OpenOrb Tutorial v.0.2

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Short introduction to OpenOrb

1.1 Theory

In the Bayesian framework, the parameters to be estimated are treated as random variables and the complete solution to the inverse problem is contained in the parameters' posterior probability densities. The posterior distribution p_p is proportional to the a priori (p_{pr}) and the observational error (p_{ϵ}) PDFs:

$$p_{\rm p}(\mathbf{P}) \propto p_{\rm pr}(\mathbf{P})p_{\epsilon}(\Delta\psi(\mathbf{P}))$$
 (1.1)

where **P** refers to the orbital elements and $\Delta\psi(\mathbf{P})$ stands for the observed minus computed (O-C) residuals (Muinonen & Bowell 1993, Virtanen 2005). The a priori often used is Jeffreys' a priori which secures the invariance of the results. For example, the collision probability does not depend on the type of orbital elements used in the analysis (Virtanen & Muinonen 2006).

If you want to transform the computed orbital-element PDF to another set of variables such as other types of orbital elements or ephemerides, you must also transform (that is, propagate) the weights to the new variables (Muinonen & Bowell 1993):

$$p(\mathbf{F}) = \int dP p(\mathbf{P}) \delta_{\mathrm{D}}(\mathbf{F} - \mathbf{F}(\mathbf{P})) = \frac{1}{\det(\frac{\delta \mathbf{F}}{\delta \mathbf{P}})_{\mathbf{F}}} p(\mathbf{P}(\mathbf{F})), \tag{1.2}$$

where $\mathbf{F}(\mathbf{P}) = (F_1(\mathbf{P}), \dots, F_k(\mathbf{P}))^T$ is a set of functions of the orbital elements, δ_{D} is Dirac's function, and $\det(\frac{\delta \mathbf{F}}{\delta \mathbf{P}})_F$ is the determinant of the Jacobian matrix for the transformation $\mathbf{P} \to \mathbf{F}$. The propagation of the weights is done automatically for the PDFs produced by the "official" OpenOrb executable, oorb.

1.2 Numerical Methods

1.2.1 Orbital inversion

Ranging

Ranging maps the non-Gaussian orbital-element PDF with a given number of sample orbits (Virtanen et al. 2001, Muinonen et al. 2001). Each sample orbit is computed using the following scheme: Two observations are chosen from the data set and a random deviate is added to all four coordinates to mimic observational noise. Next, a random topocentric distance is generated for the first observation date using a, typically, broad interval. The topocentric distance for the second observation date is generated from an interval relative to the topocentric distance on the first observation date. Since the location of the observatory with respect to the Sun is usually known, the four planeof-sky coordinates and the two topocentric distances can be transformed into two heliocentric positions corresponding to the two observation dates. Using well-established methods in celestial mechanics, an orbit can be computed using the two heliocentric positions. The generated sample orbit is then used to compute ephemerides for the other observation dates. If the residuals are acceptable and the PDF value is good enough with respect to the untilthen best-fit orbit, the sample orbit is accepted. The inversion can be sped up by iteratively adjusting the intervals for the topocentric distance either by performing the simulation for a smaller number of sample orbits before performing the full-scale inversion (Virtanen et al. 2003) or by starting with only two observations and adding more observations step by step (Granvik & Muinonen 2005).

Least-squares with linearized covariances

Least-squares with linearized covariances (LSL)...

1.2.2 Integration

- Bulirsch-Stoer extrapolation method
 - n-body dynamical model contains 8 planets + Moon + Pluto
 - leading relativistic term by the Sun (perihelion shift)

Installing OpenOrb

2.1 Software requirements

In addition to basic Unix tools such as tar and make, using OpenOrb only requires a Fortran 90/95 compiler—we are mostly using the free gfortran compiler (http://gcc.gnu.org/)—and gnuplot (http://www.gnuplot.info) for automatic generation of plots.

