

Statistical Description of Cosmological Density Perturbations

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Observational Cosmology for MACSS 2017 (as part of MexiCopas), León Guanajuato.

Bibliografía

- Cosmological Physics, John Peacock, capitulo 16, Cosmological Density Fields.
- Large-Scale Structure of the Universe and Cosmological Perturbation Theory ,Bernardeau a, S. Colombi b, E. Gaztan~aga c, R. Scoccimarro Seccion 6, <https://arxiv.org/pdf/astro-ph/0112551>
- Cosmological Principle.
 - What have we learned from observational cosmology ? Jean-Christophe Hamilton, <https://arxiv.org/abs/1304.4446>
 - A Test of the Copernican Principle, Caldwell and Stebbins <https://arxiv.org/pdf/0711.3459.pdf>

Cosmological Principle

“The Universe is spatially homogeneous and isotropic, (statistically speaking)”

Cosmological Principle

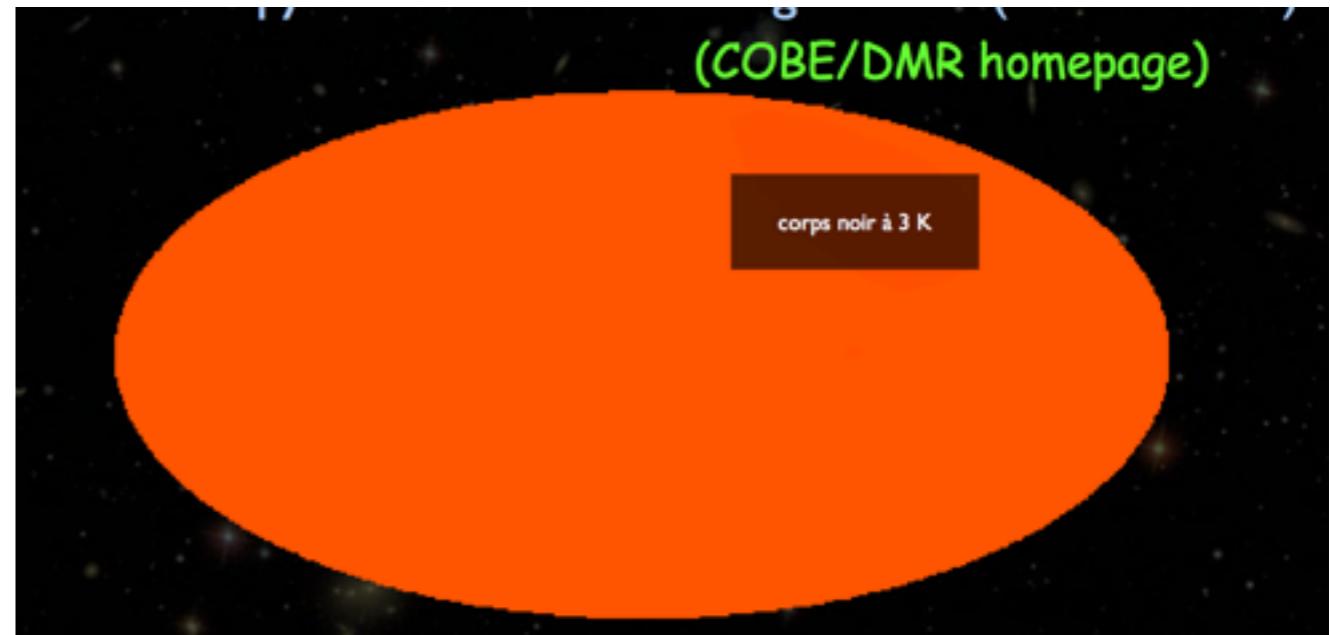
- Motivated by extending the Copernican principle to the whole Universe
- Copernican principle :

“Earth is not at a privileged place in the Universe. We are located in a region of the Universe that has nothing special, we could be living somewhere else and our observations, although not exactly the same at the anecdotic level, would be similar in average”

- **Universe is isotropic:** whatever the direction we look at on the sky, we observe similar things. Of course we are inside a galaxy that is shaped like a fried egg, so we observe more stars in the direction of the Galactic plane and even more in the direction of the Galactic center, but this is a local effect.

Isotropy

- Isotropy is nowadays well established throughout the observable Universe:
- Using modern spectroscopic surveys
- The perfect black-body nature of the CMB shows a uniform temperature over the whole celestial sphere.



Criticisms on the assumption of the Copernican principle

- Possible alternative explanation for the acceleration of the expansion **is that we live in a particularly under-dense region of the Universe (a large void)**, the faraway galaxies falling towards the walls of this void.
- Explain Dark Energy through the fact that we could be in a inhomogeneous Universe (Lemaître-Tolman-Bondi [Bondi; 1947] space–time [Nadathur and Sarkar; 2010].
- Such models, centered on ourselves, the **CMB seen by distant observers would be strongly inhomogeneous** and should result in **violations of the black- body nature of the CMB we observe** [Stebbins; 2007]. It could indeed be isotropic, but inhomogeneity would induce spectral distortions that are not compatible with the observed spectrum of the CMB [Caldwell and Stebbins; 2008] for the cases of large voids with density contrasts large enough to explain the acceleration of the expansion.



500 Mpc/h

**El Universo es homogeneo e isotropico a escalas
mayores a 100 Mpc !!!**

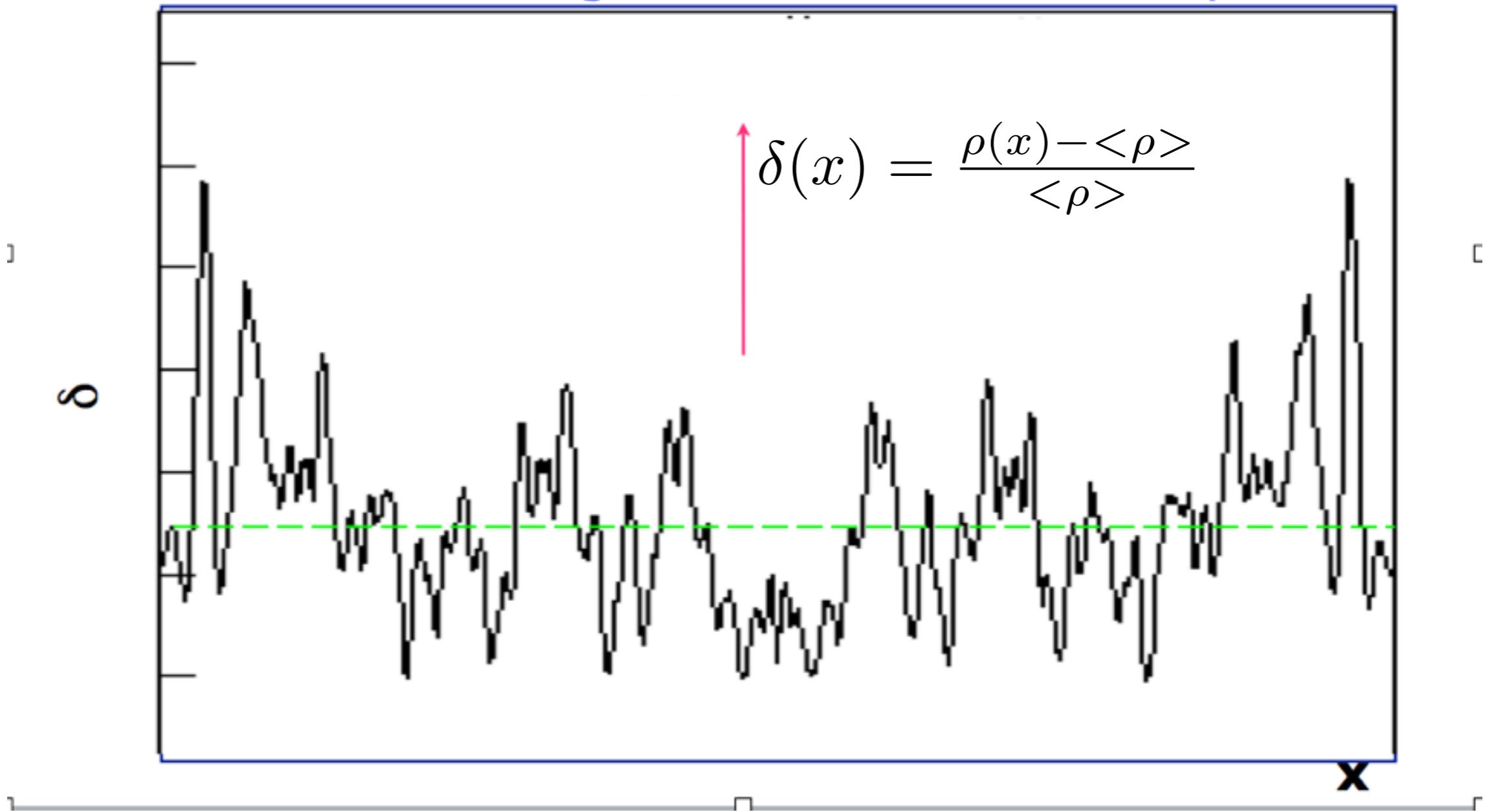
Preliminaries

- Let $\rho(x)$ be the density distribution of matter at a location x

$$\delta(x) = \frac{\rho(x) - \langle \rho \rangle}{\langle \rho \rangle}$$

- It is useful to define the corresponding over density field
 - is believed to be the outcome of some random process in the early universe (i.e. Quantum fluctuations in inflation)

Density Fluctuations



- NOTE: $\langle \cdot \rangle$ denotes an ensemble average. For instance, means the average overdensity at for many realizations of the random process

Perturbations Statistical description.

- Overdensity $\delta(t,x)$ contains all information about the LSS in the universe at any time.
- In order to characterize the structure in the universe and to compare observations of δ with theory, it is meaningful to think of δ as a **realization of a stochastic process**.
- initial inhomogeneities in the universe were created by a **stochastic process** and that this process was the same at every position.
- the mathematical theory needed here is the **theory of random fields**.

δ as a realization of a homogeneous and isotropic random field with zero mean.

Cosmological density field

- How we can describe the cosmological density field without having to specify the actual value of delta at each location in space-time.?

