

# Evaluation of probabilistic photometric redshift estimation approaches for LSST

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## ABSTRACT

Many scientific investigations of photometric galaxy surveys require redshift estimates, whose uncertainty properties are best encapsulated by photometric redshift (photo- $z$ ) posterior probability distribution functions (PDFs). A plethora of photo- $z$  PDF estimation methodologies abound, producing discrepant results with no consensus on a preferred approach. We present the results of a comprehensive experiment comparing twelve photo- $z$  algorithms applied to mock data produced for the Large Synoptic Survey Telescope (LSST) Dark Energy Science Collaboration (DESC). By supplying perfect prior information, in the form of the complete template library and a representative training set as inputs to each code, we demonstrate the impact of the assumptions underlying each technique on the output photo- $z$  PDFs. In the absence of a notion of true, unbiased photo- $z$  PDFs, we evaluate and interpret multiple metrics of the ensemble properties of the derived photo- $z$  PDFs as well as traditional reductions to photo- $z$  point estimates. We report systematic biases and overall over/under-breadth of the photo- $z$  PDFs of many popular codes, which may indicate avenues for improvement in the algorithms or implementations. Furthermore, we raise attention to the limitations of established metrics for assessing photo- $z$  PDF accuracy; though we identify the conditional density estimate (CDE) loss as a promising metric of photo- $z$  PDF performance in the case where true redshifts are available but true photo- $z$  PDFs are not, we emphasize the need for science-specific performance metrics.

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

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### 1 INTRODUCTION

The current and next generations of large-scale galaxy surveys, including the Dark Energy Survey (DES, Abbott et al. 2005), the Kilo-Degree Survey (KiDS, de Jong et al. 2013), Hyper Suprime-Cam Survey (HSC, Aihara et al. 2018a,b), 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), represent a paradigm shift to reliance on photometric, rather than solely spectroscopic, galaxy catalogues of substantially larger size at a cost of lacking complete spectroscopically confirmed redshifts ( $z$ ). Effective astrophysical inference using the catalogues resulting from these ongoing and upcoming missions, however, necessitates accurate and precise photometric redshift (photo- $z$ ) estimation methodologies.

As an example, in order for photo- $z$  systematics to not dominate the statistical noise floor of LSST’s main cosmological sample of several  $10^9$  galaxies, the LSST Science Requirements Document (SRD)<sup>1</sup> specifies that individual galaxy photo- $zs$  must have root-mean-square error  $\sigma_z < 0.02(1+z)$ ,  $3\sigma$  catastrophic outlier rate below 10 per cent, and bias below 0.003. Specific science cases may have their own requirements on photo- $z$  performance that exceed those of the survey as a whole. In that vein, the LSST Dark Energy Science Collaboration (LSST-DESC) developed a separate SRD (The LSST Dark Energy Science Collaboration et al. 2018) that conservatively forecasts the constraining power of five cosmological probes, leading to even more stringent requirements on photo- $z$  performance, including those defined in terms of tomographically binned subsample populations rather than individual galaxies.

Though the standard has long been for each galaxy in a photometric catalogue to have a photo- $z$  point estimate and Gaussian error bar, even early applications of photo- $zs$  in precision cosmology indicate the inadequacy of point estimates (Mandelbaum et al. 2008) to encapsulate the degeneracies resulting from the nontrivial mapping between broad band fluxes and redshift. Far from a hypothetical situation, such degeneracies are real consequences of the same deep imaging that enables larger galaxy catalogue sizes. The lower luminosity and higher redshift populations captured by deeper imaging introduce major physical systematics to photo- $zs$ , among them the Lyman break/Balmer break degeneracy, that did not affect shallower large area surveys like the Sloan Digital Sky Survey (SDSS, York et al. 2000) and Two Micron All Sky Survey (2MASS, Skrutskie et al. 2006).

To fully characterize such physical degeneracies, subsequent photometric galaxy catalogue data releases, (e. g. Sheldon et al. 2012; Erben et al. 2013; de Jong et al. 2017), provide a more informative photo- $z$  data product, the photo- $z$  probability density function (PDF), that describes the redshift probability, commonly denoted as  $p(z)$ , as a function of a galaxy’s redshift, conditioned on the observed photometry. Early template-based methods such as Fernández-Soto et al. (1999) approximated the likelihood of photometry conditioned on redshift with the relative  $\chi^2$

values of template spectra. Not long after, Bayesian adaptations of template-based approaches such as Benítez (2000) combined the estimated likelihoods with a prior to yield a posterior PDF of redshift conditioned on photometry. While the first data-driven photo- $z$  algorithms yielded a point estimate, Firth et al. (2003) estimated a photo- $z$  PDF using a neural net with realizations scattered within the photometric errors.

There are numerous techniques for deriving photo- $z$  PDFs, yet no one method has been established as clearly superior. Consistent experimental conditions enable the quantification if not isolation of their differences, which can be interpreted as a sort of *implicit prior* imparted by the method itself. Comprehensive comparisons of photo- $z$  methods have been made before; the Photo- $z$  Accuracy And Testing (PHAT, Hildebrandt et al. 2010) effort focused on photo- $z$  point estimates derived from many photometric bands. Rau et al. (2015) introduced a new method for improving photo- $z$  PDFs using an ordinal classification algorithm. DES compared several codes for photo- $z$  point estimates and a subset with photo- $z$  PDF information (Sánchez et al. 2014) and examined summary statistics of photo- $z$  PDFs for tomographically binned galaxy subsamples (Bonnett et al. 2016).

This paper is distinguished from other comparisons of photo- $z$  methods by its focus on the evaluation criteria for photo- $z$  PDFs and interpretation thereof. In the absence of simulated data drawn from known redshift distributions, the very concept of a “true PDF” for an individual galaxy is unavailable, and we must instead rely on measures of ensemble behaviour to characterize PDF quality (see § 4 for further discussion). We aim to perform a comprehensive sensitivity analysis of photo- $z$  PDF techniques in order to ultimately select those that will become part of the LSST-DESC pipelines, described in the Science Roadmap (SRM)<sup>2</sup>. In this initial study, we focus on evaluating the performance of photo- $z$  PDF codes using PDF-specific performance metrics in a formally controlled experiment with complete and representative prior information (template libraries and training sets) to set a baseline for subsequent investigations. This approach probes how each code considered exploits the information content of the data versus prior information from template libraries and training sets.

The outline of the paper is as follows: in § 2 we present the simulated data set; in § 3 we describe the current generation codes employed in the paper; in § 4 we discuss the interpretation of photo- $z$  PDFs in terms of metrics of accuracy; in § 5 we show our results and compare the performance of the codes; in § 6 we offer our conclusions and discuss future extensions of this work.

### 2 DATA

In order to test the current generation of photo- $z$  PDF codes, we employ an existing simulated galaxy catalogue, described in detail in Section 2.1. The experimental conditions shared among all codes are motivated by the LSST SRD requirements and implemented for machine learning and template

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

<sup>2</sup> Available at: [https://lsstdesc.org/assets/pdf/docs/DESC\\_SRM\\_latest.pdf](https://lsstdesc.org/assets/pdf/docs/DESC_SRM_latest.pdf)

113 based photo- $z$  PDF codes according to the procedures of  
 114 Sections 2.3.1 and 2.3.2 respectively.

## 115 2.1 The Buzzard-v1.0 simulation

116 Our mock catalogue is derived from the BUZZARD-highres-  
 117 v1.0 catalogue (DeRose et al. 2019, Wechsler et al., in prep.).  
 118 BUZZARD is built on a dark matter-only N-body simulation  
 119 of  $2048^3$  particles in a  $400 \text{ Mpc h}^{-1}$  box. The lightcone was  
 120 constructed from smoothing and interpolation between a set  
 121 of time snapshots. Dark matter halos were identified using  
 122 the Rockstar software package (Behroozi et al. 2013) and  
 123 then populated with galaxies with stellar masses and ab-  
 124 solute  $r$ -band magnitudes in the SDSS system determined  
 125 using a sub-halo abundance matching model constrained to  
 126 match both projected two-point galaxy clustering statistics  
 127 and an observed conditional stellar mass function (Reddick  
 128 et al. 2013).

129 To assign a spectrum to each galaxy, the Adding Den-  
 130 sity Dependent Spectral Energy Distributions (SEDs) pro-  
 131 cedure (ADDSEDS, deRose in prep.)<sup>3</sup> was used. ADDSEDS  
 132 uses a sample of  $\sim 5 \times 10^5$  galaxies from the magnitude-  
 133 limited SDSS Data Release 6 Value Added Galaxy Cata-  
 134 logue (NYU-VAGC, Blanton et al. 2005) to train an em-  
 135 pirical relation between absolute  $r$ -band magnitude, local  
 136 galaxy density, and SED. Each SDSS spectrum is param-  
 137 eterized by five weights corresponding to a weighted sum  
 138 of five basis SED components using the k-correct software  
 139 package<sup>4</sup> (Blanton & Roweis 2007).

140 Correlations between SED and galaxy environment  
 141 were included so as to preserve the colour-density relation of  
 142 galaxy environments. The distance to the spatially projected  
 143 fifth-nearest neighbour was used as a proxy for local density  
 144 in the SDSS training sample. For each simulated galaxy,  
 145 a galaxy with similar absolute  $r$ -band magnitude and local  
 146 galaxy density was chosen from the training set, and that  
 147 training galaxy's SED was assigned to the simulated galaxy.

### 148 2.1.1 Caveats

149 By necessity, BUZZARD does not contain all of the compli-  
 150 cating factors present in real data, and here we discuss the  
 151 most pertinent ways that these limitations affect our exper-  
 152 iment. BUZZARD includes only galaxies, not stars nor AGN.  
 153 The catalogue-based construction excludes image-level ef-  
 154 fects, such as deblending errors, photometric measurement  
 155 issues, contamination from sky background (Zodiacal light,  
 156 scattered light, etc.), lensing magnification, and Galactic  
 157 reddening.

158 The BUZZARD SEDs are drawn from a set of  $\sim 5 \times 10^5$   
 159 SEDs, which themselves are derived from a five-component  
 160 linear combination fit to  $\sim 5 \times 10^5$  SDSS galaxies; thus the  
 161 sample contains only galaxies that resemble linear combina-  
 162 tions of those for which SDSS obtained spectra, and there  
 163 are necessarily duplicates. The linear combination SEDs also  
 164 restrict the properties of the galaxy population to linear  
 165 combinations of the properties corresponding to five basis  
 166 templates, precluding the modeling of non-linear features

167 such as the full range of emission line fluxes relative to the  
 168 continuum. The only form of intrinsic dust reddening comes  
 169 from what is already present in the five basis SEDs via the  
 170 training set used to create the basis templates, and linear  
 171 combinations thereof do not span the full range of realistic  
 172 dust extinction observed in galaxy populations.

173 While these idealized conditions limit the realism of our  
 174 mock data, they are irrelevant to the controlled experimental  
 175 conditions of this study, if anything assuring that differentia-  
 176 tion in the performance of the photo- $z$  PDF codes is due to  
 177 the inferential techniques rather than nuances in the data.

## 178 2.2 LSST-like mock observations

179 Given the SED, absolute  $r$ -band magnitude, and true red-  
 180 shift of each simulated galaxy, we computed apparent magni-  
 181 tudes in the six LSST filter passbands,  $ugrizy$ . We assigned  
 182 magnitude errors in the six bands using the simple model of  
 183 Ivezić et al. (2008), assuming achievement of the full 10-year  
 184 depth, with a modification of fiducial LSST total numbers  
 185 of 30-second visits for photometric error generation: we as-  
 186 sume 60 visits in  $u$ -band, 80 visits in  $g$ -band, 180 visits in  
 187  $r$ -band, 180 visits in  $i$ -band, 160 visits in  $z$ -band, and 160  
 188 visits in  $y$ -band.

189 As a consequence of adding Gaussian-distributed photo-  
 190 metric errors, 2.0 per cent of our galaxies exhibit a negative  
 191 flux in one or more bands, the vast majority of which are  
 192 in the  $u$ -band. We deem such negative fluxes *non-detections*  
 193 and assign a placeholder magnitude of 99.0 in the catalogue to  
 194 indicate to the photo- $z$  PDF codes that such galaxies would  
 195 be “looked at but not seen” in multi-band forced photome-  
 196 try.

197 The full dataset thus covers 400 square degrees and con-  
 198 tains 238 million galaxies of redshift  $0 < z \leq 8.7$  down  
 199 to  $r = 29$ . Systematic inconsistencies with galaxy colors  
 200 at  $z > 2$  were observed, so the catalogue was limited to  
 201  $0 < z \leq 2.0$ . To obtain a catalogue matching the LSST  
 202 Gold Sample, we imposed a cut of  $i < 25.3$ , which gives a  
 203 signal-to-noise ratio  $\gtrsim 30$  for most galaxies. In order for sta-  
 204 tistical errors to be subdominant to the systematic errors we  
 205 aim to probe, we further reduced the sample size to  $< 10^7$   
 206 galaxies by isolating  $\sim 16.8$  square degrees selected from five  
 207 separate spatial regions of the simulation. We refer to this  
 208 final set of galaxies as DC1, for the first LSST-DESC Data  
 209 Challenge.

