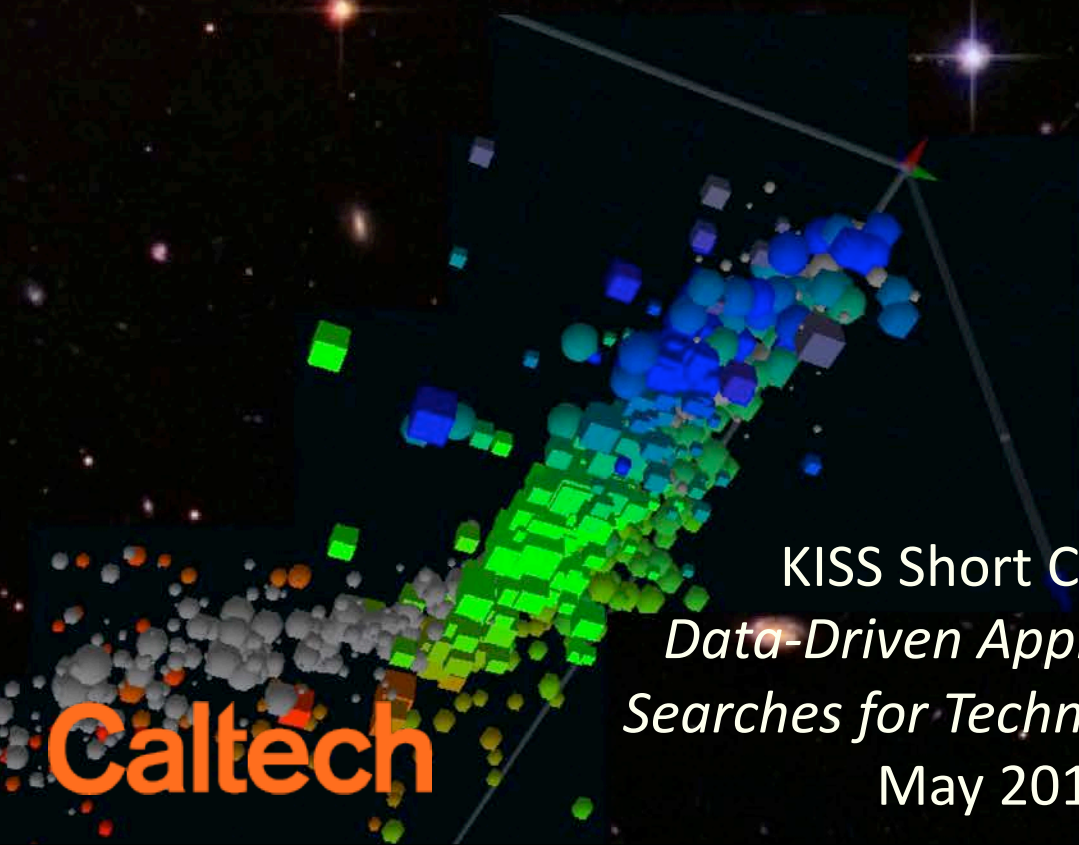


Astronomy Data Landscape and Observable Parameter Spaces

S. George Djorgovski, Caltech

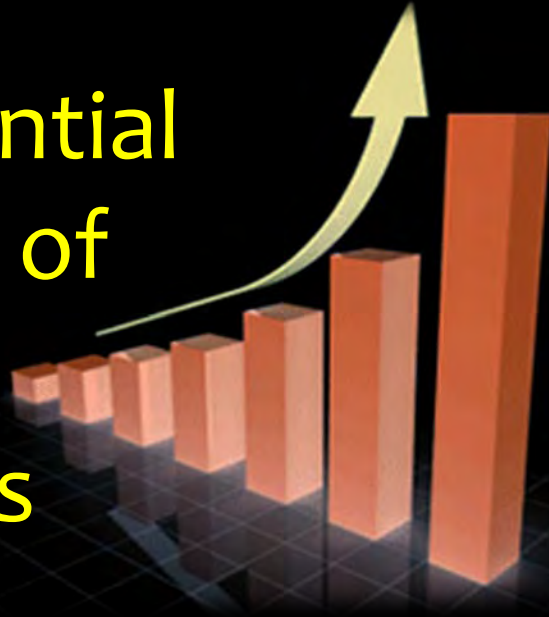


KISS Short Course
*Data-Driven Approaches to
Searches for Technosignatures*
May 2019

Caltech

Keck
INSTITUTE FOR SPACE STUDIES

Exponential Growth of Data Volumes



... and
Complexity



on Moore's law time scales

*Understanding of
complex phenomena
requires complex data!*

From data poverty to data glut

From data sets to data streams

From static to dynamic, evolving data

From anytime to real-time analysis and discovery

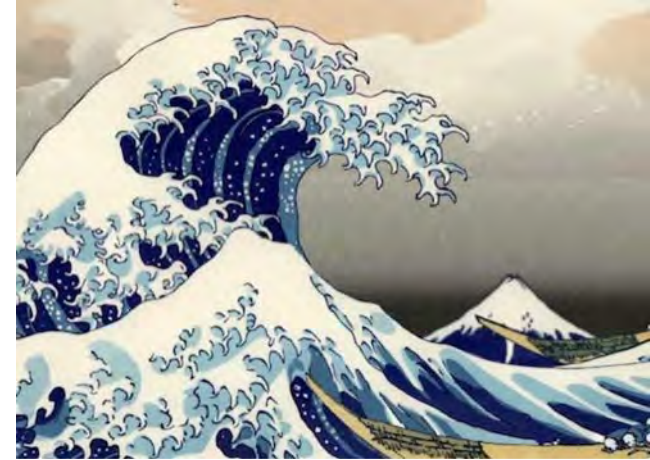
From centralized to distributed resources

From ownership of data to ownership of expertise

What is Fundamentally New Here?

- The *information volumes and rates* grow exponentially

➔ *Most data will never be seen by humans*



- A great increase in the data *information content*

➔ *Data driven vs. hypothesis driven science*

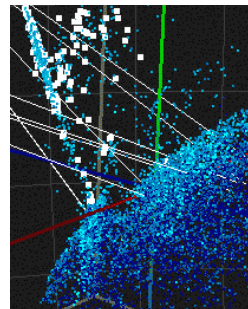
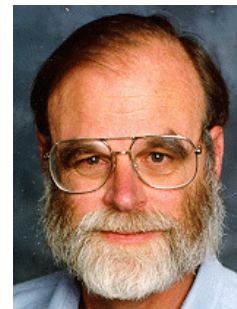
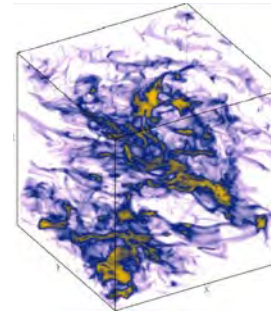
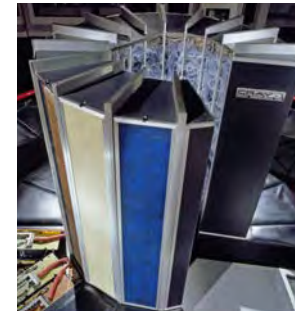
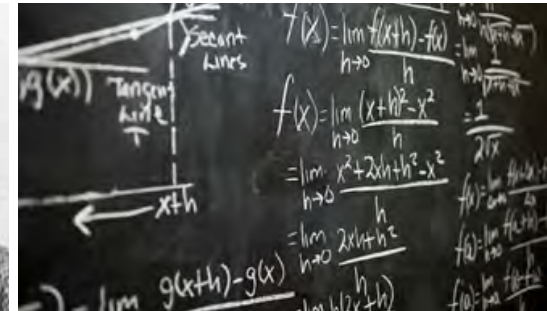
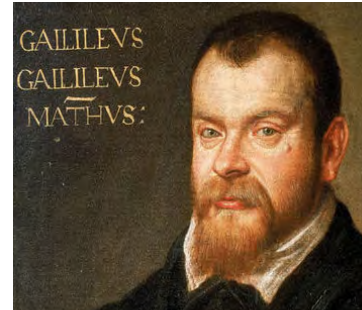
- A great increase in the *information complexity*

➔ *There are patterns in the data that cannot be comprehended by humans directly*

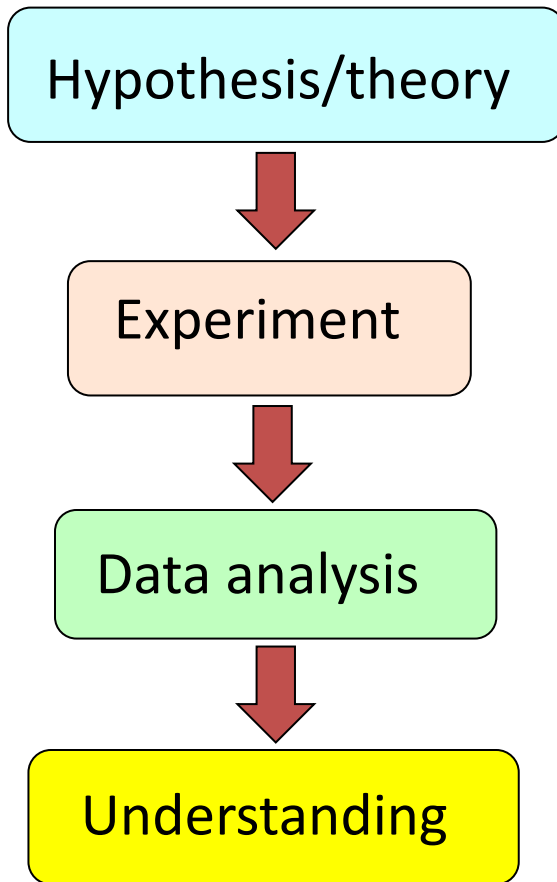


The Evolving Paths to Knowledge

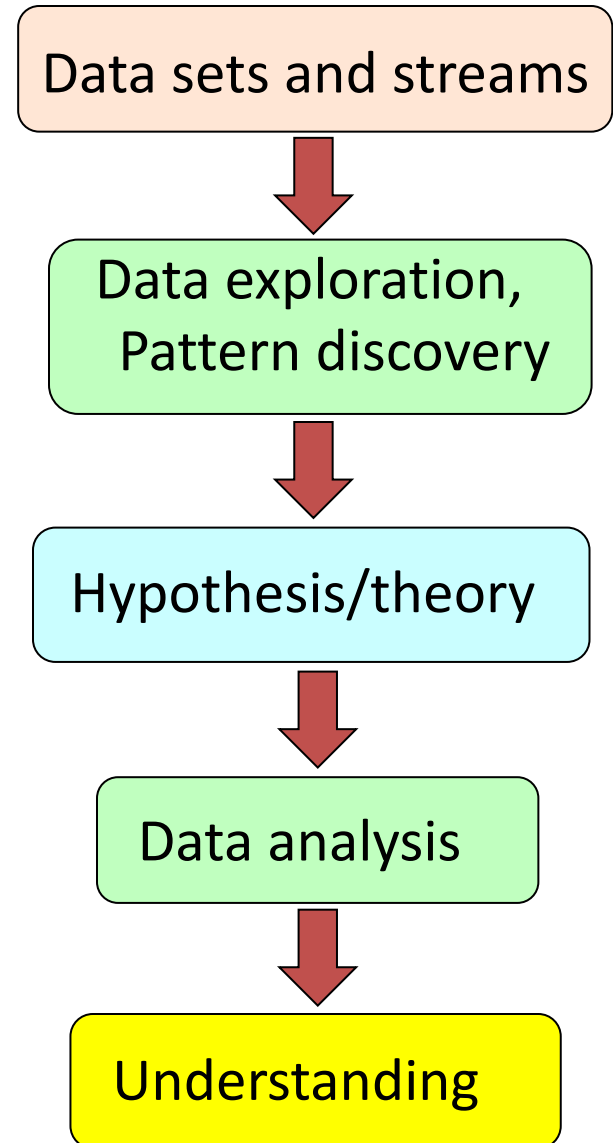
- The First Paradigm:
Experiment/Measurement
- The Second Paradigm:
Analytical Theory
- The Third Paradigm:
Numerical Simulations
- The Fourth Paradigm:
Data-Driven Science



Hypothesis-driven science



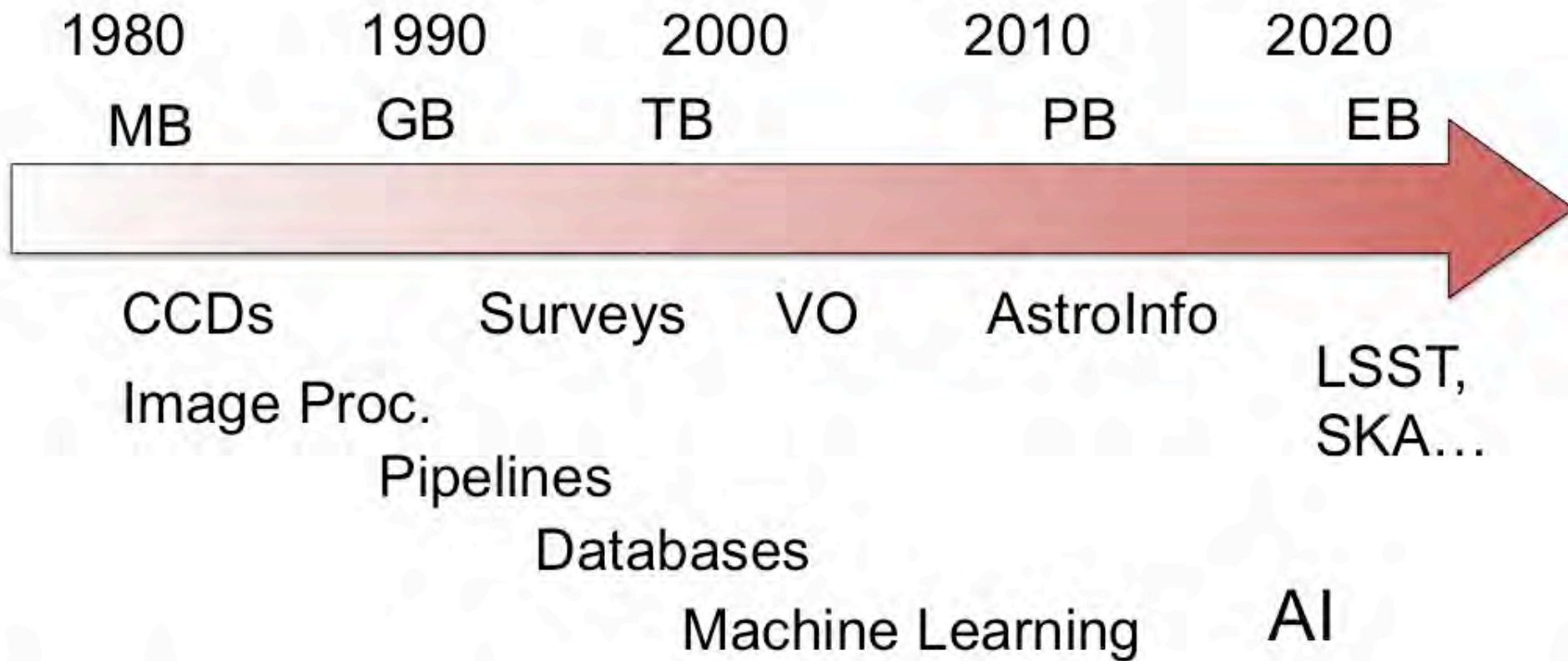
Data-driven science



The two approaches are complementary

The Evolving Data-Rich Astronomy

An example of a “Big Data” science driven by the advances in computing/information technology



Key challenges: data heterogeneity and complexity

How Much Data* is There in Astronomy?