2.2 Producing the executable

Extracting the source code archive will produce a directory called OpenOrb:

```
tar xvzf OpenOrb-vN.N.tar.gz
```

Change directory to the OpenOrb directory:

```
cd OpenOrb
```

Run configuration script to set up the chosen compiler and its commandline switches:

```
./configure [COMPILER] [opt | deb]
```

Here COMPILER can be one of the following: gfortran, g95, lahey, intel, sun, compaq, or absoft. The option opt will produce optimized code for production use, whereas deb will produce code suitable for debugging. The compiler commands and switches are explicitly given in (and should be modified through) the make.config file. Next change to the main directory and

produce the oorb executable:

cd main
make oorb

Assuming everything compiled without problems¹ the oorb executable is now in the main directory.

To allow a flexible usage of the executable, you may want to make the following changes or additions to your shell's configuration file:

export PATH=\$PATH:/path/to/oorb

If you have access to gnuplot and want to make automatic plots of the orbital-element PDFs, you should define the \$00RB_GNUPLOT_SCRIPTS_DIR environment variable:

export OORB_GNUPLOT_SCRIPTS_DIR=/path/to/OpenOrb/gnuplot/

2.3 Getting and processing required data files

Access to the following data files is required to run oorb:

- OBSCODE.dat http://www.cfa.harvard.edu/iau/lists/ObsCodes.html
- TAI-UTC.dat http://hpiers.obspm.fr/eop-pc/
- ET-UT.dat
- de405.dat

The most recent versions of the three first files are incorporated in the OpenOrb package. OBSCODE.dat is updated every night by the Minor Planet Center. However, if you do not use observations from observatories that have recently acquired an observatory code, there is no need to update this file more often than, say, once every year or so. Note that the format of the OBSCODE.dat is identical to the HTML page with the exception that all HTML tags and the header line have been deleted. TAI-UTC.dat and ET-UT.dat have to be updated manually. A suitable interval to check the availability of updates is every six months or so.

¹The only known (compatibility) issue can be found at the end of modules/cl_options.f90 and requires commenting certain lines in/out. If you are using the latest gfortran compiler, everything should compile without errors.

To generate the JPL planetary ephemeris file de405.dat, go to the OpenOrb/data/JPL_ephemeris/ directory

cd ../data/JPL_ephemeris/

and issue the following make command:

make de405

If successful, the ASCII versions of the de405 ephemerides will first be automatically downloaded from the JPL FTP server, and then built to the binary file de405.dat. Finally, de405.dat is copied to the data directory and the intermediate files are deleted. Note that you do not have to rebuild the de405.dat file every time you get a new version of OpenOrb. However, since de405.dat is a binary file, it may have to be built separately for every operating system. The correctness of the generated ephemeris file can be checked with

make de405_test

Finally, the OORB_DATA environment variable, which contains the path to the data directory (usually OpenOrb/data/), should be added to the environment:

export OORB_DATA=/path/to/data/directory/

Again, consider adding the OORB_DATA variable to your shell's configuration file.

2.4 Configuration file

The explanations and possible values for the configuration parameters are given in Table 2.4. The path to the configuration file FILE (path to default file is OpenOrb/main/oorb.conf) can either be given using the command line option --conf=FILE or using an environment variable:

export OORB_CONF=/path/to/configuration/FILE

If neither of these are used, it is assumed that the configuration file is called oorb.conf and resides in the working directory. Note that speci-

Option	Explanation						
MANY OPTIONS	NOT MUCH TIME						

Table 2.1: See configuration file. The options should be self-explanatory...

fying the path as a command-line parameter (--conf=FILE) overrides the environment variable (\$00RB_CONF) which in turn overrides the default path (./oorb.conf).

2.5 Sample configuration file

If you are using Bash, it makes life quite a bit easier if the .bashrc file contains the following entries:

```
export PATH=$PATH:/path/to/oorb
export OORB_CONF=/path/to/oorb/configuration/file
export OORB_DATA=/path/to/data/directory/
export OORB_GNUPLOT_SCRIPTS_DIR=/path/to/OpenOrb/gnuplot/
```

Using OpenOrb

The basic options (input, output, etc.) are given as command-line parameters when running oorb, but more detailed configuration parameters are defined using a configuration file.