## 210 2.3 Shared prior information

211 For the purpose of performing a controlled experiment that  
 212 compares photo- $z$  PDF codes on equal footing as a base-  
 213 line for a future sensitivity analysis, we take care to provide  
 214 each with optimal prior information. Redshift estimation ap-  
 215 proaches built upon physical modeling and machine learning  
 216 alike have a notion of prior information considered beyond  
 217 the photometry of the data for which redshift is to be con-  
 218 strained: that information is derived from a template library  
 219 for a model-based code and a training set for a data-driven  
 220 code. In this initial study, we seek to set a baseline for a  
 221 later comparison of the performance of photo- $z$  PDF codes  
 222 under incomplete and non-representative prior information  
 223 that will propagate differently in the space of data-driven

<sup>3</sup> <https://github.com/vipasu/addseds>

<sup>4</sup> <http://kcorrect.org>

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and model-based algorithms. However, for the baseline case of perfect prior information, physical modeling and machine learning codes can indeed be put on truly equal footing. We outline the equivalent ways of providing all codes perfect prior information below.

### 2.3.1 Training and test set division

Following the findings of Bernstein & Huterer (2010), Newman et al. (2015), and Masters et al. (2017) that only  $\sim 10^4$  spectra are necessary to calibrate photo- $z$ s to Stage IV requirements, we aimed to set aside a randomly selected training set of  $3 - 5 \times 10^4$  galaxies,  $\sim 10$  per cent of the full sample. After all cuts described above, we designated the *DC1 training set* of 44 404 galaxies for which observed photometry, true SEDs, and true redshifts would be provided to all codes and the blinded *DC1 test set* of 399 356 galaxies for which photometry alone would be provided to all codes and photo- $z$  PDFs would be requested. The exact form of LSST photometric filter transmission curves were also considered public information that could be used by any code.

### 2.3.2 Template library construction

We aimed to provide template-fitting codes with complete yet manageable library of templates spanning the space of SEDs of the DC1 galaxies. We constructed  $K = 100$  representative templates from the  $\sim 5 \times 10^5$  SEDs of the SDSS DR6 NYU-VAGC by using the five-dimensional vectors of SED weight coefficients described above. After regularizing the SED weight coefficients  $\in [0, 1]$ , we ran a simple K-means clustering algorithm on the five-dimensional space of regularized SED weight coefficients of the SDSS galaxy sample. The resulting clusters were used to define Voronoi cells in the space of weight coefficients, with centre positions corresponding to weights for the **k**-correct SED components, yielding the 100 SEDs that comprise the *DC1 template set* provided to all template-based codes. We did not, however, exclude from consideration template-based codes that made modifications in their use of these templates due to architecture limitations (as opposed to knowledge of the experimental conditions that could artificially boost the code's apparent performance), with deviations noted in Section 3.

## 3 METHODS

Here we summarize the twelve photo- $z$  PDF codes compared in this study, listed in Table 1, which include both established and emerging approaches in template fitting and machine learning. Though not exhaustive, this sample represents codes for which there was sufficient expertise within the LSST-DESC Photometric Redshifts Working Group. Some aspects of data treatment were left to the individual code runners, for example, whether/how to split the available data with known redshifts into separate training and validation sets.

Another key difference is the treatment of non-detections in one or more bands: some codes ignore incomplete bands, while others replace the value with either an estimate for the detection limit, the mean of other values in the training set, or another default value. There are varying

conventions among machine learning-based codes for treatment of non-detections, and no one prescription dominates in the photo- $z$  literature. However, we remind the reader that only 2.0 per cent of our sample has non-detections, almost exclusively in the  $u$ -band, and thus should not dominate the code performance differences.

The authors welcome interest from those outside LSST-DESC to have their codes assessed in future investigations that build upon this one.

We describe the algorithms and implementations of the model-based and data-driven codes in Sections 3.1 and 3.2 respectively, with a straw-person approach included in Section 3.3.

### 3.1 Template-based Approaches

We test three publicly available and commonly used template-based codes that share the standard physically motivated approach of calculating model fluxes for a set of template SEDs on a grid of redshift values and evaluating a  $\chi^2$  merit function using the observed and model fluxes:

$$\chi^2(z, T, A) = \sum_i^{N_{\text{filt}}} \left( \frac{F_{\text{obs}}^i - A F_{\text{pred}}^i(T, z)}{\sigma_{\text{obs}}^i} \right)^2 \quad (1)$$

where  $A$  is a normalization factor,  $F_{\text{pred}}^i(T, z)$  is the flux predicted for a template  $T$  at redshift  $z$ ,  $F_{\text{obs}}^i$  is the observed flux in a given band  $i$ ,  $\sigma_{\text{obs}}^i$  is the observed flux error, and  $N_{\text{filt}}$  is the total number of filters, in our case the six *ugrizy* LSST filters. The likelihood is a sum of observed flux error  $\sigma_b^{\text{obs}}$ -weighted squared differences between the observed flux  $F_b^{\text{obs}}$  and the normalized predicted flux  $F_b^{\text{mod}}(T, z)$  in  $N_{\text{filt}}$  photometric filters  $b$ , which are the LSST *ugrizy* filters in this case. Specific implementation details of each code, e. g. prior form and implementation, are described below.

#### 3.1.1 BPZ

Bayesian Photometric Redshift (BPZ, Benítez 2000) determines the likelihood  $p(C|z, T)$  of a galaxy's observed colours  $C$  for a set of SED templates  $T$  at redshifts  $z$ . The BPZ likelihood is related to the  $\chi^2$  likelihood by  $p(C|z, T) \propto \exp[-\chi^2/2]$ . Given a Bayesian prior  $p(z, T|m_0)$  over apparent magnitude  $m_0$  and type  $T$ , and assuming that the SED templates are spanning and exclusive, BPZ constructs the redshift posterior  $p(z|C, m_0)$  by marginalizing over all SED templates with the form  $p(z|C, m_0) \propto \sum_T p(C|z, T) p(z, T|m_0)$  (Eq. 3 from Benítez 2000), corresponding to setting the parameter PROBS\_LITE=TRUE in the BPZ parameter file. The BPZ prior is the product of an SED template proportion that varies with apparent magnitude  $p(T|m_0)$  and a prior  $p(z|T, m_0)$  over the expected redshift as a function of apparent magnitude and SED template. We anticipate BPZ to outperform other template-based approaches due to the prior that both comprehensively accounts for SED type and is calibrated to the training set.

Here we test BPZ-v 1.99.3 (Benítez 2000) with the DC1 template set of Section 2.3.2. To keep the number of free parameters manageable, the DC1 template set is pre-sorted by the rest-frame  $u - g$  colour and split into three broad classes of SED template, equivalent to the E, Sp and Im/SB types. The Bayesian prior term  $p(T|m_0)$  was derived directly from

**Table 1.** List of photo- $z$  PDF codes featured in this study

Published code	Type	Public source code
LePhare (Arnouts et al. 1999)	template fitting	<a href="http://www.cfht.hawaii.edu/~arnouts/lephare.html">http://www.cfht.hawaii.edu/~arnouts/lephare.html</a>
BPZ (Benítez 2000)	template fitting	<a href="http://www.stsci.edu/~dcoe/BPZ/">http://www.stsci.edu/~dcoe/BPZ/</a>
EAZY (Brammer et al. 2008)	template fitting	<a href="https://github.com/gbrammer/eazy-photoz">https://github.com/gbrammer/eazy-photoz</a>
ANNz2 (Sadeh et al. 2016)	machine learning	<a href="https://github.com/IftachSadeh/ANNZ">https://github.com/IftachSadeh/ANNZ</a>
FlexBoost (Izbicki & Lee 2017)	machine learning	<a href="https://github.com/tospis/flexcode">https://github.com/tospis/flexcode</a> ; <a href="https://github.com/rizbicki/FlexCoDE">https://github.com/rizbicki/FlexCoDE</a>
GPz (Almosallam et al. 2016b)	machine learning	<a href="https://github.com/OxfordML/GPz">https://github.com/OxfordML/GPz</a>
METAPhR (Cavuoti et al. 2017)	machine learning	<a href="http://dame.dsf.unina.it">http://dame.dsf.unina.it</a>
CMNN (Graham et al. 2018)	machine learning	N/A
SkyNet (Graff et al. 2014)	machine learning	<a href="http://ccforge.cse.rl.ac.uk/gf/project/skynet/">http://ccforge.cse.rl.ac.uk/gf/project/skynet/</a>
TPZ (Carrasco Kind & Brunner 2013)	machine learning	<a href="https://github.com/mgckind/MLZ">https://github.com/mgckind/MLZ</a>
Delight (Leistedt & Hogg 2017)	hybrid	<a href="https://github.com/ixkael/Delight">https://github.com/ixkael/Delight</a>
trainZ	machine learning	See Section 3.3

the DC1 training set, and the other term  $p(z|T, m_0)$  was chosen to be the best fit for the eleven free parameters from the functional form of Benítez (2000). We use template interpolation, creating two linearly interpolated templates between each basis SED (sorted by rest-frame  $u - g$  colour) by setting the parameter `INTERP=2`. Prior to running the code, the non-detection placeholder magnitude was replaced with an estimate of the  $1-\sigma$  detection limit for the undetected band as a proxy for a value close to the estimated sky noise threshold.

### 3.1.3 LePhare

Photometric Analysis for Redshift Estimate (LePhare, Arnouts et al. 1999; Ilbert et al. 2006) uses the  $\chi^2$  of Equation 1 to match observed colours with those predicted from a template set. The template set can be semi-empirical or entirely synthetic. The reported photo- $z$  PDF is an arbitrary normalization of the likelihood evaluated on the output redshift grid.

Here we use LePhare-v 2.2 with the DC1 template set of Section 2.3.2. Unlike both BPZ and EAZY, LePhare uses generic, SED-independent priors that are not tuned to the DC1 data set.

### 3.1.2 EAZY

Easy and Accurate Photometric Redshifts from Yale (EAZY, Brammer et al. 2008) extends the basic  $\chi^2$  fit procedure that defines template-fitting approaches. The algorithm models the observed photometry with a linear combination of template SEDs at each redshift. The best-fit SED at each redshift is found by simultaneously fitting one, two, or all of the templates via  $\chi^2$  minimization, which is distinct from marginalizing across all templates. The minimized  $\chi^2$  likelihood at each redshift is then combined with an apparent magnitude prior to obtain the redshift posterior PDF. We note that the utilization of the best-fit SED conditioned on redshift rather than a proper marginalization does not lead to the correct posterior distribution, an implementation issue that has now been identified and will be addressed by the developers in the future.

In contrast with BPZ, EAZY’s apparent magnitude prior is independent of SED, though it was derived empirically from the DC1 training set. The EAZY architecture cannot accept a template set other than the same five basis templates employed by `k-correct` when constructing the DC1 catalogue, but, for consistency with the experimental scope of perfect prior information, EAZY’s flexible `all-templates` mode was used to fit the photometric data with a linear combination of the five basis templates. Though EAZY can account for uncertainty in the template set by adding in quadrature to the flux errors an empirically derived template error as a function of redshift, we set the template error to zero since the same templates were in fact used to produce the DC1 photometry.

## 3.2 Machine Learning-based Approaches

We compared nine data-driven photo- $z$  estimation approaches, eight of which are described in this section and one of which is discussed in Section 3.3. Because the algorithms differ more from one another and the techniques are relative newcomers to the astronomical literature, we provide somewhat more detail about the implementations below.

### 3.2.1 ANNz2

ANNz2(Sadeh et al. 2016) supports several machine learning algorithms, including artificial neural networks (ANN), boosted decision tree, and k-nearest neighbour (KNN) regression. In addition to accounting for errors on the input photometry, ANNz2 uses the KNN-uncertainty estimate of Oyaizu et al. (2008) to quantify uncertainty in the choice of method over multiple runs. Using the Toolkit for Multivariate Data Analysis with ROOT<sup>5</sup>, ANNz2 can return the results of running a single machine learning algorithm, a “best” choice of the results from simultaneously running multiple algorithms (based on evaluation the cumulative distribution functions of validation set objects), or a combination of the results of multiple algorithms weighted by their method uncertainties averaged over multiple runs.

In this study, we used ANNz2-v.2.0.4 to output only the result of the ANN algorithm. Photo- $z$  PDFs were produced by running an ensemble of 5 ANNs with a 6 : 12 : 12 : 1 architecture corresponding to the 6 *ugrizy* inputs, 2 hidden layers with 12 nodes each, and 1 output of redshift. Each of

<sup>5</sup> <http://tmva.sourceforge.net/>

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413 the five ANNs was trained with different random seeds for  
 414 the initialization of input parameters, reserving half of the  
 415 training set for validation to prevent overfitting. Undetected  
 416 galaxies were excluded from the training set, and per-band  
 417 non-detections in the test set were replaced with the mean  
 418 magnitude in that band within the entire test set.

