Implemetation of an intrinsic dimension estimator for locally undersampled data

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The original model

The problem

From the original paper by Erba, Gherardi and Rotondo:

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This is particularly relevant when dealing with strongly curved manifolds, in which local sampling is required.

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Full Correlation Integral:

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

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FCI estimator:

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

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

The global ID estimator

Algorithm:

1. center and normalize data
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

The multiscale ID estimator

Algorithm:

- select a random datapoint x_0 and a *cutoff radius* r_c, and fit FCI estimator using the set of data within distance r_c from x_0
- repeat previous step for several values of r_c
- select the minimum ID estimated

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.

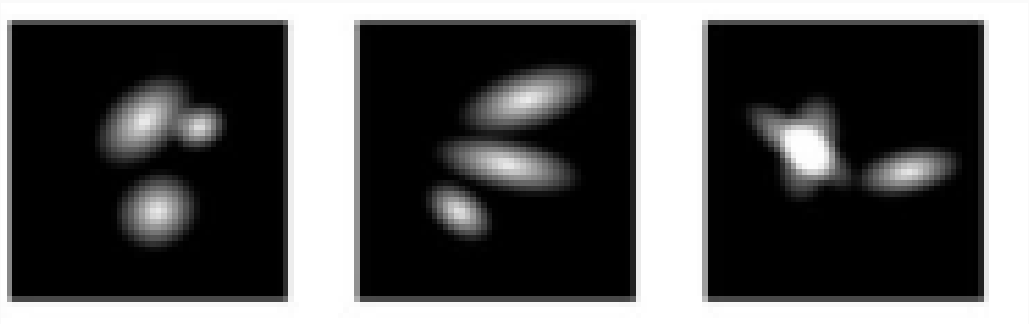
Original datasets for multiscale estimator

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

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

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

High-contrast bitmap images



Examples from high-contrast bitmap images dataset with $n = 3$ 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**
- 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.

Numerical details - hypergeometric function

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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).

Numerical details - solid angles

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

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

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

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(**Actually**, there are still numerical issues for $d > 350$, 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

Implementation - final considerations

- The algorithm is not that easy to implement, mainly because of numerical issues caused by the complexity of the hypergeometric function.