Cosmological density field

- How we can describe the cosmological density field without having to specify the actual value of delta at each location in space-time.?
- Since is believed to be the outcome of some random process in the early Universe our goal is to describe the probability distribution

$$P(\delta_1, \delta_2, \dots, \delta_N) d\delta_1, d\delta_2, \dots d\delta_N \quad \delta_1 = \delta(\vec{x}_1)$$

- For now we will focus on the cosmological density field at some particular (random) time. We will address it's time evolution later in this lecture
- This probability distribution is completely specified by the moments

$$\langle \delta_1^{l1} \delta_2^{l2} \dots \delta_N^{lN} \rangle = \int \delta_1^{l1} \delta_2^{l2} \dots \delta_N^{lN} P(\delta_1, \delta_2, \dots, \delta_N) d\delta_1, d\delta_2, \dots d\delta_N$$

Moments

- Moments are used to characterize the probability distribution.
- For now let us just introduce the moments: $\hat{\mu}_m = \langle x^m \rangle$
- and, of special interest, the central moments: $\mu_m = \langle (x - \langle x \rangle)^m \rangle$.
- Here, μ_2 is the variance, μ_3 is called the skewness, μ_4 is related to the kurtosis. To keep things as simple as possible let's just consider the Gaussian distribution as reference.
- For a Gaussian distribution all moments of order higher than 2 are specified by μ_1 and μ_2 . Or, in other words, the mean and the variance completely specify a Gaussian distribution.

Ergodic Hypothesis

- First Moment $\langle \rho = \int \rho P(\rho) d\rho \rangle$
- PROBLEM: Theory specifies ensemble average, but observationally we have only access to one realization of the random process.
- Ergodic Hypothesis: Ensemble average is equal to spatial average taken over one realization of the random field.
- Essentially, the ergodic hypothesis requires spatial correlations to decay sufficiently rapidly with increasing separation so that there exists many statistically independent volumes in one realization..

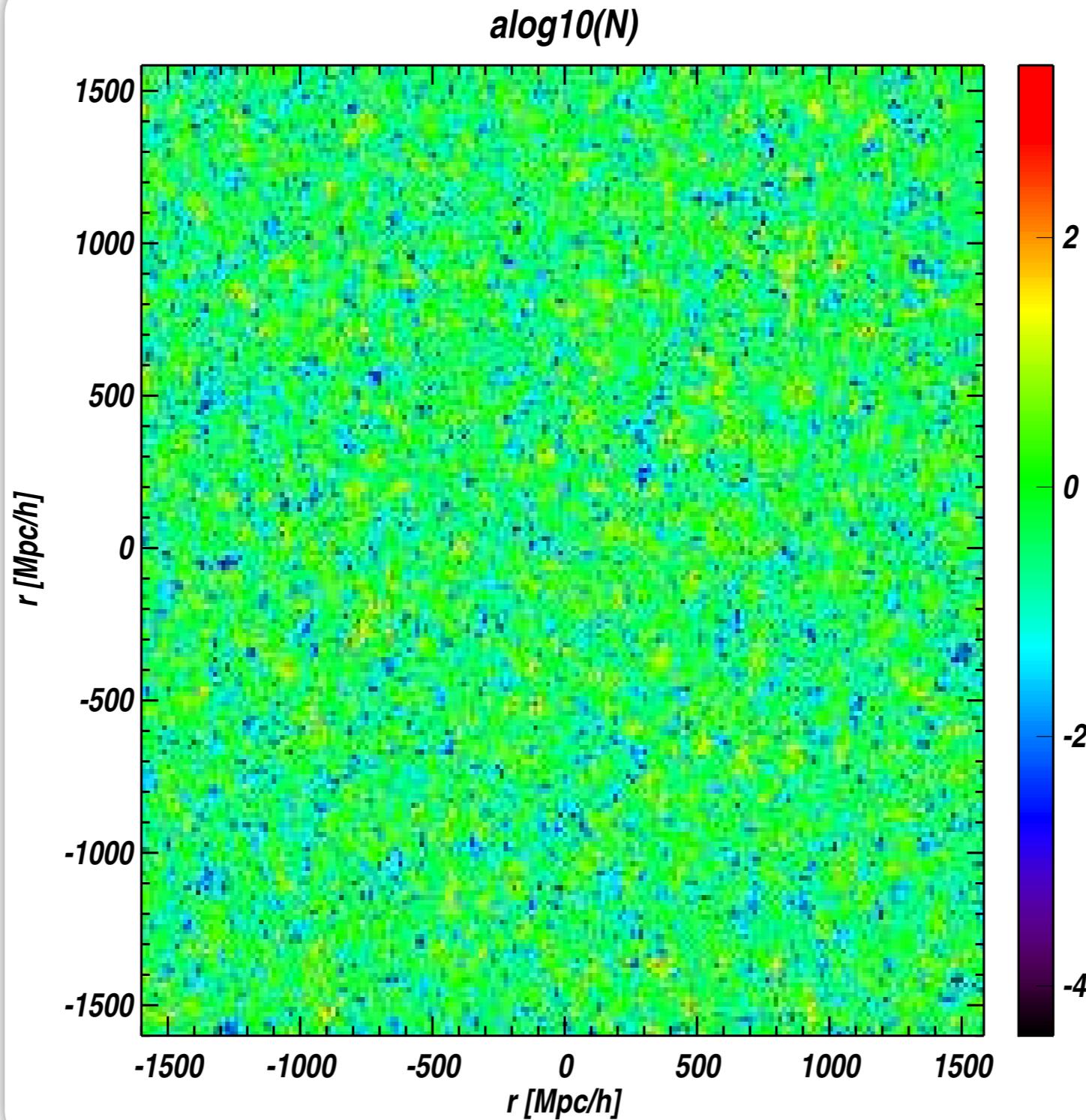
Fair Sample Hypothesis

- (Peebles 1980) states that **well separated parts of the universe can be regarded as independent realizations of the underlying stochastic process** and that the observable universe contains many such realizations.
- Most present day galaxy surveys are way too small to constitute a fair sample (especially at high redshift) and thus **averages over the volumes of such surveys are subjected to statistical fluctuations**. This phenomenon is called **sample variance** or **cosmic variance** if the sample is constrained by **the size of the observable universe** (e.g., CMB). The two terms are, however, often used interchangeably.

Moments

- First Moment $\langle \rho = \int \rho P(\rho) d\rho \rangle$
- because of the ergodic principle, that allows to exchange ensemble average over spatial average
- **QUESTION:How many moments do we need to completely specify the cosmological density field?**
- In principle infinitely many. However, there are good reasons to believe that the initial cosmological density field is special, in that it is a Gaussian random field.

Gaussian Random Field



Gaussian Random Fields

- A random field is said to be Gaussian if the distribution of the field values at an arbitrary set of N points is an N-variate Gaussian.

$$\mathcal{P}(\delta_1, \delta_2, \dots, \delta_N) = \frac{\exp(-Q)}{[(2\pi)^N \det(\mathcal{C})]^{1/2}}$$
$$Q \equiv \frac{1}{2} \sum_{i,j} \delta_i (\mathcal{C}^{-1})_{ij} \delta_j$$
$$\mathcal{C}_{ij} = \langle \delta_i \delta_j \rangle \equiv \xi(r_{ij})$$

- A random field is said to be Gaussian if the distribution of the field values at an arbitrary set of N points is an N-variate Gaussian: $\delta(x)$ where we have defined the two-point correlation function.
 - $\xi(x) = \langle \delta(x) \delta(x+r) \rangle$
 - As you can see, **for Gaussian random field the N-point probability function is completely specified by the two-point correlation function**

