DATA DRIVEN DISCOVERY IN ASTROPHYSICS





TD-403

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Giuseppe Longo – D³ in Astrophysics

BIDS'14 - Frascati

Behind the scenes in the lockers room

• Big data in Astrophysics

Data Driven Discovery

The evolving paths to knowledge

(Jim Gray)

The First Paradigm

Experiments/measurements (XVII century)

<image>

The Second Paradigm

Analytical theory (XVIII century)

The Third Paradigm Numerical simulations (early 40's)

The Fourth Paradigm Data Driven Discovery (Now)









So what are «Big Data» in Astrophysics?



Big Data is like teenage sex: Everyone talks about it, Nobody really knows about it, Everyone thinks everyone else is doing it, So everyone claims they are doing it

But astronomers definetely do it Dan Ariely

The Sloan Digital Sky Survey (in its various incarnations)

Sloan Digital Sky Survey – Sky Server

– 2.5 Terapixels of images => 5 Tpx of sky; 10 TB of raw data => 400TB processed; 0.5 TB catalogs => 35TB final

... a Prototype in 21st Century data access

– 1.2B web hits in 12 years; 200M external SQL queries; 4,000,000 distinct users vs. 15,000 astronomers

Data products (e.g. SPECTROSCOPIC and PHOTOMETRIC

catalogues) and raw data were «immediately» made available to the community

Terra Server SDSS SkyServer Hubble Turbulence Super COSMOS CASJobs SkyQuery GalaxyZoo Legacy Space Your Fee **MvDB** JHU 1K VO Open SkyQuery Pan-Paloma GALEX UKIDDS Millennium STARRS Services Genome VO INDRA Milky Way VO MHD DB Potsdam Spectrum Simulatio Laborator Footprint

The SDSS Genealogy

The right data set at the right moment

Pioneeristic yet manageable with available technology (10 TB of data products); general in purpose, flexible enough to be useful for a large variety of existing problems, yet capable to rise new ones





Courtesy of Alex Szalay

The SDSS data set Photometric

Hundreds of features for 300M galaxies and stars Quality flags

Spectr. subsample (ca. 3 Mobjects)

Equivalent widths Spectroscopic redshifts Spectral ckassification in classes and subclasses





Name	bands	Area (sq. Deg)	KB's	epochs	Size/acce ss
SDSS	Optical (5)	25.000	yes	1	20/2 Tbyte yes
KIDS	Visible (4)	1.500	Yes /no	1	20/2 TB Yes del.
VIKING	IR (5)	1.500	Yes/no	1	20/2 TB Yes. Del.
CRTS	Optical (1)	33.000 (1)	Yes	>100	100 TB growing yes
EUCLID	Optical/NI R	10.000	Yes	1	>150 PB Yes del
LSST	Optical	15.000	Yes	>>100	15 TB/night >100 PB
SKA	Radio		Yes	>100	1.5 PB/sec

Automatic processing

Hundreds of parameters

- Morphological
- Photometric
- Epoch
- ...
- Public access
- Real time processing
- Needs for real time automatic follow-up scheduling

Hundreds of different groups running hundreds of vastly different research projects

Technological challenges of big data:





Standards, interoperability, etc, ... Taken care by Virtual Observatory projects around the world





In less than a decade astronomy has moved from

... and data complexity

- 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



These data sets are so large and rich that:

- No single researcher or group can exploit them *(public access)*
- It is impossible to transfer them from the data centers to the final user (move programs and not the data)
- Their value increases with time (data re-use)
- They impose an entirely different methodological approach (Data Mining, and, eventually
- The astronomical community **needs D**³ to scientifically exploit otherwise unmanageable datasets

But ...

Does the community understand what **D³** is truly about? And...

Is the community ready to abandon old ways of thinking and traditional methods (*faster horses*)?