### 419 3.2.2 Colour-Matched Nearest-Neighbours

420 The colour-matched nearest-neighbours photometric red-  
 421 shift estimator (CMNN, [Graham et al. 2018](#)) uses a training  
 422 set of galaxies with known redshifts that has equivalent or  
 423 better photometry than the test set in terms of quality and  
 424 filter coverage. For each galaxy in the test set, CMNN identifies  
 425 a colour-matched subset of training galaxies using a thresh-  
 426 old in the Mahalanobis distance  $D_M = \sum_j^{N_{\text{colours}}} (c_j^{\text{train}} -$   
 427  $c_j^{\text{test}})^2 / \delta c_{\text{test}}^2$  in the space of available colours  $c$ , with colour  
 428 measurement errors  $\delta c_{\text{test}}$  and  $N_{\text{colours}} = 5$  colours  $j$  defined  
 429 by the *ugrizy* filters, which defines the set of colour-matched  
 430 neighbours based on a value of the percent point function  
 431 (PPF). As an example, for  $N_{\text{filt}} = 5$  with PPF= 0.95, 95 per  
 432 cent of all training galaxies consistent with the test galaxy  
 433 will have  $D_M < 11.07$ . Undetected bands are dropped,  
 434 thereby reducing the effective  $N_{\text{filt}}$  for that galaxy. The  
 435 photo-z PDF of a given test set galaxy is the normalized dis-  
 436 tribution of redshifts of its colour-matched subset of training  
 437 set galaxies.

438 Here, we make two modifications to the implementation  
 439 of [Graham et al. \(2018\)](#) to comply with the controlled exper-  
 440 imental conditions. First, we do not impose non-detections  
 441 on galaxies fainter than the expected LSST 10-year limit-  
 442 ing magnitude nor galaxies bright enough to saturate with  
 443 LSST’s CCDs, instead using all of the photometry for the  
 444 DC1 test and training sets. Second, we apply the initial  
 445 colour cut to the training set before calculating the Ma-  
 446 halanobis distance in order to accelerate processing and use a  
 447 magnitude pseudo-prior as in [Graham et al. \(2018\)](#), but for  
 448 both we use cut-off values corresponding to the DC1 training  
 449 set galaxies’ colours and magnitudes.

450 We make an additional adaptation to enable the CMNN  
 451 algorithm to yield accurate photo-z PDFs for all galaxies,  
 452 as the original [Graham et al. \(2018\)](#) algorithm is optimized  
 453 for photo-z point estimates and is susceptible to less ac-  
 454 curate photo-z PDFs for bright galaxies or those with few  
 455 matches in colour-space. We use PPF= 0.95 rather than  
 456 PPF= 0.68 to generate the subset of colour-matched train-  
 457 ing galaxies, whose redshifts are weighted by their inverse  
 458 Mahalanobis distances when composing the photo-z PDF  
 459 rather than weighting all colour-matched training galaxies  
 460 equally. Additionally, when the number of colour-matched  
 461 training set galaxies is less than 20, the nearest 20 neigh-  
 462 bours in colour-space are used instead, and the output  
 463 photo-z PDF is convolved with a Gaussian kernel of vari-  
 464 ance  $\sigma_{\text{train}}^2 (\text{PPF}_{20}/0.95)^2 - 1$  to account for the corre-  
 465 sponding growth of the effective PPF to include 20 neighbors.

### 466 3.2.3 Delight

467 Delight([Leistedt & Hogg 2017](#)) is a hybrid technique that  
 468 infers photo-zs with a data-driven model of latent SEDs and

469 a physical model of photometric fluxes as a function of red-  
 470 shift. Generally, machine learning methods rely on represen-  
 471 tative training data with shared photometric filters, while  
 472 template-based methods rely on a complete library of tem-  
 473 plates based on physical models constructed. **Delight** aims  
 474 to take the best aspects of both approaches by construct-  
 475 ing a large collection of latent SED templates (or physical  
 476 flux-redshift models) from training data, with a template  
 477 SED library as a guide to the learning of the model, thereby  
 478 circumventing the machine learning prerequisite of represen-  
 479 tative training data in the same photometric bands and the  
 480 template fitting requirement of detailed galaxy SED models.  
 481 It models noisy observed flux  $\hat{\mathbf{F}} = \mathbf{F} + F_b$  as a sum of a noise-  
 482 less flux plus a Gaussian processes  $F_b \sim \mathcal{GP}(\mu^F, k^F)$  with  
 483 zero mean function  $\mu^F$  and a physically motivated kernel  $k^F$   
 484 that induces realistic correlations in flux-redshift space.

485 From a template-fitting perspective, each test set galaxy  
 486 has a posterior  $p(z|\hat{\mathbf{F}}) \approx \sum_i p(\hat{\mathbf{F}}|z, T_i)p(z|T_i)p(T_i)$  of red-  
 487 shift  $z$  conditioned on noisy flux  $\hat{\mathbf{F}}$ , where  $p(z|T_i)p(T_i)$  cap-  
 488 tures prior information about the redshift distributions and  
 489 abundances of the galaxy templates  $T_i$ . As in traditional  
 490 template fitting, each likelihood  $p(\hat{\mathbf{F}}|\mathbf{F})$  relates the noisy flux  
 491  $\hat{\mathbf{F}}$  with the noiseless flux  $\mathbf{F}$  predicted by the model of a linear  
 492 combination of templates, carefully constructed to account  
 493 for model uncertainties and different normalization of the  
 494 same SED, plus the Gaussian process term.

495 The machine learning approach appears in the inclu-  
 496 sion of a pairwise comparison term  $p(\mathbf{F}|z, z_j, \hat{\mathbf{F}}_j)$  for the  
 497 prediction of model flux  $\mathbf{F}$  at a model redshift  $z$  with re-  
 498 spect to training set galaxy  $j$  with redshift  $z_j$  and ob-  
 499 served flux  $\hat{\mathbf{F}}_j$ . Thus the photo-z posterior  $p(\hat{\mathbf{F}}|z, T_i) =$   
 500  $\int p(\hat{\mathbf{F}}|\mathbf{F})p(\mathbf{F}|z, z_j, \hat{\mathbf{F}}_j)d\mathbf{F}$  may be interpreted as the proba-  
 501 bility that the training and the target galaxies have the same  
 502 SED at different redshifts. The flux prediction  $p(\mathbf{F}|z, z_j, \hat{\mathbf{F}}_j)$   
 503 of the training galaxy at redshift  $z$  is modeled via the Gaus-  
 504 sian process described above; more detail is provided in  
 505 [Leistedt & Hogg \(2017\)](#).

506 In this study, the default settings of **Delight** were used,  
 507 with the exception that the PDF bins were set to be linearly  
 508 spaced rather than logarithmically. The Gaussian process  
 509 was trained using the full DC1 training set. We used the  
 510 full DC1 template set with a flat prior in magnitude and  
 511 SED type. Photometric uncertainties from the inputs are  
 512 propagated into the code, while non-detections for each band  
 513 are set to the mean of the respective bands.

### 514 3.2.4 FlexZBoost

515 **FlexZBoost**([Izbicki & Lee 2017](#)) is built on **FlexCode**, a  
 516 general-purpose methodology for converting any conditional  
 517 mean point estimator of  $z$  to a conditional density estima-  
 518 tor  $p(z|\mathbf{x}) \equiv f(z|\mathbf{x})$ , where  $\mathbf{x}$  here represents our photomet-  
 519 ric covariates and errors. **FlexZBoost** expands the unknown  
 520 function  $f(z|\mathbf{x}) = \sum_i \beta_i(\mathbf{x})\phi_i(z)$  using an orthonormal basis  
 521  $\{\phi_i(z)\}_i$ . By the orthogonality property, the expansion  
 522 coefficients  $\beta_i(\mathbf{x}) = \mathbb{E}[\phi_i(z)|\mathbf{x}] \equiv \int f(z|\mathbf{x})\phi_i(z)dz$  are thus  
 523 conditional means. The expectation value  $\mathbb{E}[\phi_i(z)|\mathbf{x}]$  of the  
 524 expansion coefficients conditioned on the data is equivalent  
 525 to the regression of the space of possible redshifts on the  
 526 space of possible photometry. Thus the expansion coeffi-

cients  $\beta_i(\mathbf{x})$  can be estimated from the data via regression to yield the conditional density estimate  $\hat{f}(z|\mathbf{x})$ .

In this paper, we used `xgboost` (Chen & Guestrin 2016) for the regression; it should, however, be noted that `FlexCode-RF`<sup>6</sup>, based on Random Forests, generally performs better on smaller datasets. As our basis  $\phi_i(z)$ , we choose a standard Fourier basis. The two tuning parameters in our photo- $z$  PDF estimate are the number  $I$  of terms in the series expansion and an exponent  $\alpha$  that we use to sharpen the computed density estimates  $\tilde{f}(z|\mathbf{x}) \propto \hat{f}(z|\mathbf{x})^\alpha$ . Both  $I$  and  $\alpha$  were chosen in an automated way by minimizing the weighted  $L_2$ -loss function (Eq. 5 in Izbicki & Lee 2017) on a validation set comprised of a randomly selected 15 per cent of the DC1 training set. While `FlexCode`'s lossless native encoding stores each photo- $z$  PDF using the basis coefficients  $\beta_i(\mathbf{x})$ , we discretized the final estimates into 200 linearly spaced redshift bins  $0 < z < 2$  to match the consistent output format of the experimental conditions.

### 3.2.5 GPz

`GPz`(Almosallam et al. 2016a,b) is a sparse Gaussian process-based code, a scalable approximation of full Gaussian Processes (Rasmussen & Williams 2006), that produces input-dependent variance estimates corresponding to heteroscedastic noise. The model assumes a Gaussian posterior probability  $p(z|\mathbf{x}) = \mathcal{N}(z|\mu(\mathbf{x}), \sigma(\mathbf{x})^2)$  of the output redshift  $z$  given the input photometry  $\mathbf{x}$ . The mean  $\mu(\mathbf{x})$  and the variance  $\sigma(\mathbf{x})^2$  are modeled as functions  $f(\mathbf{x}) = \sum_{i=1}^m w_i \phi_i(\mathbf{x})$  that are linear combinations of  $m$  basis functions  $\{\phi_i(\mathbf{x})\}_{i=1}^m$  with associated weights  $\{w_i\}_{i=1}^m$ . 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). `GPz`'s variance estimate is composed of a model uncertainty term corresponding to sparsity of the training set photometry and a noise uncertainty term encompassing noisy photometric observations, enabling quantification of any need for more representative or more precise training samples. `GPz` may also weight training set samples by importance according to  $|z_{\text{spec}} - z_{\text{phot}}|/(1+z_{\text{spec}})$  to minimize the normalized photo- $z$  point estimate error. However, this function may be adapted to photo- $z$  PDFs, pressuring the model to dedicate more resources to test set galaxies that are not well-represented in the training set.

To smooth the long tail in the distribution of magnitude errors, we use the logarithm of the magnitude errors, improving numerical stability and eliminating the need for constraints on the optimization process. Unobserved magnitudes  $x_u = \mu_u + \Sigma_{uo}\Sigma_{oo}^{-1}(x_o - \mu_o)$  were imputed from observed magnitudes  $x_o$  and the training set mean  $\mu$  and covariance  $\Sigma$  using a linear model. This is the optimal expected value of the unobserved variables given the observed ones under the assumption that the distribution is jointly Gaussian; note that this reduces to a simple average if the covariates are independent with  $\Sigma_{uo} = 0$ . We reserved for validation 20 per cent of the training set and used the Variable Covariance option in `GPz` with 200 basis functions (see

Almosallam et al. (2016b) for details), and did not apply cost-sensitive learning options.

### 3.2.6 METAPhOr

Machine-learning Estimation Tool for Accurate Photometric Redshifts (`METAPhOr`, Cavuoti et al. 2017) is based on the Multi Layer Perceptron with Quasi Newton Algorithm (MLPQNA) with the least square error model and Tikhonov  $L_2$ -norm regularization (Hofmann & Mathé 2018). Photo- $z$  PDFs are generated by running  $N$  trainings on the same training set, or  $M$  trainings on  $M$  different random samplings of the training set. Upon regression of the test set, the photometry  $m_{ij}$  of each test set galaxy  $j$  in filter  $i$  is perturbed according to  $m'_{ij} = m_{ij} + \alpha_i F_{ij}\epsilon$  in terms of the standard normal random variable  $\epsilon \sim \mathcal{N}(0, 1)$ , a multiplicative constant  $\alpha_i$  permitting accommodation of multi-survey photometry, and a bimodal function  $F_{ij}$  composed of a polynomial fit of the mean magnitude errors on the binned bands plus a constant term representing the threshold below which the polynomial's noise contribution is negligible (Brescia et al. 2018).

In this work, we used a hierarchical KNN to replace non-detections with values based on their neighbors. The usual cross-validation of redshift estimates and PDFs was also omitted for this study.

### 3.2.7 SkyNet

`SkyNet`(Graff et al. 2014) employs a neural network based on a second-order conjugate gradient optimization scheme (see Graff et al. 2014, for further details). The neural network is configured as a standard multilayer perceptron with three hidden layers and one input layer with 12 nodes corresponding to the 6 photometric magnitudes and their measurement errors.

