Abstract. Systematic exploration of the observable parameter space, covered by large digital sky surveys spanning a range of wavelengths, will be one of the primary modes of research with a Virtual Observatory (VO). This will include searches for rare, unusual, or even previously unknown types of astronomical objects and phenomena, e.g., as outliers in some parameter space of measured properties, both in the catalog and image domains. Examples from current surveys include high-redshift quasars, type-2 quasars, brown dwarfs, and a small number of objects with puzzling spectra. Opening of the time domain will be especially interesting in this regard. Data-mining tools such as unsupervised clustering techniques will be essential in this task, and should become an important part of the VO toolkit.

1. Introduction: Mining the Sky

The great quantitative increases in the amount and complexity of information harvested from large digital sky surveys, with information volumes now measured in multiple Terabytes (and soon Petabytes), with billions of sources detected and tens or hundreds of parameters measured for each of them, pose some fundamental questions: Will this quantitative increase lead to a qualitative change in the way we do astronomy? Will we start asking new kinds of questions about the universe, and use new methods in answering them? How to exploit this great riches of information in a systematic and effective way, and how to extract the scientific essence and knowledge from this mass of bits and pixels? This is indeed what a Virtual Observatory (VO) idea is all about.

There may be two (or, better yet, at least two) main streams of the new, VO-enabled astronomy:

First, there will be statistical astronomy “done right”, i.e., studies such as the mapping and quantification of the large scale structure in the universe, of
the Galactic structure, construction and studies of complete samples of all kinds of objects (stars or galaxies of particular types or particular ranges of properties, AGN, clusters of galaxies, etc.). This is the “bread-and-butter” of astronomy, the way to map and quantify our universe in a systematic, statistically sound fashion, and to feed and constrain our basic theoretical models and understanding. We should never again be limited by the Poissonian errors from small samples of objects; of course, understanding of possible systematic errors and biases in the sky surveys now becomes even more important. Both the numbers of sources and the wide-angle coverage are important for such studies. In some sense, this will be a direct extrapolation of the type of astronomy we have been doing all along, but brought to a higher level of accuracy and detail by the sheer information content of the new, digital sky.

The second stream, where we may expect more novelty and surprises, is a systematic exploration of the poorly known portions of the observable parameter space, and specifically searches for rare types of astronomical objects and phenomena, both already known, and as yet unknown. Here we can use the large numbers of detected sources to look for rare events which would be unlikely to be found in smaller data sets: if some type of an interesting object is, say one in a million or a billion down to some flux limit, then we need a sample of sources numbering in many millions or billions in order to discover a reasonable sample of such rare species. Rare objects may be indistinguishable from the more common varieties in some observable parameters (e.g., quasars look just like normal stars in images), but be separable in other observable axes (e.g., the shape of the broad-band spectral energy distribution). This type of new astronomy with large digital sky surveys (and a VO) is the subject of this review.

2. Exploring the Parameter Space

Some axes of the observable parameter space are obvious and well understood: the flux limit (depth), the solid angle coverage, and the range of wavelengths covered. Others include the limiting surface brightness (over a range of angular scales), angular resolution, wavelength resolution, polarization, and especially variability over a range of time scales; all of them at any wavelength, and again as a function of the limiting flux. In some cases (e.g., the Solar system, Galactic structure) apparent and proper motions of objects are detectable, adding additional information axes. For well-resolved objects (e.g., galaxies), there should be some way to quantify the image morphology as one or more parameters. And then, then there are the non-electromagnetic information channels, e.g., neutrinos, gravity waves, cosmic rays . . . The observable parameter space is enormous.

We can thus, in principle, measure a huge amount of information arriving from the universe, and so far we have sampled well only a relatively limited set of sub-volumes of this large parameter space, much better along some axes than others: We have fairly good sky surveys in the visible, NIR, and radio; more limited all-sky surveys in the x-ray and FIR regimes; etc. For example, it would be great to have an all-sky survey at the FIR and sub-mm wavelengths, reaching to the flux levels we are accustomed to in the visible or radio surveys, and with an arcsecond-level angular resolution; this is currently technically difficult and expensive, but it is possible. The whole time domain is another great potential
growth area. Some limits are simply technological or practical (e.g., the cost issues); but some are physical, e.g., the quantum noise limits, or the opacity of the Galactic ISM.

