Model Fitting, Bootstrap, & Model Selection

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Model Fitting

- Non-linear regression
- Density (shape) estimation
- Parameter estimation of the assumed model
- Goodness of fit

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Model Selection

- Nested (In quasar spectrum, should one add a broad absorption line BAL component to a power law continuum? Are there 4 planets or 6 orbiting a star?)
- Non-nested (is the quasar emission process a mixture of blackbodies or a power law?).
- Model misspecification

- Is the underlying nature of an X-ray stellar spectrum a non-thermal power law?

Model Fitting in Astronomy

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- Are the fluctuations in the cosmic microwave background best fit by Big Bang models with dark energy?

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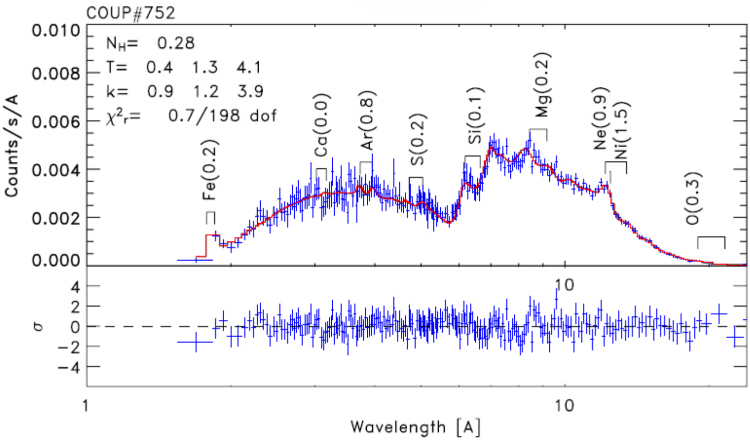
- Are the fluctuations in the cosmic microwave background best fit by Big Bang models with dark energy?
- Are there interesting correlations among the properties of objects in any given class (e.g. the Fundamental Plane of elliptical galaxies), and what are the optimal analytical expressions of such correlations?

A good model should be

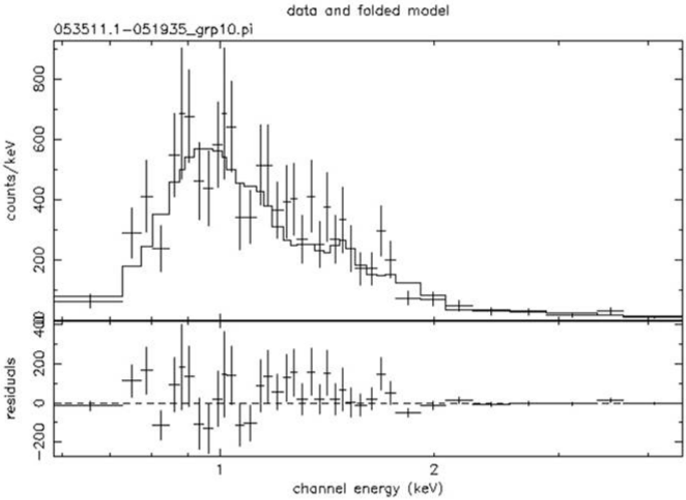
- Parsimonious (model simplicity)
- Conform fitted model to the data (goodness of fit)
- Easily generalizable.
- Not *under-fit* that excludes key variables or effects
- Not *over-fit* that is unnecessarily complex by including extraneous explanatory variables or effects.
- Under-fitting induces bias and over-fitting induces high variability.

A good model should balance the competing objectives of conformity to the data and parsimony.

What is the underlying nature of a stellar spectrum?



One of the 1616 bright sources from Chandra Orion Ultradeep Project
Successful model for high signal-to-noise X-ray spectrum.
Complicated thermal model with several temperatures
and element abundances (17 parameters)



COUP source # 410 in Orion Nebula with 468 photons
Thermal model with absorption $A_V \sim 1$ mag
Fitting binned data using χ^2

Best-fit model: A plausible emission mechanism

- Model assuming a single-temperature thermal plasma with solar abundances of elements. The model has three free parameters denoted by a vector θ.
  - plasma temperature
  - line-of-sight absorption
  - normalization
- The astrophysical model has been convolved with complicated functions representing the sensitivity of the telescope and detector.
- The model is fitted by minimizing sum of squares ('minimum chi-square') with an iterative procedure.

$$\hat{\theta} = \arg\min_{\theta} \chi^2(\theta) = \arg\min_{\theta} \sum_{i=1}^{N} \left(\frac{y_i - M_i(\theta)}{\sigma_i} \right)^2 .$$

Chi-square minimization is a misnomer.

It is parameter estimation by *weighted least squares*.

