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## Organised Randoms: learning and correcting for systematic galaxy clustering patterns in KiDS using self-organising maps

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#### ABSTRACT

We present a new method for the mitigation of observational systematic effects in angular galaxy clustering via corrective random galaxy catalogues. Real and synthetic galaxy data, from the Kilo Degree Survey's (KiDS) 4<sup>th</sup> Data Release (KiDS-1000) and the Full-sky Lognormal Astro-fields Simulation Kit (FLASK) package respectively, are used to train self-organising maps (SOMs) to learn the multivariate relationships between observed galaxy number density and up to six systematic-tracer variables, including seeing, Galactic dust extinction, and Galactic stellar density. We then create 'organised' randoms, *i.e.* random galaxy catalogues with spatially variable number densities, mimicking the learnt systematic density modes in the data. Using realistically biased mock data, we show that these organised randoms consistently subtract spurious density modes from the two-point angular correlation function  $w(\vartheta)$ , correcting biases of up to  $12\sigma$  in the mean clustering amplitude to as low as  $0.1\sigma$ , over a high signal-to-noise angular range of 7 – 100 arcmin. Their performance is also validated for angular clustering cross-correlations in a bright, flux-limited subset of KiDS-1000. comparing against an analogous sample constructed from highly-complete spectroscopic redshift data. Each organised random catalogue object is a 'clone' carrying the properties of a real galaxy, and is distributed throughout the survey footprint according to the parent galaxy's position in systematics-space. Thus, sub-sample randoms are readily derived from a single master random catalogue via the same selection as applied to the real galaxies. Our method is expected to improve in performance with increased survey area, galaxy number density, and systematic contamination, making organised randoms extremely promising for current and future clustering analyses of faint samples.

Key words. cosmology: observations, large-scale structure of Universe; methods: data analysis

#### 1. Introduction

Recent decades have seen the advent of precision cosmology, as inferred from the large-scale structures of the Universe (Ho et al. 2012; Font-Ribera et al. 2014; Anderson et al. 2014; Hildebrandt et al. 2017; Alam et al. 2017; Troxel et al. 2018; Hamana et al. 2019; eBOSS Collaboration et al. 2020; Tröster et al. 2020; Asgari et al. 2020b). We can shed light on the mysterious dark matter scaffold by examining the distribution of the galaxies supported by it, and extend these measurements across broad redshift epochs in order to study dark energy through the evolution of structures and the universal expansion history. Tensions are beginning to emerge between near-universe measures of the expansion rate and the amount/clustering of matter (Freedman 2017; Riess et al. 2019; Hildebrandt et al. 2019; Joudaki et al. 2020; Heymans et al. 2020), and those obtained through state-of-the-art cosmic microwave background (CMB) analyses (Aghanim et al. 2020). Resolving these tensions will require strict control of sources of systematic error, in the new era of statistical precision soon to be explored (Dark Energy Spectroscopic Instrument; DESI Collaboration et al. 2016, Rubin Observatory; LSST Science Collaboration et al. 2009, *Euclid*; Laureijs et al. 2011).

Currently, the most competitive large-scale structure (LSS) constraints upon the matter energy density  $\Omega_{\rm m}$  vs. normalisation of the matter power spectrum  $\sigma_8$  plane come from combined analyses of galaxy clustering and weak gravitational lensing (van Uitert et al. 2018; Joudaki et al. 2017; Abbott et al. 2018; Asgari et al. 2020a; Heymans et al. 2020), making use of wide-area galaxy survey data (*e.g.* Dark Energy Survey; Sánchez 2006, Kilo Degree Survey; de Jong et al. 2013, Hyper Suprime-Cam; Miyazaki et al. 2012). However these surveys are susceptible to complex source selection functions, which can destroy and/or mimic

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real, informative signals, such as cosmological density fluctuations. These selection functions are generally imprinted on galaxy survey data in a way that correlates with observational and physical properties of the survey on-sky. Examples of such properties, which have the propensity to introduce spurious selection effects on galaxy data, include spatial variation in: atmospheric seeing, the telescope pointspread function (PSF), stellar density, Galactic dust extinction, and more. Crucially, it is possible, or even likely, that some spurious selection functions may be introduced due to a complex confluence of many observational properties; some of which we may be unaware.

This work focuses on sources of systematic error affecting the detection of galaxies, and propagating into statistics involving galaxy positional data, e.g. correlation functions. Much work has been devoted to mitigating such errors: techniques for systematics mode deprojection – assigning large variance to spurious modes, so that they are ignored by power spectrum estimators – were developed by Leistedt et al. (2013); Leistedt & Peiris (2014) for photometric quasar clustering, and similar methods were recently applied to Hyper Suprime-Cam (HSC) data by Nicola et al. (2020). Ross et al. (2011); Ho et al. (2012) suppressed systematics in SDSS BOSS-like (Sloan Digital Sky Survey; York et al. 2000, Baryon Oscillation Spectroscopic Survey; Eisenstein et al. 2001) photometric luminous red galaxy (LRG) data by deriving per-galaxy inverse weights from number density-systematics ('1-point' or 'pixel') correlations, or by computing signal corrections (assuming systematic-tracers relate linearly to galaxy number densities) from galaxy-systematic (2-point) cross-correlations. Vakili et al. (2020) also estimated weights from 1-point functions to measure the clustering of photometric LRGs in the Kilo Degree Survey (KiDS), decomposing systematictracers in an orthogonal basis and exploring second-order polynomials to characterise cross-talk between parameters. Elvin-Poole et al. (2018) iteratively derived weights for Dark Energy Survey (DES) LRGs from linear systematicdensity fits, and Wagoner et al. (2020) recently improved upon that analysis by performing simultaneous likelihood fitting of linear coefficients to all systematics maps and the observed density contrast, and then calibrating for overcorrection of clustering correlations with mock catalogues. Rezaie et al. (2020) derived weights for emission line galaxies (ELGs) selected (following eBOSS; Raichoor et al. 2017) from the Dark Energy Camera Legacy Survey (DECaLS; Dey et al. 2019) using deep neural networks. Morrison & Hildebrandt (2015) tackled clustering biases in the Canada-France-Hawaii Telescope Lensing Survey (CFHTLenS; Erben et al. 2013), using galaxy density-systematic 1-point functions to create weight-maps from which to draw random points. Suchyta et al. (2016) went even further, simulating galaxies and injecting them into real imaging data, so as to gauge the detector-response to observational systematics. As the breadth of work (only partially summarised here) suggests, mitigating the impact of systematic galaxy density modes is crucial to maximising the potential of future large-scale structure surveys.

Upcoming surveys are likely to build upon the many weak lensing analyses that currently aim to constrain cosmology with the '3x2pt' analysis method, simultaneously fitting the 2-point functions describing the galaxy shearshear (cosmic shear), position-shear (galaxy-galaxy lensing), and position-position (galaxy clustering) correlations. Analysed simultaneously, these statistics help to constrain nuisance parameters (*e.g.* photo-*z* calibration uncertainties, or intrinsic alignments), thereby tightening cosmological constraints. However this additional constraining power also brings sensitivity to systematic biases; any bias in (for example) the galaxy clustering correlation, such as those which may be introduced by systematic variation of the galaxy density field, will propagate into the inferred (joint) cosmology in a pathological fashion.

We seek to mitigate such biases through the construction of tailored random galaxy catalogues (hereafter 'organised randoms'), which mirror systematically induced galaxy-density variations (similarly to Morrison & Hildebrandt 2015; Suchyta et al. 2016). Random galaxy catalogues (commonly referred to simply as 'randoms') are widely used when estimating galaxy clustering and galaxygalaxy lensing (GGL), whereby correlations between galaxies and random points allow for reductions in methodological bias, improved covariance properties between the statistics, removal of systematics caused by edge/masking-effects, and aid in the reduction of additional systematic correlations (Landy & Szalay 1993; Singh et al. 2017). For this task, studies typically employ high-density (relative to the survey galaxy number density), spatially uniform random points. However, while these will aid in the removal of systematic correlations with the observed galaxy distribution, they cannot account for spatial correlations stemming from systematically *unobserved* galaxies, or those systematically lost due to sample selection effects.

Our work aims to tackle this problem: we utilise a form of machine-learning assisted dimensionality reduction, the self-organising map (or 'SOM', Kohonen 1990), to infer, from the observed galaxy distribution, the high-dimensional mapping between survey systematics and galaxy number densities on-sky. We then create many 'clones' of the real galaxies (*i.e.* copies retaining all photometric/other properties, see Farrow et al. 2015) and distribute them as 'random' points throughout the survey footprint, in accordance with their systematically-derived number density on-sky. This allows any selection effects in galaxy data to be trivially mirrored in the organised randoms, thereby preserving the systematic patterns and the systematically-induced density variations for an arbitrarily defined galaxy sample.

The paper is organised as follows: In Sec. 2, we introduce our galaxy data, from Kilo Degree Survey (KiDS, Kuijken et al. 2019) observations, and from Full-sky Lognormal Astro-fields Simulation Kit (FLASK; Xavier et al. 2016) simulations. Sec. 3 describes self-organising maps, and how they are utilised in this work. In Sec. 4 we assess the capability of the self-organising map to identify artificially created systematic trends in galaxy density. Sec. 5 then turns to KiDS data-driven systematic density fluctuations, and demonstrates the utility of organised randoms in recovering unbiased clustering signals from realistically biased FLASK mocks. Final data applications are presented in Sec. 6, and we make concluding remarks in Sec. 7. Throughout this work, we quote AB magnitudes and assume a fiducial WMAP9+BAO+SN cosmology (Hinshaw et al. 2013): flat ACDM, with  $\Omega_{\rm m} = 0.2905$ ,  $\Omega_{\rm b} = 0.0473$ ,  $\sigma_8 = 0.826$ , h = $0.6898, n_s = 0.969.$ 

#### 2. Data

We validate our random catalogues using both real and synthetic galaxy data, and invoking both realistic distributions of systematic parameters on-sky (drawn from the KiDS 4<sup>th</sup> Data Release, DR4, Kuijken et al. 2019) and artificially constructed systematics distributions. For our simulations, we utilise lognormal galaxy fields simulated with FLASK (Xavier et al. 2016).

#### 2.1. KiDS

Both KiDS (de Jong et al. 2013) and its partner survey, the VISTA Kilo-Degree Infrared Galaxy (VIKING; Edge et al. 2013) survey, are now observationally complete, covering a combined area of  $1350 \deg^2$  on-sky in a total of 9 photometric bandpasses ( $ugriZYJHK_s$ ). Over 1000 deg<sup>2</sup> of this combined dataset is publically available as part of KiDS  $DR4^1$  (Kuijken et al. 2019), providing gravitational shear estimates (unused in this work), 9-band photometric redshift estimates (Hildebrandt et al. 2019; Wright et al. 2020; Hildebrandt et al. 2020), and observational information for over 100 million galaxies. This galaxy sample, typically referred to as  $KiDS-1000^2$ , samples a wide range of observing conditions over a large area, and is consequently imprinted with an unknown combination of systematic galaxy depletion and enhancement patterns. Of all the various data products provided within the KiDS DR4, we identify a selection of 'systematic-tracer' variables (detailed in Table 1, and mapped-out in Figs. 1 & 2) which trace physical phenomena that, we believe, have the greatest potential to imprint subtle galaxy selection functions on the dataset. These parameters, individually and in combination, form the dataset used to train our SOMs. Of course, whether the chosen variables all trace real observational phenomena that cause the systematic loss of galaxies is not known apriori; we therefore explore the influence of unimportant, 'distracting' variables as we test our methodology (Sec. 4).