The scientific exploitation of a multi band, multiepoch (K epochs) universe implies to search for patterns, trends, etc. among N points in a DxK dimensional parameter space:



N >10⁹, D>>100, K>10

X-parameter spaces of very high dimensionality

 \mathbb{R}^{n}

Each observation defines a point $p\{x_1, \dots, x_n\} \in \mathbb{R}^n$ Spectrophotometric Astrometric λ Domain Domain Flux F/ΔF λ/Δλ Each survey carves an Polarization Hypervolume in the parameter space Non-EM UT Surface ∆t baselines Brightness Angular Nexp Resolution Time Morphological Ω Domain Domain

DATA Mining is about rediscovering/discovering known (unknown) useful patterns in the data

DATA DRIVEN DISCOVERY is not «simply» about machine learning

D³ is a methodological and paradigmatic shift

 $D^3 \equiv \{ data mining, statistical pattern recognition, visualization \}$

 D^3 is about *letting the data to speak for themselves* with minimum use of a-priori assumed models and hypothesis

3-D is an intrinsic human limitations



A simple universe

or rather ...

... a limitation of human brain?

diagnostics



What should we do to extract ordering laws in Rⁿ а space



PPS projection of a 21-D parameter space showing as blue dots the candidate quasars.Notice better disentanglement

08 05 04 02 0 02 04 06 08



DAMEWARE (DAME Web Application REsource) v 1.0



A University Federico II, INAF-OACN & Caltech effort, recently joined by ITHS of Heidelberg, aimed at implementing a science gateway for data exploration on top of a virtualized distributed computing environment. It is multi-disciplinary platform (astronomy, bioinformatics and medical diagnostics)

End users can remotely exploit high computing and storage power to process massive datasets (in principle they can do data mining on their smartphone...) User can automatically plug-in his/her own algorithm and launch experiments through the Suite via a simple web browser



DAMEWARE is a part of the **DAME** project



Is a web-based application (FREE AND OPEN TO THE PUBLIC) for massive data mining based on a suite of machine learning methods on top of a virtualized hybrid computing infrastructure

A joint effort between University Federico II, INAF-OACN & Caltech, recently joined by ITHS of Heidelberg, aimed at implementing (as web 2.0 apps and services) a science gateway for data exploration on top of a virtualized distributed computing environment



Effective DM requires complex work-flows





		DM models	
	Functionality		Experiment
	Classification	GAME S, C,R MLPBP S, C,R MLPGA S, C,R	S
Use	Regression	MLPQNA S, C,R SVM S, C,R	1-st 2-nd
case	Clustering	K-Means U, Cl ESOM U, Cl	3-rd 4-th
	Feature selection	SOFM U, Cl SOM U, Cl PPS U, Cl, FS	 N-th

Then ... let's play a game

...

Photometric redshifts vs Spectroscopic redshifts

GETTING READY FOR EUCLID

A template case of machine learning vs «pure» D³ Photometric redshifts for quasars and galaxies

$$1 + z = \frac{\lambda_{obs}}{\lambda_0} \approx \frac{v}{c}$$



QSO; z=3.81 QSO; z=5.31

Crucial cosmological probe

- Large scale structure
- Weak lensing
- Tests of cosmological models

Only viable way to obtain distance info's for large samples of galaxies

Mathematically simple: to find the mapping function

Input vector Target vector Physical redshift

$$\left(\overline{X}_{j} \{ x_{1}, \dots, x_{n} \} j = 1, \dots m \right) \in OPPS \subset \mathbb{R}^{n}$$

$$\overline{Y} \{ y_{1}, \dots, y_{m} \} \in OPPS \subset \mathbb{R}^{n}$$

$$\overline{Y} \{ y_{1}, \dots, y_{m} \} \rightarrow \overline{Z} \in PPS \subset \mathbb{R}^{n}$$



PPS = Physical Parameter Space

Photo-z for Quasars: first attempt (by us)



Astroinformatics of galaxies and quasars: a new general method for photometric redshifts estimation, O. Laurino, R. D'Abrusco, G. Longo, and G. Riccio, MNRAS, 2011, 418, 2165 (arXiv/1107.3160);

