A note on the unbiased estimation of mutual information

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Abstract

Estimators for mutual information are typically biased. However, in the case of the Kozachenko-Leonenko estimator for metric spaces, a type of nearest neighbour estimator, it is possible to calculate the bias explicitly.

Introduction

Consider the problem of calculating the mutual information $I(X, Y)$ between a discrete random variable $X$ and a variable $Y$ which takes its value in a metric space $Y$. This is a common situation, $X$ can represent a set of labels while $Y$ represents a corresponding space of outcomes which is high-dimensional or does not have a convenient set of coordinates. Mutual information estimates for high-dimensional data are important in biomedical science [1], in blind source separation [2, 3], information bottleneck [4], the analysis of deep learning networks [5] and elsewhere and by considering mutual information estimators which use only metric information it is possible to avoid some of the difficulties that high-dimensionality present.

In [6] a Kozachenko-Leonenko estimator [7, 8, 9] is derived for this situation. As is common with estimators for mutual information this estimator has a bias; here this bias is calculated exactly to give an unbiased estimator. This calculation closely follows the calculation provided in [10] for a similar estimator for the mutual information between two random variables which both take values in a metric space.

When calculated the mutual information the data will be $(x, y)$ pairs:

$$\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$$

(1)

where $n$ is the number of data points. The estimator for mutual information is a kind of nearest-neighbours or kernel density estimator [11, 12]. It starts with a smoothing parameter, an integer $h$. For each outcome $(x_i, y_i)$ a ball is formed of the $h$ points, including $y_i$ itself, which are closest to $y_i$ in $Y$. $(x_i, y_i)$ will be called the seed point for this ball containing $h$ points. Since the data are $(x, y)$ pairs, each of these $h$ closest points, $y_j$, will have an associated label $x_j$. To estimate the mutual information the number, $h_y(i)$, of these $h$ points that has the same label as the seed is calculated:

$$h_y(i) = \# \{x_j = x_i \text{ and } y_j \text{ is one of the } h \text{ closest points to } y_i\}$$

(2)

The estimated mutual information is now

$$I_0 = \frac{1}{n} \sum_{i=1}^{n} \log_2 \frac{n_x h_y(i)}{h}$$

(3)

where $n_x$ is the number of different labels, that is, the number of different possible outcomes for $X$. This is illustrated in Fig.[1]

This estimator $I_0$ is calculated using the metric structure on $Y$; it depends only on the matrix of distances between the $y_i$ points and on their corresponding labels $x_i$. This distance matrix in turn is used to work out the near $h$ points to each of the $y_i$ in turn; the algorithm is not computationally fast because the points need to be sorted in distance order. However, since it depends only on the metric it works well for high-dimensional data.

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Result

This estimated is biased because it gives a non-zero value even if the $X$ and $Y$ are independent. However, one advantage of the Kozachenko–Leonenko is that bias can be calculated exactly. The bias is given by

$$I_b = \sum_{r=1}^{h} \mathbb{P}(h_y = r) \log_2 \frac{n_x r}{h}$$

where $\mathbb{P}(h_y = r)$ is the probability $h_y$ is $r$ if $X$ and $Y$ are independent.

Now

$$\mathbb{P}(h_y = r) = \sum_{c=1}^{n_x} \frac{n_c}{n} \mathbb{P}(h_y = r | x = x_c)$$

where the sum is over the possible labels $x_c$ of $X$. Let $n_c$ be the number of data points with label $x_c$, so

$$n = \sum_{c=1}^{n_x} n_c$$

then the bias for the data set is

$$\mathbb{P}(h_y = r) = \sum_{c=1}^{n_x} \frac{n_c}{n} \mathbb{P}(h_y = r | x = x_c)$$

Calculating $\mathbb{P}(h_y = r | x = x_c)$ is an urn problem. $\mathbb{P}(h_y = r | x = x_c)$ is the probability that there are $r - 1$ points in the set of $h - 1$ points in the ball around a ‘seed point’ that have the same label, $x_c$, as the seed. The $h - 1$ points in the ball are picked from the $n - 1$ remaining data points and, under the assumption that $X$ and $Y$ are independent, this is a random choice. As such $\mathbb{P}(h_y = r | x = x_c)$ is the probability of picking $r$ of the $n_c - 1$ distinguished point, the remaining points with label $x_c$, when selecting $h - 1$ points from $n - 1$.

This means

$$\mathbb{P}(h_y = r | x = x_c) = \frac{\binom{n_c - 1}{r - 1} \binom{n - n_c}{h - 1}}{\binom{n - 1}{h - 1}} \sim \text{Hypergeometric}(n - 1, n_c - 1, h - 1)$$

Using $u(n - 1, n_c - 1, h - 1)$ for the hypergeometric pdf, this means

$$I_b = \sum_{r=1}^{h} \sum_{c=1}^{n_x} \frac{n_c}{n} u(n - 1, n_c - 1, h - 1) \log_2 \frac{n_x r}{h}$$

and the unbiased estimator is

$$I_e = I_0 - I_b$$

One subtlety concerns draws: what to do if there are multiple points the same distance from the seed point. This can be dealt with by counting points fractionally. Draws are only problematic if they occur at

Figure 1: The calculation of $I_0$. The circles and triangle are data points and red and blue represent two labels. The dashed line is the ball around the ‘seed’ point in the center marked by a triangle $\triangle$. Here $h = 7$ so the ball has been expanded until it includes seven points. It contains four red points, the colour of the central point, so $h_y(\triangle) = 4$. For illustration the points have been drawn in a two-dimensional space, but this can be any metric space.
the boundary of the ball around a point \((x_i, y_i)\), meaning that it is not clear which \(h\) points to regard as part of the ball. Consider the case where there are \(b\) points on the boundary, so that \(b\) points are equidistant from \((x_i, y_i)\), let \(c < h\) be the number of points closer to \((x_i, y_i)\) than the boundary points. This means \(b + c > h\), and only \(h - c\) of the \(b\) boundary points are needed to fill out the ball. This is solved by counting all \(b\) points fractionally with a weight \((h - c)/b\); when calculating \(h_y(i)\) any of these \(b\) points with the same label as \(x_i\) adds this weight to the total.

This leaves open the choice of \(h\), the smoothing parameter; one approach that appears to work is picking the \(h\) that maximizes \(I_e[10]\).

**Code availability**

Code to implement this estimator is available at [github.com/EstimatingInformation/DiscreteEstimator](https://github.com/EstimatingInformation/DiscreteEstimator).

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