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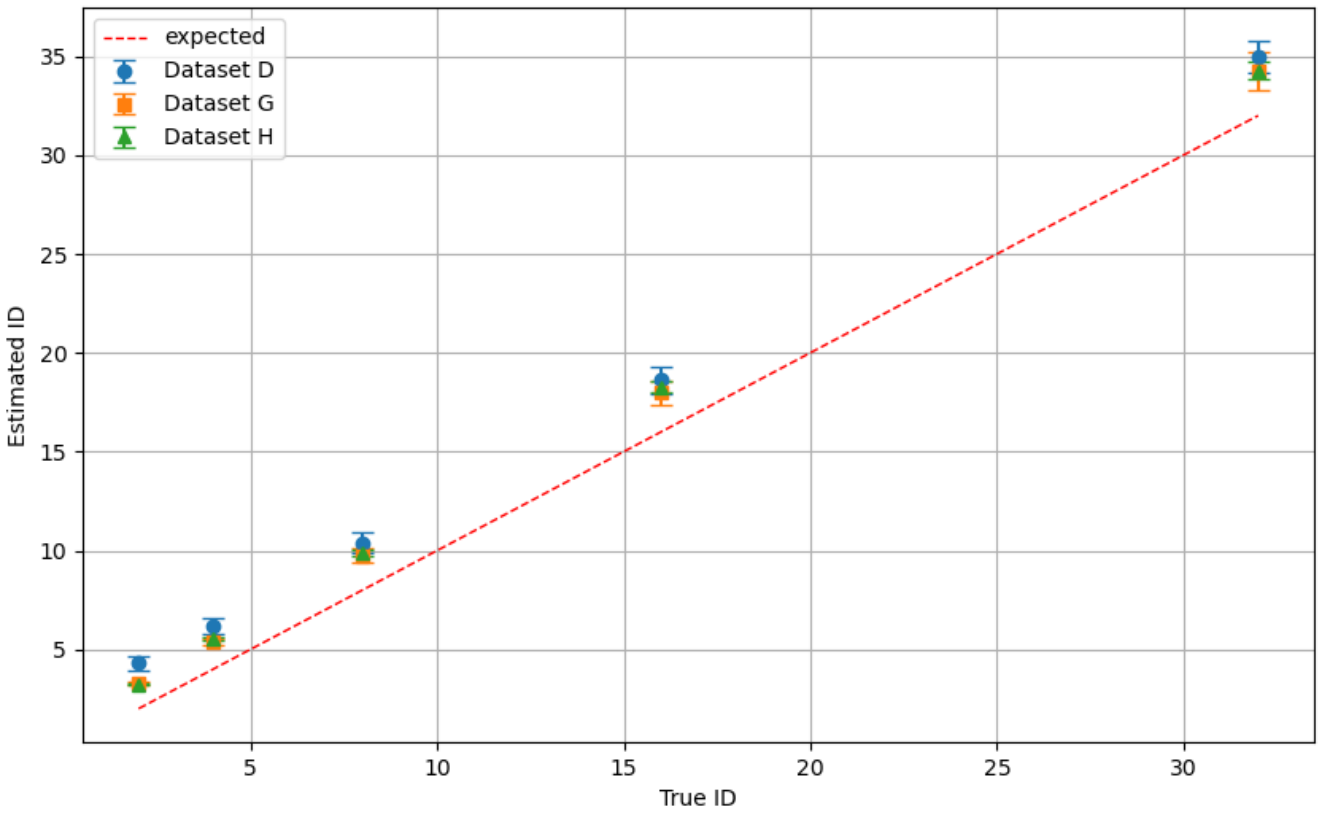
- The algorithm is not that easy to implement, mainly because of numerical issues caused by the complexity of the hypergeometric function.
- The parameter r_s turns out to be useless when the last argument of the hypergeometric is normalized, and so it can be completely removed from the model. This could result in an easier fitting procedure.

