

Improving random sampling in Python

scipy.stats.sampling and scipy.stats.qmc

Tirth Patel
Christoph Baumgarten
Matt Haberland

Pamphile T. Roy
  *PamphileRoy*



SciPy

Statistics, optimization,
interpolation,
integration, *



Random numbers you said?

>>> Draw from a set: variable

... Numbers

... Things/Variables are dimensions

... Draw/samples are independent

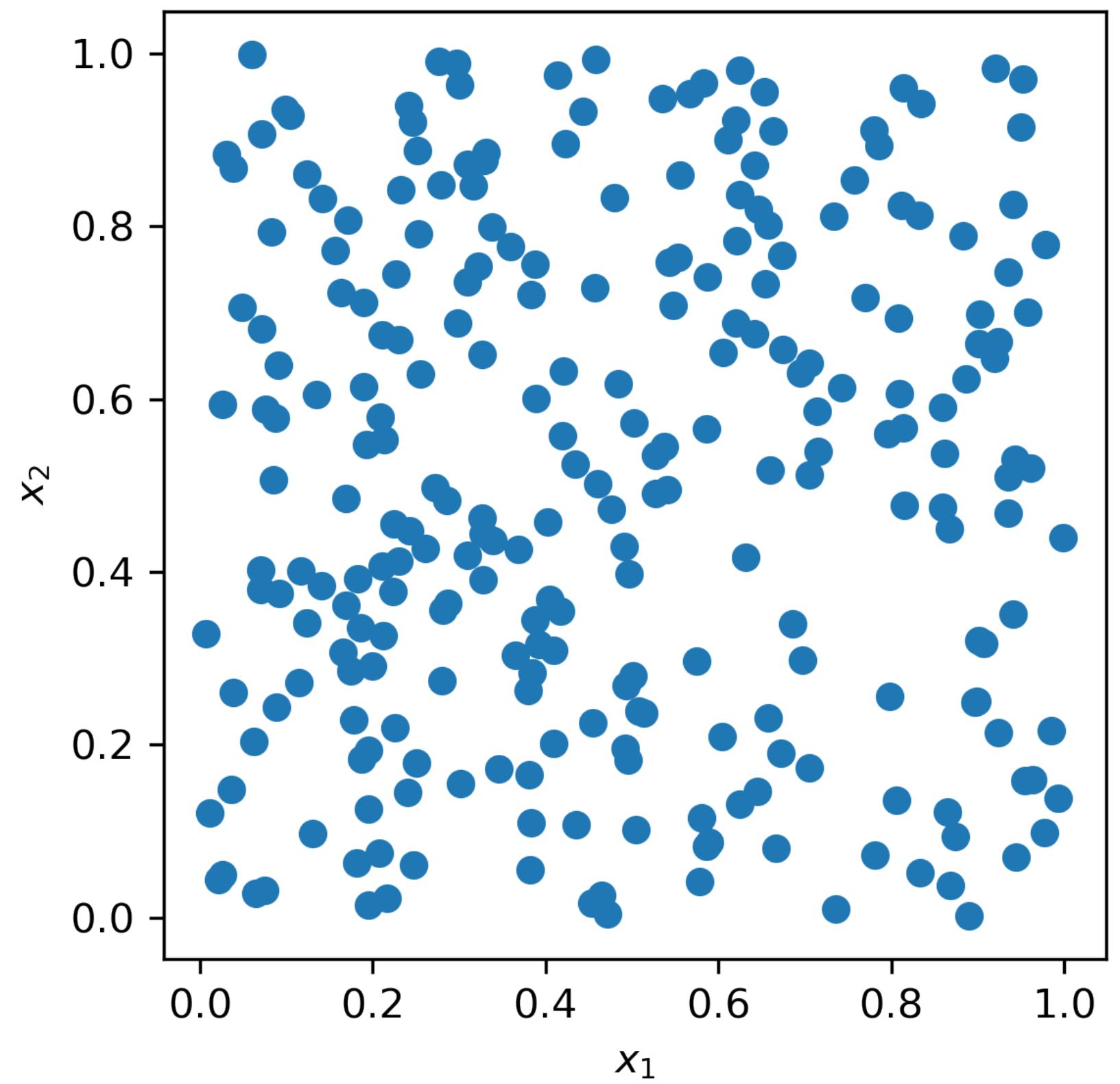
```
>>> rng = np.random.default_rng()
```

```
>>> x = rng.random(1_000)
```

```
>>> x = rng.random(size=(1_000, 10))
```

Random numbers you said?