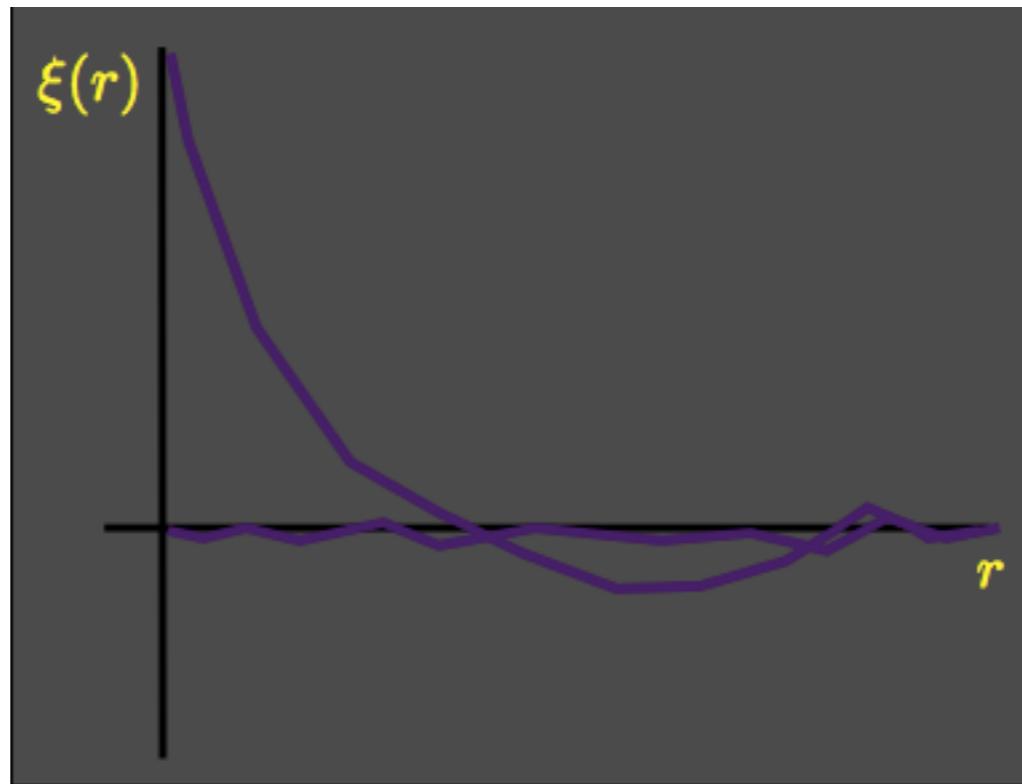
2-point Correlation Function

Second Moment

$$\langle \delta_1 \delta_2 \rangle \equiv \xi(r_{12})$$

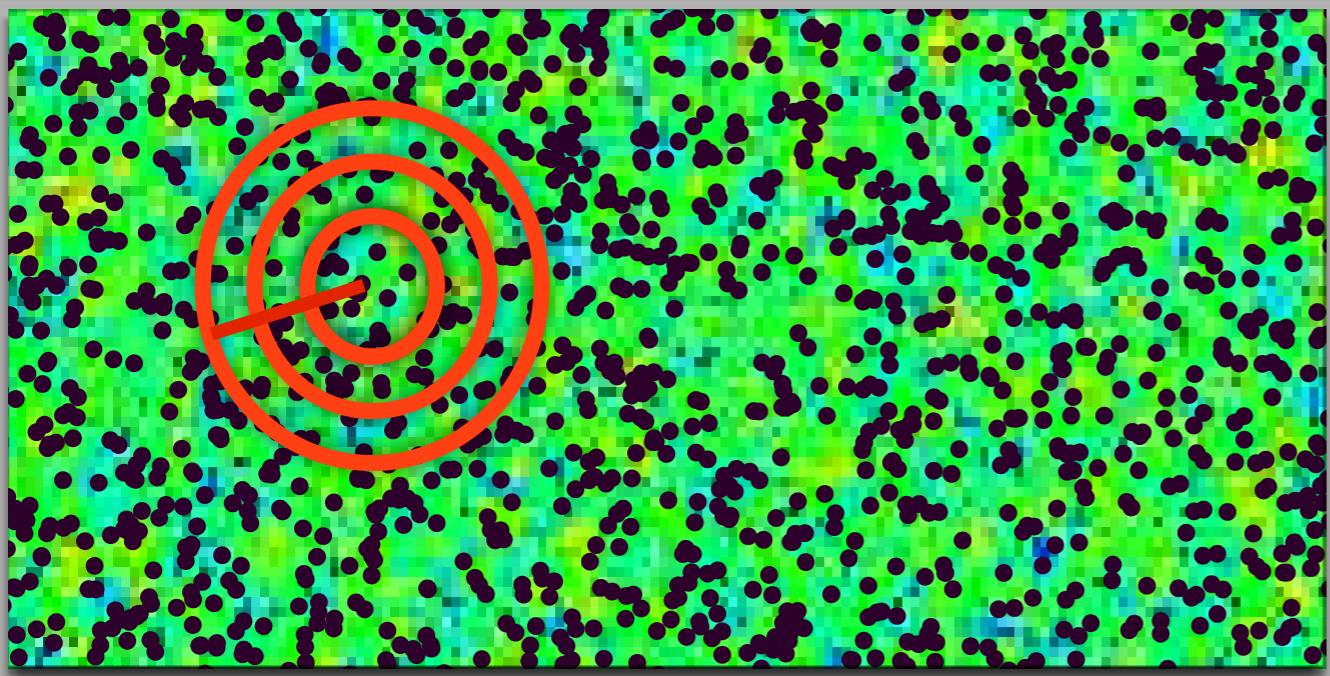
$$r_{12} = |\vec{x}_1 - \vec{x}_2|$$

- $\xi(r)$ is called the two-point correlation function
- Note that this two-point correlation function is defined for a continuous field, . However, one can also define it for a point distribution:

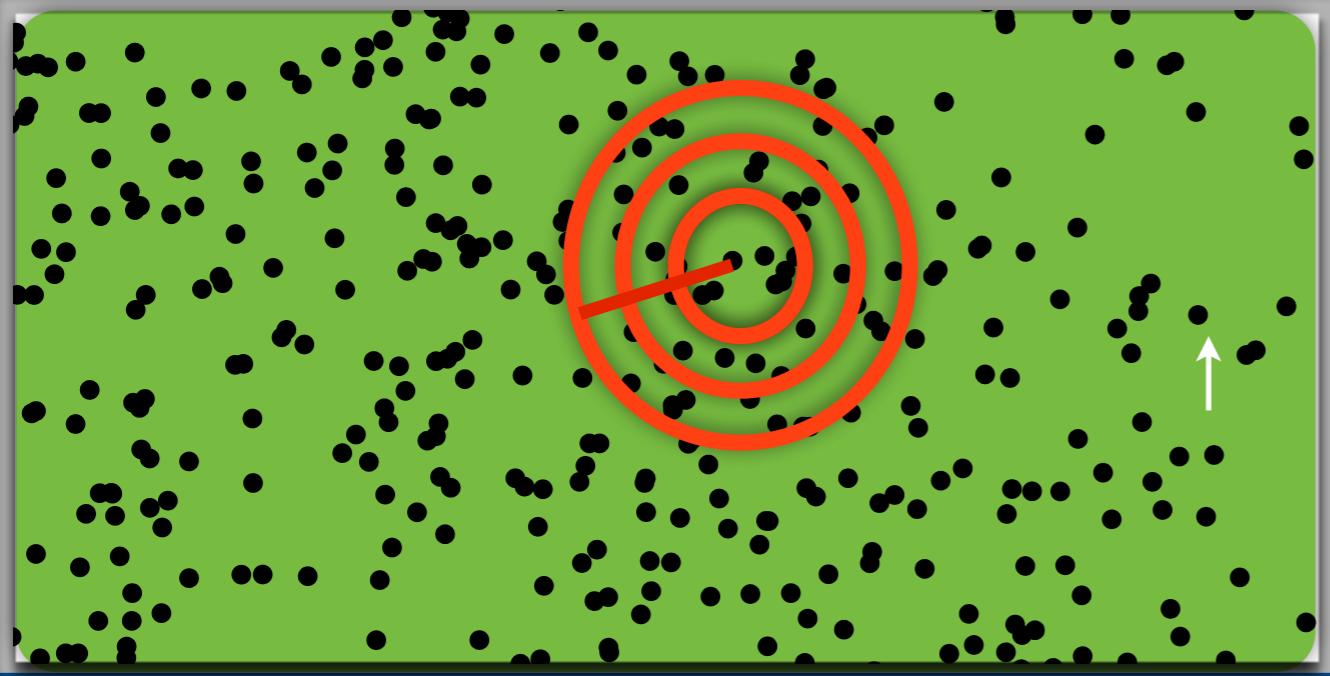


La fonction de Corrélation

Correlated Data



Random Set



- The 2PCF represents the probability excess to find a pair of galaxies in 2 volumes dV_1 and dV_2 separated by a distance r_{12} ; compared with an random sample.

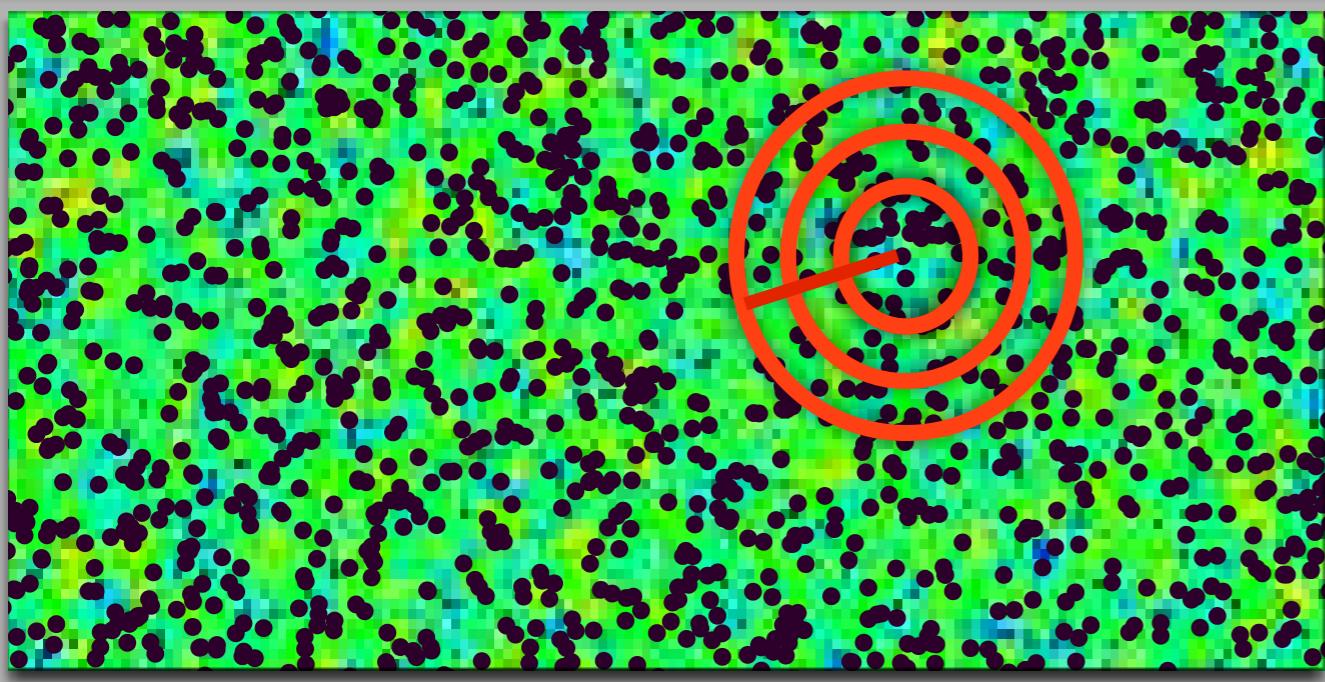
$$dP_{12} = \bar{n}_g^2 [1 + \xi(\vec{r}_{12})] dV_1 dV_2$$

$$\hat{\xi}_{PH} = \frac{DD}{RR} \quad \begin{matrix} \nearrow \\ \text{\# of pairs in DATA set at bin } r_i \end{matrix}$$