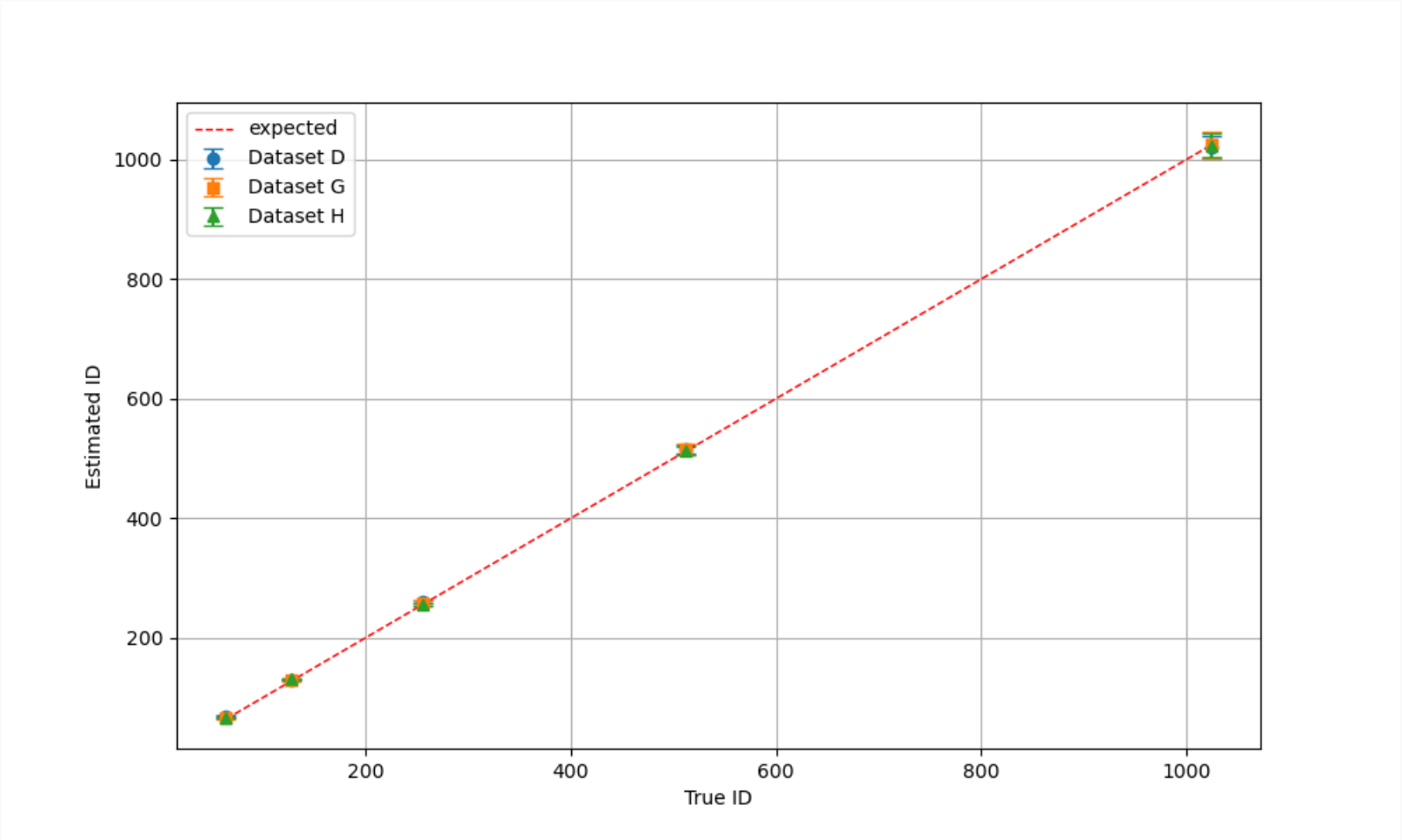
Results

Varying ID - small values



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

Varying ID - large values



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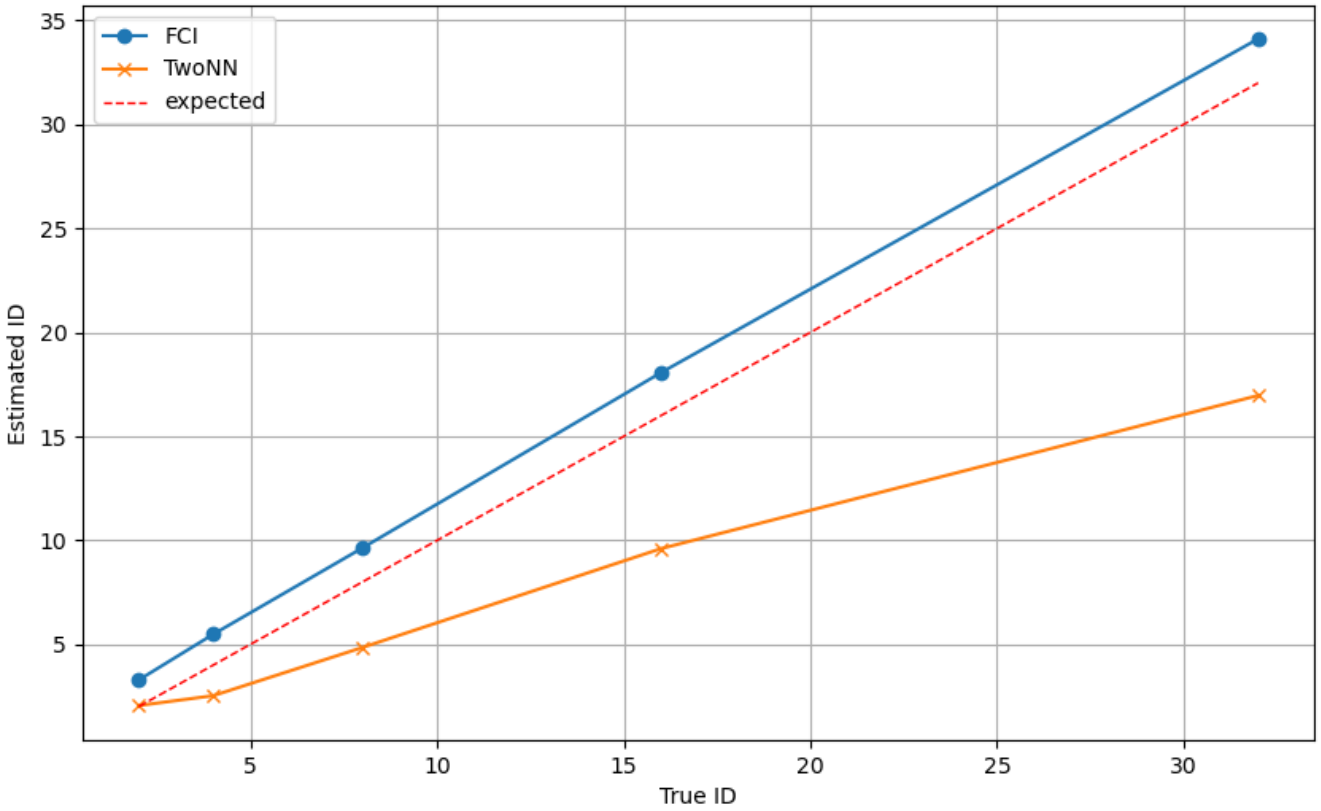
Comparison with TwoNN - small values