Limitations to *weighted least squares*

- Fails when bins have too few data points.
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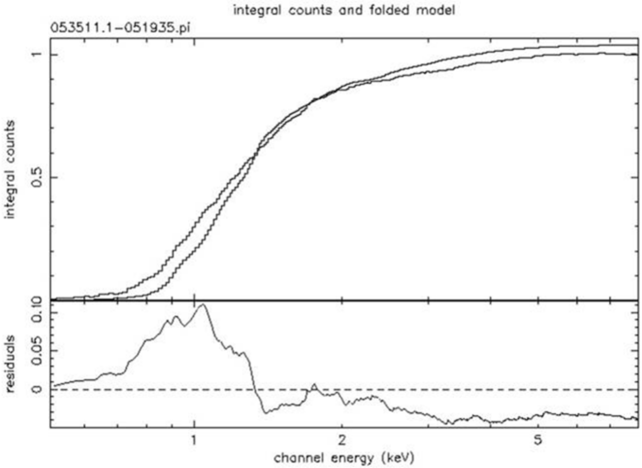
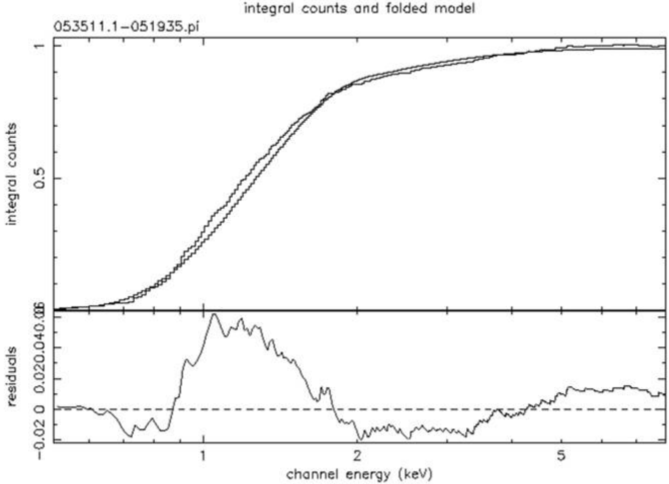
- Failure of independence assumption is common in astronomical data due to effects of the instrumental setup; *e.g.* it is typical to have ≥ 3 pixels for each telescope point spread function (in an image) or spectrograph resolution element (in a spectrum). Thus adjacent pixels are not independent.
- Does not provide clear procedures for adjudicating between models with different numbers of parameters (*e.g.* one- vs. two-temperature models) or between different acceptable models (*e.g.* local minima in $\chi^2(\theta)$ space).
- Unsuitable to obtain confidence intervals on parameters when complex correlations between the estimators of parameters are present (*e.g.* non-parabolic shape near the minimum in $\chi^2(\theta)$ space).

Alternative approach to the model fitting based on EDF



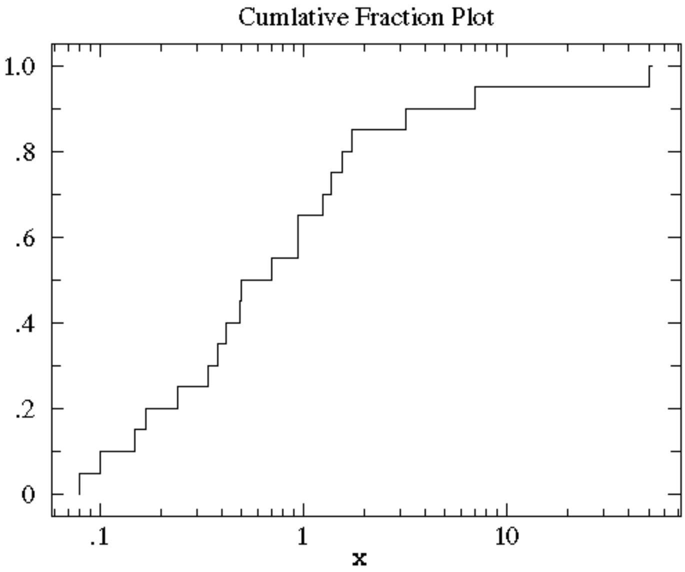
Fitting to unbinned EDF
Correct model family, incorrect parameter value
Thermal model with absorption set at $A_V \sim 10$ mag



Misspecified model family!
Power law model with absorption set at $A_V \sim 1$ mag
Can the power law model be excluded with 99% confidence

Outline

Empirical Distribution Function



Statistics based on EDF

Kolmogrov-Smirnov: $D_n = \sup_x |F_n(x) - F(x)|,$

$$H(y) = P(D_n \le y), \quad 1 - H(d_n(\alpha)) = \alpha$$

Cramér-von Mises: $\int (F_n(x) - F(x))^2 \, dF(x)$

Anderson - Darling: $\int \frac{(F_n(x) - F(x))^2}{F(x)(1 - F(x))} \, dF(x)$

is more sensitive at tails.

