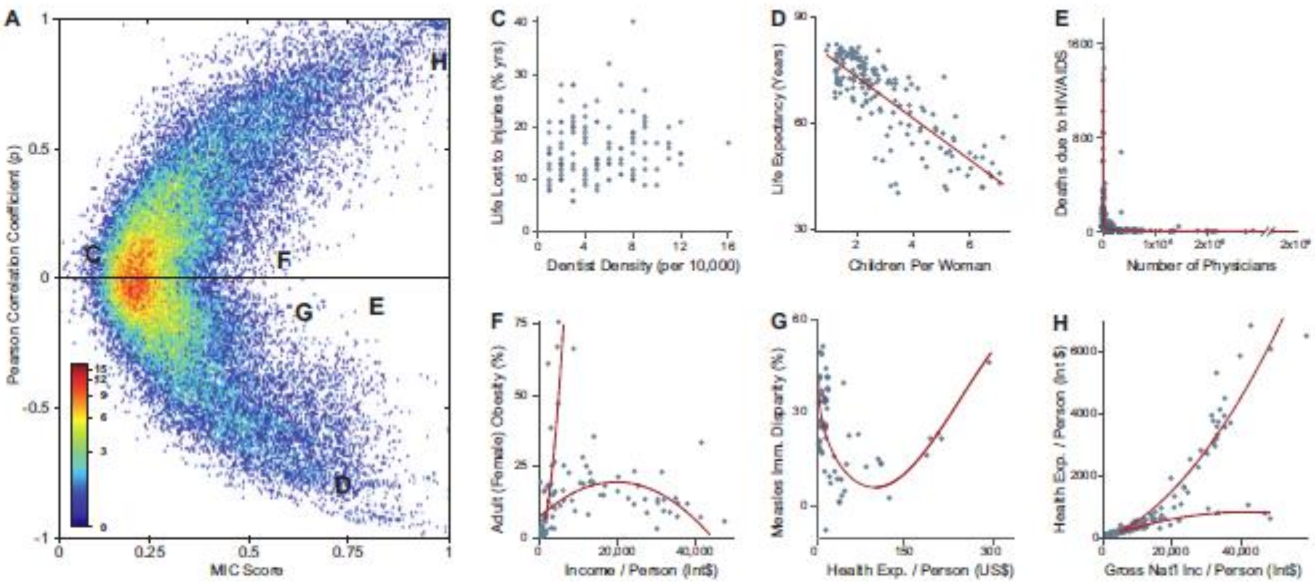
Correlation Coefficient Vs MIC



- ❑ Point marked C has a *low CC and a low MIC*. From the corresponding scatter we see that there is *no relationship between these two variables.*

- ❑ The points marked D and H have high CC (in absolute value) and high MIC and we see from the scatter plot that they represent nearly linear relationships.

Correlation Coefficient Vs MIC



- The points E, F, and G have low CC but high MIC. They correspond to non-linear (and sometimes, as in E and F, one-to-many) relationships between the variables.

- Statistics (such as MIC) based on mutual information can be used to discover interesting relationships between variables in a way that correlation coefficients cannot.