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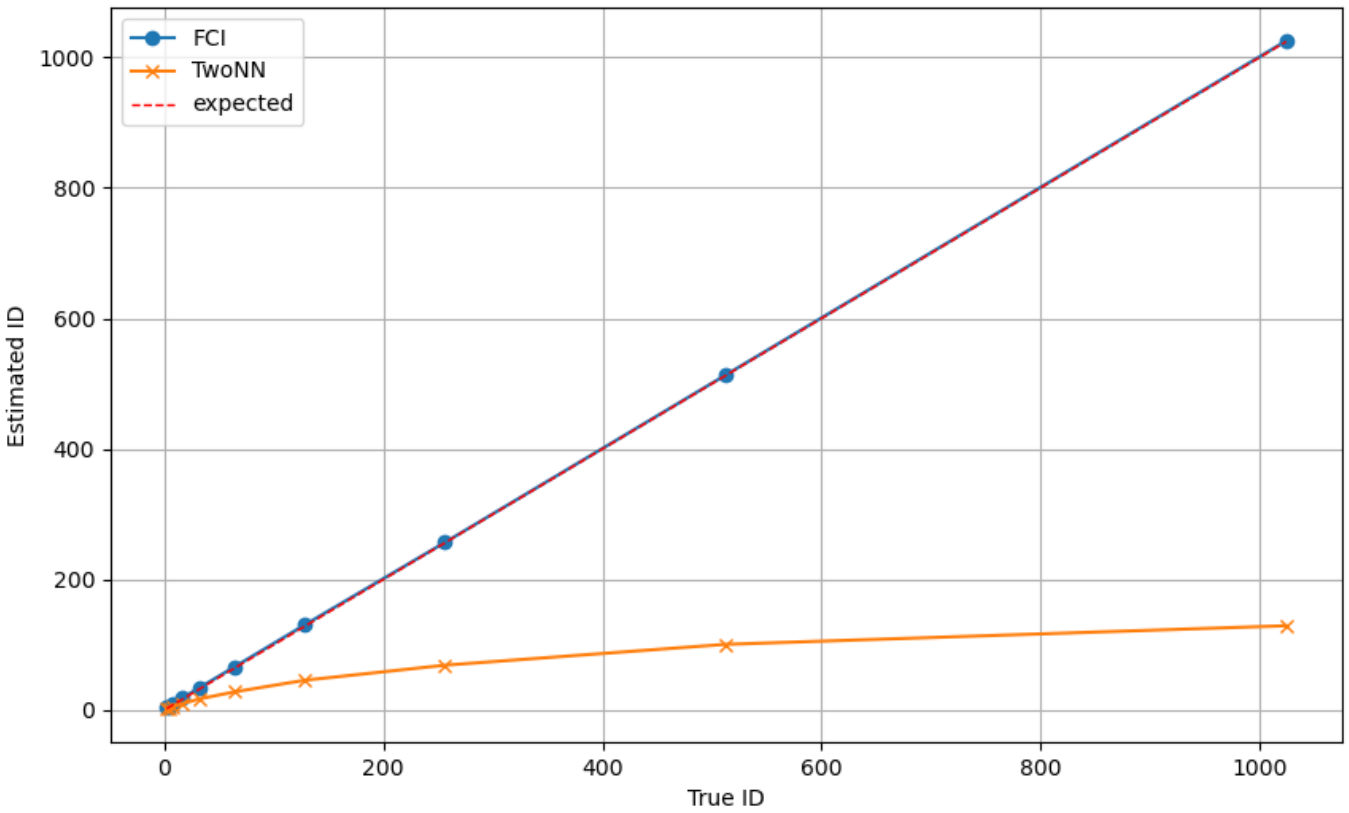

