



UNIVERSITÀ DEGLI STUDI DI MILANO  
FACOLTÀ DI SCIENZE E TECNOLOGIE

# Intrinsic dimension estimation for locally undersampled data

Vittorio Erba<sup>(1)</sup>, Marco Gherardi<sup>(1)</sup>, Pietro Rotondo<sup>(2)</sup>

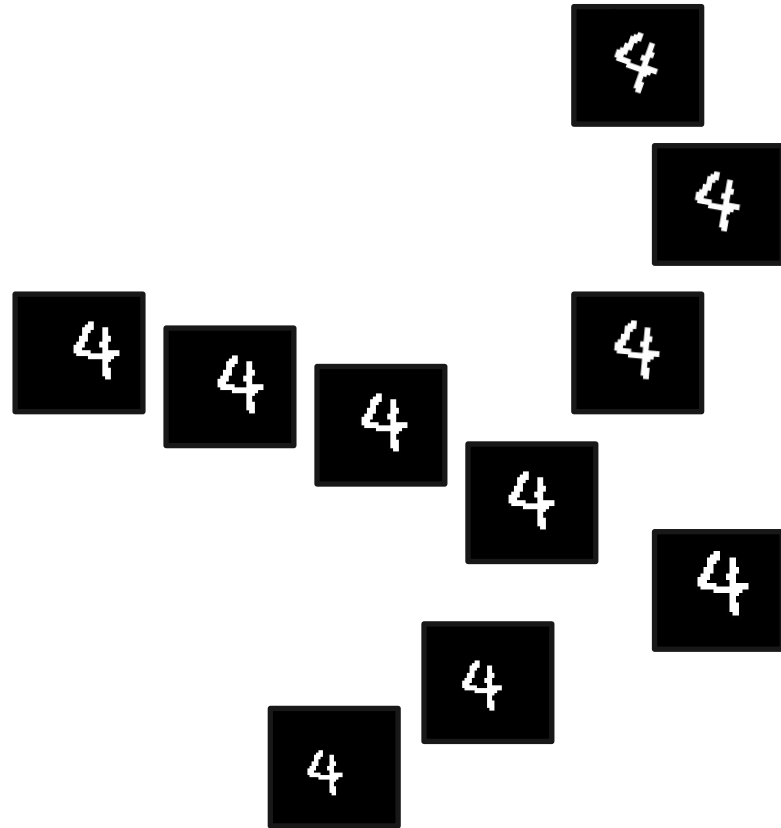
---

5th Workshop on Complex System, Università degli Studi di Milano, 31 October 2019

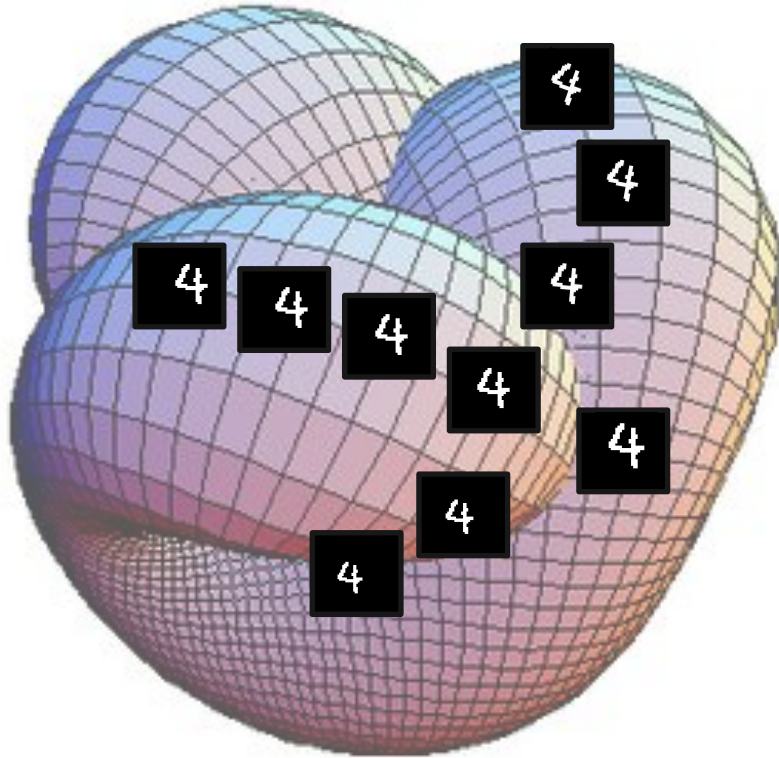
(1) Università degli Studi di Milano and INFN, Sezione di Milano

(2) School of Physics and Astronomy and Centre for the Mathematics and Theoretical Physics of Quantum Non-equilibrium Systems, Nottingham

