PlanetPack: a radial-velocity time-series analysis tool facilitating exoplanets detection, characterization, and dynamical simulations

Roman V. Baluev

Central Astronomical Observatory at Pulkovo of Russian Academy of Sciences, Pulkovskoje sh. 65, St Petersburg 196140, Russia
Sobolev Astronomical Institute, St Petersburg State University, Universitetskij pr. 28, Petrodvorets, St Petersburg 198504, Russia

Abstract
We present PlanetPack, a new software tool that we developed to facilitate and standardize the advanced analysis of radial velocity (RV) data for the goal of exoplanets detection, characterization, and basic dynamical N-body simulations. PlanetPack is a command-line interpreter, that can run either in an interactive mode or in a batch mode of automatic script interpretation.

Its major abilities include: (i) Advanced RV curve fitting with the proper maximum-likelihood treatment of unknown RV jitter; (ii) User-friendly multi-Keplerian as well as Newtonian N-body RV fits; (iii) Use of more efficient maximum-likelihood periodograms that involve the full multi-planet fitting (sometimes called as “residual” or “recursive” periodograms); (iv) Easily calculatable parametric 2D likelihood function level contours, reflecting the asymptotic confidence regions; (v) Fitting under some useful functional constraints is user-friendly; (vi) Basic tasks of short- and long-term planetary dynamical simulation using a fast Everhart-type integrator based on Gauss–Legendre spacings; (vii) Fitting the data with red noise (auto-correlated errors); (viii) Various analytical and numerical methods for the tasks of determining the statistical significance.

It is planned that further functionality may be added to PlanetPack in the future. During the development of this software, a lot of effort was made to improve the calculational speed, especially for CPU-demanding tasks. PlanetPack was written in pure C++ (standard of 1998-2003), and is expected to be compilable and usable on a wide range of platforms.

Keywords: planets and sattelites: detection, planets and satellites: dynamical evolution and stability, techniques: radial velocities, methods: data analysis, methods: statistical, surveys

1. Introduction
The new era in planetary science has started in 1990s, after the discovery of the first exoplanet orbiting a main-sequence star (Mayor and Queloz [1995]). This discovery was followed by similar ones in a continuously accelerating regime, and by now the number of known exoplanets candidates is approaching the notable milestone of thousand (see The Extrasolar Planets Encyclopaedia at exoplanet.eu).

The main method of the exoplanets detection is still the precision radial-velocity (RV) monitoring. Although with the launch of the specialized spacecrafts like CoRoT (smsc.cnes.fr/CoRoT) and Kepler (kepler.nasa.gov) the role of the photometric searches of exoplanetary transits was considerably emphasized, the RV method still remains superior in many positions. Even if the discovered transiting exoplanets will eventually outnumber the ones detected by RV monitoring, the photometric method introduces a severe bias in favour of the short-period planets. On contrary, the long-term RV monitoring allows for a detection of exoplanetary systems with architectures resembling the Solar System, e.g. con-
taining Jupiter analogs — giant planets with orbital
periods about a decade or more. Giants with short
orbital periods are easier to detect, but they would
hardly allow existence of a terrestrial planet on a
dynamically stable Earth-like orbit (although it is still
possible to have an Earth-like satellite of such a gas
giant in the habitable zone). In addition, the RV data
are typically necessary to confirm a photometric ex-
planetary detection. From only the transit photom-
etry data we can derive only the transiter’s radius,
which does not reliably imply its mass value, and
thus radial-velocity observations are needed to con-
firm its planetary nature.

Another promising exoplanets detection method
is astrometry. It looks relatively latent at present,
but it may become much more productive and effi-
cient in the near future, after the launch of GAIA.
However, we are a bit sceptical about its ability to
reliably detect and characterize long-period exoplan-
ets, because of the relatively short 5-year expected
duration of the mission. On contrary to space mis-
sions, ground-based programmes are able to accu-
mulate much longer time series. The RV exoplanet
searches have already reached the \( \sim 20 \) years bas-
eline.

Therefore, the RV technique is the main tool of
exoplanetary searches at present, and it will continue
to play at least an important, if not central, role in the
future. It is already quite obvious that efficient RV
exoplanetary detections request sophisticated meth-
ods of data analysis, which need a specialized soft-
ware: a good such software complex is the Systemic
Console (Meschiari et al., 2009). Our paper repre-
sents a scientific description of another such software
tool that we developed for similar same goals. The
need for another software tool was justified by the
following argumentation:

1. Systemic Console relies on rather simple sta-
tistical methods and models that appear inade-
quate when working with high-precision ex-
planetary RV data. For example, it relies on
the plain \( \chi^2 \) fitting and on the textbook \( F \)-test,
which are unreliable for the RV noise appear-
ing in our task (Baluev, 2009a). We needed to
implement some more intricate statistical treat-
ment, especially in what concerns peri-
odograms.

2. Systemic Console was written in JAVA to
reach cross-platform compatibility, but this
led to a dramatic decrease in the compu-
tational performance, which appears pretty ob-
vious when working with Systemic. In scient-
ific tasks the speed of calculations is usually a
more important matter than the wide compat-
bility. PlanetPack is written in standard C++,
and thus it is quick. It should be easily com-
pilable by different compilers and for various
platforms, although it was extensively tested
only with the GCC and Linux-based environ-
ments.

3. It appears that Systemic Console is targeted
to amateur astronomers: e.g. it is more fo-
cused on the graphical interface rather than on
a dense scientific content. We needed to focus
mainly on the scientific contribution and more
scripting capabilities, shifting the basis of the
software to a command-line interface, since it
allows for a more controllable and powerful
work environment.

4. According to the information in the official
Systemic web page at oklo.org, this package
was last updated in 2009.

A few more recent software tools intended for ex-
planetary data fits are available today. In particu-
lar, Wright and Howard (2009) provide an algorithm
of exoplanets RV fitting, taking into account the fact
that there are a few strictly linear parameters of Ke-
plerian RV variation, that can be efficiently elimi-
nated during the fitting of the remaining non-linear
parameters. This algorithm assumes that the gravi-
tational perturbations in the exoplanetary system are
negligible. Pál (2010) provided an RV fitting algo-
rithm for the self-perturbed exoplanetary systems,
based on the Lie integration scheme. And finally,
Eastman et al. (2013) offer an algorithm of simul-
taneous “photometry+RV” fitting, also equipped by
some Bayesian Markov chain Monte Carlo simul-
ation tools.

We have not done a “field-test” performance
comparison of these packages with PlanetPack.
Nevertheless, we may note that PlanetPack offers
some highly important algorithms that are unavail-
able in other packages (in particular, the red-noise
RV fitting and the advanced periodograms construction) and, on contrary, the mentioned packages offer some important tools that are absent in PlanetPack (in particular, the joint analysis of photometry and radial velocities, Bayesian statistics). The practical value of our new package, as we see it, is in its wide task coverage: it unites under the same umbrella a large number of very different particular tools in a single place. When developing PlanetPack the main effort was done in the direction of the data-analysis methods, rather than just in programming or optimizing computational performance. Almost all data-analysis methods that PlanetPack incorporates belong to the self-consistent theory work that we carried out over a few years.

