

Astronomical imaging: The theory of everything

David W. Hogg^{*} and Dustin Lang[†]

^{*}*Center for Cosmology and Particle Physics, Department of Physics, New York University,*

4 Washington Place, New York, New York 10012, USA

[†]*Department of Computer Science, University of Toronto,*

6 King's College Road, Toronto, Ontario, M5S 3G4 Canada

Abstract. We are developing automated systems to provide homogeneous calibration meta-data for heterogeneous imaging data, using the pixel content of the image alone where necessary. Standardized and complete calibration meta-data permit generative modeling: A good model of the sky through wavelength and time—that is, a model of the positions, motions, spectra, and variability of all stellar sources, plus an intensity map of all cosmological sources—could synthesize or generate any astronomical image ever taken at any time with any equipment in any configuration. We argue that the best-fit or highest likelihood model of the data is also the best possible astronomical catalog constructed from those data. A generative model or catalog of this form is the best possible platform for automated discovery, because it is capable of identifying informative failures of the model in new data at the pixel level, or as statistical anomalies in the joint distribution of residuals from many images. It is also, in some sense, an astronomer's “theory of everything”.

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CATALOGS AND IMAGE MODELS

Astronomers love catalogs; we have been creating catalogs of celestial sources for as long as there has been information recorded in hard copy. Why? Consider two examples.

The first is Abell [1]. He spent thousands of hours poring over images of the sky; his Catalog communicated information he found in those images, so that other workers would not have to repeat the effort. This was at a time when you couldn't just “send them the data and the code”. Indeed, Abell's Catalog wasn't constructed using code at all; there was no way to re-run the experiment, so the experiment *had* to be recorded and published in the form of the output catalog.

The second is the Sloan Digital Sky Survey (SDSS) [2]. Why did the SDSS produce a catalog rather than just releasing one enormous, five-band, terapixel image? The SDSS Collaboration produced a catalog because investigators want to search for sources and measure the fluxes of those sources, and they do this in a limited number of ways. The SDSS made it easier for them by pre-computing all these fluxes and positions and making the computation output searchable.

Importantly, however, unlike Abell, the SDSS *could have* produced a piece of fast code and a fast interface to the data, and *could have* made it easy to run the code on the data and search its output. For any user, that would have been no worse; it could even have been *identical* in user interface and query language (though—admittedly—much

harder to implement at the present day).

Astronomers use the SDSS Catalogs (instead of working directly with the image pixels) not just because they are easy to use but also because they contain all of the SDSS Collaboration's *knowledge* about the data, encoded as proper data analysis procedures and error estimates; this knowledge takes considerable time and effort to learn and implement. This is a very important aspect of a good catalog: It has made the best possible use of the data. But here it would have been *equally good*—and we would argue *more useful*—to produce a piece of shared *code* that knows about these things than an immutable data file or database that knows about these things: The code would be readable (self-documenting), re-usable, and modifiable. Code *passes on* knowledge, whereas a catalog *freezes* it.

In fact, a sufficiently persistent astronomer *can* get the code that was used to create the SDSS Catalogs, or at least parts of it. But there is still a problem in principle: The SDSS Catalogs (in common, as far as we know, with *all* widely used astronomical catalogs at the present day) have no *justified probabilistic description* or basis in the subject of *statistical inference*.

Both Abell and the SDSS Collaboration used their catalogs to describe a set of imaging data. How do we judge whether or not a particular description is a *good* description? If we have two reasonable but different descriptions of the same imaging data, how can we choose between them? We need a quantitative measure of the *quality* of the description. Fortunately, there is a standard solution to this problem, which is justified in the context of Bayesian (or frequentist) inference: The best description of the data is the one that generates the highest-posterior-likelihood *model* of the data (or, if you like, of derived features, derived from the data by a similar inferential process).

These issues are not theoretical: For example, in the SDSS Catalog, there is a sophisticated and extremely well thought-out system that performs “deblending” of overlapping sources. This system performs well. However, it makes “hard” (binary) decisions about what extended SDSS sources are groups of overlapping sources, and it separates those sources into components according to those hard decisions. An investigator who wants to question those decisions—decisions made by the code—has no way to perform any kind of hypothesis test between a catalog with a certain source deblended and another catalog that is very similar but has that same source *not* deblended. This situation comes up frequently when the SDSS Catalog is compared to data from other telescopes, where sometimes the comparison data decisively contradict the SDSS Catalog on a point of deblending, and the investigator is squeezed between either ignoring the new data (that is, sticking with the SDSS deblending decision despite the new data) or else re-analyzing the SDSS imaging data from scratch.

