

An assessment of photometric redshift PDF performance in the context of LSST

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ABSTRACT

Photometric redshift (photo- z) probability distribution functions (PDFs) are a key data product of nearly all upcoming galaxy imaging surveys. However, the photo- z PDFs resulting from different techniques are not in general consistent with one another, and an optimal method for obtaining an accurate PDF remains unclear. We present the results of an initial study of the Large Synoptic Survey Telescope Dark Energy Science Collaboration (LSST-DESC), the first in a planned series of papers testing multiple photo- z codes on simulations of upcoming LSST galaxy photometry catalogues. This initial test evaluates photo- z algorithms in the presence of representative training data and in the absence of several common sources of systematic errors that affect the procedures by which photo- z PDFs are derived. The photo- z PDFs are evaluated using multiple metrics including the Kolmogorov-Smirnov statistic, Cramer-von Mises statistic, Anderson-Darling statistic, Kullback-Leibler divergence, $N(z)$ moments, quantile-quantile plots and probability integral transform. We observe several trends, including an overall over/under-prediction in the broadness of the PDFs for several of the codes. A careful accounting of all systematics discovered will be necessary for the codes employed in upcoming analyses in order to achieve unbiased cosmological measurements.

Key words: galaxies: distances and redshifts – galaxies: statistics – methods: statistical

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1 INTRODUCTION

Large-scale photometric galaxy surveys are entering a new era with currently or soon-to-be running Stage III and Stage IV dark energy experiments like the Dark Energy Survey (DES, Abbott et al. 2005), the Kilo-Degree Survey (KiDS, de Jong et al. 2013), Large Synoptic Survey Telescope (LSST, Abell et al. 2009), Euclid (Laureijs et al. 2011), and Wide-Field Infrared Survey Telescope (WFIRST, Green et al. 2012). The move to imaging based surveys, rather than spectroscopic based, for cosmological measurements makes proper understanding of photometric redshifts (“photo- z ’s”) of paramount importance, as cosmological distance measures for statistical samples are directly dependent on photo- z measurements.

The unprecedented sample size of LSST galaxies, expected to number several billion for the main cosmological sample, necessitates stringent constraints on photo- z accuracy if systematic errors are not to dominate the statistical errors. The LSST Science Requirements Document (SRD)¹ lists the photometric redshift goals for a magnitude limited sample with $i < 25$ as: root-mean-square error with a goal of $\sigma_z < 0.02(1+z)$; 3σ “catastrophic outlier” rate below 10%; bias below 0.003².

The tremendous size of LSST’s galaxy catalog will be enabled by its exceptional depth, pushing to fainter magnitudes and deeper imaging and including galaxies of lower luminosity and higher redshift than ever before. In addition to the contribution of low signal-to-noise photometry to the systematic error of photo- z s, these populations introduce major physical degeneracies, for example the Lyman break/Balmer break degeneracy, that were not present in the populations covered in previous large area surveys like the Sloan Digital Sky Survey (SDSS, York et al. 2000) and the Two Micron All Sky Survey (2MASS, Skrutskie et al. 2006). In order to meet LSST’s demanding error budget, it will be necessary to fully characterize those degeneracies wherein multiple redshift solutions have comparable likelihood.

There is often a desire to have a single valued “point-estimate” redshift for an individual galaxy. However, the complex, non-linear (and often non-unique) nature of the mapping between broad band fluxes and redshift means that a single value is unable to capture the full redshift information encoded in a galaxy’s magnitudes. For example, a common point-estimate for a template-based method is taking the highest likelihood solution as the point photo- z . A single valued redshift ignores degenerate redshift solutions of lower probability, potentially biasing photometric redshift estimates both for individual galaxies and ensemble distributions. Storing more information is necessary, most often photo- z codes output the redshift probability density function (PDF), also often referred to as $p(z)$, describing the relative likelihood as a function of redshift. Early template methods such as Fernández-Soto et al. (1999) converted rel-

ative χ^2 values of template spectra to likelihoods to estimate $p(z)$. Soon after, codes such as Benítez (2000) added a Bayesian prior and output a posterior probability distribution. While many early machine learning based algorithms focused on a point-estimate, Firth et al. (2003) used a neural net with 1000 realizations scattered within the photometric errors to estimate a $p(z)$. As more groups began to employ photometric redshifts in their cosmological analyses, realization that point-estimate photo- z ’s were inadequate for precision cosmology measurements (Mandelbaum et al. 2008). From around this point onward, most photo- z algorithms have attempted to implement some estimate of the overall redshift probability in their outputs, and some surveys began supplying a full $p(z)$ rather than a simple redshift point-estimate and error (e. g. de Jong et al. 2017).

There are numerous techniques for deriving photo- z PDFs from photometry, yet no one method has yet been established as clearly superior. Quantitative comparisons of photo- z methods have been made before. The Photo- z Accuracy And Testing (PHAT, Hildebrandt et al. 2010) effort focused on point estimates derived from many photometric bands. DES compared several codes for point estimates (Sánchez et al. 2014) and a summary statistic of photo- z interim posteriors for tomographically binned galaxy subsamples (Bonnett et al. 2016). This paper is distinguished by its inclusion of metrics of photo- z interim posteriors themselves and consideration of both classic and state-of-the-art photo- z algorithms, comparing the performance of several of the most widely employed codes as well as some that have been developed only recently on the basis of metrics appropriate for a probabilistic data product. The results presented in this work are a major focus of the Photometric Redshift working group of the LSST Dark Energy Science Collaboration (LSST-DESC). This work is laid out in the Science Roadmap (SRM)³ as one of the critical activities to be completed in preparation for dark energy science analysis on the first year LSST data. This is the first of multiple papers by the working group, which will grow in sophistication. In this initial paper we focus on evaluating the performance of photometric redshift codes and their ability to produce accurate PDFs in the presence of representative training sets. This can be thought of as an initial test under near perfect conditions, before further complexities are added in future papers. Comparing the relative performance of the codes enables us to evaluate whether each code is using information in an optimal way, and may reveal enhancements in some codes and deficiencies in others, either in the fundamental algorithm, or in specific implementation.

Certain science cases need redshift information on individual objects, e. g. identification of host galaxy redshift for supernova classification, or identifying potential cluster membership. Other science cases need only ensemble redshift information; for instance current weak lensing techniques require the overall redshift distribution $N(z)$ for tomographic redshift samples, but do not need single galaxy estimates. In the case of the multiple types of probes of cosmology enabled by the LSST cosmology sample of several billion galaxies, the number of redshift bins and their photo-

¹ available at <https://docushare.lsstcorp.org/docushare/dsweb/Get/LPM-17>

² Note that at the time the SRD was written, these goals were stated in terms of a photo- z point estimate for each galaxy, as was standard in many previous studies, while in this paper we emphasize the importance of using a full photo- z PDF.

³ Available at: http://lsst-desc.org/sites/default/files/DESC_SRMs_V1_1.pdf

113 z requirements vary with the specific probe; 2-point angular correlations benefit from many bins, while weak lensing 114 probes do not (due to the wide lensing kernel). Large photometric surveys such as LSST must develop algorithms that 115 meet the needs of all such science cases. In order to meet 116 these ambitious goals for photo- z accuracy, every aspect of 117 photo- z estimation will have to be optimized: the algorithms 118 employed, both template and machine-learning based (both 119 in design and implementation); the spectroscopic data used 120 as a training set for machine learning algorithms or to es- 121 timate template sets and train Bayesian priors; and proba- 122 bilistic catalog compression schemes that balance informa- 123 tion retention against limited storage resources. 124

125 Before moving forward, we must address how the best 126 methods may be unique to the performance metrics and sci- 127 ence cases considered and what distinguishes photo- z PDFs 128 of different methods from one another. Though photo- z 129 PDFs are often written simply as $p(z)$, the PDF itself must 130 be an interim posterior distribution $p(z|d, I)$, the probability 131 of redshift conditioned on photometric data d that has actu- 132 ally been observed and the prior information I that guides 133 how a redshift is extracted from the photometry. If we run 134 multiple photo- z codes on a single dataset, the photo- z in- 135 terim posteriors will not be identical because each code is 136 based on assumptions in the form of an interim prior — 137 these assumptions form the premise for photo- z estimation 138 as a whole and are the only way to introduce differences in 139 estimates of what would otherwise be a shared photo- z pos- 140 terior $p(z|d)$ regardless of the code used to obtain it. Though 141 explicit knowledge of the interim prior is necessary to use 142 photo- z interim posteriors self-consistently in physical infer- 143 ence, the interim prior of a particular methodology is often 144 implicit and not necessarily shared among all galaxies in the 145 catalog.

146 This paper therefore aims (1) to constrain the impact of 147 the interim prior I by separating it into a component I_H rep- 148 resenting the method itself and a component I_D representing 149 physical information, such as a training set or SED template 150 library and (2) to present a procedure for evaluating the 151 performance of photo- z codes in generic tests that may include 152 many more systematics in the interim prior I . In order to 153 isolate the effects encapsulated by I_H of variation between 154 codes from issues with the training set or template library 155 encapsulated by I_D , we use an identical set of simulated 156 galaxies for every code and construct a template library 157 and training sample that are *complete and representative* 158 and shared among all codes; that is, our training sample for 159 machine learning codes is drawn from the same underlying 160 galaxy population as our test set, with no additional selec- 161 tions, and the SED library used for template-based codes is 162 the same as the one used to generate the photometric data. 163 We explore a number of performance metrics in this paper, 164 not to make a conclusion regarding the superiority or even 165 relative favorability of each code but to establish a method 166 for comparing photo- z PDFs derived by different methods. 167 These test conditions set the stage for addressing in a future 168 paper the crucial issue of incomplete and non-representative 169 prior information. 170

171 The outline of the paper is as follows: in § 2 we present 172 the simulated data set; in § 3 we describe the current genera- 173 tion codes employed in the paper; in § 4 we discuss the inter- 174 pretation of photo- z PDFs in terms of metrics of accuracy;

175 in § 5 we show our results and compare the performance of 176 the codes; in § 6 we offer our conclusions and discuss future 177 extensions of this work.

178 2 THE SIMULATION AND MOCK GALAXY CATALOG

180 In order to test the current generation codes, we employ 181 a simulated galaxy catalogue. The simulation is completely 182 catalogue-based, with no image construction or mock mea- 183 surements made. We describe these in detail below.

184 2.1 Buzzard-v1.0 simulation

185 The BUZZARD-HIGHRES-V1.0 186 put in cites to in prep 187 Buzzard 188 papers catalogue construction started with a dark matter 189 only simulation. This N-body simulation contained 2048^3 190 particles in a 400 Mpc h^{-1} box. 191 [N] snapshots (with smooth- 192 ing and interpolation between snapshots) were saved in 193 order to construct a lightcone. Dark matter halos were identi- 194 fied using the ROCKSTAR software package (195 Behroozi et al. 196 2013). These dark matter halos were populated with galax- 197 ies with a stellar mass and absolute r -band magnitude in 198 the SDSS system determined using a sub-halo abundance 199 matching model constrained to match both projected two- 200 point galaxy clustering statistics and an observed condi- 201 tional stellar mass function (202 Reddick et al. 203 2013).

202 To assign an SED to each galaxy, the *Adding Den- 203 sity Dependent Spectral Energy Distributions* (ADDSEDS, 204 deRose in prep.)⁴ procedure was used. This consisted of 205 training an empirical relation between absolute r -band mag- 206 nitude, local galaxy density, and SED using a sample of 207 $\sim 5e^5$ galaxies from the magnitude-limited Sloan Digital 208 Sky Survey Data Release 6 Value Added Galaxy Catalog 209 (210 Blanton et al. 211 2005)[Note: is this the proper reference to 212 SDSS-NYU VAGC? File is called combined_dr6.cooper.fits, 213 but I don't see which Cooper et al 2006 this is supposed 214 to refer to?]. Each SDSS spectrum is fit with a sum of five 215 SED components using the K-CORRECT v?216 software pack- 217 age⁵ (218 Blanton & Roweis 219 2007), thus each galaxy SED is 220 parameterized as five weights for the basis SEDs. The distance 221 to the spatial projected fifth-nearest neighbour was used as a 222 proxy for local density in the SDSS training sample. For each 223 simulated galaxy, a “random” 224 [details] galaxy with “similar” 225 [details] absolute r -band magnitude and local galaxy density 226 was chosen from the training set, and that training galaxy’s 227 SED was assigned to the simulated galaxy. Given the SED, 228 absolute r -band magnitude and redshift, we computed ap- 229 parent magnitudes in the six LSST filter passbands, $ugrizy$. 230 We assigned magnitude errors in the six bands using the 231 simple model described in 232 Ivezić et al. (2008), assuming full 233 10-year depth observations had been completed. The num- 234 ber of total 30-second visits assumed when generating the 235 photometric errors differs slightly from the fiducial numbers 236 assumed for LSST: we assume 60 visits in u-band, 80 vis- 237 its in g-band, 180 visits in r-band, 180 visits in i-band, 160 238 visits in z-band, and 160 visits in y-band.

239 ⁴ <https://github.com/vipasu/addseds>

240 ⁵ <http://kcorrect.org>

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228 2.1.1 Selection of training and test sets

229 The total catalogue covered 400 square degrees and con-
 230 tained 238 million galaxies to an apparent magnitude limit
 231 of $r = 29$ and spanning the redshift range $0 < z \leq 8.7$. This
 232 catalogue contained two orders of magnitude more galaxies
 233 than were needed for this study, so only ~ 8 square degrees
 234 were used. Systematic problems with galaxy colors above
 235 $z > 2$ were observed, so the catalogue was trimmed to in-
 236 clude only galaxies in the redshift range $0 < z \leq 2.0$. A
 237 random subset of the the remaining galaxies was chosen,
 238 and placed at random into either a “training” set (10 per
 239 cent of the sample), for which the galaxies true redshifts
 240 will be supplied, or a “test” set (the remaining 90 per cent
 241 of the sample), for which each code will need to predict a
 242 redshift PDF for each galaxy. The resulting catalogues con-
 243 tain 111 171 training galaxies and 1 000 883 test galaxies. We
 244 restrict our analysis to a sample with $i < 25.3$, which give a
 245 signal-to-noise ~ 30 for most galaxies, a cut often referred
 246 to as the expected “LSST Gold Sample”. This magnitude
 247 cut results in a training set with 44 404 galaxies and a test
 248 set containing 399 356 galaxies. All subsequent results will
 249 evaluate this “gold sample” test set.

250 2.1.2 Templates

251 As mentioned in Section 2.1, the SEDs in the Buzzard sim-
 252 ulation are drawn from an empirical set of SEDs taken from
 253 the SDSS DR6 NYU-VAGC, a sample of roughly $\sim 5e^5$
 254 galaxies with spectra in SDSS. To determine a finite set of
 255 templates to use with template fitting codes we take the five
 256 SED weight coefficients for each of the $\sim 500\,000$ galaxies in
 257 the SDSS sample and run a simple K-means clustering algo-
 258 rithm on this five dimensional space. The K-means cluster
 259 centres span the space of coefficients and properly reflect the
 260 underlying density in the coefficient space, thus providing a
 261 reasonable approximation for a spanning SED set. An ad-
 262 hoc number of $K = 100$ was chosen and the 100 K-means
 263 centre positions are taken as the weights for the K-CORRECT
 264 SED components to construct one hundred template SEDs.
 265 These 100 templates were provided, however not every tem-
 266 plate code uses this set of one hundred templates: because
 267 EAZY was designed and written to use the same five basis
 268 templates employed by K-CORRECT when constructing our
 269 mock galaxies, EAZY was run using linear combinations of
 270 these five templates rather than using the 100 discrete tem-
 271 plates.