`SkyNet`'s classifier mode uses a cross-entropy error function with a 20:40:40 node (all rectified linear units) architecture for each hidden layer and an output layer of 200 nodes corresponding to 200 bins for the PDF, with a softmax activation function to enforce the normalization condition that the probabilities sum to unity. While previous implementations of the code (see Appendix C.3 of Sánchez et al. 2014; Bonnett 2015) implement a sliding bin smoothing, no such procedure was used in this study.

We pre-whitened the data by pegging the magnitudes to (45,45,40,35,42,42) and errors to (20,20,10,5,15,15) for *ugrizy* filters, respectively. To avoid over-fitting, 30 per cent of the training set was reserved for validation, and training was halted as soon as the error rate began to increase on the validation set. The weights were randomly initialized based on normal sampling.

### 3.2.8 TPZ

Trees for Photo- $z$  (`TPZ`, Carrasco Kind & Brunner 2013; Carrasco Kind & Brunner 2014) uses prediction trees and random forest techniques to estimate photo- $z$  PDFs. `TPZ` recursively splits the training set into branch pairs based on maximizing information gain among a random subsample of

<sup>6</sup> <https://github.com/tppspisi/flexcode>;  
<https://github.com/rizbicki/FlexCoDE>

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features, to minimize correlation between the trees, terminating only when a newly created leaf meets a criterion, such as a leaf size minimum or a variance threshold. The regions in each terminal leaf node correspond to a subsample of the training set with similar properties. Bootstrap samples from the training set photometry and errors are used to build a set of prediction trees.

To run TPZ, we replaced non-detections with an approximation of the  $1\sigma$  detection threshold based on the signal-to-noise-based error forecast of the 10-year LSST data, i. e.  $dm = 2.5 \log(1 + N/S)$  where  $dm \sim 0.7526$  magnitudes for  $N/S = 1$  (where  $N$  and  $S$  are the noise and signal). We calibrated TPZ with the Out-of-Bag cross-validation technique (Breiman et al. 1984; Carrasco Kind & Brunner 2013) to evaluate its predictive validity and determine the relative importance of the different input attributes. We grew 100 trees to a minimum leaf size of 5 using the *ugri* magnitudes, all  $u - g, g - r, r - i, i - z, z - y$  colours, and the associated errors, as the  $z$  and  $y$  magnitudes did not show significant correlation with the redshift in our cross-validation. We partitioned our redshift space into 200 bins and smoothed each individual PDF with a smoothing scale of twice the bin size.

### 3.3 trainZ: a pathological photo- $z$ PDF estimator

We also consider a pathological photo- $z$  PDF estimation method, dubbed **trainZ**, which assigns each test set galaxy a photo- $z$  PDF equal to the normalized redshift distribution  $N(z)$  of the training set, according to

$$p(z|\{z_j\}) \equiv \frac{1}{N_{\text{train}}} \sum_{i=1}^{N_{\text{train}}} \begin{cases} 1 & \text{if } z_k \leq z_i < z_{k+1} \\ 0 & \text{otherwise} \end{cases}. \quad (2)$$

Unlike the other methods, the **trainZ** estimator is *independent of the photometric data*, effectively performing a KNN procedure with  $k = N_{\text{train}}$ .

Though **trainZ** is strongly vulnerable to a nonrepresentative training set, it should optimize performance metrics probing the ensemble properties of the galaxy sample, modulo Poisson error due to small sample size, as the training set and test set are drawn from the same underlying population. We will demonstrate its performance under the metrics of Section 4 and discuss it as an illustrative experimental control case in Section 6.1 to highlight the limitations of our evaluation criteria for photo- $z$  PDFs.

## 4 ANALYSIS

The goal of this study is to evaluate the degree to which photo- $z$  PDFs of each method can be trusted for a generic analysis. The overloaded “ $p(z)$ ” is a widespread abuse of notation that obfuscates this goal, so we dedicate attention to dismantling it here.

Galaxies have redshifts  $z$  and photometric data  $d$  drawn from a joint probability space  $p(z, d)$  in nature, and each observed galaxy  $i$  has a *true posterior photo- $z$  PDF*  $p(z|d_i)$ . There are a number of metrics that can be used to test the accuracy of a photo- $z$  posterior as an estimator of a true photo- $z$  posterior if the true photo- $z$  PDF is known. However, the true photo- $z$  PDF of observed data is not accessible, and existing mock catalogues produce redshift-photometry pairs  $(z, d)$  by a deterministic algorithm that

does not correspond to a joint probability density from which one can take samples. In these cases there is no “true PDF” for an individual object, and most measures of PDF fidelity will necessarily be restricted to probing the quality of the ensemble of photo- $z$  PDFs. (See §6.2 for a discussion of how one might circumvent this limitation.)

Before describing the metrics appropriate to the DC1 data set, we outline the philosophy behind our choices. A photo- $z$  PDF estimator derived by method  $H$  must be understood as a posterior probability distribution

$$\hat{p}_i^H(z) \equiv p(z|d_i, I_D, I_H), \quad (3)$$

conditioned not only on the photometric data  $d_i$  for that galaxy but also on parameters encompassing prior information  $I_D$  shared, in our experiment, among all photo- $z$  PDF codes and  $I_H$  that will differ depending on the method  $H$  used to produce it. To be concrete,  $I_D$  takes the form of a training set for the machine learning codes and a template library for the model fitting codes.

The interpretation of the information  $I_H$  is more subtle. This investigation is built upon the knowledge that two codes taking the same approach, among choices of model fitting or machine learning, are nonetheless expected to yield different results even if they take the same external prior information  $I_D$ .  $I_H$  represents the projection of the code’s architecture onto the estimated posteriors over redshift, specific to each code, and even the tunable parameters or random seeds of a specific run of a code with a random component. We refer to  $I_H$  as the *implicit prior*, in contrast with the training set or template library provided to a given code explicitly by the researcher. In simple terms, the implicit prior is the collection of the many different assumptions, coding choices, algorithm selections, and other implementation details that are specific to each code, the ensemble of which results in differing estimates of redshift when combined with the data and prior information in common to all codes.

The presence of the implicit prior in some sense makes a direct comparison of photo- $z$  PDFs produced by different methods impossible; even if they share the same external prior information  $I_D$ , by definition they cannot be conditioned on the same assumptions  $I_H$ , otherwise they would not be distinct methods at all. In this study, we isolate the effect of differences in prior information  $I_H$  specific to each method by using a single training set  $I_D^{\text{ML}}$  for all machine learning-based codes and a single template library  $I_D^T$  for all template-based codes. These sets of prior information are carefully constructed to be representative and complete, so we have  $I_D \equiv I_D^{\text{ML}} \equiv I_D^T$  for every method  $H$ . Under this assumption, a ratio of posteriors of codes is in effect a ratio of the implicit posteriors  $p(z|d_i, I_H')$  since the external prior information  $I_D$  is present in the numerator and denominator. Thus comparisons of  $\hat{p}_i^H(z)$  isolate the effect of the method used to obtain the estimator, which should enable interpretation of the differences between estimated PDFs in terms of the specifics of the method implementations.

The exact implementation of the metrics theoretically depends on the parametrization of the photo- $z$  PDFs, which may differ across codes and can affect the precision of the estimator (Malz et al. 2018). Even considering a single method under the same parametrization, such as the 200-bin  $0 < z < 2$  piecewise constant function used here, the exact

bin definitions must affect the result. The piecewise constant format is chosen because of its established presence in the literature, and the choice of 200 bins was motivated by the approximate number of columns expected to be available for storage of photo-z PDFs for the final LSST Project tables.<sup>7</sup> We will discuss the choice of photo-z PDF parameterization further in Section 6.

This analysis is conducted using the `qp`<sup>8</sup> software package (Malz & Marshall 2018) for manipulating and calculating metrics of univariate PDFs. We present the metrics of photo-z PDFs that address our goals in the sections below. Section 4.1 outlines aggregate metrics of a catalogue of photo-z PDFs, and Section 4.2 presents a metric of individual photo-z PDFs in the absence of true photo-z PDFs. Those seeking a connection to previous comparison studies will find metrics of redshift point estimate reductions of photo-z PDFs in Appendix B and metrics of a science-specific summary statistic heuristically derived from photo-z PDFs in Appendix A.

#### 4.1 Metrics of photo-z PDF ensembles

Because LSST’s photo-z PDFs will be used for many scientific applications, some of which require each individual catalogue entry to be accurate, we consider several metrics that probe the population-level performance of the photo-z PDFs. As we have the true redshifts but not true photo-z PDFs for comparison, we remind the reader of the Cumulative Distribution Function (CDF)

$$\text{CDF}[f, q] \equiv \int_{-\infty}^q f(z) dz, \quad (4)$$

of a generic univariate PDF  $f(z)$ , which is used as the basis for several of our metrics. We describe metrics based on the CDF in Section 4.1.1 and metrics of summary statistics thereof in Section 4.1.2.

##### 4.1.1 CDF-based metrics

A quantile of a distribution is the value  $q$  at which the CDF of the distribution is equal to  $Q$ ; percentiles and quartiles are familiar examples of linearly spaced sets of 100 and 4 quantiles, respectively. The quantile-quantile (QQ) plot serves as a graphical visualization for comparing two distributions, where the quantiles of one distribution are plotted against the quantiles of the other distribution, providing an intuitive way to qualitatively assess the consistency between an estimated distribution and a true distribution. The closer the QQ plot is to diagonal, the closer the match between the distributions.

The probability integral transform (PIT)

$$\text{PIT} \equiv \text{CDF}[\hat{p}, z_{true}] \quad (5)$$

is the CDF of a photo-z PDF evaluated at its true redshift, and the distribution of PIT values probes the average accuracy of the photo-z PDFs of an ensemble of galaxies. The distribution of PIT values is effectively the derivative of the

QQ plot. A catalogue of accurate photo-z PDFs should have a PIT distribution that is uniform  $U(0, 1)$ , and deviations from flatness are interpretable: overly broad photo-z PDFs induce underrepresentation of the lowest and highest PIT values, whereas overly narrow photo-z PDFs induce overrepresentation of the lowest and highest PIT values. Catastrophic outliers with a true redshift outside the support of its photo-z PDF have  $\text{PIT} \approx 0$  or  $\text{PIT} \approx 1$ .

The PIT distribution has been used to quantify the performance of photo-z PDF methods in the past (e. g. Bordoloi et al. 2010; Polsterer et al. 2016; Tanaka et al. 2018). Tanaka et al. (2018) use the histogram of PIT values as a diagnostic indicator of overall code performance, while Freeman et al. (2017) independently define the PIT and demonstrate how its individual values may be used both to perform hypothesis testing (via, e. g. the KS, CvM, and AD tests; see below) and to construct QQ plots. Following Kodra & Newman (in prep.) we define the PIT-based catastrophic outlier rate as the fraction of galaxies with  $\text{PIT} < 0.0001$  or  $\text{PIT} > 0.9999$ , which should total 0.0002 for an ideal uniform distribution.

##### 4.1.2 Summary statistics of CDF-based metrics

We evaluate a number of quantitative metrics derived from the visually interpretable QQ plot and PIT histogram, built on the Kolmogorov-Smirnov (KS) statistic

$$\text{KS} \equiv \max_z \left( \left| \text{CDF}[\hat{f}, z] - \text{CDF}[\tilde{f}, z] \right| \right), \quad (6)$$

interpretable as the maximum difference between the CDFs of the empirical distribution of PIT values for the test sample  $\hat{f}(z)$  and a reference distribution  $\tilde{f}(z)$ , in this case  $U(0, 1)$ , for the ideal distribution of PIT values. We also consider two variants of the KS statistic. A cousin of the KS statistic, the Cramer-von Mises (CvM) statistic

$$\text{CvM}^2 \equiv \int_{-\infty}^{+\infty} (\text{CDF}[\hat{f}, z] - \text{CDF}[\tilde{f}, z])^2 d\text{CDF}[\tilde{f}, z] \quad (7)$$

is the mean-squared difference between the CDFs of an approximate and true PDF. The Anderson-Darling (AD) statistic

$$\text{AD}^2 \equiv N_{tot} \int_{-\infty}^{+\infty} \frac{(\text{CDF}[\hat{f}, z] - \text{CDF}[\tilde{f}, z])^2}{\text{CDF}[\tilde{f}, z](1 - \text{CDF}[\tilde{f}, z])} d\text{CDF}[\tilde{f}, z] \quad (8)$$

is a weighted mean-squared difference featuring enhanced sensitivity to discrepancies in the tails of the distribution. In anticipation of a substantial fraction of galaxies having PIT of 0 or 1, a consequence of catastrophic outliers, we evaluate the AD statistic with modified bounds of integration (0.01, 0.99) to exclude those extremes in the name of numerical stability.