This was not just a pure theoretical investigation: we applied our tools to real exoplanetary systems, so that these data-analysis methods were evolving and improving in this process. Moreover, this allowed to obtain new results concerning the relevant exoplanetary systems, and most of these concrete results were eventually confirmed by independent authors, often based on the enlarged and/or improved datasets. Such examples include the rejection of the planet HD74156 d (disclaimed by Baluev (2009a), further retracted by Wittenmyer et al. (2009) and Meschiari et al. (2011)); the revealing of the 2/1 resonance in the HD37124 planetary system (first revealed in Baluev (2008b), later confirmed by Wright et al. (2011)), and the detection of the hints of the planet GJ876 e (as we discuss in Baluev (2008c, 2011), a good and stable orbit for this planet can be found in the old RV data, long before its announcement by Rivera et al. (2010)). We draw the reader’s attention to these examples not for bragging, but in order to highlight the potential of the software tool we applied our tools to real exoplanetary systems, and most of these concrete results were eventually confirmed by independent authors, often based on the enlarged and/or improved datasets. Such examples include the rejection of the planet HD74156 d (disclaimed by Baluev (2009a), further retracted by Wittenmyer et al. (2009) and Meschiari et al. (2011)); the revealing of the 2/1 resonance in the HD37124 planetary system (first revealed in Baluev (2008b), later confirmed by Wright et al. (2011)), and the detection of the hints of the planet GJ876 e (as we discuss in Baluev (2008c, 2011), a good and stable orbit for this planet can be found in the old RV data, long before its announcement by Rivera et al. (2010)). We draw the reader’s attention to these examples not for bragging, but in order to highlight the potential of the theory work that we collected now under the name “PlanetPack”. The demonstrated examples prove that this software tool may significantly increase the outcome of the ongoing exoplanetary RV data-analysis work, as well as to prevent us from too hasteful conclusions.

PlanetPack source, along with its technical manual, is available for download as a project at sourceforge.net/projects/planetpack. In the further sections of the present paper, we consider the main PlanetPack abilities and the related theory. This paper does not say anything about the use of PlanetPack commands, its data organization, and other technical documentation necessary to use it in practice. The mentioned technical documentation is given in a standalone file downloadable together with PlanetPack sources.

2. Data and basic models

Let us first describe the general structure of the observational data set that we deal with. Assume that we have J RV time-series, referring to the same star but to different observatories or spectrographs. A j-th such time series contains Nj elementary data packets, consisting of the time of an observation, \( t_{ij} \), of the RV measurement itself, \( v_{ij} \), and of its expected uncertainty \( \sigma_{\text{meas,}j} \). The total number of these observations is \( N = \sum_{j=1}^{J} N_j \).

In addition to this raw input data, PlanetPack uses a time reference epoch, \( T_0 \), as an unfittable parameter. Before any fitting, the values of \( t_i \) are always shifted by this quantity and divided by the total timeseries span, \( T \) (calculated internally). Therefore, the values that are actually used are \( (t_i - T_0)/T \). This process should normally remain invisible to the user, but to minimize numerical errors, it is recommended to choose \( T_0 \) close to the middle of the time series. This \( T_0 \) is also used as a reference epoch for the orbital parameters, when such a reference epoch is necessary (see below). The desired value of \( T_0 \) can be assigned explicitly by the user or it may be chosen automatically (a round number close to the weighted mean of \( t_i \)). Below we assume that \( T_0 = 0 \) for the simplicity of the formulae. The transition to the case of \( T_0 \) is obvious.

Now let us specify the general functional model of the RV curve. It is basically the same as we used in Baluev (2008b). For each of the J time series we have a separate model that can be represented as the following sum:

\[
\mu_j(t, \theta) = \mu_{\text{obs},j}(t, \theta_{\text{obs},j}) + \mu_*(t, \theta_*) \quad (1)
\]

This is a sum of two terms. The first term, \( \mu_{\text{obs},j} \), depends on the time series through the index \( j \), and it represents an observatory-specific part of the mea-
sured radial velocity:

\[ \mu_{\text{obs}, j} = c_{0,j} + \sum_{n=1}^{s_j} A_{jn} \cos \left( \frac{2\pi}{P_{jn}} (t - \tau_{jn}) \right). \]  

In this definition, the term \( c_{0,j} \) is a constant term denoting an RV offset of the \( j \)-th time series, and the remaining (periodic) terms model possible observatory-specific periodic components, e.g. systematic errors. The compound vector \( \theta_{\text{obs}, j} \) contains the variables \( c_{0,j}, A_{jn} \) (the semi-amplitude of a systematic term), and \( \tau_{jn} \) (the epoch of the maximum systematic variation, treated relatively to \( T_0 \)). The periods \( P_{jn} \) are treated as fixed parameters.

We may recall that e.g. annual systematic errors can be rather frequently met in the published exoplanetary RV data, especially in the old datasets, where they may exceed ~10 m/s (Baluev, 2008b, 2009a). Although this conclusion was first considered with some scepticism by other researchers, at present such errors have been revealed by independent teams (Wittenmyer et al., 2009; Meschiari et al., 2011) and sometimes they can be clearly and undoubtedly seen when comparing published old and revised RV data for the same star (Baluev, 2011). We believe that the existence of such errors in some of the publicly released RV data of exoplanetary systems is already proven well.

Although we must admit that in recent years the major observing teams seem to do a good job on removing this issue, the old data, which are certainly useful, may still suffer from such errors. Therefore PlanetPack still allows to deal with this issue by means of an expanded model (2).

The second term in (1) is common for all time series; it refers to the star and its planetary system and it has the general form of

\[ \mu_\star(t, \theta_\star) = \sum_{n=1}^{r} c_n t^n + \mu_{\text{pl}}(t, \theta_{\text{pl}}), \]

where \( c_n \) are coefficients of a polynomial trend modelling some long-term underlying RV variation (usually it reflects the compound RV contribution from some long-period seen or unseen bodies in the system), and \( \mu_{\text{pl}} \) describes the RV variation due to the assumed orbiting exoplanets (each with an individual and independent RV contribution). The vector \( \theta_\star \) contains the coefficients \( c_n \) and the elements of \( \theta_{\text{pl}} \).

Notice that \( c_n \) are understood in view of the reference epoch \( T_0 \).

The first published version of PlanetPack may set only a common polynomial trend for the whole time series. Sometimes it might be useful to allow for separate datasets to have different trends, reflecting e.g. some long-term instrumental drifts. This ability was not implemented in PlanetPack till now, because we have not yet faced a practical task where this would be necessary, but this may be done in the future. At present, the models with different trends may already be constructed with a help of a ruse: to obtain, e.g. an almost quadratic trend in the model of only some specific dataset, we need to specify in the relevant sum (2) a harmonic term with a very large period value (larger than the observations time span). A linear trend can be mimiced by means of setting a constraint (Sect. 5) to fix one of the two parameters of this long-period harmonic term.