272 2.1.3 Limitations

273 For our initial investigation of photometric redshift codes,
 274 we begin with a data set that is somewhat idealized, and
 275 does not contain all of the complicating factors present in
 276 real data. In several cases, the simplification is done with
 277 a purpose, with potentially confounding effects excluded
 278 in order to better isolate the differences between current-
 279 generation photo- z codes, and their causes. We list several
 280 of the simulations limitations in this section. As the sim-
 281 ulation is catalogue-based, no image level effects, such as
 282 photometric measurement effects, object blending, contami-
 283 nation from sky background (Zodiacal light, scattered light,

284 etc...), lensing magnification, or Galactic reddening are in-
 285 cluded. No stars are included in the catalogue, nor are the
 286 effects of AGN. As all SEDs are constructed from only five
 287 basis templates, properties of the galaxy population will be
 288 restricted to follow linear combinations of the characteristics
 289 of the five basis templates, so certain non-linear features, for
 290 example the full range of emission line fluxes relative to the
 291 continuum, will not be included in the model galaxy pop-
 292 ulation. No additional dust reddening intrinsic to the host
 293 galaxy is included, the only approximation of dust extinc-
 294 tion comes in the form of dust encoded in the five basis SEDs
 295 via the training set used to create the basis templates. Sim-
 296 ple linear combinations of these basis templats will, once
 297 again, not explore the full range of realistic dust extinction
 298 observed in galaxy populations.

299 3 METHODS

300 Here we outline the photo- z PDF codes tested in this study.
 301 In total, eleven distinct codes are tested. This sample is not
 302 comprehensive, but does cover a broad range of current-
 303 generation codes. Both template-based and machine learn-
 304 ing approaches are included and each are described sepa-
 305 rately in Secs. 3.1 and 3.2 respectively. The list of codes are
 306 summarized in Table. 1.

307 The questions that must be answered for each code are:
 308 what unique features are included in the specific implemen-
 309 tation that influence the output $p(z)$. What form of valida-
 310 tion was performed with the training data, how were pho-
 311 tomometric uncertainties employed in the analysis, how were
 312 negative fluxes treated, what specific prior form was em-
 313 ployed (for template based codes), or what specific machine
 314 learning architeture was used (for ML codes)?

315 3.1 Template-based Approaches

316 3.1.1 BPZ

317 BPZ⁶ (Bayesian Photometric Redshift, Benítez 2000) is a
 318 template-based photo- z code that compares the expected
 319 colors (C) calculated for a set of spectral energy distribution
 320 (SED) types/templates (T) to the observed colors to calcu-
 321 late the likelihood of observing colors at each redshift for
 322 each type, $p(C|z, T)$. The code employs an empirically deter-
 323 mined Bayesian prior in apparent magnitude (m_0) and SED-
 324 type. Assuming that the SED-types are spanning and exclu-
 325 sive, we can determine the redshift posterior $p(z|C, m_0)$ by
 326 marginalizing over all SED-types with a simple sum (Eq. 3
 327 from Benítez 2000):

$$328 p(z|C, m_0) \propto \sum_T p(z, T|m_0) p(C|z, T) \quad (1)$$

329 where the first term on the right-hand side is the Bayesian
 330 prior and the second term is the traditional likelihood.
 331 The prior is assumed to have the form: $p(z, T|m_0) =$
 332 $p(T|m_0) p(z|T, m_0)$, i.e. it parameterizes the prior as an
 333 evolving type fraction with apparent magnitude, combined

6 <http://www.stsci.edu/~dcoe/BPZ/>

Table 1. List of photo-z codes featured in this study. ML here means machine learning.

Code	Type	Paper	Website
BPZ	template	Benítez (2000)	http://www.stsci.edu/~dcoe/BPZ/
EAZY	template	Brammer et al. (2008)	https://github.com/gbrammer/eazy-photoz
LePHARE	template	Arnouts et al. (1999)	http://www.cfht.hawaii.edu/~arnouts/lephare.html
ANNz2	ML	Sadeh et al. (2016)	https://github.com/IftachSadeh/ANNz2
DELIGHT	ML/template	Leistedt & Hogg (2017)	https://github.com/ixkael/Delight
FLEXZBOOST	ML	Izbicki & Lee (2017)	https://github.com/tospisici/flexcode; https://github.com/rizbicki/FlexCoDE
GPz	ML	Almosallam et al. (2016b)	https://github.com/OxfordML/GPz
METAPhOR	ML	Cavuoti et al. (2017a)	http://dame.dsfa.unina.it
CMNN	ML	Graham et al. (2018)	-
SKYNET	ML	Graff et al. (2014)	http://ccpforge.cse.rl.ac.uk/gf/project/skynet/
TPZ	ML	Carrasco Kind & Brunner (2013)	https://github.com/mgckind/MLZ
TRAINZ	N/A	See Section 3.3	

with a prior on the expected redshift probability distribution as a function of both apparent magnitude and SED-type.

In this paper we use BPZ v 1.99.3. The template set employed here is the set of 100 discrete SEDs described in Section 2.1.2 To keep the number of free parameters to a manageable level the SEDs in the training set are sorted by the rest-frame $u-g$ colour and split into three “broad” SED classes, equivalent to the E, Sp and Im/SB types in Benítez (2000). We assume the same functional form for the Bayesian priors as used by Benítez (2000), and utilize the training-set galaxies with known SED-type, redshift, and apparent magnitude to determine the type fractions and the best fit for the eleven free parameters of the prior. For galaxies with negative flux in a measured band, the placeholder value is replaced with an estimate one σ detection limit in that particular band, i. e. a value close to the estimated sky noise threshold. The type-marginalized $p(z)$ is generated by setting the parameter PROBS_LITE=TRUE in the BPZ parameter file.

3.1.2 EAZY

EAZY⁷ (Easy and Accurate Photometric Redshifts from Yale, Brammer et al. 2008) is a template-based photo-z code that includes several features that improve on the basic χ^2 fit used in many template codes. It can fit the observed photometry with SEDs created from a linear combination of a set of templates at each redshift, and the best-fit SED is found by simultaneously fitting one, two or all of the templates by minimizing χ^2 . The minimized $\chi^2(z)$ is then combined with an apparent magnitude prior to obtain the posterior redshift probability distribution, although some argue that this is not the mathematically correct way of calculating the posteriors. EAZY can also account for the uncertainties in the templates by adding an empirically derived template error in quadrature as a function of redshift to the flux errors.

In this paper we use the all-templates mode, which fits the photometric data with a linear combination of the five basis templates. We employed the 5 basis templates described in Section 2.1, and set the template error to zero

since these same templates were used to produce the simulated catalog photometry. The likelihoods are calculated on a 200-point redshift grid spanning $0 \leq z \leq 2$, and include the application of a type-independent apparent magnitude prior estimated from the training data.

3.1.3 LePhare

LEPHARE⁸ (Photometric Analysis for Redshift Estimate, Arnouts et al. 1999; Ilbert et al. 2006) is a photo-z reconstruction code based on a χ^2 template-fitting procedure. The observed colors are matched with the colours predicted from a set of spectral energy distribution (SED) which can be either synthetic or based on a semi-empirical approach. LEPHARE has been used to produce the COSMOS2015 photo-z catalogue (Laigle et al. 2016).

Each SED is redshifted in steps of $\Delta z = 0.01$ and convolved with the simulated LSST filter transmission curves (accounting for instrument efficiency). The opacity of the inter-galactic medium has been set to zero as no additional reddening has been included in the Buzzard simulations. The computed photo-z is then the value that minimizes the merit function $\chi^2(z, T, A)$ from Arnouts et al. (1999):

$$\chi^2(z, T, A) = \sum_f^{N_f} \left(\frac{F_{\text{obs}}^f A \times F_{\text{pred}}^f(T, z)}{\sigma_{\text{obs}}^f} \right)^2 \quad (2)$$

where A is a normalization factor, $F_{\text{pred}}^f(T, z)$ is the flux predicted for a template T at redshift z . F_{obs}^f is the observed flux in a given band f and σ_{obs}^f the associated observational error. The index f refers to the considered band and N_f is the total number of filters.

In this paper we use LEPHARE v 2.2. The set of templates used for fitting the photo-z’s are the 100 discrete Buzzard SED templates as described in section 2.1.2. The full $p(z)$ corresponds to the likelihoods calculated at each point on our z -grid.

⁷ <https://github.com/gbrammer/eazy-photoz>

⁸ <http://www.cfht.hawaii.edu/~arnouts/lephare.html>

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3.2 Training-based Codes

3.2.1 ANNz2

ANNz2⁹ (Sadeh et al. 2016) is a powerful package that has the ability to employ several machine learning algorithms, including artificial neural networks (ANN), boosted decision tree (BDT) and k-nearest neighbour (KNN). Using the Toolkit for Multivariate Data Analysis (TMVA) with ROOT¹⁰, it can run multiple machine learning algorithms for a single training and outputs photo- z 's based on a weighted average of their performances.

ANNz2 is capable of producing both photo- z point estimates and redshift posterior probability distributions $p(z)$, it could also conduct classifications and supports reweighting between samples. The PDFs are produced by propagating the intrinsic uncertainty on the input parameters and the uncertainty in the machine learning method to the expected photo- z solution, averaged over multiple runs weighted based on the performance of each run. ANNz2 presents its photo- z uncertainty different from many codes by using the KNN method: it estimates the photo- z bias between each object and a fixed number of nearest neighbours in parameter space, it then takes the 68th percentile width of the distribution of the bias. This is based on the implication that objects with similar photometric properties would have similar uncertainties, and therefore the photometric errors of the inputs are not propagated into the code.

In this study, ANNz2 v. 2.0.4 was used. The full PDF for each galaxy is also produced with a linear stepsize of $z = 0.01$ for $0 \leq z \leq 2$. A set of 5 ANNs with architecture $6 : 12 : 12 : 1$ ($6 ugrizy$ inputs, 2 hidden layers with 12 nodes each, and 1 output) with different random seeds are used during each training. Half of the training set is used as a validation set to prevent overtraining. All training objects are set to have detected magnitudes, however the non-detections ($\text{mag} = -99$) in the testing set are replaced with the mean of that particular band.

3.2.2 Color-Matched Nearest-Neighbours

The nearest-neighbours color-matching photometric redshift estimator (CMNN) is presented in (Graham et al. 2018, hereafter G18). This method uses a training set of galaxies with known redshifts that has equivalent or better photometry as the test set in terms of quality and filter coverage. For each galaxy in the test set we identify a color-matched subset of training galaxies, choose one (e.g. the nearest-neighbour or a random selection), and use its known redshift as the photo- z . This color-matched subset is identified by first calculating the Mahalanobis distance D_M in color-space between the test galaxy and all training-set galaxies: the difference between the test and a training set galaxy's color divided by the photometric error, summed over all colors (i.e., $u-g$, $g-r$, $r-i$, $i-z$, and $z-y$). Then, the threshold value for D_M that define a good color match is set by the percent point function (PPF): for example, for $N_{\text{dof}} = 5$, PPF= 95 per cent of all training galaxies consistent with the test galaxy will have $D_M < 11.07$ (where N_{dof} , the number of degrees of

freedom, is the number of colors). For a given test galaxy, the $p(z)$ is the normalized distribution of the true catalogue redshifts of this color-matched subset of training galaxies, and the standard deviation of the color-matched subset is used as the photo- z uncertainty.

We have applied the nearest-neighbours color-matching photometric redshift estimator described in G18 to the simulated data. Compared to its application in G18, there are some minor differences in the application of this estimator to the Buzzard catalogue. First, we do not impose non-detections on galaxies with a magnitude fainter than the expected LSST 10-year limiting magnitude or bright enough to saturate with LSST: *all* of the photometry for all the galaxies in the test and training sets are used for this experiment. Second, as in G18 we do apply an initial cut in color to the training set before calculating the Mahalanobis distance in order to accelerate processing, and also use a magnitude pseudo-prior to improve photo- z estimates, but for both we have used different cut-off values that are appropriate for the Buzzard galaxies' colors and magnitudes. Third, we set different parameters for the identification of the color-matched subset of training galaxies and the selection of a photometric redshift estimate. In G18 we used a percent point function (PPF) value of 0.68 to identify the color-matched subset of training galaxies and used the redshift of nearest neighbour in color-space as the photo- z estimate. These choices work well when the desire is to obtain accurate photo- z estimates for most test-set galaxies, but does not return a robust $p(z)$ in all cases – especially for galaxies that are bright and/or have few matches in color-space. Since a robust estimate of $p(z)$ is desired for this work we make several changes to our implementation of the CMNN photo- z estimator. We continue to use a percent point function of PPF = 0.95 to generate the subset of color-matched training galaxies, but weight them by the inverse of their Mahalanobis distance. This weighting maintains some of the accuracy that was previously achieved by simply using the nearest neighbour in color-space. We then use the weights to create the $p(z)$ instead of having the redshift of each color-matched training-set galaxy count equally. To obtain a robust estimate of the $p(z)$ for galaxies with a small number of color-matched training set galaxies, when this number is less than 20 the nearest 20 neighbours in color-space are used instead, and we convolve the $p(z)$ with a Gaussian with a standard deviation of:

$$504 \quad \sigma = \sigma_{\text{train}} \sqrt{(\text{PPF}_{20}/0.95)^2 - 1} \quad (3)$$

to appropriately broaden it so that the $p(z)$ for these test galaxies represents the enlarged PPF value associated with it. Overall, these three changes will yield poorer accuracy photo- z compared to those presented in G18, but they will all have significantly more robust estimates of the $p(z)$, particularly for the brightest test galaxies. This is sufficient for this work because, as described in G18, the goal of the CMNN photo- z estimator was never to provide the “best” (or even competitive) estimates in the first place, given its reliance on a deep training set, but rather to provide a means for direct comparisons between LSST photometric quality and photo- z estimates. With this work we show how the input parameters should be set in order to return robust $p(z)$ estimates in addition to point value estimates.

⁹ <https://github.com/IftachSadeh/ANNZ>

¹⁰ <http://tmva.sourceforge.net/>

519 3.2.3 Delight

520 DELIGHT¹¹ (Leistedt & Hogg 2017) infers photo-z’s by using
 521 a data-driven model of latent SEDs and a physical model
 522 of photometric fluxes as a function of redshift. Generally,
 523 machine learning methods rely on representative training
 524 data with similar band passes, while template based meth-
 525 ods rely on a complete library of templates based on physi-
 526 cal models constructed. DELIGHT is constructed in attempt
 527 to combine the advantages and eliminate the disadvantages
 528 of both template-based and machine learning algorithms: it
 529 constructs a large collection of latent SED templates (or
 530 physical flux-redshift models) from training data, with a
 531 template SED library as a guide to the learning of the model.
 532 The advantage of DELIGHT is that it neither needs represen-
 533 tative training data in the same photometric bands, nor does
 534 it need detailed galaxy SED models to work.

535 This conceptually novel approach is done by using
 536 Gaussian processes operating in flux-redshift space. The pos-
 537 terior distribution on the redshift of a target galaxy is ob-
 538 tained via a pairwise comparison with training galaxies,

$$539 p(z|\hat{\mathbf{F}}) \approx \sum_i p(\hat{\mathbf{F}}|z, t_i) p(z|t_i) p(t_i), \quad (4)$$

540 where $p(z|t_i)p(t_i)$ captures prior information about the red-
 541 shift distributions and abundances of the galaxies, with t_i
 542 denoting the galaxy template; while $p(\hat{\mathbf{F}}|z, t_i)$ is the poste-
 543 rior of noisy flux $\hat{\mathbf{F}}$ at redshift z . For each training-target
 544 pair, $p(\hat{\mathbf{F}}|z, t_i)$ is evaluated as follows:

$$545 p(\hat{\mathbf{F}}|z, t_i) = \int p(\hat{\mathbf{F}}|\mathbf{F}) p(\mathbf{F}|z, z_i, \hat{\mathbf{F}}_i) d\mathbf{F}, \quad (5)$$

546 where $p(\hat{\mathbf{F}}|\mathbf{F})$ is the likelihood function, it compares the
 547 noisy real flux $\hat{\mathbf{F}}$ with the noiseless flux \mathbf{F} obtained from the
 548 linear combination of template models, carefully constructed
 549 to account for model uncertainties and different normaliza-
 550 tion of the same SED; while $p(\mathbf{F}|z, z_i, \hat{\mathbf{F}}_i)$ is the prediction
 551 of flux at a different redshift z with respect to the training
 552 object with redshift z_i and flux $\hat{\mathbf{F}}_i$. Eq. 5 is essentially the
 553 probability that the training and the target galaxies having
 554 the same SED but at a different redshift. The flux prediction
 555 $p(\mathbf{F}|z, z_i, \hat{\mathbf{F}}_i)$ of the training galaxy at redshift z is modeled
 556 via a Gaussian process,

$$557 F_b \sim \mathcal{GP}(\mu^F, k^F), \quad (6)$$

558 with mean function μ^F and kernel k^F , both imposed to
 559 capture expected correlations resulting from the known un-
 560 derlying physics (i.e., fluxes resulting from observing SEDs
 561 through filter response, and the SEDs being redshifted). The
 562 reader should refer to Leistedt & Hogg (2017) for further de-
 563 tails.