Historically, the concept of the systematic exploration of the universe through a systematic study of the observable parameter space was pioneered by Fritz Zwicky, starting in 1930’s (see, e.g., Zwicky 1957). While his methodology and approach did not find many followers, the core of the important ideas was clearly there. Zwicky was limited by the technology available to him at the time; probably he would have been a major developer and user of a VO today! Another interesting approach was taken by Harwit (1975; see also Harwit & Hildebrand 1986), who examined the limits and selection effects operating on a number of axes of the observable parameter space, and tried to estimate the number of fundamental new (“class A”) astrophysical phenomena remaining to be discovered. While one could argue with the statistics, philosophy, or details of this analysis, it poses some interesting questions and offers a very general view of our quest to understand the physical universe.

So, it is not just the space we want to study; it is the parameter space (in the cyber-space). Much of the total observable parameter space which is in principle (i.e., technologically) available to us is still very poorly sampled. This is our Terra Incognita, which we should explore systematically, and where we have our best chance to uncover some previously unknown types of objects or astrophysical phenomena — as well as reach a better understanding of the already known ones.

This is an ambitious, long-term program, but even with a relatively limited coverage of the observable parameter space we already have in hand it is possible to make some significant advances.

3. Looking for the Rare, but Known Types of Objects

Some types of astronomical objects, e.g., particular types of stars or quasars may be relatively rare, or simply be hard to find in the available data sets. But we could use some of their known or expected properties (e.g., typical broadband spectra, or variability) folded through the survey selection functions (e.g., bandpass curves) to design experiments where such objects can be distinguished from the “uninteresting” majority (e.g., normal stars or galaxies). This approach has been used very successfully in the past: most quasars have been found using some such approach, first as “radio-loud stars”, then as UV excess objects, etc.; ultraluminous IRAS galaxies have anomalously large FIR/visible flux ratios; variable stars and distant supernovae distinguish themselves with particular types of light curves; and so on.

Sometimes a simple cross-wavelength match can reveal interesting objects or phenomena by indicating those with unusual broad-band energy distributions: recall the discovery of quasars and radio-galaxies, or ULIRGs, or LMXBs, or intra-cluster x-ray gas, or the recent progress on GRBs through the study of their afterglows. This is an obvious area where a VO can be used to construct a detailed, panchromatic view of the universe, and isolate different kinds of objects, with better understanding of the observational biases and selection effects;
Lonsdale’s contribution to this volume illustrates such an approach to a general census of AGN.

If objects are spatially unresolved in some sky survey, then the only distinguishing information is in their flux ratios between different bands, e.g., colors. As an example, FIR flux ratios have been used to classify IRAS sources as probable stars or galaxies (e.g., Boller et al. 1992).

Even within a given survey with a limited wavelength baseline this approach can be used to separate physically distinct types of objects, or, through some photometric redshift indicator, objects of a given type but in different redshift ranges. This color selection technique is now the principal discovery method for quasars at $z \gtrsim 4$ (Warren et al. 1987, Irwin et al. 1991, Kennefick et al. 1995a, 1995b, Fan et al. 1999, 2000a, 2000c, etc.), or brown (L and T) dwarfs (Kirkpatrick et al. 1999, Strauss et al. 1999, Burgasser et al. 2000, Fan et al. 2000b, Leggett et al. 2000, etc.).

As an illustration, in Figure 1 we show how the color selection works with the examples of high-$z$ and type-2 quasars discovered in DPOSS (Djorgovski et al. 1998; and in preparation). Normal stars form a temperature sequence, seen here as a banana-shaped locus of points in the parameter space of colors. The spectra of these quasars, when folded through the survey filter curves (Figures 2 and 3), produce colors discrepant from those of normal stars.

