

Evaluation of probabilistic photometric redshift estimation approaches for LSST

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31 October 2019

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 $\sim 10^7$ galaxies, the LSST Science Requirements Document (SRD)¹ specifies that individual galaxy photo- zs must have root-mean-square error $\sigma_z < 0.02(1+z)$, 3σ catastrophic outlier rate below 10%, 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 subsamples 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, later 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 χ^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 pipelines, as part of a key project of the Photometric Redshifts working group of the LSST-DESC, described in the Science Roadmap (SRM)². 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

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

² Available at: http://lsst-desc.org/sites/default/files/DESC_SRMs_V1_1.pdf

among all codes are motivated by the LSST SRD requirements and implemented for machine learning and template-based photo- z PDF codes according to the procedures of Sections 2.3.1 and 2.3.2 respectively.

2.1 The Buzzard-v1.0 simulation

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

To assign a spectrum to each galaxy, the Adding Density Dependent Spectral Energy Distributions (SEDs) procedure (ADDSEDS, deRose in prep.)³ was used. ADDSEDS uses a sample of $\sim 5 \times 10^5$ galaxies from the magnitude-limited SDSS Data Release 6 Value Added Galaxy Catalogue (Blanton et al. 2005) to train an empirical relation between absolute r -band magnitude, local galaxy density, and SED. Each SDSS spectrum is parameterized by five weights corresponding to a weighted sum of five basis SED components using the k-correct software package⁴ (Blanton & Roweis 2007).

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

2.1.1 Caveats

By necessity, BUZZARD does not contain all of the complicating factors present in real data, and here we discuss the most pertinent ways that these limitations affect our experiment. BUZZARD includes only galaxies, not stars nor AGN. The catalogue-based construction excludes image-level effects, such as deblending errors, photometric measurement issues, contamination from sky background (Zodiacal light, scattered light, etc.), lensing magnification, and Galactic reddening.

The BUZZARD SEDs are drawn from a set of $\sim 5 \times 10^5$ SEDs, which themselves are derived from a five-component linear combination fit to $\sim 5 \times 10^5$ SDSS galaxies; thus the sample contains only galaxies that resemble linear combinations of those for which SDSS obtained spectra, and there are necessarily duplicates. The linear combination SEDs also restrict the properties of the galaxy population to linear combinations of the properties corresponding to five basis

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

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

2.2 LSST-like mock observations

Given the SED, absolute r -band magnitude, and true redshift of each simulated galaxy, we computed apparent magnitudes in the six LSST filter passbands, $ugrizy$. We assigned magnitude errors in the six bands using the simple model of Ivezić et al. (2008), assuming achievement of the full 10-year depth, with a modification of fiducial LSST total numbers of 30-second visits for photometric error generation: we assume 60 visits in u -band, 80 visits in g -band, 180 visits in r -band, 180 visits in i -band, 160 visits in z -band, and 160 visits in y -band.

As a consequence of adding Gaussian-distributed photometric errors, 2.0% of our galaxies exhibit a negative flux in one or more bands, the vast majority of which are in the u -band. We deem such negative fluxes *non-detections* and assign a placeholder magnitude of 99.0 in the catalogue to indicate to the photo- z PDF codes that such galaxies would be “looked at but not seen” in multi-band forced photometry.

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

2.3 Shared prior information

For the purpose of performing a controlled experiment that compares photo- z PDF codes on equal footing as a baseline for a future sensitivity analysis, we take care to provide each with maximally optimistic prior information. Redshift estimation approaches built upon physical modeling and machine learning alike have a notion of prior information considered beyond the photometry of the data for which redshift is to be constrained: that information is derived from a template library for a model-based code and a training set for a data-driven code. In this initial study, we seek to set a baseline for a later comparison of the performance of photo- z PDF codes under incomplete and non-representative prior

³ <https://github.com/vipasu/addsed>

⁴ <http://kcorrect.org>

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information that will propagate differently in the space of data-driven 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), Masters et al. (2017) that only 10^4 spectra are necessary to calibrate photo-zs to Stage IV requirements, we aimed to set aside a randomly selected training set of $3 - 5 \times 10^4$ galaxies, $\sim 10\%$ 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, also 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 χ^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_{obs}^i is the observed flux in a given band i , σ_{obs}^i is the observed flux error, and N_{filt} is the total number of filters, in our case the six *ugrizy* LSST filters. The likelihood is a sum of observed flux error σ_b^{obs} -weighted squared differences between the observed flux F_b^{obs} and the normalized predicted flux $F_b^{\text{mod}}(T, z)$ in N_{filt} photometric filters b , which is 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 (BPZ⁵, 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 χ^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

⁵ <http://www.stsci.edu/~dcoe/BPZ/>

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

329 template set of Section 2.3.2. To keep the number of free pa-
 330 rameters manageable, the DC1 template set is pre-sorted by
 331 the rest-frame $u - g$ colour and split into three broad classes
 332 of SED template, equivalent to the E, Sp and Im/SB types.
 333 The Bayesian prior term $p(T|m_0)$ was derived directly from
 334 the DC1 training set, and the other term $p(z|T, m_0)$ was
 335 chosen to be the best fit for the eleven free parameters from
 336 the functional form of Benítez (2000). We use template in-
 337 terpolation, creating two linearly interpolated templates be-
 338 tween each basis SED (sorted by rest-frame $u - g$ colour) by
 339 setting the parameter `INTERP=2`. Prior to running the code,
 340 the non-detection placeholder magnitude was replaced with
 341 an estimate of the one- σ detection limit for the undetected
 342 band as a proxy for a value close to the estimated sky noise
 343 threshold.

3.1.2 EAZY

344 Easy and Accurate Photometric Redshifts from Yale (EAZY⁶,
 345 Brammer et al. 2008) extends the basic χ^2 fit procedure that
 346 defines template-fitting approaches. The algorithm models
 347 the observed photometry with a linear combination of tem-
 348 plate SEDs at each redshift. The best-fit SED at each red-
 349 shift is found by simultaneously fitting one, two, or all of
 350 the templates via χ^2 minimization, which is distinct from
 351 marginalizing across all templates. The minimized χ^2 like-
 352 lihood at each redshift is then combined with an apparent
 353 magnitude prior to obtain the redshift posterior PDF. We
 354 note that the utilization of the best-fit SED conditioned on
 355 redshift rather than a proper marginalization does not lead
 356 to the correct posterior distribution, an implementation is-
 357 sue that has now been identified and will be addressed by
 358 the developers in the future.

359 In contrast with BPZ, EAZY’s apparent magnitude prior is
 360 independent of SED, though it was derived empirically from
 361 the DC1 training set. The EAZY architecture cannot accept
 362 a template set other than the same five basis templates em-
 363 ployed by `k-correct` when constructing the DC1 catalogue,
 364 but, for consistency with the experimental scope of perfect
 365 prior information, EAZY’s flexible `all-templates` mode was
 366 used to fit the photometric data with a linear combination
 367 of the five basis templates. Though EAZY can account for
 368 uncertainty in the template set by adding in quadrature to
 369 the flux errors an empirically derived template error as a

371 function of redshift, we set the template error to zero since
 372 the same templates were in fact used to produce the DC1
 373 photometry.