$\mathbf{x} = (x_1, \dots, x_n)$
 $x \sim \mathcal{U}(0,1)$

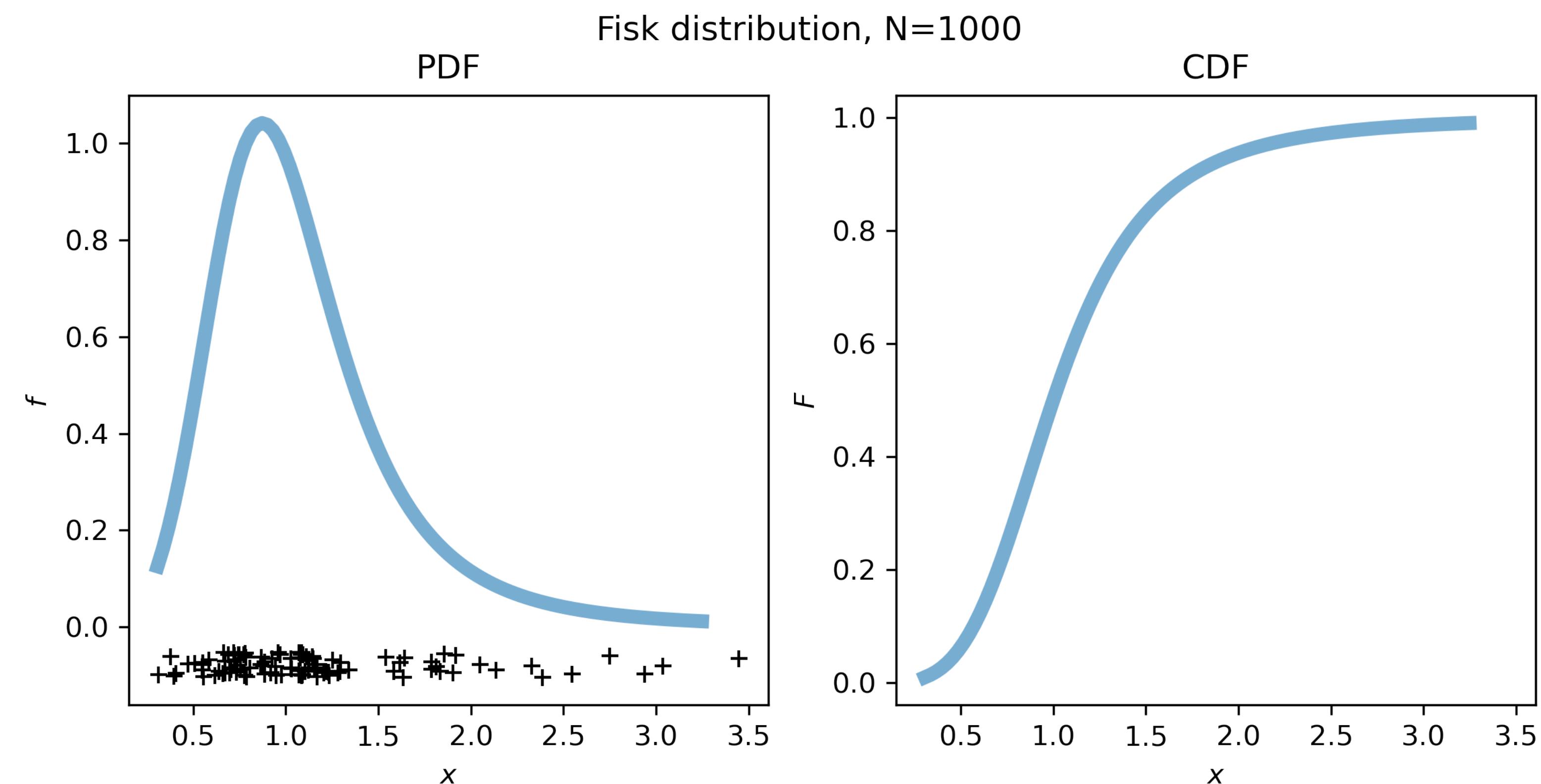


Distribution sampling is easy

```
>>> x = U~0, 1()
```

```
>>> PDF = f(x)
```

```
>>> CDF = F(x)
```