#### 4.2 Conditional Density Estimate (CDE) Loss: a metric of individual photo-z PDFs

The BUZZARD simulation process precludes testing the degree to which samples from our photo-z posteriors reconstruct the space of  $p(z, \text{data})$ . To the knowledge of the authors, there is only one metric that can be used to evaluate the performance of individual photo-z PDF estimators in the absence of true photo-z posteriors. The conditional density

<sup>7</sup> See, e. g. the LSST Data Products Definition Document, available at: <https://ls.st/dpdd>

<sup>8</sup> <http://github.com/aimalz/qp/>

estimation (CDE) loss is an analogue to the familiar root-mean-square-error used in conventional regression, defined as

$$L(f, \hat{f}) \equiv \int \int (f(z|\mathbf{x}) - \hat{f}(z|\mathbf{x}))^2 dz dP(\mathbf{x}), \quad (9)$$

where  $f(z|\mathbf{x})$  is the true photo- $z$  PDF that we do not have and  $\hat{f}(z|\mathbf{x})$  is an estimate thereof, in terms of the photometry  $\mathbf{x}$ . (See Section 3.2.4 for a review of the notation.) We estimate the CDE loss via

$$\hat{L}(f, \hat{f}) = \mathbb{E}_{\mathbf{X}} \left[ \int \hat{f}(z | \mathbf{X})^2 dz \right] - 2\mathbb{E}_{\mathbf{X}, Z} \left[ \hat{f}(Z | \mathbf{X}) \right] + K_f, \quad (10)$$

where the first term is the expectation value of the photo- $z$  posterior with respect to the marginal distribution of the photometric covariates  $\mathbf{X}$ , the second term is the expectation value with respect to the joint distribution of  $\mathbf{X}$  and the space  $Z$  of all possible redshifts, and the third term  $K_f$  is a constant depending only upon the true conditional densities  $f(z|\mathbf{x})$ . We may estimate these expectations empirically on the test or validation data (Eq. 7 in Izbicki et al. 2017) without knowledge of the true densities.

## 5 RESULTS

We begin with a demonstrative visual inspection of the photo- $z$  PDFs produced by each code for individual galaxies. Figure 1 shows the photo- $z$  PDFs for four galaxies chosen as examples of photo- $z$  PDF archetypes: a narrow unimodal PDF, a broad unimodal PDF, a bimodal PDF, and a multimodal PDF. We reiterate that under our idealized experimental conditions, differences between codes are the isolated signature of the implicit prior due to the method by which the photo- $z$  PDFs were derived.

The most striking differences between codes are the small-scale features induced by the interaction between the shared piecewise constant parameterization of 200 bins  $0 < z < 2$  of Section 4 and the smoothing conditions or lack thereof in each algorithm. The  $dz = 0.01$  redshift resolution is sufficient to capture the broad peaks of faint galaxies' photo- $z$  PDFs with large photometric errors but is too broad to resolve the narrow peaks for bright galaxies' photo- $z$  PDFs with small photometric errors. This observation is consistent with the findings of Malz et al. (2018) that the piecewise constant parameterization underperforms in the presence of small-scale structures.

However, the shared small-scale features of ANNz2, METAPhoR, CMNN, and SkyNet are a result of various weighted sums of the limited number of training set galaxies with colours similar to those of the test set galaxy in question, with behavior closer to classification than regression in the case of ANNz2. The settings used on GPz in this work forced broadening of the single Gaussian to cover the multimodal redshift solutions of the other codes.

### 5.1 Performance on photo- $z$ PDF ensembles

The histogram of PIT values, QQ plot, and QQ difference plot relative to the ideal diagonal are provided in Figure 2, showcasing the biases and trends in the average accuracy

**Table 2.** The catastrophic outlier rate as defined by extreme 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  $p(z)$ .

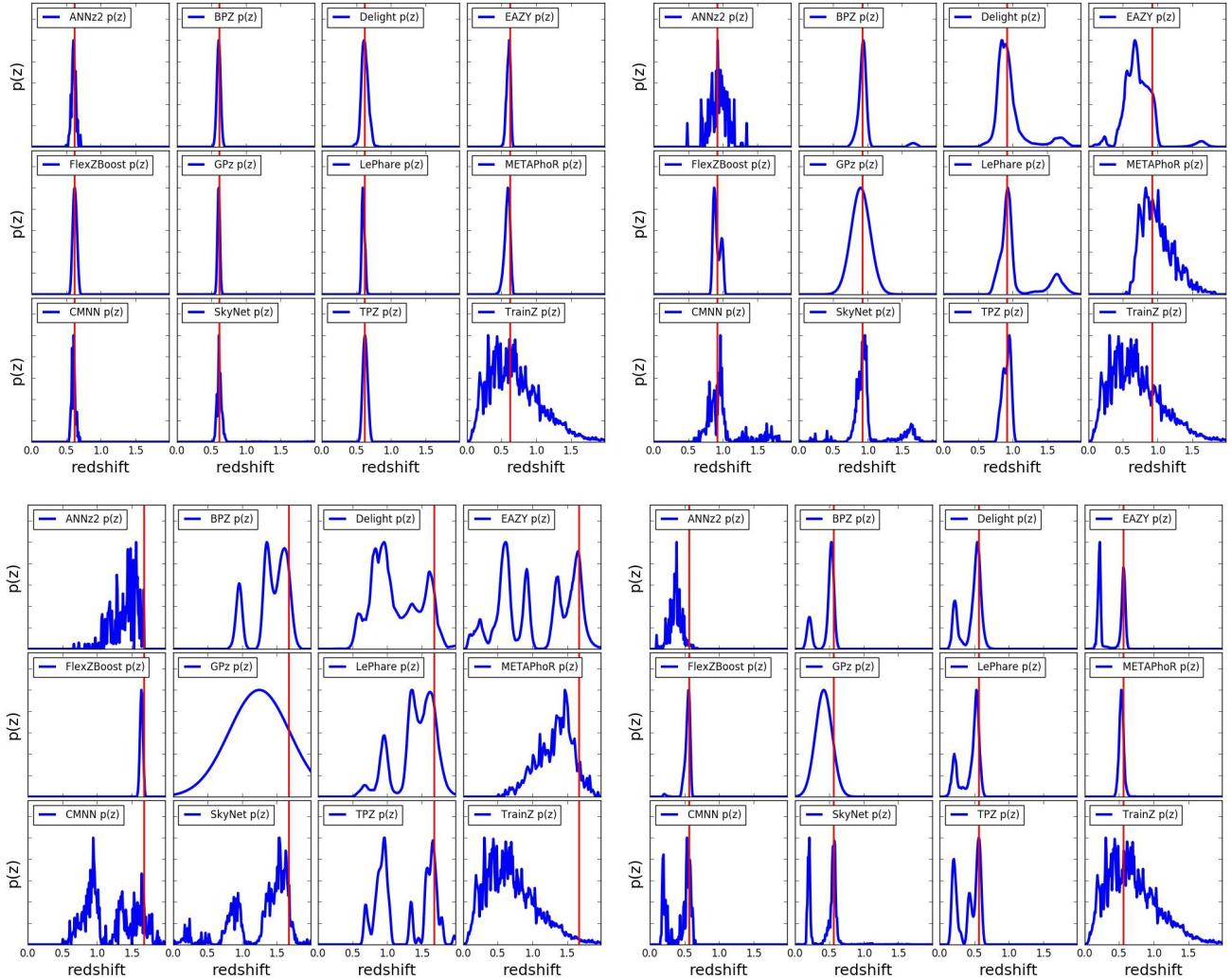
Photo- $z$ Code	fraction PIT < $10^{-4}$ or > 0.999
ANNz2	0.0265
BPZ	0.0192
Delight	0.0006
EAZY	0.0154
FlexZBoost	0.0202
GPz	0.0058
LePhare	0.0486
METAPhoR	0.0229
CMNN	0.0034
SkyNet	0.0001
TPZ	0.0130
trainZ	0.0002

of the photo- $z$  PDFs for each code. The high QQ values (i.e. more high than low PIT values) of BPZ, CMNN, Delight, EAZY, and GPz indicate photo- $z$  PDFs biased low, and the low QQ values (more low than high PIT values) of SkyNet and TPZ indicate photo- $z$  PDFs biased high. The gray shaded band marks the  $2\sigma$  variance in PIT values found using the trainZ algorithm with a bootstrap resampling of the training set and a sample size of 30,000 galaxies, representing a very conservative estimate of the representative training sample size, and thus an approximate minimal error significance compared to ideal performance. Deviations in the PIT histograms outside of this range show that significant biases are present for some codes.

The PIT histograms of Delight, CMNN, SkyNet, and TPZ feature an underrepresentation of extreme values, indicative of overly broad photo- $z$  PDFs, while the overrepresentation of extreme values for METAPhoR indicate overly narrow photo- $z$  PDFs. These five codes in particular have a free parameter for bandwidth, which may be responsible for this vulnerability, in spite of the opportunity for fine-tuning with perfect prior information. FlexZBoost's “sharpening” parameter (described in Section 3.2.4) played a key role in diagonalizing the QQ plot, indicating a common avenue for improvement in the approaches that share this type of parameter. On the other hand, the three purely template-based codes, BPZ, EAZY, and LePhare, do not exhibit much systematic broadening or narrowing, which may indicate that complete template coverage effectively defends from these effects.

Close inspection of the extremes at PIT values of 0 and 1 reveal spikes in the first and last bin of the PIT histogram for some codes in Figure 2, corresponding to catastrophic outliers where the true redshift lies outside of the support of the  $p(z)$ . The catastrophic outlier rates are provided in Table 2. As expected, trainZ achieves precisely the 0.0002 value expected of an ideal PIT distribution. ANNz2, FlexZBoost, LePhare, and METAPhoR have notably high catastrophic outlier rates  $> 0.02$ , exceeding 100 times the ideal PIT rate, meriting further investigation.

Figure 3 highlights the relative values of the KS, CvM, and AD test statistics calculated by comparing the PIT distribution and a uniform distribution  $U(0, 1)$ . METAPhoR and LePhare perform well under the AD but poorly under the



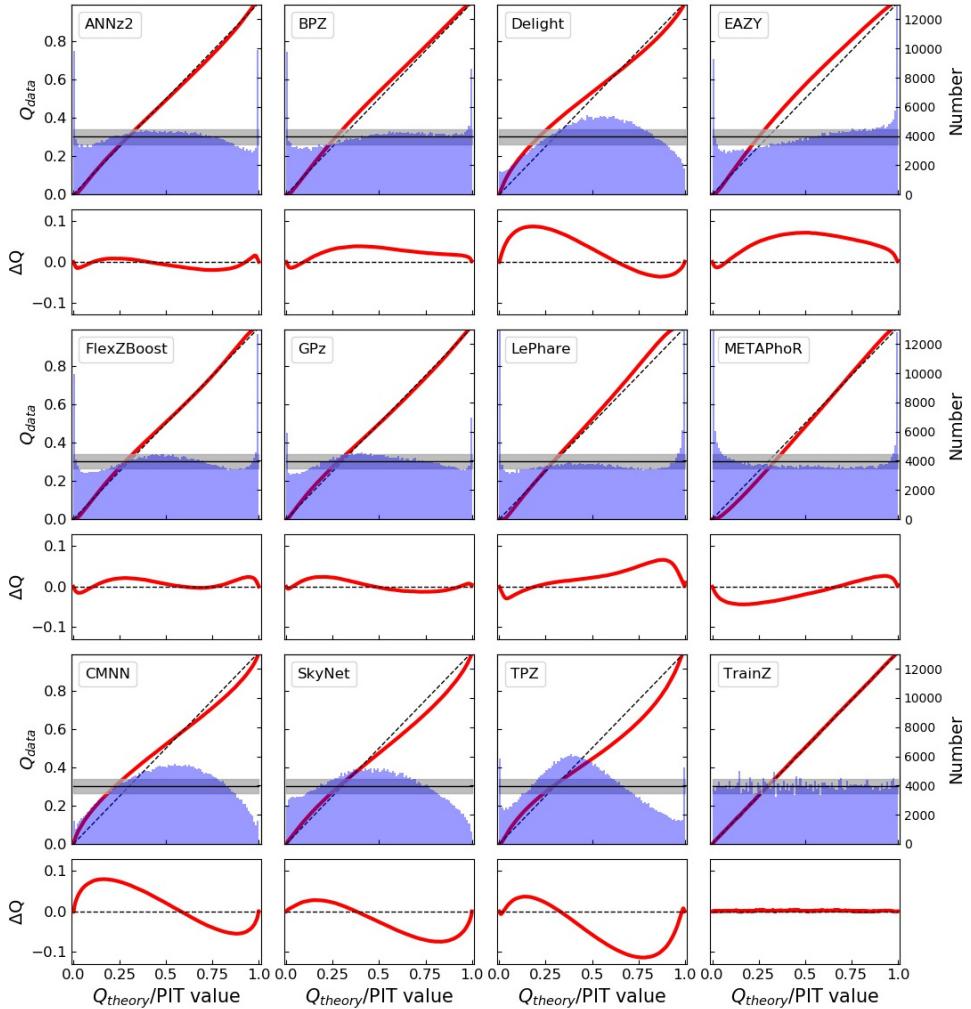
**Figure 1.** The individual photo- $z$  PDFs (blue) distributions produced by the twelve codes (small panels) on four exemplary galaxies' photometry (large panels) with different true redshifts (red). The photo- $z$  PDFs of all codes share some features for the example galaxies due to physical colour degeneracies and photometric errors: tight unimodal  $p(z)$  (upper left), broad unimodal  $p(z)$  (upper right), bimodal  $p(z)$  (lower right), and complex/multimodal  $p(z)$  (lower left). The diverse algorithms and implementations induce differences in small-scale structure and sensitivity to physical systematics.