3.1.3 LePhare

374 Photometric Analysis for Redshift Estimate (LePhare⁷,
 375 Arnouts et al. 1999; Ilbert et al. 2006) uses the χ^2 of Equa-
 376 tion 1 to match observed colors with those predicted from a
 377 template set. The template set can be semi-empirical or en-
 378 tirely synthetic. The reported photo-z PDF is an arbitrary
 379 normalization of the likelihood evaluated on the output red-
 380 shift grid.

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

3.2 Machine Learning-based Approaches

386 We compared nine data-driven photo-z estimation ap-
 387 proaches, eight of which are described in this section and one
 388 of which is discussed in Section 3.3. Because the algorithms
 389 differ more from one another and the techniques are rela-
 390 tive newcomers to the astronomical literature, we provide
 391 somewhat more detail about the implementations below.

3.2.1 ANNz2

394 ANNz2⁸ (Sadeh et al. 2016) supports several machine learn-
 395 ing algorithms, including artificial neural networks (ANN),
 396 boosted decision tree, and k-nearest neighbour (KNN) re-
 397 gression. In addition to accounting for errors on the input
 398 photometry, ANNz2 uses the KNN-uncertainty estimate of
 399 Oyaizu et al. (2008) to quantify uncertainty in the choice of
 400 method over multiple runs. Using the Toolkit for Multivariate
 401 Data Analysis with ROOT⁹, ANNz2 can return the results
 402 of running a single machine learning algorithm, a “best”
 403 choice of the results from simultaneously running multiple
 404 algorithms (based on evaluation the cumulative distribution
 405 functions of validation set objects), or a combination of the

⁷ <http://www.cfht.hawaii.edu/~arnouts/lephare.html>

⁸ <https://github.com/IftachSadeh/ANNZ>

⁹ <http://tmva.sourceforge.net/>

⁶ <https://github.com/gbrammer/eazy-photoz>

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406 results of multiple algorithms weighted by their method uncertainties averaged over multiple runs.

407 In this study, we used ANNz2-v.2.0.4 to output only the result of the ANN algorithm. Photo-z PDFs were produced
 408 by running an ensemble of 5 ANNs with a 6 : 12 : 12 : 1
 409 architecture corresponding to the 6 *ugrizy* inputs, 2 hidden
 410 layers with 12 nodes each, and 1 output of redshift. Each of
 411 the five ANNs was trained with different random seeds for
 412 the initialization of input parameters, reserving half of the
 413 training set for validation to prevent overfitting. Undetected
 414 galaxies were excluded from the training set, and per-band
 415 non-detections in the test set were replaced with the mean
 416 magnitude in that band within the entire test set.
 417

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 δc_{test} and $N_{\text{colours}} = 5$ colors 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 $N_{\text{fit}} = 5$ with PPF = 0.95, 95%
 432 of all training galaxies consistent with the test galaxy will
 433 have $D_M < 11.07$. Undetected bands are dropped, thereby
 434 reducing the effective N_{fit} for that galaxy. The photo-z PDF
 435 of a given test set galaxy is the normalized distribution of
 436 redshifts of its colour-matched subset of training set galax-
 437 ies.

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 of the when composing the photo-
 459 z PDF rather than weighting all colour-matched training
 460 galaxies equally. Additionally, when the number of colour-
 461 matched training set galaxies is less than 20, the nearest 20
 462 neighbours in color-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 correspond-
 465 ing growth of the effective PPF to include 20 neighbors.

466 3.2.3 Delight

467 [Delight](#)¹⁰ ([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 $\hat{\mathbf{F}} = \mathbf{F} + \mathbf{F}_b$ 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 μ^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 logarithmic. The Gaussian process was
 509 trained using the full DC1 training set. We used the full DC1
 510 template set with a flat prior in magnitude and SED type.
 511 Photometric uncertainties from the inputs are propagated
 512 into the code, while non-detections for each band are set to
 513 the mean of the respective bands.

514 3.2.4 FlexZBoost

515 [FlexZBoost](#)¹¹ ([Izbicki & Lee 2017](#)) is built on [FlexCode](#), a
 516 general-purpose methodology for converting any conditional

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

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

mean point estimator of z to a conditional density estimator $p(z|\mathbf{x}) \equiv f(z|\mathbf{x})$, where \mathbf{x} here represents our photometric covariates and errors. **FlexZBoost** expands the unknown function $f(z|\mathbf{x}) = \sum_i \beta_i(\mathbf{x})\phi_i(z)$ using an orthonormal basis $\{\phi_i(z)\}_i$. By the orthogonality property, the expansion coefficients $\beta_i(\mathbf{x}) = \mathbb{E}[\phi_i(z)|\mathbf{x}] \equiv \int f(z|\mathbf{x})\phi_i(z)dz$ are thus conditional means. The expectation value $\mathbb{E}[\phi_i(z)|\mathbf{x}]$ of the expansion coefficients conditioned on the data is equivalent to the regression of the space of possible redshifts on the space of possible photometry. Thus the expansion coefficients $\beta_i(\mathbf{x})$ 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**¹¹, 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 α that we use to sharpen the computed density estimates $\hat{f}(z|\mathbf{x}) \propto \hat{f}(z|\mathbf{x})^\alpha$. Both I and α 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% 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.

545 3.2.5 GP_z

546 GP_z¹² (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 547 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 548 output redshift z given the input photometry \mathbf{x} . The mean 549 $\mu(\mathbf{x})$ and the variance $\sigma(\mathbf{x})^2$ are modeled as functions 550 $f(\mathbf{x}) = \sum_{i=1}^m w_i \phi_i(\mathbf{x})$ linear combinations of m basis 551 functions $\{\phi_i(\mathbf{x})\}_{i=1}^m$ with associated weights $\{w_i\}_{i=1}^m$. The 552 details on how to learn the parameters of the model and the 553 hyper-parameters of the basis functions are described in Al- 554 mosallam et al. (2016b). GP_z's variance estimate is composed 555 of a model uncertainty term corresponding to sparsity of the 556 training set photometry and a noise uncertainty term en- 557 compassing noisy photometric observations, enabling quan- 558 tification of any need for more representative or more precise 559 training samples. GP_z may also weight training set samples 560 by importance according to $|z_{\text{spec}} - z_{\text{phot}}|/(1+z_{\text{spec}})$ to min- 561 imize the normalized photo- z point estimate error, however, 562 this function may be adapted to photo- z PDFs, pressuring 563 the model to dedicate more resources to test set galaxies 564 that are not well-represented in the training set.

To smooth the long tail in the distribution of magnitude errors, we use the log of the magnitude errors, im- 570 proving numerical stability and eliminating the need for 571 constraints on the optimization process. Unobserved mag- 572 nitudes $x_u = \mu_u + \Sigma_{uo}\Sigma_{oo}^{-1}(x_o - \mu_o)$ were imputed from

573 observed magnitudes x_o and the training set mean μ and 574 covariance Σ using a linear model. This is the optimal ex- 575 pected value of the unobserved variables given the observed 576 ones under the assumption that the distribution is jointly 577 Gaussian; note that this reduces to a simple average if the 578 covariates are independent with $\Sigma_{uo} = 0$. We reserved for 579 validation 20% of the training set and used the Variable 580 Covariance option in GP_z with 200 basis functions (see Al- 581 mosallam et al. (2016b) for details), neglecting to apply cost- 582 sensitive learning options.