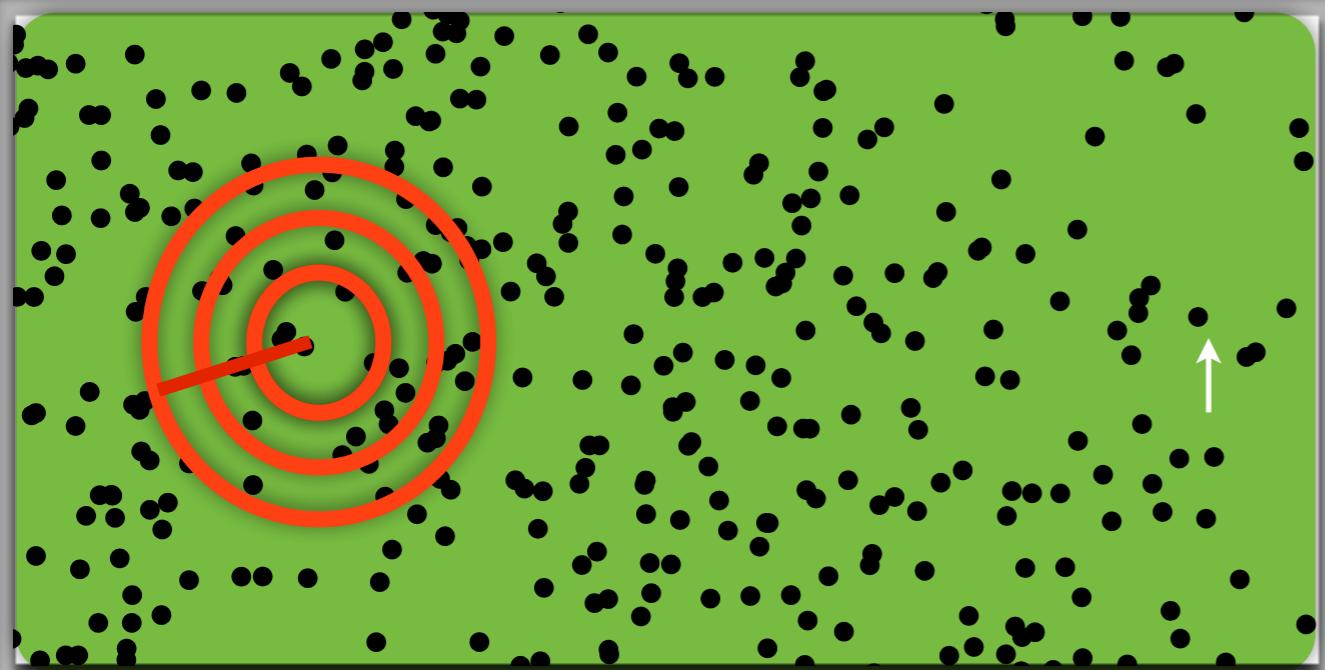
pairs at RANDOM set at bin r_i

Correlation Function

Correlated Data



Random Set



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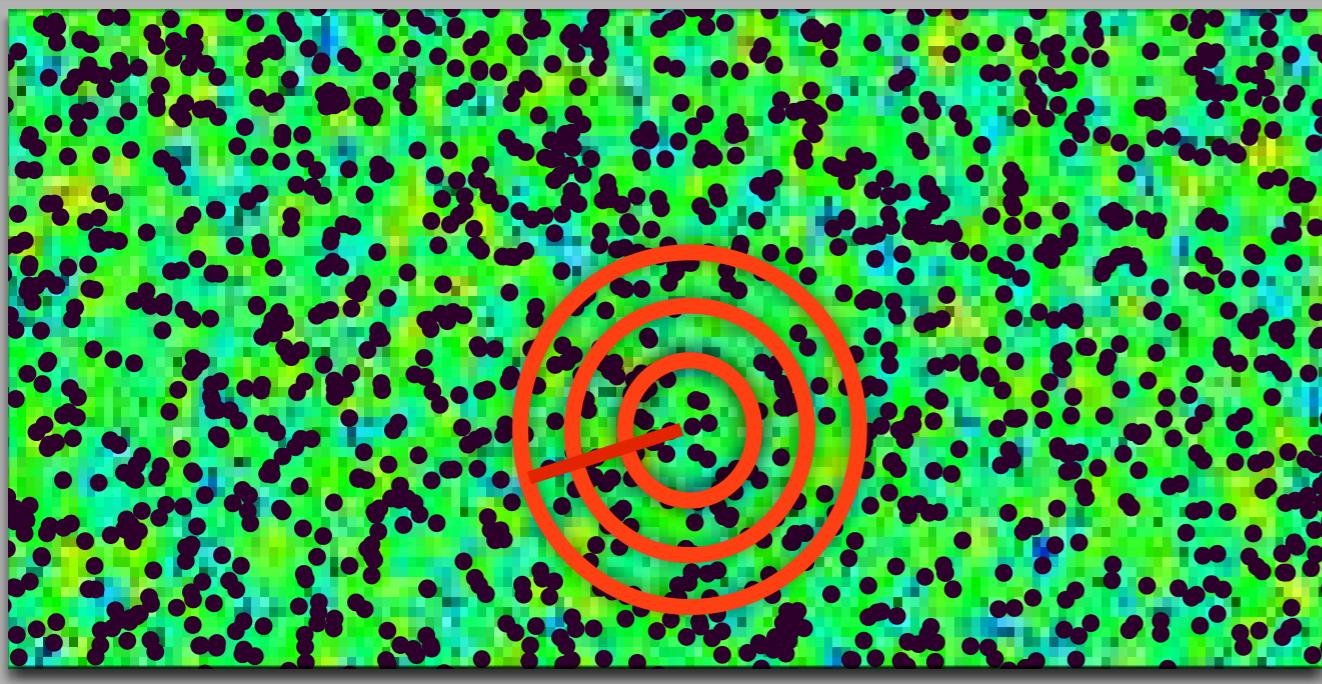
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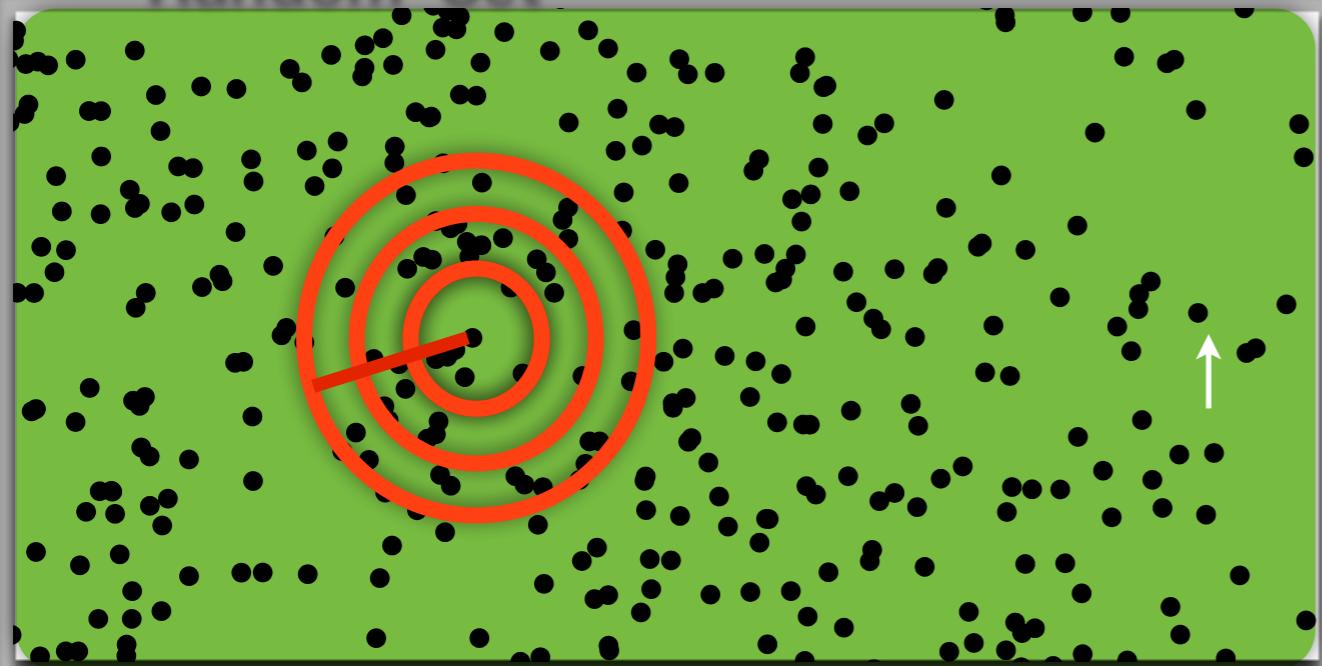
pairs at RANDOM set
at bin r_i