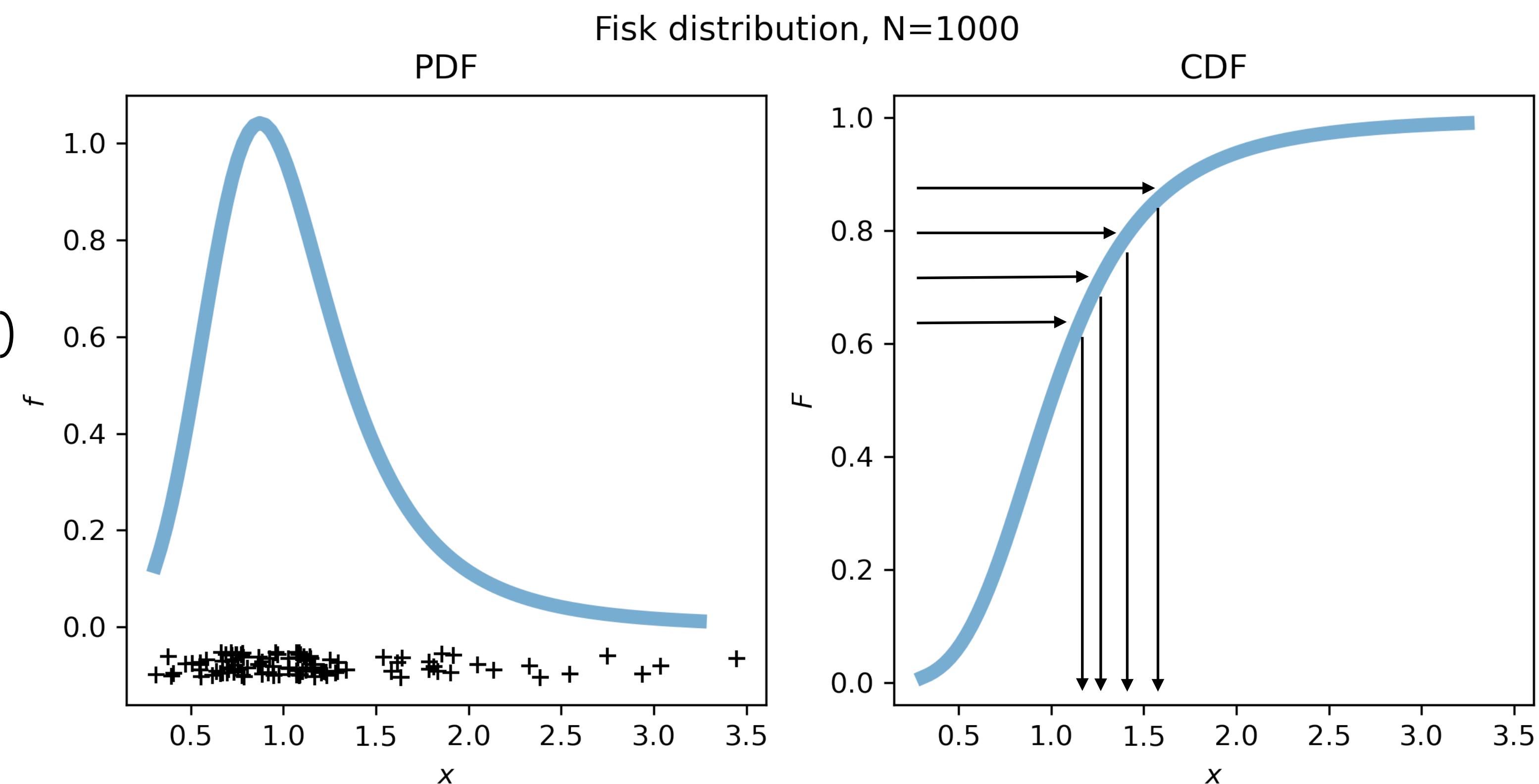
Distribution sampling is easy

Inverse CDF: $F^{-1}(x') = x$

```
>>> rng = np.random.default_rng()
```

```
>>> x_ = rng.random(1_000)
```

```
>>> x = dist.ppf(x_)
```



But it's hard

- >>> What is this PPF function?
- >>> What to do if there is no direct formula!?

```
>>> from scipy.stats import sampling
```

>>> Blackbox methods

>>> C library UNU.RAN

>>> Generate variates from non-standard distributions

>>> Inversion methods are relevant for QMC

>>> "Automatic random variate generation in Python"
in the conference proceedings

Sampling Continuous distributions

Methods for continuous distributions	Required Inputs	Optional Inputs	Setup Speed	Sampling Speed
<code>TransformedDensityRejection</code>	pdf, dpdf	none	slow	fast
<code>NumericalInverseHermite</code>	cdf	pdf, dpdf	(very) slow	(very) fast
<code>NumericalInversePolynomial</code>	pdf	cdf	(very) slow	(very) fast
<code>SimpleRatioUniforms</code>	pdf	none	fast	slow

where

- pdf: probability density function
- dpdf: derivative of the pdf
- cdf: cumulative distribution function