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EDF based fitting requires little or no probability distributional assumptions such as Gaussianity or Poisson structure.

Kolmogorov-Smirnov Table

Table 1. Limiting Distribution of the Kolmogorov-Smirnov Statistic
(from Smirnov (1948))

x	$L(x)$	x	$L(x)$	x	$L(x)$	x	$L(x)$
0.28	0.000001	0.73	0.339113	1.18	0.876548	1.76	0.995922
0.29	0.000004	0.74	0.355981	1.19	0.882258	1.78	0.996460
0.30	0.000009	0.75	0.372833	1.20	0.887750	1.80	0.996932
0.31	0.000021	0.76	0.389640	1.21	0.893030	1.82	0.997346
0.32	0.000046	0.77	0.406372	1.22	0.898104	1.84	0.997707
0.33	0.000091	0.78	0.423002	1.23	0.902972	1.86	0.998023
0.34	0.000171	0.79	0.439505	1.24	0.907648	1.88	0.998297
0.35	0.000303	0.80	0.455857	1.25	0.912132	1.90	0.998536
0.36	0.000511	0.81	0.472041	1.26	0.916432	1.92	0.998744
0.37	0.000826	0.82	0.488030	1.27	0.920556	1.94	0.998924
0.38	0.001285	0.83	0.503808	1.28	0.924505	1.96	0.999079
0.39	0.001929	0.84	0.519366	1.29	0.928288	1.98	0.999213
0.40	0.002808	0.85	0.534682	1.30	0.931908	2.00	0.999329
0.41	0.003972	0.86	0.549744	1.31	0.935370	2.02	0.999428
0.42	0.005476	0.87	0.564546	1.32	0.938682	2.04	0.999516
0.43	0.007377	0.88	0.579070	1.33	0.941848	2.06	0.999588
0.44	0.009730	0.89	0.593316	1.34	0.944872	2.08	0.999650
0.45	0.012590	0.90	0.607270	1.35	0.947756	2.10	0.999705
0.46	0.016005	0.91	0.620928	1.36	0.950512	2.12	0.999750
0.47	0.020022	0.92	0.634286	1.37	0.953142	2.14	0.999790
0.48	0.024682	0.93	0.647338	1.38	0.955650	2.16	0.999822
0.49	0.030017	0.94	0.660082	1.39	0.958040	2.18	0.999852
0.50	0.036055	0.95	0.672516	1.40	0.960318	2.20	0.999874
0.51	0.042814	0.96	0.684636	1.41	0.962486	2.22	0.999896
0.52	0.050306	0.97	0.696444	1.42	0.964552	2.24	0.999912
0.53	0.058534	0.98	0.707940	1.43	0.966516	2.26	0.999926
0.54	0.067497	0.99	0.719126	1.44	0.968382	2.28	0.999940
0.55	0.077183	1.00	0.730000	1.45	0.970158	2.30	0.999949
0.56	0.087577	1.01	0.740566	1.46	0.971846	2.32	0.999958
0.57	0.098656	1.02	0.750826	1.47	0.973448	2.34	0.999965
0.58	0.110395	1.03	0.760780	1.48	0.974970	2.36	0.999970
0.58	0.122760	1.04	0.770434	1.49	0.976412	2.38	0.999976
0.60	0.135718	1.05	0.779794	1.50	0.977782	2.40	0.999980
0.61	0.149229	1.06	0.788860	1.52	0.980310	2.42	0.999984
0.62	0.163225	1.07	0.797636	1.54	0.982578	2.44	0.999987
0.63	0.177753	1.08	0.806128	1.56	0.984610	2.46	0.999989
0.64	0.192677	1.09	0.814342	1.58	0.986426	2.48	0.999991
0.65	0.207987	1.10	0.822282	1.60	0.988048	2.58	0.999 9925
0.66	0.223637	1.11	0.829950	1.62	0.989492	2.55	0.999 9956
0.67	0.239582	1.12	0.837356	1.64	0.990777	2.60	0.999 9974
0.68	0.255780	1.13	0.844502	1.66	0.991917	2.65	0.999 9984
0.69	0.272189	1.14	0.851394	1.68	0.992928	2.70	0.999 9990
0.70	0.288765	1.15	0.858038	1.70	0.993823	2.80	0.999 9997
0.71	0.305471	1.16	0.864442	1.72	0.994612	2.90	0.999 99990
0.72	0.322265	1.17	0.870612	1.74	0.995309	3.00	0.999 99997

KS probabilities are invalid when the model parameters are estimated from the data. Some astronomers use them incorrectly.

