Implemetation of an intrinsic dimension estimator for locally undersampled data

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Original paper

Erba, V., Gherardi, M. Rotondo, P. Intrinsic dimension estimation for locally undersampled data. Sci Rep 9, 17133 (2019). https://doi.org/10.1038/s41598-019-53549-9

The algorithm

The problem

From the original paper by Erba, Gherardi and Rotondo:

"All the existing intrinsic dimension estimators are not reliable whenever the dataset is locally undersampled, and this is at the core of the so called **curse of dimensionality**".

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This is particularly relevant when dealing with high dimension or strongly curved manifolds (in which local sampling is required).

Proposed solution

We can project data on a unitary-radius hypershpere, where density can be easily estimated.

Full correlation integral ("FCI")

Empirical correlation integral:

$$\rho\left(r\right) = \frac{2}{N\left(N-1\right)} \sum_{1 \leq \mu < \nu \leq N} \theta\left(r - ||\mathbf{x}^{\mu} - \mathbf{x}^{\nu}||\right),$$

where r is the cutoff distance.

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FCI estimator for a (uniformly sampled) (d-1)-dimensional sphere of radius 1:

$$\bar{\rho}_{r_s}\left(r\right)=\frac{1}{2}+\frac{\Omega_{d-1}}{2\Omega_d}\left(\bar{r}^2-2\right)F_{2,1}\left(\frac{1}{2},1-\frac{d}{2};\frac{3}{2};\left(\bar{r}^2-2\right)^2\right),$$

where Ω_d is the d-dimensional solid angle, $F_{2,1}$ is the (2,1)-hypergeometric function and $\bar{r}=\frac{r}{r_s}$.

Global ID estimator

Algorithm:

1. center and normalize data (i.e. project on hypersphere)
2. measure empirical correlation integral as function of the radius r
3. perform a non-linear regression on the computed empirical FCI using the estimator, with d and r_s as free parameters
4. add one to the estimated d, since the normalization step removes one degree of freedom

Multiscale ID estimator

Algorithm:

1. select a random datapoint x_0 and a *number of nearest neighbors* k, and fit FCI estimator using only x_0's k nearest neighbors
2. repeat step 1 for several values of k
3. select the optimal estimate of ID

Evaluation

Original datasets for global estimator

- $D_{d,D}$: uniform sampling of $\{0,1\}^d$, linearly embedded.
- $G_{d,D}$: sampling of $\mathbb{R}^d$ with the multivariate Gaussian distribution of covariance matrix $\mathbb{I}$ and null mean, linearly embedded.
- $H_{d,D}$: uniform sampling of $[0,1]^d$, linearly embedded.

Original datasets for multiscale estimator

- $C_{d,2d}$: uniform sampling of $[0,2]^d$, embedded with the map

$$\phi\left(x_1 ... x_d\right) = \left(x_2 \cos(x_1), x_2 \sin(x_1) ... x_1 \cos(x_d), x_1 \sin(x_d)\right).$$

- $B_{5n,81^2}$: dataset of high-contrast bitmap images (81×81 pixel) of n blobs.

Implementation

Used packages

- Vectorization: **NumPy**
- Random variables: **NumPy**, **Random**
- Non-linear fit: **SciPy** (scipy.optimize.curve_fit)
- Hypergeometric computation: **SciPy**, **mpmath**
- Nearest neighbors: **scikit-learn**
- TwoNN for comparison: **DADApy**
- Data visualization: **JSON**, **Matplotlib**

Numerical details - hypergeometric function

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Solution: we use two methods:

1. scipy.special.hyp2f1
    - pros: compatible datatype with numpy
    - cons: cannot handle complex outputs and particular inputs
2. mpmath.hyp2f1
    - pros: high precision, can handle wide variety of inputs and complex outputs
    - cons: needs typecasting

We choose depending on the specific set of inputs.

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Solution: we normalize the last argument (i.e. we divide by the largest radius considered).

Apparently, the algorithm effectiveness is not greatly invalidated. Also, the parameter r_s becomes useless (always $\simeq 1$ in fitting).

