# Introduction to Astrostatistics and R

Eric Feigelson Penn State University

Harvard-Smithsonian Center for Astrophysics 2014

# My credentials

Professor of Astronomy & Astrophysics and of Statistics Assoc Director, Center for Astrostatistics at Penn State Scientific Editor (methodology), Astrophysical Journal Chair, IAU Working Group in Astrostatistics & Astroinformatics Councils, Intl Astrostatistics Assn, AAS/WGAA, LSST/ISSC Lead editor, Astrostatistics & Astroinformatics Portal Lead author, *MSMA* textbook (2012 PROSE Award)

also Harvard Ph.D. Class of '80

# Outline

Introduction to astrostatistics

- Role of statistics in astronomy
- History of astrostatistics
- Status of astrostatistics today

## Introduction to R

- History of statistical computing
- The R language & CRAN packages
- Sample R script

# What is astronomy?

**Astronomy** is the observational study of matter beyond Earth: planets in the Solar System, stars in the Milky Way Galaxy, galaxies in the Universe, and diffuse matter between these concentrations.

**Astrophysics** is the study of the intrinsic nature of astronomical bodies and the processes by which they interact and evolve. This is an indirect, inferential intellectual effort based on the assumption that physics – gravity, electromagnetism, quantum mechanics, etc – apply universally to distant cosmic phenomena.

## What is statistics? (No consensus !!)

#### Statistics characterizes and generalizes data

"... briefly, and in its most concrete form, the object of statistical methods is the reduction of data"
 (R. A. Fisher, 1922)

 "Statistics is a mathematical body of science that pertains to the collection, analysis, interpretation or explanation, and presentation of data."

(Wikipedia, 2014)

"A statistical inference carries us from observations to conclusions about the populations sampled"
 (D. R. Cox, 1958)

Does statistics relate to scientific models? The pessimists ...

"Essentially, all models are wrong, but some are useful."

(Box & Draper 1987)

"There is no need for these hypotheses to be true, or even to be at all like the truth; rather ... they should yield calculations which agree with observations" (Osiander's Preface to Copernicus' *De Revolutionibus*, quoted by C. R. Rao)

"The object [of *statistical* inference] is to provide ideas and methods for the critical analysis and, as far as feasible, the interpretation of empirical data ... The extremely challenging issues of *scientific* inference may be regarded as those of synthesising very different kinds of conclusions if possible into a coherent whole or theory ... The use, if any, in the process of simple *quantitative* notions of probability and their numerical assessment is unclear."

(D. R. Cox, 2006)

#### The optimists ...

"The goal of science is to unlock nature's secrets. ... Our understanding comes through the development of theoretical models which are capable of explaining the existing observations as well as making testable predictions. ...

"Fortunately, a variety of sophisticated mathematical and computational approaches have been developed to help us through this interface, these go under the general heading of statistical inference."

(P. C. Gregory, *Bayesian Logical Data Analysis for the Physical Sciences*, 2005)

# Recommended steps in the statistical analysis of scientific data

The application of statistics can reliably quantify information embedded in scientific data and help adjudicate the relevance of theoretical models. But this is not a straightforward, mechanical enterprise. It requires:

> exploration of the data
 > careful statement of the scientific problem
 > model formulation in mathematical form
 > choice of statistical method(s)
 > calculation of statistical quantities 
 > judicious scientific evaluation of the results

Astronomers often do not adequately pursue each step

## Some further comments

- Modern statistics is vast in its scope and methodology. It is difficult to find what may be useful (jargon problem!), and there are usually several ways to proceed. Very confusing.
- Some statistical procedures are based on mathematical proofs which determine the applicability of established results. It is perilous to violate mathematical truths! Some issues are debated among statisticians, or have no known solution.
- Scientific inferences should not depend on arbitrary choices in methodology & variable scale. Prefer nonparametric & scaleinvariant methods. Try multiple methods.
- It can be difficult to interpret the meaning of a statistical result with respect to the scientific goal. Statistics is only a tool towards understanding nature from incomplete information.

We should be knowledgeable in our use of statistics and judicious in its interpretation

## **Astronomy & Statistics: A glorious past**

For most of western history, the astronomers were the statisticians!

#### Ancient Greeks – 18th century

What is the best estimate of the length of a year from discrepant data?