In the simplest and most frequent case, when the interplanetary gravitational perturbations in the system are negligible, we may assume the multi-Keplerian model

\[ \mu_{\text{pl}} = \sum_{k=1}^{N} K_k (\cos(\omega_k + \nu_k) + e_k \cos \omega_k). \]

Here \( N \) is the number of orbiting exoplanets, \( K_k \) is the RV semi-amplitude induced by the \( k \)-th exoplanet, \( e_k \) is the relevant orbital eccentricity, \( \omega_k \) is the pericenter argument, and \( \nu_k \) is the true anomaly. The true anomaly can be represented as a function of the time \( t \), of the mean-motion \( n_k \), of \( e_k \), and of an additional phase parameter \( \lambda_k \). We choose this phase parameter to be the mean longitude at \( T_0 \). Therefore, the vector \( \theta_{\text{pl}} \) contains the variables \((n, K, \lambda, e, \omega)_k \) for each of the \( N \) planets. Notice that for an exoplanet on a circular orbit we have the relevant RV variation looking like \( K_k \cos(n_k t + \lambda_k) \).

For some time, we investigated the possibility to fit the parameters \( e \cos \omega \) and \( e \sin \omega \) instead of \( e \) and \( \omega \), since the last pair implies an undesired singularity at \( e = 0 \). However, we did not note any increase in the fitting performance after the transition to \((e \cos \omega, e \sin \omega)\). Moreover, it appeared that in the practical tests the resulting convergence rate
actually dropped after that transition, and even for small-eccentricity orbits. We therefore abandoned this idea and returned to the direct fitting of \((e, \omega)\). However, when \(e\) is small, the user should be careful with the interpretation of its uncertainty reported by PlanetPack: in this case, the uncertainty of \(e\) becomes meaningless without an accompanying uncertainty of \(\omega\) and without the correlation between \(e\) and \(\omega\). Actually, in this case the best course of action would be to look at the 2D confidence contours (Sect. 5) plotted in the plane \((e \cos \omega, e \sin \omega)\), assuming that \(e\) and \(\omega\) are polar coordinates. Such a plot would be much more informative in this case, than e.g. just an upper limit on \(e\).

The minimum mass of an exoplanet, \(m \sin i\), and the semi-major axis of its orbit, \(a\), can be expressed via the primary fit parameters using the well-known relations

\[
m \sin i \approx \tilde{K} \left( \frac{M_\star}{Gn} \right)^{1/3} = M \tilde{K} M_\star^{2/3} n^{-1/3},
\]

\[
a \approx \frac{GM_\star}{n^2} = \mathcal{A} M_\star^{1/3} n^{-2/3},
\]

(5)

where \(\tilde{K} = K \sqrt{1 - e^2}\), \(G\) is the gravitational constant, and \(M_\star\) is the mass of the star (which should be derived from some external considerations), and \(M\) and \(\mathcal{A}\) are conversion constants \((M \approx 9.077 \cdot 10^{-3}\) and \(\mathcal{A} \approx 6.664 \cdot 10^{-2}\) when the unit of \(m\) is \(M_{\text{Jup}}\), of \(M_\star\) is \(M_\odot\), of \(n\) is day\(^{-1}\), and of \(\tilde{K}\) is m/s). PlanetPack uses \(\tilde{K}\) as primary parameter instead of \(K\), since then its conversion to \(m \sin i\) does not involve the eccentricity \(e\) (which also eliminates the need to take into account the correlation with \(e\) when evaluating the uncertainty of \(m \sin i\)).

The approximate formulae (5) are valid when \(m \ll M_\star\), which is true for the most practical cases. More accurate formulae, which take into account barycenter effects, exist (Ferraz-Mello et al., 2005; Pal, 2010; Beauchêne et al., 2012) and are rather popular in practice. However, for multi-Keplerian fits we do not accept this approach due to the following reasons:

1. These formulae are implicit and therefore more difficult for practical use.
2. They involve significant dependence on the orbital inclination (the famous \(\sin i\)), which is typically unknown. Eventually we have to assume e.g. \(i = 90^\circ\), and if this assumption is wrong, the “corrected” mass value will anyway contain a remaining error comparable to the original one.
3. They are not actually more accurate than (5), unless we deal with a single-planet system. When the system contains two or more planets we should also take into account mutual gravitational perturbations, including e.g. the offset in the apparent period value (Ferraz-Mello et al., 2005), which would affect the resulting mass value too. These biases of the order of \(m/M_\star\) are typically neglected, but then there is no reason to take into account any other terms with a similar magnitude, including those due to the barycenter displacement.
4. For the unperturbed exoplanetary case the formulae (5) are more than satisfactory, because the errors due to statistical uncertainties are dominating anyway.

We may note that in the case of the Newtonian \(N\)-body fitting (Sect. 8), PlanetPack will honestly evaluate the correct planet masses, taking into account all gravitational effects and the best-fit value of \(\sin i\). This is achieved using an artificial “osculating RV semi-amplitude” parameter, see the details in (Baluev, 2011). Also, we would like to emphasize that the primary fit parameters are \(K\) and \(P\), not \(m\), and the formula used to obtain \(m\) do not affect the fitting process in any way. It only affects the value of \(m\) derived after the fit.

PlanetPack deals with the parametrized RV noise. The basic noise model assumes that the errors of all \(v_{ji}\) are independent and Gaussian with the variances expressed as

\[
\sigma_{ji}^2 = \sigma_{\text{meas},ji}^2 + \sigma_{*,ji}^2,
\]

(6)

where the quantities \(p_j = \sigma_{*,ji}^2\) represent additional unknown parameters (RV “jitter”) to be estimated from the data. These parameters can be combined in a single vector \(p\). Notice that we understand \(\sigma_{*,ji}^2\) as a solid symbol here, because in practice we may sometimes deal with the cases \(p_j < 0\), meaning that the values of \(\sigma_{\text{meas},ji}^2\) supplied by the observers possess rather poor quality, and the real errors of \(v_{ji}\) are
systematically smaller (Baluev, 2009a). As we have already discussed in that paper, in practice the apparent RV jitter often have little resemblance with the actual RV instability caused by astrophysical effects on the star itself. The instrumental errors and various spectrum reduction imperfections may introduce a comparable and even dominating contributions. We should treat \( p_j \) just as free parameters introduced to reach some degree of model consistency, avoiding to assign any concrete physical sense to them.