Angular clustering correlations are typically measured in bins of galaxy redshift, so as to constrain the galaxy bias of redshift samples, thus combining powerfully with lensing probes such as GGL (e.g. Yoon et al. 2019), and to assess the growth of large-scale structure over cosmic time. Accurate redshifts (typically from spectroscopy) are required for the optimal binning of galaxies and modelling of correlations, however these are expensive to obtain for large samples of galaxies over a wide area. Consequently, such wide-field surveys rely upon photometric redshifts (photoz), estimated from broadband photometry (such as the nine filters used in KiDS-1000) which sample the galaxies' SEDs. In this work, we focus on a subsample of KiDS-1000 with high-quality photo-z estimates: the  $\sim$  1.16M bright galaxy subsample (with  $r \leq 20$ ), whose photo-z are computed using ANNz2 neural networks (Sadeh et al. 2016), trained on spectroscopically observed galaxies from the Galaxy And Mass Assembly (GAMA) survey (Driver et al. 2009). This approach to photo-z estimation for bright KiDS galaxies was originally presented by Bilicki et al. (2018) using only optical (ugri) photometry from KiDS DR3. In our work we use the updated DR4 bright-sample described in Bilicki et al., (in prep.), which leverages the expanded 9-band photo metric dataset to achieve photo-z's of typical accuracy:  $\sigma_{z_{\text{phot}}} \sim 0.02(1+z)$ , in terms of the normalised median absolute deviation (nMAD).

The photometric redshift distribution  $n(z_{phot.})$  for this GAMA-like photometric sample is shown in the top panel of Fig. 3. Following van Uitert et al. (2018), we define 2 redshift bins for our GAMA-like sample, with edges at  $z_{\text{phot.}} = \{0.02, 0.2, 0.5\}, \text{ within (and between) which we shall}$ measure angular clustering correlations. For the purpose of additional testing, we define 2 more bins within the range of  $z_{\text{phot.}} = \{0.02, 0.5\},$  but with inner boundaries well-separated in photo-z, at  $z_{phot.} = \{0.22, 0.28\}$ . This separation minimises overlap between the bins' true redshift distributions, which are induced by photo-z scatter; we display the approximate 95% scatter  $2\sigma_{z_{\text{phot}}} \sim 0.04(1+z)$  as a red line, with values on the right-hand axis. We use these GAMA-like KiDS data, 'KiDS-Bright' henceforth, for intermediate tests and to assess the ultimate performance of our organised randoms (Sec. 5 & 6).

In our companion letter, Wright et al., (in prep.), we also explore an application of our organised randoms to measurements of galaxy clustering in the KiDS-1000 shear sample; this 'gold' sample (see Wright et al. 2020; Giblin et al. 2020; Hildebrandt et al. 2020, for details) is ~ 5 magnitudes deeper than KiDS-Bright, and a factor ~ 20 more dense on-sky. Such increased statistical power should allow for a more faithful sampling of the multivariate systematics-density relation hidden in the data, which should also be easier to disentangle from cosmic structure as the faint data are more heavily biased; we expect the performance of organised randoms to *improve* on application to faint datasets, posing intriguing possibilities for the future of deep galaxy clustering analyses.

#### 2.2. FLASK

FLASK (Xavier et al. 2016) is a public code designed to simulate lognormal (or Gaussian) random fields on the celestial sphere, with configurable tomography and preservation of all relevant correlations between galaxy density and weak lensing convergence fields, to the sub-percent level. We estimate the error on  $w(\vartheta \ge 3 \operatorname{arcmin})$  to be  $\ge 2.5\%$  for KiDS-Bright-like statistics from sample variance and Poisson noise considerations alone, hence < 1% accuracy from FLASK is sufficient for our purposes.

For the cosmology specified at the end of Sec. 1 and the  $n(z_{\text{phot.}})$  displayed in the top panel of Fig. 3, we compute a 'truth' angular power spectrum  $C_{\ell}$  with which we use FLASK to generate many mock galaxy catalogues from lognormal random fields; these form the basis of initial testing for our organised randoms, as is described in Secs. 4 & 5. The bottom panel of Fig. 3 demonstrates that measurements of  $w(\vartheta)$  in our mocks reliably recover the analytical input clustering and sample variance (plus shot-noise) over 30 realisations (see Eqs. 5.1 & 5.2), modulo noise. These statistics are for FLASK realisations with average galaxy densities  $0.36 \operatorname{arcmin}^{-2}$  (*i.e.* the same as KiDS-Bright) simulated within the true KiDS-Bright masked survey footprint, and with a galaxy bias equal to unity. We shall use these KiDS-Bright-like FLASK catalogues, as well as simpler  $10 \deg \times 100 \deg$  windows (straddling the celestial equator, to loosely mimic the KiDS survey geometry) initialised with

<sup>&</sup>lt;sup>1</sup> http://kids.strw.leidenuniv.nl/DR4/

<sup>&</sup>lt;sup>2</sup> Though the retained area after masking is  $\sim 900 \deg^2$ .

#### A&A proofs: manuscript no. main

Table 1.	KiDS:	systematic-tracer	variables f	for	training	of sel	f-organising	maps.	with	units	and	descriptions.
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Systematic-tracer variable	Unit	Description
MU_THRESHOLD (MU)	mag / arcsec <sup>2</sup>	r-band detection threshold above background; the minimum surface brightness of objects detected after background-subtraction. Fainter objects will be lost from an area of observation where the detection threshold is brighter.
psf_fwhm	arcsec	full-width at half-maximum of the <i>r</i> -band point-spread function, averaged over $n_{side} = 512$ (47 arcmin <sup>2</sup> ) HEALPIX <sup>1</sup> (Gorski et al. 2005) pixels and then interpolated to galaxy locations. The blurring of small, faint sources could cause objects to drop below detection thresholds.
psf_ell	dimensionless	ellipticity $(1 - q)$ , where $q$ is the 2D major/minor axis ratio) of the $r$ -band point-spread function, also averaged over $n_{side} = 512$ pixels and interpolated to galaxy locations. A PSF ellipticity indicates non-isotropic blurring of object isophotes, creating challenges for shape estimation and inducing a directional dependence for detections.
MAG_LIM_x	mag	x-band limiting magnitude (5 $\sigma$ above background in a 2" aperture) at the object's location, for each of the 9 bands observed by KiDS-VIKING. KiDS object detection is performed in the <i>r</i> -band.
EXTINCTION_r	mag	Galactic dust extinction in the <i>r</i> -band, derived using the Schlafly & Finkbeiner (2011) coefficients for the Schlegel et al. (1998) dust maps. Dust preferentially scatters short-wavelength light from extragalactic objects; the loss of flux could prevent detections, and the modification of galaxy spectral energy distributions (SEDs) poses other problems, <i>e.g.</i> for photo- <i>z</i> estimation.
gaia_nstar	count / arcmin <sup>2</sup>	number density of Gaia DR2 (Arenou et al. 2018) 14 < $G$ < 17 stars in $n_{side} = 512$ pixels, interpolated onto galaxy locations. High stellar densities can hamper detections as the light from stars obscures background objects, and can also result in spurious galaxy-detections through the misidentification of PSF-blurred, or blended, stars as galaxies.

<sup>1</sup> http://healpix.sourceforge.net (Gorski et al. 2005)

**Notes.** Systematic-tracer variables chosen from the KiDS DR4 data products, or from other public data *e.g.* Gaia  $n_{\text{star}}$  – these are variables thought to trace phenomena which may impact upon the observed number density of galaxies. See Kuijken et al. (2019) for details on threshold, PSF and magnitude-limit parameters. Maps of each of these quantities are displayed in Figs. 1 & 2. Where specified, pixelated systematic-tracer values are interpolated from pixel-centres onto galaxy locations via a 2-dimensional (RA/DEC) nearest-neighbour interpolation.

1 galaxy  $\operatorname{arcmin}^{-2}$ , to test our self-organising maps and random galaxy catalogues.

#### 3. Self-organising Maps

Self-organising maps (SOMs; Kohonen 1990) are a class of unsupervised neural network methods, designed to project high-dimensional data onto (typically) 2dimensional 'maps' which preserve the topological features of the input space – thus proximity on the map tends to denote proximity within the high-dimensional space. SOMs are fast, simple, and useful for problems benefiting from dimensionality-reduction, unsupervised classification, and ease of data visualisation. Their use within cosmology has included: object selection and classification for large datasets (Geach 2012); template photo-z's (Speagle & Eisenstein 2015, 2017); characterisation of galaxy properties from observables (Davidzon et al. 2019); and calibration of the colour-redshift relation (Masters et al. 2017, 2019), enabling direct photo-*z* calibration (Buchs et al. 2019; Wright et al. 2020; Hildebrandt et al. 2020).

This work makes use of SOMs for dimensionality reduction and unsupervised classification, to identify on-sky areas of observation (or simulation) with correlated observing conditions, as indicated by various 'systematic' survey variables. These variables, such as those describing atmospheric effects, Galactic foreground properties, etc., ought to correlate with phenomena causing systematic alterations to the observed galaxy number density in a wide-field survey. These variables define a systematics-vector<sup>3</sup> V per galaxy, which jointly describe an  $\mathcal{R}^n$  (where n = length(V)) dimensional space to be mapped by the SOM. While this space can hypothetically consist of all derived data within the galaxy catalogue, in practice it is beneficial to select variables from the data products available which are likely to trace the true galaxy density variations, so as to allow the

 $<sup>^3</sup>$  These are simply rows in a galaxy catalogue, where each element is a number describing the amplitude of some potential source of systematic error at the location of the galaxy.



Fig. 1. Maps of systematic-tracer variables (from Table 1) from *r*-band (the detection band) imaging in the KiDS-North (*top-panels*) and KiDS-South (*bottom-panels*) areas. Grey colours denote the 50<sup>th</sup> percentile of the systematics distribution in each case, and blue/red then denote 'good'/'bad' observing conditions, relative to the 50<sup>th</sup> percentile. As we show in Fig. 4, the majority of spatial variations in galaxy number density correlate with these parameters at  $\leq 5\%$ .

maximum density-variation information to be encoded in the SOM. We therefore explore different choices of tracers, detailing these in Table 1.

The SOM algorithm starts by instantiating a grid with user-specified dimensions, *e.g.*  $100 \times 100$  for two-dimensional SOM containing  $10^4$  cells. Each cell is then assigned a randomised weights-vector  $\boldsymbol{W}$ , of the same length as the galaxies' systematics-vectors; *i.e.* the number of systematic-tracer variables *n*. To train the SOM, galaxy systematics-vectors  $\boldsymbol{V}$  are then chosen at random and presented to the SOM lattice. At each step of training, the SOM cell with weights  $\boldsymbol{W}$  most closely matching the training galaxy's systematics-vector  $\boldsymbol{V}$  is termed the best-matching unit (BMU). The match is typically quantified via the Euclidean distance *d* between the SOM cell weights-vector  $\boldsymbol{W}$  and the galaxy systematics-vector  $\boldsymbol{V}$  as

$$d = \sqrt{\sum_{i=1}^{n} (V_i - W_i)^2} \quad , \tag{3.1}$$

where the minimum d over the grid belongs to the BMU. Next we identify SOM cells within some radius  $\sigma(t)$  (the "neighbourhood") of the BMU, and modify their weightsvectors W to be closer to V, with more significant modifications for cells nearer the BMU. The resulting weights-vectors are given by

$$W(t+1) = W(t) + L(t)\Theta(t,\sigma)\left[V(t) - W(t)\right]$$
(3.2)

where t denotes a time-step (*i.e.* the presentation of a new training galaxy to the SOM), the "learning rate" L sets the strength of modifications, and  $\Theta$  implements the distance-to-BMU dependence thereof. The final feature is that all of (i) the radius  $\sigma$  within which cell weights-vectors are to be modified, (ii) the learning rate L, and (iii) the BMU-distance dependence  $\Theta$ , are exponentially decaying with each time-step, hence their dependence upon t. In this way, the SOM converges to a final representation as the training data are exhausted. Once all galaxies have been presented to the SOM, each cell on the SOM grid carries a weights-vector describing some unique position in the n-dimensional systematics parameter space, and the full collection of 10<sup>4</sup> cells spans the entire space sampled by the galaxies.