584 3.2.6 METAPhōR

585 Machine-learning Estimation Tool for Accurate Photomet- 586 ric Redshifts (METAPhōR¹³, Cavuoti et al. 2017) is based on 587 the Multi Layer Perceptron with Quasi Newton Algorithm 588 (MLPQNA) with the least square error model and Tikhonov 589 L_2 -norm regularization (Hofmann & Mathé 2018). Photo- z 590 PDFs are generated by running N trainings on the same 591 training set, or M trainings on M different random sam- 592 plings of the training set. Upon regression of the test set, 593 the photometry m_{ij} of each test set galaxy j in filter i is 594 perturbed according to $m'_{ij} = m_{ij} + \alpha_i F_{ij} \epsilon$ in terms of 595 the standard normal random variable $\epsilon \sim \mathcal{N}(0, 1)$, a mul- 596 tiplicative constant α_i permitting accommodation of multi- 597 survey photometry, and a bimodal function F_{ij} composed of 598 a polynomial fit of the mean magnitude errors on the binned 599 bands plus a constant term representing the threshold below 600 which the polynomial's noise contribution is negligible 601 (Brescia et al. 2018).

602 In this work, we used a hierarchical KNN to replace 603 non-detections with values based on their neighbors. The 604 usual cross-validation of redshift estimates and PDFs was 605 also omitted for this study.

606 3.2.7 SkyNet

607 SkyNet¹⁴ (Graff et al. 2014) employs a neural network based 608 on a second order conjugate gradient optimization scheme 609 (see Graff et al. 2014, for further details). The neural net- 610 work is configured as a standard multilayer perceptron with 611 three hidden layers and one input layer with 12 nodes cor- 612 responding to the 6 photometric magnitudes and their mea- 613 surement errors.

614 SkyNet's classifier mode uses a cross-entropy error func- 615 tion with a 20:40:40 node (all rectified linear units) architec- 616 ture for each hidden layer and an output layer of 200 nodes 617 corresponding to 200 bins for the PDF, with a softmax acti- 618 vation function to enforce the normalization condition that 619 the probabilities sum to unity. While previous implemen- 620 tations of the code (see Appendix C.3 of Sánchez et al. 2014; 621 Bonnett 2015) implement a sliding bin smoothing, no such 622 procedure was used in this study.

623 We pre-whitened the data by pegging the magnitudes 624 to (45,45,40,35,42,42) and errors to (20,20,10,5,15,15) for 625 ugrizy filters, respectively. To avoid over-fitting, 30% of the 626 training set was reserved for validation, and training was 627 halted as soon as the error rate began to increase on the

¹² <https://github.com/OxfordML/GPz>

¹³ <http://dame.dsfa.unina.it>

¹⁴ <http://ccpforge.cse.rl.ac.uk/gf/project/skynet/>

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validation set. The weights were randomly initialized based on normal sampling.

3.2.8 TPZ

Trees for Photo- z (TPZ¹⁵, 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 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 1σ detection threshold based on the error forecast of the 10-year LSST data, i. e. $dm = 2.5 \log(1 + N/S)$ where $dm \sim 0.7526$ magnitudes for $N/S = 1$. 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 catalogs 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^{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 ra-

¹⁵ <https://github.com/mgckind/MLZ>

tio 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.¹⁶ We will discuss the choice of photo- z PDF parameterization further in Section 6.

This analysis is conducted using the `qp`¹⁷ 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. Though the outmoded practices should not be encouraged, 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 statistics 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 accuracy of each individual catalog entry, 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)

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

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 quantile-quantile 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

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

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

¹⁶ See, e. g. the LSST Data Products Definition Document, available at: <https://ls.st/dpdd>

¹⁷ <http://github.com/aimalz/qp/>

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 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,

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 $\text{PIT} < 10^{-4}$ 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

METAPhOr, CMNN, and SkyNet are a result of various weighted sums of the limited number of training set galaxies with colors 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 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 2σ 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

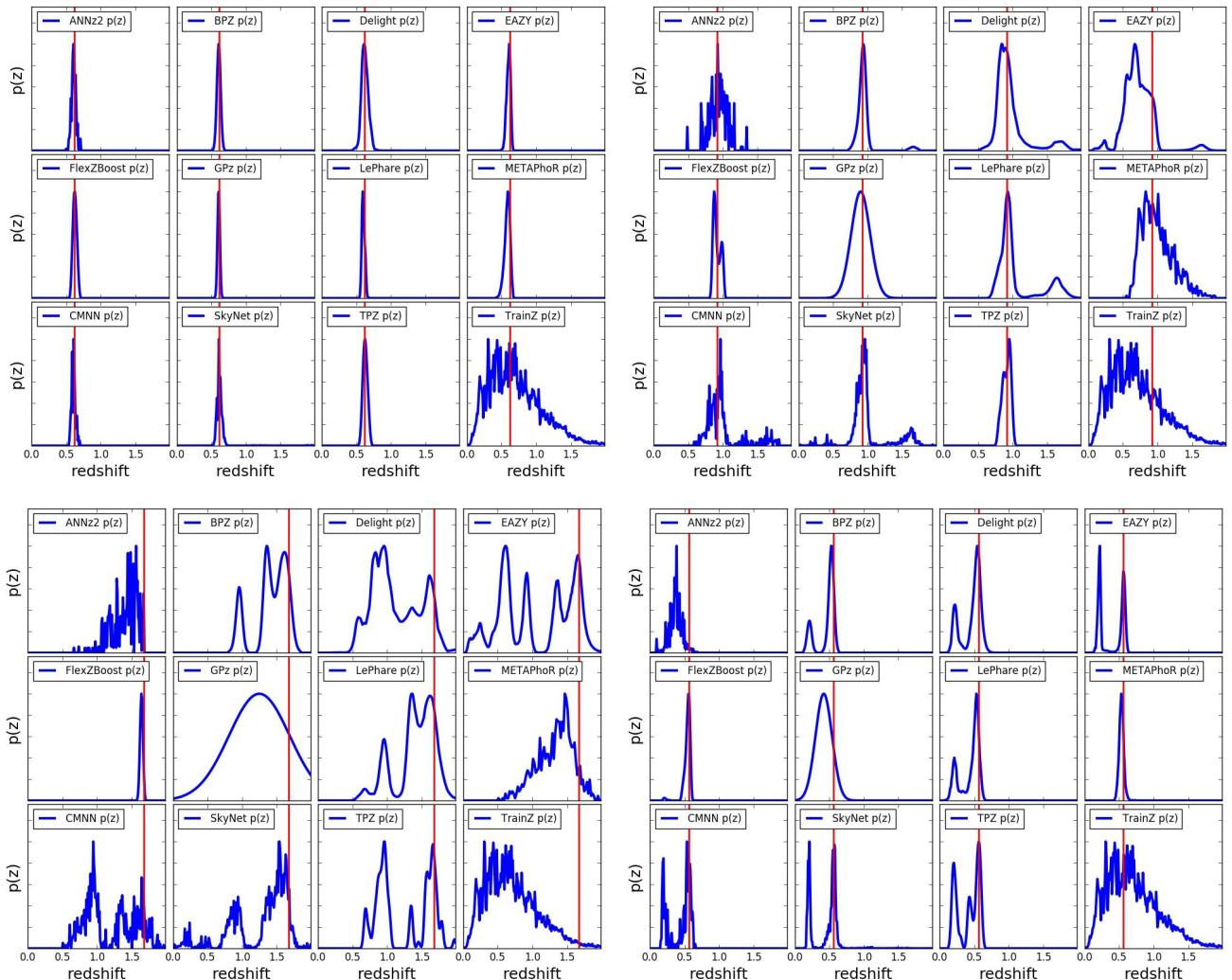


Figure 1. The individual photo- z PDFs (blue) distributions produced by the twelve codes (small panels) on four exemplary galaxies' photometry (large panels) with different true redshifts (red). The photo- z PDFs of all codes share some features for the example galaxies due to physical color degeneracies 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.