3. Maximum-likelihood RV curve fitting

Assuming the uncorrelated Gaussian distribution of RV errors, we can write down the likelihood function of the task as

\[
\ln L(\theta, p) = -\frac{1}{2} \sum_{j=1}^{J} \sum_{i=1}^{N_j} \ln \sigma_{ji}^2(p) + \frac{(v_{ji} - \mu_j(t_{ji}, \theta))^2}{\sigma_{ji}^2(p)} - \frac{N}{2} \ln 2\pi. \tag{7}
\]

The position of the maximum of (7) would yield the classic maximum-likelihood estimation of the parameters \( \theta \) and \( p \). However, PlanetPack uses a modification of the maximum-likelihood method, which is based on the following modified likelihood function:

\[
\ln \tilde{L}(\theta, p) = -\frac{1}{2} \sum_{j=1}^{J} \sum_{i=1}^{N_j} \ln \sigma_{ji}^2(p) + \frac{(v_{ji} - \mu_j(t_{ji}, \theta))^2}{\gamma \sigma_{ji}^2(p)} - \frac{N}{2} \ln 2\pi. \tag{8}
\]

The best-fitting estimations of \( \theta \) and \( p \) are obtained as the position of the maximum of \( \ln \tilde{L} \). The thing that makes the definition (8) to differ from the classic one in (7) is the correction divisor \( \gamma \). It is equal to \( \gamma = 1 - d/N \), where \( d \) is the number of the degrees of freedom of the RV model, here equal to \( \text{dim} \theta \). The purpose of the corrector \( \gamma \) is to reduce the systematic bias in the estimation of \( p \) that would otherwise appear due to the fact that the best-fit residuals are systematically smaller than the actual measurement errors. See the details in (Baluev, 2009a).

The larger is the resulting maximum value of \( \tilde{L} \), the better is the fit quality. The value of \( \tilde{L} \) is not very intuitive, however. As a numerical measure of the fit quality we offer a more useful quantity

\[
\tilde{I} = 0.2420 \tilde{L}^{-1/N}, \tag{9}
\]

because it is resembling the traditional r.m.s. measure. First, the smaller is \( \tilde{I} \), the better is the fit. Second, \( \tilde{I} \) is measured in the same units as the observations \( v_{ji} \) (i.e., in m/s). And third, the normalization of \( \tilde{I} \) is chosen so that \( \tilde{I} \) approximately reflects an average of the RV residuals.

The detailed theory and justification of this method is given in (Baluev, 2009a). PlanetPack performs the non-linear maximization of (8) using a variant of the Levenberg–Marquardt (LM) algorithm. Our implementation of this algorithm is different from e.g. the one used in the wide-spread MINPACK library, because the latter was designed to deal with only a sum-of-squares objective function, emerging in the least-squares regression task. This special structure of the objective would allow to use certain simplifying relations between its gradient and the Hessian matrix, but our objective (8) does not belong to this class. Although we describe in (Baluev, 2009a) a way to “fool” the MINPACK or MINPACK-like algorithms, forcing them to solve the task we actually need, we eventually decided to use our own variant of the LM algorithm, more general than the one used in MINPACK. Our implementation represents some hybrid method between the MINPACK variant and the classic general one described in (Bard, 1974). It does not rely on the assumption that the objective is a sum of squares.

4. Advanced periodograms

PlanetPack is equipped with improved versions of the periodograms, which have many advantages in comparison with the classic Lomb (1976)–Scargle (1982) periodogram. Their main improvements are listed below.

1. These periodograms are the likelihood-ratio periodograms. Their values basically represent the likelihood-ratio statistic associated with the modified likelihood function (8). The motivation and details of this approach are given in
In particular, such periodograms involve a built-in estimation of the RV jitter and other RV noise parameters, which allows for a self-consistent data fitting already at the period-search stage.

2. At the very beginning of the analysis, these periodograms can be used to just detect a periodic signal in a raw input time series. But they may also be used in further steps, when one or a few planets have already been extracted from the data, and we need to check whether the residuals hide an additional planet. However, these periodograms are not just the plain periodograms of the relevant pre-calculated and then frozen residuals, as it is typically done in this task. PlanetPack evaluates each value of such a periodogram by means of a full multi-planet fit, which is performed almost anew; re-adjusting e.g. the parameters of already extracted planets. The advantage of such periodograms is clearly demonstrated by Anglada-Escude and Tuomi (2012), who call them “recursive periodograms”. We prefer to call them as the “residual periodograms”, on contrary to the “periodograms of residuals”. This can also be treated as a broad extension of the generalized “floating-mean” periodogram (Ferraz-Mello, 1981; Cumming et al., 1999; Zechmeister and Kurster, 2009). The PlanetPack’s periodograms can utilize the simple sinusoidal model of the signal, as well as a more complicated periodic model representing a segment of the Fourier series (trigonometric polynomial of a given degree). The periodogram with the sinusoidal model represents an extension of the classic Lomb–Scargle periodogram, while the periodogram with the Fourier model is a similar extension of the so-called multiharmonic periodogram (Schwarzenberg-Czerny, 1996; Balvev, 2009b). The Fourier model may be more suitable for non-sinusoidal RV signals, which may appear due to planets on highly-eccentric orbits.

Therefore, the individual values of the PlanetPack’s periodograms actually represent the modified likelihood-ratio statistic $\tilde{Z}$ of Section 9 below. The base RV model describes our knowledge of the planetary system at the current step of the analysis, while the alternative one also involves a trial periodic signal modelled by a sinusoid or trigonometric polynomial (having a given basic period). The issues related to the statistical significance levels of these periodograms will be discussed in detail in Section 9.

5. Constrained fitting

PlanetPack allows to perform the maximum-likelihood fitting under some simple equality constraints. Let us denote full vector of the RV curve parameters, consisting of the RV curve parameters $\theta$ and of the noise parameters $p$, as $\xi$. Let us assume that we need to maximize (8) under a condition $\eta(\xi) = \eta_0$, where $\eta$ is a specified vector function of a vector argument, and $\eta_0$ is a vector constant. In this case we need to find

$$\tilde{L}^*(\eta_0) = \max_{\xi} \tilde{L}(\xi) \bigg|_{\eta(\xi) = \eta_0},$$

$$\xi^*(\eta_0) = \arg \max_{\xi} \tilde{L}(\xi) \bigg|_{\eta(\xi) = \eta_0}. \tag{10}$$

At present there is only rather limited, though useful, set of functions that can be chosen as constraints. Namely, it is allowed to constrain any single fit parameter (either primary or derived one, including the amplitudes $K$ and $\tilde{K}$, and the minimum mass $m \sin i$), a mutual inclination between planetary orbits (in the case when it appears constrainable from the RV data thanks to the gravitational perturbations), and the mutual inclination with an accompanying nodes line orientation angle (see Baluev, 2011 and PlanetPack manual for further details).

The procedure of the constrained fitting when one or more primary fit parameters are held fixed is trivial: we just need to ignore the relevant parameters in the LM algorithm. When a combination of two or more primary parameters is constrained, we use the method of elimination to perform this constrained fitting. That is, during the fitting we directly express some of the parameters involved in $\eta$ via the remaining ones by means of explicit formulae, and also adjust the gradient and the Hessian approximation for $\tilde{L}$ to take this elimination into account.
Notice that the constraint in (10) implies a decrease in the number of degrees of freedom of the RV model, which affects the value of the corrector γ in (8). In the constrained case we have γ = 1 − (dim θ − dim η)/N, provided that all constraints in η refer to the RV curve model (the RV noise parameters, as well as any their constraints, do not affect γ).

