An Active Learning Approach to Optimizing Astronomy

I. INTRODUCTION

Need a discussion of all the different sciences that will need some kind of automated classification in the future

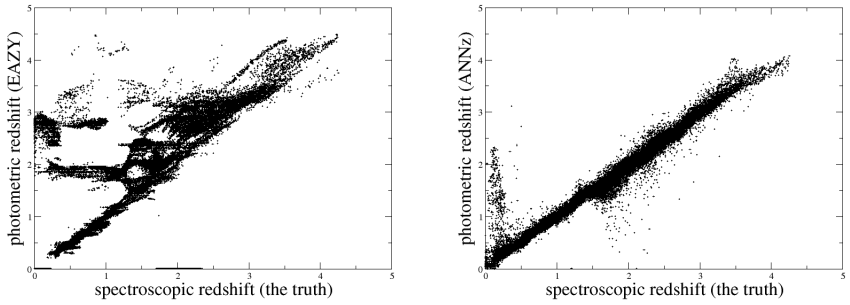
II. PHOTOMETRIC REDSHIFTS

The apparent acceleration of the rate of cosmic expansion [**CITE**] represents one of the most vexing problems in modern astrophysics. Whether it is an indication of the presence of a gravitationally-repulsive "Dark Energy" or of a break down in our General Relativistic description of gravity, answering it will require a detailed three-dimensional map of the constituents of the Universe, and how they are being moved away from us by the cosmic expansion. Traditionally, such measurements are made by taking detailed spectra of objects and measuring the Doppler shift due to cosmic expansion (the "redshift" of the object, since cosmic expansion increases the wavelength of emitted photons). Detailed spectroscopy is an expensive measurement. Photometry – measuring the brightness of objects in broad passband filters – is thousands of times less expensive. Therefore, a great deal of attention has focused on developing a method of determining "photometric redshifts": inferring a relationship between an object's photometric and spectroscopic signatures such that redshifts can be determined solely from photometric data. Presently, two broad classes of photometric redshift algorithm are typically employed: template fitting and empirical algorithms.

Template fitting methods operate by using synthetic or empirical basis spectra to reconstruct a galaxy's rest frame spectrum. The reconstructed spectrum is then redshifted and integrated over the profile of the given photometric filters until a good fit to the observed photometric data is found. The redshift of the galaxy is taken as that which produces the best fit between template and data. Many publicly available codes such as EAZY [Brammer *et al.* 2008] implement this method. While it is straightforward in principle, it requires accurate foreknowledge to select the appropriate basis spectra. If the chosen spectra are not representative of the population of observed galaxies, the algorithm will fail to give accurate redshifts and cosmological inferences will be inaccurate [Budavári 2008]. The effects of this shortcoming can be seen in Figure 1(a), which plots the results of running the publically available EAZY algorithm [Brammer *et al.* 2008] on a set of simulated galaxy observations designed to represent results expected from the Large Synoptic Survey Telescope (LSST[1]). While many of the galaxies fall near the $z_{\rm photometric} = z_{\rm spectroscopic}$ line, there is significant scatter in the results.

Empirical photometric redshift methods take a training set of galaxies for which photometric and spectroscopic information exists and construct an empirical mapping function

[1] http://www.lsst.org



(a) (b)

FIG. 1: Photometric redshift plotted against true spectroscopic redshift for 48,000 simulated LSST galaxy observations. Photometric redshifts are derived using the EAZY template-fitting algorithm in Figure 1(a) and the ANNZ neural network algorithm in Figure 1(b).

to assign redshifts to galaxies based solely on their photometric measurements. The neural network code ANNz is one example of this method [Collister and Lahav 2004]. Because the empirical photometric redshift mapping function is learned directly from actual data, there is no need to ensure perfect theoretical understanding of the spectra being inferred. In this case, the principal shortcoming the method is that present algorithms are designed only to return a photometric redshift value and an uncertainty. This leaves their results sensitive to degeneracies in the photometric data whereby low redshift galaxies look similar to high redshift galaxies, confusing the algorithm. This can be seen in Figure 1(b).

We propose to address these shortcomings by designing an empirical algorithm which treats the photometric redshift problem probabilistically. Rather than taking the spectroscopic data and learning a one-to-one photometric redshift relationship, we will use Gaussian Processes to model a probability density function in $z_{\rm photometric}$ which can characterize the probability that a given galaxy is at a given redshift. This method will not only be resilient against the pitfalls demonstrated in Figure 1, but will allow us to quantify the information content of our trainind data in such a way as to optimize the gathering of additional spectroscopic data to further improve on our results.