Imagine now that along with the SDSS Catalog, the Collaboration had released a piece of code that converts any contiguous chunk of the catalog into synthetic images or model images of that patch of sky, and—if requested—returns a likelihood or posterior probability of those model images given the imaging data and the noise model. This joint release of catalog and code would provide users with a range of new capabilities that go far beyond what is possible with the current Catalog:

- Error analyses could be performed by adjusting the catalog entries and re-evaluating the likelihood. This “non-parametric” approach to error analysis allows

non-trivial (for example, non-Gaussian and non-Poisson) error estimates to be computed and propagated easily.

- It would be possible to measure *any* element of the full “billion by billion” covariance matrix of catalog parameters by adjusting the two catalog entries at the same time and re-evaluating the likelihood.
- Catalogs from different imaging data sets (with different resolutions and at different wavelengths) could be “matched” or compared or fit jointly by finding the catalog parameters that optimize the product of likelihoods of the two data sets. (This presumes that the “language” in which catalogs are communicated is sufficiently flexible that, for example, a single catalog could be submitted to the HST, SDSS, and GALEX “synthetic image” systems without error.) If that became possible, then the entire field of “catalog matching” and the complexity found therein [3]—including issues like the deblending issue mentioned above—could disappear.
- Catalog entries could be made self-documenting, in the sense that it would be easy for investigators to see the effect in the synthetic images of making variations in the catalog parameters.
- Idiosyncratic photometric parameters or other metrics not specifically measured by the catalog makers (and there are many such requests made of the SDSS Catalog makers, even after the Catalog contains dozens of measurements per object per band) could be computed—approximately—by applying the operation to the synthetic images; and the same code could be used to compute the quantity exactly by retrieving the imaging data.

In addition, a “catalog plus code” approach gives catalog builders a way of expressing the ambiguities in the catalog. Rather than making a hard decision about each catalog entry, the catalog builders can make “soft” decisions by trying each reasonable alternative of each decision and producing a *set* of possible catalog entries that explain a particular image region. These samples can be weighted in a principled way: By using their likelihoods, the weight of a potential catalog entry corresponds to its ability to explain the observed image. In this setting, the catalog builders no longer have to set arbitrary thresholds for hard decisions, but instead must set prior probabilities to bias soft decisions. This clarifies the role of priors in the construction of the catalog, and permits other investigators to inject side information.

Finally—and we will return to this below—there is a direct relationship between (lossless) compression of data and Bayesian inference such that—if you choose the right encoding—the most posterior-probable model of a data set also provides the best possible lossless compression of those data for transmission over a channel [4]. In this context, the best possible lossless compression of, for example, the SDSS data, is—in the optimistic future in which the “catalog” is a model of the data—the catalog, the code that converts that catalog into synthetic images, and a map of the residuals. This picture gives new meaning to the idea of a catalog being the result of “data reduction”.

Of course there are many practical issues, since (as with any catalog-building), the code needs to know quite a bit about the imaging and sensitivity properties of the data set, and have a realistic noise model for computing likelihoods. In what follows, we are going to make a general proposal for such a system, deduce some of its potential capa-

bilities, and give some sense of what baby steps we are taking towards implementation.

Don't get us wrong: we love the SDSS Catalogs; one of us (DWH) was involved in a minor way in their construction and vetting [5]. Going forward, we are hoping we can do even better.

CALIBRATION AND STANDARDIZATION

We seek a catalog—which, as we have argued, is an image model—that is a good description not just of one image or one set of images, but of *every astronomical image ever taken*. We need these images to be vetted and calibrated in a consistent way, and we need the vetting and calibration meta-data to be computed and stored in a consistent way for every image. This motivates fully automated vetting and calibration.

We have built a successful system in this domain—*Astrometry.net* [6]—a reliable and robust system that takes as input an astronomical image, and returns as output the pointing, orientation, and field-of-view of that image (the astrometric calibration). The system requires no first guess, and works with the information in the image pixels alone. The success rate is > 99.9 percent for contemporary near-ultraviolet (*Galaxy Evolution Explorer* [7]) and visual (SDSS [2]) imaging survey data, with *no false positives*. We are using this system to generate consistent and standards-compliant meta-data for all public digital and digitized astronomical imaging from plate repositories, individual scientific investigators, and amateurs.