Correlation Function

Correlated Data



Random Set
Random Set



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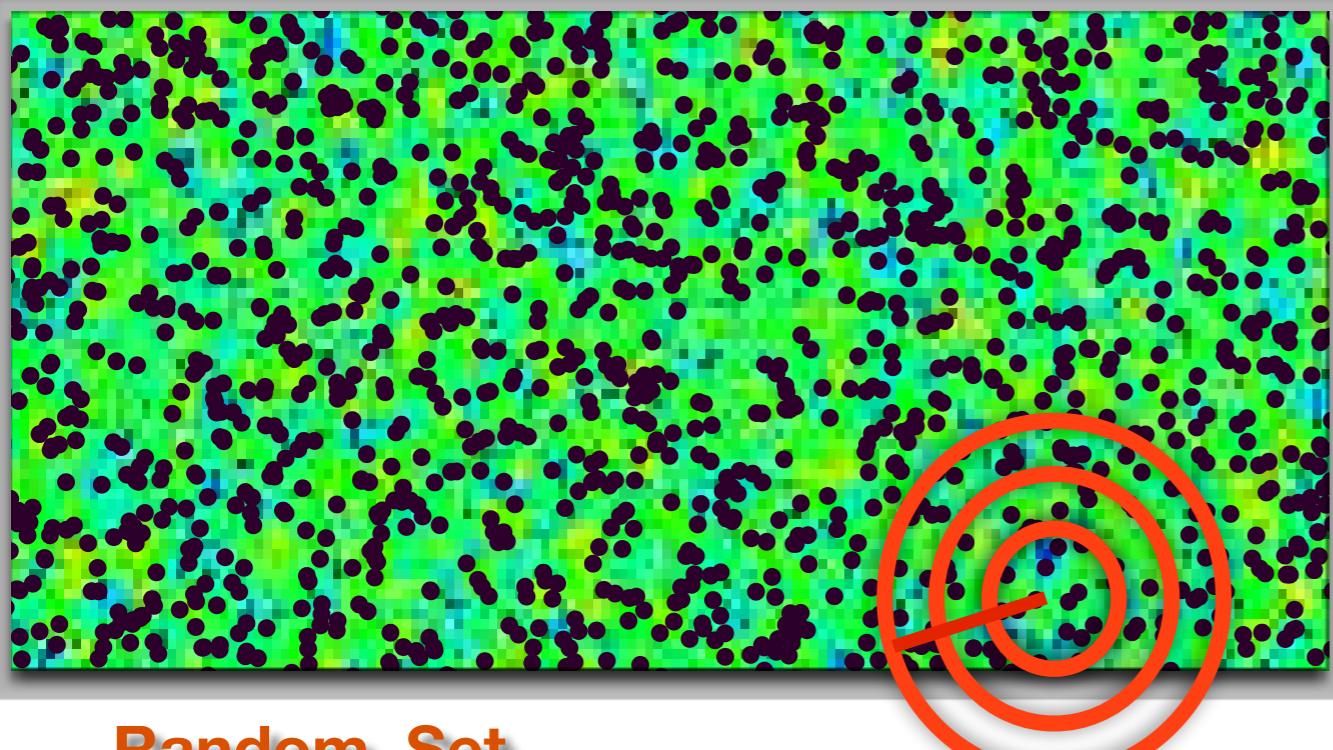
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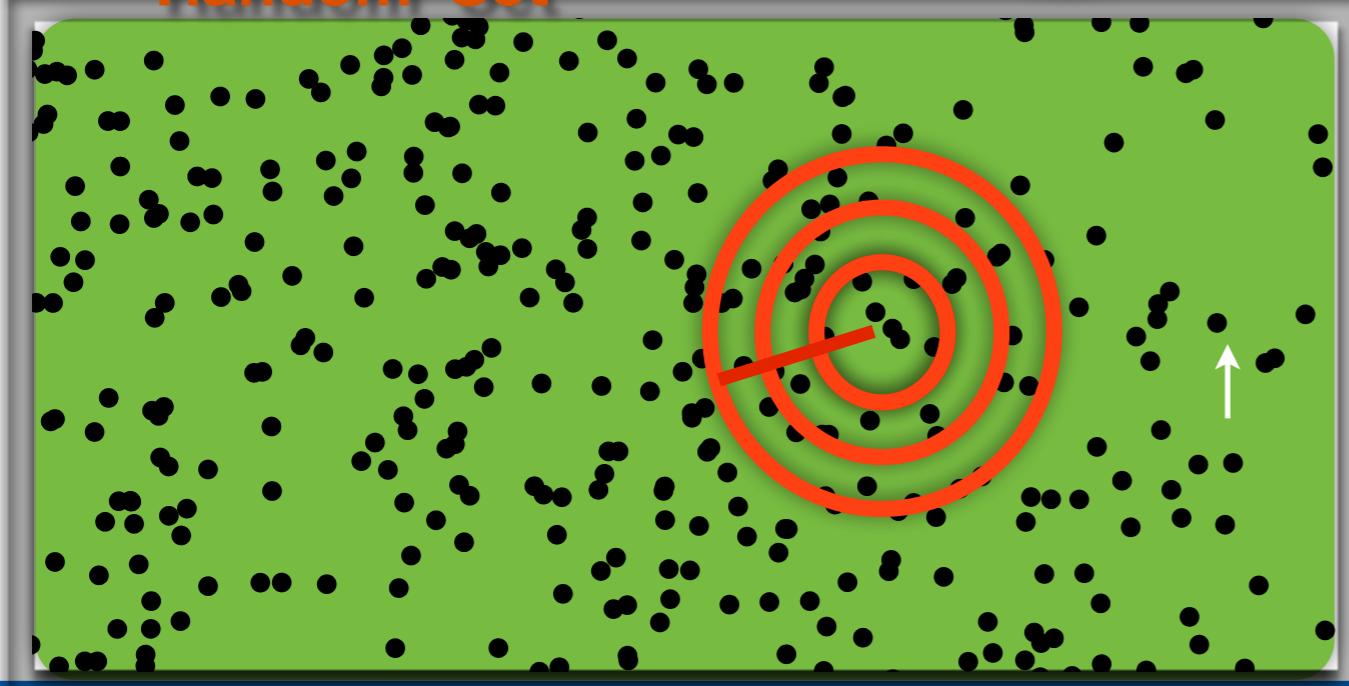
pairs at RANDOM set at bin r_i

Correlation Function

Correlated Data



Random Set
Random Set



- The 2PCF represents the probability excess to find a pair of galaxies in 2 volumes dV_1 and dV_2 separated by a distance r_{12} ; compared with an random sample.

$$dP_{12} = \bar{n}_g^2 [1 + \xi(\vec{r}_{12})] dV_1 dV_2$$

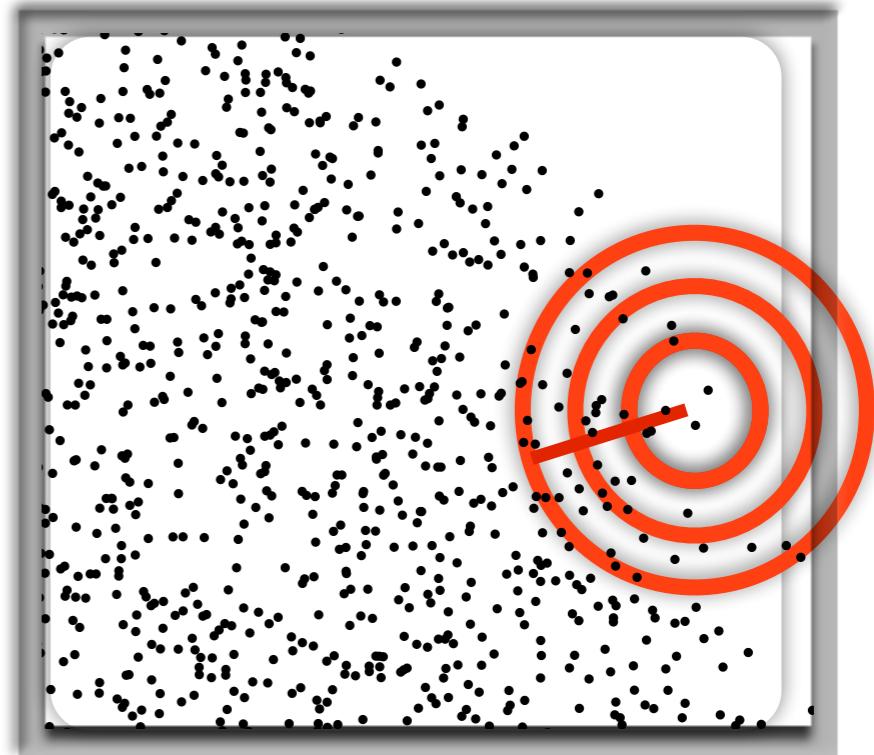
$$\hat{\xi}_{PH} = \frac{DD}{RR} \quad \begin{matrix} \nearrow \\ \# \text{ of pairs in DATA set at bin } r_i \end{matrix}$$

pairs at RANDOM set at bin r_i

Estimators

$$b_\xi = \langle \hat{\xi} \rangle - \xi_{true}$$

$$\Delta\xi^2 = \left\langle \left(\hat{\xi} - \langle \hat{\xi} \rangle \right)^2 \right\rangle$$



$$\hat{\xi}_{DP}(r) = \frac{DD}{RD} - 1$$

$$\hat{\xi}_H(r) = \frac{DD \times RR}{RD^2} - 1$$

$$\hat{\xi}_{Hew}(r) = \frac{DD - DR}{RR}$$

$$\hat{\xi}_{LS}(r) = \frac{DD - 2RD + RR}{RR}$$

Davis & Peebles(Davis1983)

Hamilton(1993)

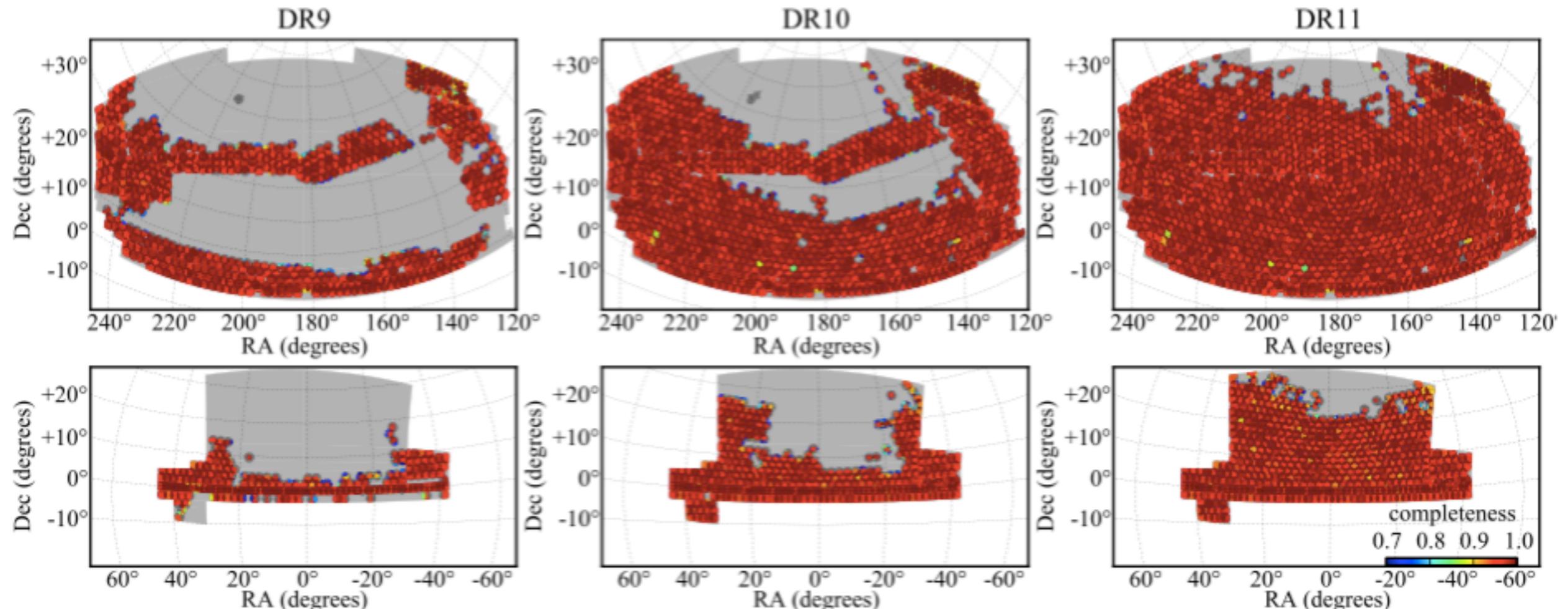
Hewett(Hewett1982)

Landy – Szalay(1993)

Window or Mask

- You can never observe a perfect (or even better infinite) squared box of the Universe . The mask is a function that usually takes values of 0 or 1and is defined on the plane of the sky (i.e. it is constant along the same line of sight).
- Window or mask
- The mask is also a real space multiplication effect. In addition sometimes in LSS studies different pixels may need to be weighted differently, and the mask is an extreme example of this where the weights are either 0 or 1. Also this operation is a real space multiplication effect.