WGE: Weak Gated Expert

Data from the unresolved objects SDSS catalogue



Table 5. Statistical diagnostics of photometric redshifts reconstruction for all the experiments discussed in this paper and for relevant papers in the literature. Column 'Exp. 1' contains the diagnostics for the experiment for the determination of the photometric redshifts of the optical galaxies from the SDSS catalogue described in Section 6.1, while columns 'Exp. 2' and 'Exp. 3' describe the diagnostics for the experiments concerning the determination of the photometric redshifts for quasars with optical and optical+UV photometry, respectively (the details can be found in Sections 6.2 and 6.3). The same statistical diagnostics are shown for some papers from the literature, respectively, D'Abrusco et al. (2007) for optical galaxies in column (1) and both Ball et al. (2008) and Richards et al. (2009) for optical and optical+UV quasars in the columns (2) and (3), respectively (as reported in Ball et al. 2008). The definitions of the statistical diagnostics and other relevant results of the literature are discussed in Section 8.

Diagnostic	Exp. 1	(1)	Exp. 2	(2)	(3)	Exp. 3	(2)	(3)	
$\langle \Delta z \rangle$	0.015	0.021	0.21	_	-	0.13	_	_	
$rms(\Delta z)$	0.021	0.074	0.35	_	_	0.25	_	-	
$\sigma^2(\Delta z)$	2.3×10^{-4}	5.0×10^{-4}	0.08	0.123	0.27	0.044	0.054	0.136	
$MAD(\Delta z)$	0.011	0.012	0.11	_	-	0.061	-	-	
$MAD'(\Delta z)$	0.012	-	0.098	-	-	0.062	-	-	
$Per cent(\Delta z_1)$	43.4	41.1	50.7	54.9	63.9	68.1	70.8	74.9	
Per cent(Δz_2)	72.4	68.4	72.3	73.3	80.2	86.5	85.8	86.9	
Per cent(Δz_3)	86.9	83.4	80.5	80.7	85.7	91.4	90.8	91.0	
$\sigma^2(\Delta z_1)$	8.2×10^{-6}	8.2×10^{-6}	7.9×10^{-4}	-	-	7.6×10^{-4}	-	-	
$\sigma^2(\Delta z_2)$	3.0×10^{-5}	3.1×10^{-5}	0.003	-	-	0.023	-	-	
$\sigma^2(\Delta z_3)$	6.1×10^{-5}	6.3×10^{-5}	0.005	_	-	0.039	-	-	
$\langle \Delta z_{\rm norm} \rangle$	0.014	0.017	0.095	0.095	0.115	0.058	0.06	0.071	
$rms(\Delta_{norm})$	0.019	0.037	0.10	_	-	0.11		-	
$\sigma^2(\Delta z_{\rm norm})$	1.8×10^{-4}	1.1×10^{-3}	0.025	0.034	0.079	0.086	0.014	0.031	5
$MAD(\Delta z_{norm})$	0.009	0.011	0.041	-	-	0.029	_	-	/
$MAD'(\Delta z_{norm})$	0.010	-	0.040			0.031	-	-	
Per cent($\Delta z_{norm,1}$)	48.3	45.6	77.3	-	-	87.4	-	-	
Per cent($\Delta z_{norm,2}$)	77.2	73.5	87.3	-	-	94.0	-	-	
$Per cent(\Delta z_{norm,3})$	90.1	87.0	91.8	-	-	96.4	-	-	
$\sigma^2(\Delta z_{\rm norm,1})$	8.3×10^{-6}	8.2×10^{-6}	6.2×10^{-4}	-	-	5.6×10^{-4}	-	-	
$\sigma^2(\Delta z_{\text{norm},2})$	3×10^{-5}	3.0×10^{-5}	0.002	-	-	0.001	-	-	
$\sigma^2(\Delta z_{\text{norm},2})$	5.8×10^{-5}	6.0×10^{-5}	0.004	-	-	0.002	-	-	

Catalogues for both experiments available on Vizier.