A. Gaussian Processes

Gaussian processes (GPs) are means for interpolating the value of a scalar function on high-dimensional coordinate spaces given noisy data [Rasmussen and Williams 2006]. An important feature of GPs is that they do not make parametric assumptions about the form of the function they are modeling. They have received attention as a means of describing physical phenomena (e.g. the expansion history of the universe) without having to assume a model of the underlying process [Shafieloo *et al.* 2012], of interpolating point spread functions across large images [Bergé *et al.* 2012], and of accelerating the search of high-dimensional likelihood functions on the cosmological parameters by efficiently selecting sample points [Daniel *et al.* 2012]. We illustrate the method below for the case of photomet-

ric redshifts.

Assume that each galaxy training set datum is of the form $\{\vec{\theta}, y\}$, where $\vec{\theta}$ is an N_p-dimensional vector respresenting the magnitude of the galaxy in each of the survey's filters (the galaxy's position in photometric color space) and $y = f(\theta)$ is the physical quantity (redshift) we are trying to infer. Gaussian processes assume that f is a probabilistic function on the N_p-dimensional space with some covariance function such as a squared exponential covariance, $K_{ij} \equiv \mathrm{Cov}\left[f(\vec{\theta^i}), f(\vec{\theta^j})\right] = \exp(-\frac{1}{2}|\vec{\theta^i} - \vec{\theta^j}|^2)$. Under those assumptions, the mean of the predicted redshift distribution for a new query point $\{\vec{\theta^q}\}$ is:

$$f(\vec{\theta^q}) = \sum_{i=1}^{n} \alpha_i k(\vec{\theta^i}, \vec{\theta^{qi}}) \tag{1}$$

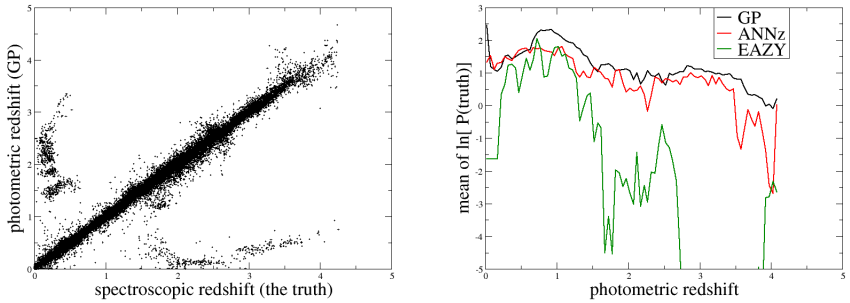
where $\vec{\alpha} = (K + \sigma^2 I)^{-1}\vec{y}$, K is the matrix of covariances between all training points, σ^2 is the variance of Gaussian noise added to each observed value of y, and $\vec{y}$ represents the training data redshifts. The variance of the predicted redshift distribution is:

$$\Sigma^q = \mathrm{Cov}(f^q) = K_{qq} - K_q^T (K + \sigma^2 I)^{-1} K_q \tag{2}$$

where K_q is the vector of covariances between the query point and all training points. Eq. 2 extends directly to the case of multiple query points by making the variables matrices as appropriate, and the result is a full covariance matrix for the query points. Readers looking for a more detailed explanation of Gaussian processes should consult Rasmussen and Williams (2006).

Gaussian processes offer two distinct advantages which render them particularly amenable to integration into active learning frameworks. Because they model the likelihood of both their inputs and their outputs, they allow us to assess both our confidence in the outputs (the probability that we have found the correct photometric redshift), and our confidence in the model as a whole. Bryan *et al.* (2007) and Daniel *et al.* (2012) use the former feature to great affect, treating the determined variances as a measure of the information that can be learned by promoting a query point to a new training point and thus learning the likelihood surface of a theory space with greater efficiency than traditional MCMC methods (see especially Figures 5-10 of Daniel *et al.* 2012). The latter feature allows us to compare PDF models with one and two modes, thus correcting for the degeneracies in the photometry-to-redshift relationship in Figure 1(b). This is the method we use to generate Figure 2.