In our implementation, the resulting 2D map then represents the landscape of possible systematics-vectors realised by the data in question. By computing the distances between points in the space, we can then divide the landscape



Fig. 2. The same as Fig. 1, but for the remaining systematic-tracer variables from Table 1.

Table 2. Analysis choices for various self-organising map/randoms-creation configurations: setup identifier, number of hierarchicalclusters, resolution on-sky & systematic-tracers for training.

setup ID	$N_{\rm HC}$	res (smth) [arcmin]	systematics
T1mock	100	5 (0)	A1,A2,A3,B1,B2,B3,C1,C2
100A	100	2.8 (0.1)	MU,psf_ell,psf_fwhm
800A	800	2.8 (0.1)	MU,psf_ell,psf_fwhm
800Ares2	800	2 (0)	MU,psf_ell,psf_fwhm
100B	100	2.8 (0.1)	MU,psf_ell,psf_fwhm,MAG_LIM_r
800B	800	2.8 (0.1)	MU,psf_ell,psf_fwhm,MAG_LIM_r
100C	100	2.8 (0.1)	MU,psf_ell,psf_fwhm,MAG_LIM_r,gaia_nstar,EXTINCTION_r
800C	800	2.8 (0.1)	MU,psf_ell,psf_fwhm,MAG_LIM_r,gaia_nstar,EXTINCTION_r

**Notes.** Various configurations for our SOM & organised randoms-creation pipeline. Throughout the text, we shall refer to these by their 'setup ID' – this shorthand typically just indicates the number of hierarchical clusters defined on the SOM, *e.g.* 800 or 100, and the number of systematic-tracer variables used in training: A is just PSF and threshold parameters, B then includes the *r*-band magnitude limit, and C further includes Galactic dust extinction and stellar density (all described in Table 1). The exception T1mock refers to the SOM trained against artificial systematic-tracers A1-3,B1-3,C1-2, which are described in Sec. 4.  $N_{HC}$  is the number of hierarchical clusters to be defined on a given SOM, 'res (smth)' are the resolution and Gaussian smoothing-width, in arcminutes, of the sky-grid used to group galaxies and populate random fields, and 'systematics' refers to the set of systematic-tracer variables presented to each SOM in training (see Table 1). All SOMs employed in our analysis have dimensions  $100 \times 100$ .

into  $N_{\rm HC}$  maximally-separated 'hierarchical clusters' (see Wright et al. 2020, for a description of this process). Briefly, hierarchical clusters are defined by assigning each SOM cell to its own 'cluster', and then iteratively combining the two least-separated clusters (in our case by Euclidean distance

between the cell weight-vectors W) into one, until only a single cluster remains. At each iteration, the cluster centres are recomputed using the Lance-Williams dissimilarity formula (see Defays 1977; Iezzi 2014), invoking complete-linkage clustering to generate the most similar clusters. This



Fig. 3. Top: The photometric redshift distribution of the 'KiDS-Bright' GAMA-like KiDS DR4 bright sample (Bilicki et al., in prep.), with the  $z_{phot.} = \{0.02, 0.2, 0.5\}$  redshift bins (dashed lines) employed in our clustering analysis (Sec. 6), and the additional bins  $z_{\text{phot},1a} = \{0.02, 0.22\}$  and  $z_{\text{phot},2a} = \{0.28, 0.5\}$  (dotted lines) defined to have minimal photo-z overlap, as reckoned by the 95% scatter (red line);  $2\sigma_{z_{\rm phot}}\sim$  0.05, at that redshift. We use this  $n(z_{\text{phot.}})$  distribution to generate angular power spectra and FLASK mock galaxy catalogues. Bottom: The full redshift-range angular clustering (red) averaged over 30 independent FLASK lognormal random field realisations of the input power spectrum itself displayed in blue (see Eq. 5.2) with the theoretical  $1\sigma$  error for a KiDS-Bright-like survey - with 0.36 galaxies per square arcminute over  $900 \text{ deg}^2$ . The galaxy bias is set to unity. Error-bars are the root-diagonal of the covariance across the 30 realisations we note that for the 30 data-points shown, the covariance over just 30 realisations of the field is quite noisy. We are clearly able to recover the analytical input cosmology with these 30 realisations from FLASK.

iterative process constructs a cell-merger dendrogram which can then trivially be sliced at the desired number of clusters  $N_{\rm HC}$ . Each cluster of cells then contains a unique subset of the total galaxy sample, which are described by similar systematics-vectors V. In this way, the combination of the SOM and hierarchical clustering is able to construct  $N_{\rm HC}$ distinct groups of sources with similar systematics properties, but which occupy non-contiguous areas of the sky. The average total area on-sky that is spanned by each of the  $N_{\rm HC}$ groups is therefore determined by the area of the dataset in question (*i.e.* ~ 900 deg<sup>2</sup> for KiDS-Bright) and  $N_{\rm HC}$ .

From the on-sky distribution and galaxy-count corresponding to each hierarchical cluster, one is able to compute an estimate of the galaxy number density associated

with each section of the high-dimensional systematics-space (*i.e.* the space of systematic-tracer variables from Table 1 and Figs. 1 & 2). Our randoms creation algorithm uses this information to populate the survey volume with variablydense but locally unclustered random points. Moreover, each random point is constructed as a copy of one of the training galaxies from the hierarchical cluster to which it belongs, carrying all of the parent galaxy's physical and photometric properties: a 'clone'. Clones are therefore scattered only within the (again, non-contiguous) areas of sky represented by the parent hierarchical cluster. As a result, galaxy sample selection effects, and associated selection of specific systematic clustering patterns, are easily reproduced in the randoms catalogue by a simple selection of clones satisfying the chosen galaxy selection function. Acting as the reference points in a galaxy clustering measurement, the randoms ought to then compensate density variations correlating with any combination of the tracked systematic variables, for any selection of galaxies used to train the SOM.

The number of clusters  $N_{\rm HC}$  is an important tuning parameter for this analysis: besides determining the area-percluster,  $N_{\rm HC}$  must also trade off against the amount of discretisation of the systematics-space to be mapped. If we invoke too few clusters in our high-dimensional space, each will span a wide range of observational (*i.e.* systematic) and cosmological regimes, and could thus lose discerning power as a result (indeed,  $N_{\rm HC} = 1$  will return completely uniform randoms, by definition). Conversely, invoking too many clusters in the same space will result in too much freedom, and begin to over-fit the number density vs. systematics relation. This over-fitting can itself be pathological, as we shall see, if the individual clusters begin to trace the cosmic (*i.e.* not systematic) structure.

Our various choices for SOMs are detailed in Table 2. and Fig. 4 displays SOMs of the configuration 100A after training on KiDS-Bright. The bottom-left, top-left and top-right panels are coloured by the MU,psf\_fwhm,psf\_ell (Table 1) values for those cells, and the bottom-right panel connects these to the galaxy density contrast,  $(n_{\rm gal} \langle n_{\rm gal} \rangle / \langle n_{\rm gal} \rangle$ , in 100 hierarchical clusters (denoted by discrete patches of colour with black borders). Inspecting any region of the density contrast map, one can easily identify correlations between density contrast and various systematic parameters. For example, one can note the upper-left quadrant of the density contrast SOM as being populated by clusters of generally below-average (*i.e.* blue) density contrast. This is clearly correlated with above-average values of the *r*-band imaging surface brightness limit MU\_THRESHOLD. The opposite effect (i.e. aboveaverage density contrast) is seen for below-average values of MU\_THRESHOLD, except for clusters where the value of the PSF FWHM is above average; in this case, the density contrast is once-again below average. Such conclusions are easily drawn from the SOM, and are a significant advantage of our method presented here.

#### 4. Validating SOMs with artificial systematics

First, we will elucidate the capabilities and limitations of SOMs in recognising galaxy density-systematic correlations, through the use of artificial systematic fields with complex correlations to the depletion of the galaxy number density. Figure 5 shows on-sky distributions of  $1 \operatorname{arcmin}^{-2}$ 



Fig. 4. Self-organising maps, with dimension  $100 \times 100$ , coloured (*top-left, top-right, bottom-left*) by the systematics values taken on by each cell during the training procedure described in Sec. 3. In the density contrast panel (*bottom-right*), colours and black borders mark the 100 hierarchical clusters (see Sec. 3) defined according to groupings of cells with similar systematics-vectors for KiDS parameters psf\_fwhm,psf\_ell,MU\_THRESHOLD (Table 1). Systematic-tracer variables are linearly mapped onto the interval [0,1] before being passed to the SOM, hence the colourbar ranges. The density contrast panel (*bottom-right*) maps clusters of SOM pixels from their vectors of systematic-tracer values back onto a relative number density on-sky, and reveals almost all systematic density fluctuations to be at  $\leq 10\%$ , as reckoned by this SOM configuration (100A; Table 2).

FLASK galaxies, colour-coded by our set of eight artificial systematics variables, which were designed to mimic realistic spatial patterns in KiDS-like wide-field observations. 'A'-type variables vary smoothly over large angles, in a manner similar to Galactic foregrounds. 'B'-type variables have a 2-dimensional Gaussian form, which varies independently and discretely in  $1 \times 1 \text{ deg}^2$  'tiles', thereby mimicking telescope and camera effects such as PSF variations over the focal plane. Finally 'C'-type variables vary discretely between tiles but are constant within them, thereby mimicking perexposure effects such as limiting depth variations that arise from the use of a step-and-stare observing strategy (meaning that each tile is only observed once, per-band, over the course of the entire survey, thereby increasing sensitivity to the variable sky brightness on any given night). Each effect varies in the range [0, 1] for simplicity. By construction, these analytic systematics have no serious outliers.

To create spurious density modes as multivariate functions of our artificial systematics, we invent an independent *depletion function* for each parameter, shown in Fig. 6 as red dashed lines. These each describe the probability that an object will be discarded from the catalogue as a function of the object's position in systematics-space, thereby 'depleting' the galaxy number density at that point in systematics space. Note that some systematic variables cause no depletion (A3,B3,C2), and act instead as dummy parameters for the SOM to navigate. In Appendix Fig. A.1 we show the spatially-variable probability of depletion resulting from the depletion functions of Fig. 6 as applied to the systematics-maps of Fig. 5.