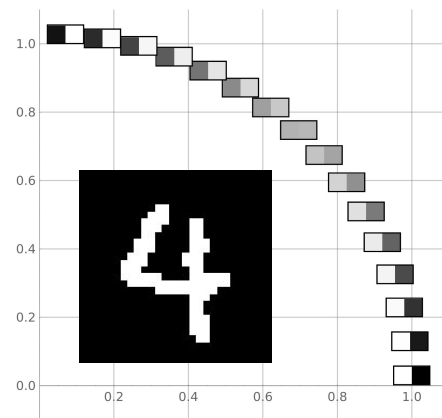
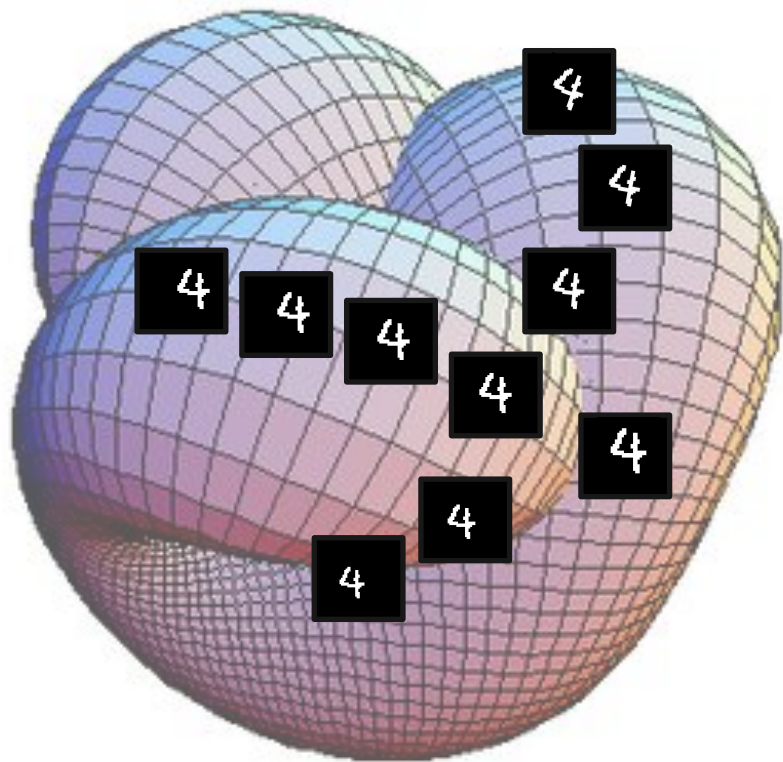
What is the structure underlying complex data?



What is the structure underlying complex data?



# What is the structure underlying complex data?



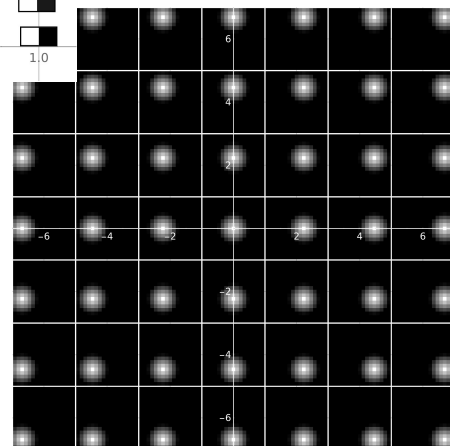
Simple embeddings for humans are complex for maths

pixel space is huge!

$\mathbb{R}^{28 \times 28}$

High dimensional embeddings are redundant:

**Intrinsic Dimensionality**



# What is the structure underlying complex data?

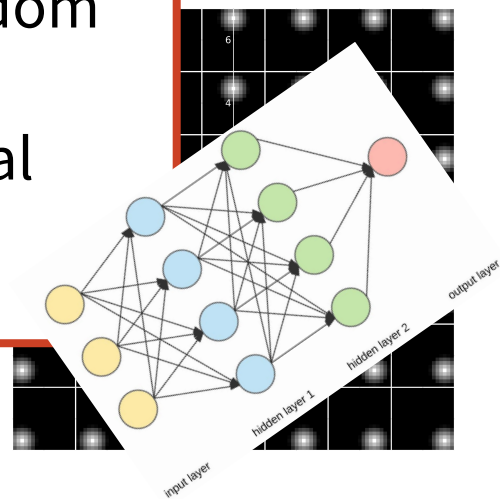
4

**Intrinsic dimension estimation:**  
given the embedded data, retrieve the  
minimum number of degrees of freedom

Unsupervised learning, dimensional  
reduction, feature extraction

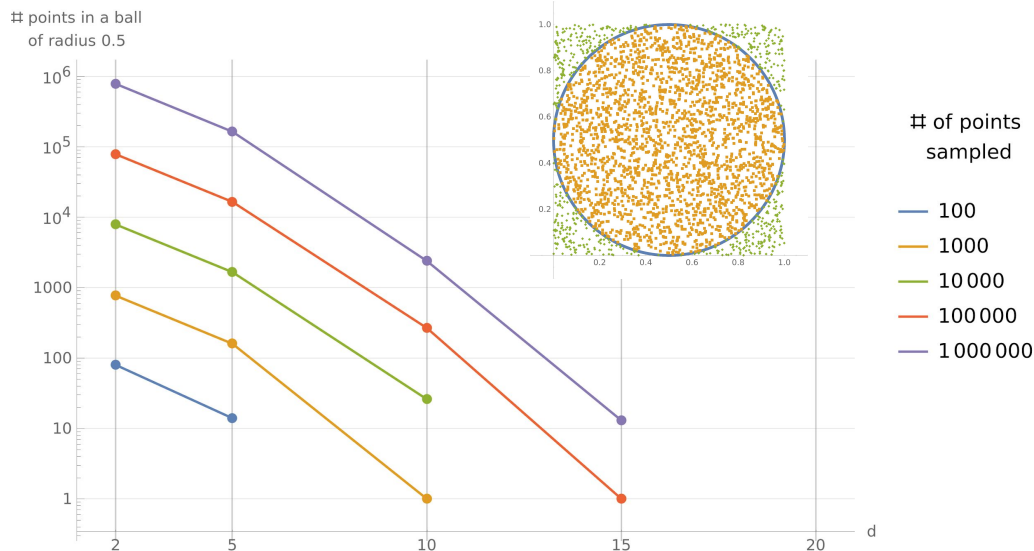
embeddings are redundant:  
**Intrinsic Dimensionality**

Simple embeddings for  
humans are  
complex for maths



# Curse of dimensionality: exponential undersampling in high dimension

How many points in a  $d$ -dim cube are  
at distance smaller than 0.5 from its center?

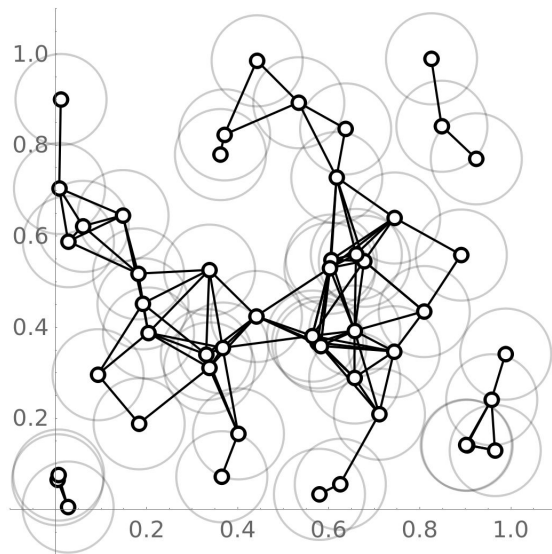


High dimension  
 $d > 6$

Eckmann, J-P., and David Ruelle.  
"Fundamental limitations for estimating  
dimensions and Lyapunov exponents in  
dynamical systems." *Physica D: Nonlinear  
Phenomena* 56.2-3 (1992): 185-187.

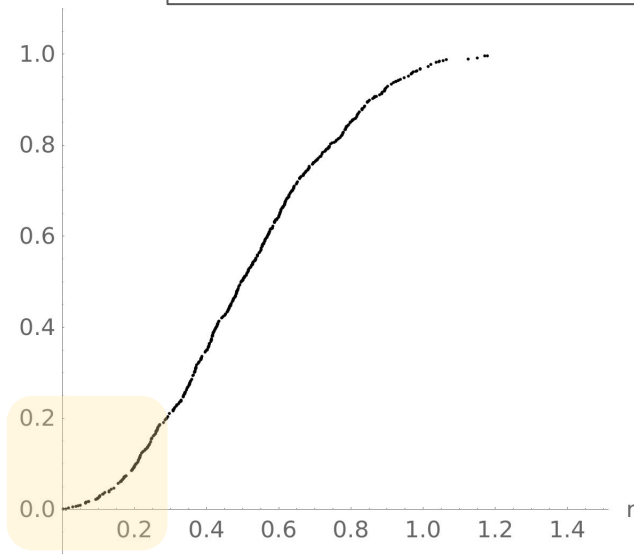
# Geometric estimators: look at the local structure of data

Locally, datasets are linear  $\Rightarrow$  Local number of neighbours scales as  $r^d$