564 In this study, all 100 ordered Buzzard templates, as
 565 described in Section 2.1.2, were used in DELIGHT, and the
 566 Gaussian process was trained with a subset of 50 000 galaxies.
 567 Photometric uncertainties from the inputs are propa-
 568 gated into the code, while non-detections for each band are
 569 set to the mean of the respective bands. Default settings

570 of DELIGHT were use, with the exception that the PDF bins
 571 were set to be linear instead of logarithmic, with 200 equally-
 572 spaced bins between $0.0 < z < 2.0$. In this study a flat prior
 573 is assumed.

574 3.2.4 FlexZBoost

575 FLEXZBOOST¹² (Izbicki & Lee 2017) is a particular realiza-
 576 tion of FlexCode, which is a general-purpose methodology
 577 for converting any conditional mean point estimator of z to
 578 a conditional density estimator $f(z|\mathbf{x})$, where \mathbf{x} here repre-
 579 sents our photometric covariates and errors.¹³ The key idea
 580 is to expand the unknown function $f(z|\mathbf{x})$ in an orthonormal
 581 basis $\{\phi_i(z)\}_i$:

$$582 f(z|\mathbf{x}) = \sum_i \beta_i(\mathbf{x}) \phi_i(z). \quad (7)$$

583 By the orthogonality property, the expansion coefficients are
 584 just conditional means

$$585 \beta_i(\mathbf{x}) = \mathbb{E}[\phi_i(z)|\mathbf{x}] \equiv \int f(z|\mathbf{x}) \phi_i(z) dz. \quad (8)$$

586 These coefficients can easily be estimated from data by re-
 587 gression.

588 In this paper, we use XGBOOST (Chen & Guestrin 2016)
 589 for the regression part as these techniques scale well for mas-
 590 sive data; it should however be noted that FLEXCODE-RF
 591 (also on GitHub), based on Random Forests, generally per-
 592 forms better for smaller data sets. As our basis, we choose a
 593 standard Fourier basis. There are two tuning parameters in
 594 our $p(z)$ estimate: (i) the number of terms, I , in the series
 595 expansion in Eq. 7, and (ii) an exponent α that we use to
 596 sharpen the computed density estimates $\hat{f}(z|\mathbf{x})$, according
 597 to $\tilde{f}(z|\mathbf{x}) \propto \hat{f}(z|\mathbf{x})^\alpha$. We split the “train data” into a train-
 598 ing set (85%) and a validation set (15%), and choose both I
 599 and α in an automated way by minimizing the weighted L_2 -
 600 loss function (Eq. 5 in Izbicki & Lee 2017) on the validation
 601 set.

602 Although FlexCode offers a *lossless compression* of the
 603 photo-z estimates (in this study, one can reconstruct $\tilde{f}(z|\mathbf{x})$
 604 exactly at any resolution from estimates of the first 35 co-
 605 efficients, Eq. 8, for a Fourier basis $\{\phi_i(z)\}_i$), we discretize
 606 our final estimates into 200 bins linearly spaced in $0 < z < 2$
 607 for easy comparison with other algorithms. Using a higher
 608 resolution may yield better results (with no added cost in
 609 storage).

610 3.2.5 GPz

611 GPz¹⁴ (Almosallam et al. 2016a,b) is a sparse Gaussian pro-
 612 cess based code, a fast and a scalable approximation of full
 613 Gaussian Processes (Rasmussen & Williams 2006), with the
 614 added feature of being able to produce input-dependent vari-
 615 ance estimations (heteroscedastic noise). The model assumes

¹² <https://github.com/tpospisi/flexcode>;
<https://github.com/rizbicki/FlexCoDE>

¹³ Instead of $p(z)$, we use the notation $f(z|\mathbf{x})$ to explicitly show the dependence on \mathbf{x} .

¹⁴ <https://github.com/OxfordML/GPz>

¹¹ <https://github.com/ixkael/Delight>

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that the probability of the output y , the redshift, given the input x , the photometry, is $p(y|x) = \mathcal{N}(y|\mu(x), \sigma(x)^2)$. The mean function, $\mu(x)$, and the variance function $\sigma(x)^2$ are both linear combinations of basis functions that take the following form:

$$f(x) = \sum_{i=1}^m \phi_i(x) w_i, \quad (9)$$

where $\{\phi_i(x)\}_{i=1}^m$ and $\{w_i\}_{i=1}^m$ are sets of m basis functions and their associated weights respectively. Basis function models (BFM), for specific classes of basis functions such as the sigmoid or the squared exponential, have the advantage of being universal approximators, i.e. there exist a function of that form that can approximate any function, with mild assumptions, to any desired degree of accuracy. The details on how to learn the parameters of the model and the hyper-parameters of the basis functions are described in Almosallam et al. (2016b).

A unique feature in GPz, is that the variance estimate is composed of two terms each quantifying a different source of uncertainty. One term (the model uncertainty) reflects how much of the uncertainty is due to lack of training samples at the location of interest, whereas the second term (the noise uncertainty) reflects how much of the uncertainty is caused from observing many noisy samples at that location. Thus, the predictive variance can determine whether we need more representative samples or more precise samples for any particular location in the input space. GPz can also emphasize the importance of some samples as weights. This weight can be for example $|z_{\text{spec}} - z_{\text{phot}}|/(1 + z_{\text{spec}})$ to target the desired objective of minimizing the normalized redshift error or as a function of their probability in the test set relative to the training set in order to pressure the model to better fit samples that are rare in the training set but are expected to be abundant during testing.

The data is prepared for GPz by taking the log of the magnitude errors, decorrelating the data set using PCA and imputing the missing values using a simple linear model that estimates the missing variables given the observed ones. The log transformation helps to smooth the long tail distribution of the magnitude errors, which is more stable numerically and makes the optimization process unconstrained. The missing values are imputed by computing the mean of the training set μ and its covariance Σ , then we use the following equation to estimate the missing values from the observed ones

$$x_u = \mu_u + \Sigma_{uo} \Sigma_{oo}^{-1} (x_o - \mu_o), \quad (10)$$

where the subscript o in x_o indexes the *observed* part of the input x , whereas the subscript u indexes the *unobserved* set (similarly for μ and Σ). This is the optimal expected value of the unobserved variables given the observed ones if the distribution is jointly Gaussian, note that if the variables are independent, i.e. $\Sigma_{uo} = 0$, this will reduce to a simple average predictor.

We use the Variable Covariance (VC) option in GPz with 200 basis functions after we note that there is no significant increase in the performance on the validation set (using 80%-20% training-validation split) and with no cost-sensitive learning applied.

3.2.6 METAPhOR

METAPHOR (Machine-learning Estimation Tool for Accurate Photometric Redshifts, Cavuoti et al. 2017a) is a pipeline designed to provide photo-z's point estimates and a reliable PDF for machine learning (ML) based techniques. It includes pre- and post-processing phases, hosting a photo-z prediction engine based on the Multi Layer Perceptron with Quasi Newton Algorithm (MLPQNA), already validated on photo-z's in several cases (de Jong et al. 2017; Cavuoti et al. 2017b, 2015; Brescia et al. 2014, 2013; Biviano et al. 2013). Due to its plug-in based modular nature, METAPHOR can be easily replaced by any other photo-z prediction kernel, regardless its implementation, by taking the I/O interface compliance as unique constrain.

At a higher level, the pipeline mainly consists of three modules: (i) *data pre-processing*, including a catalogue cross-matching sub-module (based on the tool C3, Riccio et al. 2017), a sub-module for photometric evaluation and error estimation of the multi-band catalogue used as Knowledge Base (KB), and a sub-module dedicated to the perturbation of the photometric KB, propaedeutic to the PDF estimation; (ii) *photo-z prediction*, which is the training/validation/test phase, producing the photo-z's point estimates, based on a pre-selected ML method; (iii) *PDF estimation*, specifically designed to calculate the PDF of the photo-z estimation errors. The last module includes also a post-processing tool, providing some statistics on the produced point estimates and PDFs.

The photometry perturbation law is based on the formula $m_{ij} = m_{ij} + \alpha_i F_{ij} * u_{\mu=0, \sigma=1}$, where α_i is a user selected multiplicative constant (useful in case of multi-survey photometry), $u_{\mu=0, \sigma=1}$ is a random value from the standard normal distribution and F_{ij} is a bimodal function (a constant function + polynomial fitting of the mean magnitude errors on the binned bands), heuristically tuned in such a way that the constant component is the threshold under which the polynomial function is considered too low to provide a significant noise contribution to the photometry perturbation.

As introduced, the photo-z point estimate prediction engine of METAPHOR is based on the MLPQNA model, whose photo-z regression training error, used by the quasi Newton learning rule, is based on the least square error and Tikhonov L_2 -norm regularization (Hofmann & Mathé 2018).

As main prerogative, METAPHOR is able to provide a PDF for ML methods by taking into account the photometric errors provided with data, by running N trainings on the same training set, or M trainings on M different random extractions from the KB. The different test sets, used to produce the PDF, are thus obtained by introducing a proper perturbation, parametrized from the photometric error distribution in each band, on the photometric data populating the original test set (Brescia et al. 2018).

For the present work since it was required to produce a redshift (and a PDF) for each object of the test set we decided to apply a hierarchical kNN to fill the missing detection, it goes without saying that for such points the reliability of PDFs and point estimation is lower. No cross validation has been used.

733 3.2.7 *SkyNet*

734 SKYNET¹⁵ (Graff et al. 2014) is a publicly available neural
 735 network software, based on a 2nd order conjugate gradient
 736 optimization scheme (see Graff et al. 2014, for further de-
 737 tails). It has been used efficiently for redshift PDF estimates
 738 (Sánchez et al. 2014; Bonnett 2015; Bonnett et al. 2016).

739 The neural network is configured as a standard multi-
 740 layer perceptron with three hidden layers and one input layer
 741 with 12 nodes (the 6 magnitudes and their errors). The clas-
 742 sifier is laid out such that the hidden layers have 20:40:40
 743 nodes each, all rectified linear units, and the output layer
 744 has 200 nodes (corresponding to 200 bins for the PDF) acti-
 745 vated with a “softmax” function so that they automatically
 746 sum to 1.

747 To avoid over-fitting, a 30 per cent fraction of the train-
 748 ing set is used as validation, and the training is stopped as
 749 soon as the error rate begins to increase in the validation
 750 set. The weights are randomly initialized based on normal
 751 sampling. The error function is a standard chi-square func-
 752 tion for the regressor, and a cross-entropy function for the
 753 classifier. Finally, the data are all whitened before process-
 754 ing, with magnitudes pegged to (45,45,40,35,42,42) and their
 755 errors pegged to (20,20,10,5,15,15) for *ugrizy* filters, respec-
 756 tively.

757 3.2.8 *TPZ*

758 TPZ¹⁶ (Trees for Photo-*z*, Carrasco Kind & Brunner 2013;
 759 Carrasco Kind & Brunner 2014) is a parallel machine learning
 760 algorithm that generates photometric redshift PDFs us-
 761 ing prediction trees and random forest techniques. The code
 762 recursively splits the input data (i. e. the training sample),
 763 into two branches, one after another, until a terminal leaf is
 764 created that meets a termination criterion (e. g. a minimum
 765 leaf size or a variance threshold). Bootstrap samples from
 766 the training data and associated errors are used to build a
 767 set of prediction trees. In order to minimize correlation be-
 768 tween the trees, the data is divided in such a way that the
 769 highest information gain among the random subsample of
 770 features is obtained at every point. The regions in each ter-
 771 minal leaf node corresponds to a specific subsample of the
 772 entire data that possesses similar properties.

773 The training data is examined before running TPZ.
 774 Since TPZ does not handle non-detections (magnitudes
 775 flagged as 99.0), we replace these values with an approxi-
 776 mation of the 1σ detection threshold, i. e. a signal to noise
 777 ratio of 1 in terms of magnitude uncertainty using the equa-
 778 tion $dm = 2.5 \log(1 + N/S)$ where $dm \sim 0.7526$ mag
 779 for $N/S = 1$. That is, for each band, we replace the non-
 780 detection with the magnitude corresponding to the error of
 781 0.7526 from the error model forecasted for 10-year LSST
 782 data. The Out-of-Bag (Breiman et al. 1984; Carrasco Kind
 783 & Brunner 2013) cross-validation technique is used within
 784 TPZ to evaluate its predictive validity and determine the
 785 relative importance of the different input attributes. We em-
 786 ployed this information to calibrate our algorithm.

787 In the present work, the LSST magnitudes u , g , r , i
 788 and colors $u-g$, $g-r$, $r-i$, $i-z$, $z-y$ and their associated

789 errors are used in the process of growing 100 trees with a
 790 minimum leaf size of 5 (the z and y magnitudes did not
 791 show significant correlation with the redshift in our cross-
 792 validation, so we did not use them when constructing our
 793 trees). We partitioned our redshift space into 100 bins from
 794 $z = 0.005$ to $z = 2.0$ and smoothed each individual PDF
 795 with a smoothing scale of twice the bin size.

796 3.3 Simple Ensemble Estimator

797 In addition to the main photo- z algorithms described above
 798 we also include a very simple method. For TRAINZ, as we will
 799 we call this simple estimator, we well define $p(z)$ as simply:

$$800 p(z) = \frac{1}{N_{train}} \sum_{i=1}^{N_{train}} z_{train} \quad (11)$$

801 That is, we simply set the redshift PDF of every galaxy equal
 802 to the normalized $N(z)$ of the training sample. As the train-
 803 ing sample is drawn from the same underlying distribution
 804 as the test sample, modulo small deviations due to sam-
 805 ple size, the quantiles of the training and test distributions
 806 should be identical. This is a wildly unrealistic estimator, as
 807 it assigns all galaxies, no matter their apparent magnitude,
 808 colour, or true redshift, the same redshift PDF, and is thus
 809 uninformative at the level of individual object redshifts, but
 810 is designed to perform very well for the ensemble of all ob-
 811 jects. We will discuss this method and cautions relative to
 812 metrics in Section 5.3.

813 4 METRICS FOR QUANTIFYING PDF
814 COMPARISONS

815 The overloaded “ $p(z)$ ” is a widespread abuse of notation;
 816 we would like the outputs of photo- z PDF codes to be in-
 817 terpretable as probabilities. Obviously photo- z PDFs must
 818 not take negative values and must integrate to unity over
 819 the range of possible redshifts. Additionally, an estimator
 820 derived by method H for the photo- z PDF of galaxy i must
 821 be understood as a posterior probability distribution

$$822 \hat{p}_j(z_i) = p(z|d_i, I_D, I_H), \quad (12)$$

823 conditioned not only on the photometric data d_i for that
 824 galaxy but also on parameters encompassing a number of
 825 things that will differ depending on the method H used to
 826 produce it, namely the assumptions I_H necessary for the
 827 method to be valid and any inputs I_D it takes as prior infor-
 828 mation, such as a template library or training set. Because of
 829 this, direct comparison of photo- z PDFs produced by differ-
 830 ent methods is in some sense impossible; even if they share
 831 the same prior information I_D , by definition they cannot
 832 be conditioned on the same assumptions I_H , otherwise they
 833 would not be distinct methods at all.