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Solution: we use the *Stirling approximation* of the Γ function to approximate the angle ratio:

$$\frac{\Omega_{d-1}}{\Omega_d} = \frac{2\pi^{\frac{d-1}{2}}}{\Gamma\left(\frac{d-1}{2}\right)} \frac{\Gamma\left(\frac{d}{2}\right)}{2\pi^{\frac{d}{2}}} \simeq \dots = \frac{1}{2\pi e} \frac{(d-2)^{\frac{d-1}{2}}}{(d-3)^{\frac{d-2}{2}}},$$

where we used $\Gamma(x) \simeq \sqrt{2\pi(x-1)}\left(\frac{x-1}{e}\right)^{x-1}$.

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where we used $\Gamma(x) \simeq \sqrt{2\pi(x-1)} \left(\frac{x-1}{e}\right)^{x-1}$.

(**Actually**, there are still numerical issues for $d > 350$ (overflow), so we have to use a "log-exp" trick to compute the approximation)

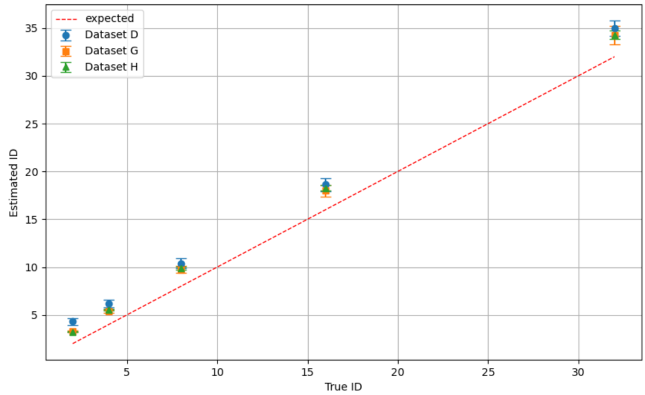
Linear embedding

For linear embedding of the datasets we used the following procedure:

1. add 0-padding to each datapoint until the embedding dimension is reached
2. choose a random hyperplane described by two random vectors in the embedding space (orthonormalized by Gram-Schmidt), and a random angle
3. rotate each datapoint of the extracted angle along the extracted hyperplane

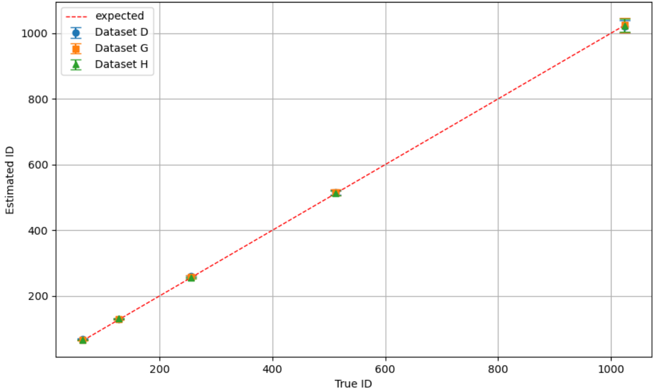
Results

Varying ID - small values



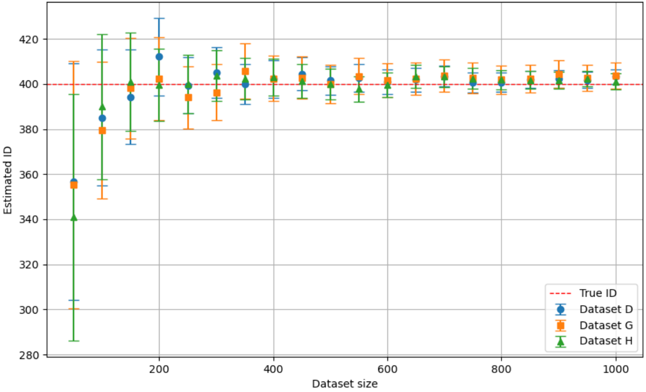
Increasing ID - embedding dimension = 1500, dataset size = 700

Varying ID - large values



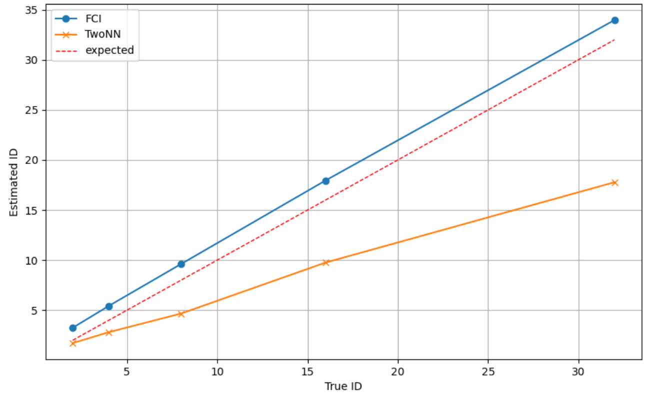
Increasing ID - embedding dimension = 1500, dataset size = 700