– Lillifors (1964)

Uses and misuses of Kolmogorov-Smirnov

The KS statistic is used in $\sim$500 astronomical papers/yr, but often incorrectly or with less efficiency than an alternative statistic.

The 1-sample KS test (data vs. model comparison) is distribution-free only in 1-dimension and when the model is not derived from the dataset (i.e., probabilities can be used for hypothesis testing).

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See the viral page
Beware the Kolmogorov-Smirnov test!
at http://asaip.psu.edu

Monte Carlo simulation

- Astronomers have often used *Monte Carlo methods* to simulate datasets from uniform or Gaussian populations. While helpful in some cases, this does not avoid the assumption of a simple underlying distribution.

- Instead, what if we take the observed data as hypothetical 'population' and use Monte Carlo simulation on it. Can simulate many 'datasets' and, each of these can be analyzed in the same way to see how the estimates depend on plausible random variations in the data.

  (No costly observations for 'new/additional' data).

What is Bootstrap?

- Bootstrap (a resampling procedure) is a Monte Carlo method of simulating ‘datasets’ from an observed/given data, without any assumption on the underlying population.
- Resampling the original data preserves (adaptively) whatever distributions are truly present, including selection effects such as truncation (flux limits or saturation).
- Bootstrap helps evaluate statistical properties using data rather than an assumed Gaussian or power law or other distributions.
- Bootstrap procedures are supported by solid theoretical foundations.

Bootstrap Procedure

$\mathbf{X} = (X_1, \ldots, X_n)$ - a sample from F

$\mathbf{X}^* = (X_1^*, \ldots, X_n^*)$ - a simple random sample from the data.

$\hat{\theta}$ is an estimator of θ

θ^* is based on X_i^*

Examples:

$\hat{\theta} = \bar{X}_n,$ $\qquad \theta^* = \bar{X}_n^*$

$\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2,$ $\qquad \theta^* = \frac{1}{n}\sum_{i=1}^{n}(X_i^* - \bar{X}_n^*)^2$

$\theta^* - \hat{\theta}$ behaves like $\hat{\theta} - \theta$

Nonparametric and Parametric Bootstrap

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Example of Parametric Bootstrap:

$X_1, \ldots, X_n \; i.i.d. \sim N(\mu, \sigma^2)$

$X_1^*, \ldots, X_n^* \; i.i.d. \sim N(\bar{X}_n, s_n^2); \quad s_n^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \bar{X}_n)^2$

$N(\bar{X}_n, s_n^2)$ is a good estimator of the distribution $N(\mu, \sigma^2)$

Bootstrap Variance

$\hat{\theta}$ is an estimator of θ based on $X_1, \ldots, X_n$.

θ^* denotes the bootstrap estimator based on $X_1^*, \ldots, X_n^*$.

$$\mathrm{Var}^*(\hat{\theta}) = E^* \left(\theta^* - E(\theta^*)\right)^2$$

In practice, generate N bootstrap samples of size n.
Compute $\theta_1^*, \ldots, \theta_N^*$ for each of the N samples.

$$\bar{\theta^*} = \frac{1}{N} \sum_{i=1}^{N} \theta_i^*$$

$$\mathrm{Var}(\hat{\theta}) \approx \frac{1}{N} \sum_{i=1}^{N} \left(\theta_i^* - \bar{\theta^*}\right)^2$$

Bootstrap Distribution

Statistical inference requires sampling distribution G_n,
given by $G_n(x) = \mathrm{P}(\sqrt{n}(\bar{X} - \mu)/\sigma \leq x)$

statistic	bootstrap version
$\sqrt{n}(\bar{X} - \mu)/\sigma$	$\sqrt{n}(\bar{X}^* - \bar{X})/s_n$
$\sqrt{n}(\bar{X} - \mu)/s_n$	$\sqrt{n}(\bar{X}^* - \bar{X})/s_n^*$

where $s_n^2 = \frac{1}{n}\sum_{i=1}^n (X_i - \bar{X})^2$ and $s_n^{*2} = \frac{1}{n}\sum_{i=1}^n (X_i^* - \bar{X}^*)^2$

For a given data, the bootstrap distribution G_B is given by

$$G_B(x) = \mathrm{P}^*(\sqrt{n}(\bar{X}^* - \bar{X})/s_n \leq x|\mathbf{X})$$

G_B is completely known and $G_n \approx G_B$.