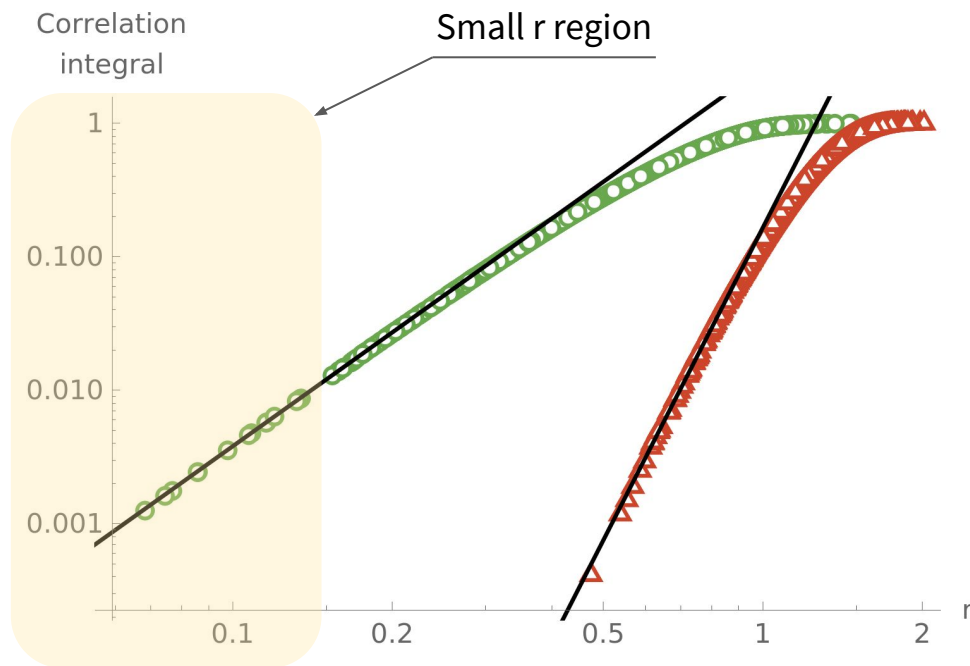
Correlation  
Integral

$$\rho(r) = \frac{2}{N(N-1)} \sum_{1 \leq i < j \leq N} \theta(r - \|\vec{x}_i - \vec{x}_j\|)$$



# Data undersampling $\Rightarrow$ ID underestimation

The intrinsic dimension can be extracted by a linear fit on the log-log plot in the region of small  $r$



$N = 1000$

- Cube  $d = 3$  | Slope = 2.9 ✓
- △ Cube  $d = 10$  | Slope = 7.9 ✗

Grassberger, Peter, and Itamar Procaccia. "Measuring the strangeness of strange attractors." *Physica D: Nonlinear Phenomena* 9.1-2 (1983): 189-208.



# A tradeoff between non-linearity and undersampling

	Geometric local estimators	Projective global estimators	???
Non linear	✓	✗	✓
High dimension	✗ (exp d)	✓ (d log d)	✓

Grassberger, Peter, and Itamar Procaccia. "Measuring the strangeness of strange attractors." *Physica D: Nonlinear Phenomena* 9.1-2 (1983): 189-208.

Ceruti, Claudio, et al. "Danco: An intrinsic dimensionality estimator exploiting angle and norm concentration." *Pattern recognition* 47.8 (2014): 2569-2581.

Hein, Matthias, and Jean-Yves Audibert. "Intrinsic dimensionality estimation of submanifolds in  $\mathbb{R}^d$ ." *Proceedings of the 22nd international conference on Machine learning*. ACM, 2005.

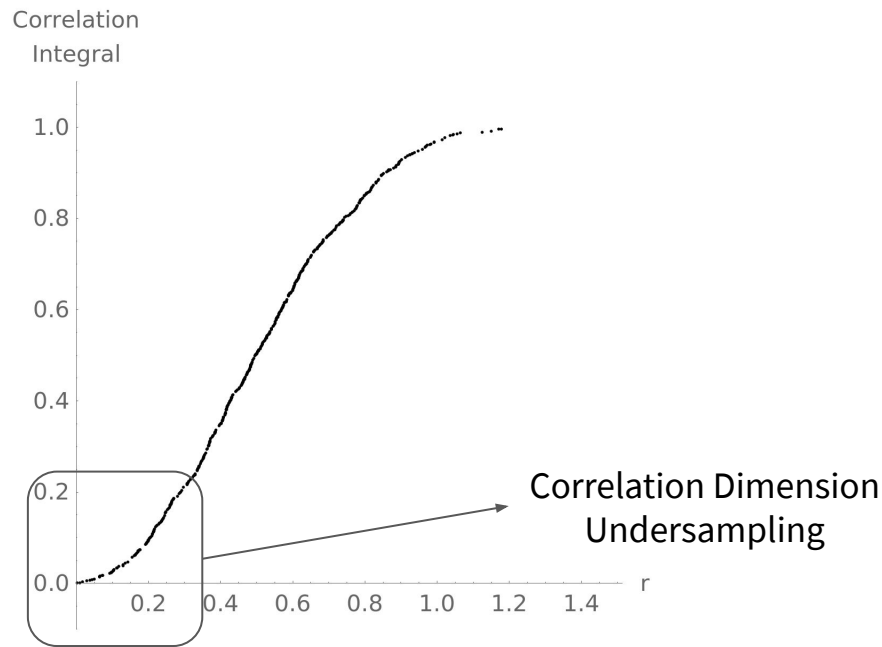
Correlation  
dimension  
DANCO  
Hein  
...