In the case of high-$z$ quasars, absorption by the intergalactic hydrogen (the Lyα forest) produces a strong drop blueward of the quasar’s own Lyα emission line center, and thus a very red $(g − r)$ color, while the observed $(r − i)$ color reflects the intrinsically blue spectrum of the quasars: these objects are red in the blue part of the spectrum, and blue in the red part of the spectrum — unlike any stars. To date, $\sim 100$ such quasars have been found in DPOSS; we make them publicly available through our webpage\textsuperscript{1}. At intermediate Galactic latitudes, there is about one of them per million stars, down to $r \sim 19.5$ magnitude. Thus a good color discrimination and a good star-galaxy separation are essential in order to avoid an excessive contamination of the spectroscopic follow-up samples by mismeasured stars or misclassified galaxies. A variant of this technique (based also on the Lyman-limit drop) is now used to find galaxies at $z \sim 3$ (e.g., Steidel et al. 1999, Dickinson et al. 2000, and references therein).

A similar “convex spectrum” effect can be caused by the presence of strong emission lines in the middle band (r), as shown here in the example of type-2 quasars discovered in DPOSS (Djorgovski et al. 1999, and in prep.). We found a whole population of these long-sought objects (which are now also appearing in considerable numbers in the CXO x-ray data), selected through their peculiar colors. The selection effects are complex, depending both on the [O III] line fluxes and equivalent widths, so we find only a subset of them, those with a mostly unobscured narrow-line region, in the redshift interval given by the width of the DPOSS r band ($z \sim 0.31–0.38$ for the [O III] lines). These objects are sufficiently rare, with surface density $\lesssim 10^{-2}$ per square degree for our selection criteria, that one must have a survey covering a very large area, yet go sufficiently deep to detect the host galaxies (in our survey most of the light in the g and i

\textsuperscript{1}http://www.astro.caltech.edu/~george/z4.qsos
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Figure 1. A representative color-color plot for objects classified as PSF-like in DPOSS. The dots are normal stars with \( r \approx 19 \) mag. Solid circles are some of the \( z > 4 \) quasars, and open circles are some of the type-2 quasars found in this survey. While quasars are morphologically indistinguishable from ordinary stars, this color parameter space offers a good discrimination among these types of objects. Similar methodology is now also used to discover brown dwarfs in SDSS and 2MASS.

bands is from the hosts). This is why this population was missed in the past, with surveys lacking either the necessary depth or the area coverage.

This simple, but very efficient and demonstrably successful method can be used to isolate other kinds of sources as well, e.g., stars of a particular spectral type, to be used as tracers of Galactic structure, or the samples of mostly unobscured quasars in general (cf. Wolf et al. 1999 or Warren et al. 2000). Multiplicity of bandpasses and the dynamical range of the wavelength baseline help; after all, multicolor photometry can be viewed as an extremely low resolution spectroscopy.

Analogous techniques could be used in other parameter spaces, for example for an objective classification and selection of galaxies of a particular type, when image morphology can be quantified appropriately.

4. Looking for New Kinds of Objects

Perhaps the most intriguing new scientific prospect for a VO is the possibility of discovery of previously unknown types of astronomical objects and phenomena.
Figure 2. A spectrum of a typical $z > 4$ quasar, with the DPOSS bandpasses shown as dotted lines. The mean flux drop blueward of the Lyα line, caused by the absorption by Lyα forest and sometimes a Lyman-limit system, gives these objects a very red $(g - r)$ color, while their intrinsic blue color is retained in $(r - i)$. This places them in the portion of the color parameter space indicated in Figure 1.

Figure 3. A spectrum of a typical type-2 quasar, with the DPOSS bandpasses shown as dotted lines. The presence of the strong [O III] lines is the $r$ band places such objects in the portion of the color parameter space indicated in Figure 1.

Such things might have been missed so far either because they are rare, or because they would require a novel combination or a way of looking at the data.
A thorough, large-scale, unbiased, multi-wavelength census of the universe will uncover them, if they do exist (and surely we have not yet found all there is out there). Methodology similar to that used to find known rare types of objects, i.e., as outliers in some suitably chosen, discriminative parameter space, can be used to search for the possible new species. This “organized serendipity” can lead to some exciting new discoveries.