Mask Examples: Angular Selection Function



Radial selection Function $n(r)$

2.1 Correlation Function

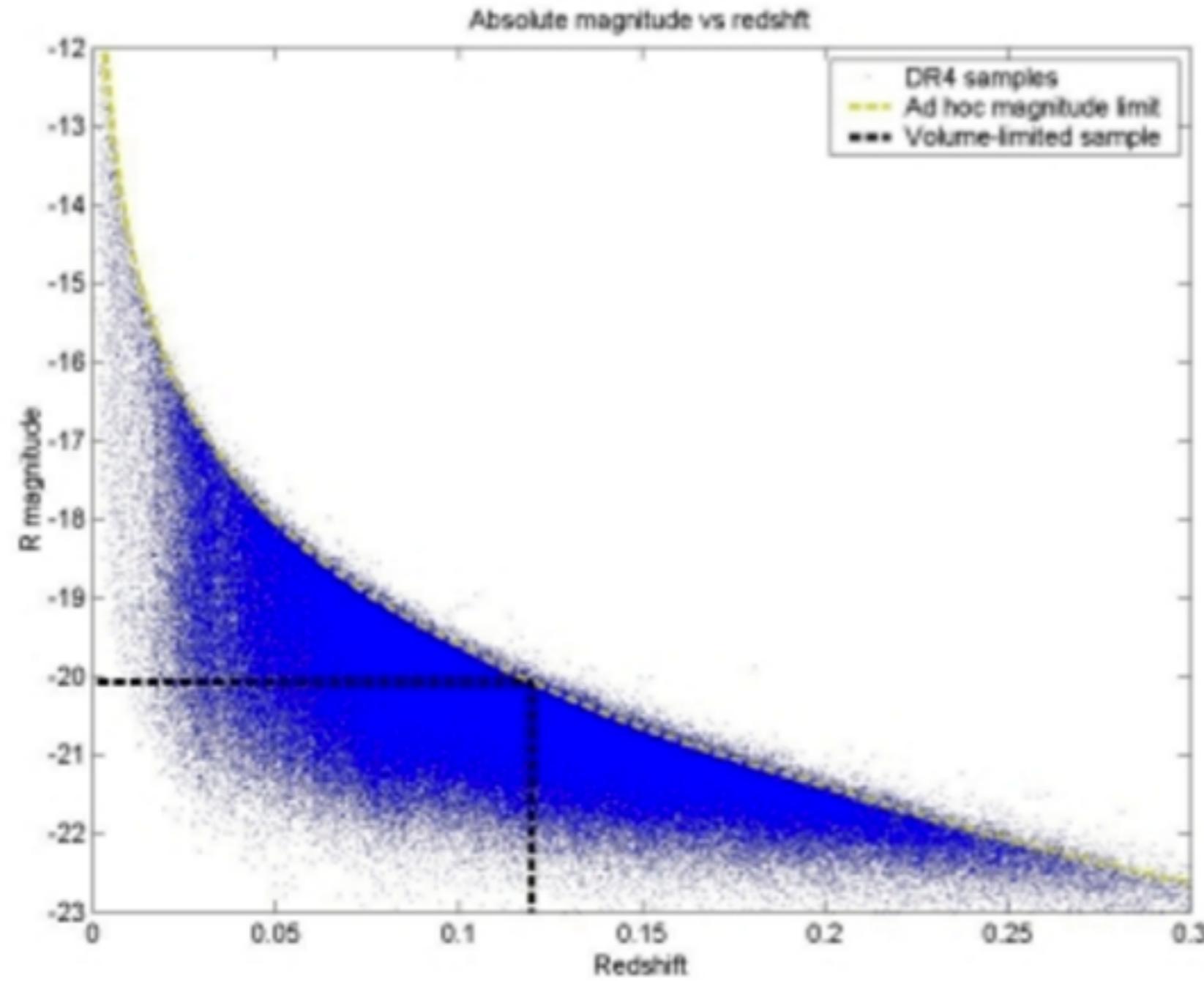
Let $n(\mathbf{r})$ denote the observed number **density** of particles (galaxies) at position \mathbf{r} in a survey.

Let $\bar{n}(\mathbf{r})$ denote the **selection function**, the expected mean number of particles (galaxies) at position \mathbf{r} given the selection criteria of the survey. Often but not always, the selection function is separable into a product of an **angular selection function** $\bar{n}(\hat{\mathbf{r}})$ and a **radial selection function** $\bar{n}(r)$. The determination or measurement of the angular and radial selection functions of a survey is a non-trivial enterprise which is an essential prerequisite for measuring correlation functions or power spectra.

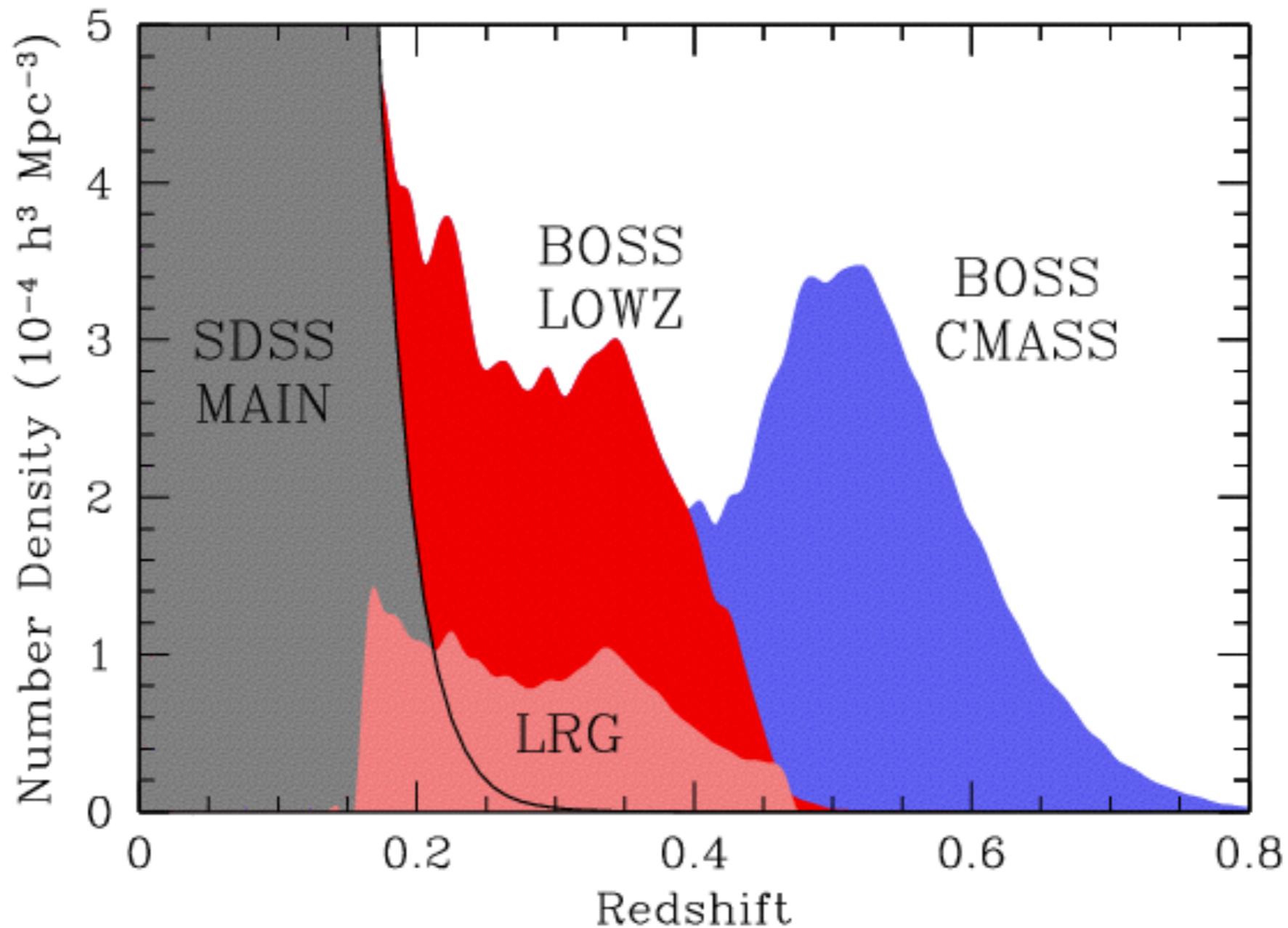
Example: Magnitud limited Samples

- Galaxy surveys are usually magnitude limited, which means that as you look further away you start missing some galaxies. The selection function tells you the probability for a galaxy at a given distance (or redshift z) to enter the survey
- One way to avoid these effects is through use of a volume-limited sample, in which a maximum redshift and minimum absolute magnitude are chosen so that every galaxy in this redshift and magnitude range will be observed.

Example: Magnitud limited Samples



Example: Magnitud limited Samples



Discreteness

- While the dark matter distribution is almost a continuous one the galaxy distribution is discrete. We usually assume that the galaxy distribution is a sampling of the dark matter distribution.
- The discreteness effect give the galaxy distribution a Poisson contribution (also called shot noise contribution).
- Note that the Poisson contribution is non Gaussian: it is only in the limit of large number of objects (or of modes) that it approximates a Gaussian.