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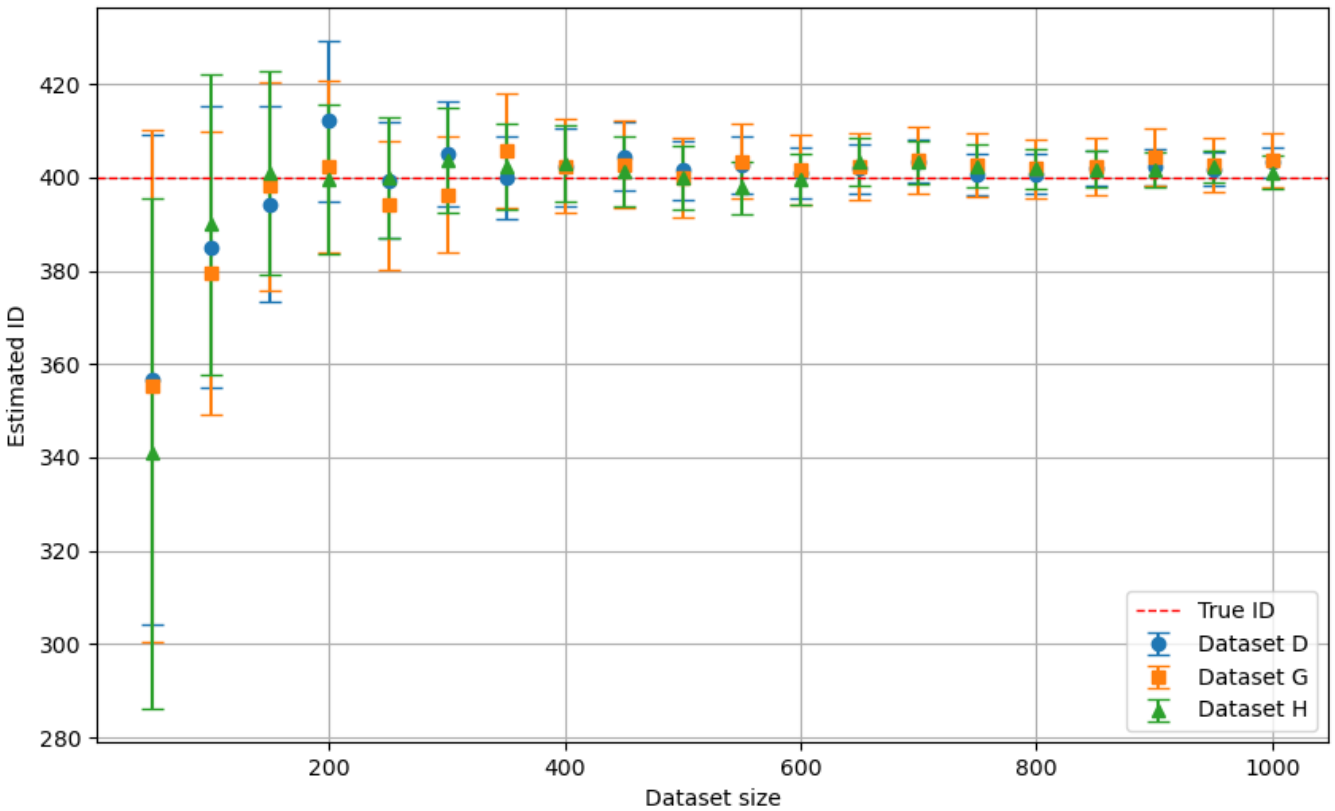
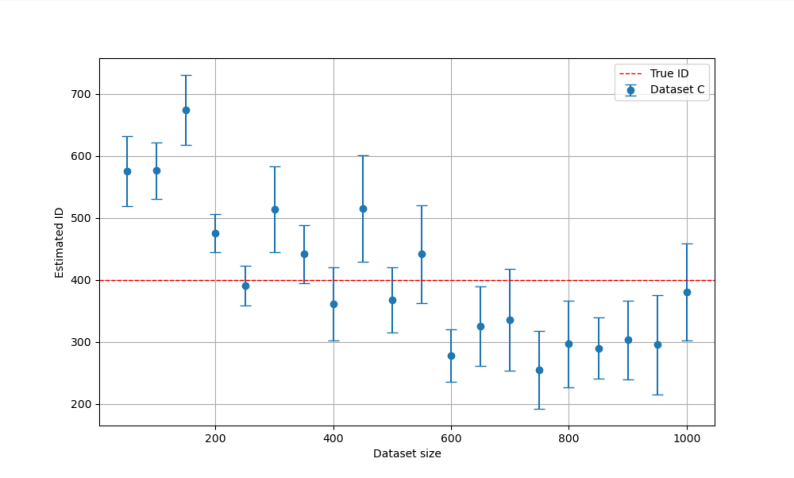
Varying size