Possible examples of new kinds of objects (or at least extremely rare or peculiar sub-species of known types of objects) have been found in the course of high-z quasar searches by both SDSS (Fan & Strauss, private communication) and DPOSS groups. Two examples from DPOSS are shown in Figures 4 and 5. These objects have most unusual, and as yet not fully (or not at all) understood spectra, which cause them to have peculiar broad-band colors. Their colors places them in the designated portions of the color space where high-z quasars are to be found, and clearly other, as yet unexplored portions of this parameter space may contain additional peculiar objects. While some may simply turn out to be little more than curiosities, others may be representative of genuine new astrophysical phenomena.

Figure 4. A spectrum of a peculiar object PSS 1537+1227, obtained at Palomar. The object was initially selected as a high-z quasar candidate due to its colors, in a manner illustrated in Figure 1. It turned out to be an extreme case of a rare type of a low-ionization, Fe-rich, BAL QSO, at \( z \approx 1.2 \). A prototype case (but with a spectrum not quite as extreme as this) is FIRST 0840+3633, discovered by Becker et al. (1997).
Figure 5. A spectrum of another peculiar object, PSS 0052+2405, obtained at Keck. This object was also initially selected as a high-$z$ quasar candidate. Its nature is still uncertain, but it may be another example of a peculiar BAL QSO — or something completely different.

In order to tackle this problem right, we need proper computational and statistical tools, generally falling in the area of unsupervised clustering or classification, which is a part of the more general and rapidly growing field of Data Mining (DM) and Knowledge Discovery in Databases (KDD). This opens up great opportunities for collaborations with computer scientists and statisticians. For an overview of some of the issues and methods, see the volume edited by Fayyad et al. (1996b), as well as several papers in this volume. Good visualization tools are also essential for this task.

If applied in the catalog domain, the data can be viewed as a set of $n$ points or vectors in an $m$-dimensional parameter space, where $n$ can be in the range of many millions or even billions, and $m$ in the range of a few tens to hundreds. The data may be clustered in $k$ statistically distinct classes, which could be modeled, e.g., as multivariate Gaussian clouds in the parameter space, and which hopefully correspond to physically distinct classes of objects (e.g., stars, galaxies, quasars, etc.). This is a computationally highly non-trivial problem, approaching Terascale supercomputing, and it calls for some novel and efficient implementations of clustering algorithms. However, not all parameters may be equally interesting or discriminating, and lowering this dimensionality to some more appropriate subset of parameters would be an important task for the scientists actually using such tools to explore the data.

If the number of object classes $k$ is known (or declared) a priori, and training data set of representative objects is available, the problem reduces to supervised classification, where tools such as Artificial Neural Nets (ANN) or Decision Trees
(DT) can be used. This is now commonly done for star-galaxy separation in the optical or NIR sky surveys (e.g., Odewahn et al. 1992, or Weir et al. 1995), and searches for known types of objects with predictable signatures in the parameter space (e.g., high-$z$ quasars) can be also cast in this way.

However, a more interesting and less biased approach is where the number of classes $k$ is not known, and it has to be derived from the data themselves. The problem of unsupervised classification is to determine this number in some objective and statistically sound manner, and then to associate class membership probabilities for all objects. Majority of objects may fall into a small number of classes, e.g., normal stars or galaxies. What is of special interest are objects which belong to much less populated clusters, or even individual outliers with low membership probabilities for any major class. Some initial experiments with unsupervised clustering algorithms in the astronomical context include, e.g., Goebel et al. (1989), Weir et al. (1995), de Carvalho et al. (1995), and Yoo et al. (1996), but a full-scale application to major digital sky surveys yet remains to be done. An array of good unsupervised classification techniques will be an essential part of a VO toolkit.

5. Other Domains of the Parameter Space

Most of the work described so far involved searches in the catalog domain, and specifically in the parameter spaces of colors measured in optical and NIR sky surveys. However, many other domains of the observable parameter space are still wide open and waiting to be fully explored.