We apply each depletion function individually<sup>4</sup> to a set of 30 FLASK mocks. We then train a SOM using each depleted mock galaxy sample with the T1mock configuration from Table 2, and create a hierarchy of cell-clusters on each trained SOM. The number densities of the clusters should then reflect the input depletion functions, per individual systematic from Fig. 6. This test is thus a simple verification of the SOM's ability to characterise galaxy-density

 $<sup>^4</sup>$  The case of multiple, potentially correlated, systematic biases working in confluence is more realistic, however a SOM could then only infer the combined, multivariate depletion function, making an assessment of success more complicated. We shall explore the consequences of multiple biases when we turn to data-driven systematic density fluctuations in the next section.



Fig. 5. A FLASK-generated uniform random field, binned hexagonally (cell scale  $\sim 10 \, \mathrm{arcmin}$ ) in RA/DEC and coloured according to our various artificial systematic-tracer variables. A-types vary smoothly over large angles, B-types vary over  $1 \, \mathrm{deg}^2$  tiles with a 2D-Gaussian form, and C-types are single-valued for each tile. Iso-contours (white lines) are lain over A-type variables for clarity, and to illustrate the subtle difference between A2 and A3.

variations as a function of some systematic effect, with a particular pattern on-sky. Further, we can use this test to explore possible systematic patterns that may cause the SOM to fail in its corrective pursuit.

#### 4.1. Characterisation of artificial systematic fluctuations

We find that the SOMs are able to recover individual depletion functions with good accuracy. Figure 7 displays number densities vs. systematic-values for hierarchical clusters defined on the T1mock SOM (Table 2), along with our input depletion functions in red. Errorbars are the root-diagonal of the covariance over 30 realisations, and we display the result for both lognormal (green) and uniform (orange) random fields (GRF and URF respectively). The extra noise seen in  $n_{\rm gal}$  for the GRF case is due to the simulated cosmic structure, and can be seen to correlate with systematics that localise finite regions on-sky (*i.e.* A and C types). In contrast, B-type parameters show little difference between uniform and lognormal random fields, as individual systematics clusters cover a much less localised on-sky area; thus having much less sensitivity to (local) variations in cosmic number density. We also verify that the SOM does not 'create' depletion functions where none exist; Appendix Fig. A.2 shows that the SOM recovers the mean galaxy density in all cases, when training the SOM on the same parameters but without any depletion of galaxy number densities.

We note and address the presence of some irregularities in the distributions of Fig. 7, bearing in mind that the test here is merely to recover the form of depletions, and that these will be superseded by 2-point statistics in the next section. In extrema, A-type parameters appear to have outlier clusters with very high/low number density. These are artefacts from binning galaxies on the 5 arcmin Cartesian grid – at the footprint-edges, some grid-cells are only partially filled, resulting in seemingly under/overdense clusters. The B1 clusters are also affected by footprint-edges, where B1 is predominantly low (Fig. 5), and the amplitude of recovered fluctuations is suppressed with respect to the expectation for decreasing values of B1. The distribution of B1 (Fig. 6; blue histogram) drops sharply below values of  $\sim 0.5$ , whilst the probability of depletion rises (Fig. 6; red dashed line), resulting in a thin, sparsely-populated, grid-like distribution of objects across the footprint that begins to noisily sample the mean density, and causes further suppression of inferred fluctuations when the periodicities of the B1 fluctuation and the on-sky grid are misaligned. We verify that such effects can be mitigated by modifying the on-sky grid used to discretise the galaxy sample, however we caution that a reduction in the grid size can cause artificial masking of 'empty' patches of sky, given sparse galaxy data. In practice, these effects can be mitigated by ensuring mutual masking of the randoms and galaxy catalogues, and by tuning the on-sky grid size and grid-smoothing parameters to account for the range of number densities in the dataset under investigation. We further note that these artefacts are also seen in Appendix Fig. A.2, demonstrating that they are not related to the applied systematic density fluctuations.

Given our experience with this test, we settle on a fiducial setup with an on-sky resolution of 2.8 arcmin, and invoke a Gaussian smoothing kernel with a standard deviation of 0.1 arcmin. This allows empty grid-cells on the sky to be influenced by their populated neighbours, thus ensuring that the randoms respect the survey mask even for sparsely distributed galaxy data (such as the KiDS-Bright sample).

# 5. Validating Organised Randoms with data-driven systematics

The ultimate goal for our organised randoms is to provide a simple and unsupervised method with which to debias galaxy clustering signals upon measurement. In the previous section, we demonstrated that self-organising maps are capable of identifying systematic density fluctuations in data; we shall now use the SOMs to infer realistic systematic fluctuations from KiDS-Bright data, and apply these to simulated FLASK catalogues. Training organised randoms



Fig. 6. Histograms – each normalised to a maximum of unity – of the artificial model systematics (see Fig. 5) we impose upon our FLASK lognormal random field galaxies, both before (blue) and after (orange) applying our probabilistic depletion functions, shown as red dashed lines. Dummy-variables (A3,B3,C2) have no depletion applied – these are intended to 'distract' the SOMs.

against these biased data, we can then assess their ability to recover unbiased 2-point statistics.

We first note that many typical approaches to systematics-handling for galaxy clustering feature the correction of pixel density-systematics 1-point correlations (e.g. Suchyta et al. 2016; Elvin-Poole et al. 2018; Rezaie et al. 2020; Kitanidis et al. 2020; Vakili et al. 2020). We find this approach to be unsuitable for validation of our own methods, where the successful correction of pixel correlations is neither necessary for the recovery of unbiased 2-point functions, nor robust to the possibility of overcorrection; in fact, a perfect performance with regard to 1-point correlations could mask a total failure of our methods at the 2-point level, featuring a dramatic suppression of real clustering signals – for further details, see Appendix B.

#### 5.1. Galaxy clustering

For all measurements of galaxy clustering 2-point correlations, we consider the angular correlation function  $w(\vartheta)$ , and make use of the public software TREECORR<sup>5</sup> (Jarvis et al. 2004). The standard Landy-Szalay (Landy & Szalay 1993) estimator for angular galaxy clustering is given as

$$\hat{w}^{ij}(\vartheta) = \frac{\Theta(\vartheta) \left\{ D_i D_j - D_i R_j - R_i D_j + R_i R_j \right\}}{\Theta(\vartheta) \left\{ R_i R_j \right\}} \quad , \tag{5.1}$$

where i, j denote the galaxy samples being correlated – photo-z bins, in this work – while DD, DR and RR denote normalised<sup>6</sup> pair-counts between galaxies D and randoms R, and the bin-filter operator  $\Theta(\vartheta)$  rejects pairs with separations falling outside of the angular bin centred at  $\vartheta$ . We will consider both auto- (i = j) and cross-correlations  $(i \neq j)$  when evaluating our organised randoms.

Assuming a flat universe and a linear galaxy bias, and under the Limber and flat-sky approximations, one obtains a theoretical expectation for  $w(\vartheta)$ , between galaxy samples *i* and *j*, as follows (Limber 1953; Loverde & Afshordi 2008)

$$w^{ij}(\vartheta) = 2\pi b_g^i b_g^j \times \int_0^\infty \frac{\mathrm{d}\ell}{\ell} J_0(\ell\vartheta) \int_0^{\chi_{\mathrm{h}}} \mathrm{d}\chi \, \frac{p^i(\chi)p^j(\chi)}{\chi^2} \, P_\delta\!\left(\frac{\ell+1/2}{\chi},\chi\right),$$
(5.2)

where  $b_g$  denotes the linear galaxy bias,  $\ell$  the angular frequency,  $J_0$  the zeroth-order Bessel function of the first kind,  $\chi$  the comoving distance to a given redshift,  $p(\chi)$  the normalised comoving distance distribution of the sample, and  $P_{\delta}$  the matter power spectrum with non-linear corrections (for which we employ the halofit model of Smith et al. 2003; Takahashi et al. 2012). The right-most integral is equal to the (Limber-approximate) angular power spectrum  $C_{\ell}$ .

#### 5.2. Realistic biasing of FLASK fields

An application of SOMs to real data lacks a clear notion of 'truth' - we do not know exactly how our tracer variables relate to the deprecation of observed galaxy densities. Thus we cannot know whether or not the systematicdensity relations inferred by the SOMs are contaminated by cosmological density variations; for example, it could be that a real, local North-to-South galaxy density gradient happens to correlate with some systematic-tracer the SOMs could falsely identify such a variable to be tracing the *source* of the density gradient. Any randoms organised accordingly would then act to erase real, cosmological clustering signals. Moreover, we do not know the true underlying clustering signal – if our corrections were already sufficient to recover the unbiased clustering, but 1-point pixel density-systematics correlations (e.g. Elvin-Poole et al. 2018; Rezaie et al. 2020, see Appendix B) still revealed correlations with systematics, how would we know to stop?

Here we assess the performance of organised randoms in recovering unbiased clustering signals, and also address the question of 'over-fitting' to spatial, possibly cosmological,

<sup>&</sup>lt;sup>5</sup> https://github.com/rmjarvis/TreeCorr

<sup>&</sup>lt;sup>6</sup> Normalisation is by the product of total-counts  $N_iN_j$  for samples *i* and *j*, i.e. the count of all possible pairs. For autocorrelations, *N* is subtracted from the product, as a galaxy cannot be paired with itself.



**Fig. 7.** A recovery by the SOM of the artificial biases applied to 30 FLASK realisations (see Figs. 5 & 6) of random fields. Panels show the galaxy number density (arcmin<sup>-2</sup>) of 100 hierarchical clusters, defined on the SOM, against the median systematic value in each said cluster. Green points give the results for SOMs trained against depleted lognormal random fields (GRF), and orange points give the same for uniform random fields (URF), each generated using FLASK. The functions describing systematic galaxy depletion relative to our artificial systematic parameters (from Fig. 6) are converted into expected number densities and shown here as red dashed lines ('input DF'; depletion function). The solid horizontal lines indicate the global average number densities expected per systematic after depletion. We see that the SOM correctly recovers the expected number densities in all cases, demonstrating that none of the systematics models tested are unable to be recovered by the SOM. Points where both our URF and GRF data sit systematically away from the expected values are artefacts due to footprint edge-effects in our FLASK simulations, and do not affect the conclusions of this test (see Sec. 4.1).



Fig. 8. The systematic density contrast  $\delta_{\text{OR}}$  (Eq. 5.3) inferred, for the KiDS-North (*top-panel*) and KiDS-South (*bottom-panel*) areas of the KiDS-1000 bright sample (KiDS-Bright), by the 800C SOM setup. We use these maps to construct our organised randoms, populating the footprint to mirror the systematic density modes.

trends in galaxy density. For the reasons detailed above, this is difficult to do for real galaxy data such as KiDS-Bright, where any biases are already present. We sidestep these concerns with synthetic galaxy distributions from FLASK. The test method is as follows: we feed real galaxies and systematics data to a SOM, and infer the spatial pattern of depletion – whether the pattern is contaminated by LSS or not is, at this stage, unimportant. We perform a nearestneighbour interpolation in RA/DEC to port the real spatial distributions of systematics from KiDS-Bright onto FLASK galaxies simulated within the same mask. We then apply the SOM-inferred, systematic density patterns to the mocks, probabilistically, as

$$P_{\text{depl.}}(\boldsymbol{x}) = 1 - \frac{n_{\text{gal}}}{n'_{\text{gal}}} [1 + m \,\delta_{\text{OR}}(\boldsymbol{x})] \quad , \tag{5.3}$$

where  $P_{depl.}(\mathbf{x})$  is the probability that a galaxy at position  $\mathbf{x}$  will be 'lost'; a uniform random draw in the range [0, 1] must exceed  $P_{depl.}(\mathbf{x})$  for the galaxy to be retained.  $n_{gal}$  and  $n'_{gal}$  are the target and initial FLASK number density – we can only remove galaxies from the mocks, so we initialise the FLASK realisations with  $n'_{gal} = 0.72$  galaxies

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arcmin<sup>-2</sup> and then generate systematic under/overdensities with respect to the mean (target) KiDS-Bright density of  $n_{\rm gal} = 0.36 \, {\rm arcmin}^{-2}$ .  $\delta_{\rm OR}(x)$  is the density contrast at position x sourced by systematics<sup>7</sup> according to the SOM, and m is a scalar variable which we can use to manually modify the amplitude of the applied depletion, whilst retaining its functional relationship to the KiDS-Bright systematics distribution. Taking m > 1 would intensify the depletion, relative to that present in KiDS-Bright, whilst m < 1 would yield a comparatively soft depletion. We display an example map of  $\delta_{\rm OR}$ , inferred from KiDS-Bright galaxies, in Fig. 8.