Example

If G_n denotes the sampling distribution of $\sqrt{n}(\bar{X} - \mu)/\sigma$ then the corresponding *bootstrap distribution* G_B is given by

$$G_B(x) = \mathrm{P}^*(\sqrt{n}(\bar{X}^* - \bar{X})/s_n \leq x|\mathbf{X}).$$

Construction of Bootstrap Histogram

$M = n^n$ bootstrap samples possible

$$\begin{array}{cc}
X_1^{*(1)}, \ldots, X_n^{*(1)} & r_1 = \sqrt{n}(\bar{X}^{*(1)} - \bar{X})/s_n \\
X_1^{*(2)}, \ldots, X_n^{*(2)} & r_2 = \sqrt{n}(\bar{X}^{*(2)} - \bar{X})/s_n \\
\ddots \quad \ddots & \ddots \quad \ddots \\
X_1^{*(M)}, \ldots, X_n^{*(M)} & r_M = \sqrt{n}(\bar{X}^{*(M)} - \bar{X})/s_n
\end{array}$$

Frequency table or histogram based on $r_1, \ldots, r_M$ gives G_B.

$$G_B(x) = \frac{1}{M}\#(r_i \leq x).$$

Confidence Interval for the mean

For $n = 10$ data points, $M =$ ten billion

$N \sim n(\log n)^2$ bootstrap replications suffice
N is much smaller than n^n.

– Babu and Singh (1983) Ann. Stat.

Compute $\sqrt{n}(\bar{X}^{*(j)} - \bar{X})/s_n$ for N bootstrap samples

Arrange them in increasing order

$r_1 < r_2 < \cdots < r_N \qquad k = [0.05N],\ m = [0.95N]$

90% Confidence Interval for μ is

$$\bar{X} - r_m \frac{s_n}{\sqrt{n}} \leq \mu < \bar{X} - r_k \frac{s_n}{\sqrt{n}}$$

Bootstrap at its best

Pearson's correlation coefficient and its bootstrap version

$$\hat{\rho} = \frac{\frac{1}{n}\sum_{i=1}^{n}(X_i Y_i - \bar{X}\bar{Y})}{\sqrt{\left(\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2\right)\left(\frac{1}{n}\sum_{i=1}^{n}(Y_i - \bar{Y})^2\right)}}$$

$$\rho^* = \frac{\frac{1}{n}\sum_{i=1}^{n}(X_i^* Y_i^* - \bar{X}_n^* \bar{Y}_n^*)}{\sqrt{\left(\frac{1}{n}\sum_{i=1}^{n}(X_i^* - \bar{X}_n^*)^2\right)\left(\frac{1}{n}\sum_{i=1}^{n}(Y_i^* - \bar{Y}_n^*)^2\right)}}$$

Smooth Functional Model

$$\hat{\rho} = H(\bar{\mathbf{Z}}), \quad \text{where} \quad \mathbf{Z}_i = (X_i Y_i, X_i^2, Y_i^2, X_i, Y_i)$$

$$H(a_1, a_2, a_3, a_4, a_5) = \frac{(a_1 - a_4 a_5)}{\sqrt{((a_2 - a_4^2)(a_3 - a_5^2))}}$$

$$\rho^* = H(\bar{\mathbf{Z}}^*), \quad \text{where} \quad \mathbf{Z}_i^* = (X_i^* Y_i^*, X_i^{*2}, Y_i^{*2}, X_i^*, Y_i^*)$$

Smooth Functional Model: General case

H is a smooth function and $\mathbf{Z}_1$ is a random vector.
$\hat{\theta} = H(\bar{\mathbf{Z}})$ is an estimator of the parameter $\theta = H(\mathrm{E}(\mathbf{Z}_1))$

Division (normalization) of $\sqrt{n}(H(\bar{\mathbf{Z}}) - H(\mathrm{E}(\mathbf{Z}_1))$ by its standard deviation makes them units free.
Studentization, if estimates of standard deviations are used.
Under some regularity conditions Bootstrap distribution gives a very good approximation to the sampling distribution of such normalized statistics.

The theory works for both *parametric and nonparametric Bootstrap*.

– Babu and Singh (1983) Ann. Stat.
– Babu and Singh (1984) Sankhyā
– Singh and Babu (1990) Scand J. Stat.