KS and CvM due to their high catastrophic outlier rates. ANNz2 and FlexZBoost are the top scorers under these metrics of the PIT distribution. ANNz2's strong performance can be attributed to an aspect of the training process in which training set galaxies with a PIT that more closely matches the percentiles of the DC1 training set's redshift distribution are upweighted; in effect, these quantile-based metrics were part of the algorithm itself that may or may not serve it well under more realistic experimental conditions. Similar to what was done for the PIT histograms in Figure 2, we create bootstrap training samples of 30,000 galaxies for use with trainZ in order to estimate a conservative statistical floor that we would expect in real data. No code reaches this idealized floor, indicating that all codes suffer some degradation from the ideal when employing their implicit priors, though ANNz2, FlexZBoost, and GPz are within a factor of two.

## 5.2 Performance on individual photo- $z$ PDFs

The values of the CDE loss statistic of individual photo- $z$  PDF accuracy are provided in Table 3. It is worth noting that strong performance on the CDE loss, corresponding to lower values of the metric, should imply strong performance on the other metrics, though the inverse is not necessarily true. Thus the CDE loss is the most effective metric for generic science cases.

Of the metrics we were able to consider in this experiment, the **CDE Loss is the only metric that can appropriately penalize the pathological trainZ**. Additionally, it favors CMNN and FlexZBoost, the latter of which is optimized for this metric.



**Figure 2.** The QQ plot (red) and PIT histogram (blue) of the photo- $z$  PDF codes (panels) along with the ideal QQ (black dashed diagonal) and ideal PIT (gray horizontal) curves, as well as a difference plot for the QQ difference from the ideal diagonal (lower inset). The gray shaded region indicates the  $2\sigma$  range from a bootstrap resampling of the training set with a size of 30,000 galaxies using `trainZ`. The twelve codes exhibit varying degrees of four deviations from perfection: an overabundance of PIT values at the centre of the distribution indicate a catalogue of overly broad photo- $z$  PDFs, an excess of PIT values at the extrema indicates a catalogue of overly narrow photo- $z$  PDFs, catastrophic outliers manifest as overabundances at PIT values of 0 and 1, and asymmetry indicates systematic bias, a form of model misspecification. Values in excess of the  $2\sigma$  shaded region show that for some codes these errors will be significant given expected training sample sizes.

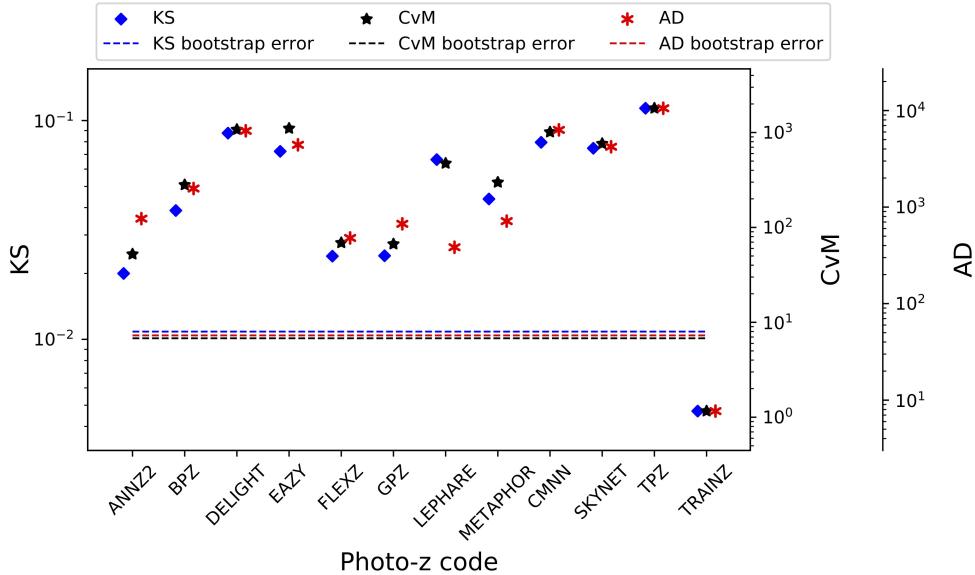
## 979 6 DISCUSSION AND FUTURE WORK

980 In contrast with other photo- $z$  PDF comparison papers that  
 981 have aimed to identify the “best” code for a given survey, we  
 982 have focused on the somewhat more philosophical questions  
 983 of how to assess photo- $z$  PDF methods and how to interpret  
 984 differences between codes in terms of photo- $z$  PDF per-  
 985 formance. In Section 6.1, we reframe the strong performance of  
 986 our pathological photo- $z$  PDF technique, `trainZ`, as a cau-  
 987 tionary tale about the importance of choosing appropriate  
 988 comparison metrics. In Section 6.2, we outline the experi-  
 989 ments we intend to build upon this study. In Section 6.3, we  
 990 discuss the enhancements of the mock data set that will be  
 991 necessary to enable the future experiments.

### 992 6.1 Interpretation of metrics

993 We remind the reader that contributed codes were given a  
 994 goal of obtaining accurate photo- $z$  PDFs, not an accurate  
 995 stacked estimator of the redshift distribution, so we do not  
 996 expect the same codes to necessarily perform well for both  
 997 classes of metrics. Indeed, the codes were optimized for their  
 998 interpretation of our request for “accurate photo- $z$  PDFs,”  
 999 and we expect that the implementations would have been  
 1000 adjusted had we requested optimization of the traditional  
 1001 metrics of Appendices A and B.

1002 Furthermore, our metrics are not necessarily able to as-  
 1003 sess the fidelity of individual photo- $z$  PDFs relative to true  
 1004 posteriors: in the absence of a “true PDF” from which  
 1005 redshifts are drawn, it is difficult to construct metrics to mea-  
 1006 sure performance for individual galaxies rather than ensem-



**Figure 3.** A visualization of the Kolmogorov-Smirnov (KS, blue diamond), Cramer-von Mises (CvM, black star), and Anderson-Darling (AD, red asterisk) statistics for the PIT distributions. There is generally good agreement between these statistics, with differences corresponding to the codes with outstanding catastrophic outlier rates, a reflection in the differences in how each statistic weights the tails of the distribution. Horizontal lines indicate the level of uncertainty found by bootstrapping a training set sample of 30,000 galaxies using `trainZ`; none of the codes reach this conservative ideal floor in expected uncertainty.

**Table 3.** CDE loss statistic of the individual photo- $z$  PDFs for each code. A lower value of the CDE loss indicates more accurate individual photo- $z$  PDFs, with CMNN and FlexZBoost performing best under this metric.

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
<code>trainZ</code>	-0.83

the experimental control, outperforms all codes on the CDF-based metrics, and all but one code on the  $N(z)$  based statistics. The PIT and other CDF-based metrics upon which modern photo- $z$  PDF comparisons are built (Bordoloi et al. 2010; Polsterer et al. 2016; Tanaka et al. 2018) can be gamed by a trivial estimator that yields only an affirmation of prior knowledge uninformed by the data. In other words, such ensemble metrics are not appropriate for the task of selecting photo- $z$  PDF codes for analysis pipelines.

The CDE loss and point estimate metrics appropriately penalize `trainZ`'s naivete. As shown in Appendix B, `trainZ` has identical  $ZPEAK$  and  $ZWEIGHT$  values for every galaxy, and thus the photo- $z$  point estimates are constant as a function of true redshift, 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 5.2, distinguishes this metric from those of the photo- $z$  PDF ensemble and stacked estimator of the redshift distribution, despite their prevalence in the photo- $z$  literature.

bles. (The CDE Loss metric of section 4.2 is an exception to this rule.) A lack of appropriate metrics more sophisticated than the CDE Loss remains an open issue for science cases requiring accurate individual galaxy PDFs. The metric-specific performance demonstrated in this paper implies that we may need multiple photo- $z$  PDF approaches tuned to each metric in order to maximize returns over all science cases in large upcoming surveys.

The `trainZ` estimator of Section 3.3, which assigns every galaxy a photo- $z$  PDF equal to  $N(z)$  of the training set, is introduced as an experimental control or null test to demonstrate this point via *reductio ad absurdum*. Because our training set is perfectly representative of the test set,  $N(z)$  should be identical for both sets down to statistical noise. We make the alarming observation that `trainZ`,

In summary, context is crucial to defend against deceptively strong performers such as `trainZ`; the best photo- $z$  PDF method is the one that most effectively achieves our science goals, not the one that performs best on a metric that does not reflect those goals. In the absence of a single scientific motivation or the information necessary for a principled metric definition, we must consider many metrics and be critical of the information transmitted by each.

## 1052 6.2 Extensions to the experimental design

1053 The work presented in this paper is only a first step in assessing photo- $z$  PDF approaches and moving toward an improved photometric redshift estimator. Here we discuss the next steps for subsequent investigations.

1057 This initial paper explores photo- $z$  PDF code performance in idealized conditions with perfect catalogue-based photometry and representative training data, but the resilience of each code to such realistic imperfections in prior information has not yet been evaluated. A top priority for a follow-up study is to test realistic forms of incomplete, erroneous, and non-representative template libraries and training sets as well as the impact of other forms of external priors that must be ingested by the codes, major concerns in Newman et al. (2015); Masters et al. (2017). Outright redshift failures due to emission line misidentification or noise spikes may be modeled by the inclusion of a small number of high-confidence yet false redshifts. We plan to perform a full sensitivity analysis on a realistically incomplete training set of spectroscopic galaxies, modeling the performance of spectrographs, emission-line properties, and expected signal-to-noise to determine which potential training set galaxies are most likely to be excluded.

1075 Appendix A only addresses the stacked estimator of the redshift distribution of the entire galaxy catalogue rather than subsets in bins, tomographic or otherwise. The effects of tomographic binning scheme will be explored in a dedicated future paper, including propagation of redshift uncertainties in a set of fiducial tomographic redshift bins in order to estimate impact on cosmological parameter estimation.

1082 Sequels to this study will also address some shortcomings of our experimental procedure. The fixed redshift grid shared between the codes may have unfairly penalized codes with a different native parameterization, as precision is lost when converting between formats. Performance on the (admittedly small) population of sharply peaked photo- $z$  PDFs may have been suppressed across all codes due to the insufficient resolution of the redshift grid. In light of the results of Malz et al. (2018), in future analyses we plan to switch from a fixed grid to the quantile parameterization or to permit each code to use its native storage format under a shared number of parameters.

1094 Section 4 discussed the difficulty in evaluating PDF accuracy for individual objects with known  $(z, d)$  information but without a known  $p(z, d)$ . In a follow-up study, we will generate mock data probabilistically, yielding true PDFs in addition to true redshifts and photometric data. This future data set will enable tests of PDF accuracy for individual galaxies rather than solely ensembles.

## 1101 6.3 Realistic mock data

1102 To make optimal use of the LSST data for cosmological and other astrophysical analyses of the LSST-DESC Science Roadmap, future investigations that build upon this one will require a more sophisticated set of galaxy photometry and redshifts. This initial paper explored a data set that was constructed at the catalogue level, with no inclusion of the complications that come from measuring photometry from images. Future data challenges will move to catalogues constructed from mock images, including the complications

1111 of deblending, sensor inefficiencies, and heterogeneous observing conditions, all anticipated to affect the measured colours of LSST’s galaxy sample (Dawson et al. 2016).

1112 The DC1 galaxy SEDs were linear combinations of just five basis SED templates, but a next generation of data for photo- $z$  PDF investigations must include a broader range of physical properties. Though we only considered  $z < 2$  here, LSST 10-year data will contain  $z > 2$  galaxies, plagued by fainter apparent magnitudes and anomalous colours due to stellar evolution. A subsequent study must also have a data set that includes low-level active galactic nuclei (AGN) features in the SEDs, which perturb colours and other host galaxy properties. An observational degeneracy between the Lyman break of a  $z \sim 2 - 3$  galaxy from the Balmer break of a  $z \sim 0.2 - 0.3$  galaxy is a known source of catastrophic outliers (Massarotti et al. 2001) that was not effectively included in this study. To gauge the sensitivity of photo- $z$  PDF estimators to catastrophic outliers, our data set must include realistic high-redshift galaxy populations.

1113 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).

## 7 CONCLUSION

1131 This paper compares twelve photo- $z$  PDF codes under controlled experimental conditions of representative and complete prior information to set a baseline for an upcoming sensitivity analysis. This work isolates the impact on metrics of photo- $z$  PDF accuracy due to the estimation technique as opposed to the complications of realistic physical systematics of the photometry. Though the mock data set of this investigation did not include true photo- $z$  posteriors for comparison, we interpret deviations from perfect results given perfect prior information as the imprint of the implicit assumptions underlying the estimation approach.

