Measuring Dependency via Intrinsic Dimensionality

SUPPLEMENTARY MATERIAL

PROOFS OF PROPOSITIONS AND THEOREMS

Theorem 1. Let X be a set of D continuous variables, f(x) the p.d.f. of the distribution from which X is drawn, and ID(x) the local intrinsic dimension at the locality x. The α -Rényi dimension can be expressed as:

$$\dim_{\alpha}(X) = \frac{\int f^{\alpha}(x) \operatorname{ID}(x) \, \mathrm{d}x}{\int f^{\alpha}(x) \, \mathrm{d}x}.$$

Proof. We first note that the following holds true for the generalized correlation integral in Equation (4):

$$C_{\alpha}(X,r) = \left(\int \left(\int f(y)\bar{\mathbf{1}}(x,y,r) \,\mathrm{d}y \right)^{\alpha-1} f(x) \,\mathrm{d}x \right)^{\frac{1}{\alpha-1}}$$
$$= \left(\int F_R^{\alpha-1}(x,r)f(x) \,\mathrm{d}x \right)^{\frac{1}{\alpha-1}},$$

where $F_R(x,r) = \int f(y)\bar{\mathbf{1}}(x,y,r) \, dy$ is the number of points at distance smaller than r from x. Then, we use l'Hôpital's rule on the definition of $\dim_{\alpha}(X)$ in Equation (3):

$$\dim_{\alpha}(X) = \lim_{r \to 0^{+}} \frac{\log\left(\int F_{R}^{\alpha-1}(x,r)f(x)\,\mathrm{d}x\right)}{(\alpha-1)\log r}$$

$$\stackrel{\mathrm{H}}{=} \lim_{r \to 0^{+}} \frac{r\int(\alpha-1)F_{R}^{\alpha-2}(x,r)f_{R}(x,r)f(x)\,\mathrm{d}x}{(\alpha-1)\int F_{R}^{\alpha-1}(x,r)f(x)\,\mathrm{d}x}$$

$$= \lim_{r \to 0^{+}} \frac{\int F_{R}^{\alpha-1}(x,r)\frac{rf_{R}(x,r)}{F_{R}^{\alpha-1}(x,r)f(x)\,\mathrm{d}x}}{\int F_{R}^{\alpha-1}(x,r)f(x)\,\mathrm{d}x}$$

$$= \lim_{r \to 0^{+}} \frac{\int F_{R}^{\alpha-1}(x,r)\mathrm{ID}(x,r)f(x)\,\mathrm{d}x}{\int F_{R}^{\alpha-1}(x,r)f(x)\,\mathrm{d}x}.$$

As r tends to 0^+ , $F_R(x, r)$ tends to f(x). Therefore:

$$\dim_{\alpha}(X) = \frac{\int f^{\alpha}(x) \mathrm{ID}(x) \,\mathrm{d}x}{\int f^{\alpha}(x) \,\mathrm{d}x}$$

Theorem 2. The kNN estimator of $\dim_{\alpha}(X)$ is:

$$\widehat{\dim_{\alpha}}(X) = \frac{\sum_{i=1}^{n} \widehat{\mathrm{ID}}(x_i) (d_k(x_i)^{-D})^{\alpha - 1}}{\sum_{i=1}^{n} (d_k(x_i)^{-D})^{\alpha - 1}}.$$

Proof. We first prove a more general result: if $K(\cdot)$ is a kernel function with width h, then for $\alpha \ge 1$,

$$\widehat{\dim}_{\alpha}(X) = \frac{\sum_{i=1}^{n} \widehat{\mathrm{ID}}(x_{i}) \left(\sum_{j=1}^{n} K(\|x_{i} - x_{j}\|, h)\right)^{\alpha - 1}}{\sum_{i=1}^{n} \left(\sum_{j=1}^{n} K(\|x_{i} - x_{j}\|, h)\right)^{\alpha - 1}}.$$
(8)

To prove this, note that for $\alpha \geq 1$, $\dim_{\alpha}(X) = \frac{\int f(x)f(x)^{\alpha-1}\mathrm{ID}(x)\,\mathrm{d}x}{\int f(x)f(x)^{\alpha-1}\,\mathrm{d}x}$. The p.d.f. f(x) of X can be es-

timated with kernel functions $K(\cdot)$ via summation over all data points x_i : $\hat{f}(x) = \frac{1}{n} \sum_{j=1}^n \frac{1}{h} K(||x - x_j||, h)$. If we have a reliable sample of n i.i.d data points from X, the expected value $\int f(x)g(x) \, dx$ of any function g(x) over the p.d.f. f(x) can be estimated using the formula: $\frac{1}{n} \sum_{i=1}^n g(x_i)$. Therefore the denominator of $\dim_{\alpha}(X)$ can be estimated with $\frac{1}{n} \sum_{i=1}^n \hat{f}(x_i)^{\alpha-1} = \frac{1}{n} \sum_{i=1}^n (\frac{1}{n} \sum_{j=1}^n \frac{1}{h} K(||x_i - x_j||, h))^{\alpha-1}$. The numerator is instead equal to $\frac{1}{n} \sum_{i=1}^n \widehat{ID}(x_i)(\frac{1}{n} \sum_{j=1}^n \frac{1}{h} K(||x_i - x_j||, h))^{\alpha-1}$. The formula in Eq. (8) can be easily obtained with algebraic simplifications.