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 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

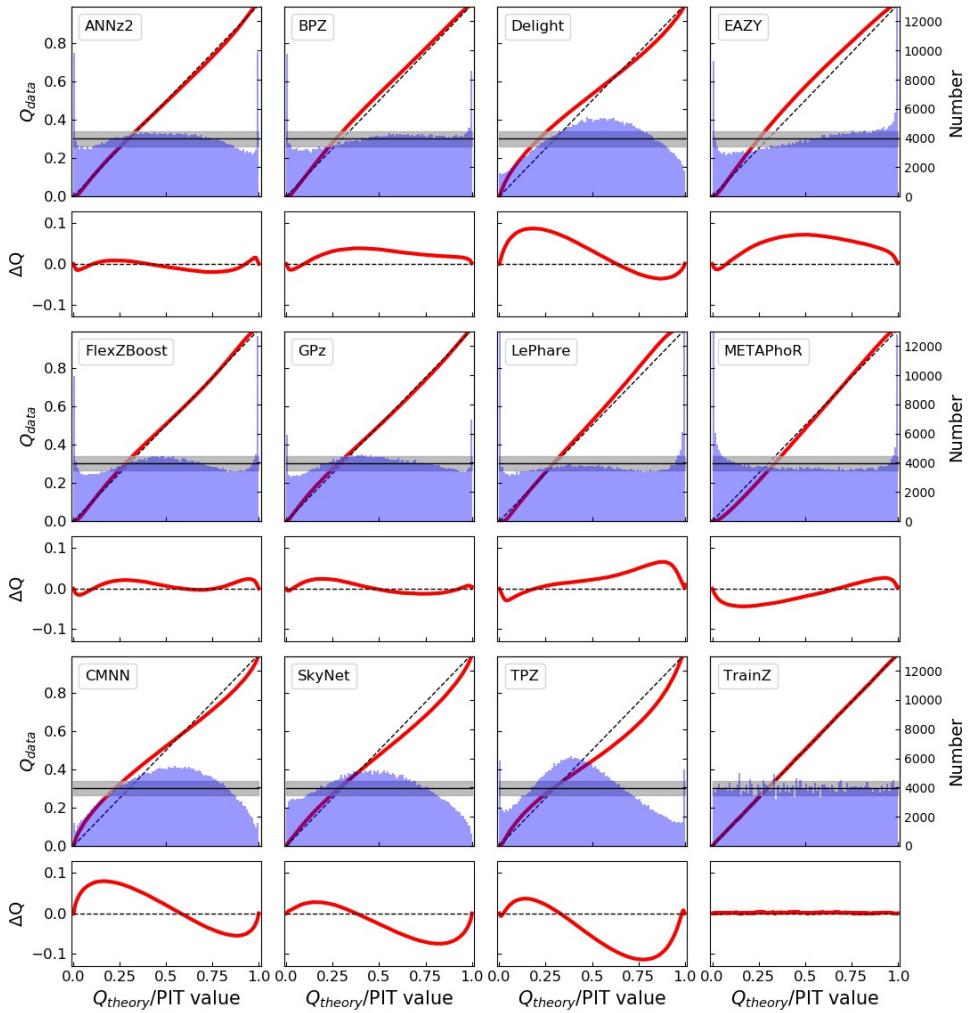


Figure 2. The QQ plot (red) and PIT histogram (blue) of the photo- z PDF codes (panels) along with the ideal QQ (black dashed) and ideal PIT (gray horizontal) curves, as well as a difference plot for the QQ difference from the ideal diagonal (lower inset). The gray shaded region indicates the 2σ range 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 2σ shaded region show that for some codes these errors will be significant given expected training sample sizes.

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.

of how to assess photo- z PDF methods and how to interpret differences between codes in terms of photo- z PDF performance. In Section 6.1, we reframe the strong performance of our pathological photo- z PDF technique, `trainZ`, as a cautionary tale about the importance of choosing appropriate comparison metrics. In Section 6.2, we outline the experiments we intend to build upon this study. In Section 6.3, we discuss the enhancements of the mock data set that will be necessary to enable the future experiments.

979 6 DISCUSSION AND FUTURE WORK

In contrast with other photo- z PDF comparison papers that have aimed to identify the “best” code for a given survey, we have focused on the somewhat more philosophical questions

992 6.1 Interpretation of metrics

We remind the reader that contributed codes were given a goal of obtaining accurate photo- z PDFs, not an accurate stacked estimator of the redshift distribution, so we do not

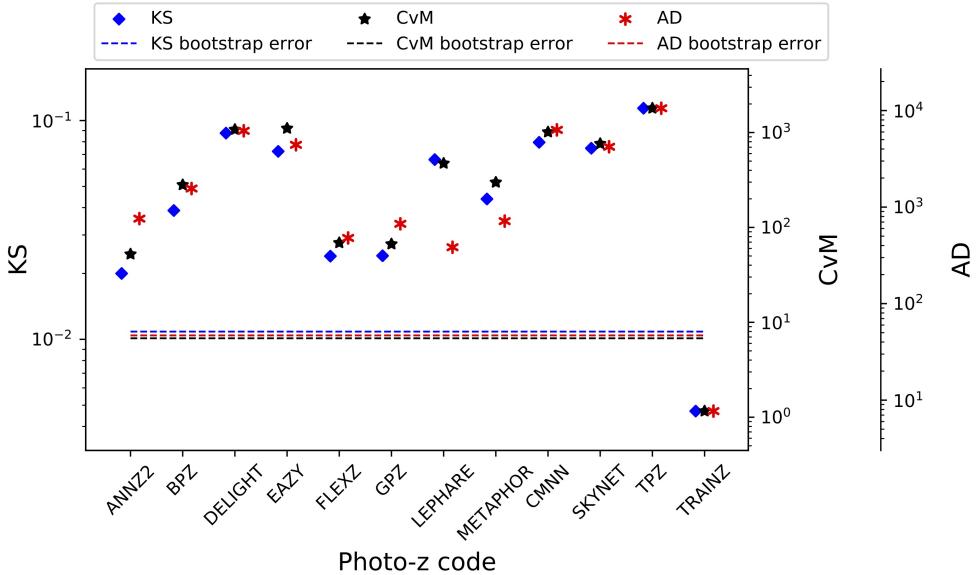


Figure 3. A visualization of the Kolmogorov-Smirnov (KS, blue diamond), Cramer-von Mises (CvM, black star), and Anderson-Darling (AD, red asterisk) statistics for the PIT distributions. There is generally good agreement between these statistics, with differences corresponding to the codes with outstanding catastrophic outlier rates, a reflection in the 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

expect the same codes to necessarily perform well for both classes of metrics. Indeed, the codes were optimized for their interpretation of our request for “accurate photo- z PDFs,” and we expect that the implementations would have been adjusted had we requested optimization of the traditional metrics of Appendices A and B.