6. Parametric confidence regions

PlanetPack makes it easy to construct the level contours of the function (8), which can serve as asymptotic parametric confidence regions. The method is generally similar to the one described in (Balucnev, 2008b). Let our full vector of the RV curve parameters be ξ, and we need to to construct the confidence region for the variables η = η(ξ). This new vector η has necessarily smaller dimension than ξ (in practice usually there are only one or two parameters in η) and it may represent just a subset of ξ or some simple function of ξ (among those described in Section 5). Then, for a given trial η0 from a multi-dimensional grid, we perform the following constrained fitting (10).

The partly-maximized function \( \bar{L}^* \) in (10) can be plotted on a multi-dimensional grid of η, and its level contours will represent the necessary confidence regions. We need to notice that PlanetPack does not contain any graphical plotting facilities; it only generates a table of the quantities \( \eta, \bar{L}^*(η), \xi^*(η) \), which is supposed to be used later by an external graphical plotter (like e.g. GNUPLOT).

We still need to calibrate these level contours with the actual significance probability. For this goal, we also need to define the following quantities, produced by the usual unconstrained fitting:

\[
\hat{L}^* = \max_\xi \bar{L}(\xi), \\
\xi^* = \arg \max_\xi \bar{L}(\xi). \tag{11}
\]

Then, following (Balucnev, 2009a), we can pose a hypothesis testing task, with the encompassing (alternative) hypothesis \( K \): “ξ is arbitrary” (implying the best-fitting estimation \( \hat{\xi} = \xi^* \) and \( \hat{\xi}_K = \hat{\xi}^* \)), and the restricted (base) hypothesis \( H \): “ξ satisfies the constraint \( \eta(\xi) = \text{const} \)” (implying \( \hat{\xi} = \xi^*(\eta) \) and \( \hat{\xi}_H = \bar{L}^*(\eta) \)). The numbers of the degrees of freedom in the relevant models are now \( d_H = \dim \xi - \dim \eta \) and \( d_K = \dim \xi \). Note that due to the divisor γ in (8), which depends on the number of free parameters (hence, on the number of constraints too), the function \( \hat{L} \) is a bit different in (10) and in (11). This means, e.g., that \( \hat{L}^* = \max_\eta \hat{L}^*(\eta) \) in our case.

The confidence level for a given likelihood contour \( \hat{L}^*(\eta) = \text{const} \) can be mapped with the relevant likelihood-ratio statistic \( \hat{Z} \) of the below Section 9 with \( \hat{L}_H = \hat{L}^* \) and \( \hat{L}_K = \hat{L}^* \). From the well-known classical results it follows that when \( N \to \infty \), the quantity 2\( \hat{Z} \) asymptotically follows the \( \chi^2 \) distribution with \( d = d_K - d_H = \dim \eta \) degrees of freedom.

Therefore, the overall sequence to obtain the asymptotic confidence regions for the parameters η looks like the following:

1. Obtain the necessary table of \( \bar{L}^* \).
2. For a selected contour value \( \hat{L}^* \) and pre-calculated \( \xi^*(\eta) \), construct the statistic \( \hat{Z} \).
3. Evaluate the corresponding asymptotic confidence probability as \( P_{\hat{Z}}(\hat{Z}) \), where \( P_{\hat{Z}}(\hat{Z}) = \Gamma_{\frac{1}{2}}\left(\frac{1}{2}\right) \Gamma\left(\frac{1}{2}\right) \), with \( \Gamma_{\frac{1}{2}} \) being the incomplete gamma function.

The step two is actually done by PlanetPack automatically: the relevant value of \( \hat{Z} \) is written in the output table along with the other data. The probability \( P_{\hat{Z}}(\hat{Z}) \) is not evaluated by PlanetPack, because it would require an access to non-standard math libraries, which we try to avoid. However, the necessary gamma function is available in GNUPLOT, which we recommend to use when plotting the relevant probability contours in a graph.

7. Red-noise analysis

PlanetPack can deal with the RV data contaminated by the correlated (“red”) noise. This red noise appears rather frequently in practice and imposes a lot of misleading effects without proper treatment (Balucnev, 2011, 2013b). PlanetPack uses the

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1Possible constraints set on the parameters of the RV noise (rather than curve) model, do not affect the corrector γ, but still affect the asymptotic \( \chi^2 \) distribution of \( \hat{Z} \), increasing its number of degrees of freedom. PlanetPack is aware of this subtle issue and deals with it properly.
maximum-likelihood algorithm of the red-noise reduction, which is described in (Baluev, 2013b) in full details. The RV noise model is now more complicated than the basic white-noise one described in Section 2. It is modelled by a Gaussian random process with an exponentially decreasing correlation function. In the white-noise case we had only a single noise parameter, \( \sigma_x^2 \) (or a few such parameters for different time series). The free parameters of the correlated RV noise model are: the variance of the “white” noise component \( \sigma_{\text{white}}^2 \), the variance of the “red” noise component \( \sigma_{\text{red}}^2 \), and the noise correlation timescale \( \tau_{\text{red}} \), such that the covariance coefficient between two RV measurements separated by the time gap \( \Delta \) is equal to \( \sigma_{\text{red}}^2 \exp(-\Delta/\tau_{\text{red}}) \). This parameter \( \tau_{\text{red}} \) should not be mixed with \( \tau_{\text{fr}} \) from (2).

PlanetPack allows for two types of the red-noise models: the model with a “shared” red noise and with a “separated” red noise. In the shared model, PlanetPack deals with only a single pair of the red-noise parameters \( (\sigma_{\text{red}}^2, \tau_{\text{red}}) \), and the red component of the noise is the same for all RV data points of the joint time series. This model means that the red noise is generated by the star itself, and not by individual instruments. The white parts of the noise are still assumed different for individual data sets of the compound time series. In the second, separated, model, the red noise is treated separately for to each individual datasets, and the number of the red-noise parameters is increased accordingly. The correlations between RV data points belonging to different datasets (i.e., different spectrographs) are set to zero in such a case. It is also possible to specify red-noise component to only some of the datasets, leaving the others purely white. It is not allowed to specify one or more separated red-noise component when a shared red noise is defined, because such a model would be very close to the degeneracy.

Although this method of red-noise reduction is rather new, it have proven its high practical efficiency in the case of the exoplanetary systems of GJ876 (Baluev, 2011) and GJ581 (Baluev, 2013b). We believe that it should appear useful in other cases too, so we offer its implementation in PlanetPack.

8. Newtonian N-body fitting and dynamics

Some exoplanetary systems show detectable hints of non-Keplerian dynamics due to interplanetary perturbations. In this case a more complicated RV curve model should be used, which should be based on the numerical integration of the relevant N-body task. The algorithm of N-body fitting used by PlanetPack is the one described in (Baluev, 2011) in all details. This algorithm involves an integration of the N-body equations for the planetary coordinates and velocities together with the associated differential equations for their partial derivatives with respect to the osculating orbital elements (i.e., the variational or sensitivity equations). This method allows to calculate the necessary objective function, its gradient, and its Hessian matrix with much better speed/error ratio then e.g. evaluating the gradient via finite differences. The osculating orbital parameters are referenced in the Jacobi coordinate system. Please see (Baluev, 2011) for the explanation of the method, coordinate system, and other details.