Our basic approach involves two components. The first is an indexing system for asterisms, which can examine a query image and very quickly generate candidate explanations for that image, where each explanation consists of a proposed location, orientation and field-of-view on the celestial sphere. The second component is a verification criterion that judges any proposed explanation. Calibration proceeds by extracting the two-dimensional positions of stars in a query image, typically yielding a few hundred stars localized to pixel accuracy or better. Then, using subsets of stars (asterisms, usually of four stars, but the system is general), the indexing system generates *hypotheses*—proposed alignments of the query image to the sky. We assign a score to each hypothesis by measuring its ability to predict the locations of other stars in the image (taking into account that we cannot expect the image and catalog stars to overlap exactly). This “score” is a well-posed probability, under some justifiable assumptions; it permits us to reasonably estimate the chance of the hypothesis being a false match; we output a result only when this chance is vanishingly small (of order 10^{-9}). We continue generating and testing asterism-inspired hypotheses until we find one with sufficient confidence and output it as a confident match and therefore calibration. In some cases, we never find a hypothesis with sufficient confidence (or we give up searching before we find one), but our thresholds are set such that we essentially never produce a false positive match.

The astrometric calibration locates the image on the sky, and also identifies sources in the image with known sources in established catalogs. This permits other kinds of calibration. We have shown, for example, that comparison of the precise positions of the stars in the image with their positions and proper motions tabulated in current catalogs determines the *date* at which the image is taken, to an accuracy of years in typical

data [8]. We are currently working on other kinds of calibration:

- Analysis of sources known in previous catalogs to be stars provides an estimate of the point-spread function and its variation over the field. Right now there is no widely agreed-upon method for storing or communicating point-spread function meta-data, but certainly this is essential.
- Comparison of the brightness ordering of sources in the image with brightness ordering in other multi-band catalogs provides a reliable estimate of the broad-band wavelength bandpass.
- Comparison with tabulated magnitudes or flux densities provides an estimate of the sensitivity or zero-point.
- Statistics of the dark and bright parts of the image can be used to infer aspects of the noise model and saturation or nonlinearity effects. Some of these can be pathological, even for science-grade data. Since right now these kinds of problems are usually handled with expert systems built on observer “folklore”, this is the area in which we have the least confidence in our ability to work automatically.

We seek to remove astronomers from the calibration step. Of course one problem with the limited approaches we are taking with *Astrometry.net* is that the system is taking the images *independently* and not using the *joint* information about calibration from many images that can far exceed the information in any individual image. Think, for example, of all the images from the SDSS Telescope; we understand the world coordinate systems and its variations and the point-spread function and its variations much better by considering all of the images *simultaneously* than we do by considering them one at a time.

The quality of system we need for the “theory of everything” is such that it must be able to *discover* these groups of similar and related data, and discover that there are synergies to the joint analysis. (There is an alternative, which is to “hard-code” these synergies, but we are imagining an optimistic future in which this is not possible given the eventual scale.)

Another problem with our current approaches is that we don’t have good strategies for calibrating truly raw data streams; that is, for inferring the pixel-by-pixel relative sensitivities, for inferring additive components like bias and zero-exposure data (think hot pixels and charge sources). These steps *require* that we successfully group input data by source and use it jointly. Similarly, we don’t have good strategies for inferring non-trivial noise models or saturation and nonlinearity problems. There are many important problems here, all of which must be solved if we are going to model the entirety of the available data.

Finally, we have a problem of *reliable data*. Our approach assumes that all data are equally unreliable, and must be calibrated from scratch by our robots. For some data sets this may be unnecessary or even counter-productive, where instrument or survey calibration teams have done a wonderful job. How do we detect these situations automatically—and inject correct priors—or do we really have to calibrate everything from scratch? Will automatic calibration *really* be better than calibration by the best craftspeople? What we have going for us is that CCDs (and equivalent detectors) and telescopes have a limited range of properties and faults. What we have going against us

is that there are some beautifully understood telescopes and cameras, calibrated as well as their entire data outputs allow.

We have emphasized *scale* here, but we also need automated calibration to enforce *standards*: The procedures by which calibration is performed, and the language in which the calibration meta-data are communicated, must be standardized across all the data if joint simultaneous modeling is going to be successful and reliable. This might argue for going with automated calibration *even* in situations where it costs us some precision. That's a quantitative question.

AUTOMATED DISCOVERY

In our world, a catalog is a probabilistic model of the data; indeed, it *generates* a synthetic version of every image upon which it is based. In our optimistic future, every new piece of imaging data can be *explained* by this catalog/model and is also used to *improve* this catalog/model.

The synthetic-image or generative aspect of this model relies completely on reliable and standardized calibration meta-data for each image. Hence the relevance of our automated calibration efforts. These meta-data, at a minimum, must include the astrometric calibration (world coordinate system), the point-spread function as a function of position, the bandpass and sensitivity (zeropoint) of the image (also possibly as a function of position), and whatever is necessary about flatfielding, saturation, defects, and other data complexities. Each incoming image can be synthesized by the catalog, given these calibration meta-data. Preferably, image synthesis happens as close to the “raw data” (original instrument read-out) as possible, but there is a well-posed version of this problem at the “flat-fielded” level also, provided that the calibration was found by a justifiable inferential process. Of course, in the long run, the model comparison with the incoming image and the calibration of the incoming image ought to be performed *simultaneously*, of course.