Repeating this procedure for many realisations of the underlying cosmology, we have created the 'truth' case of a single, global pattern of galaxy-depletion. Running the SOMs again, now against the depleted FLASK mocks, we can assess how consistently they are able to recover this truth for many different realisations of the constant cosmological background. If the SOMs are able to retrieve the fixed systematic depletion pattern from many independent realisations of the cosmic structure, then we can assert that the inferred  $\delta_{OR}(\mathbf{x})$  is uncontaminated by cosmology.

Having thus created many realisations of KiDS-Brightlike data for which we can turn systematic biases on or off, we can now run our SOMs and assess the corrective performance of our organised randoms with various measurements of  $w(\vartheta)$ . A caveat is that our depletion of the FLASK galaxies is derived from runs of the SOM against KiDS-Bright, thus the bias can be said not to be *entirely* realistic (although far more so than the artificial systematics of the previous section, for which the accuracy of capture was excellent) but dependent upon the configuration of the initial SOM. As such, we consider many different configurations along with modifications (via the *m* parameter from Eq. 5.3) to the intensity of depletion that we apply to the FLASK mocks.

Over the course of testing, we recognised that systematic-tracer set B (Table 1) transpires to be a relatively uninformative yardstick between sets A and C; as such, we limit our discussion from here to parameter sets A, C, which are instructive for our work with the relatively unbiased KiDS-1000 bright sample.

#### 5.3. Correction of data-driven systematic fluctuations

We devise a battery of  $w(\vartheta)$  tests to assess the performance of our organised randoms at the 2-point level. The key variables that we change are (i) the parameters used to train a SOM against KiDS-Bright, and (ii) the number of hierarchical clusters  $N_{\rm HC}$  defined on that KiDS-Bright SOM. These determine the spatial depletion to be ported onto FLASK realisations, as described in Sec. 5. We also change (iii) the parameters used to train a second SOM against biased FLASK realisations, and (iv) the number of hierarchical clusters  $N_{\rm HC}$  defined on that FLASK SOM – these allow us to break any circularity by comparing independent SOMs. Finally, we also experiment with (v) intensifying the depletion via the *m* parameter (Eq. 5.3).

We find that the performance and flexibility of our organised randoms are excellent. The randoms are able to

consistently mitigate biases in FLASK fields, even when having limited sensitivity to smaller scales (via reduced  $N_{\rm HC}$ w.r.t the SOM used to infer systematic modes), or when trained on incomplete systematics information. Fig. 9 displays some examples of organised randoms' performance, which we continue to explore in Appendix C. Panel-titles in these figures give the SOM setups trained (i – 'bias') against KiDS-Bright to infer the clustering bias, and (ii 'recovery') against the biased FLASK mocks to recover the true clustering with organised randoms. Multiplicative factors in the panel-titles indicate where  $m \neq 1$ . Black points and dashed curves give the unbiased clustering signal  $\pm 1\sigma$ errors from 30 FLASK realisations (equivalent to red points in Fig. 3). Triangles and hatched curves are the measured (biased) clustering after depletion of the FLASK fields, and solid-filled curves show the corrected clustering, measured with organised randoms. In all meaningful (see Appendix B, where we present a deliberate failure mode: 800Ares2) bias/recovery cases considered, our organised randoms yield clustering correlations that are more consistent with the truth than the biased signals (*i.e.* those measured with uniform randoms).

In Fig. 9, one sees that the recovery:100C organised randoms yield an effective correction of clustering biases from the bias:800C SOM (blue panel), with the recovered signal much closer to the unbiased measurement (mean absolute deviation over 7 – 100 arcmin:  $1.48\sigma \rightarrow 0.31\sigma$ , where  $\sigma$ is the uncertainty in the unbiased signal) – this indicates that a relatively insensitive SOM setup (100C) is able to characterise the more complex biases inferred from a SOM with greater sensitivity to small-scale systematic structure (800C). We see an even better correction  $(1.43\sigma \rightarrow 0.09\sigma)$ when passing incomplete systematics information to the SOM, as demonstrated by bias:800C vs. recovery:100A (orange panel). This demonstrates that our SOM methods are able to correctly infer systematic density fluctuation patterns even when the patterns are sourced by systematictracers unknown to the SOM: thus inter-parameter correlations serve to make organised randoms robust against 'missing' training variables, and the additional freedom afforded to  $N_{\rm HC}$  clusters in a systematics-space of reduced dimensionality can actually improve the accuracy of the correction. Homogenising the scale-sensitivity (via  $N_{\rm HC}$ ) between bias/recovery SOMs, but keeping the incomplete systematics set for recovery (100C vs. 100A; green panel), we still see an excellent recovery of the unbiased clustering signature  $(0.94\sigma \rightarrow 0.28\sigma)$ ; as we might expect for a less complex bias. For identical bias/recovery setups 100C (red panel), we begin to see a slight over-correction by the organised randoms; this comes about as clusters on the SOM begin to over-fit to the cosmic structure around the density-systematics relation.

Whilst the recovery is still preferable to the biased statistic here  $(0.96\sigma \rightarrow 0.54\sigma)$ , we acknowledge that overcorrections could be problematic for cosmological inference (see Wagoner et al. 2020). However, the KiDS-Bright sample is a bright subset of the KiDS-1000 photometric sample, specifically chosen to be ~ 5 magnitudes shallower than the survey flux-limit, and thus less sensitive to systematic detection failures; these data are relatively unbiased already. For more pathological biases, resulting in a higher amplitude of systematic density contrast, such over-fitting to cosmic structure is less likely to occur. Thus we expect our randoms to perform even better for samples with stronger sys-

<sup>&</sup>lt;sup>7</sup> This inferred density contrast from systematics forms the basis for our organised randoms generation algorithm, though for this test we create organised randoms only after training separate SOMs against the depleted FLASK mocks.



**Fig. 9.** Angular clustering correlation functions  $w(\vartheta)$  measured in FLASK fields, after they have been depleted (as described in Sec. 5.2; Eq. 5.3) according to the output of various SOMs trained against the KiDS-1000 bright sample (KiDS-Bright). For each configuration, panel-titles give the 'bias:SOM' trained against KiDS-Bright, and the 'recovery:SOM' trained against biased FLASK data to create organised randoms. *Top:* ratios of measured clustering signals to the true, unbiased clustering. *Bottom:* the unbiased angular clustering signature (black points and dashed curves; measured with uniform randoms on unbiased FLASK fields), compared with biased (triangles and hatching; measured with uniform randoms) and recovered (coloured points and shading; measured with organised randoms) clustering signals measured in the depleted fields. Errors are the root-diagonal of the covariance over 30 FLASK realisations, and all are given to  $\pm 1\sigma$ . From left-to-right, the FLASK fields are biased according to  $\delta_{OR}$  from the 800C,800C,100C,100C,100C SOMs, trained against KiDS-Bright. The *m*-parameter (Eq. 5.3) is set to unity in all but the purple panel (where m = 4), and each correlation measured in the depleted fields using organised randoms displays greater consistency with the unbiased signal, as compared with the signal measured using uniform randoms.

tematics imprints, *e.g.* the KiDS-1000 shear sample, dominated by faint galaxies. We test this assertion using the same setup, but setting m = 4 in Eq. 5.3. In this case  $[100C(\times 4) \text{ vs. } 100C; \text{ purple panel}]$ , a massively inflated bias of  $12.17\sigma$  is once again reliably corrected to  $0.34\sigma$ .

This result is particularly important, as measuring accurate clustering statistics for faint, systematics-dominated samples has historically been extremely challenging; hence why we often choose bright subsamples for clustering analyses (also for typically more reliable estimation of galaxies' photo-z; see Porredon et al. 2020). Our companion letter, Wright et al., (in prep.), thus presents an application of our organised randoms pipeline to the KiDS-1000 shear sample, finding excellent and robust performance in correcting for systematic clustering bias. Moreover, the shear sample is a factor of  $\sim 20$  denser on-sky than the bright sample, enabling us to increase the resolution of the cartesian RA/DEC grid whilst still respecting the survey mask (see Sec. 4.1); in this way, we become more sensitive to smallscale systematic density fluctuations at fixed  $N_{\rm HC}$ , which Wright et al., (in prep.) show is important for those faint data.

#### 6. Clustering in the KiDS-1000 bright sample

Having validated the performance of our SOMs/organised randoms in recognising systematic trends in galaxy density, and removing their traces from synthetic galaxy 2-point correlations, we apply our methods to measurements of galaxy clustering in the KiDS-Bright sample, and compare tomographic cross-correlations with analogous signals measured in the highly-complete GAMA (Driver et al. 2009; Liske et al. 2015) sample.

We make use of randoms organised by the SOM configuration 100A (detailed in Table 2), which we show (in Figs. 9 & C.1) to robustly improve the fidelity of signal recovery in all bias:SOM scenarios from our FLASK tests (which vary in scale-sensitivity via  $N_{\rm HC}$ , and in the systematic-tracer parameters) – thus we expect a reasonable correction even if the additional systematictracers (MAG\_LIM\_r, EXTINCTION\_r, gaia\_nstar) are in reality uncorrelated with the KiDS-Bright systematic density contrast. Moreover, the bias:800C / recovery:100A test case (Fig. 9; orange panel) demonstrates that the bias inferred from all parameters (set C: threshold, PSF FWHM/ellipticity, limiting magnitude, Galactic density of stars and extinction), with high small-scale sensitivity  $(N_{\rm HC} = 800)$ , is corrected with great precision by 100A organised randoms, having a residual bias of  $< 0.1\sigma$ . Table C.1 summarises the performance of differently configured organised randoms, and reveals 100A to be the net-best performer across all bias:SOMs.

We note that these particular SOM setups and parameter-sets may not be the ideal for other surveys with different areas, geometries, systematics imprints etc., and that any organised randoms should be thoroughly tested with simulations, as we have done (in Sec. 5).