1132 We evaluate the twelve codes under science-agnostic metrics both established and emerging to stress-test the ensemble properties of photo- $z$  PDF catalogues derived by each method. In appendices, we also present metrics of point estimates and a prevalent summary statistic of photo- $z$  PDF catalogues used in cosmological analyses to enable the reader to relate this work to studies of similar scope. We observe that no one code dominates in all metrics, and that the standard metrics of photo- $z$  PDFs and the stacked estimator of the redshift distribution can be gamed by a very simplistic procedure that asserts the prior over the data. We emphasize to the photo- $z$  community that metrics used to vet photo- $z$  PDF methods must be scrutinized to ensure they correspond to the quantities that matter to our science.

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1163 Author contributions are listed below.  
S.J. Schmidt: Co-led the project. (conceptualization, data curation, formal analysis, investigation, methodology,

1168 project administration, resources, software, supervision, 1229  
 1169 visualization, writing – original draft, writing – review & 1230  
 1170 editing) 1231  
 1171 A.I. Malz: Co-led the project, contributed to choice of 1232  
 1172 metrics, implementation in code, and writing. (conceptu- 1233  
 1173 alization, methodology, project administration, resources, 1234  
 1174 software, visualization, writing – original draft, writing – 1235  
 1175 review & editing) 1236  
 1176 J.Y.H. Soo: Ran ANNz2 and Delight, updated abstract, 1237  
 1177 edited sections 1 through 6, added tables in Methods 1238  
 1178 and Results, updated references.bib and added references 1239  
 1179 throughout the paper 1240  
 1180 I.A. Almosallam: vetted the early versions of the data set 1241  
 1181 and ran many photo-z codes on it, applied GPz to the final 1242  
 1182 version and wrote the GPz subsection 1243  
 1183 M. Brescianini: main ideator of METAPHOR and of MLPQNA; 1244  
 1184 modification of METAPHOR pipeline to fit the LSST data 1245  
 1185 structure and requirements 1246  
 1186 S. Cavaudi: Contributed to choice and test of metrics, ran 1247  
 1187 METAPHOR, minor text editing 1248  
 1188 J. Cohen-Tanugi: contributed to running code, analysis 1249  
 1189 discussion, and editing, reviewing the paper 1250  
 1190 A.J. Connolly: Developed the colour-matched nearest- 1251  
 1191 neighbours photo-z code; participated in discussions of the 1252  
 1192 analysis. 1253  
 1193 P.E. Freeman: Contributed to choice of CDE metrics and 1254  
 1194 to implementation of FlexZBoost 1255  
 1195 M.L. Graham: Ran the colour-matched nearest-neighbours 1256  
 1196 photo-z code on the Buzzard catalogue and wrote the 1257  
 1197 relevant piece of Section 2; participated in discussions of 1258  
 1198 the analysis. 1259  
 1199 K. Iyer: assisted in writing metric functions used to evaluate 1260  
 1200 codes 1261  
 1201 M.J. Jarvis: Contributed text on AGN to Discussion section 1262  
 1202 and portions of GPz work 1263  
 1203 J.B. Kalmbach: Worked on preparing the figures for the 1264  
 1204 paper. 1265  
 1205 E. Kovacs: Ran simulations, discussed data format and 1266  
 1206 properties for SEDs, dust, and ELG corrections 1267  
 1207 A.B. Lee: Co-developed FlexZBoost and the CDE loss 1268  
 1208 statistic, wrote text on the work, and supervised the 1269  
 1209 development of FlexZBoost software packages 1270  
 1210 G. Longo: Scientific advise, test and validation of the 1271  
 1211 modified METAPHOR pipeline, text of the METAPHOR 1272  
 1212 section 1273  
 1213 C. B. Morrison: Managerial support; Discussions with au- 1274  
 1214 thors regarding metrics and style; Some coding contribution 1275  
 1215 to metric computation. 1276  
 1216 J. Newman: Contributions to overall strategy, design of 1277  
 1217 metrics, and supervision of work done by Rongpu Zhou 1278  
 1218 E. Nourbakhsh: Ran and optimized TPZ code and wrote a 1279  
 1219 subsection of Section 2 for TPZ 1280  
 1220 E. Nuss: contributed to running code, analysis discussion, 1281  
 1221 and editing, reviewing the paper 1282  
 1222 T. Pospisil: Co-developed FlexZBoost software and CDE 1283  
 1223 loss calculation code 1284  
 1224 H. Tramin: contributed to providing SkyNet results and 1285  
 1225 writing the relevant section 1286  
 1226 R. Zhou: Optimized and ran EAZY and contributed to the 1287  
 1227 draft 1288  
 1228 R. Izbicki: Co-developed FlexZBoost and the CDE loss 1289  
 1229 1290

statistic, and wrote software for FlexZBoost

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In addition to packages cited in the text, analyses performed in this paper used the following software packages: **Numpy** and **Scipy** (Oliphant 2007), **Matplotlib** (Hunter 2007), **Seaborn** (Waskom et al. 2017), **minFunc** (Schmidt 2005), **qp** (Malz & Marshall 2018; Malz et al. 2018), **pySkyNet** (Bonnett 2016), and **photUtils** from the LSST simulations package (Connolly et al. 2014).

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## APPENDIX A: EVALUATION OF THE REDSHIFT DISTRIBUTION

Perhaps the most popular application of photo-z PDFs is the estimation of the overall redshift distribution  $N(z)$ , a quantity that enters some cosmological calculations and the true value of which is known for the DC1 data set and will be denoted as  $\tilde{N}(z)$ . In terms of the prior information provided to each method, the true redshift distribution satisfies the tautology  $\tilde{N}(z) = p(z|I_D)$  due to our experimental set-up; because the DC1 training and template sets are representative and complete,  $I_D$  represents a prior that is also equal to the truth. In this ideal case of complete and representative prior information, the method that would give the best approximation to  $\tilde{N}(z)$  would be one that neglects all the information contained in the photometry  $\{d_i\}_{N_{tot}}$  and gives every galaxy the same photo-z PDF  $\hat{p}_i(z) = \tilde{N}(z)$  for all  $i$ ; the inclusion of any information from the photometry would only introduce noise to the optimal result of returning the prior. This is the exact estimator, **trainZ**, that we have described in Section 3.3, and which will serve as an experimental control.

1287   **A1 Metrics of the stacked estimator of the  
1288    redshift distribution**

1289   “Stacking” according to

$$1290 \quad \hat{N}^H(z) \equiv \frac{1}{N_{tot}} \sum_i^{N_{tot}} \hat{p}_i^H(z) \quad (A1)$$

1291   is the most widely used method for obtaining  $\hat{N}^H(z)$  as an  
1292   estimator of the redshift distribution from photo- $z$  PDFs  
1293   derived by a method  $H$ . While the stacked estimator of the  
1294   redshift distribution violates the mathematical definition of  
1295   statistical independence and is thus not formally correct<sup>9</sup>,  
1296   we use it as a basis for comparison of photo- $z$  PDF methods  
1297   under the untested assumption that the response of our met-  
1298   rics of  $\hat{N}^H(z)$  will be analogous to the same metrics applied  
1299   to a principled estimator of the redshift distribution.

1300   As  $N(z)$  is itself a univariate PDF, we apply the met-  
1301   rics of the previous sections to it as well. We additionally  
1302   calculate the first three moments

$$1303 \quad \langle z^m \rangle \equiv \int_{-\infty}^{\infty} z^m N(z) dz \quad (A2)$$

1304   of the estimated redshift distribution  $\hat{N}^H(z)$  for each code  
1305   and compare them to the moments of the true redshift distri-  
1306   bution  $\tilde{N}(z)$ . Under the assumption that the stacked estima-  
1307   tor is unbiased, a superior method minimizes the difference  
1308   between the true and estimated moments.

1309   **A2 Performance on the stacked estimator of the  
1310    redshift distribution**

1311   Figure A1 shows the stacked estimator  $\hat{N}(z)$  of the redshift  
1312   distribution for each code compared to the true redshift  
1313   distribution  $\tilde{N}(z)$ , where the stacked estimator has been  
1314   smoothed for each code in the plot using a kernel density  
1315   estimate (KDE) with a bandwidth chosen by Scott’s Rule  
1316   (Scott 1992) in order to minimize visual differences in small-  
1317   scale features; the quantitative statistics, however, are calcu-  
1318   lated using the empirical CDF which is not smoothed.

1319   Many of the codes, including all the model-fitting app-  
1320   roaches and ANNz2, GPz, METAPhoR, and SkyNet from the  
1321   data-driven camp, overestimate the redshift density at  $z \sim$   
1322   1.4. This behavior is a consequence of the 4000 Å break  
1323   passing through the gap between the  $z$  and  $y$  filters, which  
1324   induces a genuine discontinuity in the  $z - y$  colour as a func-  
1325   tion of redshift that can sway the photo- $z$  PDF estimates in  
1326   the absence of bluer spectral features.

1327   ANNz2, GPz, and METAPhoR feature exaggerated peaks  
1328   and troughs relative to the training set, a potential sign  
1329   of overtraining. Further investigation on overtraining is  
1330   needed, if present this is an obstacle that may be overcome  
1331   with adjustment of the implementation.

1332   As expected, trainZ perfectly recovers the true redshift  
1333   distribution: as the training sample is selected from the same  
1334   underlying distribution as the test set, the redshift distribu-  
1335   tions are identical, up to Poisson fluctuations due to the  
1336   finite number of sample galaxies. CMNN is also in excellent

<sup>9</sup> Malz & Hogg (prep) shows how the stacking procedure can lead to bias in the estimate of  $N(z)$  and presents a principled alternative to this commonly employed method.

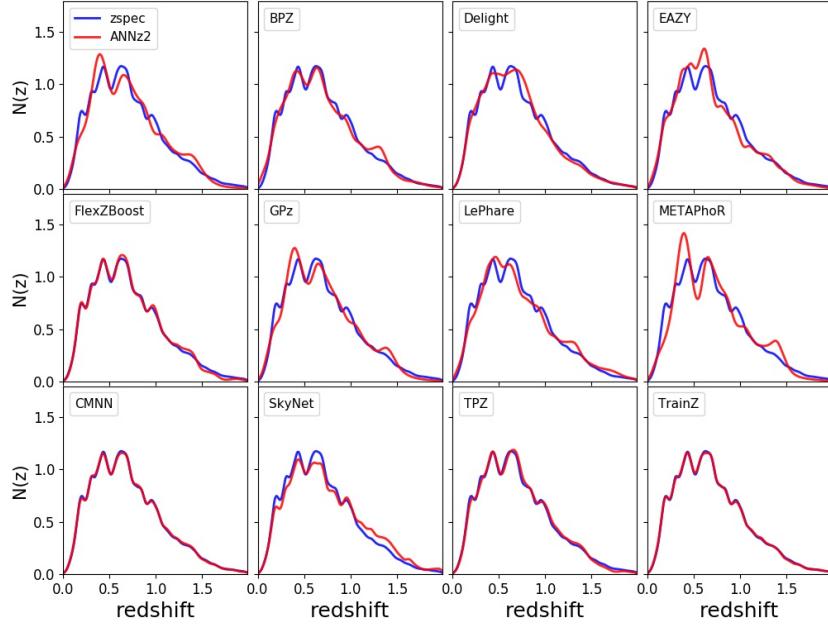
1337   agreement for similar reasons: with a representative train-  
1338   ing sample of galaxies spanning the colour-space, the sum  
1339   of the colour-matched neighbour redshifts should return the  
1340   true redshift distribution. FlexZBoost and TPZ also perform  
1341   superb recovery of the true redshift distribution, with only  
1342   a slight deviation at  $z \sim 1.4$ . Our metrics, however, cannot  
1343   discern whether these four approaches, as well as Delight,  
1344   are spared the  $z \sim 1.4$  degeneracy in  $\hat{N}(z)$  because they have  
1345   more effectively used information in the data or if the impact  
1346   is simply washed out by the stacked estimator’s effective av-  
1347   erage over the test set galaxy sample. See Appendix B for  
1348   further discussion of the  $z \sim 1.4$  issue.

1349   Figure A2 shows the quantitative Kolmogorov-Smirnov  
1350   (KS), Cramer-Von Mises (CvM), and Anderson Darling  
1351   (AD) test statistics for each of the codes for the  $\hat{N}(z)$  based  
1352   measures. The horizontal lines show the the result of a boot-  
1353   strap resampling of the training set using 30,000 samples for  
1354   trainZ, representing a conservative idealized limit on ex-  
1355   pected performance for a modest-sized representative train-  
1356   ing set of galaxies, as mentioned in Section 5.1. The AD  
1357   bootstrap statistic is elevated due to its sensitivity to the  
1358   tails of distributions. The stacked estimators of the redshift  
1359   distribution for CMNN and trainZ best estimate  $\hat{N}(z)$  under  
1360   these metrics, whereas EAZY, LePhare, METAPhoR, and  
1361   SkyNet underperform; BPZ, GPz, and TPZ are within a factor  
1362   of two of the conservative limit for all statistics. It is un-  
1363   surprising that CMNN scores well, as with a nearly complete  
1364   and representative training set choosing neighbouring points  
1365   in colour/magnitude space to construct an estimator should  
1366   lead to excellent agreement in the final  $\hat{N}(z)$ .