Shot noise

- As long as a galaxy number density is high enough and we have enough modes, we say that we will have a superposition of our random field (say the dark matter one characterized by its $P(k)$)
- plus a white noise contribution coming from the discreteness which amplitude depends on the average number density of galaxies (and should go to zero as this go to infinity)

Fourier space

- Often it is useful to describe the matter field in Fourier space

$$\delta_{\vec{k}} = \frac{1}{V} \int \delta(\vec{x}) e^{-i\vec{k} \cdot \vec{x}}$$

- Here V is the volume over which the Universe is assumed to be periodic
- The perturbed density field can be written as a sum of plane waves of different wave numbers k , that we call modes.
- For $\delta \ll 1$, each mode evolves independently $\delta_k(t)$

$$\delta(\vec{x}) = \sum_k \delta_{\vec{k}} e^{+i\vec{k} \cdot \vec{x}}$$

Notation and convention

- Throughout this lecture we adopt the following convention for Fourier Transforms:
- Fourier Space $\delta(\vec{x}) = \frac{1}{(2\pi)^3} \int \delta(\vec{k}) e^{+i\vec{k}\cdot\vec{x}} d^3\tilde{\mathbf{k}}$
- Configuration Space $\delta(\vec{k}) = \int \delta(\vec{x}) e^{-i\vec{k}\cdot\vec{x}} d^3\tilde{\mathbf{x}}$

Finite (periodic) Fourier Transform

- Rather than working in infinite space, we assume an finite (but large) volume where the Universe is assumed to be periodic, this implies discrete modes, and the FT becomes.

$$\delta_{\vec{k}} = \frac{1}{V} \int \delta(\vec{x}) e^{-i\vec{k}\cdot\vec{x}} d^3\tilde{x}$$

$$\delta(\vec{x}) = \sum \delta(k) e^{+i\vec{k}\cdot\vec{x}}$$

$F[x]$ is the Discrete Fourier Transform of the sequence $f(k)$

$$F[n] = \sum_{k=0}^{N-1} f[k] e^{-j\frac{2\pi}{N}nk} \quad (n = 0 : N - 1)$$

FFT in Python



[Scipy.org](#) [Docs](#) [NumPy v1.15 Manual](#) [NumPy Reference](#) [Routines](#)

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Discrete Fourier Transform (numpy.fft)

Standard FFTs

- `fft(a[, n, axis, norm])` Compute the one-dimensional discrete Fourier Transform.
- `ifft(a[, n, axis, norm])` Compute the one-dimensional inverse discrete Fourier Transform.
- `fft2(a[, s, axes, norm])` Compute the 2-dimensional discrete Fourier Transform
- `ifft2(a[, s, axes, norm])` Compute the 2-dimensional inverse discrete Fourier Transform.
- `fftn(a[, s, axes, norm])` Compute the N-dimensional discrete Fourier Transform.
- `ifftn(a[, s, axes, norm])` Compute the N-dimensional inverse discrete Fourier Transform.

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Power Spectrum

- The Fourier transform (FT) of the two-point correlation function is called the power spectrum and is given by

$$\begin{aligned} P(\vec{k}) &\equiv V \langle |\delta_{\vec{k}}|^2 \rangle \\ &= \int \xi(\vec{x}) e^{-i\vec{k}\cdot\vec{x}} d^3x \\ &= 4\pi \int \xi(r) \frac{\sin kr}{kr} r^2 dr \end{aligned}$$

- A Gaussian random field is completely specified by either the two-point correlation function , or, equivalently, the power spectrum

Variance of the density Field

Mean Density Field

$$\langle \delta \rangle = \frac{1}{V} \int \delta(\vec{x}) d^3\vec{x}$$

Variance Density Field

$$\sigma^2 = \langle \delta^2 \rangle = \frac{1}{V} \int \delta^2(\vec{x}) d^3\vec{x}$$

$$\xi(r) = \langle \delta(\vec{x}) \delta(\vec{x} + \vec{r}) \rangle = \frac{1}{(2\pi)^3} \int P(k) e^{+i\vec{k}\vec{r}} d^3\vec{k}$$

- The power spectrum is defined as

$$\langle \delta(\mathbf{k}_1) \delta(\mathbf{k}_2) \rangle = (2\pi)^3 P(k_1) \delta^D(\mathbf{k}_1 + \mathbf{k}_2)$$

Power Spectrum

- The power spectrum is defined as

$$\langle \delta(\mathbf{k}_1) \delta(\mathbf{k}_2) \rangle = (2\pi)^3 P(k_1) \delta^D(\mathbf{k}_1 + \mathbf{k}_2)$$

- With this definition, σ_8 is

$$\sigma_8^2 = \int \frac{d^3k}{(2\pi)^3} P(k) |W(kR)|^2 = \int \frac{dk}{k} \Delta^2(k) |W(kR)|^2$$

- with $R = 8\text{Mpc}/h$, and $\Delta^2(k) = P(k)k^3/2\pi^2$ is the dimensionless power spectrum. One can check the normalization of the power spectrum by calculating σ_8 .

Power spectrum (and Bispectrum) from N-body simulation

- Estimating power spectrum (and bispectrum) from the N-body simulation data is less complicated as N-body simulations have 1) the cubic box, 2) the constant mean number density. We divide the general procedure of measuring power spectrum from N-body simulation by following five steps:
 1. Distributing particles onto the regular grid
 2. Fourier transformation
 3. Estimating power spectrum
 4. Deconvolving window function
 5. Subtracting shot noise

Density estimation and effect on P(k)

- In order to apply the Fast Fourier Transform technique, we have to assign the density field onto each point in the regular grid. The way we distribute a particle to the nearby grid points is called a ‘particle distribution scheme.’
- For a given distribution scheme, we can define an associated ‘shape function’, which quantifies how a quantity (mass, number, luminosity, etc) of particle is distributed. After this process, the sampling we made from the particle distribution is not a mere sampling of the underlying density field, but a sampling convolved with the ‘window function’ of particle distribution scheme.
- There are different ways of placing galaxies (or particle in your simulation) on a grid:
 - Nearest grid point, NGP.
 - Cloud in cell, CIC.
 - triangular shaped cloud, TSC.
- For each of these we need to deconvolve the resulting P(k) for their effect. **For our course we consider NGP.**

Particle Distribution Scheme

- Nearest Grid Point (NGP) scheme assigns particles to their nearest grid points. Therefore, the number density changes discontinuously when particles cross cell boundaries. The one dimensional window function for NGP is proportional to the Heaviside step function:

$$W_{NGP}(x) \equiv \frac{1}{H} \mathcal{T}\left(\frac{x}{H}\right) = \begin{cases} 1/H & \text{if } |x| < H/2 \\ 1/(2H) & \text{if } |x| = H/2 \\ 0 & \text{if otherwise} \end{cases}$$

$$W_{NGP}(k) = \text{FT}[\mathcal{T}](Hk) = \text{sinc}\left(\frac{Hk}{2}\right) = \text{sinc}\left(\frac{\pi k}{2k_N}\right)$$

- Cloud In Cell (CIC) assignment is the first order distribution scheme which uniformly distributes the particle with top-hat spreading function.

$$W_{CIC}(x) = \frac{1}{H} \begin{cases} 1 - |x|/H & \text{if } |x| < H \\ 0 & \text{otherwise} \end{cases}$$

$$W_{CIC}(k) = W_{NGP}(k)^2 = \text{sinc}^2\left(\frac{\pi k}{2k_N}\right).$$

- Triangular Shaped Cloud (TSC) scheme is the second order distribution scheme.

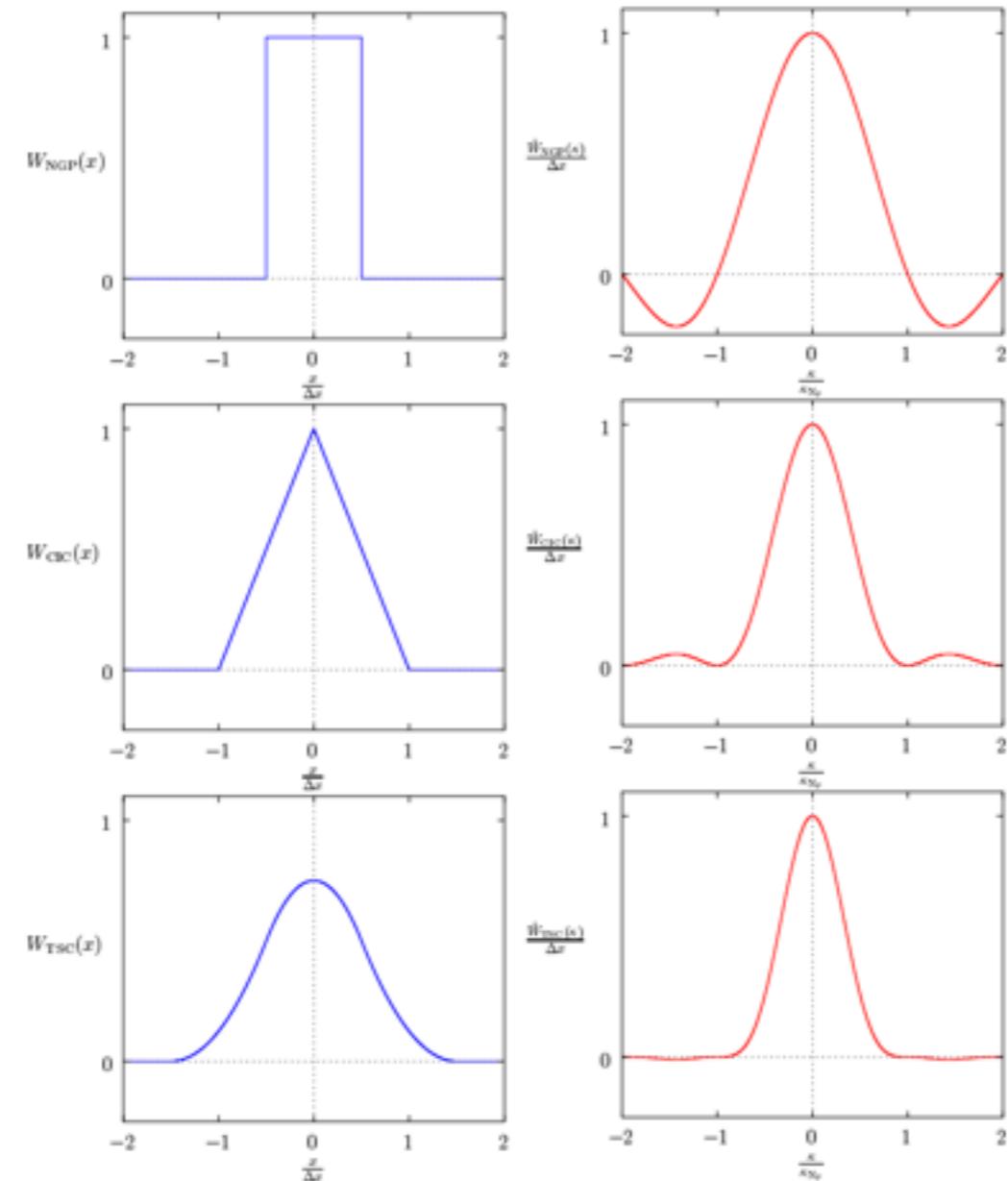
$$W_{TSC}(x) = \frac{1}{H} \begin{cases} \frac{3}{4} - \left(\frac{x}{H}\right)^2 & \text{if } |x| \leq \frac{H}{2} \\ \frac{1}{2} \left(\frac{3}{2} - \frac{|x|}{H}\right)^2 & \text{if } \frac{H}{2} \leq |x| \leq \frac{3H}{2} \\ 0 & \text{otherwise} \end{cases}$$

$$W_{TSC}(k) = W_{NGP}(k)^3 = \text{sinc}^3\left(\frac{\pi k}{2k_N}\right).$$

$kN = \pi/H$ is the Nyquist frequency

Density estimation

the density assignment wider in configuration space.