Figure 10 hints at the advantages of creating 'cloned' galaxy randoms, wherein each random point is a clone of a real object used in training of the SOM, and clones are spatially restricted to on-sky areas occupying similar positions in the systematics-space. The figure illustrates how



**Fig. 10.** Galaxy number density contrast  $\delta$  in 2D bins of photometric redshift vs. RA for uniform randoms (*left*), the KiDS-1000 bright sample (KiDS-Bright; *middle*), and relevant clones from **800Ares2** organised randoms (*right*). Rows display blue (*top*) and red (*bottom*) galaxies, according to a cut at observer-frame u - i = 2.66. We only show galaxies in the range 172 < RA < 205, 2 < DEC < 3 in order to reveal systematic density variations in the data and randoms. Unlike for uniform randoms, the organised randoms can be seen to reproduce the systematic trends in the KiDS-Bright data, namely under-densities over different pointings (*e.g.* RA = 175.5, 197.5), visible as vertical bands of fainter pixels, and the differential evolution of samples' densities with redshift, as evidenced by the boxes (highlighting a specific volume with differential density as a function of sample colour) and horizontal lines (dashed lines give the  $z_{phot}$  corresponding to the 3<sup>rd</sup> and 97<sup>th</sup> percentile number counts for uniform randoms, and dotted lines give these for KiDS-Bright data). We elect to display 800Ares2 randoms here for a clearer illustration of the cloning mechanism, which is more subtle in our other, favoured randoms (see Sec. 5.3).

we reproduce systematic density variations in a strip of KiDS-Bright (172 < RA < 205, 2 < DEC < 3 degrees) for a coarse red/blue (bottom/top) sample selection<sup>8</sup>, merely by restricting our organised randoms to the relevant clones. The figure shows the density contrast of 1 degree columns in RA, and we expand the radial dimension  $(z_{phot.})$  to draw attention to non-physical density modes -i.e. underdensities which are localised to single pointings, seen as fainter vertical strips of colour in the right-most column (e.g. at  $RA \in [175.5, 197.5]$  – and to the redshift evolution of galaxy number density, which varies for red/blue galaxies; these trends are mirrored in the 800Ares2<sup>9</sup> organised randoms (right-column), in contrast with the uniform randoms (left-column). The cloning utility will be fully realised in future work; systematics which differentially affect arbitrary galaxy selections can be automatically compensated, allowing for easy splitting of analyses into, e.g. red and blue galaxies, or into bins of galaxy luminosity. For now, we focus only on redshift tomography.

In addition to the tomographic bins '1' and '2', with edges at  $z_{\text{phot.}} = \{0.02, 0.2, 0.5\}$ , we cross-correlate two additional, non-overlapping bins, '1a' and '2a', with edges at  $z_{\text{phot.}} = \{0.02, 0.22\}$  and  $z_{\text{phot.}} = \{0.28, 0.5\}$ , respectively; the gap between the inner-edges of the 2 bins is more than the typical 95% photo-z scatter at this redshift (Fig. 3, red line in top-panel), thus we test for a null cross-correlation

between them. Barring the auto-correlations of the full ('total') sample, we refer to correlations between bins 'i' and 'j' as 'i-j', *i.e.* '1-1' is the auto-correlation of tomographic bin '1'; '1-2' is the cross-correlation between bins '1' and '2', etc.

We generate organised randoms with  $20\times$  the number density of KiDS-Bright, so as to combat Poisson-noise in the relevant pair-counts (see Eq. 5.1). Our measurements of angular clustering auto-correlations, within the 2 primary redshift bins and across the full KiDS-Bright sample, are displayed in Fig. 11. Fig. 12 displays the redshift-bin crosscorrelations, in comparison with equivalently binned signals measured in the GAMA sample – we use our ANNZ2 photoz estimates to define these GAMA bins, and employ the spatially uniform, windowed, cloned-galaxy randoms presented by Farrow et al. (2015). As we discuss in Appendix D, auto-correlations in GAMA are not suitable for validating KiDS-Bright correlations here, hence they are not displayed in Fig. 11.

For all  $w(\vartheta)$  correlations in Figs. 11 & 12, we estimate errors with the delete-one jackknife technique. We divide the KiDS-Bright/GAMA footprints into  $N_{\text{patch}}$  roughly equalarea patches, and compute  $w(\vartheta)$  upon the successive removal of individual patches. For these  $N_{\text{patch}}$  signals  $w_{\alpha}$ , the covariance is then

$$\hat{C}_{\text{jack.}} = \frac{N_{\text{patch}} - 1}{N_{\text{patch}}} \sum_{\alpha=1}^{N_{\text{patch}}} (w_{\alpha} - \bar{w})(w_{\alpha} - \bar{w})^{\text{T}} \quad , \qquad (6.1)$$

where T denotes the conjugate transpose of a vector and  $\bar{w}$  is the average of the  $N_{\text{patch}}$  measurements  $w_{\alpha}$ . For KiDS-

<sup>&</sup>lt;sup>8</sup> We define the red/blue boundary at observer-frame u-i = 2.66, which sits in the trough of the bimodal colour distribution of KiDS-Bright.

<sup>&</sup>lt;sup>9</sup> Chosen for illustrative purposes, as the inferred  $\delta_{OR}$  is wider for this setup – see Appendix B.1 – and the increased resolution results in more clearly visible systematic density modes in the organised randoms (discussed in Appendices B & C).



**Fig. 11.** Angular auto-correlation functions  $w(\vartheta)$  measured in the 'total' (*i.e.* un-selected) KiDS-1000 bright sample (*bottom*), and within redshift bins '1' ('1-1'; *top*) and '2' ('2-2'; *middle*), with edges  $\in [0.02, 0.2, 0.5]$ , as shown in Fig. 3. Measurements using uniform randoms are shown in red, and those made with 100A organised randoms are shown in blue. Errors are estimated via a 2D delete-one jackknife with 31 pseudo-independent patches of the footprint. Points are horizontally offset to aid with clarity. The total sample correlation is more clearly visible in Appendix Fig. D.1.

Bright,  $N_{\text{patch}} = 31$ , and  $N_{\text{patch}} = 20$  for GAMA<sup>10</sup>. We note that for our chosen binning – 30 log-spaced bins in the range  $3 \le \vartheta \le 300 \operatorname{arcmin}$  – so few jackknife samples will yield singular covariance matrices (see Hartlap et al. 2007). We are only interested in measurement errors (the square-root of the matrix diagonal) here, and since we are not performing any fitting we proceed as such.

In Fig. 11, we see that the 100A organised randoms make more sizeable corrections (blue points) to the measured 'total' and '2-2' correlations (red points), than to the '1-1' correlation. This is perhaps to be expected, since at higher redshifts the objects with faint apparent magnitudes, and predominantly small angular extents, will be more prone to dipping below the detection threshold (or out of sample selection criteria) as a result of observational effects; the smaller correction to '1-1' could then be the opposite man-



**Fig. 12.** Angular cross-correlation functions  $w(\vartheta)$  measured between KiDS-1000 bright sample (KiDS-Bright) redshift bins '1' and '2' (top), with edges  $\in [0.02, 0.2, 0.5]$ , and '1a' and '2a' (bottom), with edges  $\in [0.02, 0.22]$  and [0.28, 0.5], as shown in Fig. 3. Measurements using uniform randoms are shown in red, and those made with 100A organised randoms are shown in blue. Errors are estimated via a 2D delete-one jackknife with 31 pseudoindependent patches of the footprint. Grey points and shading give the equivalently-binned (by ANNZ2 photo-z) correlations measured for the GAMA sample, with errors estimated again via jackknife but from 20 sub-regions of the GAMA window – errors on scales  $\vartheta \gtrsim 180$  arcmin are thus likely to be underestimated for GAMA correlations.

if estation of this effect, wherein apparently brighter/larger galaxies are more robustly detected. The large-scale corrections to cross-correlations (Fig. 12) are also small – this is the desired behaviour, particularly in the case of disjoint bins '1a-2a', as the cross-correlation is expected to be zero. In fact, the rising 1a-2a signals at small values of  $\vartheta$  (red points) are largely corrected by the organised randoms. Given the vast gap ( $\delta z = 0.06$ ) between the disjoint bins, these small- $\vartheta$  signals are highly unlikely to correspond to real structures; the organised randoms are compensating for small-scale systematic density modes, shared across the redshift range.

We note the (still relatively small) amplitude of the  $w(\vartheta)$  correction at  $\vartheta \ge 10$  arcmin in the 'total' sample correlation (in Fig. 11), and its similarity to the signal recoveries displayed in Fig. 9. This is encouraging as we can intuit that our extraction and replication of depletion patterns, from KiDS-Bright and in FLASK realisations (Sec. 5.2), is realistic enough to result in consistent inferences of the required correction to  $w(\vartheta)$ . Thus we can expect that the corrected 'total' signal is closer to the true clustering, as is the case for the correlations from Fig. 9. In the intermediate range  $7 < \vartheta < 100$  arcmin, the mean corrections to  $w(\vartheta)$  for each correlation are:  $\{1-1: -5.6\%, 1-2: -30.0\%, 2-2: -10.9\%, total: -9.4\%\}$ .

In order that analyses be conducted free of any confirmation bias, it has become common in large-scale structure

<sup>&</sup>lt;sup>10</sup> Since the total equatorial GAMA area ~ 180 deg<sup>2</sup>, each of the 20 patches is ~  $9 \deg^2 \equiv [180 \operatorname{arcmin}]^2$  in size, hence errors on  $w(\vartheta \gtrsim 180 \operatorname{arcmin})$  are likely to be under-estimated.

analyses to practice *blinding* (e.g. Kuijken et al. 2015), wherein several modified versions of key statistics are produced<sup>11</sup> from the data alongside the true version. The truth is revealed to the team by an independent entity only after the entire analysis is complete, such that no critical decisions can be taken in favour of some expected result. At the time of writing, we were blind to the truth of our KiDS data, and thus chose not to compare with theoretical models for galaxy clustering; our companion work (Wright et al., in prep.) considers the best-fit cosmological model from the latest KiDS 3x2-point analysis (Heymans et al. 2020) for comparison with corrected clustering statistics measured in the KiDS-1000 shear sample.

A direct comparison of GAMA clustering autocorrelations with our own also transpires to be unsuitable here, for reasons we discuss in Appendix D. As such, we consider only the redshift bin cross-correlations from GAMA (in Fig. 12) for validation; with the alignment of sample properties less important here, these correlations instead probe (i) the photo-z scatter and (ii) any systematic correlations shared across the KiDS-Bright redshift bins, where the former should be negligible in the 1a-2a correlation owing to the large gap (Fig. 3) between the bins. We see that the rising signals at small- $\vartheta$  (Fig. 12; red points) are not present in GAMA (grey), and that our organised randoms' corrections (blue) result in greater consistency between GAMA and KiDS-Bright. This is also true of the slightly negative (but not significant) 1a-2a blue data-points in the  $\vartheta \sim 10 \operatorname{arcmin}$ range, where the negative GAMA points indicate possible LSS fluctuations to be at play. The GAMA data are highly complete (> 98%; Liske et al. 2015) and can be considered as the unbiased 'truth' here; they are what we expect for photo-z of this quality, in the absence of systematic galaxy density patterns. We thus argue that our corrections to the redshift bin cross-correlations are successfully removing systematic correlations from KiDS-Bright data.

#### 7. Summary

We have developed and tested methodology for the construction of 'organised randoms', which mirror systematic trends in galaxy density, using self-organising maps. We made extensive use of lognormal random field simulations from FLASK to test the abilities of SOMs to recognise both artificial and real systematic loss of galaxies, and demonstrated that organised randoms constructed using this information are able to reliably correct the measurable angular clustering of the synthetic data.