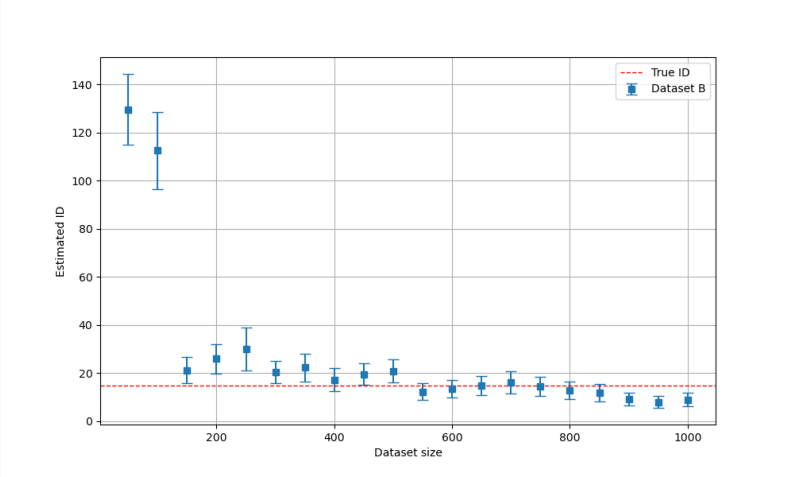


Increasing dataset size - ID = 400, embedding dimension = 1000

Multiscale estimator



(a) Dataset C - increasing dataset size, ID = 400, embedding dimension = 800



(b) High-contrast images dataset - increasing dataset size, ID = 15, embedding dimension = 6561

References

Thank you!