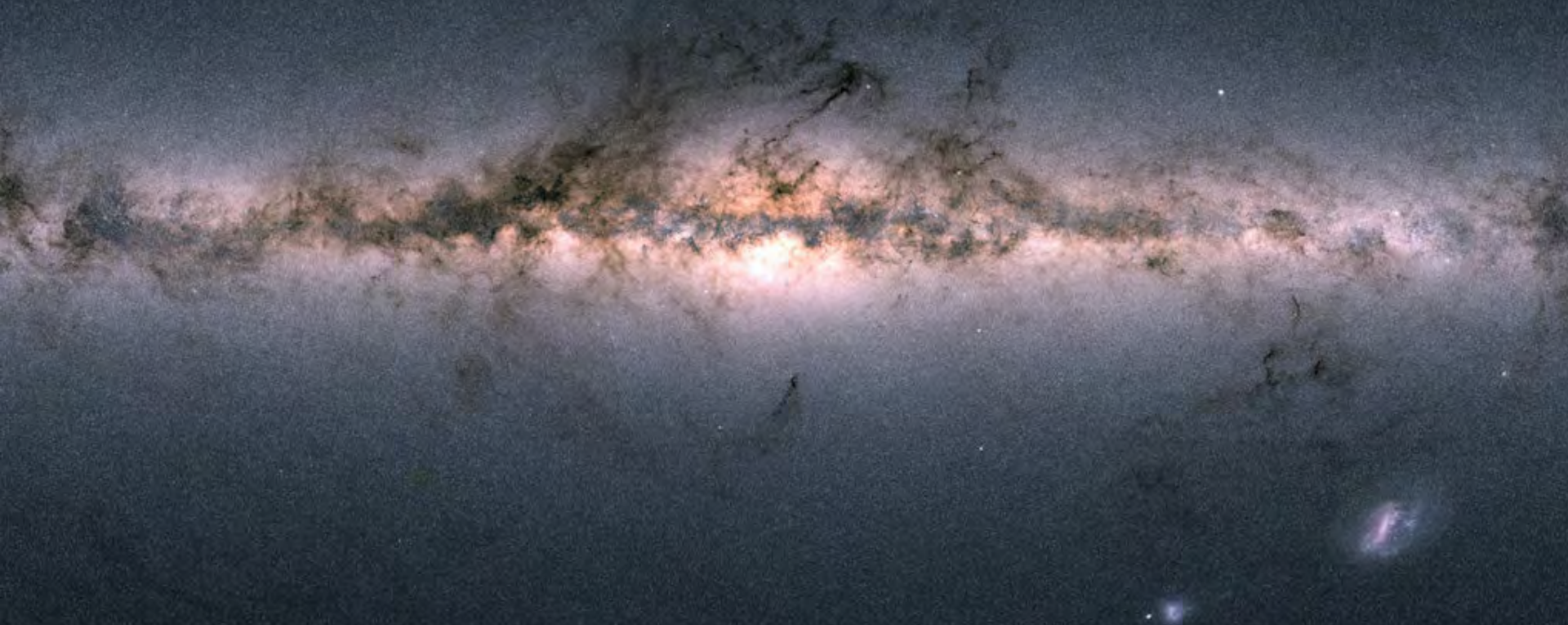
* Archived, curated, accessible

- My best guesstimate (early/mid 2019): $\sim 200 \text{ PB} \times 2^{\pm 1}$
 - Estimated data rate $> 100 \text{ TB/day}$
- Most data come from sky surveys
- Both data volumes and data rates grow exponentially, with a **doubling time $\sim 1.5 \text{ years}$**
- Even more important is the growth of **data complexity** and **data quality** (information content)
- For comparison:
 - Human Genome $< 1 \text{ GB}$
 - Human Memory $< 1 \text{ GB} (?)$
 - 1 TB $\sim 2 \text{ million books}$
 - Human Bandwidth $\sim 1 \text{ TB / year} (\pm)$



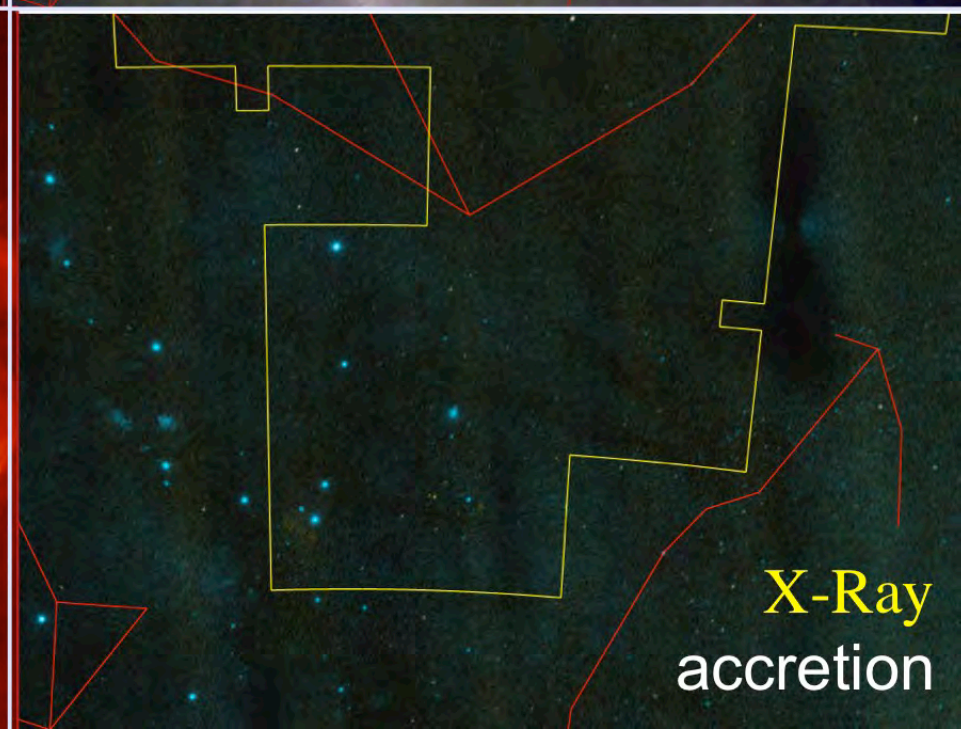
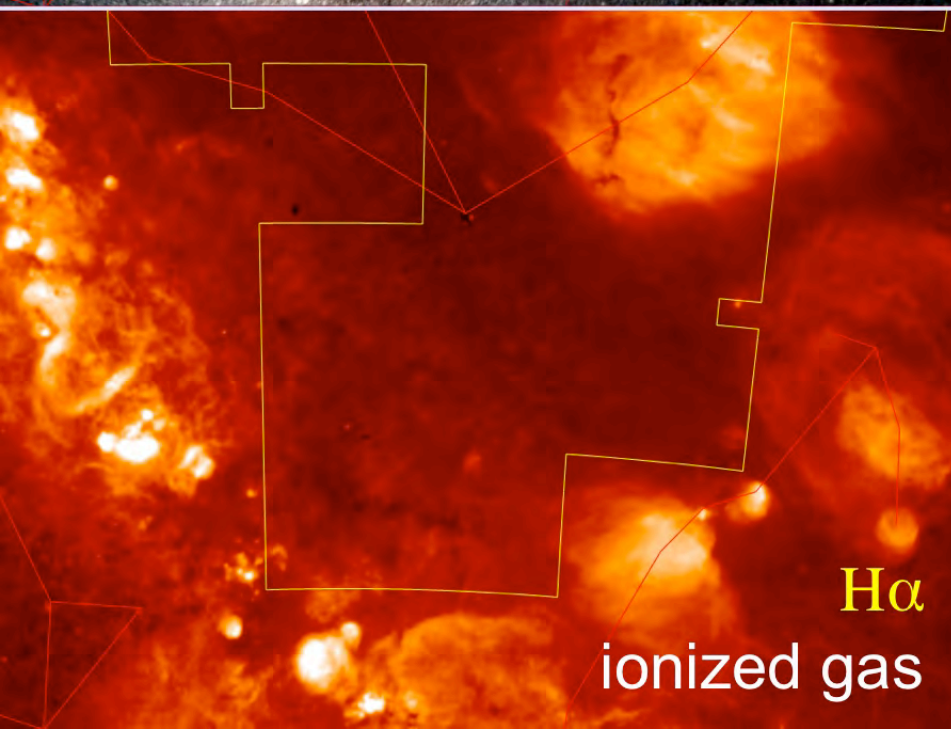
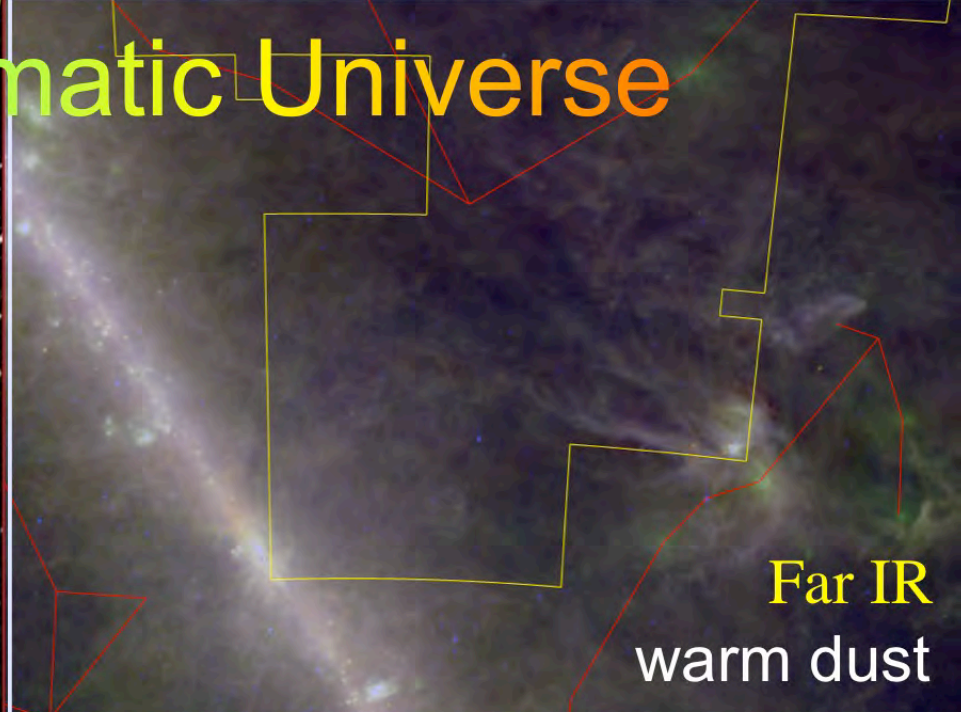
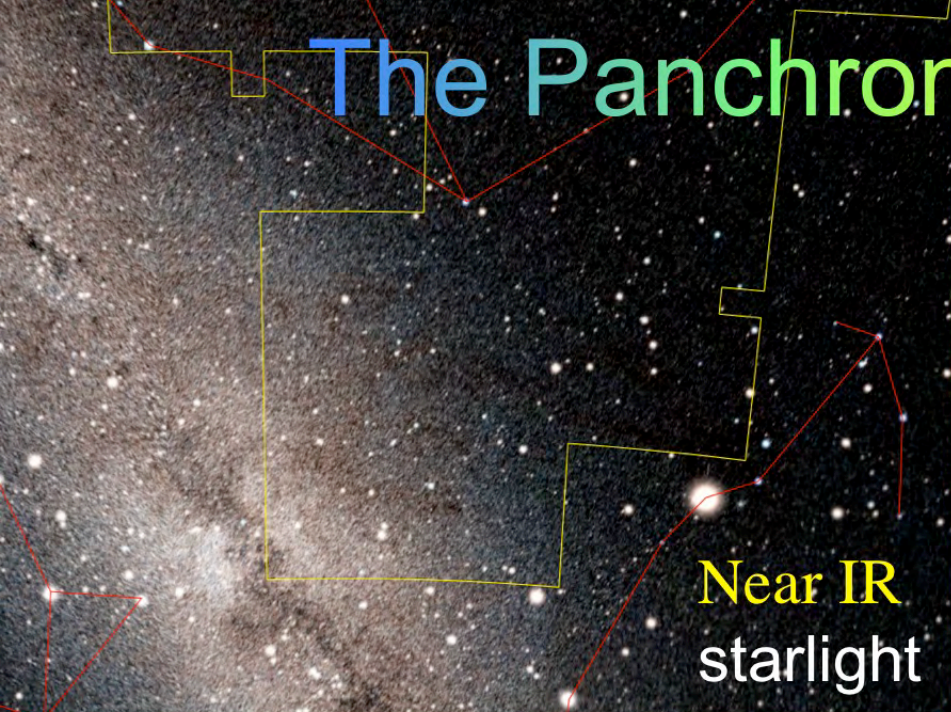
There Are Lots Of Stars In The Sky...