And Discrete distributions

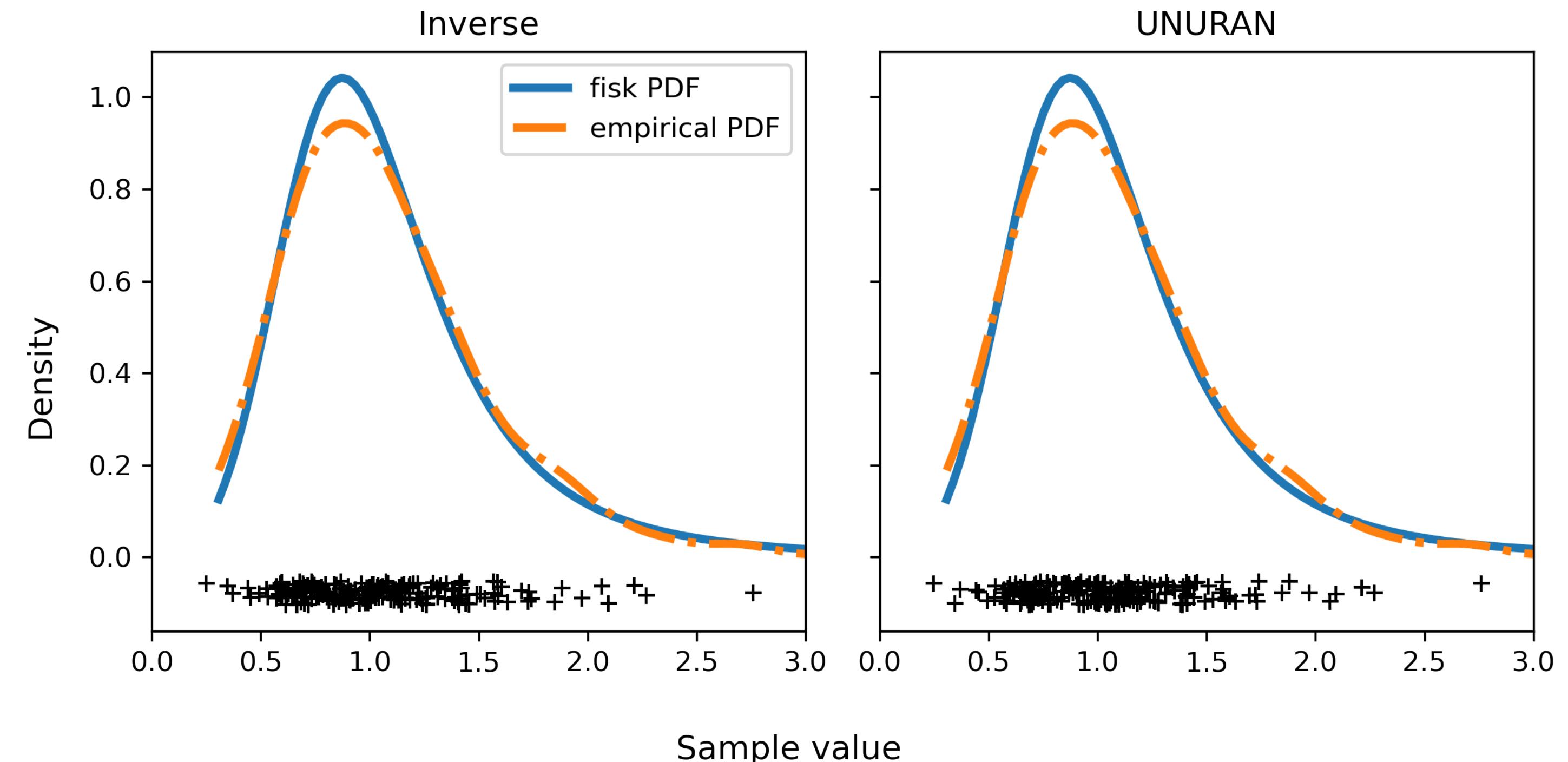
Methods for discrete distributions	Required Inputs	Optional Inputs	Setup Speed	Sampling Speed
DiscreteAliasUrn	pv	pmf	slow	very fast
DiscreteGuideTable	pv	pmf	slow	very fast

