Lower bounds on mutual information

David V. Foster[1] and Peter Grassberger[2,3]

[1]*Complexity Science Group, University of Calgary, Calgary, Canada T2N 1N4*
[2]*Complexity Science Group, University of Calgary, Calgary, Canada*
[3]*John von Neumann Institut für Computing, FZ Jülich, D-52425 Jülich, Germany*

We correct claims about lower bounds on mutual information (MI) between real-valued random variables made by Kraskov *et al.*, Phys. Rev. E **69**, 066138 (2004). We show that non-trivial lower bounds on MI in terms of linear correlations depend on the marginal (single variable) distributions. This is so in spite of the invariance of MI under reparametrizations, because linear correlations are not invariant under them. The simplest bounds are obtained for Gaussians, but the most interesting ones for practical purposes are obtained for uniform marginal distributions. The latter can be enforced in general by using the ranks of the individual variables instead of their actual values, in which case one obtains bounds on MI in terms of Spearman correlation coefficients. We show with gene expression data that these bounds are in general nontrivial, and the degree of their (non)saturation yields valuable insight.

Mutual information [1] between two objects is the difference between the combined lengths of their individual descriptions and the length of a joint description, all descriptions being "optimal," i.e. lossless and redundancy-free. In the framework of algorithmic information theory [2], this is taken literally, i.e. the "objects" are sequences of letters of some alphabet, and "description" means a compression of the sequence on some specified but otherwise arbitrary universal Turing machine. In the framework of Shannon theory, in contrast, we deal with random variables, and "description length" is to be understood as the minimal *average* information needed to specify their realizations, given the probability distributions.

In the following we shall only use the Shannon framework, but we shall not forget entirely about individual objects. When confronted with them, we make some (explicit or implicit) estimate about the probability distribution (assuming that the observed objects are in some sense "typical"); computing their MI is actually a problem of statistical inference.

More precisely, consider two random variables X and Y with realizations x and y and probability densities $p_X(x)$ and $p_Y(y)$. For simplicity we shall assume that x and y are both scalars taken either from a finite interval or from the interval $[-\infty,\infty]$. In both cases p_X and p_y are normalized to 1. The joint distribution is $p(x,y)$. The MI is then defined as

$$I(X:Y) = \int dxdy\, p(x,y) \log \frac{p(x,y)}{p_X(x)p_Y(y)}, \qquad (1)$$

where the base of the logarithm specifies the units in which information is measured. Bits correspond to logarithm base 2.

From this one sees that I is symmetrical, $I(X:Y) = I(Y:X)$, and positive definite: $I(X:Y) = 0$ if and only if X and Y are strictly independent. Thus $I(X:Y)$ is a universal measure of dependency, being nonzero whenever X and Y have anything in common. This can also be seen in the following way: the (differential) entropy $H(X) = -\int dx p_X(x) \log p_X(x)$ is

the (negative) average log-likelihood of x, and

$$I(X:Y) = H(X) - H(X|Y) \qquad (2)$$

is the logarithm of the ratio between the unconditioned likelihood of x and the posterior likelihood conditioned on the value y of Y.

For the differential entropy, there is a well-known upper bound in terms of the variance: $H(X)$ is maximal for a Gaussian with the same variance as the data [1]. Indeed, this is true also for multivariate distributions. In the Appendix of [3], a formal proof based on Lagrangian multipliers was given that analogous bounds hold also for the MI. According to [3], a given covariance matrix implies a lower bound on the MI. Unfortunately, this proof is wrong, and the claim made in [3] is incorrect (see also the Erratum [4]). The error in [3] was subtle: The unique solution of the Lagrangian variational problem was given correctly, but the fact was missed that this solution is in general a saddle point, the correct bound being an infimum which is not reached by any actual distribution (at least not by a distribution in the class admitted in the variational problem).