Principal  
Component  
Analysis

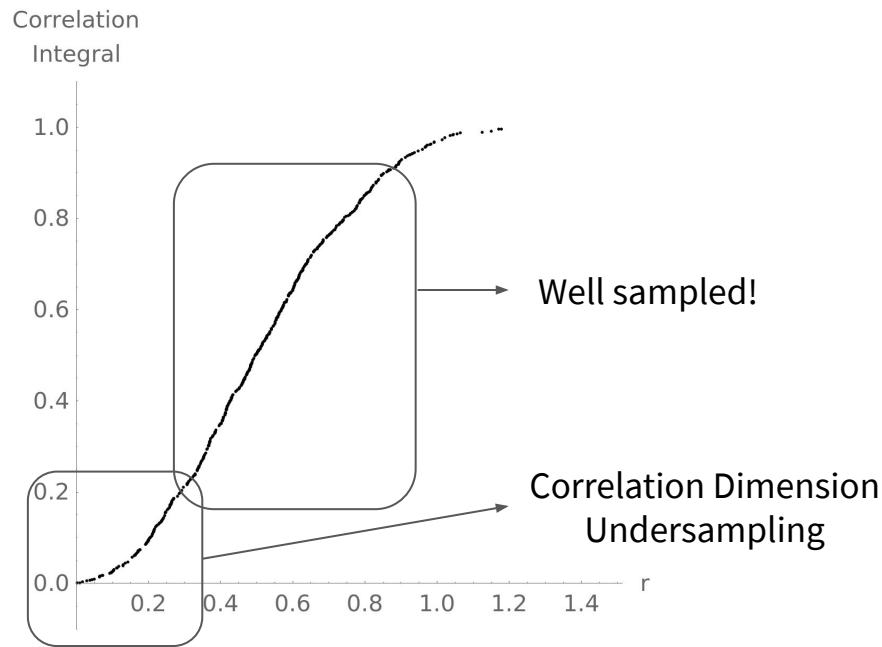
Pearson, Karl. "LIII. On lines and planes of closest fit to systems of points in space." *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 2.11 (1901): 559-572.

Anna V. Little, Jason Lee, Yoon-Mo Jung, and Mauro Maggioni. Estimation of intrinsic dimensionality of samples from noisy low-dimensional manifolds in high dimensions with multiscale SVD. In 2009 IEEE/SP 15th Workshop on Statistical Signal Processing. IEEE, 2009.

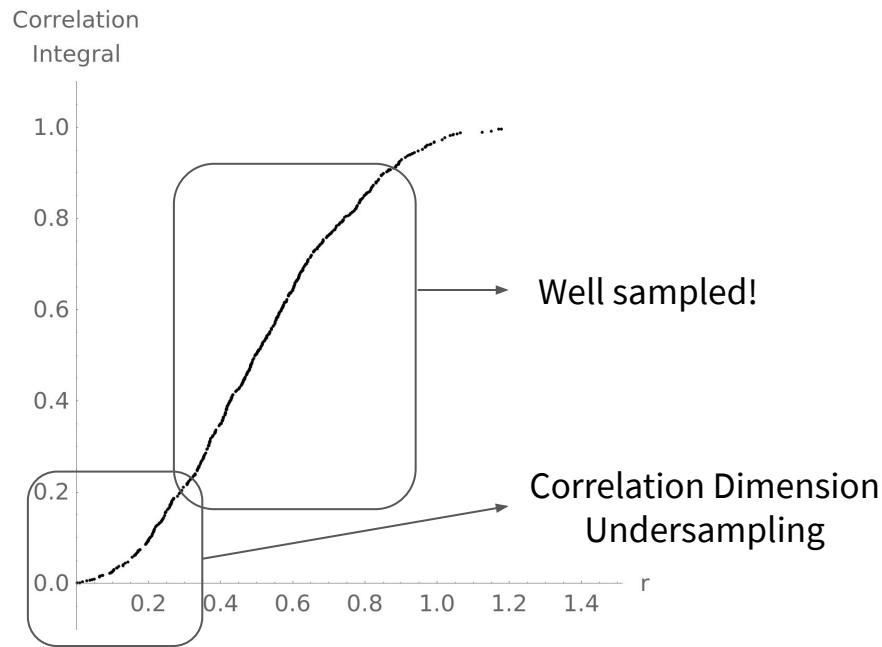
# The Full Correlation Integral Estimator (FCI)