The second advantage of Gaussian processes is their indifference to the physical meaning of the inputs and outputs. There is nothing to prevent us from adding other variables into $\vec{\theta^i}$ and including them into the covariance structure of K_{ij}. As presented, K_{ij} was the redshift-redshift correlation function. We could just as easily include redshift-magnitude and magnitude-magnitude correlation functions. Indeed, Gaussian processes allow us to incorporate any measured attribute (e.g. morphology, nearest-neighbor distance) of our galaxies in a principled manner and use those attributes to control the spread and bias in our redshift determination. In this way, we can incorporate the measurement uncertainties in our photometric colors and propagate them consistently through to uncertainties in the



(a) (b)

FIG. 2: Figure 2(a) plots photometric redshift determined by our probabilistic Gaussian Process model as a function of spectroscopic redshift. Figure 2(b) shows the mean value of ln[P(truth)] as a function of photometric redshift (the vertical axes in Figures 1 and 2(a)) for all three algorithms under consideration. Note that, even though Figure 2(a) shows the same degeneracy seen in Figure 1(b), it gives a consistently higher value of ln[P(truth)] in that range of photometric redshift.

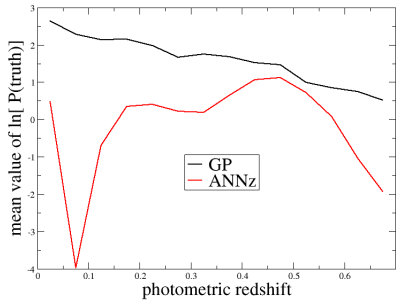


FIG. 3: The mean value of ln[P(truth)] as a function of photometric redshift for 715,000 galaxies taken from the Sloan Digital Sky Survey.

determined photometric redshifts. This would directly address the shortcomings of present Gaussian Process methods identified by Bonfield *et al.* (2010) vis-à-vis error propagation.

Figure 2 shows preliminary results of our proposed probabilistic Gaussian Process algorithm. Figure 2(a) plots photometric redshift versus spectroscopic redshift for the same simulated galaxy observations used in Figure 1. According to this metric, Gaussian Processes perform better than the EAZY algorithm and comparably to the neural network of ANNz. However, if we instead measure performancy by considering ln[P(truth)], i.e. the logarithm of the value of the posterior probability density function at the known spectroscopic redshift of our galaxies, we see that Gaussian Processes consistently outperform neural networks (see Figure 2(b)). Figure 3 recreates Figure 2(b) using actual data taken from the Sloan Digital Sky Survey [Abazajian *et al.* 2009].

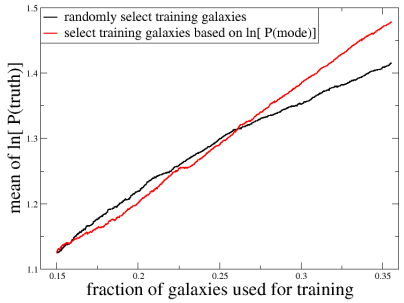


FIG. 4: A demonstration of the efficacy of Active Learning. 15% of the 97,000 simulated LSST galaxy observations are randomly assigned to the training data for our Gaussian Process algorithm. The black curve shows the performance of the algorithm as more galaxies are assigned at random to the training data. The red curve shows the performace of the algorithm as galaxies are chosen which maximize $-\ln[P(\mathrm{mode})]$ and added to the training data. Judiciously choosing training galaxies ultimately improves the performance of our learning algorithm.

B. Active Learning and Photometric Redshifts

The discussion above illustrates how the appropriate choice of machine learning algorithm can affect the fidelity of one's photometric redshift determinations. Further gains can be made if one is similarly judicious in choosing a training set. While next generation surveys like the LSST will be exclusively photometric, they will present us with large numbers of galaxies which we will have the option to follow-up with off-site spectroscopy. It behooves us, therefore, to develop a quantitative way of determining which galaxies represent the most effective use of these limited follow-up resources. Such methods fall in the field of active learning and we will develop novel algorithms for this purpose.

Active learning algorithms iteratively decide which data points they will collect outputs on and add to the training set. The goal is to choose the points that will most improve the model being learned. At each step, they consider the current training data, the potential training data that could be collected, and the current learned model, and evalute each potential new point according to some objective criterion. After selecting one or more new points, the outputs for those points are collected and added to the training set and the process repeats. The key to the active learning algorithm is the specification of the objective criterion used for selection. Settles (2009) presents a survey of such criteria.

Figure 4 demonstrates the effect that active learning can have on an automatic classifier, like our Gaussian Process photometric redshift algorithm. Initially, 15% of our 97,000 simulated LSST galaxy observations are randomly chosen to be training (spectroscopic) data. After that, we attempt two schemes to grow our training set. The black curve represents random selection of training data. The red curve represents training data chosen such that, at each iteration, the galaxy with the maximum value of of $F \equiv -\ln[P(\mathrm{mode})]$ is added to the training data. Choosing to follow up on galaxies about which the least is known (those with maximum F) ultimately produces a more effective classifier.