The choice of the Jacobi system is motivated by the fact that it allows much more smooth switching between perturbed and unperturbed RV models. The main difficulty in such a transition comes from the planetary orbital period estimations: the apparent period (the one seen in an RV periodogram) is different from the osculating period. The first-order formula for this displacement is given in (Ferraz-Mello et al., 2005). This offset appears due to the secular perturbations in the planetary mean longitude, and it has the following bad consequence. Assume we performed a non-perturbed fit and found a best-fit (apparent, or periodogram) period for some planet. After that, we may wish to see what will change if we add the interplanetary perturbations. When making a perturbed fit, we have no other option than to treat the apparent period value as the osculating one, but these values are different by their definition! In other words, feeding the N-body model with the observed period value generates a biased actual (averaged) model period; it is displaced from the observed period that we have just substituted as the osculating one. In the worst cases, we may discover that our fitting algorithm refuses to converge to anything reasonable at all, because the relevant frequency dis-
placement exceeds (even significantly exceeds) the periodogram resolution \( \sim 1/T \). This was the case for the planet GJ876 d (Baluk, 2011), for example. Ideally, we should first reduce this displacement between the periods, e.g., according to the formulæ by Ferraz-Mello et al. (2005). However, in our previous works we have established (rather empirically) that the use of the Jacobi coordinates practically eliminates the need of such a period correction: the osculating Jacobi periods appear much closer to the apparent periods, than the osculating periods referenced in other coordinate systems. Such an effect is achieved because we refer the osculating orbital periods to an increased star mass value, incorporating the mass of the planet, whose osculating period we want to define, and also of the planets below it (among those included in the integration). Again, see Baluk (2011) for the details.

To make such N-body fitting to work we obviously need a numerical integrator. PlanetPack uses an extension of the old Everhart (1974) integrator for this goal. As it was discussed by Avdushev (2010), the Everhart integrator is, basically, an implicit Runge-Kutta integrator, equipped by an efficient predictor evaluation. The original Everhart integrator was based on the Gauss–Radau or Gauss–Lobatto splitting of each integration step. Avdushev (2010) gives the general formulæ suitable for an arbitrary sequence of the splitting nodes. In particular, the Gauss–Legendre and Gauss–Lobatto spacings generate an integrator with a useful symplectic property (when the integration step is constant). The integrator used in PlanetPack is an 16-th order integrator, based on 8 Gauss–Legendre nodes. In comparision with the Avdushev (2010) implementation, we introduced some changes to increase the calculation speed:

1. The formulæ given in Avdushev (2010) are valid for a system of first-order equations \( \dot{x} = F(x) \). We extended them to the second-order case which we actually deal with, \( \ddot{x} = F(x) \). This allowed to increase the integrator performance roughly twice, in comparison with the trivial substitution \( \dot{y} = \{x, \dot{x}\} \) leading to the first-order system \( \ddot{y} = G(y) = \{\dot{x}, F(x)\} \). The necessary corrections are fairly obvious when comparing the formulæ of the original Everhart method with the general formulæ by Avdushev. We do not detail these changes here, since this would require to replicate a large part of the Avdushev’s paper.

2. On contrary to Avdushev (2010), in the source code we define the integration nodes as compile-time constants. All other derived coefficients and constants of the scheme are pre-calculated at the compilation stage as well (i.e., before the execution of PlanetPack itself). This also improves the calculation speed significantly. However, this goal was reached by means of rather sophisticated template metaprogramming tools of C++, which requires a fully standard-compliant compiler with a clever code optimization. For example, GCC or Intel C++ Compiler work well (when proper optimization options are turned on), while with MS Visual C++ compiler we failed to achieve the same fast code.

3. The step-size control method of the original Everhart integrator is imperfect. If \( s \) stands for the number of integration nodes, the step size is adjusted as if the integrator had the order of \( s \), but for the specific node systems like, e.g., Lobatto, Radau, or Legendre ones, the actual integrator order is equal to \( 2s - 2 \), \( 2s - 1 \), or \( 2s \), respectively. In case of our 16-th order integrator, the step would be chosen in a very pessimistic manner, as if the integration order was only 8. Then the resulting integration errors would be much smaller than what we request. We have established empirically that the actual integration error appears roughly equal to the square of the requested one. Therefore, we correct the step-size control procedure by passing the square root of the desired relative precision, instead of the desired relative precision itself. In practice this simple method works nicely: the step is scaled according to the actual integrator order (16), and the actual precision of the integrator is in much better agreement with the requested one (1 – 2 orders in magnitude).

All these changes leaded to a significant cumulative increase in the speed of the calculations, in
comparison with the FORTRAN code provided by Avdyshev (2010), as well as in comparison with the RADAU15, a traditional wide-spread FORTRAN implementation of the Everhart integrator.

In addition to the N-body fitting, which requires a short-term N-body integration, PlanetPack can perform the traditional long-term numeric integration. The integration scheme is the same for both cases — it is the one based on 8 Gauss–Legendre nodes. The difference is in the step-size controlling: for short-term integrations we use a variable step-size (aimed to achieve the maximum performance), while for long-term integrations we use constant step (aimed to preserve the symplectic property).

9. Statistical issues: analytical methods

Statistics is an important component of PlanetPack. It includes some theoretical results (classic and recent ones), as well as tools for numerical Monte Carlo simulations. The newly-developed statistical theory implemented in PlanetPack mainly concerns the significance levels of the periodograms. PlanetPack calculates the false alarm probability (FAP) of individual periodogram peaks using the method explained in (Baliev, 2008a, 2009a,b), which is based on theory of extreme values of random processes (the generalized Rice method). For a periodogram where the signal is modelled by a trigonometric polynomial of degree \(n\), the main FAP estimation formula derived in the works by Baliev (2008a, 2009b) looks like

\[
\text{FAP}(z) \lesssim M(z) \approx \frac{W \alpha_n e^{-z^{n-1/2}}}{(2n-1)!! \sum_{k=1}^{n} (-1)^{n-k} k^{2n+1} (n+k)!(n-k)!},
\]

where \(z\) is the observed maximum peak on the periodogram, \(\Delta f\) is the width of the frequency band, and \(T_{\text{eff}}\) is the effective length of the time series. The latter quantity is defined as \(\sqrt{4\pi \Delta f^2}\), where \(\Delta f\) is the weighted variance of the times \(t_{ji}\) (with the weights taken as \(1/\sigma_j^2\) at the best-fit \(p\)). This effective length is usually close to the plain time span of the time series. The sign ‘\(\lesssim\)’ in (12) means that \(M(z)\) represents an upper bound for \(\text{FAP}(z)\) and simultaneously an asymptotic approximation for \(\text{FAP}(z)\) when \(z \to \infty\). The approximation for the function \(M(z)\) in (12) was obtained using the so-called “assumption of the uniform phase coverage”. Regardless of so apparently restrictive name, for the stated FAP evaluation task this assumption works well in the majority of the practical cases, as we have shown, even for ultimately strong spectral leakage (aliasing).