# The Full Correlation Integral Estimator (FCI)



# The Full Correlation Integral Estimator (FCI)

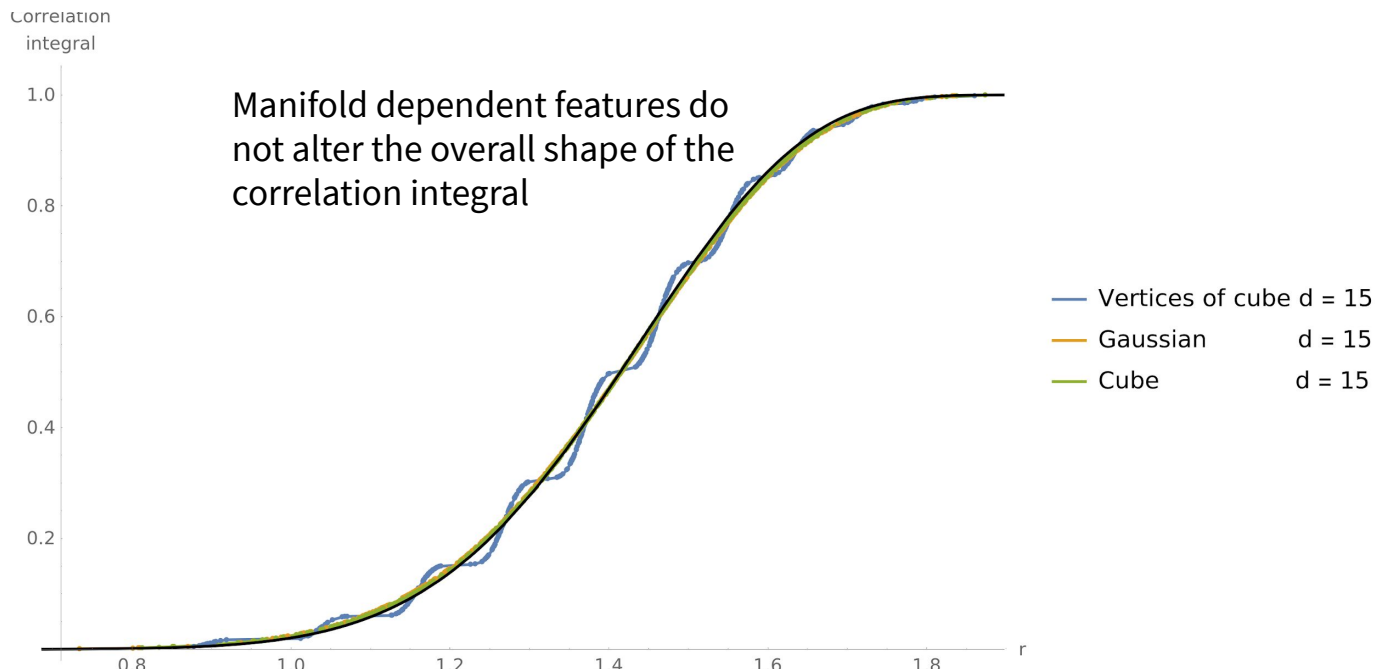


Linear manifolds  
Isotropic sampling measure  
Linear embeddings

$\Rightarrow$

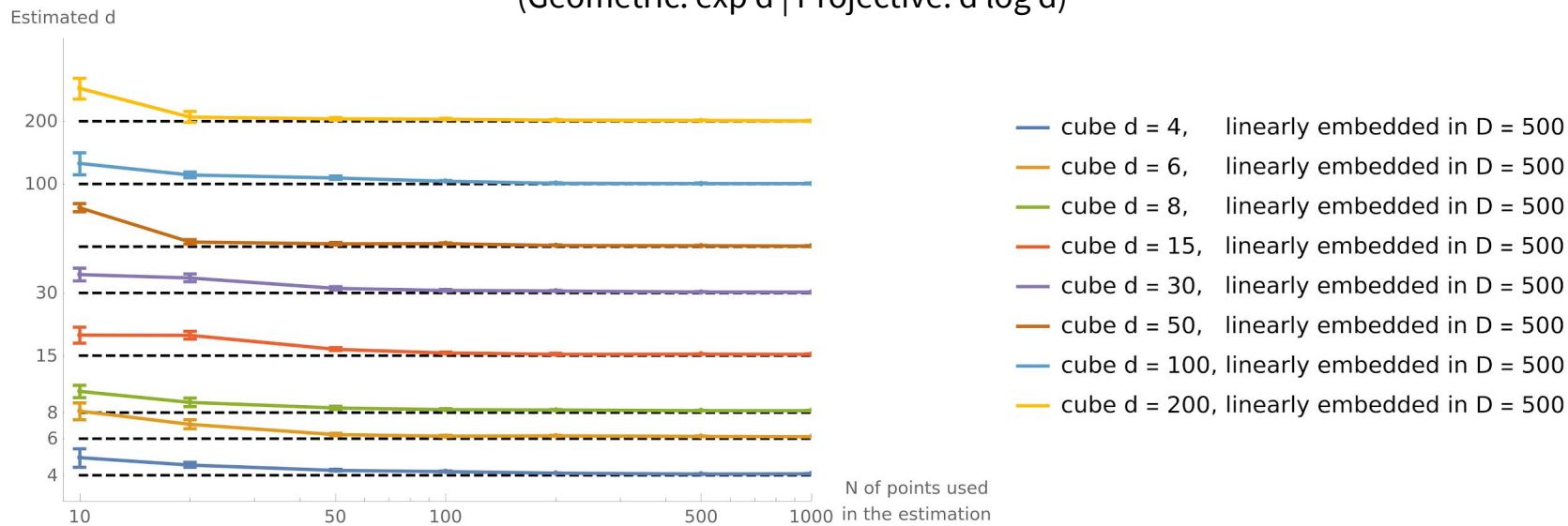
$$\rho(r; d) = \frac{1}{2} + \frac{\Omega_{d-1}}{\Omega_d} (r^2 - 2) {}_2F_1 \left( \frac{1}{2}, 1 - \frac{d}{2} \middle| \frac{3}{2} \middle| (r^2 - 2)^2 \right)$$