The method demonstrated above was the simplest possible active learning scheme. At each iteration, the algorithm "greedily" chose the galaxy with the least-constraining PDF (measured by the vaule of the PDF at its mode). More advanced active learning algorithms explored by our group in other contexts [Garnett *et al.* 2011, Garnett *et al.* 2012a] choose follow-up candidates by "looking ahead" and determining the effect of a follow-up measurement on the expected accuracy of the classification after both the immediate next iteration and the iteration to follow. This algorithm was originally implemented in the case of a binary classification ("benign" versus "malicious" inputs). In the current context, we will extend this analysis to incorporate the full posterior PDF over redshift.

We will test our algorithms using both real (as in Figure 3) and simulated (as in Figures 2 and 4) data. Connolly is the LSST lead for simulation. Validation of these techniques will utilize existing data sets comprising spectroscopic redshifts and five band photometry for one million galaxies taken from the SDSS (for low redshift galaxies) and 30,000 galaxies from the DEEP2[2] survey (for high redshift galaxies). We will extend these datasets to include multiple narrow band observations to evaluate how well we can measure redshifts with narrow band photometry.

III. TRANSIENT CLASSIFICATION

In addition to the unknown constituents of cosmology, future surveys promise to yield observations of unknown sources within our own galaxy. Most exciting among these will be the variable sources: stars whose luminosity changes either periodically or cataclysmically. Some such sources are already known and well-understood, such as type II supernovae. Some are known, but mysterious, such as the afterglows of Gamma Ray Bursts. Many others are still waiting to be discovered [LSST Science Collaborations 2009]. As with cosmological redshift, it would be ideal if we could take detailed spectra and time-series photometry of each source in order to understand its physical nature. This is unrealistic. The LSST is projected to detect as many as one million variable sources every night [LSST Collaboration 2011]. There are not sufficient follow-up resources to target every one of these sources with a detailed observation. Astronomers must develop algorithms to identify, in real time, using sparse observations which transients are novel and which are well-understood and what follow-up observations would yield the most information about the novel sources. These algorithms must be rapid and robust, as the decision to follow-up a given transient must be made before the transient fades back into quiescence. In addition to their impact on future surveys, such as the LSST, these algorithms will find immediate application characterizing observations taken by The Palomar Transient Factory[3] and Catalina Sky Survey[4].

Real-time automatic classification of objects is already widely acknowledged as a necessary support technology for the forthcoming age of survey astronomy [Djorgovski *et al.* 2011, Richards *et al.* 2011, Richards *et al.* 2012, Graham *et al.* 2012, Mahabal *et al.* 2008a,

[2] http://deep.ps.uci.edu
[3] http://www.astro.caltech.edu/ptf/
[4] http://www.lpl.arizona.edu/css/

Mahabal *et al.* 2011a]. Objects will need to be categorized into known science classes so that novel or rare objects can be flagged for detailed follow-up observations. For transient events, algorithms must be able to make rapid decisions so that sources can be targeted for follow-up and classifications learned before objects return to their quiescent phases. A great deal of work has already been done developing algorithms that can learn the classification of an object given a fixed set of observations and training data. Mahabal *et al.* (2008a,2011a,2011b) propose to break down the observations of a given object into $\{\Delta m, \Delta t\}$ pairs (where m is magnitude and t is time) and use the density of observations in this two-dimensional space as the basis for a Bayesian classification algorithm. Mahabal *et al.* (2008b) alternatively propose to use those same $\{\Delta m, \Delta t\}$ pairs as the input to a Gaussian process regression by which they will reconstruct the object's entire light curve as a function of time, and then classify the object based on that reconstruction. Richards *et al.* (2011) use observations of transient objects to extract periodic (e.g. the amplitude and frequency of the first two Fourier modes of the object's light curve) and non-periodic (e.g. the variance and skewness of all of the magnitude observations taken, regardless of their separation in time) and feed those features into several tree-based classifiers. They find misclassification rates lower than 30% with their best method yielding a misclassification rate of 22.8%. Using only non-periodic features, which will be especially easy for survey telescopes to gather, rather than full light curves, they find a misclassification rate of between 26% and 28%. Bloom *et al.* (2011) also use a tree-based automatic classifier on Palomar Transient Factory data and find a 3.8% error rate when discriminating between four major classifications. Richards *et al.* consider a more complete set of 25 possible classifications. Clearly, many possibile approaches are available for the automated classification of transient objects, and not all of them rely upon highly detailed observations to function.