Furthermore, our metrics are not necessarily able to assess the fidelity of individual photo- z PDFs relative to true posteriors: in the absence of a “true PDF” from which redshifts are drawn, it is difficult to construct metrics to measure performance for individual galaxies rather than ensembles. (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`, 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.

In summary, context is crucial to defend against deceptively strong performers such as `trainZ`; **the best photo-**

1045 ***z* PDF method is the one that most effectively** 1103
 1046 **achieves our science goals**, not the one that performs 1104
 1047 best on a metric that does not reflect those goals. In the 1105
 1048 absence of a single scientific motivation or the information 1106
 1049 necessary for a principled metric definition, we must consider 1107
 1050 many metrics and be critical of the information transmitted 1108
 1051 by each. 1109
 1110
 1111

1052 6.2 Extensions to the experimental design 1112

1053 The work presented in this paper is only a first step in as- 1113
 1054 sessing photo-*z* PDF approaches and moving toward an im- 1114
 1055 proved photometric redshift estimator. Here we discuss the 1115
 1056 next steps for subsequent investigations. 1116

1057 This initial paper explores photo-*z* PDF code perfor- 1117
 1058 mance in idealized conditions with perfect catalog-based 1118
 1059 photometry and representative training data, but the re- 1119
 1060 silience of each code to such realistic imperfections in prior 1120
 1061 information has not yet been evaluated. A top priority for a 1121
 1062 follow-up study is to test realistic forms of incomplete, erro- 1122
 1063 neous, and non-representative template libraries and train- 1123
 1064 ing sets as well as the impact of other forms of external 1124
 1065 priors that must be ingested by the codes, major concerns 1125
 1066 in [Newman et al. \(2015\)](#); [Masters et al. \(2017\)](#). Outright red- 1126
 1067 shift failures due to emission line misidentification or noise 1127
 1068 spikes may be modeled by the inclusion of a small number 1128
 1069 of high-confidence yet false redshifts. We plan to perform a 1129
 1070 full sensitivity analysis on a realistically incomplete training 1130
 1071 set of spectroscopic galaxies, modeling the performance of 1131
 1072 spectrographs, emission-line properties, and expected signal- 1132
 1073 to-noise to determine which potential training set galaxies 1133
 1074 are most likely to be excluded.

1075 Appendix A only addresses the stacked estimator of the 1134
 1076 redshift distribution of the entire galaxy catalogue rather 1135
 1077 than subsets in bins, tomographic or otherwise. The effects 1136
 1078 of tomographic binning scheme will be explored in a dedi- 1137
 1079 cated future paper, including propagation of redshift uncer- 1138
 1080 tainties in a set of fiducial tomographic redshift bins in order 1139
 1081 to estimate impact on cosmological parameter estimation. 1140

1082 Sequels to this study will also address some shortcom- 1141
 1083 ings of our experimental procedure. The fixed redshift grid 1142
 1084 shared between the codes may have unfairly penalized codes 1143
 1085 with a different native parameterization, as precision is lost 1144
 1086 when converting between formats. Performance on the (ad- 1145
 1087 mittedly small) population of sharply peaked photo-*z* PDFs 1146
 1088 may have been suppressed across all codes due to the insuffi- 1147
 1089 cient resolution of the redshift grid. In light of the results of 1148
[Malz et al. \(2018\)](#), in future analyses we plan to switch from 1149
 1090 a fixed grid to the quantile parameterization or to permit 1150
 1091 each code to use its native storage format under a shared 1151
 1092 number of parameters. 1152

1093 Section 4 discussed the difficulty in evaluating PDF ac- 1153
 1094 curacy for individual objects. In a follow-up study, we will 1154
 1095 generate “true PDF” distributions, yielding a dataset that 1155
 1096 enables a test of PDF accuracy for individual galaxies rather 1156
 1097 than solely ensembles. 1157

1098 6.3 Realistic mock data 1158

1099 To make optimal use of the LSST data for cosmological 1156
 1100 and other astrophysical analyses of the LSST-DESC Sci- 1157
 1101 ence Roadmap, future investigations that build upon this 1158

one will require a more sophisticated set of galaxy photometry and redshifts. This initial paper explored a data set that was constructed at the catalog level, with no inclusion of the complications that come from measuring photometry from images. Future data challenges will move to catalogs constructed from mock images, including the complications of deblending, sensor inefficiencies, and heterogeneous observing conditions, all anticipated to affect the measured colours of LSST’s galaxy sample ([Dawson et al. 2016](#)).

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.

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

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**.

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**.

1159 **Acknowledgments**

1160 This paper has undergone internal review in the LSST Dark
 1161 Energy Science Collaboration, the internal reviewers were:
 1162 Daniel Gruen, Markus Rau, and Michael Troxel.

1163 Author contributions are listed below.

1164 S.J. Schmidt: Co-led the project. (conceptualization, data
 1165 curation, formal analysis, investigation, methodology,
 1166 project administration, resources, software, supervision,
 1167 visualization, writing – original draft, writing – review &
 1168 editing)

1169 A.I. Malz: Co-led the project, contributed to choice of
 1170 metrics, implementation in code, and writing. (conceptu-
 1171 alization, methodology, project administration, resources,
 1172 software, visualization, writing – original draft, writing –
 1173 review & editing)

1174 J.Y.H. Soo: Ran ANNz2 and Delight, updated abstract,
 1175 edited sections 1 through 6, added tables in Methods
 1176 and Results, updated references.bib and added references
 1177 throughout the paper

1178 I.A. Almosallam: vetted the early versions of the data set
 1179 and ran many photo-z codes on it, applied GPz to the final
 1180 version and wrote the GPz subsection

1181 M. Brescia: main ideator of METAPHOR and of MLPQNA;
 1182 modification of METAPHOR pipeline to fit the LSST data

1183 structure and requirements

1184 S. Cavaudi: Contributed to choice and test of metrics, ran
 1185 METAPHOR, minor text editing

1186 J. Cohen-Tanugi: contributed to running code, analysis
 1187 discussion, and editing, reviewing the paper

1188 A.J. Connolly: Developed the colour-matched nearest-
 1189 neighbours photo-z code; participated in discussions of the
 1190 analysis.

1191 P.E. Freeman: Contributed to choice of CDE metrics and
 1192 to implementation of FlexZBoost

1193 M.L. Graham: Ran the colour-matched nearest-neighbours
 1194 photo-z code on the Buzzard catalog and wrote the relevant
 1195 piece of Section 2; participated in discussions of the analysis.

1196 K. Iyer: assisted in writing metric functions used to evaluate
 1197 codes

1198 M.J. Jarvis: Contributed text on AGN to Discussion section
 1199 and portions of GPz work

1200 J.B. Kalmbach: Worked on preparing the figures for the
 1201 paper.

1202 E. Kovacs: Ran simulations, discussed data format and
 1203 properties for SEDs, dust, and ELG corrections

1204 A.B. Lee: Co-developed FlexZBoost and the CDE loss
 1205 statistic, wrote text on the work, and supervised the
 1206 development of FlexZBoost software packages

1207 G. Longo: Scientific advise, test and validation of the
 1208 modified METAPHOR pipeline, text of the METAPHOR
 1209 section

1210 C. B. Morrison: Managerial support; Discussions with au-
 1211 thors regarding metrics and style; Some coding contribu-
 1212 tion to metric computation.