- Middle of range: Hipparcos (4<sup>th</sup> century B.C.)
- Observe only once! (medieval)
- Mean: Brahe (16<sup>th</sup> c), Galileo (17<sup>th</sup> c), Simpson (18<sup>th</sup> c)
- Median (20<sup>th</sup> c)

#### 19<sup>th</sup> century

Discrepant observations of planets/moons/comets used to estimate orbital parameters using Newtonian celestial mechanics

- Legendre, Laplace & Gauss develop least-squares regression and normal error theory (c.1800-1820)
- Prominent astronomers contribute to least-squares theory (c.1850-1900)

#### **On Professor Airy's Objections to Peirce's Criterion**

We have the right to expect such large errors in an extended series, where their effect is unimportant, and counterbalanced with similar errors with opposite signs; but when we find them irregularly in small groups, we have reason to fear that their effect may be prejudicial to the mean. But we are not required to use the same care to avoid rejection of a good observation (that is, one than False Negative affected only by ordinary causes of error) as the retention of a bad one.

Outlier rejection Autocorrelated residuals False Positive

more important

Joseph Winlock, *Astron. J.*, 4, 145, 1856 **US Navy Almanac Office** later Director, Harvard College Observatory

#### The lost century of astrostatistics....

In the late-19th and 20th centuries, statistics moved towards human sciences (demography, economics, psychology, medicine, politics) and industrial applications (agriculture, mining, manufacturing).

During this time, astronomy recognized the power of modern physics: electromagnetism, thermodynamics, quantum mechanics, relativity. Astronomy & physics were wedded into astrophysics.

Thus, astronomers and statisticians substantially broke contact; e.g. the curriculum of astronomers heavily involved physics but little statistics. Statisticians today know little modern astronomy.

# The state of astrostatistics today (not good!)

The typical astronomical study uses:

- Fourier transform for temporal analysis (Fourier 1807)
- Least squares regression for model fits (Legendre 1805, Pearson 1901)
- Kolmogorov-Smirnov goodness-of-fit test (Kolmogorov, 1933)
- Principal components analysis for tables (Hotelling 1936)

Even traditional methods are often misused:

see Friday's lecture Common Statistical Mistakes in the Astronomical Literature'

#### Under-utilized methodology:

- modeling (MLE, EM Algorithm, BIC, bootstrap)
- multivariate classification (LDA, SVM, CART, RFs)
- time series (autoregressive models, state space models)
- spatial point processes (Ripley's K, kriging)
- nondetections (survival analysis)
- image analysis (computer vision methods, False Detection Rate)
- statistical computing (R)

Advertisement ....

#### **Modern Statistical Methods for Astronomy**

#### with R Applications

E. D. Feigelson & G. J. Babu, Cambridge Univ Press, 2012

## Cosmology

## ↔ Statistics

Galaxy clustering Galaxy morphology Galaxy luminosity fn Power law relationships Strong lensing morphology <--> Shape statistics Strong lensing timing  $\leftarrow$  Time series with lag 

- ←→ Spatial point processes, clustering
- $\leftarrow$  Regression, mixture models
- ←→ Gamma distribution
- ←→ Pareto distribution
- Weak lensing morphology *Constantiation*

- $\Lambda$ CDM parameters  $\iff$  Bayesian inference & model selection

## **Recent resurgence in astrostatistics**

• Improved access to statistical software. R/CRAN public-domain statistical software environment with thousands of functions. Increasing capability in Python (http://www.astro.cornell.edu/staff/loredo/statpy/essentials.html).

• Papers in astronomical literature doubled to ~500/yr in past decade ("Methods: statistical" papers in NASA-Smithsonian Astrophysics Data System)

• Short training courses (Penn State, India, Brazil, Spain, USA, Greece, China ... here)

• Cross-disciplinary research collaborations (Harvard/ICHASC, Carnegie-Mellon, Penn State, NASA-Ames/Stanford, CEA-Saclay/Stanford, Cornell, UC-Berkeley, Michigan, Imperial College London, LSST Statistics & Informatics Science Collaboration, ...)

• Cross-disciplinary conferences (*Statistical Challenges in Modern Astronomy, Astronomical Data Analysis 1991-2011, PhysStat*, SAMSI 2012, *Astroinformatics 2012*)

• Scholarly society working groups and a new integrated Web portal <u>http://asaip.psu.edu</u> serving: Int'l Stat Institute's Int'l Astrostatistical Assn, Int'l Astro Union Working Group, Amer Astro Soc Working Group, LSST Science Collaboration)

### Textbooks

Bayesian Logical Data Analysis for the Physical Sciences: A Comparative Approach with Mathematica Support, Gregory, 2005

*Practical Statistics for Astronomers,* Wall & Jenkins, 2<sup>nd</sup> ed 2012

*Modern Statistical Methods for Astronomy with R Applications,* Feigelson & Babu, 2012

Statistics, Data Mining, and Machine Learning in Astronomy: A Practical Python Guide for the Analysis of Survey Data,