3D window function

- As we use the regular cubic grid, the three dimensional window function is simply given as the multiplication of three one dimensional window functions.

$$W(\mathbf{x}) = W(x_1)W(x_2)W(x_3)$$

- Therefore, its Fourier transformation is

$$W(\mathbf{k}) = \left[\text{sinc}\left(\frac{\pi k_1}{2k_N}\right) \text{sinc}\left(\frac{\pi k_2}{2k_N}\right) \text{sinc}\left(\frac{\pi k_3}{2k_N}\right) \right]^p,$$

- where $p = 1, 2, 3$ for NGP, CIC and TSC, respectively.

$P(k)$ using FFTW

- We shall find the proper normalization to the power spectrum estimators which use the unnormalized **Fast Fourier Transformation (FFT)** such as FFTW. For denote the unnormalized discrete Fourier transform result by superscript 'FFTW'.

$$P(k_F n_1) = \frac{V}{N^6} \left\langle |\delta^{FFTW}(\mathbf{n}_1)|^2 \right\rangle = \frac{V}{N^6} \left(\frac{1}{N_k} \sum_{|\mathbf{n}_k - \mathbf{n}_1| \leq \frac{1}{2}} |\delta^{FFTW}(\mathbf{n}_k)|^2 \right),$$

- where V is the volume of survey, N is number of one-dimensional grid, $H^3 = V/N^3$ and $k_F^3 = (2\pi)^3/V$. where we sum over all Fourier modes within $k_1 - k_F/2 < |k| < k_1 + k_F/2$ to estimate the power spectrum at $k = k_1 = k_F n_1$.

Deconvolution of Window Function

- We have the estimator for the power spectrum. However, as we have employed the distribution scheme, the power spectrum we would measure with those estimators are not the same as the power of the ‘real’ density contrast, but the **power of density contrast convolved with the window function**.
- Therefore, the power spectrum we estimate will show the **artificial power suppression on small scales**. Therefore, we have to **deconvolve the window function due to the particle distribution scheme** in order to estimate the power spectrum of the true density contrast.
- As we know the exact shape of the window function in Fourier space, we can simply divide the resulting density contrast in Fourier space by the window function. That is, we deconvolve each \mathbf{k} mode of density contrast as
 - or, deconvolve the estimated power spectrum by
 - for $\mathbf{k} < \mathbf{k}_N$. Again, $p = 1, 2, 3$ for NGP, CIC and TSC scheme, respectively. Here, superscript m denote the measured quantity.

$$\delta(\mathbf{k}) = \frac{\delta^m(\mathbf{k})}{W(\mathbf{k})},$$

$$P(\mathbf{k}) = \left| \frac{\delta^m(\mathbf{k})}{W(\mathbf{k})} \right|^2 = P^m(k_1, k_2, k_3) \left[\text{sinc}\left(\frac{\pi k_1}{2k_N}\right) \text{sinc}\left(\frac{\pi k_2}{2k_N}\right) \text{sinc}\left(\frac{\pi k_3}{2k_N}\right) \right]^{-2p},$$

Windows

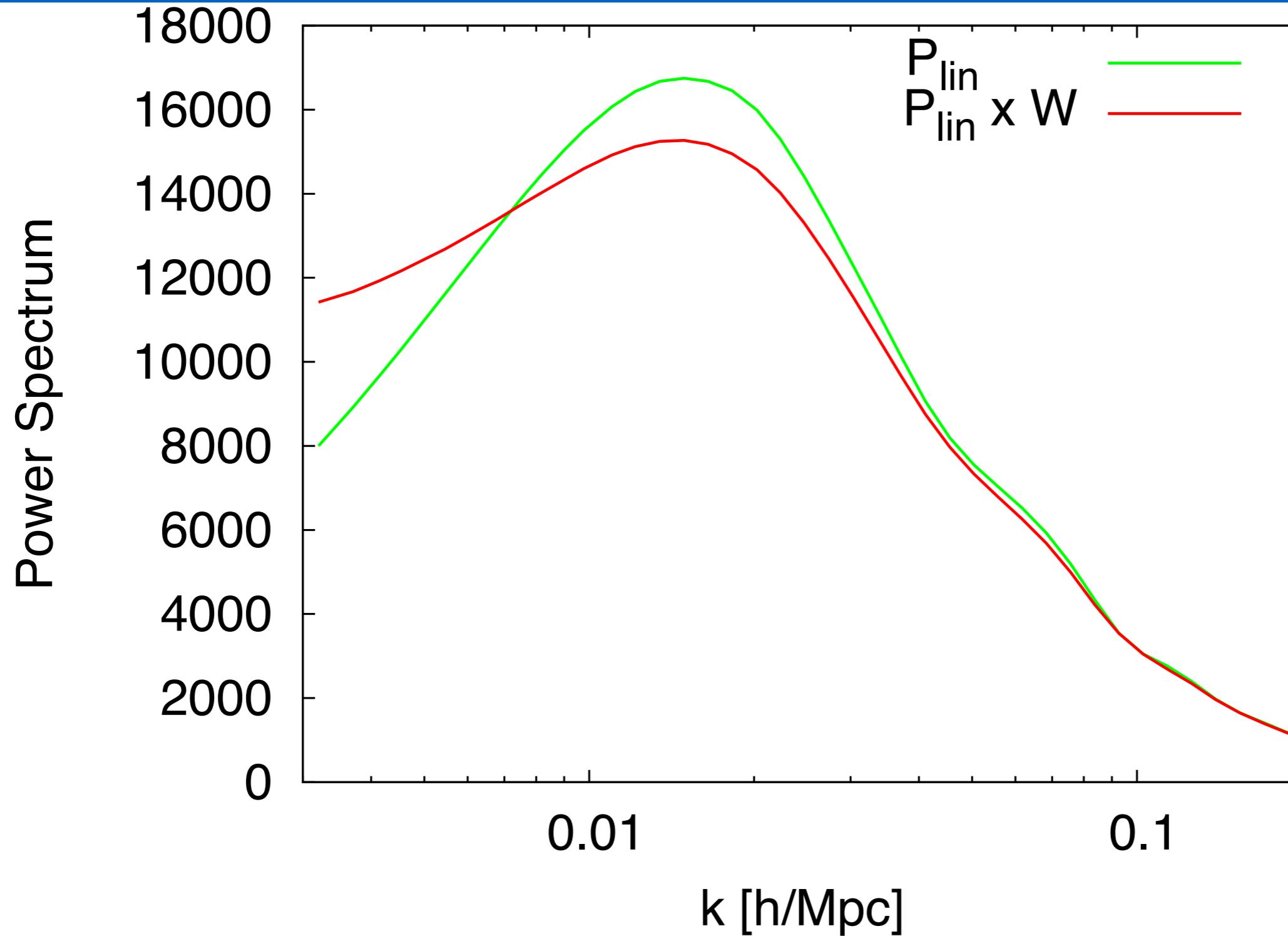
Let's recall that a multiplicaton in real space (where $W(\vec{x})$ denotes the effects of window and selection functions)

$$\delta^{true}(\vec{x}) \longrightarrow \delta^{obs}(\vec{x}) = \delta^{true}(\vec{x})W(\vec{x}) \quad (50)$$

is a convolution in Fourier space:

$$\delta^{true}(\vec{k}) \longrightarrow \delta^{obs}(\vec{k}) = \delta^{true}(\vec{k}) * W(\vec{k}) \quad (51)$$

the sharper $W(\sim r)$ is the messier and delocalized $W(\sim k)$ is. As a result it will couple different k modes even if the underlying ones were not correlated!



Shot NOISE

- As long as a galaxy number density is high enough (which will need to be quantified and checked for any practical application) and we have enough modes, we say that we will **have a superposition of our random field (say the dark matter one characterized by its $P(k)$) plus a white noise contribution coming from the discreteness which amplitude depends on the average number density of galaxies** (and should go to zero as this go to infinity), and we treat this additional contribution as if it has the same statistical properties as the underlying density field (which is an approximation).

$$\langle \delta_{k_1} \delta_{k_2} \rangle^d = (2\pi)^3 \left(P(k) + \frac{1}{\bar{n}} \right) \delta^d(\vec{k}_1 + \vec{k}_2)$$

$P(k)$ from a realistic galaxy catalog

- In the real world when you go and take the FT of your survey or even of your simulation box you will be using something like a **Fast Fourier transform code (FFT) which is a discrete Fourier transform**.
- If your box has side of size L , even if $\delta(r)$ in the box is continuous, δ_k will be discrete. The k -modes sampled will be given by

$$\vec{k} = \left(\frac{2\pi}{L} \right) (i, j, k) \quad \text{where} \quad \Delta_k = \frac{2\pi}{L}$$

- The discrete Fourier transform is obtained by placing the $\delta(x)$ on a lattice of N^3 grid points with spacing L/N . Then:

$$\begin{aligned}\delta_k^{DFT} &= \frac{1}{N^3} \sum_r \exp[-i\vec{k} \cdot \vec{r}] \delta(\vec{r}) \\ \delta^{DFT}(\vec{r}) &= \sum_k \exp[i\vec{k} \cdot \vec{r}] \delta_k^{DFT}\end{aligned}$$

kmax and kmin

- The Nyquist frequency (**maximal k**):

$$k_{Ny} = 2\pi N / 2L$$

- is that of a mode which is sampled by 2 grid points. **Higher frequencies cannot be properly sampled and give aliasing (spurious transfer of power)** effects. You should always work at **$k < k_{Ny}$** .
- There is also a **minimum k** (largest possible scale) that your finite box can test :

$$k_{min} > 2\pi / L.$$

- In addition DFT **assume periodic boundary conditions**, if you do not have periodic boundary conditions then this also introduces aliasing.