# The FCI estimator is robust to non idealities



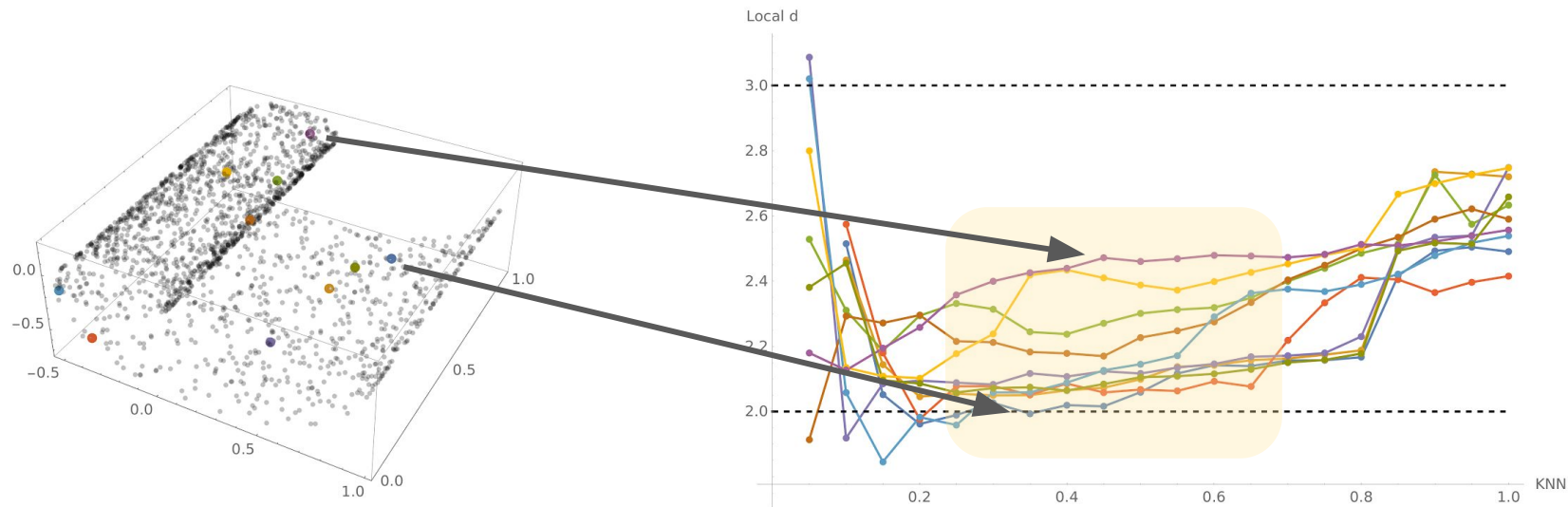
# The FCI estimator is robust to undersampling

Able to estimate in the extreme  
undersampled regime  $N < d$   
(Geometric:  $\exp d$  | Projective:  $d \log d$ )



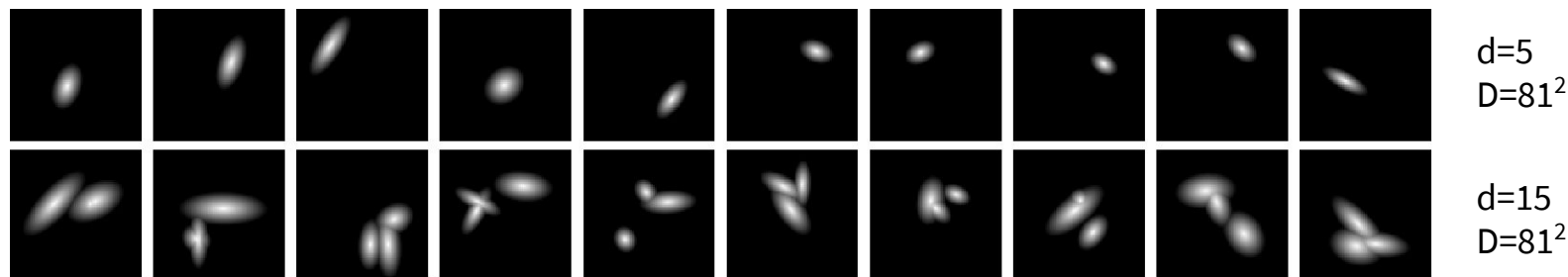
# A multiscale generalization of the FCI