834 In this study, we isolate the differences in prior infor-
 835 mation specific to each method by using a single training set
 836 I_D^{ML} for all machine learning-based codes and a single tem-
 837 plate library I_D^T for all template-based codes, and these sets

15 <http://ccpforge.cse.rl.ac.uk/gf/project/skynet/>

16 <https://github.com/mgckind/MLZ>

838 of prior information are carefully constructed to be represen-
 839 tative and complete, we have $I_D^{ML} \equiv I_D^T$ for every method
 840 H . Thus, we are saying

$$841 \frac{\hat{p}_{i,H}(z)}{\hat{p}_{i,H'}(z)} \approx \frac{p(z|d_i, I_H)}{p(z|d_i, I_{H'})}, \quad (13)$$

842 meaning that we assume comparisons of $\hat{p}_{i,H}(z)$ isolate the
 843 effect of the method used to obtain the estimator, which
 844 should make examination of differences caused by specifics
 845 of the method implementations easier to isolate.

846 As mentioned previously, there are cosmology probes
 847 that require knowledge of individual galaxy $p(z)$ and others
 848 that require only knowledge of the ensemble redshift distri-
 849 bution, $N(z)$. Due to the paucity of principled techniques
 850 for using and validating photo- z PDFs, there are few alter-
 851 natives to the common practice of reducing photo- z PDFs
 852 to point estimates. Though this practice should not be en-
 853 couraged, we also calculate traditional metrics based on the
 854 most common point estimators derived from photo- z PDFs.
 855 Those seeking to establish a connection to traditional ways
 856 of thinking about redshift estimation may consult the Ap-
 857 pendix for these results.

858 There are a number of metrics that can be used to test
 859 the accuracy of a photo- z interim posterior as an estimator
 860 of a true photo- z posterior if it is known. Even for simulated
 861 data, the true photo- z PDF is in general not accessible un-
 862 less the redshifts are in fact drawn from the true photo- z
 863 PDFs, a mock catalogue generation procedure that has not
 864 yet appeared in the literature. Furthermore, only limited ap-
 865 plications of photo- z PDFs that could be used as the basis
 866 for a metric have been presented in the literature. The most
 867 popular application by far is the calculation of the overall
 868 redshift distribution $N(z)$, the true value of which is known
 869 for the BUZZARD simulation and will be denoted as $N'(z)$.
 870 Though alternatives exist (Malz & Hogg prep), stacking ac-
 871 cording to

$$872 \hat{N}^H(z) \approx \frac{1}{N_{tot}} \sum_i^{N_{tot}} \hat{p}_i^H(z) \quad (14)$$

873 is the most widely accepted method for estimating the red-
 874 shift distribution from photo- z PDFs. If we assume that
 875 the response of estimators of $N(z)$ is uniform across all ap-
 876 proaches H , then we may interpret metrics on the accuracy
 877 of $\hat{N}(z)$ obtained in this way. We must note, however, that
 878 this is a poor assumption in general. Under the setup of this
 879 paper, the true redshift distribution $N'(z) = p(z|I_D)$ (i.e.
 880 because our training data is representative, the interim prior
 881 is the truth). In this ideal case, the method that would give
 882 the best approximation to $N'(z)$ would be one that neglects
 883 all the information contained in the photometry $\{d_i\}_{N_{tot}}$
 884 and gives every galaxy the same photo- z PDF $\hat{p}_i(z) = N'(z)$
 885 for all i . This is the exact estimator, TRAINZ, that we have
 886 described in Section 3.3, and which will serve as a point of
 887 reference for the other codes.

888 The exact implementation of the stacked estimator
 889 $\hat{N}^H(z)$ will depend on the parametrization of the photo- z
 890 PDFs, which may differ across codes and can affect the pre-
 891 cision of the estimator (Malz et al. 2018); even considering a
 892 single method under the same parametrization, say a piece-
 893 wise constant function over bins or a set of samples from

894 the posterior, an estimator using $2N$ bins or samples will
 895 trivially be more precise than an estimator using N bins or
 896 samples. In order to minimize the effects of such choices,
 897 we asked those running all eleven codes to output $p(z)$ pa-
 898 rameterized with a generous ≈ 200 piecewise constant bins
 899 spanning $0 < z < 2$. The piecewise constant format is chosen
 900 because of its established presence in the literature, and the
 901 choice of 200 bins was motivated by the approximate number
 902 of columns expected to be available for storage of $p(z)$ for
 903 the final LSST Project tables.¹⁷ All $p(z)$ catalogues are pro-
 904 cessed using the QP software package (Malz et al. 2018)¹⁸
 905 for manipulating and calculating metrics of 1-dimensional
 906 PDFs. We will discuss the choice of $p(z)$ parameterization
 907 further in Section 5.

908 4.1 Metrics of an ensemble of photo- z interim 909 posteriors

910 4.1.1 Probability integral transform (PIT)

911 The probability integral transform (PIT) (Polsterer et al.
 912 2016) is defined for each individual galaxy as:

$$913 \text{PIT} = \int_{-\infty}^{z_{\text{true}}} p(z) dz. \quad (15)$$

915 The distribution of PIT values quantifies the behavior of the
 916 ensemble of photo- z PDFs, enabling us to evaluate whether
 917 the $p(z)$ is, on average, accurate: The PIT value is the Cumu-
 918 lative Distribution Function (CDF) of the $p(z)$ evaluated at
 919 the true redshift. A catalogue of photo- z PDFs that are accu-
 920 rate should have a flat PIT histogram (i.e., the individual
 921 PIT values as samples from each CDF should match a Uni-
 922 form(0,1) distribution if the CDFs are accurate). Specific
 923 deviations from flatness indicate inaccuracy: overly broad
 924 photo- z PDFs would manifest as underrepresentation of the
 925 lowest and highest PIT values, whereas overly narrow photo-
 926 z PDFs would manifest as over-representation of the lowest
 927 and highest PIT values. High frequency at only PIT ≈ 0
 928 and PIT ≈ 1 indicates the presence of catastrophic outliers
 929 with highly inaccurate photo- z PDFs where the true red-
 930 shift is outside of the support of $p(z)$. Tanaka et al. (2017)
 931 use the histogram of PIT values as a diagnostic indicator of
 932 overall code performance, while Freeman et al. (2017) inde-
 933 pendently define the PIT and demonstrate how its individ-
 934 ual values may be used both to perform hypothesis testing
 935 (via, e.g., the KS, CvM, and AD tests; see below) and to
 936 construct quantile-quantile plots.

937 4.1.2 Quantile-quantile (QQ) plot

938 The quantile-quantile (QQ) plot is a graphical method for
 939 comparing two distributions, where the quantiles of one dis-
 940 tribution are plotted against the quantiles of the other distri-
 941 bution (A quantile being defined by partitioning a distribu-
 942 tion into consecutive intervals containing equal amounts of
 943 probability, or equal numbers of objects in each interval). In
 944 this paper we show the quantiles of the PIT values compared

¹⁷ See, e. g. the LSST Data Products Definition Document, available at: <https://ls.st/dpdd>

¹⁸ available at: <http://github.com/aimalz/qp>

to the quantiles of the Uniform distribution that we expect the PIT values to match if $p(z)$ is an accurate probability distribution for all objects. The QQ plot provides an easy way to qualitatively assess the differences in various properties such as the moments of an estimating distribution relative to a true distribution. In this paper, QQ plots are used for two purposes: (1) for comparing $N(z)$ from photo- z PDFs (estimated using Eq. 14) with the true $N(z)$, i.e. comparing the estimated distribution of redshifts with the true redshift distribution, and (2) for assessing the overall consistency of an ensemble of photo- z PDFs with their true redshifts on a population level, where the distribution of the PIT values (see previous section) is compared to a uniform distribution between 0 and 1. The QQ plot contains very similar information to that shown in the PIT histogram plot, we include both forms, as visually they each convey the information in a somewhat distinct manner.

4.1.3 Conditional density estimation loss

With the conditional density estimation loss (CDE loss) we can compare how well different methods estimate individual PDFs for photometric covariates \mathbf{x} rather than looking only at the ensemble distribution. As in Section 3.2.4, we use the notation $f(z|\mathbf{x})$ instead of $p(z)$ to explicitly show the dependence on \mathbf{x} .

The CDE loss is defined as:

$$L(f, \hat{f}) = \int \int (f(z|\mathbf{x}) - \hat{f}(z|\mathbf{x}))^2 dz dP(\mathbf{x}) \quad (16)$$

This loss is the CDE equivalent of the RMSE in regression.

To estimate this loss we rewrite the loss as

$$\mathbb{E}_{\mathbf{X}} \left[\int \hat{f}(z|\mathbf{X})^2 dz \right] - 2\mathbb{E}_{\mathbf{X}, Z} \left[\hat{f}(Z|\mathbf{X}) \right] + K_f, \quad (17)$$

where the first expectation is with respect to the marginal distribution of the covariates \mathbf{X} , the second expectation is with respect to the joint distribution of \mathbf{X} and Z , and K_f is a constant depending only upon the true conditional densities $f(z|\mathbf{x})$. For each method we can estimate these expectations as empirical expectations on the test or validation data (Eq. 7 in Izbicki et al. 2017) without knowledge of the true densities.

4.2 Metrics over estimated probability distributions

In tandem with the QQ and PIT metrics introduced above, we additionally compute the following metrics comparing the empirical CDF of a distribution to the true or expected distribution. These metrics give a more quantitative measure of the departure from ideal than the more visual PIT histogram and QQ plot. We compute metrics comparing the CDF of PIT values to a the CDF of a Uniform distribution, and also compute the CDF of the true redshift distribution $N'(z)$ compared the $\hat{N}(z)$ distribution derived from summing the $p(z)$ as described in Eq. 14.

4.2.1 Root-mean-square error (RMSE)

We employ the familiar root-mean-square error:

$$\text{RMSE} = \sqrt{\int_{-\infty}^{\infty} (\hat{f}(z) - f'(z))^2 dz}, \quad (18)$$

Though this metric does not account for the fact that the redshift distribution function is, in fact, a probability distribution, it can still be interpreted as a measure of the integrated difference between the estimated distribution and the true distribution, and it can be used to quantify the otherwise qualitative metrics.

4.2.2 Kolmogorov-Smirnov (KS) and related statistics

The *Kolmogorov-Smirnov statistic* N_{KS} is the maximum difference between $F_{\text{phot}}(z)$ and $F_{\text{spec}}(z)$, the CDFs of the photo- z and spectroscopic redshift respectively:

$$N_{\text{KS}} = \max_z (|F_{\text{phot}}(z) - F_{\text{spec}}(z)|). \quad (19)$$

The KS test quantifies the similarity between two distributions, independent of binning. A lower N_{KS} value corresponds to more similar distributions.

We also consider two variants of the KS statistic: the Cramer-von Mises (CvM) and Anderson-Darling (AD) statistics. The CvM statistic is similar to the KS statistic as it is also computed from the distance between the measured CDF and the ideal CDF, but instead of the maximum distance, the CvM statistic calculates the average of the distance squared:

$$\omega^2 = \int_{-\infty}^{+\infty} (F_{\text{meas.}}(x) - F_{\text{ideal}}(x))^2 dF_{\text{ideal}} \quad (20)$$

The AD statistic is a weighted version of the CvM statistic, making it more sensitive to the tails of the distribution:

$$A^2 = n \int_{-\infty}^{+\infty} \frac{(F_{\text{meas.}}(x) - F_{\text{ideal}}(x))^2}{F_{\text{ideal}}(x)(1 - F_{\text{ideal}}(x))} dF_{\text{ideal}} \quad (21)$$

where n is the sample size.

4.2.3 Moments

For the $\hat{N}(z)$ distributions we additionally calculate the first three moments of the estimated redshift distribution for each code and compare them to the moments of the true redshift distribution $N'(z)$. The m th moment of a distribution is defined as

$$\langle z^m \rangle = \int_{-\infty}^{\infty} z^m N(z) dz. \quad (22)$$

Here, we use the moments of the stacked estimator of the redshift distribution function as the basis for a metric. The closer the moments of $\hat{N}(z)$ for a photo- z PDF method are to the moments of the true redshift distribution function $N'(z)$, the better the photo- z PDF method.

1035 5 RESULTS

1036 5.1 Ensembles of photo-z interim posteriors

1037 Fig. 1 Shows the $p(z)$ produced by each of our twelve photo-
 1038 z codes for four example galaxies which exemplify some
 1039 prominent cases that arise when estimating photo- z PDFs: a
 1040 narrow, unimodal redshift solution, a broader unimodal so-
 1041 lution, a bimodal distribution, and a complex, multimodal
 1042 distribution. The red vertical line represents the true red-
 1043 shift of the individual galaxy, and the blue curve repre-
 1044 sents the redshift probability. Several features are obvious
 1045 even in these illustrative examples. ANNz2, METAPHOR,
 1046 NN, and SKYNET all show an excess of small-scale features,
 1047 which appear to be print-through of the underlying training
 1048 set galaxies. For example, in CMNN the $p(z)$ are a simply
 1049 a weighted histogram of all spectroscopic training galaxies
 1050 in nearby colour space with no smoothing applied, so the
 1051 substructure is due to the finite number of neighbours, and
 1052 is not unexpected. GPZ (in its current implementation), on
 1053 the other hand, always produces a single Gaussian, which
 1054 broadens to cover the multi-modal redshift solutions seen in
 1055 other codes.

1056 As stated in Section 4, $p(z)$ is parameterized as 200
 1057 piecewise constant bins covering $0 < z < 2$ for all twelve
 1058 codes, giving a grid size of $\delta z = 0.01$ for each code. A piece-
 1059 wise constant grid was a natural choice for some photo- z
 1060 codes, for instance most template-based codes compute like-
 1061 lihoods on a fixed grid. In contrast, FlexZBoost, for exam-
 1062 ple, can return estimates on any grid without compres-
 1063 sion errors as its a basis expansion method where only the ex-
 1064 pansion coefficients need to be stored. Codes with a native
 1065 output format other than the shared piecewise constant bin-
 1066 ning scheme (or one that can be losslessly converted to it)
 1067 may suffer from loss of information when converting to it,
 1068 which could artificially favor some codes over others in a lim-
 1069 ited number of cases, for example bright galaxies with very
 1070 narrow $p(z)$ where the true peak falls between grid points.
 1071 We will discuss PDF storage in Section 6.

1072 Furthermore, the fidelity of photo- z interim posteriors
 1073 in this format varies with the quality of the photometry. For
 1074 faint galaxies, this redshift resolution is sufficient to capture
 1075 the shape of $p(z)$ for the majority of the test sample, where
 1076 photometric errors on the faint galaxies lead to somewhat
 1077 broad peaks in the redshift posterior. However, as can be
 1078 seen in e. g. the top left panel of Fig. 1, for bright galaxies
 1079 with narrow $p(z)$ the grid spacing of $\delta z = 0.01$ is not suffi-
 1080 cient to resolve the peak. This is consistent with the results
 1081 described in Malz et al. (2018), who find that quantiles (and,
 1082 to a lesser degree, samples) often outperform gridded $p(z)$,
 1083 particularly for bright objects and in the presence of harsher
 1084 storage constraints. With a full 200 numbers to capture the
 1085 information of each photo- z PDF, any parametrization will
 1086 perform adequately, but other storage parametrizations and
 1087 limits on storage resources may be considered in future work.
 1088 We will discuss this further in Section 6.