Indeed, it is easily seen that the MI can be arbitrarily small for any value of the correlation. Assume that the joint distribution is a sum of a δ peak with weight $1 - \epsilon$ centered at $(x,y) = (1,1)$ and a two-dimensional (2D) Gaussian with weight ϵ centered at the origin,

$$p(x,y) = (1-\epsilon)\delta(x-1)\delta(y-1) + \frac{\epsilon}{2\pi\sigma^2}e^{-\frac{x^2+y^2}{2\sigma^2}}. \qquad (3)$$

Then the correlation between X and Y varies between zero and one as the width σ shrinks to zero, for any fixed $\epsilon > 0$. But the MI is bounded for all σ by $I(X:Y) \leqslant -\epsilon \log \epsilon - (1-\epsilon)\log(1-\epsilon)$, which tends to zero as $\epsilon \to 0$. Thus the MI can be arbitrarily close to zero, even when the correlation is arbitrarily close to 1—although this is unlikely to appear in real applications, except for outliers.

It is the purpose of the present paper to present correct bounds replacing those given in [3]. As we shall see, to obtain nontrivial bounds for the MI, one needs both the covariance matrix and the marginal distributions. But the latter can be

chosen arbitrarily to a large extent, since $I(X : Y)$ as defined in Eq. (1) is invariant under homeomorphism. Let $\phi(x)$ be a continuous and monotonic function, such that its inverse $\phi^{-1}(x)$ is also continuous and monotonic, and let X' be a random variable with realization $x' = \phi(x)$ if X has realization x. Then

$$p_X(x) = \left| \frac{d\phi(x)}{dx} \right| p_{X'}(x'), \qquad (4)$$

and $I(X : Y) = I(X' : Y)$. By symmetry, the same holds for homeomorphisms of Y.

This leads to the following strategy for obtaining bounds on $I(X : Y)$: One first transforms X and Y independently so that they have a given distribution, e.g., a Gaussian or a uniform distribution. Notice that the first and second moments in general will change during such a transformation. After that is done, one applies the bound suitable for the chosen marginal distributions.

The case of Gaussian marginal distributions is the simplest to treat theoretically. In that case the arguments given in the Appendix of [3] apply, and the MI is bounded from below by the MI of a joint Gaussian with the observed first and second moments. But this is not the most practical choice, because it is nontrivial to transform any empirical distribution into a Gaussian.

For practical purposes much more suitable is transformation to uniform distributions over finite intervals, say $x' \in [-1,1]$ and $y' \in [-1,1]$. This transformation, which also leads usually to improved MI estimates, is *de facto* achieved by using for x' and y' their normalized ranks. Assume that the empirical data consist of N pairs (x_i, y_i), $i = 1, \ldots, N$. Then the rank r_i of x_i is defined as the number of values x_j which are less than or equal to x_i (here we assume that all x_i are different, as is true with probability 1 if X is drawn from a continuous distribution; if there are degeneracies due, e.g., to discretization, we remove them by adding small random fluctuations to x_i). Finally,

$$x_i' = 2r_i/N - 1. \qquad (5)$$

and analogously for y. Notice that this does not, strictly speaking, define X', as it defines the homeomorphism ϕ only at the discrete values x_i, but this does not pose a practical problem. Furthermore, in the limit $N \to \infty$ the "empirical $\phi(x)$" tends with probability 1 toward a true homeomorphism. The linear correlation between the ranks of x and y is by definition the Spearman coefficient $S = C_{X'Y'}$ [5].

To obtain a bound on the MI for given marginal distributions and given first and second moments, we use the Lagrangian method. Without loss of generality we assume that the data are centered, i.e., $\langle X \rangle = \langle Y \rangle = 0$. We use $p(x,y)$ as independent variables, and

$$p_X(x) = \int dy\, p(x,y), \quad p_Y(y) = \int dx\, p(x,y);$$
$$C_{XY} = \iint dx\, dy\, xy\, p(x,y)/[\sigma_X \sigma_Y] \qquad (6)$$

as constraints. The Lagrangian function is

$$\begin{aligned} L = &\iint dx\, dy\, p(x,y) \log \frac{p(x,y)}{p_X(x) p_Y(y)} \\ &+ \int dx\, \nu_X(x) \left[p_X(x) - \int dy\, p(x,y) \right] \\ &+ \int dy\, \nu_Y(y) \left[p_Y(y) - \int dx\, p(x,y) \right] \\ &+ \lambda \left[\sigma_X \sigma_Y C_{XY} - \iint dx\, dy\, xy p(x,y) \right], \qquad (7) \end{aligned}$$

where $\nu_X(x)$, $\nu_Y(y)$, and λ are Lagrangian parameters. The variational equations are