Strictly speaking, the formula (12) was derived for the case when the RV models are linear (except for the frequency parameter), and the noise uncertainties are known a priori (no noise models involved). However, for more practical cases, including weakly non-linear models and parametrized noise, the same formulae can be used in the asymptotic sense for \(N \to \infty\). See (Baliev, 2009a, 2013a) for the details. Unfortunately, for the periodograms involving models with correlated noise of Section 7, we have not yet developed a reliable theory of the significance levels. In this case PlanetPack will evaluate an approximation of the FAP according to some suggestive generalization of (12) to the red-noise models, but at present Monte Carlo simulations must be considered superior in this case.

PlanetPack is tuned to utilize the likelihood-ratio test for comparison of nested models. Given two rival RV models: a base (more simple one) \(\mu_H\) and an alternative (more complicated one) \(\mu_K\), we have the classical hypothesis testing task: is the base hypothesis \(H\) consistent with the data, or it should be rejected in favour of its alternative \(K\)? This question can be answered after calculation of the classic likelihood-ratio statistic

\[
Z = \ln L^*_{\mathrm{HR}} - \ln L^*_{\mathrm{HK}},
\]

\[
L^*_{\mathrm{HR}} = \max_{\xi_H} L^*(\xi_H), \quad L^*_{\mathrm{HK}} = \max_{\xi_K} L^*(\xi_K), \quad (13)
\]

The larger is \(Z\), the greater is the observable advantage of \(K\) over \(H\). PlanetPack, however, should honour the bias-reducing modification (8), which leads to a modified likelihood-ratio by Baliev (2009a), which is defined as

\[
\hat{Z} = \frac{N_K}{N} \left( \ln \hat{L}^*_{\mathrm{HR}} - \ln \hat{L}^*_{\mathrm{HK}} \right) + \frac{N_K}{2} \ln \frac{N_H}{N_K},
\]

\[
\hat{L}^*_{\mathrm{HR}} = \max_{\xi_H} \hat{L}^*(\xi_H), \quad \hat{L}^*_{\mathrm{HK}} = \max_{\xi_K} \hat{L}^*(\xi_K), \quad (14)
\]

where \(N_{H,K} = N - d_{H,K}\) with \(d_{H,K}\) being the numbers of the degrees of freedom in the RV models to compare.
The quantity $\tilde{Z}$ represents a critical quantity for the decision: the larger is $\tilde{Z}$, the less likely is $\mathcal{H}$ in comparison with $\mathcal{K}$. When the RV models are linearisable, the asymptotic distribution of $2\tilde{Z}$ (for $N \to \infty$) is the $\chi^2$-distribution with $d = d_K - d_H$ degrees of freedom (under $\mathcal{H}$). This framework is used in PlanetPack to define the generalized periodograms (Section 4) and the asymptotic confidence regions (Section 6). In practice, at least for the confidence regions determination task, the asymptotic $\chi^2$ distribution may work well, even when the RV model is pretty complicated and non-linear (Baluev, 2013a). For the periodograms we however should use the formulae (12) and the related statistical theory, rather than the classical $\chi^2$ distribution. This is because the models involved in the periodogram definition are not entirely linearisable (Baluev, 2013a).

The definition (13) differs from the classic one in (13) in the normalization and offset which were introduced to compensate for the corrector $\gamma$ in (8). This $\gamma$ is different for the model $\mathcal{H}$ or $\mathcal{K}$, so we needed to introduce the bias of $(N_K/2) \ln(N_H/N_K) \approx d/2$ to make $Z$ asymptotically equivalent to $Z$ (with a possible residual error of $\sim 1/N$). The normalizing factor $N_K/N$ does not alter the asymptotic properties of $\tilde{Z}$ and it has only rather cosmetic purpose: it was chosen so that for the multiplicative noise model, $\sigma_i^2 = \kappa/w_i$ with fixed weights $w_i$, the statistic $\tilde{Z}$ appears equal to the statistic $z_i$ from (Baluev, 2008a).

It is important that the model $\mathcal{K}$ includes $\mathcal{H}$ as a partial case or a subset of lesser dimension, i.e. these models are nested. This implies, in particular, that $d_H < d_K$ and the fit parameters of $\xi_H$ represent a subset of $\xi_K$.

Another small but useful statistical method, implemented in PlanetPack, is the Vuong test for the comparison of non-nested rival models (Baluev, 2012). It can be used to resolve the period ambiguity due to the aliasing, or other types of ambiguity involving peer (non-nested) models.

10. Statistical issues: simulations

For more intricate statistical tasks, PlanetPack allows to perform numerical Monte Carlo simulations in a user-friendly manner. There are a few Monte Carlo algorithms that are implemented in PlanetPack.

10.1. Plain Monte Carlo assuming Gaussian noise and a single nominal model

This is a classical Monte Carlo scheme, which is used to model the distribution function of the statistic $\tilde{Z}$ or the probability density of the best-fit estimations $\xi^*$. In this algorithm we assume that the true values of the parameters are more or less known.

The relevant simulated distribution functions, $P(\tilde{Z}|\hat{\xi})$ and $p(\xi^*|\hat{\xi})$ depend on the assumed nominal values $\hat{\xi}$, which a considered as true.

1. First of all, select some “nominal” (assumed “true”) values $\hat{\xi}$ somewhere in the region of interest. We may select e.g. the best-fitting model for this goal, although such choice is not mandatory.

2. Given the chosen nominal vector $\hat{\xi}$, evaluate the implied nominal RV values and the RV errors variances $\sigma_i$ (or, for the red-noise framework, the full noise covariance matrix).

3. Construct a simulated RV dataset by means of adding to the nominal RV curve the simulated Gaussian errors, generated on the basis of previously evaluated uncertainties and correlations.

4. Based on the simulated dataset, evaluate the value of the likelihood function at the nominal parameter values from step 1, and the maximum value of $\tilde{L}$ for this trial. Based on these two values, evaluate the necessary modified likelihood ratio statistic $\tilde{Z}$ for this trial.

5. Save this value of $\tilde{Z}$, as well as the set of the simulated best fitting parameters (when necessary), and return to step 3, if the desired number of trials has not been accumulated yet.

Therefore, this classical method is not self-closed: we should feed the simulation with the nominal vector $\hat{\xi}$. Due to this weakness, the results of the simulation are usable when the functions $P(\tilde{Z}|\hat{\xi})$ and $p(\xi^*|\hat{\xi})$ do not demonstrate large dependence on $\hat{\xi}$ (at least for the expected realistic values of $\hat{\xi}$, e.g. the ones covering the uncertainty region).