where

- pv: probability vector
- pmf: probability mass function

Sample various distributions

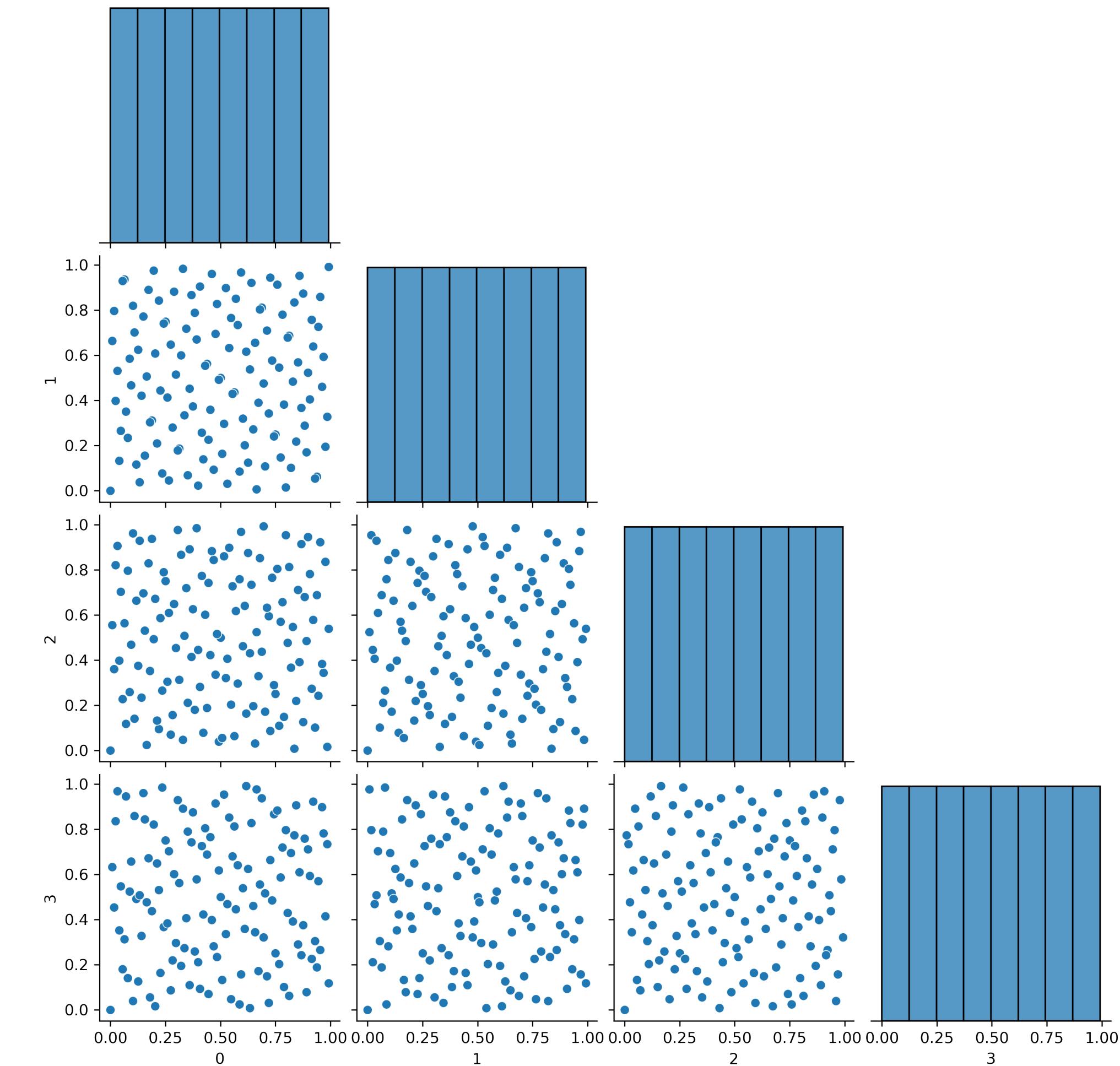
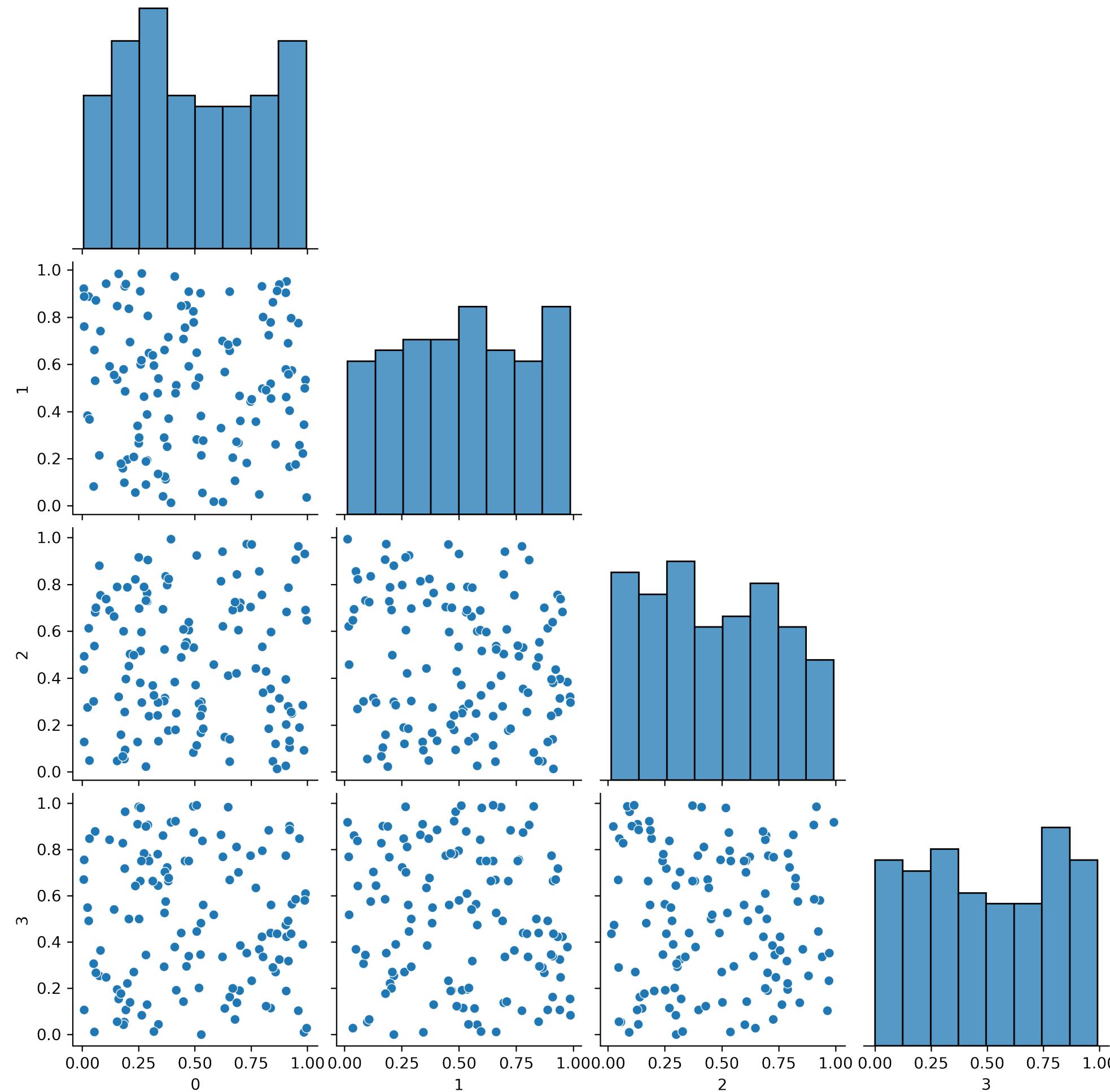
```
>>> import scipy.stats as stats  
  
>>> dist = stats.fisk(c=3.9)  
  
>>> rng_dist = stats.sampling.NumericalInverseHermite(dist)  
  
>>> sample_qmc = rng_dist.rvs(128)
```