Ivecic, Connolly, VanderPlas & Gray, 2014

## Two advertisements !

Attend the first IAU conference on astrostatistics: **Statistical Challenges in 21<sup>st</sup> Century Cosmology** IAU Symposium 306, Lisbon PT, May 2014

Join the Astrostatistics and Astroinformatics Portal and organizations (IAA, IAU/WGAA, AAS/WGAA & LSST/ISSC): http://asaip.psu.edu



You are here: Home

#### Welcome to ASAIP

The Astrostatistics and Astroinformatics Portal (http://asaip.psu.edu) is a new Web site serving the cross-disciplinary communities of astronomers, statisticians and computer scientists. It is intended to foster research into advanced methodologies for astronomical research, and to promulgate such methods into the broader astronomy community. The WWW public is welcome to read materials in ASAIP. Use the navigation bar above, or the search box at the upper right, to find material throughout the ASAIP Web site.

Prelude to R ....

## A brief history of statistical computing

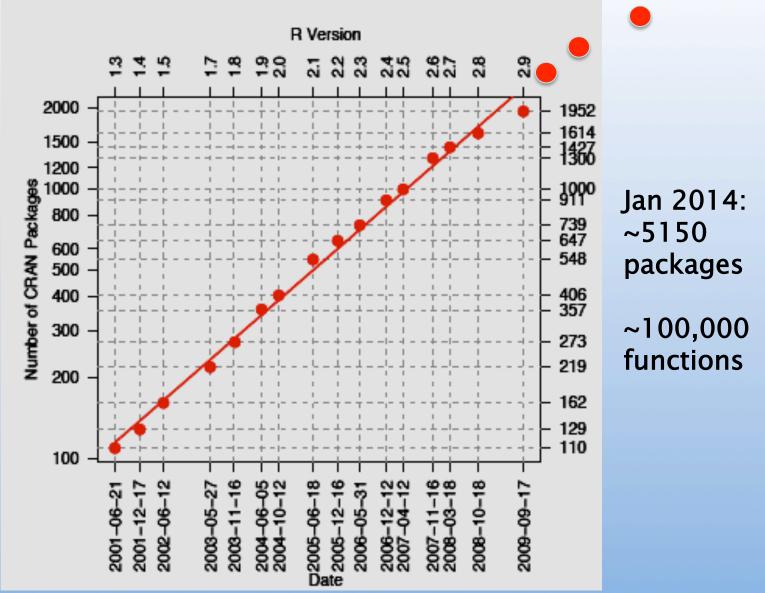
1960s – c2003: Statistical analysis developed by academic statisticians, but implementation relegated to commercial companies (SAS, BMDP, Statistica, Stata, Minitab, etc).

1980s: John Chambers (ATT, USA)) develops S system, C-like command line interface.

1990s: Ross Ihaka & Robert Gentleman (Univ Auckland NZ) mimic S in an open source system, R. Expands to ~15 Core Team members, GNU GPL release.

Early-2000s: Comprehensive R Analysis Network (CRAN) for user-provided specialized packages grows exponentially. Important packages incorporated into base-R.

#### Growth of CRAN contributed packages



See The Popularity of Data Analysis Software, R. A. Muenchen, http://r4stats.com

## The R statistical computing environment

- R integrates data manipulation, graphics and extensive statistical analysis. Uniform documentation and coding standards. But quality control is limited.
- Fully programmable C-like language, similar to IDL. Specializes in vector/matrix inputs.
- Easy download from <a href="http://www.r-project.org">http://www.r-project.org</a> for Windows, Mac or linux. On-the-fly installation of CRAN packages.
- >5000 user-provided add-on CRAN packages, tens of thousands of statistical functions

 Many resources: R help files (3500p for base R), CRAN Task Views and vignette files, on-line tutorials, >140 books, >400 blogs, Use R! conferences, galleries, blogs, companies, The R Journal & J. Stat. Software

#### **Principal steps:**

- Knowing what you want
- Finding what you want
- Writing R scripts
- Understanding what you find

[education & thought] [Google, Rseek, crantastic, ...] [R Help files, books] [education & consulting]

## Some functionalities of R

arithmetic & linear algebra bootstrap resampling empirical distribution tests exploratory data analysis generalized linear modeling graphics robust statistics linear programming local and ridge regression max likelihood estimation multivariate analysis multivariate clustering neural networks smoothing spatial point processes statistical distributions statistical tests survival analysis time series analysis