Modern sky surveys obtain $\sim 10^{15} - 10^{16}$ bytes of images,
catalog $\sim 10^9$ objects (stars, galaxies, etc.),
and measure $\sim 10^2 - 10^3$ numbers for each



... and then do it again, and again, ...

The Panchromatic Universe



Sky Surveys: Data Volumes

Sky Survey Projects	Data Volume
DPOSS (The Palomar Digital Sky Survey)	3 TB
2MASS (The Two Micron All-Sky Survey)	10 TB
GBT (Green Bank Telescope)	20 PB
GALEX (The Galaxy Evolution Explorer)	30 TB
SDSS (The Sloan Digital Sky Survey) 170 TB (DR15)	40 TB
SkyMapper Southern Sky Survey	500 TB
PanSTARRS (The Panoramic Survey Telescope and Rapid Response System)	~ 40 PB expected
LSST (The Large Synoptic Survey Telescope)	~ 200 PB expected
SKA (The Square Kilometer Array)	~ 4.6 EB expected

1990s

2000s

2010s

ZTF: ~ 1 PB/yr

2020s

(from Zhang 2015)

Some “Local” Producers:

- CRTS (all surveys, per A. Drake):
 - ~ 100 TB total to date
 - Current data rate ~ 25 TB/yr
- ZTF (3 year survey, per F. Masci):
 - ~ 3.2 PB total archived
 - Current data rate ~ 1 TB/night (images), real-time data products ~ 4 TB/night
- OVRO (per G. Hallinan):
 - LWA: Raw data rate ~ 12 PB/day, archived ~ 50 TB/day ~ 18 PB/yr
 - MWA: ~ Raw data rate ~ 0.65 PB/day, archived ~ 27 PB/yr
 - DSA: Raw data rate ~ 7 PB/day, much less archived

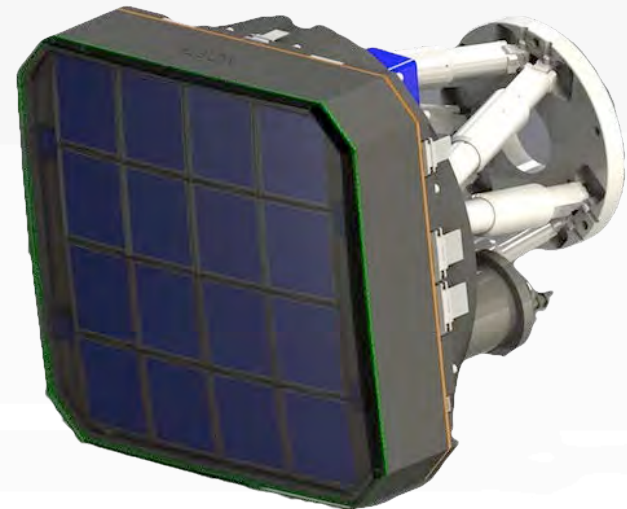
Some space missions:

- ✧ Kepler ~ 20 TB
- ✧ GALEX ~ 30 TB
- ✧ Gaia, 5-yr mission: ~ 200 TB



Zwicky Transient Facility (2017-)



- New camera on Palomar Oschin 48" with 47 deg² field of view
- 3750 deg² / hr to 20.5-21 mag (1.2 TB / night)
- Full northern sky ($\sim 12,000$ deg²) every three nights
- Galactic Plane every night
- Over 3 years: 3 PB, 750 billion detections, ~ 1000 detections / src
- First megaevent survey: 10^6 alerts per night (Apr 2018)





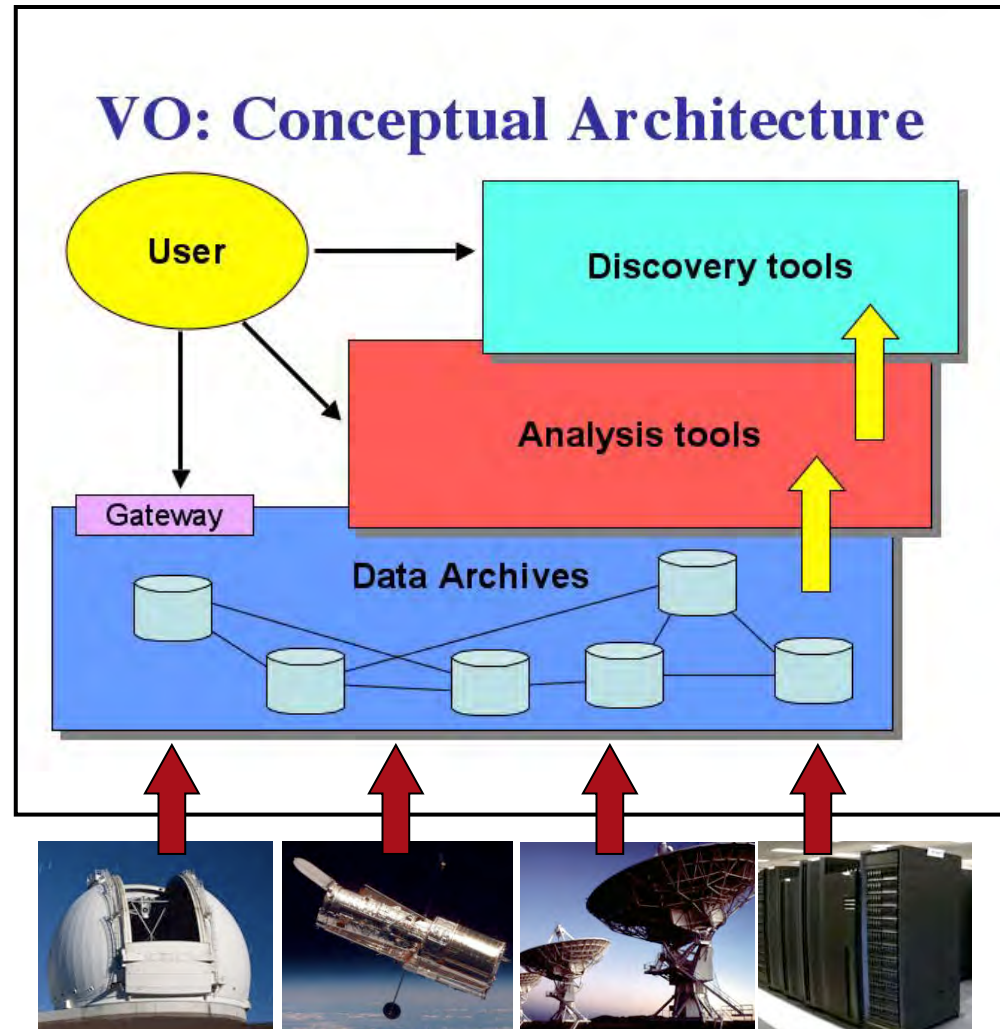
ZTF = 0.1 LSST



		
No. of sources	1 billion	37 billion
No. of detections	1 trillion	37 trillion
Annual visits per source	1000 (2+1 filters)	100 (6 filters)
No. of pixels	600 million (1320 cm ² CCDs)	3.2 billion (3200 cm ² CCDs)
Field of view	47 deg ²	9 deg ²
Hourly survey rate	3750 deg ²	1000 deg ²
Nightly alert rate	1 million	10 million
Nightly data rate	1.4 TB	15 TB

The Virtual Observatory Concept

- Envisioned as a complete, dynamical, distributed, open *research environment for the new astronomy with massive and complex data sets*
 - Provide and federate content (data, metadata) services, standards, and analysis/compute services
 - Develop and provide data exploration and discovery tools (...)
 - Today it is the global data grid of astronomy
 - A successful example of a science Cyber-Infrastructure



IVOA: The Virtual Observatory Reified

- Formed in 2002 to facilitate the international collaborative effort needed to enable integrated access to astronomical archives
- 21 international members
- Working Groups and Interest Groups overseen by Technical Coordination Group reporting to Executive Committee:
 - Applications
 - Data Access Layer
 - Data Models
 - Grid and Web Services
 - Registry
 - Semantics
 - Data Curation and Preservation
 - Knowledge Discovery in Databases
 - Education
 - Operations
 - Solar System
 - Theory
 - Time Domain
- Committee for Science Priorities
- Engage with big projects

IVOA.net



Resources at <http://ivoa.net>

INTERNATIONAL VIRTUAL OBSERVATORY ALLIANCE

[Home](#)[Astronomers](#)[Deployers](#)[Members](#)[About](#)

VO Applications for Astronomers

In this section, scientists can find available VO-compatible applications for their immediate use to do science. The level of maturity of the applications depends on a high degree on the level of maturity of the corresponding IVOA protocols and standards.. As a consequence of the flexibility of the standards, several of the applications might overlap in functionality. **The IVOA does not manage or guarantee these services/tools.**



Applications (in alphabetical order)

Aladin
AppLauncher
CASSIS
CDS Xmatch Service
Data Discovery Tool
Filter Profile Service
Iris
Montage
Octet
SkyView
Specview
SPLAT
TAPHandle

Functionality

Search for Images:

Aladin, Datascope,
SkyView, VODesktop,
Data Discovery Tool

Search for Spectra:

Aladin,
CASSIS, Datascope,
SPLAT, Specview,
VOServices, VOSpec,
Data Discovery Tool

Search for Catalogues:

Aladin, Datascope,
TOPCAT, VODesktop,
Data Discovery Tool

Search for Time Series

VO-compliant Tools & Services

DS9: Image visualiasation
GOSSIP: SED fitting
VirGO: Search for Images
and Spectra
IRAF: Image Reduction &
Analysis
World Wide Telescope
Gaia - Graphical
Astronomy and Image
Analysis
SIMBAD
TESELA
VizieR

A compilation of tools
and services

IVOA is now mainly
a standards
coordination body

...

...

...

AstroInformatics

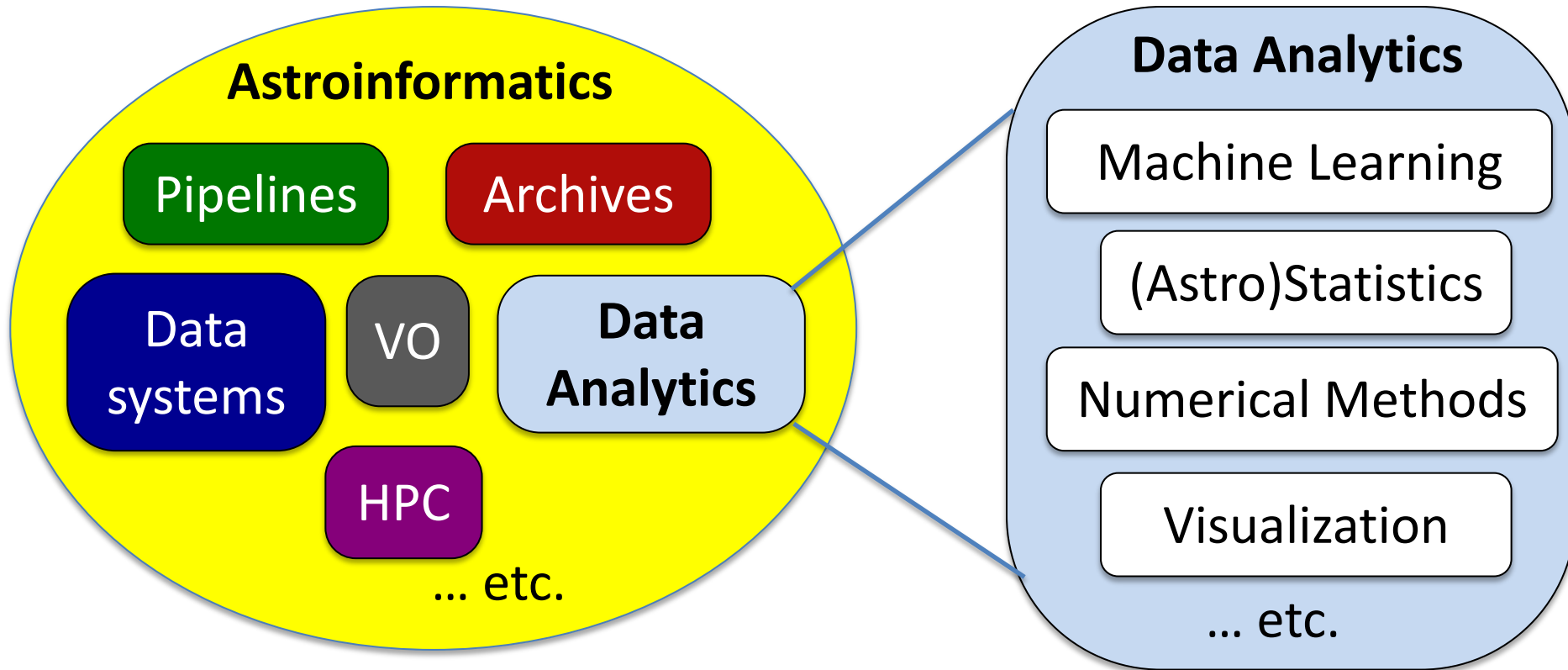
is essentially astronomical applications of Data Science



- While VO became a global data grid of astronomy, astroinformatics focuses on the **knowledge discovery tools**
- It includes a growing community of scientists, both as contributors and as users
- Like other X-Informatics (X = bio, geo, ...) it is a bridge between astronomy and data science, and for the methodology sharing with other fields.