With the present data volume, constructing effective organised randoms relies upon a balance between the area of sky probed by each hierarchical cluster (essentially an *n*dimensional bin) defined on the SOM, the variables and dimensionality of the systematics-space given to the SOM, and the width of the distribution of *systematic* density contrast – as we have demonstrated, this balance is readily assessed with simulations. If systematic modes are very much smaller than cosmological modes, organised randoms become more prone to over-correction of clustering biases – though our SOM methods are able to test for the necessity of any correction, as they estimate the distribution of systematic density contrast  $\delta_{OR}$ . Conversely, for strong pathological density modes, our randoms are highly effective. Moreover, regardless of our analysis choices when testing with FLASK simulations, our recovered clustering results are always consistent with the underlying truth, having an average bias correction across all meaningful runs of  $2.31\sigma \rightarrow 0.34\sigma$ . Our recovery of the truth is particularly striking in the amplified bias (m = 4) case, where we shift from catastrophic bias with uniform randoms  $(12.2\sigma)$  to full consistency with the truth  $(0.34\sigma)$ .

We found that the importance of certain systematicstracing variables, at the level of the 2-point correlation function, is not necessarily determined by the strength of the 1-point (pixel) correlation of the tracer with galaxy density (see Appendix B). Whilst this finding may only ring true for the KiDS-1000 bright sample (KiDS-Bright), we note that simply correcting these 1-point correlations may yet be problematic for the general goal of recovering unbiased galaxy clustering 2-point functions – the amount of 1-point correction required to achieve this goal is not necessarily clear, and further complicated by correlations between systematic-tracer parameters. We recommend the use of principle component analysis (PCA) to alleviate the latter concern, however 2-point functions should also be considered for validation in analyses of this type.

We worked with FLASK simulations, modelling the footprint and number density of the KiDS-1000 bright sample, to create realistically-biased synthetic galaxy fields within which to test the performance of our organised randoms. We inferred the field of systematic galaxy density contrast directly from KiDS-1000 bright sample data, under various assumptions modifying sensitivity to angular scales and to different systematic-tracers, and modifying the amplitude of systematic fluctuations; applying these data-driven systematic clustering imprints to many independent realisations from FLASK, we then generated organised randoms by training against the biased FLASK fields, again varying the scales/tracers utilised. Under several scenarios of biasing due to the spatially variable PSF, detection threshold, survey depth, and Galactic stellar density and extinction, we found that training upon the psf\_fwhm,psf\_ell,MU\_THRESHOLD parameters, and defining 100 hierarchical clusters on the trained SOM (setup 100A), was sufficient to yield organised randoms that consistently remove the various, realistic systematic density modes from the FLASK galaxy fields. These 100A organised randoms recovered clustering signals deviating on average from the unbiased signal at ~  $0.3\sigma$ , over the relevant FLASKtesting setups with average bias ~  $1.1\sigma$ . For the most pessimistic clustering bias scenarios, where un-corrected signals deviate from the truth at up to ~  $12\sigma$ , the performance of organised randoms remains robust, with the bias of recovery at ~  $0.3\sigma$ .

We presented the first measurement of photometric galaxy clustering from the Kilo Degree Survey, for bright, GAMA-like galaxies from the 1000 deg<sup>2</sup> 4<sup>th</sup> Data Release. Defining 2 tomographic bins, with edges  $z_{\text{phot.}} = [0.02, 0.2, 0.5]$ , we measured the angular auto- and cross-correlation functions over  $3 < \vartheta < 300$  arcmin with uniform and organised randoms. We saw that our organised randoms make variable corrections to tomographic auto- and cross-correlations, editing amplitudes at intermediate angular scales ( $7 \leq \vartheta \leq 100$  arcmin) by up to ~ 10% (~ 1 $\sigma$ ) in the auto-correlations, and ~ 30% in the cross-correlations.

<sup>&</sup>lt;sup>11</sup> Note that the best methods for blinding are active areas of research; see *e.g.* Muir et al. (2020); Sellentin (2020); Brieden et al. (2020).

We implemented our randoms such that each random point is a 'clone' of a real galaxy, scattered within regions of the survey footprint that are similar to the location of the parent galaxy in terms of the position it occupies in systematics-space. Thus by mimicking galaxy sample selections in the randoms, we compensate for distinct, samplespecific systematic correlations; e.g. those induced by selections in galaxy photo-z. For tomographic cross-correlations, our randoms were found to correct significant systematic density modes at small- $\vartheta$ , which are shared between disparate redshift populations, whilst making nearly negligible corrections throughout the remaining angular range; indicating similar small-scale, but distinct larger-scale systematic clustering imprints for the different redshift populations. This utility is easily generalised to any galaxy sample selections in e.q. luminosity, colour etc.

An extension of this work to increased areas and galaxy number densities is extremely promising; larger areas will result in better handling of large- $\vartheta$  systematic density modes, due to more redundant sampling, and a smoother distribution of density contrast, which will minimise contamination of the randoms by cosmic structure. Higher galaxy densities offer better sampling of small- $\vartheta$  modes, a smoother description of the systematics-space, and the chance to raise the resolution of the randoms without fear of greater contamination by structure. Thus the performance of organised randoms should improve on all scales with next-generation datasets; our companion letter (Wright et al., in prep.) moves to verify our assertions here, applying our testing pipeline to measurements of clustering in the faint KiDS-1000 shear sample, thus exploring a deep survey, high number density scenario.

Upon acceptance of this article, we will make our code and methods public, such that independent teams can experiment with the handling of systematic density variations using organised random clones. Future surveys that will make powerful use of galaxy clustering (e.g. the Rubin Observatory, Euclid) can then include the construction of organised randoms as a pipeline module, adding to the panoply of complementary means for the accurate measurement of galaxy positional statistics.

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campaign using the Anglo-Australian Telescope. Our GAMA catalogue is based on data taken from the Sloan Digital Sky Survey and the UKIRT Infrared Deep Sky Survey. Complementary imaging of the GAMA regions is being obtained by a number of independent survey programmes including GALEX MIS, VST KiDS, VISTA VIKING, WISE, Herschel-ATLAS, GMRT and ASKAP providing UV to radio coverage. GAMA is funded by the STFC (UK), the ARC (Australia), the AAO, and the participating institutions. The GAMA website is http://www.gama-survey.org/.

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#### **Appendix A: Artificial systematics**

Here we extend our discussion of characterisation of artificial systematic density fluctuations with self-organising maps (Sec. 4). We created artificial systematic-tracer variables (Fig. 5) with arbitrary depletion functions (Fig. 6) to apply to FLASK mock data (the excess probability of depletion for each artificial variable is given in Fig. A.1), finding the T1mock SOM (Table 2) to be capable of characterising the depletion functions directly from the mock catalogue (Fig. 7). As a sanity-check, we also run the same SOM against the 30 FLASK catalogues before applying any depletion - the SOM should not find any density-systematic correlations where none exist. The results are shown in Fig. A.2, where the depletion functions from Fig. 6 are included for reference, and we see the desired behaviour; the SOM recognises no significant, systematic trends in galaxy density (barring some of the irregularities related to gridresolution, discussed in Sec. 4.1).

# Appendix B: Pixel density-systematic 1-point correlations

Here we consider correlations between the densities of galaxies in pixels on-sky and the values of systematic-tracer variables in those pixels. Many incarnations of these statistics appear in the literature, often as metrics to demonstrate successful decorrelation of galaxy densities and systematics by other methods (*e.g.* Suchyta et al. 2016; Rezaie et al. 2020; Kitanidis et al. 2020) and occasionally in order to derive the corrections themselves (Elvin-Poole et al. 2018; Vakili et al. 2020). For these tests, we construct galaxy density and systematics maps using healpy with  $n_{\text{side}} = 256$ , corresponding to on-sky pixels of roughly  $14 \times 14 \operatorname{arcmin}$  in size. We compute the mean systematics in each pixel, applying requisite scaling to pixels that are only partially sampled by the survey window.

This approach is somewhat analogous to that of Elvin-Poole et al. (2018), who used 1-point functions directly to derive per-galaxy weights in order to mitigate clustering systematics. In our case, however, the 1-point correlations serve only as a diagnostic; our SOM approach improves on pixel-correlation methods by dropping some commonlymade approximations: in particular we map the galaxy depletion function through a higher-dimensional systematicsspace, correcting galaxies directly in this space, rather than iteratively suppressing only the worst correlations until crossing some threshold. Additionally, whilst usually approximated as linear in the density contrast, the depletion of galaxies as a function of systematics in our method can be arbitrarily non-linear, allowing greater freedom to correct for more complex systematic modes.

We make some changes to the typical formulation of the galaxy density vs. systematic pixel correlations. First, we normalise per-pixel number-counts (or 'pixel-counts') of galaxies,  $N_{\rm gal}$ , not by the global average galaxy pixel-counts,  $\langle N_{\rm gal} \rangle$ , but instead by pixel-counts for a uniform random field,  $N_{\rm rand}$  (given the same on-sky pixelisation). This minimises any influence of inhomogeneity (*e.g.* cosmic structure) across the galaxy data, and correctly accounts for survey mask effects. The two estimators are generally equivalent in the limit of large area, modulo normalisation between the average random and galaxy number densities.

Second, for the 'corrected' case we normalise the galaxy pixel-counts by the organised randoms' pixel-counts; any systematic correlations in the data should thus be cancelled by the mirrored trends in the organised randoms.

We note here, though, that the erasure of such trends can be a misleading measure of performance. Inter-tracer correlations can induce trends in the  $N_{gal} / N_{rand}$  distribution, as a function of systematics, that make individual systematics appear more/less significant than they truly are. Furthermore, the strength of correlation per systematic that is needed to introduce a significant clustering bias is also an open question, but is likely dependent upon the sample being analysed, the systematic parameter's distribution and dynamic range, and the ultimate angular scales of interest. Finally, these distributions can behave particularly pathologically when correcting systematic density variations using variable randoms, as we are doing. As a simple demonstration, should the organised randoms produce a catalogue that exactly reproduced the input galaxy catalogue (*i.e.* the randoms encoded all galaxy density fluctuations, systematic and cosmological), then these correlations would appear perfectly flat. This would constitute the most abject failure of our corrective method, and yet this diagnostic would be labelled a success.

These concerns lead us to derive and consider orthogonal principle component maps (*i.e.* principle component analysis, or PCA; see Jolliffe 2002, for a comprehensive text on PCA) alongside our systematics maps (see also Wagoner et al. 2020, who apply such a decomposition to their systematics maps). Principle components are defined as new, orthogonal basis vectors for *n*-dimensional data, constructed from linear combinations of the original dimensions. The new basis then describes – in order, from component 1 to component n – the directions of greatest variance in the data. As the basis vectors are orthogonal, principle components have no covariance and are thus more instructive for assessing the significance of density-systematic correlations, although they are more difficult to interpret physically.

Lastly, we assess the expected spread of pixel density-PCA component (or density-systematic) correlations for individual, unbiased realisations of the large-scale structure within our survey parameters – these are given in Fig. B.1, where solid lines give the  $1\sigma$  and  $2\sigma$  widths of the  $N_{\rm gal} / N_{\rm rand}$  vs. systematic-tracer distributions from 100 individual FLASK realisations. As Fig. B.1 shows, the intrinsic spread of galaxy number density vs. systematic-tracers over 100 independent realisations of KiDS-Bright-like synthetic data is often around a few percent, and rises for more longvarying tracers -e.q. Galactic extinction and stellar density. Thus, for our data, galaxy density-component/systematic correlations within a few percent of unity cannot be distinguished from those arising stochastically. These are the 'limits' of useful bias-correction dictated by sample variance, and we shall mark them as purple shading in the following pixel-correlation figures.