The low surface brightness universe (at any wavelength!) is one of the obvious frontiers, and is addressed elsewhere in this volume by Schombert and by Brunner et al.; see also the review by Impey & Bothun (1997), and references therein. Conversely, we may be missing some compact, high surface brightness galaxies (a possibility envisioned by Zwicky many decades ago): cf. Drinkwater et al. (1999); however, a field spectroscopic survey of almost-unresolved DPOSS objects at Palomar (Odewahn et al., in prep.) failed to turn up a substantial number of such objects. In any case, expanding the dynamical range of the limiting surface brightness and angular resolution in digital sky surveys at any wavelength is likely to be one of the key area of research in a VO.

Perhaps the most promising new domain for exploration is the time domain: variability at all time scales, and all wavelengths, be it periodic, eruptive, or chaotic in nature. The subject is addressed by Diercks elsewhere in this volume, and by Paczyński (2000). The importance and the scientific promise of the exploration of the time domain has been recognized through the high recommendation of the NAS Decadal Report, *Astronomy and Astrophysics in the New Millennium*, of the Large Synoptic Survey Telescope (LSST). Other large-scale sky monitoring program are already in progress (e.g., Akerlof et al. 2000, Groot et al. 2000, Everett et al. 2000, and the many searches for the Solar system objects reviewed by Pravdo elsewhere in this volume). Synoptic monitoring of the sky over a range of wavelengths, and mining of the resulting multi-Petabyte data sets may be the most technically demanding and among the most scientifically productive areas for a VO.
Figure 6. An example of a serendipitously discovered optical transient event from DPOSS. The left panel shows a portion of a DPOSS \( F \) plate image with an \( r \sim 18.5 \) magnitude, starlike object circled. The object was selected due to its apparent peculiar color (bright in \( r \), extremely faint in the other two DPOSS bands); however, this was simply a consequence of the plates taken at different times, with one of them catching it in a bright state. The right panel shows a portion of the corresponding Keck \( R \) band image. The DPOSS transient was positionally coincident with an \( R \sim 24.5 \) magnitude galaxy, with an estimated probable \( z \sim 1 \). At such a redshift, this object would have been a few hundred times brighter than a supernova at its peak. It may be an example of a GRB “orphan afterglow”, or possibly some other, new type of a transient.

Most of the studies described so far involve searches in some parameter or feature space, \textit{i.e.}, catalogs derived from survey images. However, we can also contemplate a direct exploration of sky surveys in the image (pixel) domain. Automated pattern recognition and classification tools can be used to discover sources with a particular image morphology (\textit{e.g.}, galaxies of a certain type). An example from planetary science, an automated discovery of volcanos in Magellan Venus radar images, was described in Fayyad \textit{et al.} (1996a) and Burl \textit{et al.} (1998). An even more interesting approach would be to employ AI techniques to search through panoramic images (perhaps matched from multiple wavelengths) for unusual image patterns. For example, it may be possible for a program to discover gravitationally lensed arcs in rich clusters, and possibly some other, as yet unknown phenomena.
Finally, an unsupervised classification search for unusual patterns or signals in astronomical data represents a natural generalization of the SETI problem (Djorgovski 2000).

6. Concluding Comments

A VO, applied on the plethora of large, digital sky surveys would enable a thorough and systematic exploration of the observable parameter space, leading to a more complete understanding of the physical universe. Introduction of novel DM and KDD techniques, developed in collaboration with computer scientists will be essential. In addition to the construction of significant samples of various rare types of astronomical objects which can be used for further studies, we are likely to find some completely new things. In this way, a VO will be a unique tool of astronomical discovery.

There is, however, one significant bottleneck which we can already anticipate in this type of studies: the follow-up spectroscopy of interesting sources selected from imaging surveys. While there seems to be a vigorous ongoing and planned activity to map and monitor the sky in many ways and many wavelengths, spectroscopic surveys will be necessary in order to interpret and understand the likely overabundance of interesting objects found. This is something we have to consider in our plans.

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