Bootstrap Percentile-t Confidence Interval

In practice

- Randomly generate $N \sim n(\log n)^2$ bootstrap samples
- Compute $t_n^{*(j)}$ for each bootstrap sample
- Arrange them in increasing order
  $u_1 < u_2 < \cdots < u_N, \;\; k = [0.05N], \;\; m = [0.95N]$
- 90% Confidence Interval for the parameter θ is

$$\hat{\theta} - u_m \frac{\hat{\sigma}_n}{\sqrt{n}} \leq \theta < \hat{\theta} - u_k \frac{\hat{\sigma}_n}{\sqrt{n}}$$

This is called bootstrap PERCENTILE-t confidence interval

When does bootstrap work well

- Sample Means
- Sample Variances
- Central and Non-central t-statistics
  (with possibly non-normal populations)
- Sample Coefficient of Variation
- Maximum Likelihood Estimators
- Least Squares Estimators
- Correlation Coefficients
- Regression Coefficients
- Smooth transforms of these statistics

When does Bootstrap fail

- $\hat{\theta} = \max_{1 \le i \le n} X_i$ Non-smooth estimator
  - Bickel and Freedman (1981) Ann. Stat.

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  - Babu (1984) Sankhyā
  - Athreya (1987) Ann. Stat.

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- $\hat{\theta} - \theta = H(\bar{\mathbf{Z}}) - H(\mathrm{E}(\mathbf{Z}_1))$ and $\partial H(\mathrm{E}(\mathbf{Z}_1)) = 0$

  Limit distribution is like linear combinations of Chi-squares.
  But here a modified version works.

  – Babu (1984) Sankhyā

Non-independent case

$X_1, \ldots X_n$ are identically distributed but not independent

- Straight forward bootstrap does not work in the dependent case. Variances of sums of random variables do not match.
- A clear knowledge of the dependent structure is needed to replicate resampling procedure.
- Classical bootstrap fails in the case of Time Series data.
- If the process is auto-regressive or moving-average one can replicate resampling procedure.
- In the general time-series case the *moving block bootstrap* is suggested.

Moving Block Bootstrap

$X_1, \cdots, X_n$ is a stationary sequence.

1. The sequence is split into overlapping blocks $B_1, \cdots, B_{n-b+1}$, of length b, where B_j consists of b consecutive observations starting from X_j, i.e., $B_j = \{X_j, X_{j+1}, \cdots, X_{j+b-1}\}$.
   Observation 1 to b will be block 1, observation 2 to b+1 will be block 2 etc.
2. From these n-b+1 blocks, n/b blocks will be drawn at random with replacement.
3. Align these n/b blocks in the order they were picked.

This bootstrap procedure works with dependent data.
By construction, the resampled data will not be stationary.

Varying randomly the block length can avoid this problem.
However, the moving block bootstrap is still to be preferred.
– Lahiri (1999) Annals of Statistics

Linear Regression

$Y_i = \alpha + \beta X_i + \epsilon_i$

$\mathrm{E}(\epsilon_i) = 0$ and $\mathrm{Var}(\epsilon_i) = \sigma_i^2$

Least squares estimators of β and α

$$\hat{\beta} = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^n (X_i - \bar{X})^2}$$

$$\hat{\alpha} = \bar{Y} - \hat{\beta}\bar{X}$$

$$\mathrm{Var}(\hat{\beta}) = \frac{\sum_{i=1}^n (X_i - \bar{X})^2 \sigma_i^2}{L_n^2}$$

$$L_n = \sum_{i=1}^n (X_i - \bar{X})^2$$

Classical Bootstrap

Estimate the residuals $\quad e_i = Y_i - \hat{\alpha} - \hat{\beta} X_i$

Draw $e_1^*, \ldots, e_n^*$ from $\hat{e}_1, \ldots, \hat{e}_n$, where $\hat{e}_i = e_i - \frac{1}{n}\sum_{j=1}^n e_j$.

Bootstrap estimators

$$\beta^* = \hat{\beta} + \frac{\sum_{i=1}^n (X_i - \bar{X})(e_i^* - \bar{e}^*)}{\sum_{i=1}^n (X_i - \bar{X})^2}$$

$$\alpha^* = \hat{\alpha} + (\hat{\beta} - \beta^*)\bar{X} + \bar{e}^*$$

$\mathrm{V}_B = \mathrm{E}_B(\beta^* - \hat{\beta})^2 \approx \mathrm{Var}(\hat{\beta})$ efficient if $\sigma_i = \sigma$

V_B does not approximate the variance of $\hat{\beta}$ under heteroscedasticity (*i.e.* unequal variances σ_i)

Paired Bootstrap

Resample the pairs $(X_1, Y_1), \dots, (X_n, Y_n)$
$(\tilde{X}_1, \tilde{Y}_1), \dots, (\tilde{X}_n, \tilde{Y}_n)$

$$\tilde{\beta} = \frac{\sum_{i=1}^{n} (\tilde{X}_i - \bar{\tilde{X}})(\tilde{Y}_i - \bar{\tilde{Y}})}{\sum_{i=1}^{n} (\tilde{X}_i - \bar{\tilde{X}})^2}, \qquad \tilde{\alpha} = \bar{\tilde{Y}} - \tilde{\beta}\bar{\tilde{X}}$$