AstroInformatics

It contains all of the components of Data Science, in their astronomical applications, and their interconnections



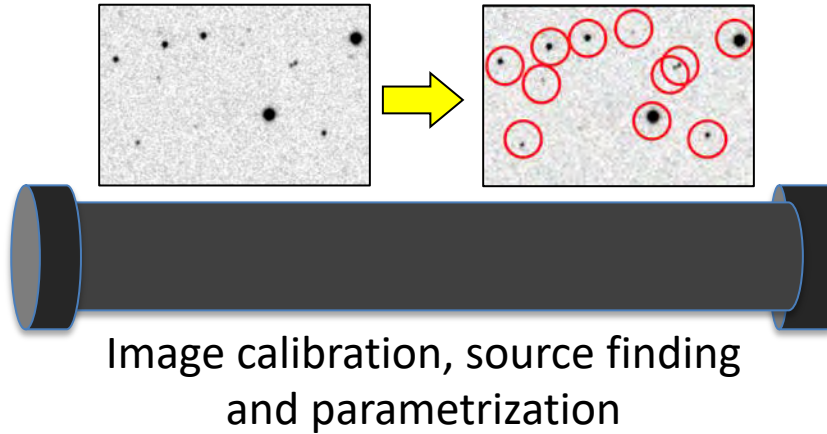
The 10th international conference,
astroinformatics2019.org, at Caltech, June 24-27, 2019

Survey-Based Astronomy

Survey Telescopes



Data Reduction Pipeline

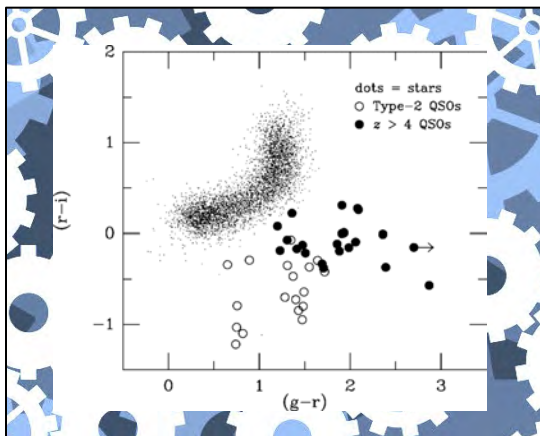


Archive Database

CSS171012:095944+641448	149.93362	64.24678	20171012.47	19.36	yes	2018-06-08	16377
CSS171012:075222+652857	118.09216	65.48244	20171012.41	18.49	yes	2018-05-17	19128
CSS171012:072652+630200	111.71466	63.03323	20171012.39	18.77	no	2018-05-09	14639
CSS171012:084704+593309	131.76754	59.55244	20171012.43	19.37	yes	2018-05-25	15507
CSS171012:172358+530024	260.99323	53.00658	20171012.12	18.73	yes	2018-06-19	11012
CSS171012:084412+531251	131.04870	53.21413	20171012.43	17.29	yes	2018-05-25	11414
CSS171012:164452+443846	251.21538	44.66291	20171012.10	17.80	yes	2018-06-19	12124
CSS171012:235710+401134	359.29246	40.19289	20171012.23	18.44	no	2018-06-19	12739
CSS171012:235703+395916	359.26183	39.98778	20171012.23	14.90	no	2018-06-19	12034
CSS171012:010541+431030	16.42287	43.17505	20171012.28	19.03	yes	2018-06-19	23148
CSS171012:003812+401052	9.55193	40.18108	20171012.25	19.76	yes	2018-06-19	12674
CSS171012:001439+425157	3.66175	42.86579	20171012.26	18.25	no	2018-06-19	21801

Source catalogs define
feature spaces

Data Analysis, Target Selection



Modeling, Machine Learning...

Follow-up Telescopes



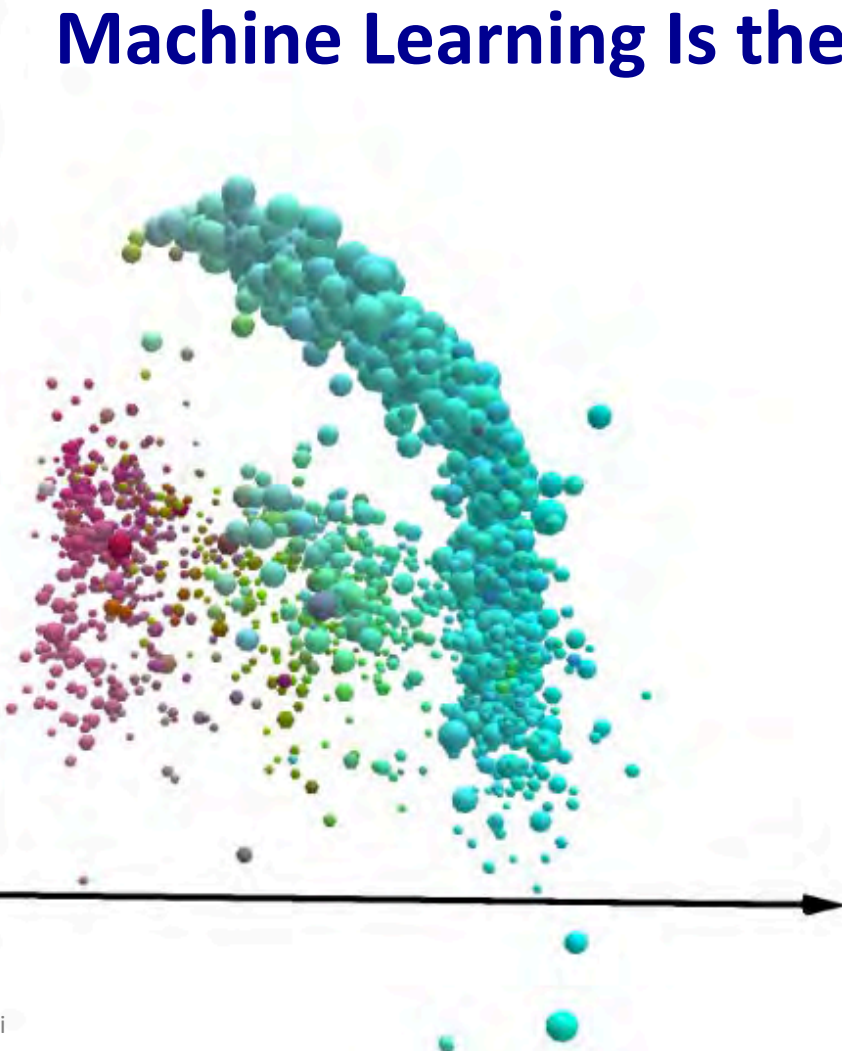
Exploration of Parameter Spaces is a Central Problem of Data Science

Clustering, classification, correlation and outlier searches, ...

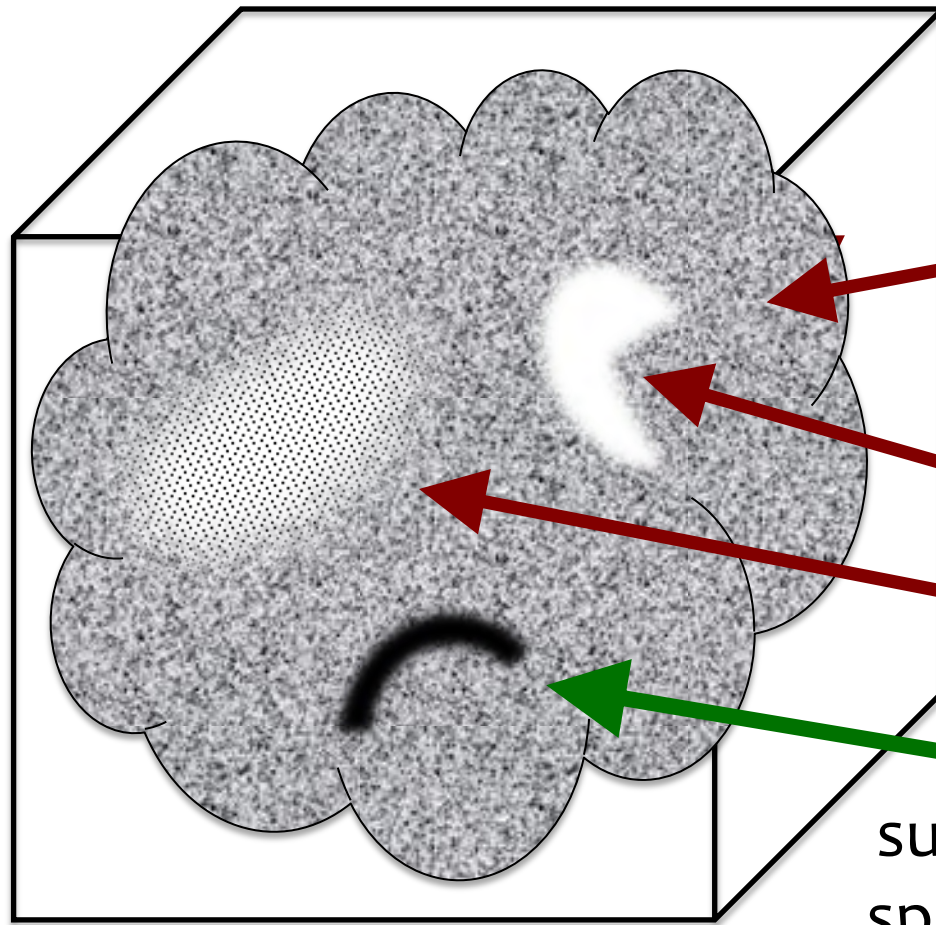
Machine Learning Is the Key Methodology

Challenges:

- Algorithm and data model choices
 - Data incompleteness
 - Feature selection and dimensionality reduction
 - Uncertainty estimation
 - Scalability
 - Visualization
 - ... etc.
- } Especially with the data dimensionality



Pattern or structure (Correlations, Clustering, Outliers, etc.) Discovery in High-Dimensional Parameter Spaces



$D \gg 3$ parameter/feature space hypercube

High-D data cloud: mostly noise, with an arbitrary PDF distribution

Missing data

Data heterogeneity

But in some corner of some subset of dimensions of this data space, there is ***something* \neq noise**, i.e., a statistically significant structure with an unknown form

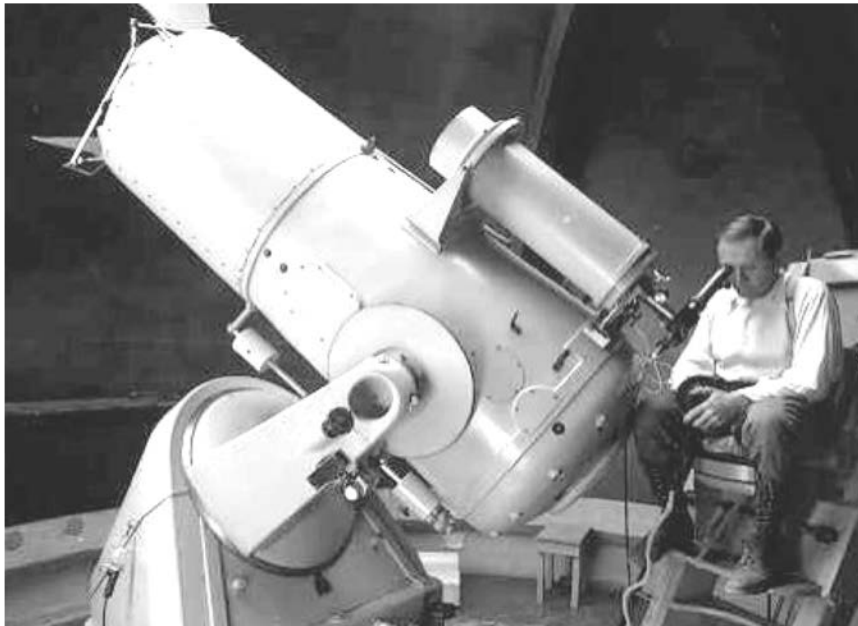
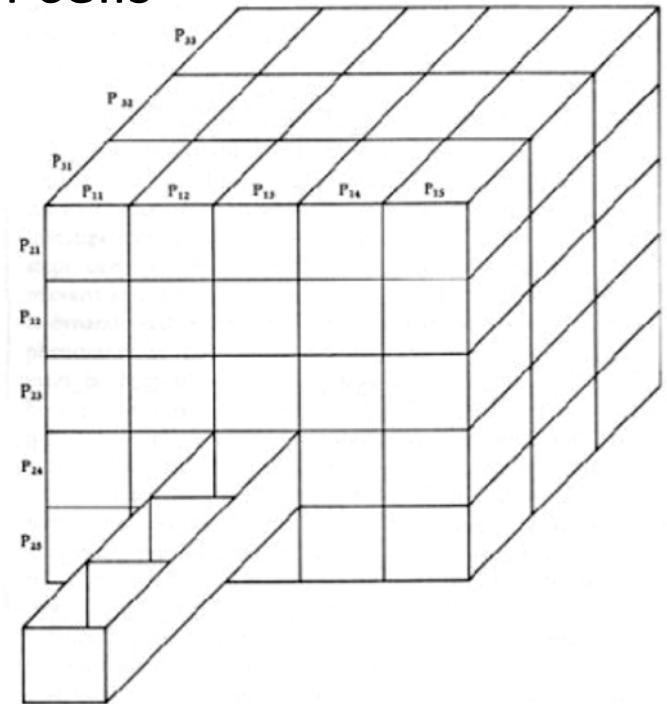
Mapping the Entropy of Large Data Spaces?