With regards to the kNN estimator, it is possible to prove that $K(||x_i - x_j||) = \frac{1(||x_i - x_j|| \le r)}{V_D(r)}$ is a proper kernel, where r is a given radius and $V_D(r) = \frac{\pi^{D/2}}{\Gamma(D/2+1)}r^D$ is the volume of a D-dimensional sphere with radius r. A valid choice for the radius r is the distance $d_k(x_i)$ from x_i to its kth nearest neighbor. Given that the number of data points at distance less than or equal to $d_k(x_i)$ from x_i is exactly k, we have $\frac{1}{n}\sum_{i=1}^n \frac{1(||x_i - x_j|| \le d_k(x_j))}{V_D(d_k(x_j))} = \frac{1}{n} \frac{k}{V_D(d_k(x_j))} = \frac{1}{n} \frac{k\Gamma(D/2+1)d_k(x_i)^{-D}}{\pi^{D/2}}$. The result follows from algebraic manipulations.

Proposition 1. Let X be a set of D continuous variables:

- 1) $0 \leq \text{IDD}(X) \leq 1;$
- 2) IDD(X) = 0 iff all X_i are independent;
- 3) IDD(X) = 1 if there exist one or more manifolds of dimension 1 whose union embeds X;
- 4) IDD(X) = 1 if there exists 1 ≤ i ≤ D such that for all j ≠ i, X_j is a a function or multivalued function of X_i.

Proof.

Point 1: By definition, $\dim(X) = \lim_{\delta \to 0^+} \frac{H(X,\delta)}{\log 1/\delta}$. Then regarding the lower bound of IDD, $\sum_{i=1}^{D} \dim(X_i) - \dim(X)$ is equal to:

$$= \sum_{i=1}^{D} \lim_{\delta \to 0^+} \frac{H(X_i, \delta)}{\log 1/\delta} - \lim_{\delta \to 0^+} \frac{H(X, \delta)}{\log 1/\delta}$$
$$= \lim_{\delta \to 0^+} \frac{1}{\log 1/\delta} \Big(\sum_{i=1}^{D} H(X_i, \delta) - H(X, \delta) \Big)$$
$$= \lim_{\delta \to 0^+} \frac{1}{\log 1/\delta} \operatorname{KL} \Big(p_X(x, \delta) || p_{X_1}(x_1, \delta) \cdots p_{X_D}(x_D, \delta) \Big),$$

where KL is the Kullback-Leibler divergence, which is greater or equal to 0 for any $\delta > 0$. Regarding the upper bound of IDD, we use the known fact that the Shannon entropy satisfies $H(X) \ge \max_i H(X_i)$ to prove the following inequalities for

$$\sum_{i=1}^{D} \dim(X_i) - \dim(X):$$

$$= \sum_{i=1}^{D} \lim_{\delta \to 0^+} \frac{H(X_i, \delta)}{\log 1/\delta} - \lim_{\delta \to 0^+} \frac{H(X, \delta)}{\log 1/\delta}$$

$$\leq \sum_{i=1}^{D} \lim_{\delta \to 0^+} \frac{H(X_i, \delta)}{\log 1/\delta} - \lim_{\delta \to 0^+} \frac{\max_i H(X_i, \delta)}{\log 1/\delta}$$

$$= \sum_{i=1}^{D} \lim_{\delta \to 0^+} \frac{H(X_i, \delta)}{\log 1/\delta} - \max_i \lim_{\delta \to 0^+} \frac{H(X_i, \delta)}{\log 1/\delta}$$

$$= \sum_{i=1}^{D} \lim_{\delta \to 0^+} \frac{H(X_i, \delta)}{\log 1/\delta} - \max_i \dim(X_i).$$

Since the Shannon entropy is a continuous function, and since X is continuous, it is possible to interchange the limit and max operations.

Point 2: As shown for Point 1 above, $\sum_{i=1}^{D} \dim(X_i) - IDD(X)$ is equal to

$$\lim_{\delta \to 0^+} \frac{1}{\log 1/\delta} \mathrm{KL}\bigg(p_X(x,\delta) \| p_{X_1}(x_1,\delta) \cdots p_{X_D}(x_D,\delta) \bigg).$$

The result follows from the fact that for any $\delta > 0$, the KL divergence is equal to 0 iff all variables X are independent. Point 3: If there exist at least a manifold of dimension 1 embedded in X, then ID(x) = 1 for any locality x. With $\dim(X) = 1$ being the expected ID over the p.d.f. of X, we have that DID(X) = 1. According to Theorem 1 in [10] if X_i is a continuous random variable, $\dim(X_i) = 1$. Given that we are considering continuous random variables X_i , $\max_i \dim(X_i) = 1$, and therefore IDD(X) = 1. Point 4: follows immediately from Point 3.