1213 J. Newman: Contributions to overall strategy, design of
 1214 metrics, and supervision of work done by Rongpu Zhou

1215 E. Nourbakhsh: Ran and optimized TPZ code and wrote a
 1216 subsection of Section 2 for TPZ

1217 E. Nuss: contributed to running code, analysis discussion,
 1218 and editing, reviewing the paper

1219 T. Pospisil: Co-developed FlexZBoost software and CDE

1220 loss calculation code

1221 H. Tranin: contributed to providing SkyNet results and
 1222 writing the relevant section

1223 R. Zhou: Optimized and ran EAZY and contributed to the
 1224 draft

1225 R. Izbicki: Co-developed FlexZBoost and the CDE loss
 1226 statistic, and wrote software for FlexZBoost

The authors would like to thank their LSST-DESC publication review committee for comments that improved the paper draft.

personal funding sources SJS acknowledges support from DOE grant DE-SC0009999 and NSF/AURA grant N56981C. AIM acknowledges support from the Max Planck Society and the Alexander von Humboldt Foundation in the framework of the Max Planck-Humboldt Research Award endowed by the Federal Ministry of Education and Research. During the completion of this work, AIM was advised by David W. Hogg and was supported by National Science Foundation grant AST-1517237.

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).

The DESC acknowledges ongoing support from the Institut National de Physique Nucléaire et de Physique des Particules in France; the Science & Technology Facilities Council in the United Kingdom; and the Department of Energy, the National Science Foundation, and the LSST Corporation in the United States. DESC uses resources of the IN2P3 Computing Center (CC-IN2P3–Lyon/Villeurbanne - France) funded by the Centre National de la Recherche Scientifique; the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231; STFC DiRAC HPC Facilities, funded by UK BIS National E-infrastructure capital grants; and the UK particle physics grid, supported by the GridPP Collaboration. This work was performed in part under DOE Contract DE-AC02-76SF00515.

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 $\hat{N}(z)$. In terms of the prior information provided to each method, the true redshift distribution satisfies the tautology $\hat{N}(z) = p(z|I_D)$ 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 $\hat{N}(z)$ 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 $\hat{p}_i(z) = \hat{N}(z)$ 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.

A1 Metrics of the stacked estimator of the redshift distribution

“Stacking” according to

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

is the most widely accepted method for obtaining $\hat{N}^H(z)$ as an estimator of the redshift distribution from photo- z PDFs derived by a method H . Though the use of the stacked estimator of the redshift distribution is not formally correct (Malz & Hogg prep), we use it under the untested assumption that the response of our metrics of $\hat{N}^H(z)$ will be analogous to the same metrics applied to a principled estimator of the redshift distribution.

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

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

of the estimated redshift distribution $\hat{N}^H(z)$ for each code and compare them to the moments of the true redshift distribution $\tilde{N}(z)$. Under the assumption that the stacked estimator is unbiased, a superior method minimizes the difference between the true and estimated moments.

A2 Performance on the stacked estimator of the redshift distribution

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

Many of the codes, including all the model-fitting approaches and `ANNz2`, `GPz`, `METAPhR`, and `SkyNet` from the data-driven camp, overestimate the redshift density at $z \sim 1.4$. This behavior is a consequence of the 4000 Åbreak passing through the gap between the z and y filters, which induces a genuine discontinuity in the $z-y$ colour as a function of redshift that can sway the photo- z PDF estimates in the absence of bluer spectral features.

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

As expected, `trainZ` perfectly recovers the true redshift distribution: as the training sample is selected from the same underlying distribution as the test set, the redshift distributions are identical, up to Poisson fluctuations due to the

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

Figure A2 shows the quantitative Kolmogorov-Smirnov (KS), Cramer-Von Mises (CvM), and Anderson Darling (AD) test statistics for each of the codes for the $\hat{N}(z)$ based measures. The horizontal lines show the the result of a bootstrap resampling of the training set using 30,000 samples for `trainZ`, representing a conservative idealized limit on expected performance for a modest-sized representative training set of galaxies, as mentioned in Section 5.1. The AD bootstrap statistic is elevated due to its sensitivity to the tails of distributions. The stacked estimators of the redshift distribution for `CMNN` and `trainZ` best estimate $\tilde{N}(z)$ under these metrics, whereas `EAZY`, `LePhare`, `METAPhR`, and `SkyNet` underperform; `BPZ`, `GPz`, and `TPZ` are within a factor of two of the conservative limit for all statistics. It is unsurprising that `CMNN` scores well, as with a nearly complete and representative training set choosing neighbouring points in color/magnitude space to construct an estimator should lead to excellent agreement in the final $\hat{N}(z)$.

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

We calculated the first three moments of the stacked $\hat{N}(z)$ distribution of all galaxies and compared it to the moments of the true redshift distribution. Figure A3 shows the residuals of the moments for all codes. Accuracy of the moments varies widely between codes, raising concerns about the propagation to cosmological analyses. The DESC SRD (The LSST Dark Energy Science Collaboration et al. 2018) lists stringent requirements on how well the mean and variance of tomographic redshift bins must be known for each of the main DESC science cases. We indicate the Year 1 requirements assuming our true mean redshift of $z = 0.701$ as dashed lines. In this study with representative training data, `ANNz2`, `BPZ`, `CMNN`, `TPZ`, and our pathological `trainZ` estimator meet the Y1 requirement on the mean redshift. Only `ANNz2`, `BPZ`, `CMNN`, and `trainZ` meet both requirements. One should be concerned that many codes fail to meet this ambitious limit under perfect prior information because all codes are anticipated to do no better under realistically imperfect prior information, and indicates that additional calibration to remove these systematic offsets (e. g. Newman 2008) will likely be necessary in order to meet these stringent goals.

`SkyNet` exhibits redshift bias in Figure A1 and is a clear

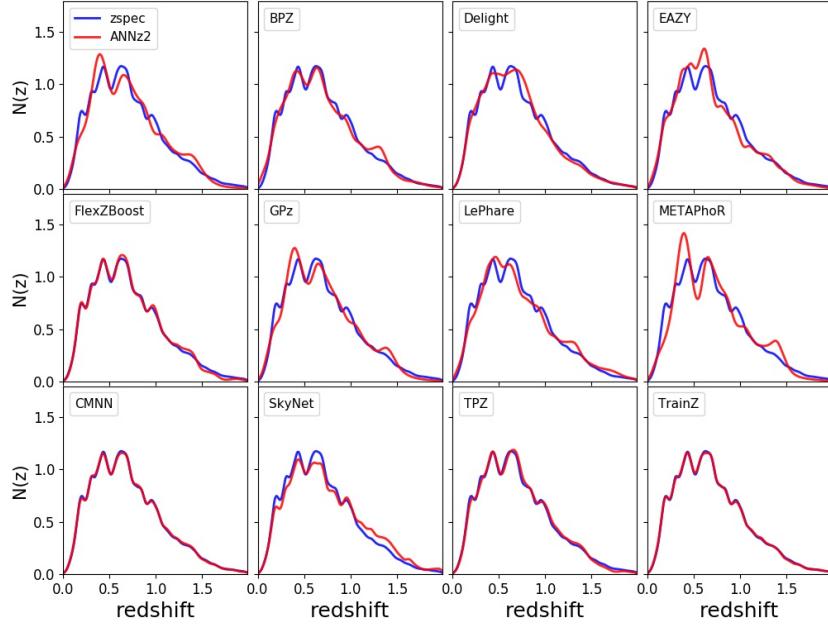


Figure A1. The smoothed stacked estimator $\hat{N}(z)$ of the redshift distribution (red) produced by each code (panels) compared to the true redshift distribution $\tilde{N}(z)$ (blue). Varying levels of agreement are seen among the codes, with the smallest deviations for CMNN, FlexZBoost, TPZ, and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