What is Quasi-Monte Carlo?

- >>> Deterministic methods
- >>> Not **i**ndependent and **i**dentially **distributed (IID)**
- >>> Better space filling
- >>> Better convergence

What is Quasi-Monte Carlo?



What is Quasi-Monte Carlo?

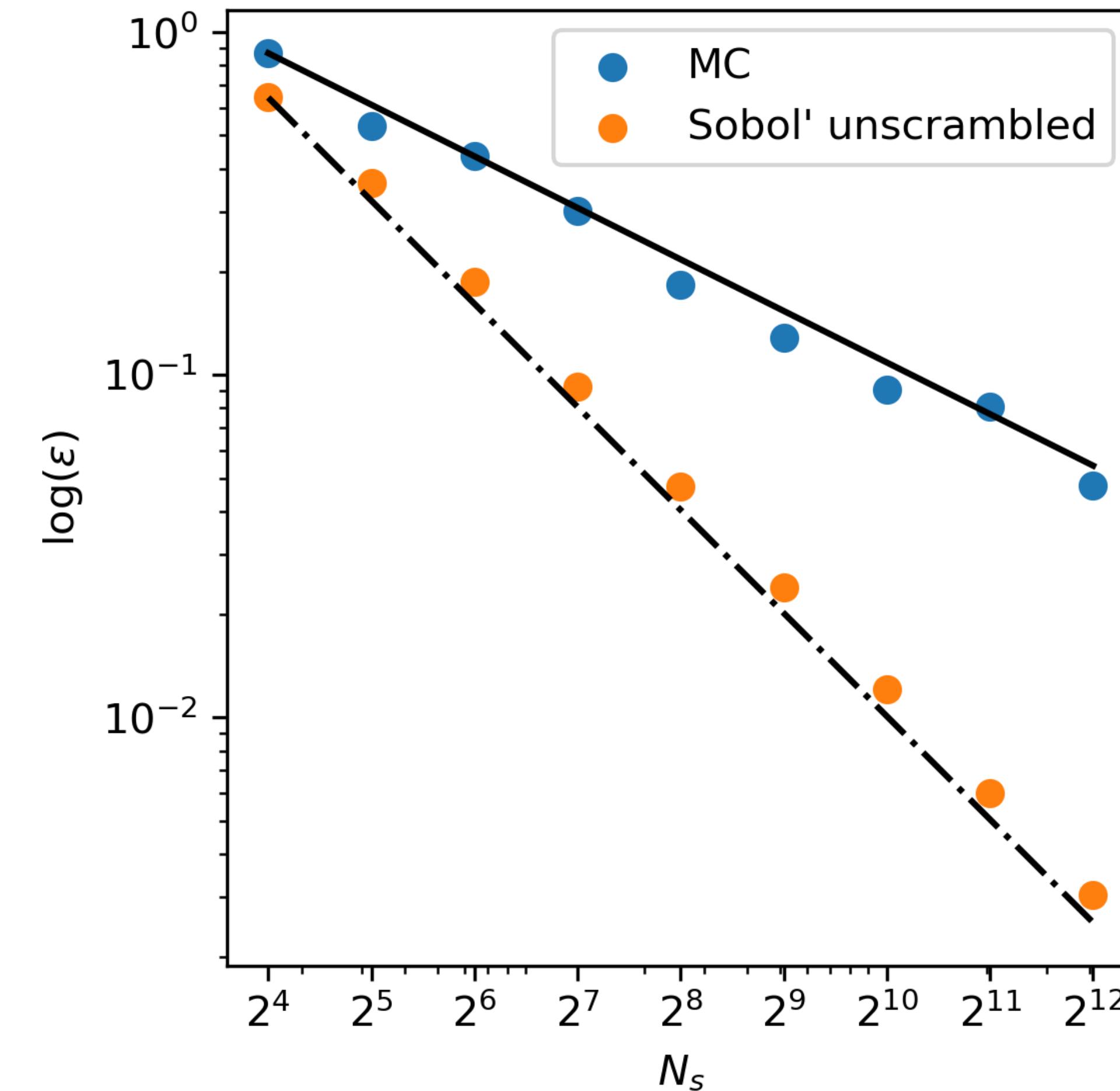
$$f(\mathbf{x}) = \left(\sum_{j=1}^5 x_j \right)^2$$