Varying dataset size



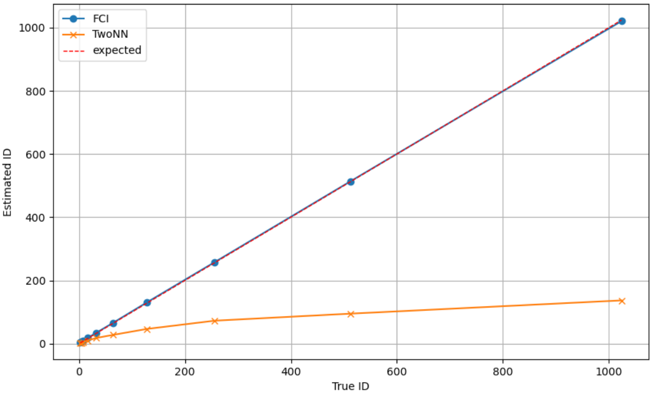
Increasing dataset size - ID = 400, embedding dimension = 1000

Comparison with TwoNN - small values



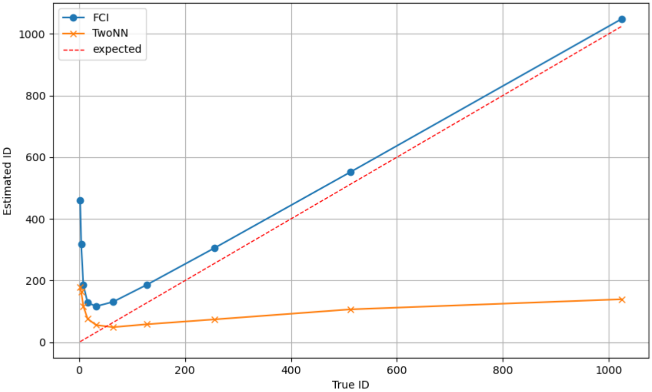
Increasing ID - dataset H with embedding dimension = 1500, dataset size = 700

Comparison with TwoNN - large values



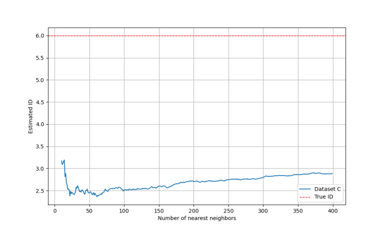
Increasing ID - dataset H with embedding dimension = 1500, dataset size = 700

Comparison with TwoNN - with noise

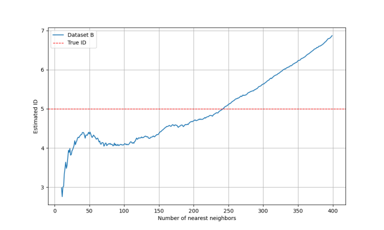


Increasing ID - dataset H with embedding dimension = 1500, dataset size = 700, with Gaussian noise ($\sigma = 0.08$).

Multiscale estimator



(a) Dataset C - increasing k, ID $= 6$, embedding dimension $= 12$, dataset size $= 10000$



(b) High-contrast images dataset - increasing k, ID $= 5$, embedding dimension $= 6561$, dataset size $= 10000$

Results - final considerations

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Results - final considerations

- The estimator is not particularly effective for low dimensions ($\simeq$ constant overestimation), but extremely accurate for large ones.
- The estimator is pretty robust to Gaussian noise.
- The multiscale version (at least my implementation!) does not seem to work in many cases.
- No clear criterion to choose optimal estimation in multiscale version.

References

- Erba, V., Gherardi, M. Rotondo, P. Intrinsic dimension estimation for locally undersampled data. Sci Rep 9, 17133 (2019). https://doi.org/10.1038/s41598-019-53549-9
- https://github.com/TommasoTarchi/My_UL_library
- https://github.com/davidmickisch/torch-rot/blob/main/torch_rot/rotations.py

Thank you!