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Subject: **Is there a mutual information for three random variables?**
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Consider three discrete "random variables" X, Y, and Z. According to the diagram of intersecting circles, the information shared in common by all three quantities—the three-variable mutual information—ought to be

$$H(X:Y:Z) \equiv H(X:Y) - H(X:Y|Z) = H(X) - H(X|Y) - H(X|Z) + H(X|Y,Z) \,. \quad (1)$$

This three-variable mutual information is manifestly symmetric under interchange of any two variables and thus can also be written as (in accordance with the diagram)

$$H(X:Y:Z) = H(X:Z) - H(X:Z|Y) = H(Y:Z) - H(Y:Z|X) \,. \quad (2)$$

The problem with $H(X:Y:Z)$ is that it can be negative when the amount of information X and Y share (i.e., the tightness of their correlation) is greater when Z is known than when it is not. An example follows

Suppose X, Y, and Z are binary variables, each taking on values 0 and 1. Let the three-variable joint probabilities be given by

$$p_{000} = p_{111} = 0 \,, \quad p_{001} = p_{010} = p_{100} = \tfrac{1}{3}p \,, \quad p_{110} = p_{101} = p_{011} = \tfrac{1}{3}q \,, \quad (3)$$

where $p+q=1$. This joint distribution is symmetric under interchange of any two variables and symmetric under the simultaneous interchange of 0 and 1 and p and q. The marginal probabilities are given by

$$p_{00} = \tfrac{1}{3}p \,, \quad p_{11} = \tfrac{1}{3}q \,, \quad p_{01} = p_{10} = \tfrac{1}{3} \,, \quad (4)$$

$$p_0 = \tfrac{2}{3}p + \tfrac{1}{3}q = \tfrac{1}{3}(1+p) \,, \quad p_1 = \tfrac{1}{3}p + \tfrac{2}{3}q = \tfrac{1}{3}(2-p) \,, \quad (5)$$

and the conditional probabilities by

$$\begin{aligned}
&p_{00|0} = 0 && p_{11|1} = 0 \\
&p_{01|0} = p_{10|0} = \frac{p}{2p+q} = \frac{p}{1+p} \,, && p_{10|1} = p_{01|1} = \frac{q}{2q+p} = \frac{1-p}{2-p} \,, \\
&p_{11|0} = \frac{q}{2p+q} = \frac{1-p}{1+p} && p_{00|1} = \frac{p}{2q+p} = \frac{p}{2-p}
\end{aligned} \quad (6)$$

$$\begin{matrix} p_{0|00} = 0 \\ p_{1|00} = 1 \end{matrix} \,, \quad \begin{matrix} p_{0|01} = p \\ p_{1|01} = q \end{matrix} \,, \quad \begin{matrix} p_{0|10} = p \\ p_{1|10} = q \end{matrix} \,, \quad \begin{matrix} p_{0|11} = 1 \\ p_{1|11} = 0 \end{matrix} \,, \quad (7)$$

$$\begin{matrix} p_{0|0} = \dfrac{p}{2p+q} = \dfrac{p}{1+p} \\ p_{1|0} = \dfrac{1}{2p+q} = \dfrac{1}{1+p} \end{matrix} \,, \quad \begin{matrix} p_{0|1} = \dfrac{1}{p+2q} = \dfrac{1}{2-p} \\ p_{1|1} = \dfrac{q}{p+2q} = \dfrac{1-p}{2-p} \end{matrix} \,. \quad (8)$$

The symmetry under exchange of any two variables means that these probabilities apply in the obvious way to any choice of the random variables.

The correlations between X and Y when Z is known are given by the probabilities in Eq. (6), and the correlations between X and Y when Z is averaged over are given by the probabilities in Eq. (4). When $p = 1$, X and Y are perfectly correlated for $z = 1$, i.e., $p_{00|1} = 1$, and they are half that strongly correlated when $z = 0$, i.e., $p_{01|0} = p_{10|0} = \frac{1}{2}$. When we average over Z to get the marginal probabilities (4), these correlations get spread out over the three possibilities, 00, 01, and 10, thus giving a weaker correlation. The tighter correlation when Z is known than when it is not gives rise to the negative value for the proposed mutual information of the three variables.

The information quantities that go into $H(X:Y:Z)$ become

$$H(X) = H(p_0, p_1) = H\big(\tfrac{1}{3}(1+p), \tfrac{1}{3}(2-p)\big)\;, \tag{9}$$

$$\begin{aligned} H(X|Y) = H(X|Z) &= p_0 H(p_{0|0}, p_{1|0}) + p_1 H(p_{0|1}, p_{1|1}) \\ &= \tfrac{1}{3}(1+p) H\left(\frac{p}{1+p}, \frac{1}{1+p}\right) + \tfrac{1}{3}(2-p) H\left(\frac{1}{2-p}, \frac{1-p}{2-p}\right)\;, \end{aligned} \tag{10}$$

$$\begin{aligned} H(X|Y,Z) &= p_{00} H(p_{0|00}, p_{1|00}) + p_{01} H(p_{0|01}, p_{1|01}) \\ &\quad + p_{10} H(p_{0|10}, p_{1|10}) + p_{11} H(p_{0|11}, p_{1|11}) \\ &= \tfrac{2}{3} H(p, 1-p)\;, \end{aligned} \tag{11}$$

$$\begin{aligned} H(X:Y) &= H(X) - H(X|Y) \\ &= H\big(\tfrac{1}{3}(1+p), \tfrac{1}{3}(2-p)\big) \\ &\quad - \tfrac{1}{3}(1+p) H\left(\frac{p}{1+p}, \frac{1}{1+p}\right) - \tfrac{1}{3}(2-p) H\left(\frac{1}{2-p}, \frac{1-p}{2-p}\right)\;, \end{aligned} \tag{12}$$

$$\begin{aligned} H(X:Y|Z) &= H(X|Z) - H(X|Y,Z) \\ &= \tfrac{1}{3}(1+p) H\left(\frac{p}{1+p}, \frac{1}{1+p}\right) + \tfrac{1}{3}(2-p) H\left(\frac{1}{2-p}, \frac{1-p}{2-p}\right) - \tfrac{2}{3} H(p, 1-p)\;. \end{aligned} \tag{13}$$

For the special case $p = 1$ and $q = 0$, these expressions reduce to

$$\begin{aligned} H(X) &= H\big(\tfrac{2}{3}, \tfrac{1}{3}\big) = \log 3 - \tfrac{2}{3} = 0.9183\;, \\ H(X|Y) = H(X|Z) &= \tfrac{2}{3} H\big(\tfrac{1}{2}, \tfrac{1}{2}\big) = \tfrac{2}{3}\;, \\ H(X|Y,Z) &= 0\;, \end{aligned} \tag{14}$$

$$H(X:Y) = H\big(\tfrac{2}{3}, \tfrac{1}{3}\big) - \tfrac{2}{3} = \log 3 - \tfrac{4}{3} = 0.2516\;, \quad H(X:Y|Z) = \tfrac{2}{3}\;, \tag{15}$$

implying that

$$H(X:Y:Z) = H\big(\tfrac{2}{3}, \tfrac{1}{3}\big) - \tfrac{4}{3} = \log 3 - 2 = -0.4150\;. \tag{16}$$