Figure 15. In the upper panel, it is shown the scatter plot of the spectroscopic versus photometric redshifts evaluated with the WGE method for the members of the KB of the experiment for the quasars extracted from the SDSS catalogue with optical photometry, while in the lower panel the scatter plot of the spectroscopic redshift z_{spec} versus Δz variable is shown for the same sources. All points are colour coded according to the value of the errors σ_{shout} as evaluated but the WGE. The vertical dashed lines represent the redshift at which the most luminous emission lines characterizing quasars spectra shift off the SDSS photometric filters due to redshift. Most of the features of the plot are associated to one or more of these lines.



Photo-z for SDSS QSOs with MLPQNA

Lenghty feature selection procedure

Survey	Bands	Name of feature	Synthetic description
GALEX	nuv, fuv	mag, mag iso mag.Aper_1 mag.Aper_2 mag.Aper_3 mag.auto and kron.radius	Near and Far UV total and isophotal mags phot. through 3, 4.5 and 7.5 arcsec apertures magnitudes and Kron radius in units of A or B
SDSS	u, g, r, i, z	psfMag	PSF fitting magnitude in the u g, r, i, z bands.
UKIDSS	Y, J, H, K	PsfMag	PSF fitting magnitude in Y, J, H, K bands
		AperMag3, AperMag4, AperMag6	aperture photometry through 2, 2.8 & 5.7" circular aperture in each band
		HallMag, PetroMag	Calibrated magnitude within circular
			aperture r_hall and Petrosian magnitude
			in Y, J, H, K bands
WISE	W1, W2, W3, W4	W1mpro, W2mpro, W3mpro, W4mpro	W1: 3.4 μm and 6.1" angular resolution; W2: 4.6 μm and 6.4" angular resolution;
			W3: 12 µm and 6.5" angular resolution;
			W4: 22 µm and 12" angular resolution.
			Magnitudes measured with profile-fitting photometry at the 95% level. Brightness upper limit if the flux
			measurement has SNR< 2
SDSS	-	Z spec	Spectroscopic redshift

Photometric redshifts for quasars in multiband surveys,

M. Brescia, S. Cavuoti, R. D'Abrusco, A. Mercurio, G. Longo 2013, ApJ, 772, 140

Table 6. Catastrophic outliers evaluation and comparison between the residual $\sigma_{dean}(\Delta z_{norm})$ and $NMAD(\Delta z_{norm})$. The reported number of objects, for each cross-matched catalog, is referred to the test sets only. Catastrophic outliers are defined as objects where $|\Delta z_{norm}| > 2\sigma (\Delta z_{norm})$. The standard deviation $\sigma_{dean}(\Delta z_{norm})$ is calculated after having removed the catastrophic outliers, i.e. on the data sample for which

 $|\Delta z_{norm}| \le 2\sigma (\Delta z_{norm})$

Exp	n. obj.	$\sigma\left(\Delta z_{norm} ight)$	% catas. outliers	$\sigma_{clean} \left(\Delta z_{norm} \right)$	$NMAD(\Delta z_{norm})$
SDSS	41431	0.15	6.53	0.062	0.058
SDSS + GALEX	17876	0.11	4.57	0.045	0.043
SDSS+UKIDSS	12438	0.11	3.82	0.041	0.040
SDSS+GALEX+UKIDSS	5836	0.087	3.05	0.040	0.032
SDSS+GALEX+UKIDSS+WISE	5716	0.069	2.88	0.035	0.029



Table 4. Comparison among the performances of the different references. MLPQNA is related to our experiments, based on a four-layers network, trained on the mixed (colors + reference magnitudes) datasets. In some cases the comparison references are not reported, due to the missing statistics. Column 1: reference; columns 2-6, respectively: bias, standard deviation, MAD, RMS and NMAD calculated on $\Delta z_{norm} = (z_{spec} - z_{phot}) / (1 + z_{spec})$ related to the test sets. For the definition of the parameters and for discussion see text.