1089 Fig. 2 shows both the quantile-quantile plots (red) and
 1090 the histogram of PIT values (blue) summarizing the results
 1091 from each photo- z code. The red line shows the measured
 1092 quantiles, while the black diagonal represents the ideal QQ
 1093 values if the distribution were perfectly reproduced. A sec-
 1094 ond panel below the main panel for each code shows the dif-
 1095 ference between Q_{data} and Q_{theory} , i. e. the departure from

1096 the diagonal, for clarity. Biases and trends in whether the
 1097 average width of the $p(z)$ values being over/under-predicted
 1098 are evident. An overall bias where the predicted redshift
 1099 is systematically low manifests as the measured QQ value
 1100 falling above the diagonal, as is the case for BPZ and EAZY,
 1101 while a systematic overprediction shows up as the measured
 1102 QQ value falling below the diagonal, as seen in TPZ. In
 1103 terms of PIT histograms, a systematic underprediction of
 1104 redshift corresponds to fewer PIT values at $PIT < 0.5$ and
 1105 more at $PIT > 0.5$, while a systematic overprediction will
 1106 show the opposite.

1107 Examination of the PIT histograms and QQ plots shows
 1108 that there are fairly generic issues with the width of $p(z)$ un-
 1109 certainties: DELIGHT, CMNN, SkyNET and TPZ all show a
 1110 PIT histogram with a dearth of low values and an excess of
 1111 high values, signs that, on average, their $p(z)$ are more
 1112 broad than the true distribution of redshifts. METAPHOR
 1113 shows the opposite trend, indicating the $p(z)$ are more
 1114 narrow than the distributions given by the true redshifts.
 1115 In all of these code cases there is a free parameter or band-
 1116 width that can be used to tune uncertainties. The sensitivity
 1117 of multiple codes to this bandwidth choice emphasizes the
 1118 fact that great care must be taken in setting user-defined
 1119 parameters in photo- z codes, even in the presence of rep-
 1120 resentative training/validation data. for FLEXZBOOST the
 1121 “sharpening” parameter (described in Section 3.2.4) plays
 1122 a key role in improving the results, resulting in a QQ plot
 1123 that is very nearly diagonal. A similar sharpening procedure
 1124 could be beneficial for several codes. Interestingly, the three
 1125 purely template-based codes, BPZ, EAZY, and LEPHARE,
 1126 show relatively well behaved $p(z)$ statistics (albeit with some
 1127 bias), which may indicate that the likelihood estimation with
 1128 representative templates is accurately capturing the uncer-
 1129 tainties on individual redshifts.

1130 The ideal PIT histogram would follow the black dashed
 1131 line, representing a uniform distribution of PIT values,
 1132 equivalent to the diagonal line in the QQ plot. Overly broad
 1133 $p(z)$ values show up as an excess of PIT values near 0.5
 1134 and a dearth of values at the edges, while overly narrow
 1135 $p(z)$ will have an excess at the edges and will be missing
 1136 values at the centre. Another feature evident in the PIT
 1137 histograms is the number of “catastrophic outlier” values
 1138 where the true redshift falls outside of the non-zero support
 1139 of $p(z)$, corresponding to $PIT = 0.0$ or 1.0 is more apparent
 1140 than in the QQ plots. Following Kodra & Newman (in prep.)
 1141 we define f_0 as the fraction of objects with $PIT < 0.0001$
 1142 or $PIT > 0.9999$. Table 2 lists these fractions for each of
 1143 the codes. For a proper Uniform distribution we expect a
 1144 value of 0.0002. Several codes show a marked excess, with
 1145 ANNz2, FLEXZBOOST, LEPHARE, AND METAPHOR with
 1146 $f_0 > 0.02$, indicating a sizeable number of catastrophic red-
 1147 shift solutions where the true redshift is not covered by the
 1148 extent of $p(z)$. For METAPHOR this may be partially due
 1149 to an overall underprediction of the $p(z)$ width, however this
 1150 is not the case for the other codes. LEPHARE is a particular
 1151 outlier with nearly 5 per cent of objects outside of $p(z)$ sup-
 1152 port. Further study will be necessary to determine what is
 1153 causing these misclassifications for LEPHARE. As expected,
 1154 and by design, TRAINZ has the proper fraction of outliers
 1155 for the f_0 statistic.

1156 Fig. 3 shows comparative metric values for the quantita-
 1157 tive Kolmogorov-Smirnoff (KS), Cramer-Von Mises (CvM),

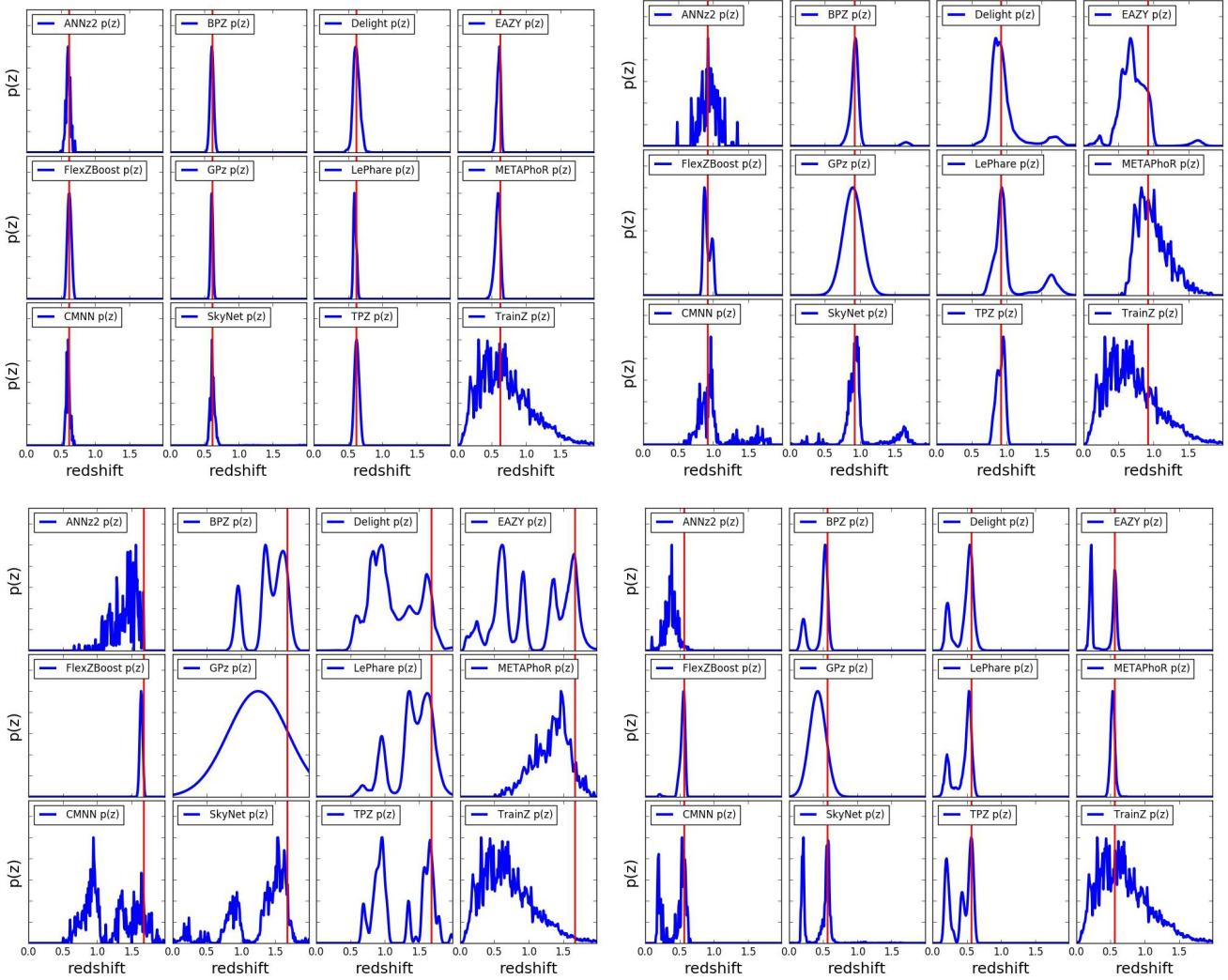


Figure 1. Four illustrative examples of individual $p(z)$ distributions produced by the codes. The red vertical line represents the true redshift. Examples are chosen with common features seen in PDFs: tight unimodal $p(z)$ (upper left), broad unimodal $p(z)$ (upper right), bimodal $p(z)$ (lower right), and complex/multimodal $p(z)$ (lower left). Codes show varying amounts of small-scale structure in their reconstruction of the posterior distribution. We see varying responses from the codes in the presence of color degeneracies and photometric errors, resulting in narrow and broad unimodal, bimodal, and multi-modal $p(z)$ curves.

and Anderson Darling (AD) test statistics for each of the 1156 codes based on comparing the distribution of their PIT val- 1157 ues to the expected uniform distribution over the interval 1158 $[0,1]$. The individual values of the statistic are not as impor- 1159 tant as the comparative score between the different codes. 1160 The AD test statistic diverges for values that include the ex- 1161 tremal, and thus is calculated by excluding the edges of the 1162 distribution. We calculate the AD statistic over the range 1163 of PIT values $v = [0.01, 0.99]$. ANNz2 and FLEXZBOOST 1164 score very well for the PIT metrics. METAPHOR and LEP- 1165 HARE score very well in the PIT AD statistic, but both have 1166 a large number of catastrophic outliers, resulting in higher 1167 KS and CvM scores.

Given the near-perfect training data, examining the individual codes for explanations for departures from the expected behaviour will be instructive in avoiding similar problems in future tests. ANNz2 performs quite well in $p(z)$ based metrics. In the specific implementation employed in

this paper, the final $p(z)$ is a weighted average of five neural-nets. During the training process ANNz2 compares the percentiles of the redshift training sample against the CDFs of the $p(z)$ sample. Distributions that more closely match are given extra weight, and the final weights are designed to produce accurate percentiles. Given that our metrics are focused on the percentile distributions, it is unsurprising that ANNz2 performs well in the given metrics. The discreteness in the individual $p(z)$ estimated by ANNz2 can be attributed to the fact that the code was run as a classifier, assigning weights to discrete bins of redshift. While multiple bins may receive weight, the bins themselves will still be discretized, and no additional smoothing was performed. Overall, FLEXZBOOST and ANNz2 show the best ensemble agreement in their distribution of PIT values.

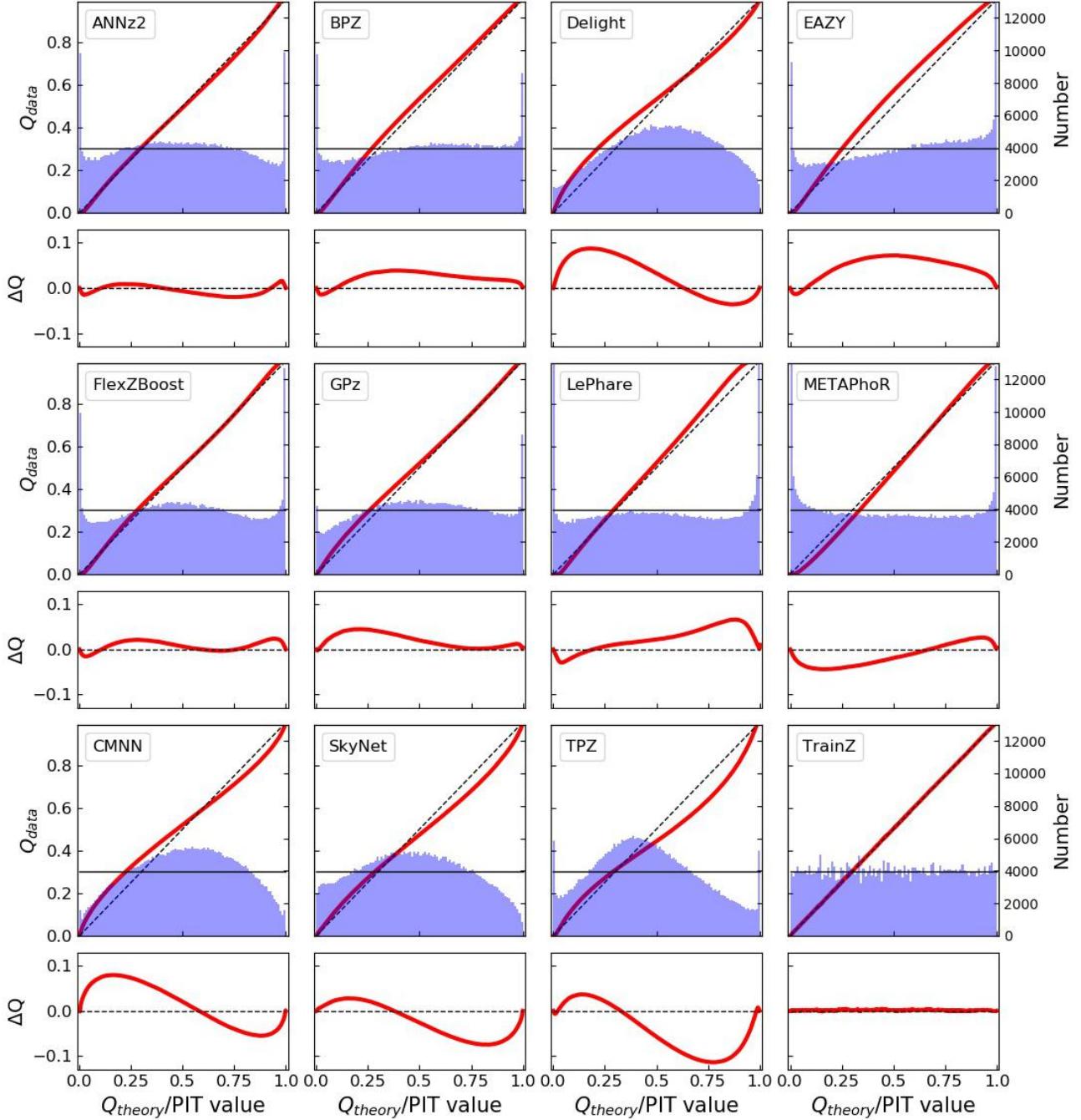


Figure 2. Summary plots for all twelve photo-z codes illustrating performance for the interim posterior statistics. The top panel of each pair shows both the Quantile-Quantile (QQ) plot (red) and the histogram of PIT values (blue). The desired behavior is a QQ plot that matches the diagonal dashed line, and a PIT histogram that matches a uniform distribution matching the thin horizontal black line. The bottom panel of each pair shows the difference between the QQ quantile and the diagonal, illustrating departure from the desired performance. Histograms with an overabundance of PIT values at the centre of the distribution indicate $p(z)$ distributions that are overly broad, while an excess of values at the extrema indicate $p(z)$ distributions that are overly narrow. Values of PIT=0 and PIT=1 indicate “catastrophic failures” where the true redshift is completely outside the support of $p(z)$. Asymmetric features are indicative of systematic bias in the redshift predictions. A variety of behaviors are evident, and specific details are discussed in the text.