Thanks to robustness + extreme undersampling



Use the “most persistent” minimum as the estimator of the Intrinsic Dimension

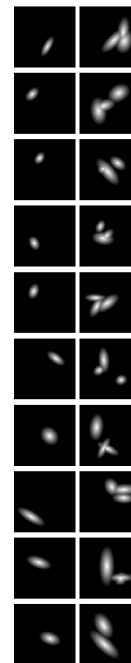
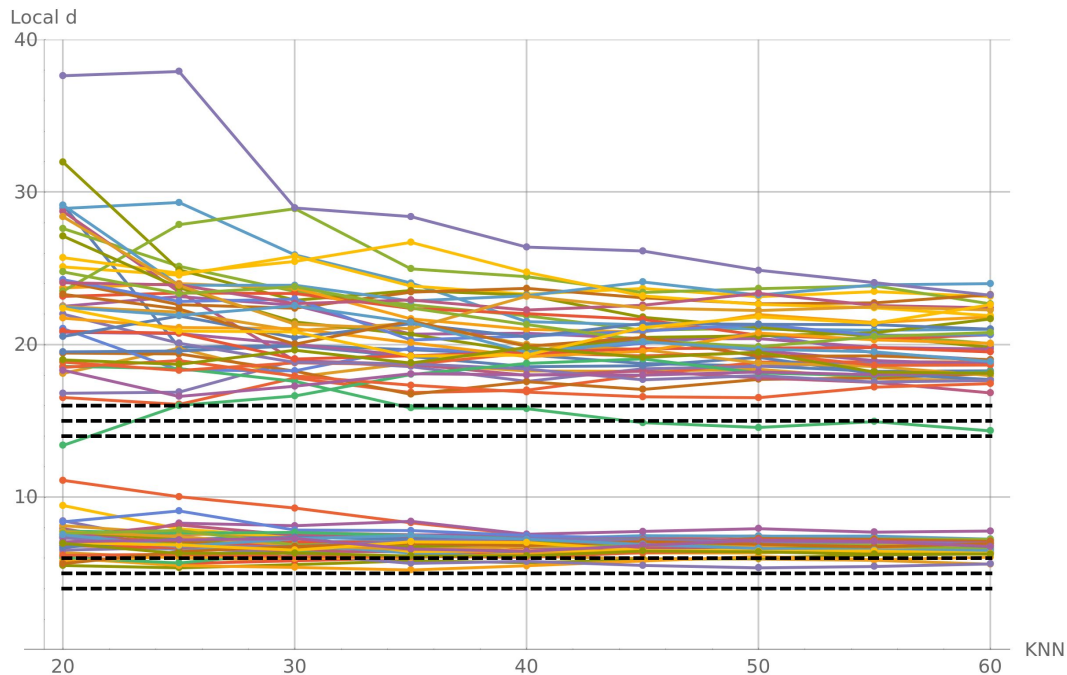
# The multiscale FCI estimator can deal with complex bitmap images



5 degrees of freedom per blob:  
translation x, translation y, eccentricity,  
scale, tilt



# The multiscale FCI estimator can deal with complex bitmap images



# The multiscale FCI is more versatile than other estimators

Estimator	$\mathcal{SR}_{2,3}$	$\mathcal{H}_{20,50}$ $\cup$ $\mathcal{H}_{30,50}$	$\mathcal{C}_{6,12}$	$\mathcal{B}_{5,81^2}$	$\mathcal{B}_{15,81^2}$
CorrDim [8]	1.98	12.53	5.93	5	13.5
Takens [10]	1.97	12.01	5.77	N.A.	N.A.
Hein et al. [13]	2	13	6	N.A.	N.A.
PCA	3	20 & 30	12	40	40
mPCA [24]	3	20 & 30	[9,12]	[2,10]	[6,31]
Multiscale FCI	2	20 & 30	6	5	15

Non linear	✓	✗	✓	✓	✓
High dimension	✗	✓	✗	✗	✓
Multidimensional	✗	✓	✗	✗	✗

Hybrid between local  
geometric methods and  
projective global methods

Easy multiscale  
generalization

Performant in a wide  
variety of situations

# Thank you for your attention!

Learn more:

V.E., Marco Gherardi, Pietro Rotondo, “Intrinsic dimension estimation for locally undersampled data”  
<https://arxiv.org/abs/1906.07670> (accepted in Scientific Reports)