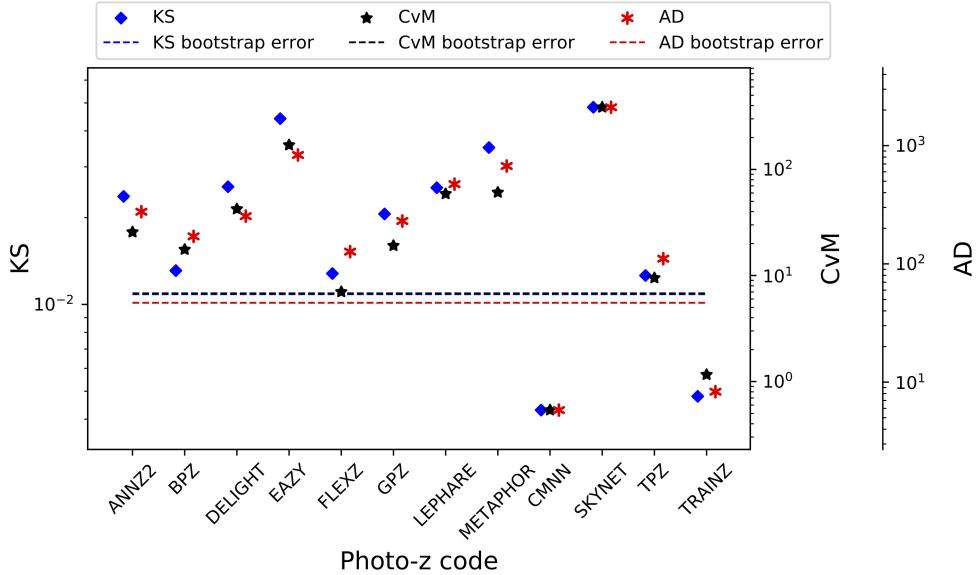


Figure A2. A visualization of the Kolmogorov-Smirnov (KS, blue diamond), Cramer-von Mises (CvM, black star), and Anderson-Darling (AD, red asterisk) statistics for the $\hat{N}(z)$ distributions. Horizontal lines indicate the statistic values (including uncertainty) achieved using `trainZ` via bootstrap 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.

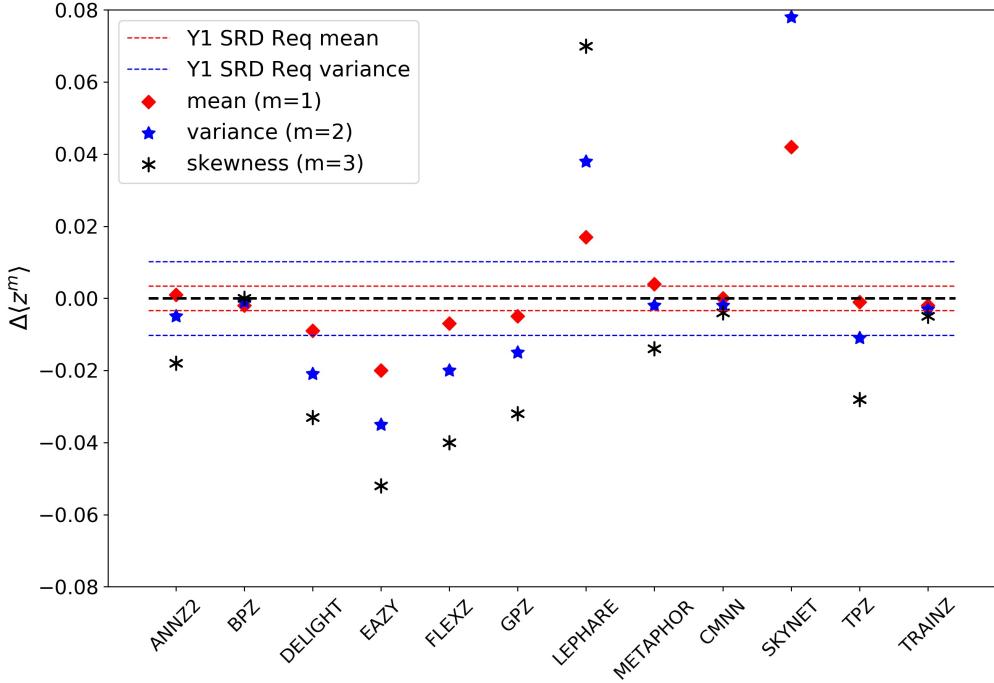


Figure A3. Residuals of the first three moments of the stacked $\hat{N}(z)$ distribution. Red and blue horizontal lines indicate the Year 1 DESC SRD requirements on accuracy of the mean and variance respectively. Only a small number of codes are able to meet these specifications even with perfect training data.

outlier in the first moment of $\hat{N}(z)$ in Figure A3. The SkyNet 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.

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 $e_z \equiv (z_{\text{PEAK}} - z_{\text{true}})/(1 + z_{\text{true}})$. 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 $\sigma_{\text{IQR}} = \text{IQR}/1.349$ to ensure that the area within σ_{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 $\max(3\sigma_{\text{IQR}}, 0.06)$.

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

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 $p(z) - 0.05 \times z_{\text{PEAK}}$. 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.

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 $z_{\text{phot}} = z_{\text{spec}}$ 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

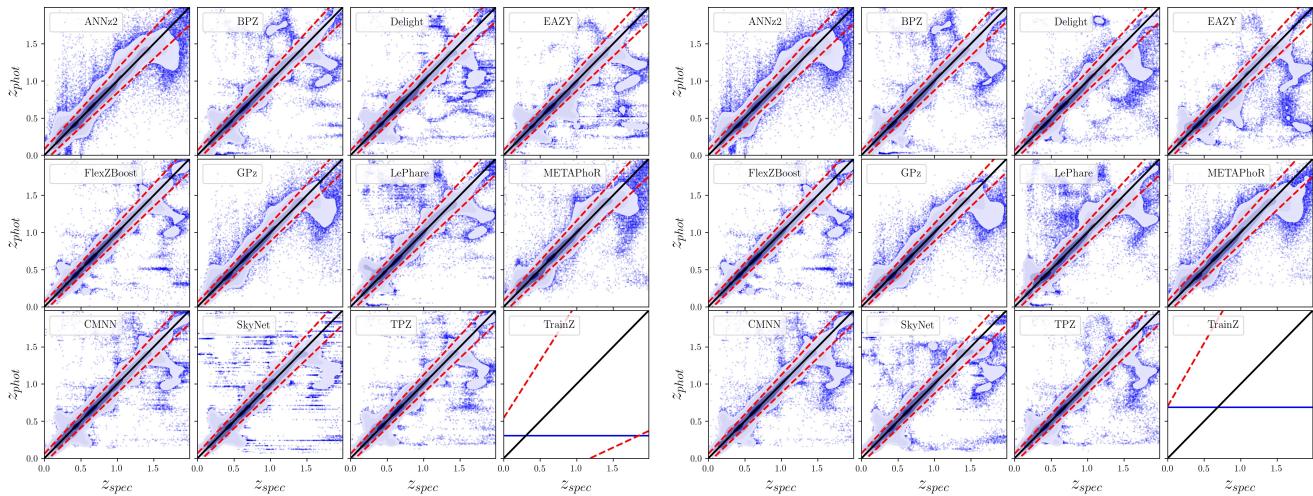


Figure B1. The density of photo- z point estimates (contours) reduced from the photo- z PDFs with outliers (blue) beyond the outlier cutoff (red dashed lines), via the mode (z_{PEAK} , left panel) and main-peak-mean (z_{WEIGHT} , right panel). The `trainZ` estimator (lower right sub-panels) has a shared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

to the $z_{phot} = z_{spec}$ line are due to the 4000 Åbreak 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 Document¹⁸ and Graham et al. (2018), which is encouraging if not unexpected for $i < 25.3$.