The key idea is that the *residuals* of the incoming image against the catalog's synthetic image—the image pixels minus the model image pixels—contain information that *improves* the model. These improvements can take several form:

- The residuals could suggest making small adjustments to the positions, fluxes, morphologies, or time-dependence of known sources. Small adjustments can be made to existing model parameters so that the overall posterior probability of the entire data set (prior data plus incoming data) is improved.
- A source that was previously modeled as not moving or not varying or of some particular type could produce residuals in the incoming image that are dramatically reduced if the source is permitted to move or vary or be of another type. New parameters can be spawned in the model that provide the freedom to make these changes and then be set to values that optimize the overall posterior probability.
- A concentrated collection of positive residuals (in image minus model) could be found to be consistent with the morphology of a point-source (or typical extended source, but inconsistent with being a cosmic ray or a detector defect) in the incoming image. A new source can be added to the model to explain these residuals, and

its parameters can be set to optimize the overall posterior probability, perhaps also simultaneously adjusting some of the parameters of nearby or overlapping sources.

- The residuals in the incoming image, when considered *in concert* with the residuals in all of the other overlapping images, might make it such that the posterior probability is improved by adding a new *faint* source. This would be a source that is too faint to detect in any individual image, but appears when one considers the joint information in all of the overlapping images. This could be a well-posed version of what astronomers do when they “co-add” their data (co-addition is rarely the right thing to do with real data, which don’t tend to have purely Poisson errors or be uncontaminated by cosmic rays and other nonlinear defects).

Notice that all four of these scenarios are scenarios of “automated discovery”. The first is least interesting, because the “discovery” is simply that the model needs a tweak. However, the following three count as true discoveries, in that the inclusion of the incoming image has made a *qualitative change* to the catalog, and therefore a qualitative change to our description of the data. The theory of everything is a *framework for automated discovery*.

Our description makes many mentions of the “posterior probability”. This is the probability that is obtained by multiplying, in a Bayesian scheme, the prior probability of the model by the likelihood of the data given the model (and normalizing sensibly). Here the priors matter, deeply: After all, how do you compare one model that does a good job, and another that does a better job, but requires more stars, or more of the stars to move? The frequentist answer is to use χ^2 (the total of the squared residuals in units of the uncertainties) divided by the number of degrees of freedom (the number of data points less the number of parameters). This is not insane, but it is only truly justified in the case of a linear model and Gaussian errors. We don’t have *either* of these in general, certainly not here.

We advocate a *communication* prior: We prefer the model that, when put into a suitably-encoded message along with the residuals of the image against the model, makes for the shortest total message. The posterior probability is, in this case, essentially the total number of bits required to communicate the model parameters *and* the residuals. A better model is better either because it reduces the dynamic range of the residuals (so the residuals require fewer bits) or because it reduces the number of parameters (so the model requires fewer bits). In the case of a linear problem with Gaussian errors, this reduces to the model that minimizes χ^2 per degree of freedom, more-or-less. We prefer this kind of prior for the simple reasons that it has *some* justification in terms of *data reduction*, it reduces to the frequentist answer in the trivial case, and it is easy to apply in real situations. It implements what is essentially the “minimum message length criterion” [9] for Bayesian model selection.

We have taken a step towards this kind of automated discovery with a small project in the SDSS Southern Stripe [10], where the SDSS Telescope has imaged 300 deg² repeatedly—30 to 50 times—in five bands over five years, and produced a calibrated time series of images. We performed image modeling of extremely red sources that are detected in the combined data but too faint to be detected in any individual epoch [11]. We find, as expected, that we can reliably determine proper motions of these faint sources despite the fact that we can’t centroid them at any epoch. The moving sources

we find are consistent with being extremely low-mass sub-stellar objects, discovered “automatically” in the sense we have used it here.

The larger problem—the theory of everything—is an immense problem in data management, calibration, and optimization. However, the model and the data are both extremely “sparse”: Widely separated parts of the sky have almost completely independent parameters, and images from different cameras on different telescopes share very little in their calibration. This means that the model can, in principle, be updated in a local or atomic way. We are confident that—without substantial new technology and in a timescale of years (not decades)—the entirety of preserved, digitized or digital astronomical imaging *can* be assembled and calibrated, and we are confident that an enormously parameterized model of the type we envision *can* be adjusted to optimize a posterior probability that is sensitive to every pixel in that imaging. This, truly, would be an astronomer’s “theory of everything”.

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