A. Active Learning for Transient Objects

The input features for transient object classification will be photometric and morphologic measures taken at different increments in time. The output is a categorical variable indicating the class. This is in contrast to photometric redshifts where the output is continuous. Fortunately, the underlying covariance for Gaussian process classification is the same as for regression and we will adopt a similar prediction model.

The active learning problem for transient objects contains three subproblems, active learning, active search, and active feature acquisition. Finally, one additional difference between the transient object method and the photometric redshift method is that transient object decisions must be made in an online, streaming fashion. Rather than considering an entire pool of test objects, they appear one at a time as they are detected and the algorithm must decide whether and how to follow up on each immediately as they are detected. We first describe algorithms for each of the three pieces and then how to combine them into a single algorithm for streaming transient detections.

Active Learning. In order to get a ground-truth class for a transient object, repeated observations are taken to estimate a full light curve. A human expert then assigns a class label. Both the repeated telescope observations and human time are expensive and thus

we want to learn a good classification model using limited training data. We propose a corresponding trace and survey criteria for active learning on transients as in Section II B.

Active Feature Acquisition. When considering photometric redshifts, we assumed that all photometric inputs were observed for every object of interest. For transients this will not be the case. A large component of the problem is deciding for each object, whether observations of additional colors and/or additional times would be valuable in classifying or characterizing the object.

We propose to extend our recent work on using GPs to detect damped lyman-alpha (DLA) systems [Garnett *et al.* 2012b]. In that work GP regression was used on each observed, noisy spectrum to infer the latent spectrum. The single independent (input) variable was wavelength. For transient objects we will have 5 color magnitudes that are a function of time and are coupled to each other. In the DLA work, a different model was learned for spectra with and without a DLA. DLAs were classified by recognizing which model fit best. In the proposed work, we will learn a different model for each class of object and will estimate class probabilities using Bayes rule for combining the prior probability for each class and how well the respective models fit the observations. The key advantage of this approach is that the GPs naturally provide a mean and covariance for future unobserved colors. This uncertainty propagates through to class labels and we can use it to estimate the reduction in class uncertainty that will be gained by observing a certain color at a certain time. The observation yielding the greatest reduction in entropy for the class and the light curves for this object will be taken.

Active Search. Many transient objects will be from common and/or well-understood classes that do not have much observational value. The ultimate objective in following up detected transients is to maximize the number of interesting transients classified and characterized while staying within a budget of follow-up observations. This is an active search problem. The problem and the Bayesian optimal algorithm for it are described in our recent work [Garnett *et al.* 2011, Garnett *et al.* 2012a]. As in active learning, the acquisition of class labels is expensive and we need to learn a model to predict these labels from limited input data. However, the final performance objective is not the accuracy of the classifier, but rather the number of positives (i.e. objects from interesting classes) identified. We propose to use the simple myopic algorithm described in that work. It computes the probability of each point belonging to the positive class and chooses the largest.

A combined streaming method. The three goals above will be combined in a staged set of decisions. When a new transient is detected, the light curve model will be used to provide estimated light curves for the object. Those light curves are the input variables for this object in the active learning and active search algorithms. In parallel, the active learning and active search methods will decide whether to follow up on this object. If either of them selects the object, it is advanced to active feature acquisition. There additional observations on the object are selected and the process for this object repeats. An object that initially seemed interesting to one algorithm may cease to be so after additional observations or may be adopted by the other one. The process for one object terminates when neither active learning nor active search remains interested in it or the object class and light curves are characterized well enough that no more observations are required.

The active search and active learning algorithms each compute an objective criterion score

for each object. For photometric redshifts the scores are used to create a ranked list and observations are scheduled proceeding down the list. When a budget is given for follow-ups on each batch of newly detected transients, going down a ranked list in each batch until that budget is exhausted is appropriate.

However, when the budget is an aggregate over a longer time period a streaming decision on how much of the budget to spend on each batch must be made on that batch in isolation. This will be done by choosing a score threshold. The threshold will be set by evaluating the historical stream and setting it at a value that would yield a number of follow ups equal to an available budget for following up. The threshold will be adjusted continuously as more observations are taken and the models and scientific goals change (e.g. the object types designated as "interesting" are changed).

Since all of the algorithm components are based on GP models, it is possible to merge them together into a single model. We hypothesize that additional performance improvements can be made through an integrated model and decision algorithm. For example, an object with a modest active learning score that can be easily characterized with only one more follow up might be promoted over one with a higher score that can not be easily characterized even with many more observations. After we have implemented the staged method described above, we will investigate and compare an integrated model.

IV. ON-LINE LEARNING ALGORITHMS

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