Repeat the resampling N times and get

$$\beta_{PB}^{(1)}, \dots, \beta_{PB}^{(N)}$$

$$\frac{1}{N} \sum_{i=1}^{N} (\beta_{PB}^{(i)} - \hat{\beta})^2 \approx Var(\hat{\beta})$$

even when not all σ_i are the same

Comparison

- *The Classical Bootstrap*
  - Efficient when $\sigma_i = \sigma$
  - But inconsistent when σ_i's differ
- *The Paired Bootstrap*
  - Robust against heteroscedasticity
  - Works well even when σ_i are all different

Bootstrap References

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- Michael R. Chernick (2007). *Bootstrap Methods - A guide for Practitioners and Researchers*, (2nd Ed.) Wiley Inter-Science.
- Michael R. Chernick and Robert A. LaBudde (2011) *An Introduction to Bootstrap Methods with Applications to R*, Wiley.
- Abdelhak M. Zoubir and D. Robert Iskander (2004) *Bootstrap Techniques for Signal Processing*, Cambridge Univ Press.

A handbook on 'bootstrap' for engineers to analyze complicated data with little or no model assumptions. Includes applications to radar and sonar signal processing.

We shall now get back to

Goodness of Fit

when parameters are estimated.

Parametric bootstrap

$X_1, \ldots, X_n$ sample from $F \in \{F(.;\theta) : \theta \in \Theta\}$ – a family of continuous distributions. Θ is p-dimensional.

$X_1^*, \ldots, X_n^*$ sample generated from $F(.;\hat{\theta}_n)$

Both

$$\sqrt{n} \sup_x |F_n(x) - F(x;\hat{\theta}_n)| \quad \text{and} \quad \sqrt{n} \sup_x |F_n^*(x) - F(x;\hat{\theta}_n^*)|$$

have the same limiting distribution.

In XSPEC package, the parametric bootstrap is command FAKEIT, which makes Monte Carlo simulation of specified spectral model.

In Gaussian case $\hat{\theta}_n^* = (\bar{X}_n^*, s_n^{*2})$.

Numerical Recipes describes a parametric bootstrap (random sampling of a specified pdf) as the ‘transformation method’ of generating random deviates.

Nonparametric bootstrap

$X_1^*, \ldots, X_n^*$ sample from F_n
i.e., a simple random sample from $X_1, \ldots, X_n$.

Bias correction

$$B_n(x) = \sqrt{n}(F_n(x) - F(x; \hat{\theta}_n))$$

is needed. Both

$$\sqrt{n} \sup_x |F_n(x) - F(x; \hat{\theta}_n)| \quad \text{and} \quad \sup_x |\sqrt{n}\left(F_n^*(x) - F(x; \hat{\theta}_n^*)\right) - B_n(x)|$$

have the same limiting distribution.

XSPEC does not provide a nonparametric bootstrap capability

Need for such bias corrections in special situations are well documented in the bootstrap literature.

χ^2 **type statistics** – (Babu, 1984, Statistics with linear combinations of chi-squares as weak limit. *Sankhyā*, Series A, **46**, 85-93.)

U-**statistics** – (Arcones and Giné, 1992, On the bootstrap of *U* and *V* statistics. *The Ann. of Statist.*, **20**, 655–674.)

Model misspecification

$X_1, \dots, X_n$ data from unknown H.

H may or may not belong to the family $\{F(.;\theta) : \theta \in \Theta\}$

H is closest to $F(., \theta_0)$

Kullback-Leibler (information) divergence

$\int h(x) \log \left(h(x)/f(x;\theta)\right) d\nu(x) \geq 0$

$\int |\log h(x)| h(x) d\nu(x) < \infty$

$\int h(x) \log f(x;\theta_0) d\nu(x) = \max_{\theta \in \Theta} \int h(x) \log f(x;\theta) d\nu(x)$

Confidence limits under model misspecification

For any $0 < \alpha < 1$,

$$P\left(\sqrt{n}\sup_x |F_n(x) - F(x;\hat{\theta}_n) - (H(x) - F(x;\theta_0))| \leq C^*_\alpha\right) - \alpha \to 0$$

C^*_α is the α-th quantile of

$$\sup_x |\sqrt{n}\left(F^*_n(x) - F(x;\hat{\theta}^*_n)\right) - \sqrt{n}\left(F_n(x) - F(x;\hat{\theta}_n)\right)|$$

This provide an estimate of the distance between the true distribution and the family of distributions under consideration.