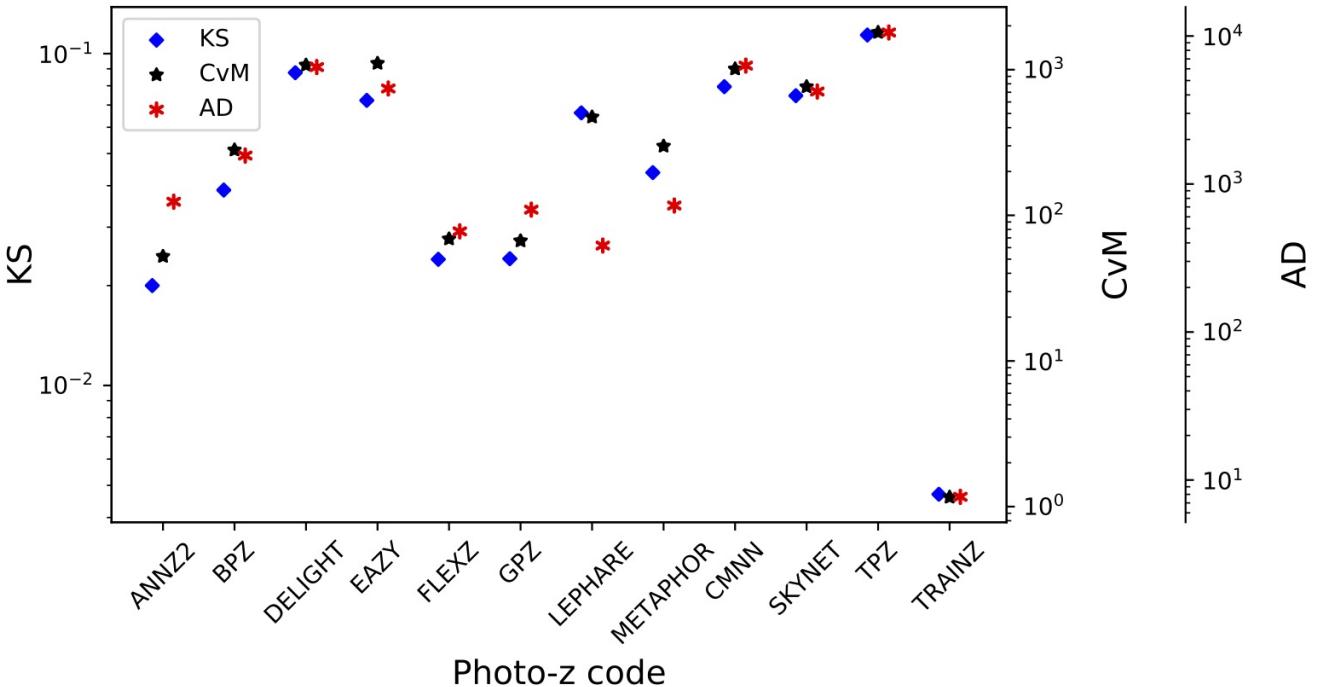


Figure 3. A visual representation of the Kolmogorov-Smirnov (KS, blue diamond), Cramer-von Mises (CvM, black star), and Anderson-Darling (AD, red asterisk) statistics for the PIT distributions. The statistics are often highly correlated, with similar relative values between metrics for each code; however, the AD statistic excludes some values at the extrema of the distributions, and can have disparate values compared to KS and CvM.

Table 2. The fraction of “catastrophic outlier” PIT values. We expect a value of 0.0002 for a proper Uniform distribution. An excess over this small value indicates true redshifts that fall outside the non-zero support of the $p(z)$.

“catastrophic outlier”	
PIT fraction	
Photo-z Code	fraction $\text{PIT} < 10^{-4}$ or > 0.9999
ANN22	0.0265
BPZ	0.0192
DELIGHT	0.0006
EAZY	0.0154
FLEXZBOOST	0.0202
GPZ	0.0058
LEPHARE	0.0486
METAPHOR	0.0229
CMNN	0.0034
SKYNET	0.0001
TPZ	0.0130
TRAINZ	0.0002

5.2 Metrics of the stacked estimator of the redshift distribution

Fig. 4 shows the stacked $\hat{N}(z)$ distribution compared to the true redshift distribution $N'(z)$ for all tested codes. The red line indicates the summed $p(z)$ for each code, while the blue line shows the true redshift distribution. All distributions are smoothed via kernel density estimation (KDE) with a com-

mon bandwidth chosen via Scott’s rule (Scott 1992) in order to minimize differences in small-scale features and make for a more uniform comparison between codes. While Scott’s rule is used to display $N'(z)$ in the figure, all quantitative statistics are computed via the empirical CDF, and are thus unaffected by bandwidth/smoothing choice. As expected, TRAINZ is in excellent agreement with the true redshift distribution: as the training sample is selected from the same underlying distribution as the test set, the redshift distributions are identical, up to Poisson fluctuations due to the finite number of sample galaxies. CMNN is also in excellent agreement for similar reasons: with a representative training sample of galaxies spanning the colour-space, the sum of the colour-matched neighbour redshifts should return the true redshift distribution. FLEXZBOOST and TPZ also show very good agreement, with only slight departures, with an over/under-prediction in the high redshift tail of $\hat{N}(z)$ evident around $z \sim 1.4$. In fact, several of the other codes show an excess at $z \sim 1.4$, particularly the template-based codes BPZ, EAZY, and LEPHARE. This is likely due to the 4000 Å break passing through the gap between the z and y filters, resulting in a drastic change in $z - y$ colour for galaxies in this redshift range. With a relative dearth of strong features blue-ward of the 4000 Å break in most galaxy SEDs, the colour change in the two reddest filter bandpasses of a survey has a large influence on the redshift determination. The $z \sim 1.4$ feature is one of the most prominent sources of larger uncertainty in individual galaxy $p(z)$. In our sample individual galaxy $p(z)$ ’s tend to be broader around $z \sim 1.4$ and point estimates are more uncertain in this regime, as

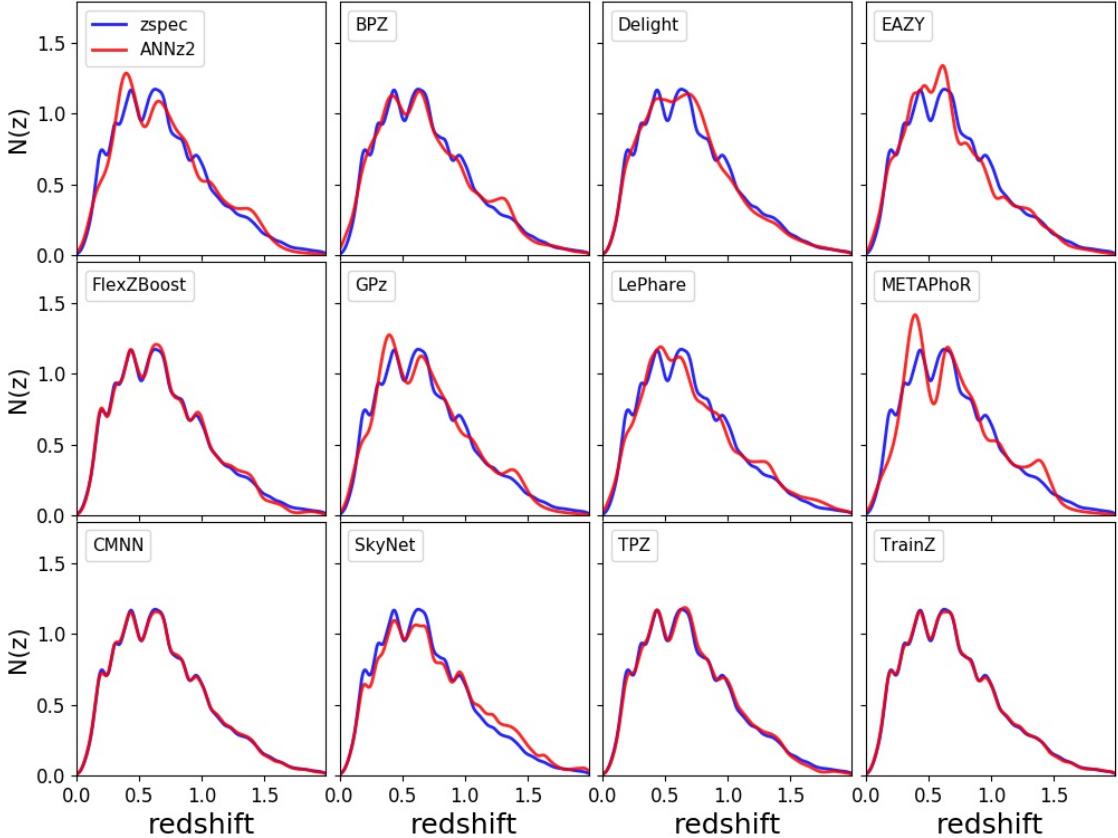


Figure 4. The stacked $p(z)$ produced by each photo- z code ($\hat{N}(z)$, red) compared to the spectroscopic redshift distribution ($N'(z)$, blue). Varying levels of agreement are seen in the codes. Both $\hat{N}(z)$ and $N'(z)$ in all codes are smoothed using a single bandwidth chosen via Scott's rule.

is readily seen in the point-estimate plots shown in Fig. A1 and described in the Appendix. This feature is not unique to this dataset, it is a common occurrence in photo- z estimation. The fact that similar excesses appear in Figure 4 for ANNz2 and METAPHOR shows that the effect is not limited to template-based codes. However, the lack of such a feature in the other codes shows that it is possible to eliminate the degeneracies. Further study on this issue may provide a solution for codes that suffer from this shortcoming.

Two of the machine learning based codes, ANNz2 and METAPHOR, appear to be over-trained, adding excess galaxy probability to the redshift peaks with the largest number of training galaxies, and missing probability in the troughs where training galaxies are of fewer number. Given that our training data is drawn from the same galaxy population as the test set, and our data has prominent peaks in $N'(z)$, perhaps it is not unexpected that such overtraining occurs in some codes, though the fact that it does not occur in all training-based codes indicates that it may be due to specifics of the implementations and bandwidth choices of ANNz2 and METAPHOR. This, once again, emphasizes

that care much be taken in choice of bandwidth parameters in individual codes in order to avoid such overtraining. SKYNET shows an obvious redshift bias, evident both visually in Figure 4 and in the first moment of $N(z)$ listed in Table 5, where it is clearly an outlier. SKYNET employed a method where a random sample of training galaxies was chosen, but there was no test that the subset was completely representative of the overall redshift distribution. Unlike the previous implementation of SKYNET in Bonnett (2015), no effort was made to add extra weight to more rare low and high redshift galaxies. Either of these decisions could be the cause of the bias seen in our results. Future runs of SKYNET will explore these implementation choices and their effects.

Figure 5 shows the quantitative Kolmogorov-Smirnoff (KS), Cramer-Von Mises (CvM), and Anderson Darling (AD) test statistics for each of the codes for the $\hat{N}(z)$ based measures. FLEXZBOOST, CMNN, and TPZ outperform the other codes in the $\hat{N}(z)$ metrics. It is unsurprising that CMNN scores well, as with a near perfectly representative training set means that choosing neighbouring points in color/magnitude space should lead to excellent agreement

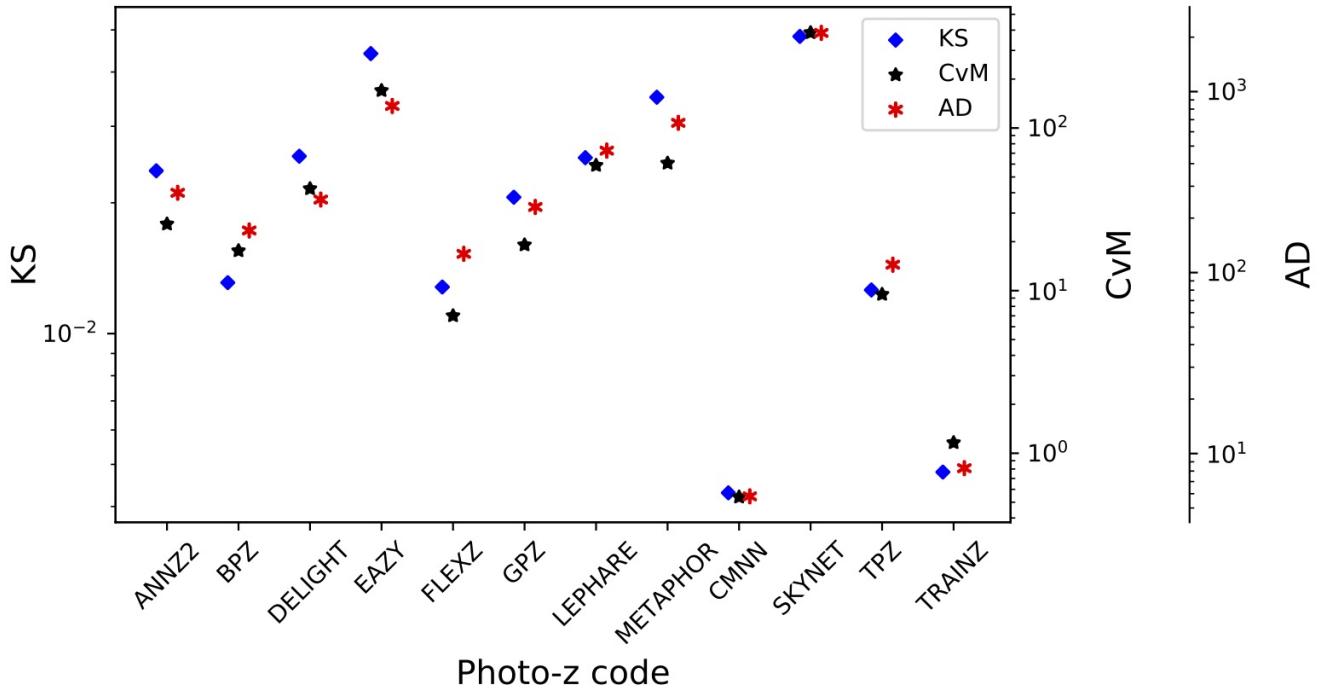


Figure 5. A visual representation of the Kolmogorov-Smirnov (KS, blue diamond), Cramer-von Mises (CvM, black star), and Anderson-Darling (AD, red asterisk) statistics for the $\hat{N}(z)$ distributions. The statistics are correlated, the codes with the lowest KS statistics tend to have the lowest CvM and AD statistics. CMNN performs markedly better than the others in reconstructing the overall $N(z)$ distribution, while SKYNET scores poorly due to an overall bias in its redshift predictions.

in the final $\hat{N}(z)$ estimate. TPZ performed quite poorly in $p(z)$ statistics, but results in a good fit to the overall $N(z)$. This is somewhat surprising, as performance was optimized for accurate $p(z)$, not $\hat{N}(z)$. During the validation stage for TPZ, there was a trade off between the width of the $p(z)$ when adjusting a smoothing parameter and overall redshift bias. The optimal result in the PIT metrics, as illustrated in the shape of the QQ plot, does contain some level of bias as well as a slight underprediction of mean $p(z)$ width, which translates to poor metric scores. This is something that will be looked into for TPZ in the future.

Table 3 shows the CDE loss statistic for each photo-z code. Once again FLEXZBOOST and CMNN score very well for the stacked $\hat{N}(z)$ metrics, as do GPZ and TPZ. The CDE loss measures how well individual PDFs are estimated, and codes with a low CDE loss tend to have good $\hat{N}(z)$ estimates (though the reverse is not necessarily true). FLEXZBOOST is optimized to minimize CDE loss which may explain why the method has good ensemble metrics as well. Note from Table 3 that both FLEXZBOOST and CMNN have low CDE losses. Empirically, we have found that PIT RMSE is not as closely correlated to CDE loss as it is to the $N(z)$ statistics. As CDE loss is a better measure of individual redshift performance, rather than ensemble distribution performance, this statistic is a better indicator of which codes will be most likely to perform well for science cases where single objects are employed.

Table 4 gives the root-mean-square-error (RMSE) statistics for both the PIT and $N(z)$ estimators. The PIT value calculates the RMSE between the quantiles shown in

the QQ plot in Figure 2 and the diagonal, while the $N(z)$ calculates the RMSE between the cumulative distribution of the stacked $\hat{N}(z)$ and the true redshift distribution $N'(z)$.

Table 5 lists the first three moments of the stacked $\hat{N}(z)$ distribution, including the moments of the “truth” distribution for comparison. Several codes are able to reproduce the mean and variance of the distribution to less than a per cent, while several codes do not, which may be a cause for concern, given that mean and variance of the redshift distribution are key properties in cosmological analyses. We note that this stated goal of the study as defined for participants was to accurately reproduce $p(z)$, the “stacking” of the probability distributions to estimate $\hat{N}(z)$ was not the focus as stated to the participants. This explains why some of the best-performing empirical codes in terms of $p(z)$ measures (e.g. FLEXZBOOST) do not do as well at reproducing $\hat{N}(z)$ moments. Had we defined a different parameter to optimize, in this case overall accuracy of $\hat{N}(z)$ rather than individual $p(z)$, would result in improved performance in a particular metric. That is, optimizing photo-z performance for one metric does not automatically give optimal performance for other metrics. As previously stated, there are a variety of scientific use cases for photo-z’s in large upcoming surveys, and care must be taken in how the metrics used to optimize catalog photometric redshifts are defined as well as in how they are used. This implies that we may need multiple photo-z estimators, tuned to the particular metric, in order to maximize science returns in upcoming surveys. In addition, very few scientific use cases will employ the overall $\hat{N}(z)$ with no cuts, as we explore in this paper. We discuss

more realistic tomographic bin selections that will be explored in a follow-up paper in Section 6.1.