From “Morphological Box” to the Observable Parameter Spaces



Fritz Zwicky

Zwicky’s concept: explore all possible combinations of the relevant parameters in a given problem; these correspond to the individual cells in a “Morphological Box”

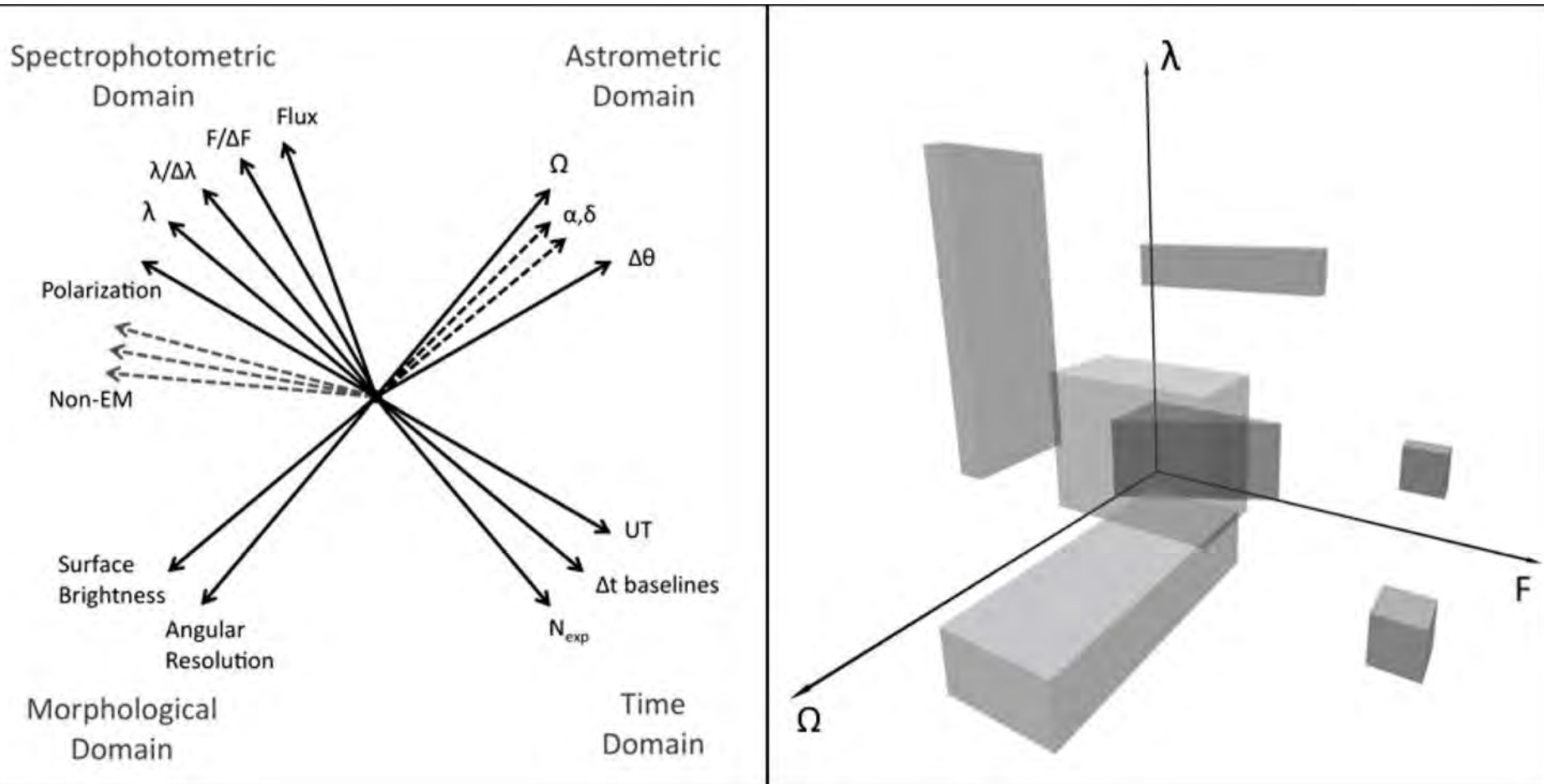


Example: Zwicky’s discovery of the compact star-forming dwarfs

Systematic Exploration of the Observable Parameter Spaces (OPS)

Its axes are defined by the
observable quantities

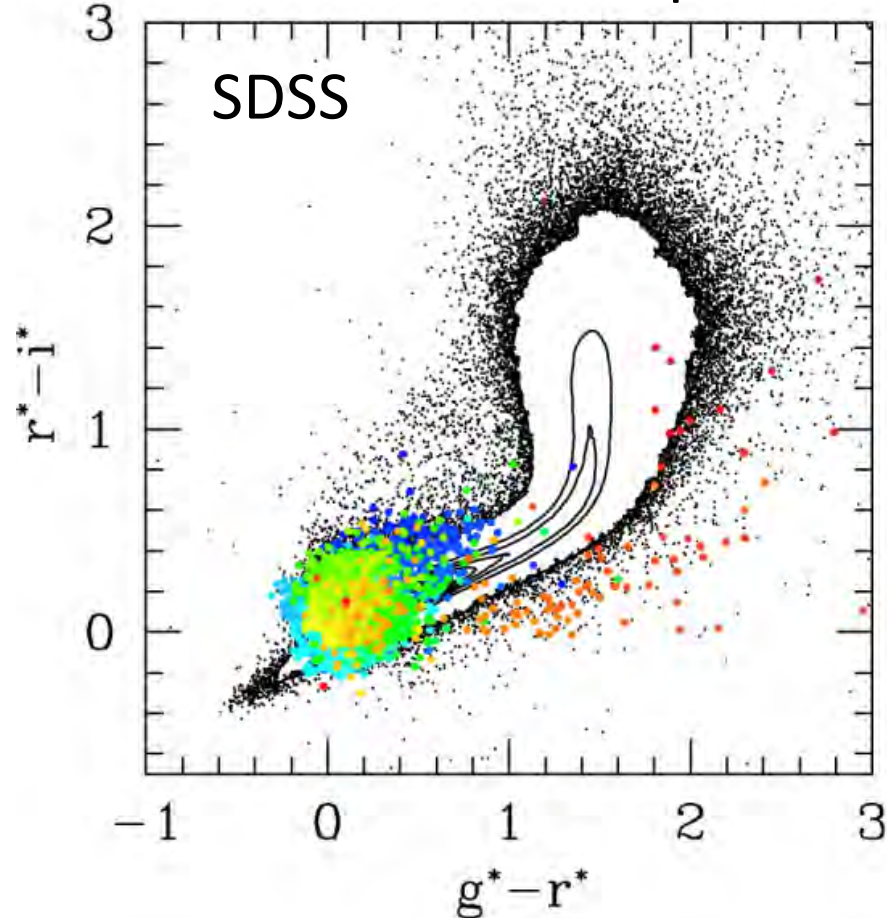
Every observation, surveys
included, carves out a
hypervolume in the OPS



Technology opens new domains of the OPS → New discoveries

Measurements Parameter Space

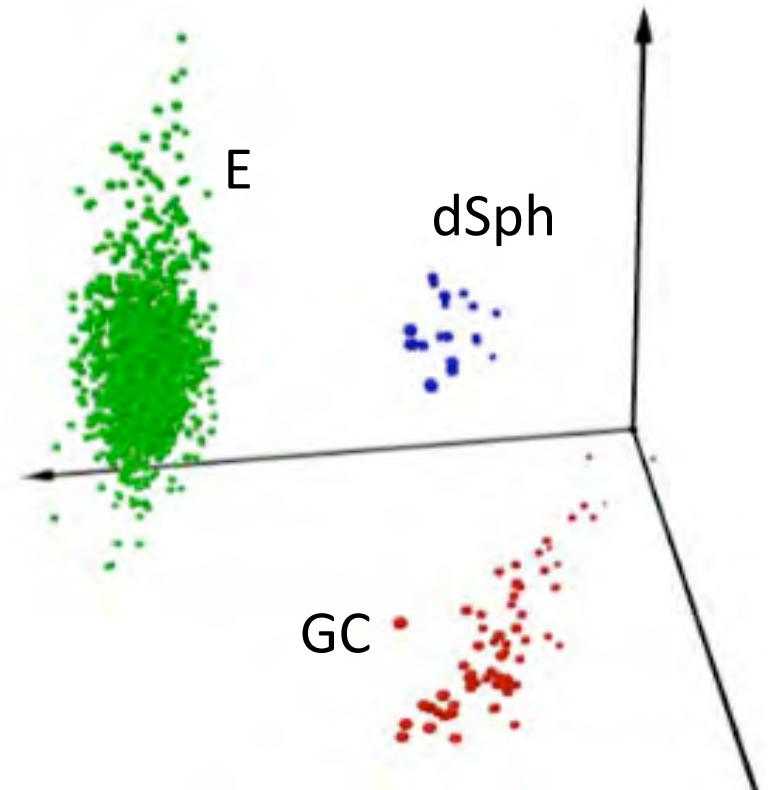
Colors of stars and quasars



Dimensionality \leq the number of
observed quantities

Physical Parameter Space

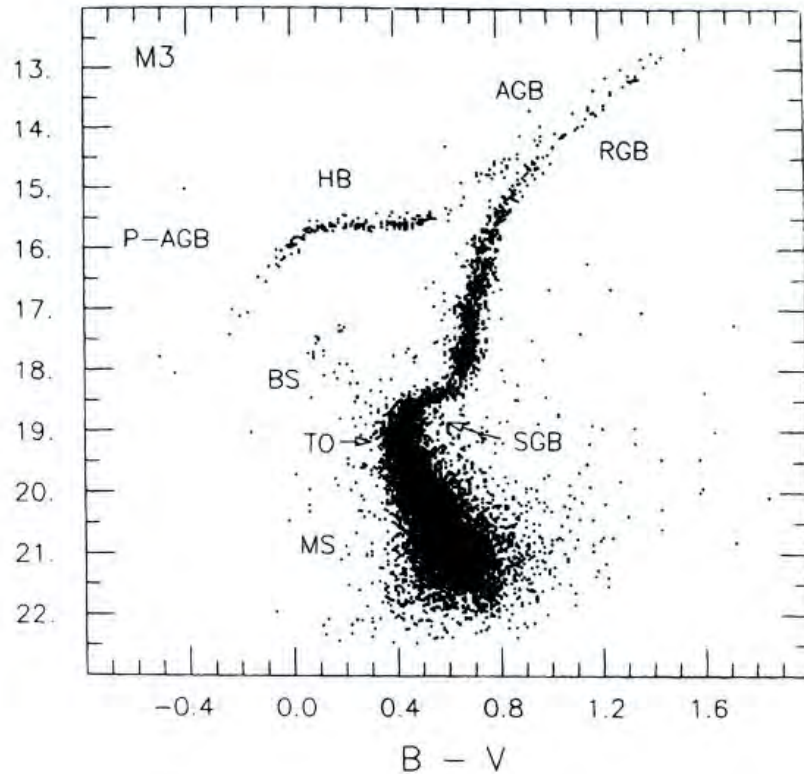
Fundamental Plane of hot
stellar systems