$$x_j \sim \mathcal{U}(0,1)$$

$$\mu = 5/3 + 5(5 - 1)/4$$

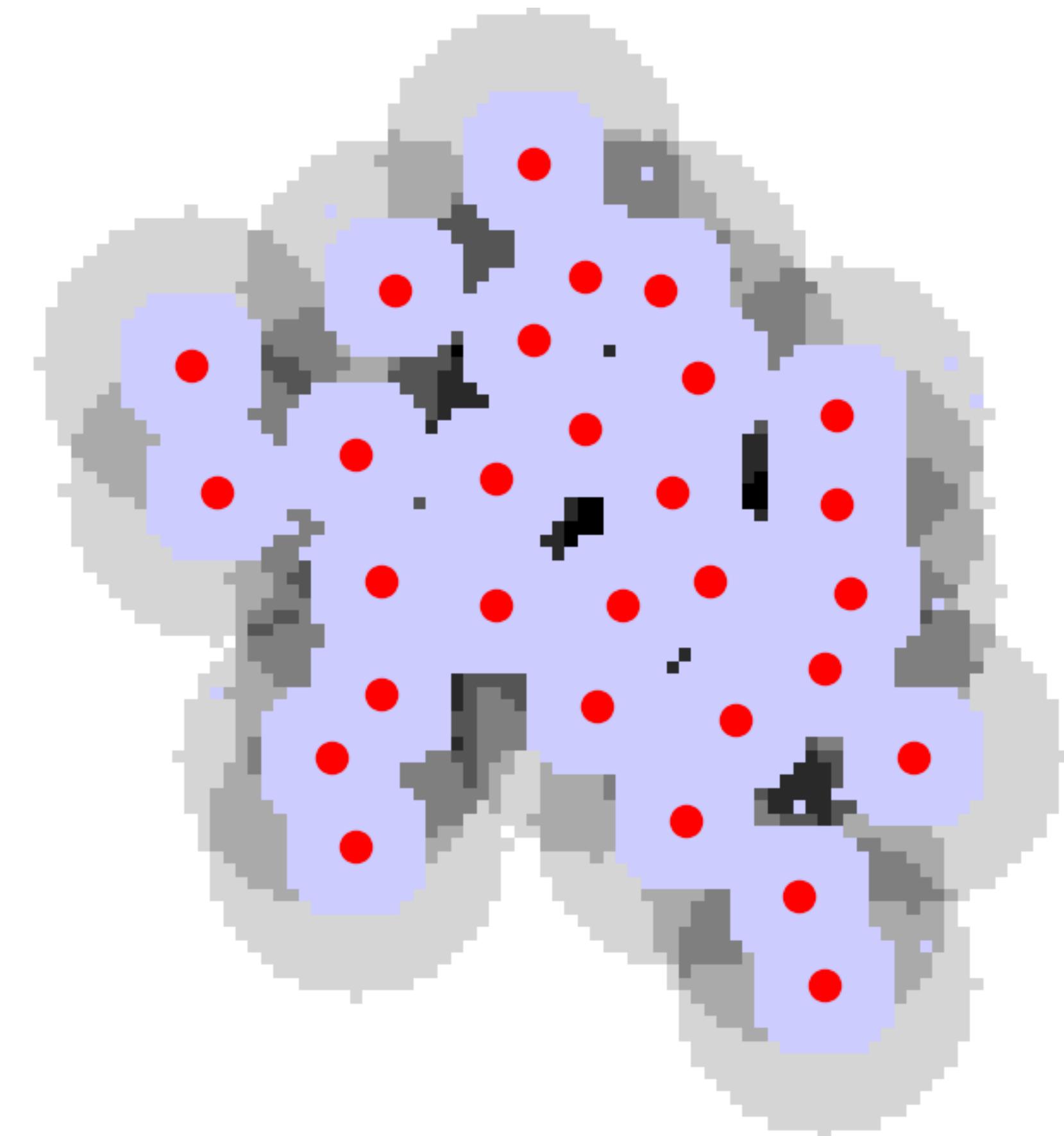
>>> Faster convergence
integration

... $\mathcal{O}(n^{-1/2})$ to $\mathcal{O}(n^{-1})$



```
>>> from scipy.stats import qmc
```

```
>>> Sobol'  
>>> Halton  
>>> LHS and Orthogonal LHS  
>>> Poisson disk (new!)  
>>> Multinomial  
>>> Multivariate normal  
>>> Discrepancy
```