Breiman L., Friedman J. H., Olshen R. A., Stone C. J., 1984, Classification and Regression Trees, Statistics/Probability Series.

Wadsworth Publishing Company, Belmont, California, U.S.A

Brescia M., Cavuoti S., Amaro V., Riccio G., Angora G., Vellucci C., Longo G., 2018, preprint, ([arXiv:1802.07683](https://arxiv.org/abs/1802.07683))

Carrasco Kind M., Brunner R. J., 2013, *MNRAS*, 432, 1483

Carrasco Kind M., Brunner R. J., 2014, *MNRAS*, 442, 3380

Cavuoti S., Amaro V., Brescia M., Vellucci C., Tortora C., Longo G., 2017, *MNRAS*, 465, 1959

Chen T., Guestrin C., 2016, in Proceedings of the 22Nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD '16. ACM, New York, NY, USA, pp 785–794, doi:10.1145/2939672.2939785, <http://doi.acm.org/10.1145/2939672.2939785>

Connolly A. J., et al., 2014, in Angeli G. Z., Dierickx P., eds, Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series Vol. 9150, Modeling, Systems Engineering, and Project Management for Astronomy VI. p. 14, doi:10.1117/12.2054953

Dahlen T., et al., 2013, *ApJ*, 775, 93

Dawson W. A., Schneider M. D., Tyson J. A., Jee M. J., 2016, *ApJ*, 816, 11

DeRose J., et al., 2019, arXiv e-prints, p. arXiv:1901.02401

Erben T., et al., 2013, *MNRAS*, 433, 2545

Fernández-Soto A., Lanzetta K. M., Yahil A., 1999, *ApJ*, 513, 34

Firth A. E., Lahav O., Somerville R. S., 2003, *MNRAS*, 339, 1195

Freeman P. E., Izbicki R., Lee A. B., 2017, *MNRAS*, 468, 4556

Graff P., Feroz F., Hobson M. P., Lasenby A., 2014, *MNRAS*, 441, 1741

Graham M. L., Connolly A. J., Ivezić Ž., Schmidt S. J., Jones R. L., Jurić M., Daniel S. F., Yoachim P., 2018, *AJ*, 155, 1

Green J., et al., 2012, preprint (arXiv:1208.4012),

Hildebrandt H., et al., 2010, *A&A*, 523, A31

Hofmann B., Mathé P., 2018, *Inverse Problems*, 34, 015007

Hunter J. D., 2007, Matplotlib: A 2D Graphics Environment, doi:10.1109/MCSE.2007.55

Ilbert O., et al., 2006, *A&A*, 457, 841

Ivezić Ž., et al., 2008, preprint (arXiv:0805.2366),

Izbicki R., Lee A. B., 2017, *Electron. J. Statist.*, 11, 2800

Izbicki R., Lee A. B., Freeman P. E., 2017, *Ann. Appl. Stat.*, 11, 698

Laureijs R., et al., 2011, preprint (1110.3193),

Leistedt B., Hogg D. W., 2017, *ApJ*, 838, 5

¹⁸ 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
METAPhORe	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

- 1527 Malz A., Hogg D., in prep., CHIPPR, chippr, <https://github.com/aimalz/chippr>
- 1528 Malz A., Marshall P., 2018, qp: Quantile parametrization for probability distribution functions (ascl:1809.011)
- 1529 Malz A. I., Marshall P. J., DeRose J., Graham M. L., Schmidt S. J., Wechsler R., (LSST Dark Energy Science Collaboration 2018, *AJ*, **156**, 35)
- 1530 Mandelbaum R., et al., 2008, *MNRAS*, **386**, 781
- 1531 Massarotti M., Iovino A., Buzzoni A., 2001, *A&A*, **368**, 74
- 1532 Masters D. C., Stern D. K., Cohen J. G., Capak P. L., Rhodes J. D., Castander F. J., Paltani S., 2017, *ApJ*, **841**, 111
- 1533 Newman J. A., 2008, *ApJ*, **684**, 88
- 1534 Newman J. A., et al., 2015, *Astroparticle Physics*, **63**, 81
- 1535 Oliphant T., 2007, Python for Scientific Computing, doi:10.1109/MCSE.2007.58
- 1536 Oyaizu H., Lima M., Cunha C. E., Lin H., Frieman J., 2008, *ApJ*, **689**, 709
- 1537 Polsterer K. L., D'Isanto A., Gieseke F., 2016, preprint (arXiv:1608.08016),
- 1538 Rasmussen C., Williams C., 2006, Gaussian Processes for Machine Learning. Adaptative computation and machine learning series, MIT Press, Cambridge, MA
- 1539 Rau M. M., Seitz S., Brimiouille F., Frank E., Friedrich O., Gruen D., Hoyle B., 2015, *MNRAS*, **452**, 3710
- 1540 Reddick R. M., Wechsler R. H., Tinker J. L., Behroozi P. S., 2013, *ApJ*, **771**, 30
- 1541 Sadeh I., Abdalla F. B., Lahav O., 2016, *PASP*, **128**, 104502
- 1542 Sánchez C., et al., 2014, *MNRAS*, **445**, 1482
- 1543 Schmidt M., 2005, minFunc: Unconstrained Differentiable Multivariate Optimization in Matlab, <http://www.cs.ubc.ca/~schmidtm/Software/minFunc.html>
- 1544 Scott D. W., 1992, Multivariate Density Estimation. Theory, Practice, and Visualization. Wiley
- 1545 Sheldon E. S., Cunha C. E., Mandelbaum R., Brinkmann J., Weaver B. A., 2012, *The Astrophysical Journal Supplement Series*, **201**, 32
- 1546 Skrutskie M. F., et al., 2006, *AJ*, **131**, 1163
- 1547 Tanaka M., et al., 2018, *PASJ*, **70**, S9
- 1548 The LSST Dark Energy Science Collaboration et al., 2018, preprint, (<arXiv:1809.01669>)
- 1549 Waskom M., et al., 2017, doi:10.5281/zenodo.824567
- 1550 York D. G., et al., 2000, *AJ*, **120**, 1579
- 1551 de Jong J. T. A., Verdoes Kleijn G. A., Kuijken K. H., Valentijn E. A., 2013, *Exp. Astron.*, **35**, 25
- 1552 de Jong J. T. A., et al., 2017, *A&A*, **604**, A134