Exp	$BIAS(\Delta z_{norm})$	$\sigma(\Delta z_{norm})$	$MAD(\Delta z_{norm})$	$RMS(\Delta z_{norm})$	$NMAD(\Delta z_{norm})$
			SDSS		
MLPQNA	0.032	0.15	0.039	0.17	0.058
Laurino et al.	0.095	0.16	0.041	0.19	-
Ball et al.	0.095	0.18	-	-	-
Richards et al.	0.115	0.28	-	-	-
		SDS	S + GALEX		
MLPQNA	0.012	0.11	0.029	0.11	0.043
Laurino et al.	0.058	0.29	0.029	0.11	-
Ball et al.	0.06	0.12	-	-	-
Richards et al.	0.071	0.18	-	-	-
		SDS	S + UKIDSS		
MLPQNA	0.008	0.11	0.027	0.11	0.040
		SDSS + G	ALEX + UKIDSS		
MLPQNA	0.005	0.087	0.022	0.088	0.032
		SDSS + GALE	X + UKIDSS + W	ISE	
MLPQNA	0.004	0.069	0.020	0.069	0.029

Table 5. Comparison in terms of outliers percentages among the different references. In some cases the comparison references are not reported, due to the missing statistics. Column 1: reference: Column 2-3 are fractions of outliers at different σ based on

Column 1: reference; Column 2-3 are fractions of outliers at different σ based on $\Delta z = (z_{spec} - z_{phot})$; Column 4-5 are the fractions of outliers at different σ based on $\Delta z_{norm} = (z_{spec} - z_{phot}) / (1 + z_{spec})$. The column 4 reports our catastrophic outliers, defined as $|\Delta z_{norm}| > 2\sigma(\Delta z_{norm})$.

Exp	Outliers (Δz)		Outliers (Δz_{norm})	
	$> 2\sigma(\Delta z)$	$> 4\sigma(\Delta z)$	$> 2\sigma(\Delta z_{norm})$	$> 4\sigma(\Delta z_{norm})$
	SDSS			
MLPQNA	7.68	0.38	6.53	1.24
Bovy et al.		0.51		
	SDSS + GALEX			
MLPQNA	4.88	1.61	4.57	1.37
Bovy et al.		1.86		
	SDSS + UKIDSS			
MLPQNA	4.00	1.73	3.82	1,38
Bovy et al.		1.92		
SDSS	S + GALEX + UK	IDSS		
MLPQNA	2.86	1.47	3.05	0.23
Bovy et al.		1.13		
SDSS + 0	GALEX + UKIDS	+ WISE		
MLPQNA	2.57	0.87	2.88	0.91

Different Machine Learning methods of different complexity (MLPQNA is conceptually simpler than WGE) lead to similar results with a slight edge for MLPQNA

Photometric redshifts for QSO's ... a data driven approach (from K. Polsterer, Heidelberg)

One does not know a-priori which features are the most relevant

 $\frac{n!}{(n-r)!r!}, with n = 55, r = 4$ $\rightarrow 341,055 \ combinations$

Use all 55 significant photometric features to select the most significant 4



Photometric redshifts for SDSS QSO

PSF, Petrosian, Total magnitudes + extinction + errors 585 features.... 1,197,308,441,345,108,200,000 combinazioni

1.2 sextilions of combinations



Photometric redshifts for SDSS QSO

PSF, Petrosian, Total magnitudes + extinction + errors 585 features.... 1,197,308,441,345,108,200,000 combinazioni

1.2 sextilions of combinations



Hence features addition.....

Catastrophic outliers

MLPQNA, same KB and same features as in Brescia et al. 2013



How about quality flags?

SDSS provides a complete set of quality flags extrapolated from astronomers expertise

PSF_FLUX_INTERP	8%	21%
INTERP_CENTER	10%	29%
DEBLEND_NOPEAK	0%	3%
$science_primary=0$	11%	24%
nuv_flags	11%	18%
fuv_artifact	18%	24%

Inspection of flags for CO's shows that these flag are practically useless to discriminate CO's

Crosscorrelation with other catalogues to check for variability (e.g. CRTS)

NO clear effect on CO's induced by variability of sources.