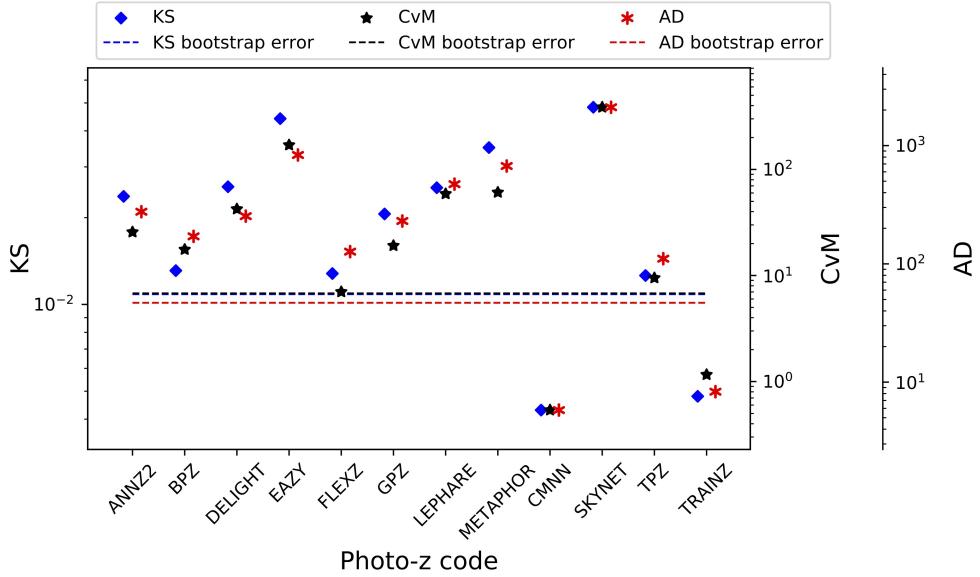
1367   It is, however, surprising that TPZ does well on  $\hat{N}(z)$   
1368   given its poor performance on the ensemble photo- $z$  PDFs,  
1369   especially knowing that TPZ was optimized for photo- $z$  PDF  
1370   ensemble metrics rather than the stacked estimator of the  
1371   redshift distribution. A possible explanation is the choice of  
1372   smoothing parameter chosen during validation, which affects  
1373   photo- $z$  PDF widths as well as overall redshift bias and could  
1374   be modified to improve performance under the photo- $z$  PDF  
1375   metrics.

1376   We calculated the first three moments of the stacked  
1377    $\hat{N}(z)$  distribution of all galaxies and compared it to the mo-  
1378   ments of the true redshift distribution. Figure A3 shows the  
1379   residuals of the moments for all codes. Accuracy of the  
1380   moments varies widely between codes, raising concerns about  
1381   the propagation to cosmological analyses. The DESC SRD  
1382   (The LSST Dark Energy Science Collaboration et al. 2018)  
1383   lists stringent requirements on how well the mean and varia-  
1384   nce of tomographic redshift bins must be known for each of  
1385   the main DESC science cases. We indicate the Year 10 (Y10)  
1386   requirements assuming our true mean redshift of  $z = 0.701$   
1387   as dashed lines. In this study with representative training  
1388   data, ANNz2, CMNN, TPZ, and our pathological trainZ es-  
1389   timator meet the Y10 requirement on the mean redshift.  
1390   Only ANNz2, CMNN, and trainZ meet both requirements. One  
1391   should be concerned that many codes fail to meet this ambi-  
1392   tious limit under perfect prior information because all codes  
1393   are anticipated to do no better under realistically imperfect  
1394   prior information, and indicates that additional calibration  
1395   to remove these systematic offsets (e. g. Newman 2008) will  
1396   likely be necessary in order to meet these stringent goals.

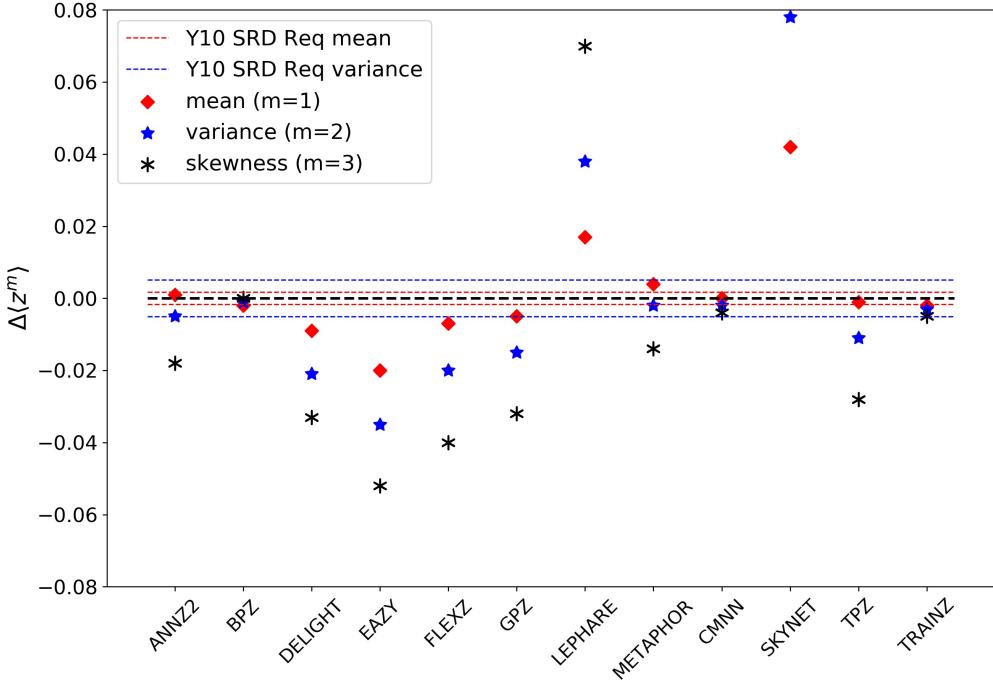
1397   SkyNet exhibits redshift bias in Figure A1 and is a clear  
1398   outlier in the first moment of  $\hat{N}(z)$  in Figure A3. The SkyNet



**Figure A1.** The smoothed stacked estimator  $\hat{N}(z)$  of the redshift distribution (red) produced by each code (panels) compared to the true redshift distribution  $\tilde{N}(z)$  (blue). Varying levels of agreement are seen among the codes, with the smallest deviations for CMNN, FlexZBoost, TPZ, and trainZ.



**Figure A2.** A visualization 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. Horizontal lines indicate the statistic values (including uncertainty) achieved using `trainZ` via bootstrap resampling a training set containing 30,000 redshifts. We make the reassuring observation that these related statistics do not disagree significantly with one another. CMNN outperforms the control case, `trainZ`, and several codes are within a factor of two of this conservative idealized limit. SkyNet scores poorly due to an overall bias in its redshift predictions.



**Figure A3.** Residuals of the first three moments of the stacked  $\hat{N}(z)$  distribution. Red and blue horizontal lines indicate the Year 10 DESC SRD requirements on accuracy of the mean and variance respectively. Only a small number of codes are able to meet these specifications even with perfect training data.

algorithm employs a random subsampling of the training set without testing that the subset is representative of the full population, and the implementation used here does not upweight rarer low- and high-redshift galaxies, as in Bonnett (2015), suggesting a possible cause that may be addressed in future work.

## APPENDIX B: Photo- $z$ POINT ESTIMATION AND METRICS

While this work assumes that science applications value the information of the full photo- $z$  PDF, we present conventional metrics of photo- $z$  point estimates as a quick and dirty visual diagnostic tool and to facilitate direct comparisons to historical studies.

### B1 Reduction of photo- $z$ PDFs to point estimates

Though we acknowledge that many of the codes can also return a native photo- $z$  point estimate, we put all codes on equal footing by considering two generic photo- $z$  point estimators, the mode  $z_{PEAK}$  and main-peak-mean  $z_{WEIGHT}$  (Dahlen et al. 2013), a weighted mean within the bounds of the main peak, as identified by the roots of  $p(z) - 0.05 \times z_{PEAK}$ . Though  $z_{WEIGHT}$  neglects information in a secondary peak of e.g. a bimodal distribution, it avoids the pitfall of reducing the photo- $z$  PDF to a redshift between peaks where there is low probability.

### B2 Metrics of photo- $z$ point estimates

We calculate the commonly used point estimate metrics of the overall intrinsic scatter, bias, and catastrophic outlier rate, defined in terms of the standard error  $e_z \equiv (z_{PEAK} - z_{true})/(1 + z_{true})$ . Because the standard deviation of the photo- $z$  residuals is sensitive to outliers, we define the scatter in terms of the Interquartile Range (IQR), the difference between the 75th and 25th percentiles of the distribution of  $e_z$ , imposing the scaling  $\sigma_{IQR} = IQR/1.349$  to ensure that the area within  $\sigma_{IQR}$  is the same as that within one standard deviation from a standard Normal distribution. We also resist the effect of catastrophic outliers by defining the bias  $b_z$  as the median rather than mean value of  $e_z$ . The catastrophic outlier rate  $f_{out}$  is defined as the fraction of galaxies with  $e_z$  greater than  $\max(3\sigma_{IQR}, 0.06)$ .

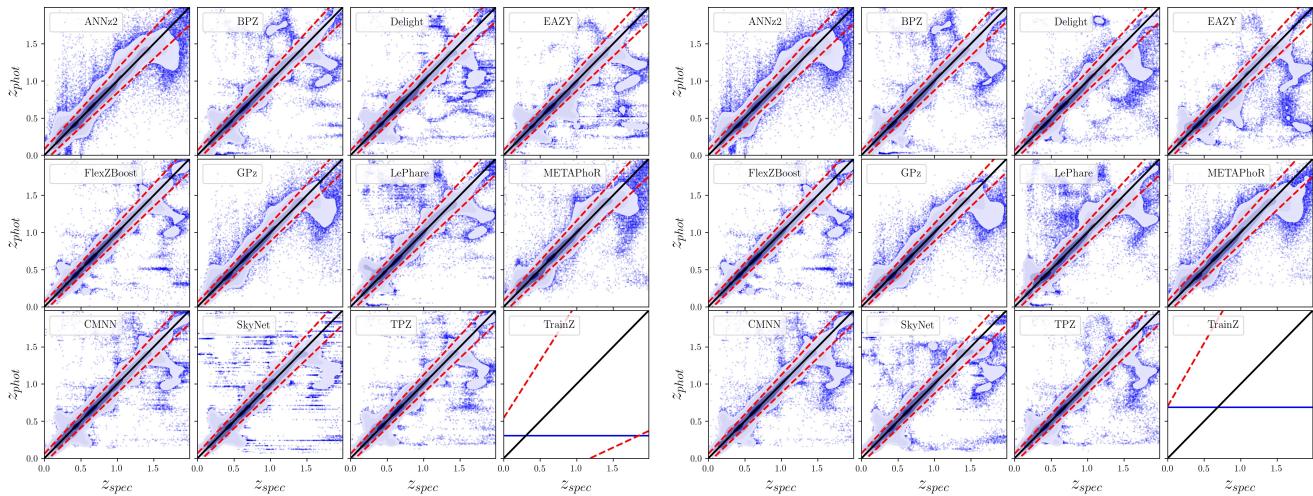
For reference, Section 3.8 of the LSST Science Book (Abell et al. 2009) uses the standard definitions of these parameters in requiring

- RMS scatter  $\sigma < 0.02(1 + z_{true})$
- bias  $b_z < 0.003$
- catastrophic outlier rate  $f_{out} < 10$  per cent .

### B3 Comparison of photo- $z$ point estimate metrics

Figure B1 shows both point estimates for all codes both  $z_{PEAK}$  and  $z_{WEIGHT}$ . Point density is shown with mixed contours to emphasize that most of the galaxies do fall close to the  $z_{phot} = z_{spec}$  line, while points trace the details of the catastrophic outlier populations.

The finite grid spacing of the photo- $z$  PDFs induces some discretization in  $z_{PEAK}$ . The features perpendicular



**Figure B1.** The density of photo- $z$  point estimates (contours) reduced from the photo- $z$  PDFs with outliers (blue) beyond the outlier cutoff (red dashed lines), via the mode ( $z_{PEAK}$ , left panel) and main-peak-mean ( $z_{WEIGHT}$ , right panel). The `trainZ` estimator (lower right sub-panels) has a shared  $z_{PEAK}$  and  $z_{WEIGHT}$  for the entire test set galaxy sample.

to the  $z_{phot} = z_{spec}$  line are due to the 4000 Å break passing through the gaps between adjacent filters. Even the strongest codes feature populations far from the  $z_{phot} = z_{spec}$  line representing a degeneracy in the space of colours and redshifts.

The intrinsic scatter, bias, and catastrophic outlier rate are given in Table B1. Perhaps unsurprisingly, performance under these metrics largely tracks that of the metrics of Section 4 of the photo- $z$  PDFs from which the point estimates were derived. All twelve codes perform at or near the goals of the LSST Science Requirements Document<sup>10</sup> and Graham et al. (2018), which is encouraging if not unexpected for  $i < 25.3$ .

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<sup>10</sup> available at: <http://ls.st/srd>

**Table B1.** Photo- $z$  point estimate statistics

Photo- $z$ PDF 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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