We actually recommend this simulation in practice only to detect a significant non-linearity of the
task specified, or, vice versa, to show that a particular task can be dealt with by means of the linear asymptotic methods discussed in previous sections. This is achieved by means of the comparison of the asymptotic confidence regions or of the asymptotic $\chi^2$ likelihood-ratio distribution with the results of simulations. We must note, that e.g. non-elliptic shape of the parametric confidence regions (asymptotic or Monte Carlo ones) does not yet imply any genuine non-linearity at all. Although such a deviation from ellipticity is usually deemed as an indicator of the non-linearity, it may be often caused by other reasons like, e.g. an uncareful choice of the parametrization (Baluev, 2013b). To check that the non-linearity is indeed genuine (“endogeneous”) and that it really requests the use of complicated non-asymptotic treatment, it is necessary to verify the agreement between the asymptotic results and the results of the classic Monte Carlo simulation.

When the model is proven to be significantly non-linear, the classic Monte Carlo scheme does not offer more realistic confidence regions or confidence probabilities, so it should not be used for this goal either. The naive interpretation of the classic Monte Carlo results leads to some caveats. For example, it may double the statistical bias of the maximum-likelihood estimations, rather than to compensate it: the Monte Carlo trials will generate “mock” best-fit parametric solutions that are biased relatively to the actual best-fit one in the same manner as this actual best-fit configuration is biased relatively to the truth.

10.2. Bootstrap simulation

The bootstrap is used when there is a danger that the RV errors are not really Gaussian, although we must note that the actual practical profit from the bootstrap in the exoplanet searches still remains without detailed investigation.

1. Evaluate the best fitting model and the resulting RV residuals.
2. Apply random shuffling procedure of the residuals (we do this separately to each sub-dataset of our combined time series).
3. Evaluate the statistic $\tilde{Z}$ and best fitting parameters in the same manner as in the plain Monte Carlo simulation.
4. Save the resulting value of $\tilde{Z}$ and parameters and return to step 2.

The bootstrap shares all weaknesses of the classical Monte Carlo scheme, except for the assumption of the noise Gaussianity. In addition, it possesses extra disadvantages, for example it is meaningful only with a white-noise RV model, because random shuffling of the residuals basically destroys any correlational structure of the RV noise, which a red-noise model tries to deal with.

Another weakness of the bootstrap simulation is that it does not work well for the noise parameters (Baluev, 2013b). Their bootstrap-simulated values are concentrated in an unexpectedly small region, much smaller than the real uncertainty domain. Consequently, the result of such a simulation looks roughly as if these noise parameters were held fixed during the simulation. This also results in a different and rather unpredictable behaviour of the statistic $\tilde{Z}$ obtained using such a simulation.

10.3. Genuinely frequentist Monte Carlo simulation

The existing criticism of the above-described Monte Carlo algorithms is due to their sensitivity to some assumed constant “true” or “nominal” vector of the fit parameters. This is one of the main arguments of many statisticians, which they often use to highlight the advantages of the Bayesian approach. The Bayesian methods do not rely on a single nominal vector: instead, they deal with a scattered prior distributions covering a large parametric domain. However, it appears that this led us to an unjustified opposing the Bayesian methods with the frequentist ones. Although the above simulation schemes do suffer from the issue of constant nominal values, this issue can be eliminated in the genuinely frequentist framework. Leaving aside the philosophy, the main technical difference between the Bayesian and frequentist methods is in how they treat the uncertainty of the nominal values of the fit parameter. While the Bayesian methods use weighted averaging with some pre-set prior probability density, the genuine frequentist approach is based on the worst-case principle, and uses the maximization or minimization in place of the averaging. If in the simplified frequentist approach we dealt with the distribution function $P(\tilde{Z}|\hat{\xi})$, in the genuine frequentist
treatment we should replace it with

$$P_{\text{worst}}(\hat{Z}) = \min_{\xi \in \Xi} P(\hat{Z}|\xi), \quad (15)$$

which means the worst-case confidence probability. Standing on the Bayesian positions with probabilistic \(\xi\), the distribution of \(\hat{Z}\) would be expressed as

$$P_{\text{mean}}(\hat{Z}) = \int_{\Xi} P(\hat{Z}|\xi) p(\xi) d\xi \quad (16)$$

with \(p(\xi)\) being the prior distribution of the parameters. Obviously, the difference between (15) and (16) is crucial, but we cannot say that one of them is generally better, or on contrary deprecated. Each approach has its own advantages and disadvantages in concrete special circumstances; some of them are briefly discussed in (Baluev, 2013b). Obviously, in the frequentist approach we need only to outline a parametric domain \(\Xi\), and any prior density inside this domain does not play any role when we find the minimum.

The entire algorithm of the genuine frequentist simulation would look as the following:

1. Select an \(i\)th trial point \(\hat{\xi}_i\) (possibly, residing inside a given parametric domain \(\Xi\)).
2. Run the plain Monte Carlo algorithm of Sect. 10.1 assuming that the true parameters correspond to the selected point.
3. Save the simulated distribution \(P(\hat{Z}|\hat{\xi}_i)\) of the test statistic of interest (\(\hat{Z}\) in our case) and return to step 1.
4. When a sufficiently dense coverage of the mentioned in step 1 parametric domain is reached, evaluate the function\( P_{\text{worst}}(\hat{Z}) = \min_{\xi \in \Xi} P(\hat{Z}|\xi)\).

After that, the rigorous frequentist false alarm probability associated with an observed value \(\hat{Z}_s\) (which was obtained using exactly the same models that were used during the simulation) can be calculated as \(1 - P_{\text{worst}}(\hat{Z}_s)\).

At present, PlanetPack does not incorporate Bayesian tools, but the genuine frequentist simulation can be organized by means of calling it subsequently from an external shell script. To do this we should first generate some set of \(\hat{\xi}_i\), saving it in a file. This can be done with PlanetPack by means of the plain Monte Carlo algorithm, or using another preferred external procedure. After that, PlanetPack can be subsequently executed for each saved \(\hat{\xi}_i\) to perform the simulation of step 2, saving the relevant distribution \(P(\hat{Z}|\hat{\xi}_i)\). Then these distributions should be processed externally to generate \(P_{\text{worst}}(\hat{Z})\). This is exactly how we estimated the significance of the planet GJ 581 e in (Baluev, 2013b).

11. Conclusions

We have a hope that PlanetPack functionality will grow further in future, not limited by the things that we have described in the paper. In particular, it would be tempting to add some algorithms of Bayesian simulations, and to have some capabilities of dealing with astrometric data, because of the forthcoming domination of GAIA astrometry. Among more technical things, we would like to make PlanetPack able to work in a multi-threaded mode, profiting from the full capabilities of modern multicore CPUs or even from GPU computing (at present, PlanetPack is single-threaded).

PlanetPack is a free and open-source software. We do not set any limitation on the use of itself or of its source code (except for providing a proper reference to the present paper). Anyone who is interested is allowed to freely modify its code to improve it or to adapt it to their specific needs, although it would be of course preferrable to incorporate a significant and worthy improvement in PlanetPack itself rather than to make an independent fork.

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