Discussion so far

- K-S goodness of fit is often better than Chi-square test.
- K-S cannot handle heteroscadastic errors
- Anderson-Darling is better in handling the tail part of the distributions.
- K-S probabilities are incorrect if the model parameters are estimated from the same data.
- K-S does not work in more than one dimension.
- Bootstrap helps in the last two cases.

So far we considered model fitting part.

We shall now discuss model selection issues.

MLE and Model Selection

1. Model Selection Framework
2. Hypothesis testing for model selection: Nested models
3. Limitations
4. Penalized likelihood
5. Information Criteria based model selection
    - Akaike Information Criterion (AIC)
    - Bayesian Information Criterion (BIC)

Model Selection Framework (based on likelihoods)

- Observed data D
- $M_1, \dots, M_k$ are models for D under consideration
- Likelihood $f(D|\boldsymbol{\theta}_j; M_j)$ and loglikelihood $\ell(\boldsymbol{\theta}_j) = \log f(D|\boldsymbol{\theta}_j; M_j)$ for model M_j.
  - $f(D|\boldsymbol{\theta}_j; M_j)$ is the probability density function (in the continuous case) or probability mass function (in the discrete case) evaluated at data D.
  - $\boldsymbol{\theta}_j$ is a k_j dimensional parameter vector.

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Example

$D = (X_1, \ldots, X_n)$, X_i, i.i.d. $N(\mu, \sigma^2)$ r.v. Likelihood

$$f(D|\mu, \sigma^2) = (2\pi\sigma^2)^{-n/2} \exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(X_i - \mu)^2\right\}$$

Most of the methodology can be framed as a comparison between two models M_1 and M_2.

Hypothesis testing for model selection: Nested models

The model M_1 is said to be nested in M_2, if some coordinates of $\boldsymbol{\theta}_1$ are fixed, *i.e.* the parameter vector is partitioned as

- $\boldsymbol{\theta}_2 = (\alpha, \gamma)$ and $\boldsymbol{\theta}_1 = (\alpha, \gamma_0)$
- γ_0 is some known fixed constant vector.

Comparison of M_1 and M_2 can be viewed as a classical hypothesis testing problem of $H_0 : \gamma = \gamma_0$.

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Example

M_2 Gaussian with mean μ and variance σ^2
M_1 Gaussian with mean 0 and variance σ^2

The model selection problem here can be framed in terms of statistical hypothesis testing $H_0 : \mu = 0$, with free parameter σ.

Hypothesis testing is a criteria used for comparing two models. Classical testing methods are generally used for nested models.

Limitations

Caution/Objections

- M_1 and M_2 are not treated symmetrically as the null hypothesis is M_1.
- Cannot *accept* H_0
- Can only reject or fail to reject H_0.
- Larger samples can detect the discrepancies and more likely to lead to rejection of the null hypothesis.

Penalized likelihood

- If M_1 is nested in M_2, then the largest likelihood achievable by M_2 will always be larger than that of M_1.
- Adding a penalty on larger models would achieve a balance between over-fitting and under-fitting, leading to the so called Penalized Likelihood approach.
- Information criteria based model selection procedures are penalized likelihood procedures.

Akaike Information Criterion – (AIC)

- Grounding in the concept of entropy, Akaike proposed an information criterion (AIC), now popularly known as Akaike Information Criterion, where both model estimation and selection could be simultaneously accomplished.

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- The penalty term increase as the complexity of the model grows.
- AIC is generally regarded as the first model selection criterion.
- It continues to be the most widely known and used model selection tool among practitioners.

Advantages of AIC

- Does not require the assumption that one of the candidate models is the "true" or "correct" model.
- All the models are treated symmetrically, unlike hypothesis testing.
- Can be used to compare nested as well as non-nested models.
- Can be used to compare models based on different families of probability distributions.

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Disadvantages of AIC

- Large data are required especially in complex modeling frameworks.
- Leads to an *inconsistent model selection* if there exists a true model of finite order. That is, if k_0 is the correct number of parameters, and $\hat{k} = k_i \;\; (i = \arg\min_j \, (-2\ell(\hat{\boldsymbol{\theta}}_j) + 2k_j))$, then $\lim_{n\to\infty} P(\hat{k} > k_0) > 0$. That is even if we have very large number of observations, $\hat{k}$ does not approach the true value.

Bayesian Information Criterion (BIC)

BIC is also known as the Schwarz Bayesian Criterion

$$-2\ell(\hat{\boldsymbol{\theta}}_j) + k_j \log n$$

- BIC is consistent unlike AIC
- Like AIC, the models need not be nested to use BIC
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Caution: *Sometimes these criteria are multiplied by -1 so the goal changes to finding the maximizer.*

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