$$\frac{\delta L}{\delta p(x,y)} = \log \frac{p(x,y)}{p_X(x) p_Y(y)} + 1 - \nu_X(x) - \nu_Y(y) - \lambda xy = 0, \qquad (8)$$

which can also be written as

$$p(x,y) = f_X(x) f_Y(y) e^{-\lambda(x-y)^2} \qquad (9)$$

with unknown functions f_X, f_Y and unknown λ, all of which are determined by the constraints. The Kolmogorov consistency condition for $p_X(x)$, in particular, gives

$$\frac{p_X(x)}{f_X(x)} = \int dy f_Y(y) e^{-\lambda(x-y)^2}. \qquad (10)$$

In the following we shall discuss only the two cases of Gaussian and uniform marginals. For Gaussian marginals, one finds that $p(x,y)$ is also Gaussian, and thus the results of [3] are obtained,

$$I(X : Y) \geqslant I_{\text{Gauss}}^-(C_{XY}) \equiv -\tfrac{1}{2} \log\left(1 - C_{XY}^2\right). \qquad (11)$$

For uniform marginals, we indeed do not solve the problem of finding a bound I_{unif}^- on the MI for given S, but we solve the easier implicit problem of finding both I_{unif}^- and S for given λ. We do this recursively, starting with the zeroth approximation

$$f_X^{(0)}(x) = f_Y^{(0)}(y) = 1/2. \qquad (12)$$

From the kth approximation of f_X and f_Y we obtain the $(k+1)$st approximations by means of

$$\frac{1}{f_X^{(k+1)}(x)} = 2 \int_{-1}^{1} dy f_Y^{(k)}(y) e^{-\lambda(x-y)^2}, \qquad (13)$$

$$\frac{1}{f_Y^{(k+1)}(y)} = 2 \int_{-1}^{1} dx f_X^{(k)}(x) e^{-\lambda(x-y)^2}. \qquad (14)$$

When doing this, we observe that $f_X^{(k)}$ and $f_Y^{(k)}$ are even functions for each k, and that both indeed are equal. We can thus drop the subscripts and write the recursion as

$$f^{(k+1)}(x) = \left[2 \int_{-1}^{1} dy f^{(k)}(y) e^{-\lambda(x-y)^2} \right]^{-1}. \qquad (15)$$

TABLE I. Spearman coefficient and lower bound on the MI (in natural units).

λ	S	I_{unif}^{-}
0.00	0.0000	0.0000
0.25	0.0829	0.0034
0.50	0.1633	0.0135
0.75	0.2390	0.0292
1.00	0.3086	0.0495
1.25	0.3713	0.0729
1.50	0.4270	0.0984
2.00	0.5189	0.1517
2.50	0.5897	0.2040
3.00	0.6428	0.2531
4.00	0.7177	0.3396
5.00	0.7666	0.4123
6.00	0.8007	0.4746
7.00	0.8260	0.5292
8.00	0.8455	0.5777
9.00	0.8610	0.6215
10.00	0.8736	0.6614
11.50	0.8887	0.7156
13.00	0.9005	0.7636
15.00	0.9128	0.8208
17.00	0.9224	0.8717
20.00	0.9333	0.9389
23.00	0.9415	0.9975
27.00	0.9498	1.0657
32.00	0.9572	1.1393
40.00	0.9654	1.2366
50.00	0.9721	1.3357

After convergence, the joint density is obtained as

$$p(x,y) \propto \lim_{k \to \infty} f^{(k)}(x) f^{(k)}(y) e^{-\lambda(x-y)^2}. \quad (16)$$

Here we have left the normalization open, in order to allow for errors in the numerical integration which might have accumulated during the recursion. The proportionality constant is thus fixed by the normalization condition $\int p = 1$. Finally, S and the lower bound $I_{\text{unif}}^{-}(S)$ on $I(X:Y)$ are obtained by using Eq. (1) and

$$S = 3 \iint_{-1}^{1} dx\, dy\, xy\, p(x,y) e^{-\lambda(x-y)^2}. \quad (17)$$

Numerical results for several values of λ, obtained by using Gaussian quadrature for the integrals, are given in Table I. Except for values of S close to ± 1, $I_{\text{unif}}^{-}(S)$ is well approximated by

$$I_{\text{unif}}^{-}(S) \approx -\tfrac{1}{2}(1 - 0.122 S^2 + 0.053 S^{12}) \log(1 - S^2). \quad (18)$$

The two bounds for Gaussians [Eq. (11)] and for uniform distributions [Eq. (18)] are shown in Fig. 1.