5.3 Interpretation of metrics

Samples from accurate photo- z posteriors should reproduce the space of $p(z, \text{data})$. However, it is difficult to test this reconstruction given our data set, as the galaxy distributions arise from mock objects pasted on to an underlying dark matter halo catalogue with properties designed to match empirical relations, rather than being drawn from statistical distributions in redshift. In previous sections we have mentioned that optimizing for a specific metric does not guarantee good performance on other metrics, nor is there any guarantee that good performance by our metrics corresponds to *accurate* photo- z posteriors. In other words, we can construct photo- z estimators that provide good coverage in many of our tests, but which have very little predictive power.

The TRAINZ estimator, which assigns every galaxy a $p(z)$ equal to $N(z)$ of the training set as described in Section 3.3, is introduced as a “null test” to demonstrate this point via *reductio ad absurdum*. TRAINZ outperforms all codes on the PIT-based metrics, and all but one code on the $N(z)$ based statistics. Because our training set is perfectly representative of the test set, $N(z)$ should be identical for both sets down to statistical noise.

The CDE loss and point estimate metrics, however, successfully identify problems with TRAINZ. As shown in Appendix A, TRAINZ has identical $ZPEAK$ and $ZWEIGHT$ values for every galaxy, and thus the photo- zs are constant as a function of spec- zs , i.e. a horizontal line at the mode and mean of the training set distribution respectively. The explicit dependence on the *individual posteriors in the calculation of the CDE loss, described in Section 4.1.3, distinguishes this metric from the other $p(z)$ metrics that test the overall ensemble of $p(z)$ distributions. With a representative training set, TRAINZ will score well on the ensemble metrics, but fails miserably for metrics tied to individual redshifts. We note that many of the ensemble-based metrics are prominent in the photo- z literature despite their inability to identify problems such as those exemplified by TRAINZ.*

In summary, context is crucial to interpreting metrics and defending against the likes of TRAINZ. The best photo- z method is the one that most effectively achieves our science goals, not the one that performs best on a metric that does not accurately reflect those goals. In the absence of clear goals or the information necessary for a principled metric definition, we must think carefully before choosing a single metric

6 DISCUSSION

In this paper we presented results evaluating the photometric redshift PDF computation for eleven photo- z codes. As discussed in Section 4 the $p(z)$ should accurately reflect the relative likelihood as a function of redshift for each galaxy. All codes were provided a set of representative training data and tested on an idealized set of model galaxies with high signal-to-noise and photometry with no confounding effects due to blending, instrumental effects, the night sky, etc...

Table 3. CDE loss statistic for each photo- z code.

Photo- z Code	CDE Loss
ANNz2	-6.88
BPZ	-7.82
DELIGHT	-8.33
EAZY	-7.07
FLEXZBOOST	-10.60
GPz	-9.93
LEPHARE	-1.66
METAPHOR	-6.28
CMNN	-10.43
SKYNET	-7.89
TPZ	-9.55
TRAINZ	-0.83

Table 4. Root-Mean-Square-Error (RMSE) statistics for the twelve photo- z codes for both PIT and $\hat{N}(z)$ distributions.

Photo- z Code	Root-Mean-Square-Error (RMSE) statistics	
	PIT RMSE	$N(z)$ RMSE
ANNz2	0.019	0.0054
BPZ	0.032	0.0050
DELIGHT	0.111	0.0056
EAZY	0.054	0.0102
FLEXZBOOST	0.021	0.0022
GPz	0.027	0.0042
LEPHARE	0.028	0.0062
METAPHOR	0.064	0.0081
CMNN	0.108	0.0009
SKYNET	0.054	0.0144
TPZ	0.082	0.0031
TRAINZ	0.0025	0.0013

Table 5. Moments of the stacked $\hat{N}(z)$ distribution

Stacked $n(z)$ Moments			
	1st Moment	2nd Moment	3rd Moment
TRUTH	0.701	0.630	0.671
Photo- z Code	1st Moment	2nd Moment	3rd Moment
ANNz2	0.702	0.625	0.653
BPZ	0.699	0.629	0.671
DELIGHT	0.692	0.609	0.638
EAZY	0.681	0.595	0.619
FLEXZBOOST	0.694	0.610	0.631
GPz	0.696	0.615	0.639
LEPHARE	0.718	0.668	0.741
METAPHOR	0.705	0.628	0.657
CMNN	0.701	0.628	0.667
SKYNET	0.743	0.708	0.797
TPZ	0.700	0.619	0.643
TRAINZ	0.699	0.627	0.666

1387 included. The goal was not to determine a “best” photo-z 1446
 1388 code: in many ways, this was a baseline test of a “best case 1447
 1389 scenario” to predict the expected photo-z performance if a 1448
 1390 stage IV dark energy survey was to obtain complete training 1449
 1391 samples and perfectly calibrated their multi-band photome- 1450
 1392 try. Given these idealized conditions, any deficiencies ob- 1451
 1393 served in a photo-z code’s performance should be a cause for 1452
 1394 concern, and may be evidence in a problem with either/both 1453
 1395 of the specific code implementation or the underlying algo- 1454
 1396 rithm. In order to meet the stringent LSST requirements on 1455
 1397 photo-z performance, identifying and correcting such prob- 1456
 1398 lems is an important first step before tackling more realistic 1457
 1399 data in future challenges. Most of the codes tested performed 1458
 1400 well, however, several did not meet the stringent goals that 1459
 1401 have been laid out for LSST photometric redshift perfor- 1460
 1402 mance. This is a cause for concern, given the idealized con- 1461
 1403 ditions, and the individual code responses will be studied in 1462
 1404 detail moving forward. One obvious trend in several of the 1463
 1405 codes tested was an overall over or underprediction of the 1464
 1406 widths of $p(z)$, as evidenced by the QQ plots and PIT his- 1465
 1407 tograms shown in Fig. 2. A more careful tuning of bandwidth 1466
 1408 or smoothing during the validation process appears to be nec- 1467
 1409 essary for many of the machine learning based codes in order 1468
 1410 to improve the accuracy of $p(z)$. For narrow peaked $p(z)$ the 1469
 1411 parameterization of the PDF as evaluated on a fixed redshift 1470
 1412 grid could also have contributed to some overestimates of 1471
 1413 $p(z)$ width simply due to the finite resolution. After evalua- 1472
 1414 ting results such as those presented in Malz et al. (2018), 1473
 1415 in future analyses we plan to switch from a fixed grid to 1474
 1416 quantile-based storage of $p(z)$ in order to more efficiently 1475
 1417 and accurately store redshift PDF results. 1476

1418 Another important factor to keep in mind when exam- 1477
 1419 ining the results presented in this paper is the fact that they 1478
 1420 are at some level dependent on the metrics that we aim to 1479
 1421 optimize: in this case code participants were asked to submit 1480
 1422 their optimal measures of an accurate $p(z)$, so participants 1481
 1423 used the training/validation data to optimize their codes ac- 1482
 1424 cordingly. Had we, instead, asked for an optimal $\hat{N}(z)$ the 1483
 1425 resulting metrics would be different for most, if not all, of 1484
 1426 the codes, as they would optimize toward a different goal. 1485
 1427 Specific metric choice can affect which codes are among the 1486
 1428 “best” codes. As stated earlier, there are cosmological science 1487
 1429 cases that require either individual galaxy photo-z measures, 1488
 1430 or ensemble $\hat{N}(z)$ measures. We must be aware of that the 1489
 1431 optimal method for one is not necessarily optimal for the 1490
 1432 other, and in fact several photo-z algorithms may be nec- 1491
 1433 essary in the final cosmological analysis in order to satisfy 1492
 1434 the requirements of all science use cases. The example of 1493
 1435 the simple TRAINZ estimator described in Section 5.3 shows 1494
 1436 a simple model with a $p(z)$ that is unrealistic for individual 1495
 1437 objects can still score very well on many of our metrics. It 1496
 1438 is important to look at all metrics, and keep in mind what 1497
 1439 information each metric conveys. We re-emphasize that the 1498
 1440 dataset tested was quite idealized, and discuss enhancements 1499
 1441 that will be added in future simulations to test photo-z codes 1500
 1442 on increasingly realistic conditions in the following section. 1501
 1502
 1503

1443 6.1 Future work

1444 The work presented in this paper is only the first step in 1506
 1445 characterizing current photo-z codes and moving toward an 1507

improved photometric redshift estimator. This initial paper 1508 explored code performance in idealized conditions with 1509 perfect catalog-based photometry and representative training 1510 data. As mentioned in Section 5.2 for the stacked $N(z)$ met- 1511 rics we examined only the entire galaxy population with no 1512 selections in either photo-z “quality” or redshift. The cos- 1513 mological analyses for weak lensing and large scale struc- 1514 ture based measures plan to break galaxy samples into to- 1515 mographic redshift bins, using photo-z $p(z)$ to infer the red- 1516 shift distribution for each bin. The specific selection used 1517 to determine these bins, both algorithmically and the specific 1518 bin boundaries, could induce biases due to indirect selections 1519 inherent in the photo-z or other bin selection parameters. 1520 The effects of tomographic bin selection will be explored in 1521 a dedicated future paper. [are there any references for this? 1522 I remember Gary Bernstein talking about this at a photo-z 1523 workshop in Japan, but I don’t know that it was published. 1524 I believe Michael Troxel has discussed this as well.] We also 1525 plan to propagate the uncertainties measured in a set of fidu- 1526 cial tomographic redshift bins in order to estimate impact on 1527 cosmological parameter estimation.

In future papers we will add more and more complexity 1528 to our simulated data in order to test photo-z algorithms in 1529 increasingly realistic conditions. The most pressing concern 1530 is the impact of incomplete spectroscopic training samples. 1531 As discussed extensively in Newman et al. (2015) a rep- 1532 resentative set of spectroscopically confirmed galaxies spanning 1533 the full range of both redshift and apparent magnitude is nec- 1534 essary as a training set to characterize the mapping from 1535 broad-band fluxes to photometric redshifts. However, due to a 1536 combination of factors due to both the galaxy SEDs and lim- 1537 itations of spectrographic instruments, redshift samples are 1538 known to be systematically incomplete, where certain galaxy 1539 types and redshift intervals fail to yield a redshift even at the 1540 longest integration times on current and near-future instru- 1541 ments. The more representative the training data, the better 1542 the performance of photo-z algorithms will be. Current and 1543 upcoming surveys are putting in significant effort into obtain- 1544 ing these training samples (e.g. Masters et al. 2017), 1545 however we still expect significant incompleteness for LSST- 1546 like samples, particularly at faint magnitudes. One major 1547 focus of an upcoming LSST Dark Energy Science Collabora- 1548 tion Photo-z Working Group data challenge is to produce a 1549 realistically incomplete training set of spectroscopic galaxies, 1550 modeling the performance of spectrographs, emission- 1551 line properties, and expected signal-to-noise to determine 1552 which galaxies will fail to yield a secure redshift. In addition 1553 to outright redshift failures we will model the inclusion 1554 of a small number of falsely identified secure redshifts where 1555 misidentified emission lines or noise spikes cause an incor- 1556 rect redshift solution to be marked as a high quality iden- 1557 tification. Even sub-per cent level contamination by false 1558 redshifts can impact photo-z solutions at levels comparable 1559 to the stringent requirements of some LSST science cases. 1560 We expect different systematics to occur in different photo-z 1561 codes in response to training on incomplete data, particularly 1562 some of the machine learning methods. The response of the 1563 codes will inform future directions of code development.

This initial paper explored a data set that was con- 1564 structed at the catalog level, with no inclusion of the compli- 1565 cations that come from measuring photometry from images. 1566 Future data challenges will move to catalogs constructed 1567

from mock images, including effects that will have great impact on photo-z measurements. Object blending will be a major area of investigation, as the mixing of flux from multiple objects and the resultant change in measured colours is predicted to affect a large fraction of LSST galaxies (Dawson *et al.* 2016), and will be one of the major contributing systematics for photo-z's. Inclusion of differing observing conditions (seeing, clouds, variations in filter curves, Galactic dust, ...), as well as models for instrumental and system effects, sky masks, will all impact object photometry, and will be explored in the upcoming data challenge and their impacts described in upcoming papers. All underlying SEDs were parameterized as a weighted combination of five basis SEDs, with no additional accounting for host galaxy dust obscuration beyond what was encoded in the basis templates. This, in effect, limited the simulation to a very simple model of internal obscuration. Future simulations will include a more complicated and realistic treatment of host galaxy dust.

The underlying simulation used in this work was based on a light-cone constructed to a maximum redshift of $z = 2$. LSST imaging after 10 years of observations will include a significant number of $z > 2$ galaxies in expected cosmology samples, and their inclusion does have potential significant implications for photo-z measures: the high redshift galaxies lie at fainter apparent magnitudes and can have anomalous colours due to evolution of stellar populations and the shift to rest-frame magnitudes probing UV features of the underlying SED. More importantly, one of the most common “catastrophic outlier” degeneracies observed in deep photometric samples occurs when the Lyman break is mistaken for the Balmer break, leading to multiple redshift solutions at $z \sim 0.2 - 0.3$ and $z \sim 2 - 3$ (Massarotti *et al.* 2001). This degeneracy, along with other potential degeneracies, are currently not covered by the limited redshift range of this initial paper, which could mean that we are not probing the full range of potential extreme outlier populations and how our photo-z estimators respond to them. Extending simulations to include the high-redshift galaxy population will be a priority in future data challenges.

7 CONCLUSION

In this study we have not accounted for the presence of Active Galactic Nuclei (AGN) contributions to galaxy fluxes. In some cases, AGN will be easily identified from the colors and morphologies, i.e. the case of the brightest quasars where the nuclear activity outshines the host galaxy, and numerous studies have utilized color selection to create large samples of quasars (e.g. Richards *et al.* 2006; Maddox *et al.* 2008; Richards *et al.* 2015). In current deep fields, similar in depth to what we expect from LSST, variability information and multi-wavelength data have been critical to not only identify AGN dominated galaxies, but also obtain more accurate photometric redshifts (e.g Salvato *et al.* 2011).

In addition to AGN dominated galaxies, those with lower levels of nuclear activity present a more insidious problem, where AGN features may not be apparent, but the colors and other host galaxy properties are perturbed relative to galaxies with an inactive nucleus. In such cases, the presence of the AGN may induce a bias if the template SEDs or empirical datasets do not include low-level AGN counterparts.

For LSST, we will need to identify and obtain accurate photometric redshifts of all types of AGN for a range of science goals, whether it is to eliminate such objects from cosmology experiments, or to use them with confidence, all the way through to understanding galaxy evolution and the role that AGN may play in influencing galaxy properties over cosmic time.

A promising route to classifying and obtaining accurate photometric redshifts for the AGN population is by combining machine learning with template-fitting techniques, as has recently been demonstrated by Duncan *et al.* (2018) for radio-selected AGN. This is because AGN are relatively easy to obtain spectroscopic redshifts for over all redshifts due to the strong emission lines that they exhibit, allowing very good training sets for machine learning algorithms to use. Whereas for those galaxies where the AGN is sub-dominant the galaxy templates are still adequate for obtaining reasonable photometric redshifts.