SDSS is almost simultaeous in all optical bands but other surveys are not

What are these Catastrophic outliers?

Petrillo C.E., Longo G., Brescia M., Cavuoti G., in preparation; Petrillo Laurea Thesis 2013, University of Naples)



So, if you apply a rejection criteria based on the σ of the different predictions.....

-		initial	average	low sd
	Dataset	14284	14284	(14284 - 487)
	$BIAS(\Delta z)$	0.002	0.0001	0.0007
	$\sigma(\Delta z)$	0.14	0.12	0.077
Ţ	$\overline{MAD}(\Delta z)$	0.043	0.036	0.034
ł	$RMS(\Delta z)$	0.14	0.12	0.077
ί	$\underline{NMAD}(\Delta z)$	0.063	0.054	0.050
	$> 2\sigma \left(\Delta z\right)$	2.94%	3.17%	3.67%
	$>4\sigma\left(\Delta z\right)$	1.14%	0.10%	0.40%
-	BIAS (Δz_{norm})	0.003	0.003	0.0005
	$\sigma\left(\Delta z_{norm} ight)$	0.070	0.059	0.037
	$MAD(\Delta z_{norm})$	0.021	0.018	0.017
	$RMS(\Delta z_{norm})$	0.070	0.060	0.037
	$\mathrm{NMAD}(\Delta z_{norm})$	0.031	0.027	0.025
	$> 2\sigma \left(\Delta z_{norm}\right)$	2.66%	2.98%	3.87%
	$> 4\sigma \left(\Delta z_{norm}\right)$	0.84%	0.89%	0.57%

 $\sigma \ge \sigma_{treshold} = 0.125$

By rejecting all objects which have

Loss in completeness

Gain in

 $\sigma \sim 2$

~ 5%

Drastic reduction in number of catastrophic outliers

Selection biases

SDSS – Data Release 10

OPPS		OSPS	
3x10 ⁸	objects	3x10 ⁶	objects
> 100	features	>50	features
> 100	flags	>50	flags

Problem:

To evaluate Photo-z for all SDSS objects using the spectroscopic z's in the KB

The KB is the result of selection criterias and is biased

Not all selections and biases can be mapped in the OPPS



A less biased approach: 3 class classification

Brescia M, Cavuoti S., Longo G., 2014 submitted

Model: MLPQNA

Features:

type	parameters
Identification	objID, specObjID, RA, DEC
psfMag	ugriz mag and mag_err
fiberMag	ugriz mag and mag_err
modelMag	ugriz mag and mag_err
cmodelMag	ugriz mag and mag_err
deredMag	ugriz mag
extinction	ugriz
spec redshift	z, zWarning
classification	type, class, subclass, flags

Table 2. Description of the parameters (features and targets) used in this work. The first part of the table lists the photometric parameters in the OPPS, the second one the spectroscopic data and targets. Column 1: collective name of a given set of parameter; column 2: the corresponding SDSS parameters.



Results:

CLASS	$\% e_{tot}$	$%C_A$	$\% P_A$	$%Co_A$
GALAXY STAR QSO	91.31	97.02 86.40 90.49	93.49 93.82 86.90	$\begin{array}{c} 6.51 \\ 6.18 \\ 13.10 \end{array}$

Table 5. Summary of the results of the best three-class experiment (3*a*), referred to the parameter space composed by the 10 magnitudes (psfMag and magModel) for each object. The training and test sets are respectively 12% and 88% of the given dataset. The columns are referred to equations from 1 to 4. All the quantities reported in the table are percentages.

Conclusions

- Large (Big) data are coming...
- Slow but steady adoption of advanced tools
- Computing infrastructures are only a part (small) of the history
- Most of the work so far consisted in extracting known information Using existing data models with automatic techniques
- New set of features specifically designed for ML need to be adopted
 Data Driven Discovery is still (and rightly) in its infancy
- A change in methodology is taking place

XXI Century Astronomy world cup (LSST, EUCLID, SKA)