As an application we show in Fig. 2 gene expression data obtained from human B lymphocyte cells [6]. In that experiment, the expressions of 12 600 different gene loci were
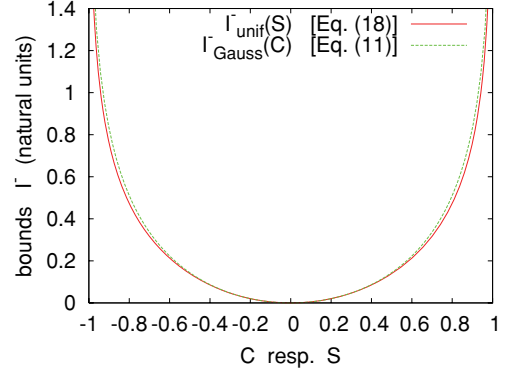

FIG. 1. (Color online) Lower bounds of MI in terms of the Spearman correlation coefficient (continuous line, red) and in terms of the Pearson correlation coefficient in the case of Gaussian marginals (dashed, green). For both curves, the MI is measured in natural units.

measured in 336 different conditions, with special interest in tumor cells. For each pair of genes the data can thus be represented as 336 points in a two-dimensional plane. Spearman coefficients were obtained by ranking both coordinates (after disambiguating degeneracies by adding low-level noise as explained above). Mutual informations were estimated using the k-nearest-neighbor method of [3] with $k = 40$. Although this was done for all $12\,600 \times 12\,599/2$ pairs, only results for the 12 599 pairs involving the important cancer gene BCL6 are shown in Fig. 2. We can make the following observations:

(a) The bound is respected by most pairs, and it forms roughly a lower envelope for the distribution.

(b) There are several pairs for which the bound is violated, mostly for small values of S. This reflects the fact that the MI estimator is not perfect. Indeed, no MI estimator can be perfect. Most estimators are chosen such that they never
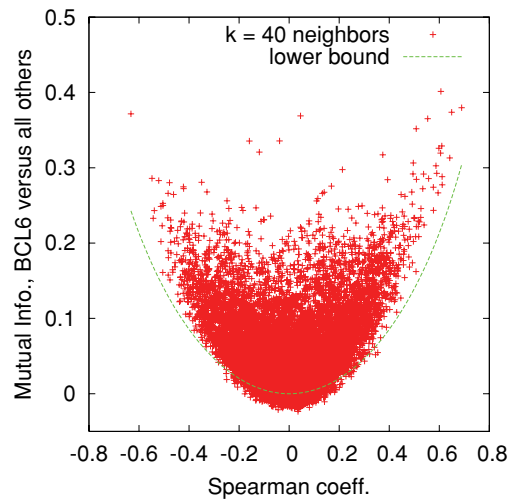