#### Selected methods in Comprehensive R Archive Network (CRAN)

Bayesian computation & MCMC, classification & regression trees, genetic algorithms, geostatistical modeling, hidden Markov models, irregular time series, kernel-based machine learning, least-angle & lasso regression, likelihood ratios, map projections, mixture models & modelbased clustering, nonlinear least squares, multidimensional analysis, multimodality test, multivariate time series, multivariate outlier detection, neural networks, non-linear time series analysis, nonparametric multiple comparisons, omnibus tests for normality, orientation data, parallel coordinates plots, partial least squares, periodic autoregression analysis, principal curve fits, projection pursuit, quantile regression, random fields, Random Forest classification, ridge regression, robust regression, Self-Organizing Maps, shape analysis, space-time ecological analysis, spatial analysis & kriging, spline regressions, tessellations, three-dimensional visualization, wavelet toolbox

### CRAN Task Views (http://cran.r-project.org/web/views)

CRAN Task Views provide brief overviews of CRAN packages by topic & functionality. Maintained be expert volunteers. Partial list:

- Bayesian ~110 packages
- ChemPhys ~60 packages (incl. 11 for astronomy)
- Cluster ~90 packages
- Graphics ~40 packages
- HighPerformanceComputing ~80 packages
- Machine Learning
- ~70 packages

~25 packages

~25 packages

- Medical imaging
- Robust
- Spatial
- Survival

~175 packages

~125 packages

• TimeSeries

~140 packages

Interfaces: BUGS, C, C++, Fortran, Java, Perl, Python, Xlisp, XML *This is very important for astronomers. R* scripts can ingest subroutines from these languages. *Packages exist for two-way communication for C, Fortran, Python & Ruby: you can ingest R functions in your legacy codes or vice versa.* 

I/O: ASCII, binary, bitmap, cgi, FITS, ftp, gzip, HTML, SOAP, URL

**Graphics & emulators:** Grace, GRASS, Gtk, Matlab, OpenGL, Tcl/ Tk, Xgobi

Math packages: GSL, Isoda, LAPACK, PVM

Text processor: LaTeX

Since c.2005, R has been the premier public-domain statistical computing package with >2M users.

# Some features of R

- Designed for individual use on workstation, exploring data interactively with advanced methodology and graphics. But it can be used for automated pipeline analysis. Very similar experience to IDL.
- R objects placed into `classes': numeric, character, logical, vector, matrix, factor, data.frame, list, and dozens of others designed by CRAN packages. plot, print, summary functions are adapted to class objects. The list class allows a hierarchical structure of heterogeneous objects (like IDL sav file).
- Extensive graphics based on SVG, RGTK2, JGD, and other GUIs.
  See graphics gallery at <u>http://www.oga-lab.net/RGM2</u> and <u>http://gallery.r-enthusiasts.com/</u>

## **Computational aspects of R**

R scripts can be very compact **IDL:** temp = mags(where(vels le 200. and vels gt 100, n)) upper\_quartile = temp((sort(temp))(ceil(n\*0.75))) **R:** upper\_quartile <- quantile(mags[vels>100. & vels<200.], probs=0.75)

Vector/matrix functionalities are fast (like C); e.g. a million random numbers generated in 0.1 sec, a million-element FFT in 0.3 sec.

Some **R** functions are much slower; e.g. for (i in 2:1000000) x[i] = x[i-1] + 1

The **R** compiler rewritten in 2012 from `parse tree' to `byte code' (similar to Java & Python) leading to several-fold speedup.

Several dozen **CRAN** packages are devoted to high-performance computing, parallelization, data streams, grid computing, GPUs, (PVM, MPI, NWS, Hadoop, etc). See **CRAN** HPC Task View.

While originally designed for an individual exploring small datasets, R can be pipelined and can treat megadatsets

## Projects at Penn State to promulgate R in astronomy

- VOStat (http://vostat.org) Web-service to ~50 simple R functions.
- Summer School in Statistics for Astronomy Since 2005 (U.S., India, ...) teaches established statistical methods to ~10% of world's astronomy graduate students.
- Modern Statistical Methods for Astronomy with R Applications (Feigelson & Babu, Cambridge Univ Press, 2012). Comprehensive textbook.
- Astrostatistics & Astroinformatics Portal (<u>http://asaip.psu.edu</u>) Recent papers, discussion forums, and other resources
- Infrastructure CRAN packages CFITSIO, IDL's astrolib, datasets

#### A vision of astrostatistics in 2025 ...

- Astronomy curriculum has 1 year of statistical inference and methodology
- A few percent of young astronomers have M.S. degrees in statistics and computer science
- Astrostatistics and astroinformatics is a well-funded, cross-disciplinary research field involving a few percent of astronomers (cf. astrochemists, instrumentalists) pushing the frontiers of methodology.
- Astronomers regularly use dozens of methods coded in P, the successor to Q and R.
- Statistical Challenges in Modern Astronomy meetings are held annually with ~250 participants