Sample various distributions with QMC

>>> Easy API

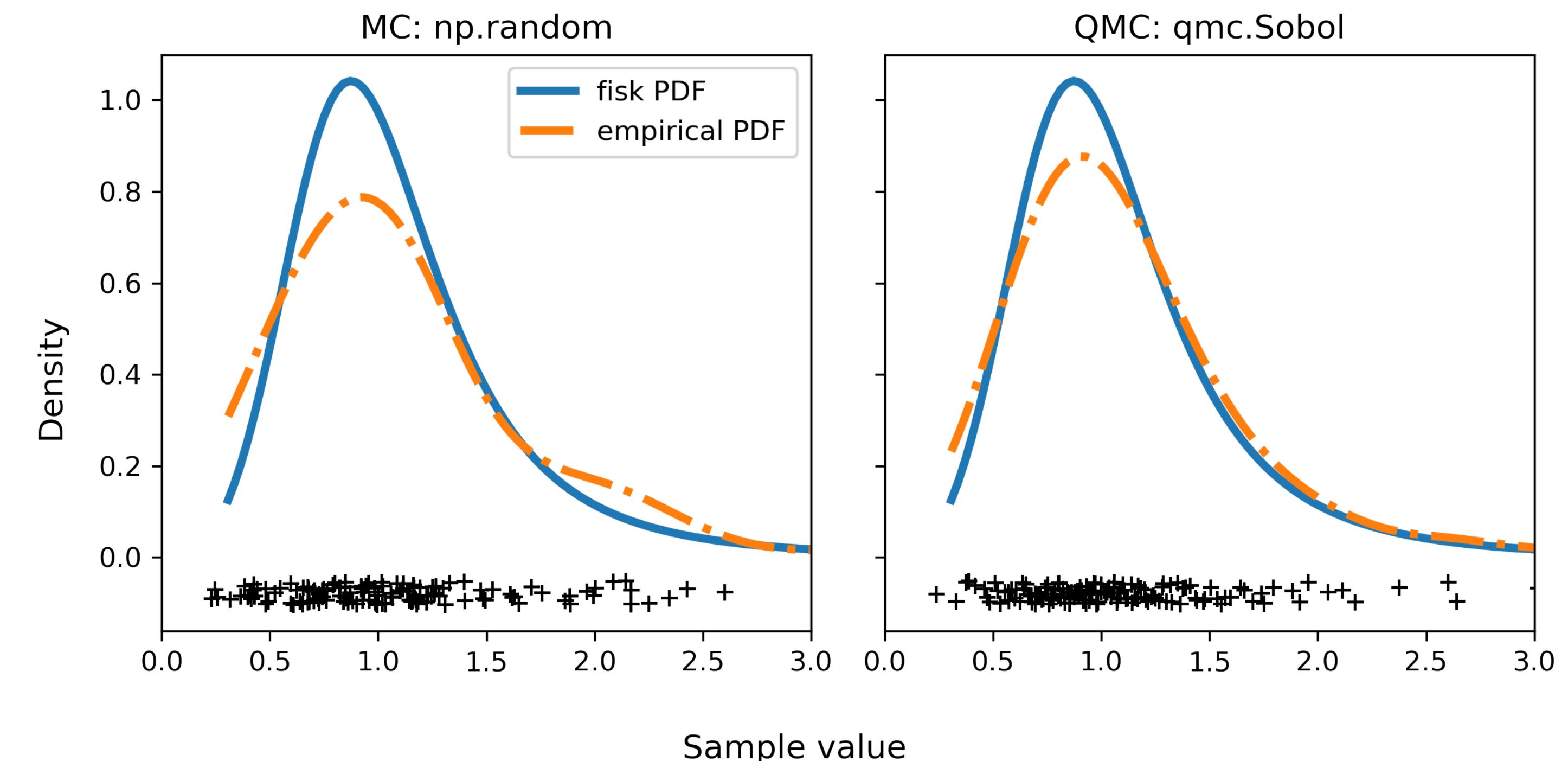
>>> sampling

```
>>> import scipy.stats as stats
```

```
>>> dist = stats.fisk(c=3.9)
```

```
>>> rng_dist = stats.sampling.NumericalInverseHermite(dist)
```

```
>>> sample_qmc = rng_dist.qrvs(128)
```



Do's and don'ts

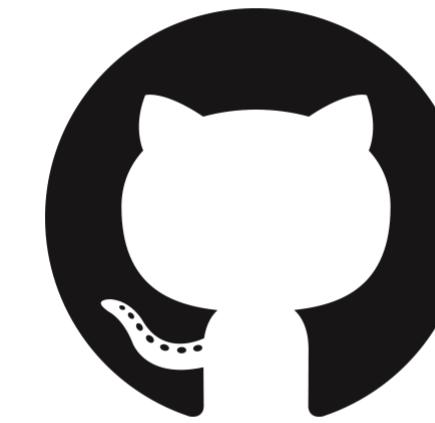
- >>> Know where speed matters: sampling/init
- >>> Use QMC!
- >>> Don't modify the sequences
- >>> Don't use a seed (ready to die on this hill)

Demo

<https://gist.github.com/tupui/9c61591395da3a0b008e4be0ebb465d7>

You help[ed] make it happen...

Issues, PR, reviews, discussions, issue management: *every contribution matters, even a star on the repository...* Join us!



scipy/scipy

Thank You!