FIG. 2. (Color online) Mutual informations (in nats) between gene BCL6 and all the other 12 599 genes as measured in the microarray gene expression experiment of [6]. Values of the MI were estimated by means of k nearest neighbors with $k = 40$. The green line is the lower bound discussed in this paper.
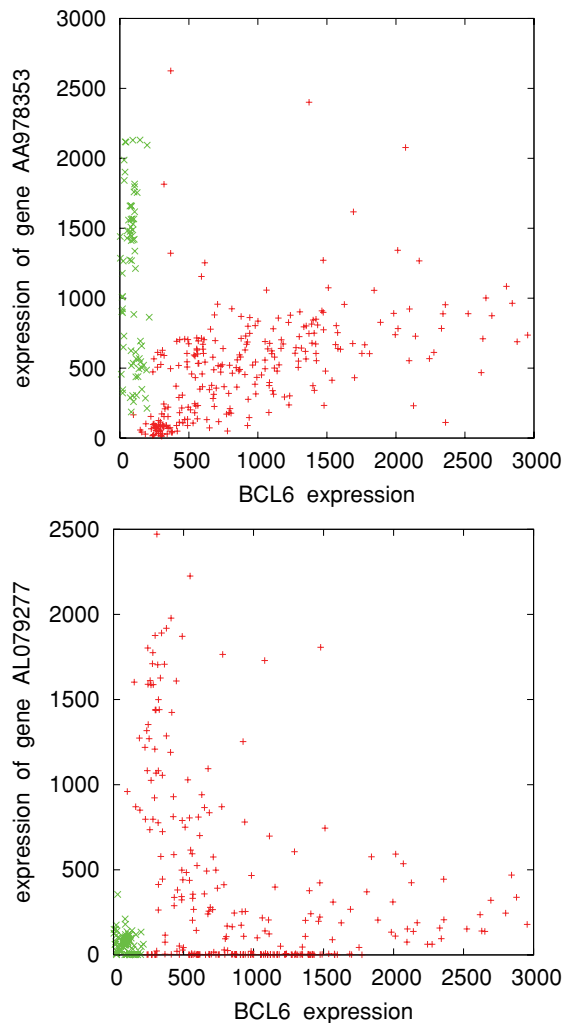
FIG. 3. (Color online) Each panel shows the gene expression intensities (arbitrary units) of two genes, one of which is BCL6 (x axis). The other gene (y axis) was chosen such as to have very large MI with BCL6, but very small Spearman coefficient (the uppermost two points in Fig. 2 with $|S| < 0.1$). The color coding (green for BCL6 expression <200 and AL079277 expression <500, red otherwise) is such that the same cell conditions have in both panels the same color. It suggests that the observed nonlinear correlations are related to the existence of two cell populations with very different properties. The two genes correspond to accession numbers AA978353 (top) and AL079277 (bottom).

produce negative MI, which is achieved by tolerating a positive bias. The estimator of [3] was constructed such that the bias is minimized, at the cost of obtaining occasionally negative values due to statistical fluctuations.

(c) For most pairs the bound is not saturated, showing that there are important nonlinear dependencies between these pairs. As an illustration for the latter we take the two points with $|S| < 0.1$ and $I > 0.3$ and plot their gene expression vectors in Fig. 3. They show the coexpression of BCL6 with the genes with GenBank accession numbers AA978353 (top) and AL079277 (bottom). In both panels of Fig. 3 we see very strong dependencies which cannot be approximated by linear correlations. Neither of these two genes is known to be related to BCL6, maybe because such relations were overlooked because of the small linear correlations. The data suggest the presence of (at least) two different subpopulations of cells, marked in Fig. 3 by different colors. In the subpopulation in which BCL6 is strongly expressed (red points in Fig. 3) there are also significant linear correlations.

In summary, we have derived lower bounds on the MI between real-valued variables in terms of linear correlation coefficients. We have seen that such bounds are not independent of the marginal distribution, in contrast to the claims made in the Appendix of [3]. But one can use the homeomorphism invariance of the MI to transform the variables to new variables with uniform distribution, in which case the linear correlation coefficient becomes equal to the Spearman coefficient S. At least in one specific and scientifically relevant example, the resulting bound of the MI in terms of S was found to be numerically nontrivial. In particular, large discrepancies between the bound and the actual values gave hints at specific structures in the data which then could be investigated in more detail. The bound can also be useful in testing MI estimators. Usually, an estimator is deemed unacceptable if it violates the bound $I(X : Y) \geqslant 0$. But it will be equally unacceptable if it violates the stronger bound $I(X : Y) \geqslant I^{-}$.

Finally, our results also answer the question of how linear correlations change under reparametrizations. There is no reason to expect a universal exact answer, but approximately they should change such that the numerical values of the bounds I^{-} stay the same.

[1] T. M. Cover and J. A. Thomas, *Elements of Information Theory*, 2nd edition (John Wiley & Sons, New York, 2006).

[2] M. Li and P. M. B. Vitányi, *An Introduction to Kolmogorov Complexity and Its Applications*, 3rd ed. (Springer, Berlin, 2008).

[3] A. Kraskov, H. Stögbauer, and P. Grassberger, Phys. Rev. E **69**, 066138 (2004).

[4] A. Kraskov, H. Stögbauer, and P. Grassberger, Phys. Rev. E **83**, 019903(E) (2011).

[5] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes: The Art of Scientific Computing*, 3rd ed. (Cambridge University Press, Cambridge, 2007).

[6] K. Basso, A. A. Margolin, G. Stolovitzky, U. Klein, R. Dalla-Favera, and A. Califano, Nat. Genet. **37**, 382 (2005).