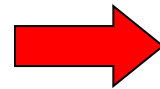
Both are populated by
objects or events

A Familiar Example: HR Diagram

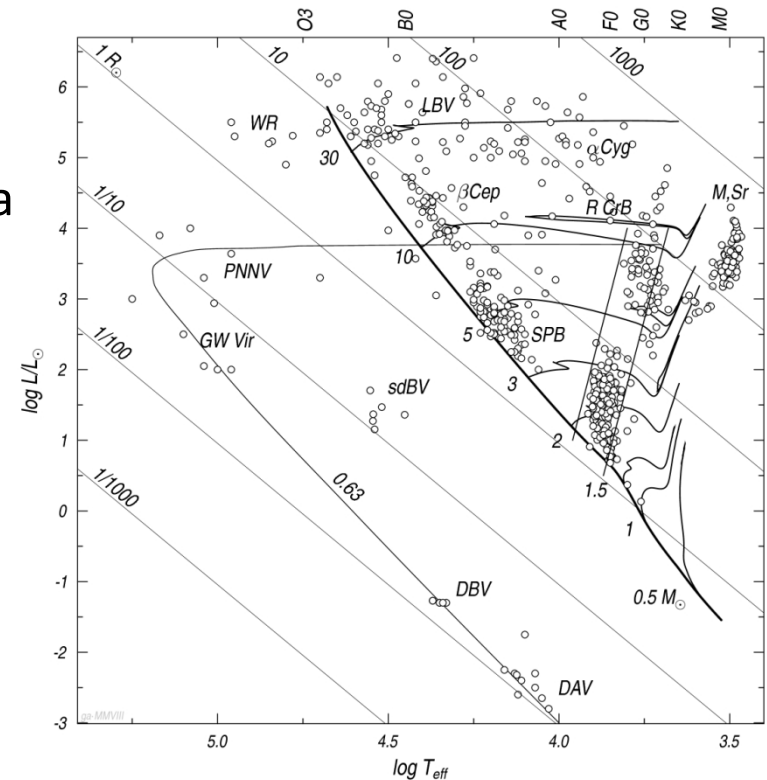
Observable
Color-magnitude diagram



Theory
+
Other data



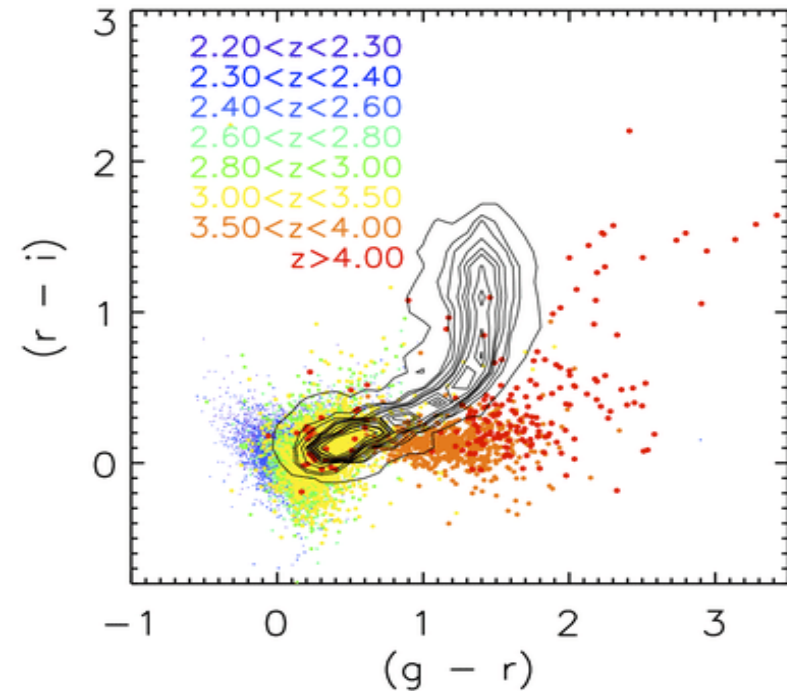
Theoretical
Temperature-Luminosity Space



- Not filled uniformly: clustering indicates different families
- Empty regions may be due to selection effects or physics
- Clustering + dimensionality reduction = correlations

Mapping the Data Parameter Spaces

- Objects of a particular type (e.g., stars, galaxies, SNe, Quasars, ...) may occupy only specific regions of a parameter space, and form clusters
- If enough known, training examples are known, this can be used for an automated, ***supervised classification***, or the searches for the rare, but known objects (e.g., quasars)
- **Unsupervised clustering** (let the data tell you what clusters are present) may reveal previously unknown types of objects, as outliers from the known clusters

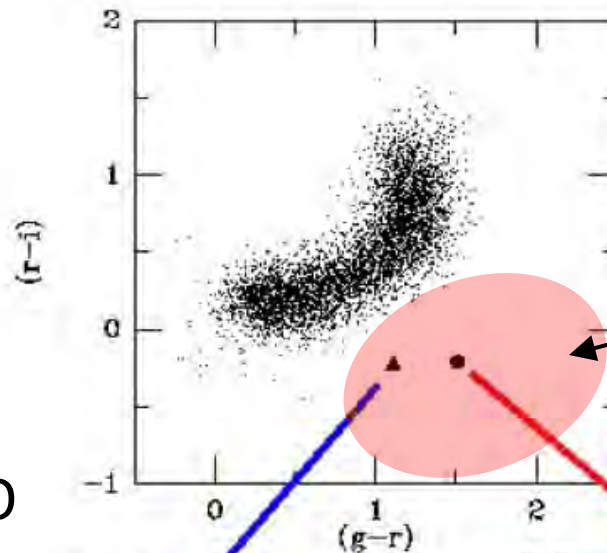


Model-Based Outlier Search and Surprises

Sometimes we know where to look for outliers on the basis of a prior knowledge, e.g., quasars or brown dwarfs in a color space

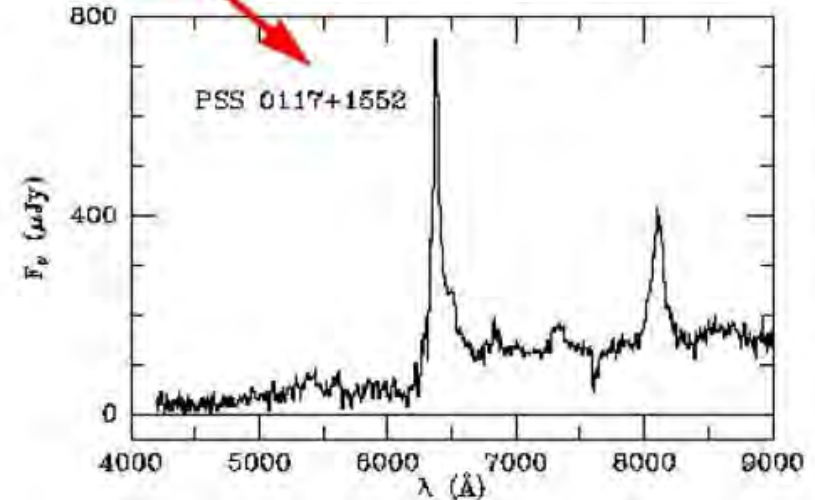
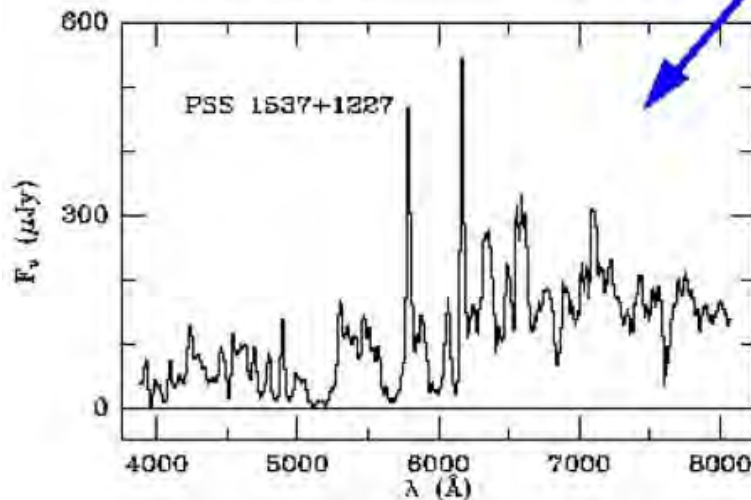
... but sometimes
you find
something
unexpected:

Peculiar Lo-BAL QSO



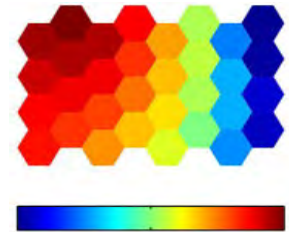
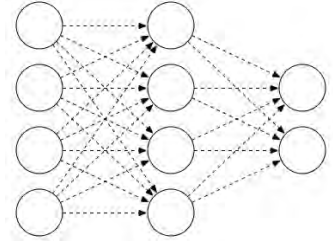
Expected high-z
quasar region

Typical $z > 4$ Quasar



Classification, Clustering, and Outliers

- **Supervised learning (classification):** use a known set of objects to train a classifier
 - Hard to find previously unknown things
- **Unsupervised learning (clustering):** let the data tell you how many different kinds of things are there
 - Could find previously unknown types as outliers



Supervised Algorithms

Neural Networks (MLP)

Boltzmann Machines

RBM

Decision Trees

Nearest Neighbor

Naive Bayes Classifiers

Bayesian Networks

Gaussian Processes

Regression

...

There is **no** “one
size fits all”:
different choices
for different
problems

Unsupervised Algorithms

K-Means

Self-Organizing Maps

RDF

Fuzzy Clustering

CURE

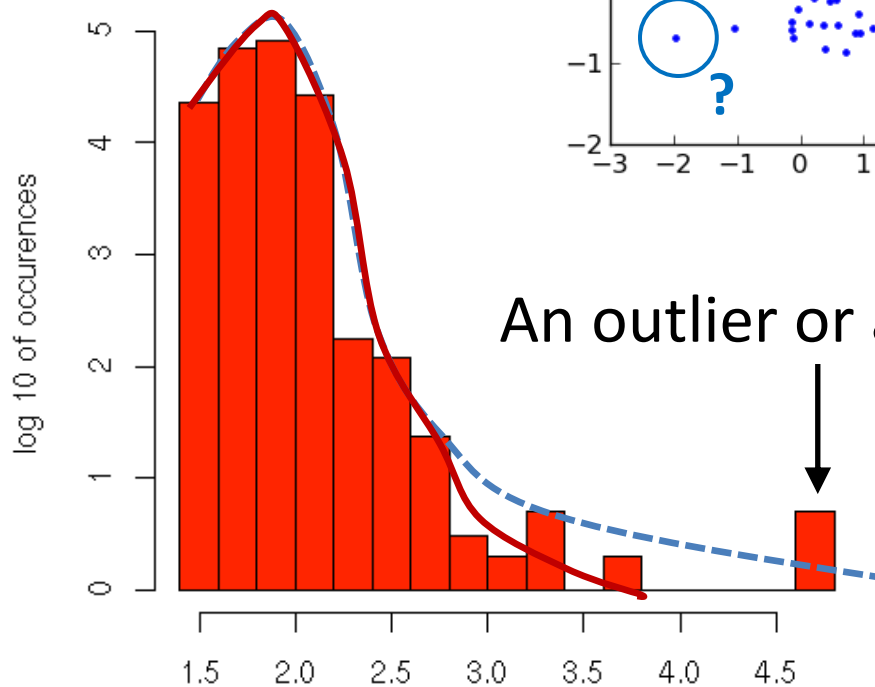
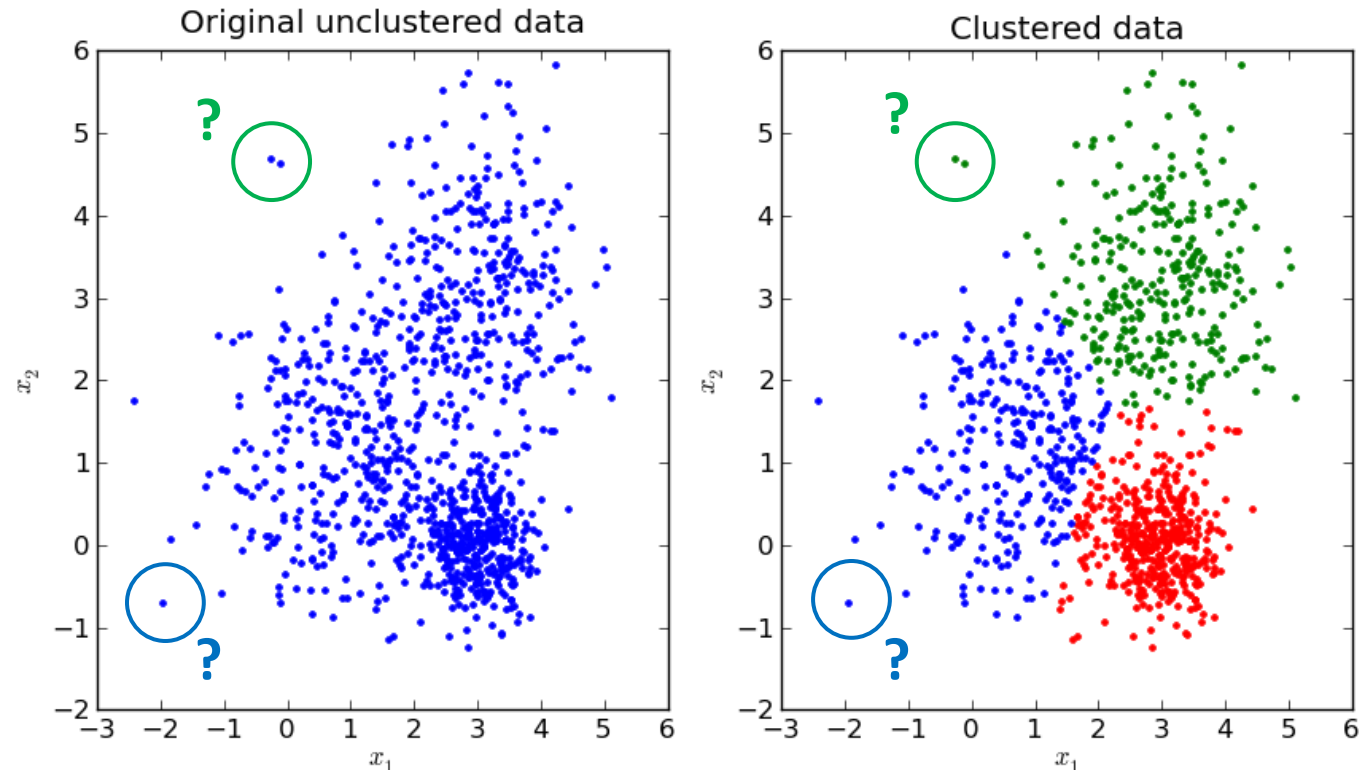
ROCK

Vector Quantization

Probabilistic Principal
Surfaces

...