#### Appendix B.1: Correction of 1-point correlations

Having created maps of each of the systematic-tracers listed in Table 1, we mask pixels in the  $1^{st}$  and  $99^{th}$  percentile tails of each distribution and make additional cuts by hand, excluding the few sparse pixels with extreme outlier values for systematic-tracers – these would otherwise contaminate correlations with poorly sampled, unrepresentative



**Fig. A.1.** The same as Fig. 5, but only for parameters with non-zero depletion functions. The colouring now denotes the *excess* probability of depletion, as a function of each artificial systematic; a galaxy with an excess probability of 1 is 100% more (or twice as) likely to be depleted when compared with an excess probability of zero.



Fig. A.2. The same as Fig. 7, but for a SOM trained on an unbiased FLASK field. The depletion functions are again shown as red dashed lines, though no depletions were applied. Irregularities, *e.g.* in the A3 panel, are discussed in Sec. 4.1. Data-points derived from lognormal random fields (green) are on average higher in  $n_{gal}$  than those from uniform fields (orange) because of the clustering of galaxies; the Cartesian grid, used to estimate the area of the sample, has more empty cells for the GRF, hence the area is under-estimated and  $n_{gal}$  is over-reported.

galaxy counts. We then 'whiten' the parameter distributions (transforming each to zero-mean and unit-variance) before retrieving 14 orthogonal principle component maps. The matrix of linear coefficients connecting PCA components to systematics tracers is shown in Fig. B.2.

Figs. B.3 & B.4 illustrate why these 1-point correlation metrics are unsuitable for assessing the performance of our corrective randoms. In Fig. B.3, we select the subset of 4 component-density pixel correlations in bias:800C FLASK realisations that are best-corrected to unity after normalisation by the 100A organised randoms' density in those pixels (one sees from Fig. B.2 that these components are closely

related to the PSF/threshold training variables from parameter set A). The implication is that residual correlations will cause 2-point clustering correlations to be biased, as the 100A SOM is insufficiently tracing systematic density fluctuations at the pixel-level. However, we also see on the right-hand side in Fig. B.3 that these organised randoms are, in fact, capable of recovering unbiased clustering 2-point functions.

Conversely, when we raise the grid-resolution of our organised randoms (setup 800Ares2 from Table 2), we see that the systematic-density 1-point correlations in Fig. B.4 are almost perfectly corrected (we show systematic-tracers



Fig. B.1. The intrinsic scatter of  $N_{gal} / N_{rand}$  vs. various systematics tracer variables (Table 1), as measured over 100 FLASK realisations with the KiDS-Bright survey parameters/footprint. Without any biases applied to the FLASK realisations, the blue (1 $\sigma$ ) curves give half the difference between the 16<sup>th</sup> and 84<sup>th</sup> percentiles of the distribution of 100 individual  $N_{gal} / N_{rand}$  vs. systematics correlations.  $2\sigma$  (orange) curves give half the difference between the 2.5<sup>th</sup> and 97.5<sup>th</sup> percentiles. Galaxy/random counts and mean-systematics are taken in  $n_{side} = 256$  pixels, about 14 arcmin in size.



Fig. B.2. Linear coefficients, as indicated by the colourbar, describing the transformation of systematic-tracer variable maps into principle component maps, for  $n_{\rm side} = 256$ .

in this figure as they are easier to interpret, and since the component corrections are similarly near-perfect), whilst the 2-point functions reveal a pathological over-correction of the clustering signature. This is because the 800Ares2 randoms are too-closely reproducing the real, cosmic struc-

ture in the data (demonstrated by the unbiased dataorganised randoms cross-correlation, which is at ~ 50% of the unbiased signal), and thus acting to destroy real clustering signals. As such, we restrict our validation of organised randoms to 2-point correlation statistics, which offer insight into potential over-corrections as organised randoms become contaminated by cosmic structure.

#### Appendix C: Data-driven systematics

Fig. C.1 presents additional configurations of the bias: [800A, 100A] / recovery: [100A, 100C] 2-point correlations. As stated in the main text, each meaningful case yields a recovered clustering signal that is more consistent with the unbiased clustering. For bias:800A cases, where the bias is slightly weaker than for bias:800C (Fig. 9) due to the omission of MAG\_LIM\_r, EXTINCTION\_r, gaia\_nstar parameters from training, the performance of organised randoms is similarly strong, and a slight preference for recovery:100A over 100C is negligible with respect to the noise-level (~  $0.1\sigma$ ). When clustering biases are particularly weak, as for the bias:100A case, our methods become more prone to over-correction. Still, the mean absolute deviation from the unbiased case (in units of the standard deviation of the unbiased clustering; summarised for all configurations in Table C.1) is improved in the recovery with respect to the biased case here, primarily due to the success of corrections at smaller values of  $\vartheta$ . We note that the bias:100A case constitutes our most optimistic bias sce-



Fig. B.3. Left: pixel (1-point) correlations between the galaxy number density  $N_{gal}/N_{rand}$  in biased (according to the 800C SOM) FLASK mocks and the mean PCA components in those same pixels (see Appendix B). Correlations normalised by uniform randoms' counts-in-pixels are given in blue, and those normalised (corrected) by the pixel-counts of 100A organised randoms are given in orange. Correlations and errors are the mean, and the root-diagonal of the covariance, over 30 FLASK realisations, respectively. Purple shading indicates the expected, intrinsic  $1\sigma$  spread in these correlations, as calculated over 100 unbiased FLASK realisations (Fig. B.1). Shown here are the 4 (out of 14) correlations for which the organised randoms correction most improves consistency with unity. Right: the corresponding biased/recovered 2-point angular clustering correlations  $w(\vartheta)$ , shown in ratio to (top), and overlaid on (bottom), the unbiased clustering signature, as in Fig. 9. We also show the cross-correlation between organised randoms and the unbiased data, and its ratio to the unbiased clustering signal, in orange. Correlations and errors are again the mean, and the root-diagonal of the covariance, over 30 FLASK realisations, respectively.

nario, having low sensitivity to small- $\vartheta$  (via small  $N_{\rm HC}$ ) and the minimal set of systematic-tracer training variables (psf\_fwhm,psf\_ell,MU\_THRESHOLD) – for more pessimistic scenarios, the organised randoms' performance is consistently improved. As also stated in the text, this bodes extremely well for the potential salvage of unbiased clustering signals from heavily systematics-contaminated data, such as the faint KiDS-1000 shear sample (see Wright et al., in prep.).

#### Appendix D: GAMA comparisons

As discussed in Sec. 2.1, our KiDS-Bright selection is deliberately GAMA-like for the training of photo-*z* estimation (Bilicki et al., in prep.). Thus we might expect a similar clustering signature from KiDS-Bright, but for a reduction in amplitude due to photometric redshift scatter; scattering dis/connected galaxies in/out of each bin will dilute the measurable clustering signals. To replicate this effect in the spectroscopic GAMA sample, we cross-matched GAMA with KiDS-Bright and defined redshift bins using the KiDS ANNZ2 photo-*z*. The resulting 'total' correlations, shown as grey points and shading in the top-panel of Fig. D.1, exceeded even the un-corrected KiDS-Bright correlations in amplitude. We determined that KiDS-Bright is not sufficiently GAMA-like to expect agreement here by re-measuring correlations for *all* KiDS-Bright galaxies in the GAMA window (Fig. D.1; middle-panel), and finding a reduced clustering amplitude which is more consistent with the corrected (by organised randoms) correlation. We measured correlations once more for KiDS-Bright in the GAMA window, now with a flux-limit r < 19.8 applied to KiDS magnitudes<sup>12</sup> (Fig. D.1; bottom-panel), and again see the clustering amplitude rise to exceed all KiDS-Bright signals. We conclude that a comparison with the GAMA auto-clustering signals is not entirely valid for KiDS-Bright, noting also that, with only  $\sim 1/5$  of the KiDS-Bright area, the impacts of increased sample variance in GAMA present further complications.

<sup>&</sup>lt;sup>12</sup> KiDS magnitudes are not equivalent to the Petrosian magnitudes against which GAMA targets were selected, so this fluxlimit is only approximately GAMA-like – see Bilicki et al. (2018).

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Fig. B.4. The same as Fig. B.3, now for bias:800Ares2 / recovery:800Ares2 – *i.e.* the high-resolution setup – and considering systematic-tracers rather than PCA components. One sees that near-perfect 1-point correlation corrections (*left*) are accompanied by the cross-correlation, between unbiased FLASK data and organised randoms (*right;* orange), rising to ~ 50% of the unbiased clustering signature, compared with the negligible cross-correlation in Fig. B.3.



Fig. C.1. The same as Fig. 9, now for some additional bias:SOM / recovery:SOM configurations, as indicated by panel-titles (with reference to Table 2).

**Table C.1.** The relative performance of corrections to angular clustering correlations  $w(\vartheta)$  on the intermediate scales  $7 < \vartheta < 100$  arcmin, for differently configured clustering biases and organised randoms.

bias:SOM	recovery:SOM	biased	recovered
100A	100A	$0.69\sigma$	0.61 $\sigma$
100A	100C	$0.79\sigma$	$0.35\sigma$
100C	100A	$0.94\sigma$	$0.28\sigma$
100C	100C	$0.96\sigma$	$0.54\sigma$
100C(x4)	100C	$12.17\sigma$	$0.34\sigma$
800A	100A	$1.13\sigma$	$0.27\sigma$
800A	100C	$1.19\sigma$	$0.31\sigma$
800Ares2	800Ares2	$7.62\sigma$	$9.58\sigma$
800C	100A	$1.43\sigma$	$0.09\sigma$
800C	100C	$1.48\sigma$	$0.31\sigma$

Notes. With reference to Table 2, the 'bias:SOM' column gives the SOM trained against KiDS-Bright to infer  $\delta_{OR}$  (Eq. 5.3) and inform the density-field bias applied to 30 FLASK realisations of KiDS-Bright-like data; the 'recovery:SOM' column gives the SOM trained against those biased FLASK mocks to produce organised randoms (see Sec. 5.2 for details). On average over the 30 FLASK realisations, the 'biased' and 'recovered' columns then give the absolute deviation from the unbiased signal  $|w_{\text{biased/recovered}} - w_{\text{unbiased}}|$ , in units of the uncertainty in the unbiased signals  $\sigma$ , averaged over the intermediate scales 7-100 arcmin. Non-uniformity of 'biased' column values, with self-similar 'bias:SOM' setups, arises stochastically due to our probabilistic application of biases to FLASK realisations, and all variations are at  $< 0.1\sigma$ . The 800Ares2 configuration illustrates a failure mode of our organised randoms methods, where the resolution and scale-sensitivity of the setup are too high, resulting in over-fitting to cosmic structure and a consequent over-correction of the clustering signal.



Fig. D.1. A comparison of different clustering measurements in the GAMA area, and how they compare with the KiDS-Bright correlations measured with (blue) and without (red) 100A organised randoms. Red/blue data-points are the same in all rows, whilst grey points and shading are the angular clustering measured with uniform randoms for (top) the KiDS-Bright-GAMA cross-matched catalogue, (middle) KiDS-Bright galaxies within the GAMA window, and (bottom) KiDS-Bright galaxies within the GAMA window, and with r < 19.8. Errors are estimated via delete-one jackknifes, from 31 sub-regions of KiDS-Bright, or 20 sub-regions of the GAMA window – errors on scales  $\vartheta \gtrsim 180 \, \rm arcmin$  (the approximate scale of each sub-region) are thus likely to be underestimated for the GAMA-area correlations.