In addition to these improvements, the DESC Photo-z group plans to look at all potential methods to combine the results from multiple photo-z codes to improve $p(z)$ accuracy, similar to the work presented in Dahlen *et al.* (2013); Carrasco Kind & Brunner (2014); Duncan *et al.* (2018). Taking advantage of multiple algorithms that use observables in slightly different ways has shown promise, however we must be very conscious of whether a potential combination properly treats the covariance between the methods, given that they are estimating quantities based on the same underlying observables. Several science cases wish to estimate physical quantities along with redshift, for example galaxy stellar mass and star formation rate. Proper joint estimation of redshift and physical quantities requires an in depth understanding of galaxy evolution, and progress on accurate bivariate redshift probability distributions will go hand in hand with progress on understanding galaxies themselves. Parameterization and storage of a complex 2-dimensional probability surface for potentially billions of galaxies (or even subsets of hundreds of thousand of particular interest) pose a potential challenge. These issues will be examined in another future paper.

Finally, while this paper and future papers discussed above focus on photometric redshift codes and estimating accurate $p(z)$ from training data, we plan a separate, but complementary, project to examine calibration of the resultant redshifts via spatial cross-correlations (Newman 2008), which will be explored in a separate series of future papers. The overarching plan describing everything laid out in this section is described in more detail in the LSST DESC Science Roadmap (see Footnote in Section 1). These plans will require significant effort, but they are necessary if we are to make optimal use of the LSST data for astrophysical and cosmological analyses.

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S.J. Schmidt: Led the project. (conceptualization, data curation, formal analysis, investigation, methodology, project administration, resources, software, supervision, visualization, writing – original draft, writing – review & editing)

A.I. Malz: Contributed to choice of metrics, implementation

in code, and writing. (conceptualization, methodology, 1689
 project administration, resources, software, visualization, 1690
 writing – original draft, writing – review & editing) 1691
 J.Y.H. Soo: Ran ANNz2 and Delight, updated abstract, 1692
 edited sections 1 through 6, added tables in Methods 1693
 and Results, updated references.bib and added references 1694
 throughout the paper 1695
 M. Brescia: main ideator of METAPHOR and of MLPQNA; 1696
 modification of METAPHOR pipeline to fit the LSST data 1697
 structure and requirements 1698
 S. Cavaudi: Contributed to choice and test of metrics, ran 1699
 METAPHOR, minor text editing 1700
 G. Longo: Scientific advise, test and validation of the 1701
 modified METAPHOR pipeline, text of the METAPHOR 1702
 section

I.A. Almosallam: vetted the early versions of the data set 1703
 and ran many photo-z codes on it, applied GPz to the final 1704
 version and wrote the GPz subsection

M.L. Graham: Ran the colour-matched nearest-neighbours 1705
 photo-z code on the Buzzard catalog and wrote the relevant 1706
 piece of Section 2; participated in discussions of the analy- 1707
 sis.

A.J. Connolly: Developed the colour-matched nearest- 1708
 neighbours photo-z code; participated in discussions of the 1709
 analysis.

E. Nourbakhsh: Ran and optimized TPZ code on the 1710
 Buzzard catalog and wrote a subsection of Section 2 for that 1711
 J. Cohen-Tanugi: contributed to running code, analysis 1712
 discussion, and editing, reviewing the paper 1713
 H. Tranin: contributed to providing SkyNet results and 1714
 writing the relevant section 1715
 P.E. Freeman: Contributed to choice of CDE metrics and 1716
 to implementation of FlexZBoost 1717
 K. Iyer: assisted in writing metric functions used to evaluate 1718
 codes 1719
 J.B. Kalmbach: Worked on preparing the figures for the 1720
 paper. 1721
 E. Kovacs: Ran simulations, discussed data format and 1722
 properties for SEDs, dust, and ELG corrections 1723
 A.B. Lee: Co-developed FlexZBoost and the CDE loss statis- 1724
 tic, wrote text on the work, and supervised the development 1725
 of FlexZBoost software packages 1726
 C. Morrison: Managerial support; Discussions with authors 1727
 regarding metrics and style; Some coding contribution to 1728
 metric computation. 1729
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 metrics, and supervision of work done by Rongpu Zhou 1731
 E. Nuss: contributed to running code, analysis discussion, 1732
 and editing, reviewing the paper 1733
 T. Pospisil: Co-developed FlexZBoost software and CDE 1734
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APPENDIX A: POINT ESTIMATE PHOTOMETRIC REDSHIFTS

While we do not recommend the use of single point estimates of redshift for most science applications, plots of the point estimates can be a useful qualitative diagnostic of photo-z code performance, i. e. examining point photo-z vs. spec-z plots visually can give a quick impression of some common trends in different codes. Computing point estimate statistics may also be useful for more direct comparisons with previous photo-z evaluations. If a point-estimate is preferred for a specific science case, it is fairly simple to compute the mean, mode, or some other simple estimator from each $p(z)$, so these point estimates can be easily derived from the stored $p(z)$.

There are several common point estimators of photo-z posteriors employed by different codes, e. g. the mode, mean, median of the $p(z)$ distribution. In addition, many of the machine learning based estimators can be set up to return a single redshift solution. For example, SkyNet can be configured to run as a regressor that returns a single float rather than a classifier that returns a 200-bin $p(z)$ estimate. The single value returned by a machine learning based code may not correspond to a particular measure such as the mode or mean, and so to avoid interpretation of results that might be introduced by variations in choice of specific point-estimate implementation per code, we discard the code-specific point estimates. We instead calculate point estimates more uniformly across the codes directly from the $p(z)$ using two measures, z_{PEAK} and z_{WEIGHT} . z_{PEAK} is simply the maximum value attained for each galaxy $p(z)$, the mode of the probability distribution. z_{WEIGHT} is defined similarly to how it is defined in Dahlen et al. (2013), as the weighted mean of the redshift over the main peak of $p(z)$ containing the z_{PEAK} value. The main peak is defined by subtracting $0.05 \times z_{\text{PEAK}}$ from $p(z)$ and identifying the roots to isolate the peak containing z_{PEAK} , z_{WEIGHT} is defined as the weighted mean redshift within this peak. We restrict to a single peak in order to avoid confusion from bimodal and multimodal $p(z)$ such as those shown in bottom panels of Figure 1. For example, for a bimodal probability distribution a weighted mean calculated over both peaks would fall between the peaks, at a redshift where the probability is minimal. Restricting the weighting to a single peak ensures that the point estimate will fall in the region of maximum redshift probability.

1747 A1 Point Estimate Metrics

1748 We calculate the commonly used point estimate metrics of
 1749 the overall photo-z scatter (σ_z , the standard deviation of
 1750 the photo-z residuals), bias, and “catastrophic outlier rate”.
 1751 Specifically, we calculate the metrics as follows: we define e_z
 1752 as

$$1753 e_z = \frac{z_p - z_s}{1 + z_s} \quad (A1)$$

1754 where z_p is the point estimate and z_s is the true redshift. In
 1755 practice, because the standard deviation calculation is quite
 1756 sensitive to the outliers, we define the photo-z scatter, σ in
 1757 terms of the Interquartile Range (IQR), the difference be-
 1758 between the 75th and 25th percentiles of the e_z distribution.
 1759 In order to match the usual meaning of a 1σ interval, we
 1805 scale the IQR and define $\sigma_{IQR} = IQR/1.349$, as there is
 1810 a factor of 1.349 difference between the IQR and the stan-
 1811 dard deviation of a Normal distribution. While many other
 1812 studies define the bias based on the mean offset between true
 1813 and estimated redshift, in this study we define the bias as
 1814 the median value of e_z for the sample. We use median as
 1815 it is, once again, less sensitive to outliers than the mean.
 1816 The catastrophic outlier fraction is defined as the fraction
 1817 of galaxies with e_z greater than the larger of $3\sigma_{IQR}$ or 0.06,
 1818 i.e. 3σ outliers with a floor of $\sigma_{IQR}=0.02$. For reference, the
 1819 goals stated in Section 3.8 of the LSST Science Book (Abell
 1820 et al. 2009) for photo-z performance in these metrics, as-
 1821 suming perfect training knowledge (as we are testing in this
 1822 paper) are:

- 1823 • RMS scatter < $0.02(1 + z)$
- 1824 • bias < 0.003
- 1825 • catastrophic outlier rate < 10%

1826 These definitions are similar, but not exactly the same, as
 1827 the σ_{IQR} and median bias calculated here, but are similar
 1828 enough for qualitative comparisons to the LSST goals.

1829 Fig. A1 shows the point estimates for both z_{PEAK} and
 1830 z_{WEIGHT} . Point density is shown with mixed contours to
 1831 emphasize that most of the galaxies do fall close to the
 1832 $z_{phot} = z_{spec}$ line, while blue points show differing char-
 1833 acteristics of the outlier populations. The red dashed lines
 1834 indicated the cutoff for catastrophic outliers, defined as:
 1835 $\max(0.06, 3\sigma_{IQR})$. As with the full $p(z)$ results, a variety
 1836 of behaviours are evident in the different codes. Table A1
 1837 lists the scatter, bias, and catastrophic outlier fractions for
 1838 the codes. The performance of the codes for point metrics is
 1839 highly correlated with performance on $p(z)$ based tests, which
 1840 is to be expected, given that the point-estimates were derived
 1841 from the $p(z)$. Some discretization is evident in z_{PEAK} , par-
 1842 ticularly for SKYNET, due to the finite grid spacing of the
 1843 reported $p(z)$. These discreteness effects are mitigated by the
 1844 weighting of z_{WEIGHT} , resulting in a smoother distribution
 1845 of redshift estimates. Several features perpendicular to the
 1846 main $z_{phot} = z_{spec}$ line are evident. These features are due
 1847 to the 4000 angstrom break passing through the gaps between
 1848 adjacent LSST filters. These features are most prominent in
 1849 template-based codes, but appear to some degree in all codes
 1850 tested.

1851 In even the best performing codes, there are visible occu-
 1852 pied regions away from the $z_{phot} = z_{spec}$ line, corresponding
 1853 to degenerate redshift solutions for certain LSST magnitudes

1854 and colors. While use of the full information available via
 1855 $p(z)$ mitigates their impact, a full understanding of the out-
 1856 lier population is critical for LSST science, particularly in
 1857 tomographic applications

1858 Finally, we note that all eleven codes are at or near the
 1859 goals for point-estimates as outlined in the LSST Science
 1860 Requirements Document¹⁹ and Graham et al. (2018). This
 1861 is to be expected, given that the requirements were designed
 1862 such that a point estimate photo-z would meet these require-
 1863 ments for perfect training data to a depth of $i < 25$. But, it
 1864 is still an encouraging sign, given an updated mock galaxy
 1865 simulation and the expanded set of photo-z codes tested.

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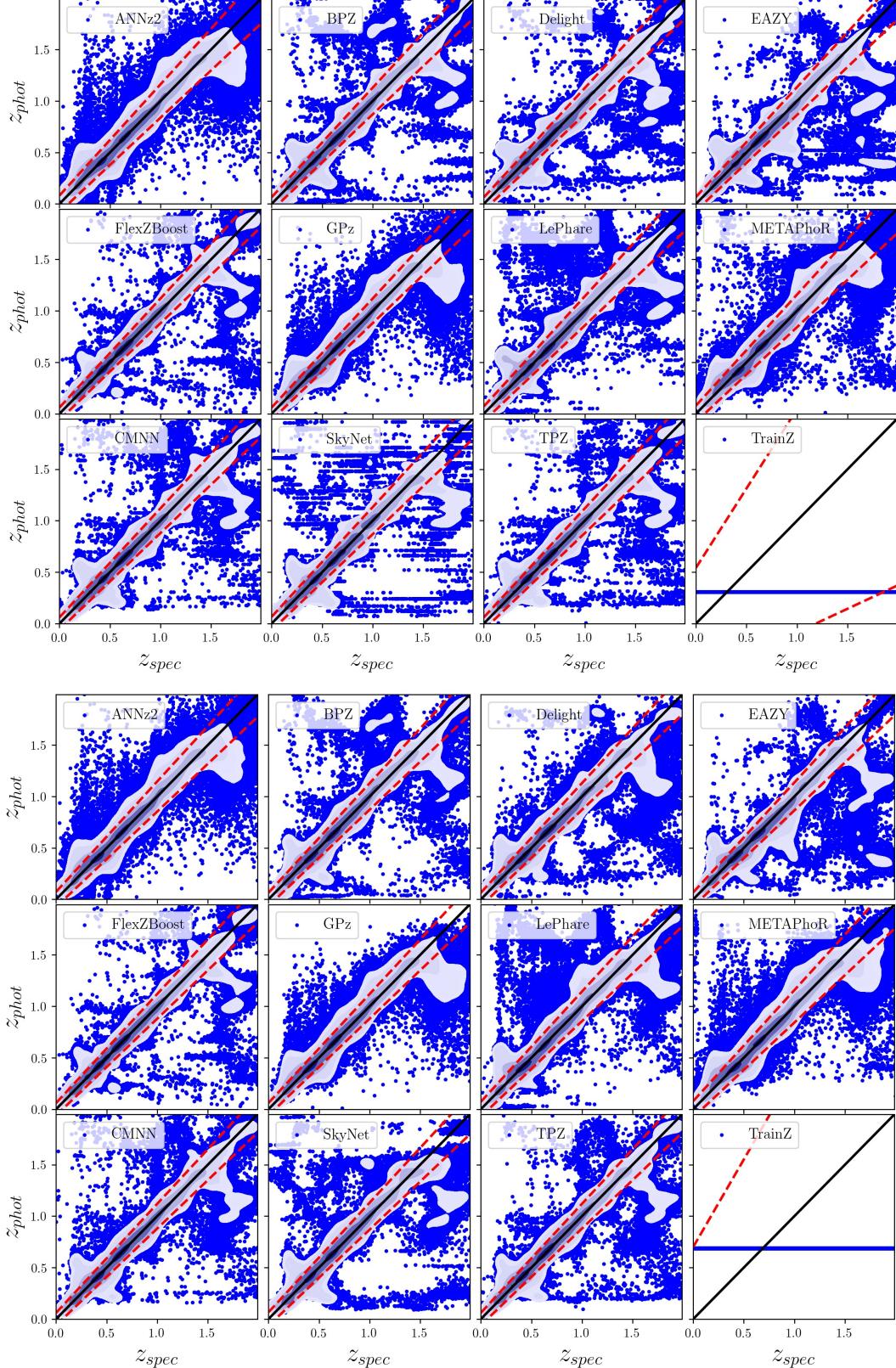


Figure A1. Point estimate photo-z's derived from the posteriors. Top panel shows z_{PEAK} , while bottom panel shows z_{WEIGHT} . Point estimate density is represented with fixed density contours, while outliers at lower density are represented by blue points. While use of point-estimate photo-z's is not recommended, they do make for useful comparative and visual diagnostics. In the lower-right panel of each plot, the TRAINZ estimator results in identical photo-z estimates at the mode and mean of the training set $N'(z)$ distribution for all galaxies.

Table A1. Point estimate statistics

Photo-z Code	Z _{PEAK}			Z _{WEIGHT}		
	$\frac{\sigma_{IQR}}{(1+z)}$	median	outlier fraction	$\frac{\sigma_{IQR}}{(1+z)}$	median	outlier fraction
ANNz2	0.0270	0.00063	0.044	0.0244	0.000307	0.047
BPZ	0.0215	-0.00175	0.035	0.0215	-0.002005	0.032
DELIGHT	0.0212	-0.00185	0.038	0.0216	-0.002158	0.038
EAZY	0.0225	-0.00218	0.034	0.0226	-0.003765	0.029
FLEXZBOOST	0.0154	-0.00027	0.020	0.0148	-0.000211	0.017
GPz	0.0197	-0.00000	0.052	0.0195	0.000113	0.051
LEPHARE	0.0236	-0.00161	0.058	0.0239	-0.002007	0.056
METAPHOR	0.0264	0.00000	0.037	0.0262	0.001333	0.048
CMNN	0.0184	-0.00132	0.035	0.0170	-0.001049	0.034
SKYNET	0.0219	-0.00167	0.036	0.0218	0.000174	0.037
TPZ	0.0161	0.00309	0.033	0.0166	0.003048	0.031
TRAINZ	0.1808	-0.2086	0.000	0.2335	0.022135	0.000

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