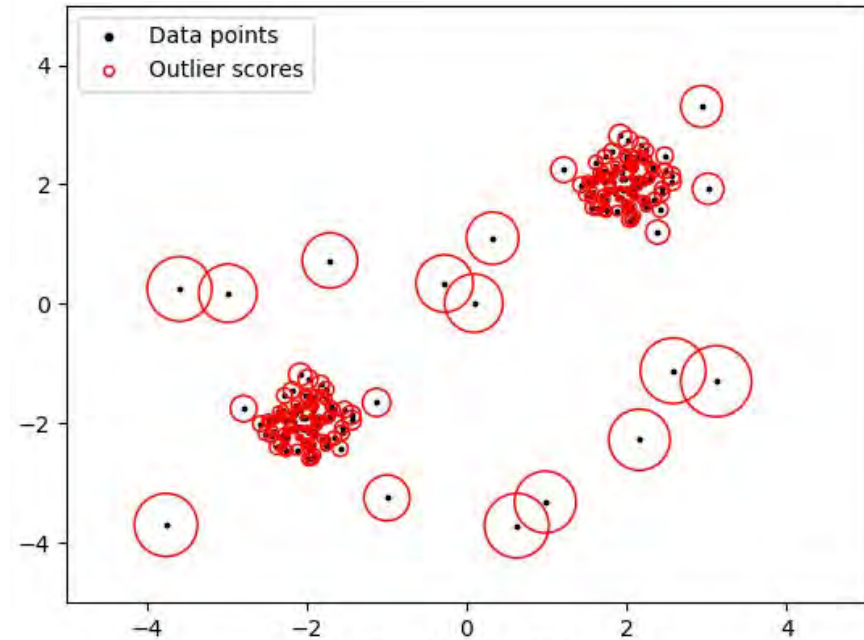
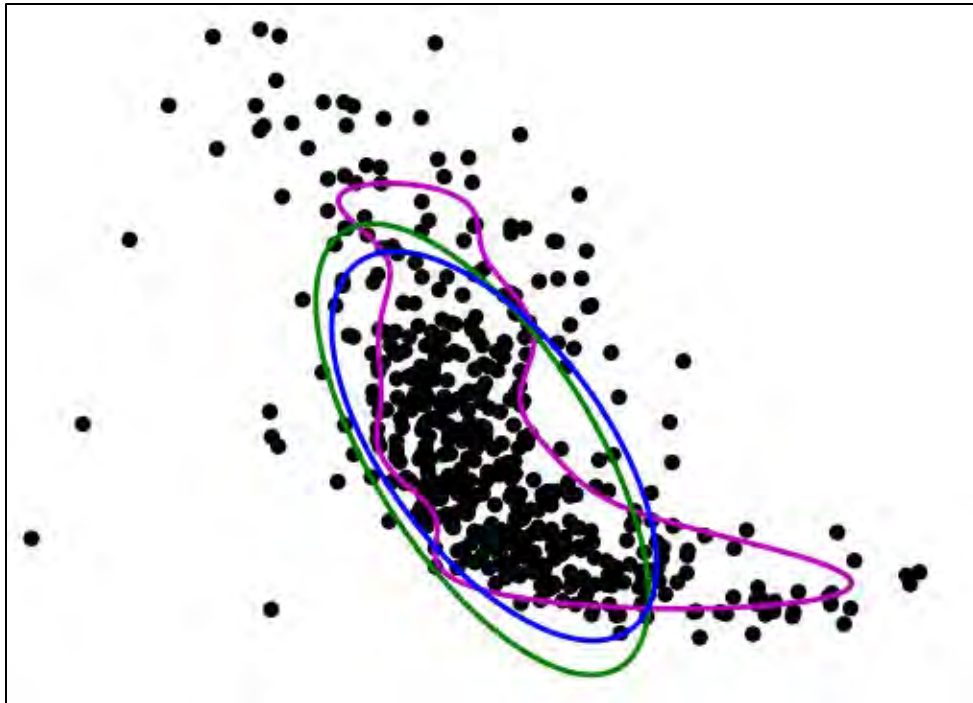
What is an Outlier?



It depends on the underlying probability distribution, and they are seldom Gaussian

Clustering and Searches for Outliers

Sometimes this is easy, not critically dependent on the assumed probability density distributions of the clusters



But sometimes it isn't

Having the right cluster descriptors, number of clusters, and metric of this feature space is crucial

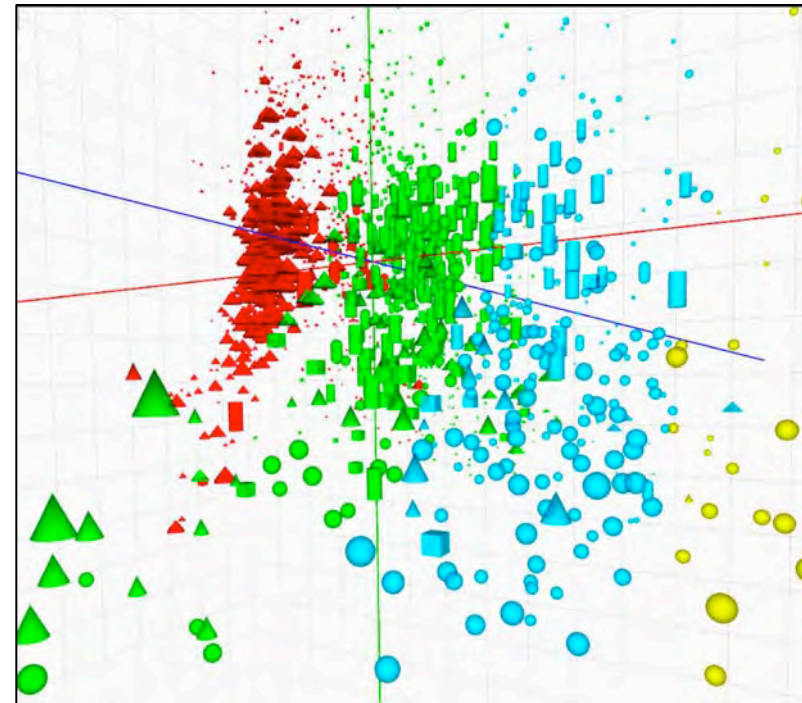
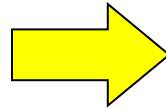
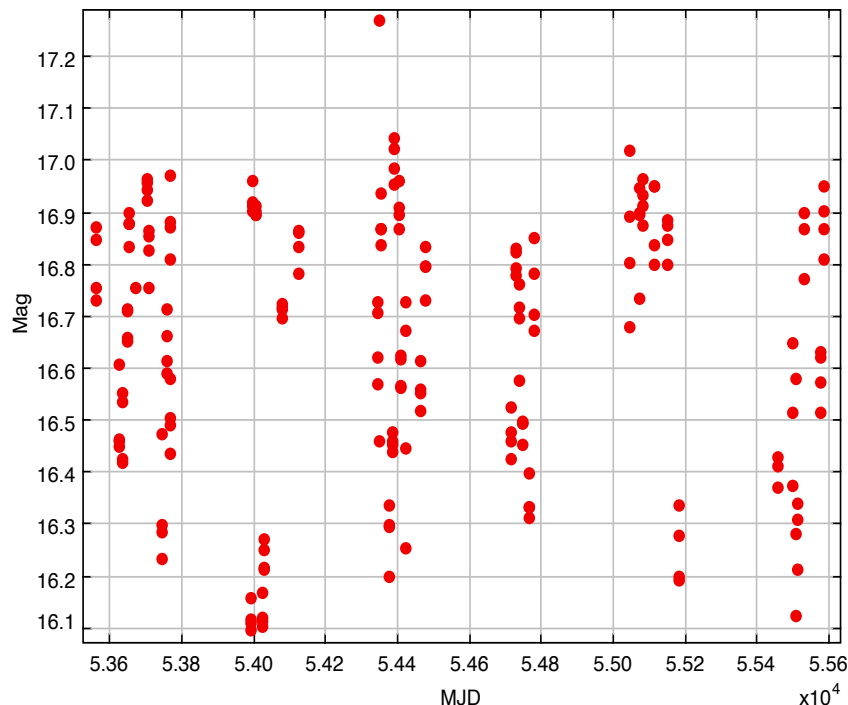
Parameter Spaces for the Time Domain

(in addition to everything else: flux, wavelength, etc.)

- For ***surveys***:
 - Total exposure per pointing
 - Number of exposures per pointing
 - How to characterize the cadence?
 - ↪ Window function(s)
 - ↪ Inevitable biases
- For ***objects/events*** ~ light curves:
 - Significance of periodicity, periods
 - Descriptors of the power spectrum (e.g., power law)
 - Amplitudes and their statistical descriptors
 - ... etc. – over 70 parameters defined so far, but which ones are the minimum / optimal set?

From Light Curves to Feature Vectors

- We compute ~ 70 parameters and statistical measures for each light curve: amplitudes, moments, periodicity, etc.
- This turns *heterogeneous* light curves into *homogeneous feature vectors* in the parameter space
- Apply a variety of automated classification methods



Variability Feature Space

- Generate homogeneous representation of time series by defining a number of **descriptive parameters**:
 - Morphology (shape): skew, kurtosis
 - Scale: Median absolute deviation, biweight midvar.
 - Variability: Stetson, Abbe, von Neumann
 - Timescale: periodicity, coherence, characteristic
 - Trends: Thiel-Sen
 - Autocorrelation: Durbin-Watson
 - Long-term memory: Hurst exponent
 - Nonlinearity: Teraesvirta
 - Chaos: Lyapunov exponent
 - Models: HMM, CAR, Fourier decomposition, wavelets
- Defines a **high-dimensional feature space** to characterize the temporal behavior

Feature Selection Algorithms

Most clustering and classification algorithms scale poorly with the dimensionality of the feature spaces. Feature selection is one set of **dimensionality reduction** techniques.

- **Filter methods** apply a statistical measure to assign a scoring to each feature, usually independently (univariate). The features are ranked by the score.
- **Wrapper methods** look for a set of features where different feature combinations are evaluated and compared to other combinations.
- **Embedded methods** learn which features best contribute to the accuracy of the model while the model is being created.
- The **scoring criterion** depends on the goal, e.g.:
 - Accurate predictions for the regression searches
 - Classification discrimination power for clustering

Feature Selection Algorithms

Optimal sets of features may be different for

- Different regression target variables:
e.g., $y_1 = f_1(x_i, x_j, x_k, \dots)$, $y_2 = f_2(x_p, x_q, x_r, \dots)$, etc.
- Different classification tasks:
e.g., $\text{Class}(A, B) = f(x_a, x_b, x_c, \dots)$, $\text{Class}(A, B, C) = f(x_d, x_e, x_f, \dots)$
- Different regression or classification algorithms:
e.g., ANN, DT, RF, SVM, ...
... so they have to be optimized in each individual case

See:

Donalek et al., IEEE BigData 2013, p. 35 = arxiv/1310.1976

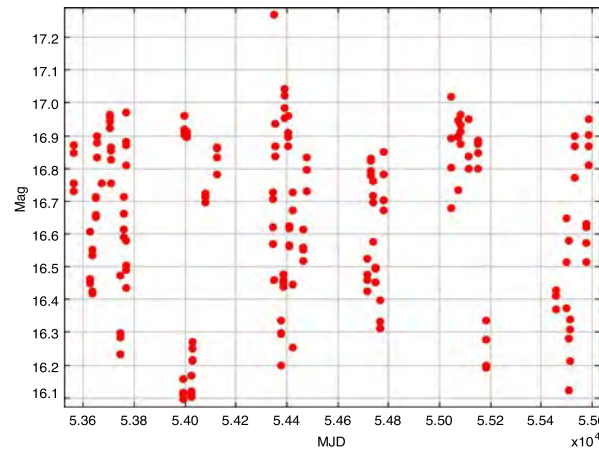
D'Isanto et al. 2016, MNRAS, 457, 3119

Feature Selection Algorithms: Examples

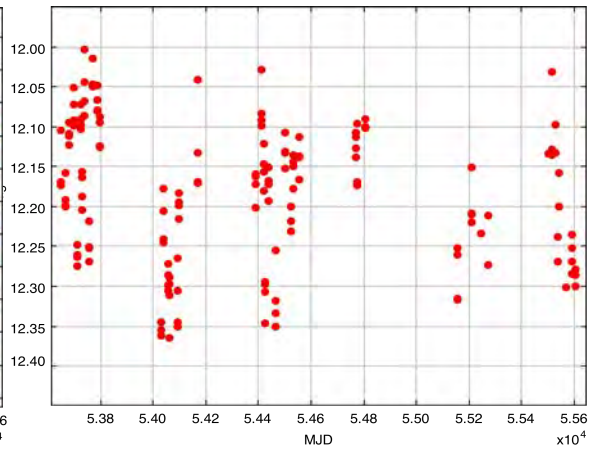
- **Fast Relief Algorithm** (aka ReliefF) ranks features according to how well their values distinguish between instances.
- **Fisher Discriminant Ratio** (FDR) ranks features according to their classification discriminatory power. It can be applied only to binary classification problems.
- **Correlation-based Feature Selection** (CFS) is a wrapper method which selects features that have low redundancy (i.e., not correlated with each other) and is strongly predictive of a class.
- **Fast Correlation Based Filter** (FCBF) is a supervised filter algorithm, similar to the CFS. Searches for features that have predominant correlation with the class . Can be computationally efficient with very high dimensional data.
- **Multi Class Feature Selection** (MCFS) is an unsupervised method based on the spectral analysis of the data. ... etc.

Optimizing Feature Selection

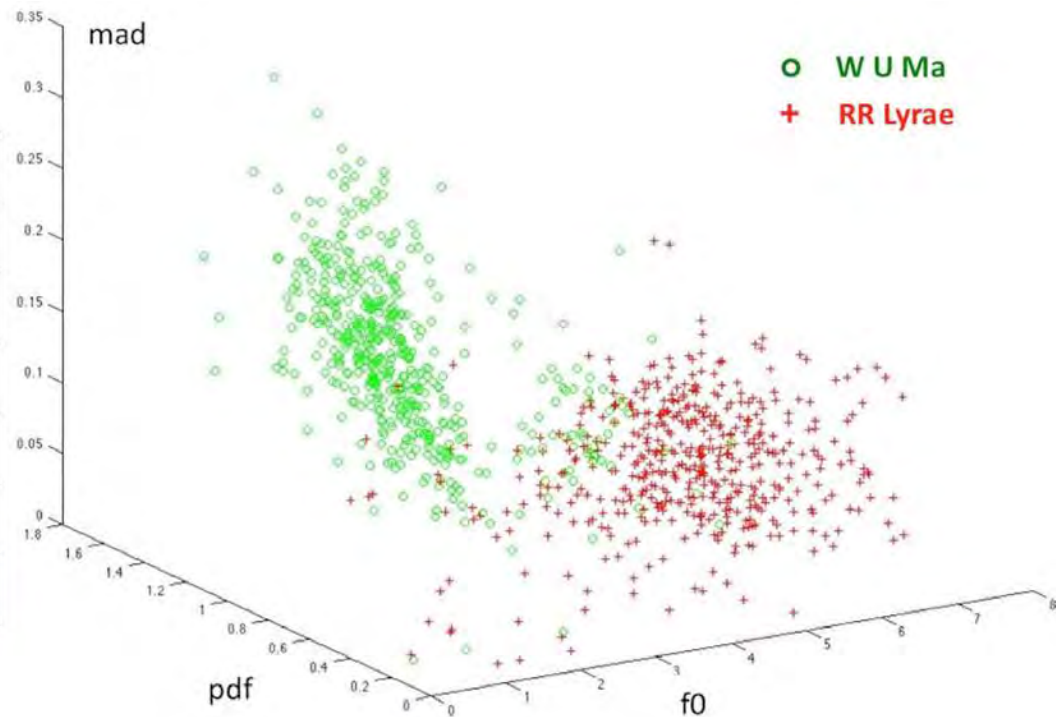
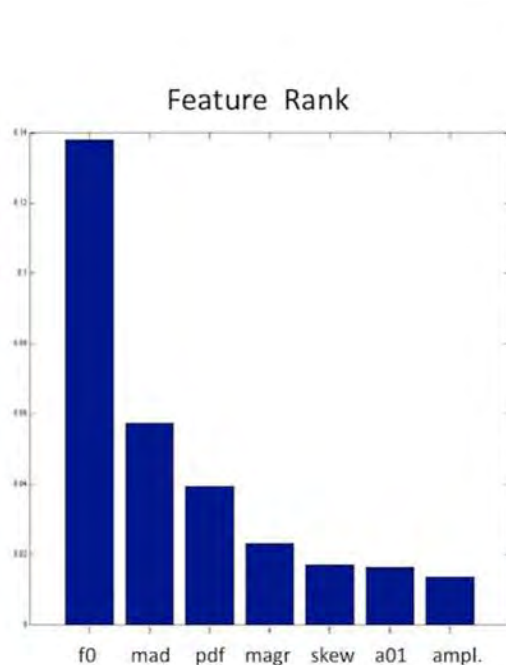
Rank features in the order of classification quality for a given classification problem, e.g., RR Lyrae vs. WUMa



RR Lyrae

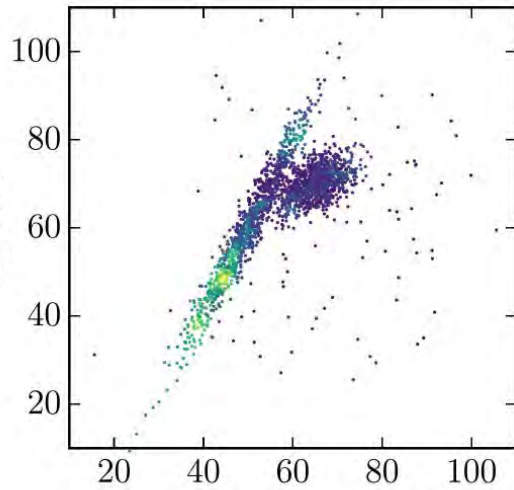


Eclipsing binary (W U Ma)

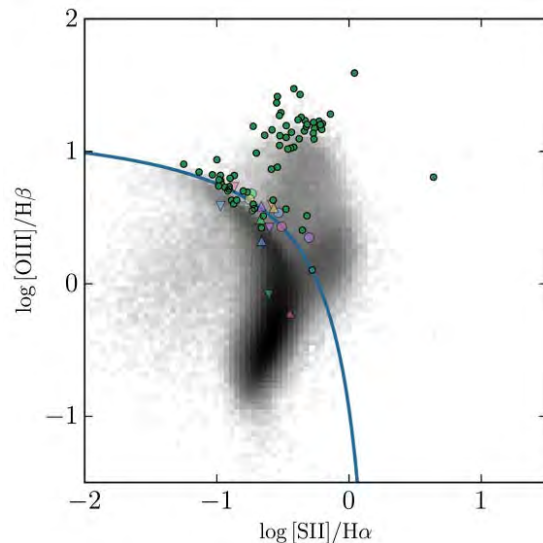


Examples from Astronomy:

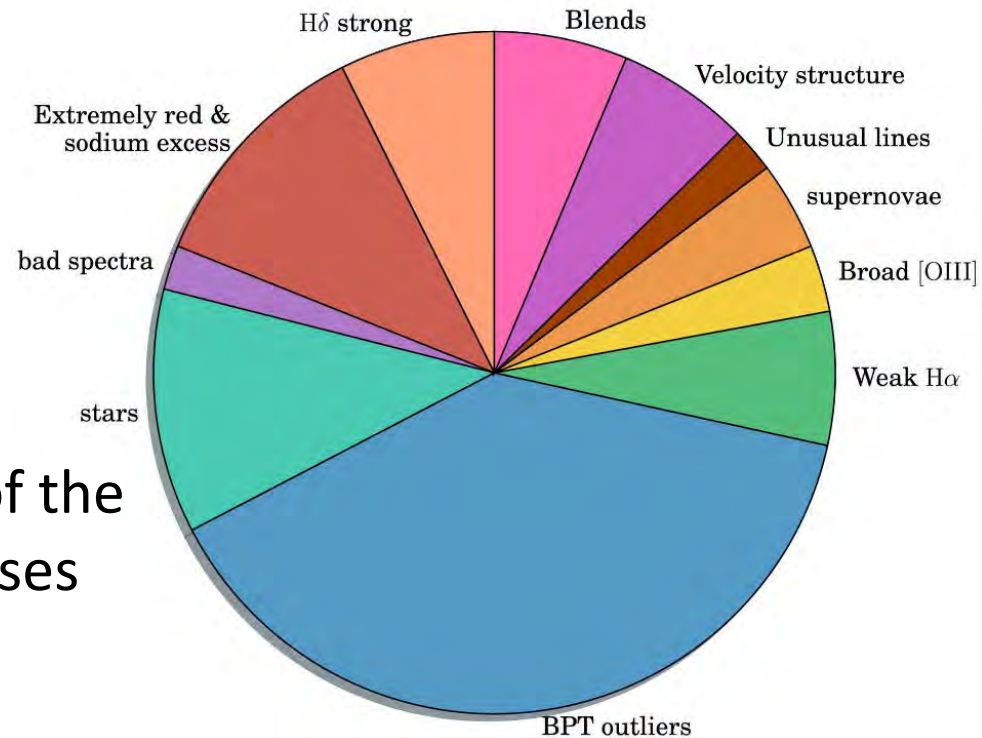
"The weirdest SDSS galaxies: results from an outlier detection algorithm", D. Baron & D. Poznanski 2017, MNRAS 465, 4530



Used Random Forests algorithm to classify SDSS galaxies using spectroscopic properties. Defined a “Weirdness” parameter to quantify the outliers.

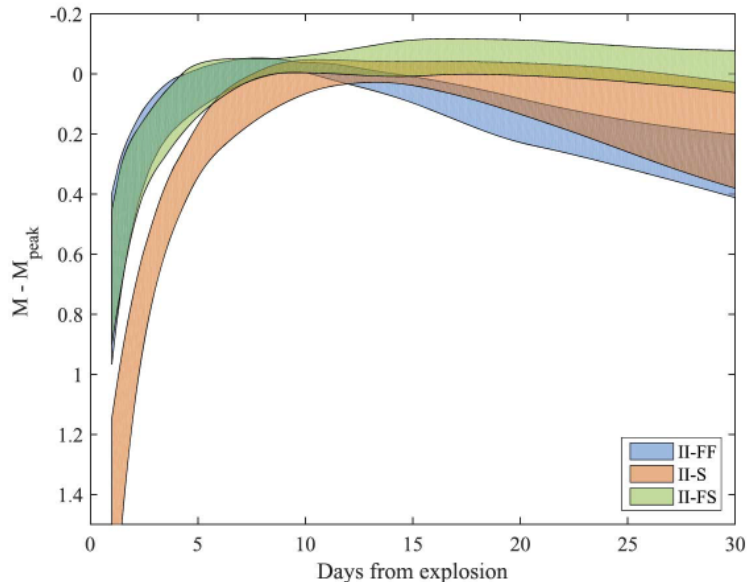
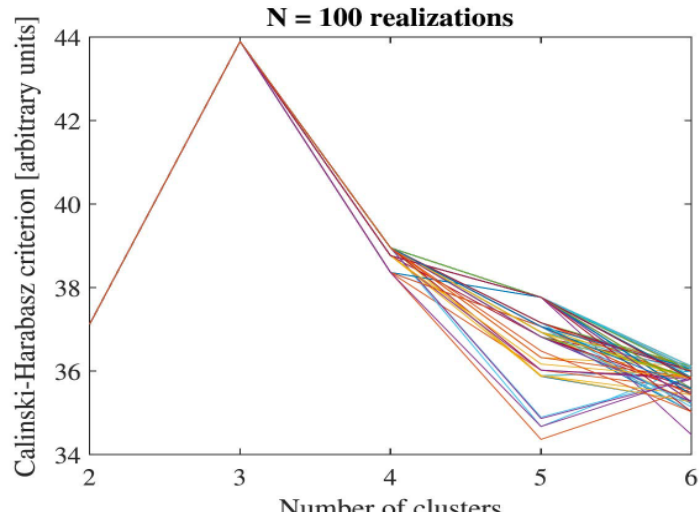


All outliers found are members of the known classes of objects.

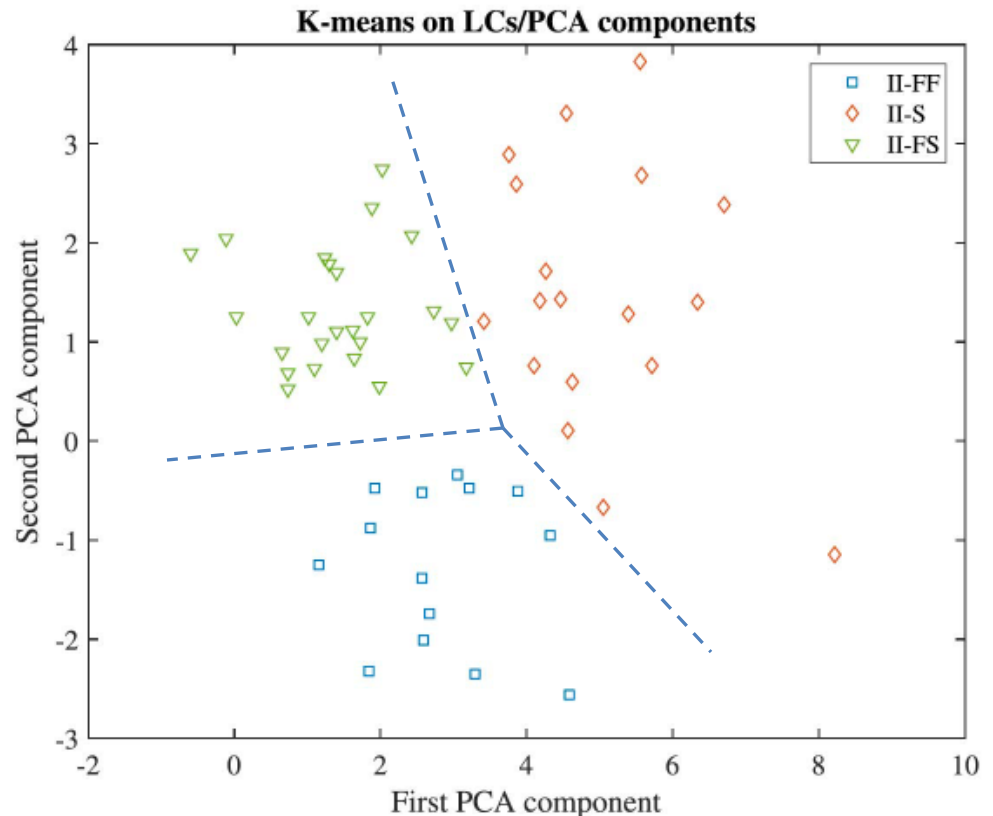


Examples from Astronomy:

"Unsupervised Clustering of Type II Supernova Light Curves",
A. Rubin & A. Gal-Yam 2016, ApJ, 828, 111



Used the K-Means algorithm to identify 3 principal clusters: slow rise, fast rise – fast decay, and fast rise – slow decay



To Recap:

- Astronomy is now well into the **Petascale data regime**, and data volumes and rates grow exponentially according to Moore's Law
 - Most data come from the large surveys
 - The biggest growth now is in the time domain
 - This is true across all wavelengths
 - Growth of **data complexity** and **information content**
- Derived source catalogs typically contain **$\sim 10^9$ objects**, with **$\sim 10^2 - 10^3$ parameters** (features) each
 - Data fusion of different surveys increases the data complexity and discovery potential
 - We use **Machine Learning** to process and analyze the data, including source classification and selection of **interesting targets** for the follow-up studies