3.1 File formats

3.1.1 Observations

- Current MPC format (.mpc).
- New MPC format (.mpc3).

In the future, OpenOrb will be able to use the format which Pan-STARRS will be using.

3.1.2 Orbits

Current OpenOrb format (.orb).

3.1.3 Ephemeris

Current OpenOrb format (.eph).

3.2 Computing orbital-elements based on observed positions

The oorb executable currently has to ways of obtaining the orbital-element PDF based on the observed positions, Ranging (--task=ranging) and LSL

(--task=lsl). Whereas Ranging maps the PDF rigorously, that is, without prior assumptions of its shape, LSL assumes that the PDF is Gaussian and derives a so-called single-point estimate for the orbital-element PDF. In practice, the single-point estimate consists of the nominal orbit and the corresponding hyperellipsoid which describes the uncertainty of the orbit. In general, Ranging is optimized for situations with scarce data. LSL, on the other hand, should only be used when there is enough data available to assume that the *true* shape of the orbital-element PDF is indeed more or less Gaussian. The orbital inversion is performed by using either one of the following commands:

```
oorb --task=ranging --obs-in=FILE.mpc [ --orb-out=OUTFILE ]
   [ --orb-out-separately ]

oorb --task=lsl --obs-in=FILE.mpc --orb-in=INFILE
   [ --orb-out=OUTFILE ] [ --orb-out-separately ]
```

Here FILE.mpc contains the observed positions in the Minor Planet Center (MPC) format, and the file may contain more than one object in which case the number or temporary designation separates different sets. The observational uncertainty is specified in the configuration file. Currently, OpenOrb also allows observations to be fed using the "New MPC Format" the fate of which is still uncertain. In the New MPC Format (OpenOrb recognizes it by the suffix .mpc3) observations are, among other things, allowed to have individual uncertainties. For LSL, oorb needs at least one starting point which is supplied using INFILE. If --orb-out=0UTFILE is omitted, the resulting orbital-element PDF is written to standard out. With the --orb-out-separately option the orbit or orbits for each separate observation set is written to separate file the name of which is defined by the designation or number of the observation set.

3.2.1 Tips for using Ranging

- Make a reasonable assumption for the observational uncertainty σ_{obs} , e.g., the observatory's historical RMS for O-C residuals.
- If using relative weights for sample orbits (non-uniform sampling), make sure the acceptance window ($[-c_{\rm acc} \times \sigma_{\rm obs}, +c_{\rm acc} \times \sigma_{\rm obs}]$, where $c_{\rm acc}$ is the acceptance-window multiplier) is large enough to allow sampling without cut-offs due to residuals. In practice, make sure the residual stamps figure do not show cut-offs.

- The generation window ($[-c_{\text{gen}} \times \sigma_{\text{obs}}, +c_{\text{gen}} \times \sigma_{\text{obs}}]$, where c_{gen} is the generation-window multiplier) should not be larger than the acceptance window. Typically, they have the same size, that is, $c_{\text{acc}} = c_{\text{gen}}$.
- Use a number of sample orbits which is enough to do statistics, but is still not overkill considering running time. Typically, 2,000–10,000 sample orbits is enough.
- As rule of thumb, use the two-body approximation for Ranging. The *n*-body corrections are usually only required for special cases such as collision-probability estimation.

3.3 Propagation of orbital elements from one epoch to another

The orbital-element PDF can be propagated to another epoch using the command

```
oorb --task=propagation --epoch-mjd-tt=MJD --orb-in=INFILE
  [ --orb-out=OUTFILE ]
```

The mode of propagation, that is, analytical two-body propagation or numerical *n*-body propagation using an integrator, can be defined in the configuration file. If --orb-out=OUTFILE is omitted, the resulting orbital-element PDF is written to standard out.

3.4 Computing ephemerides

Topocentric ephemerides and their uncertainties are computed based on the orbital-element PDF using the command

where CODE is the observatory code assigned by MPC and MJD is the Modified Julian Date of the desired ephemerides either in UTC or TT. DT1 is the timespan (in days) over which ephemerides should be computed when starting from the epoch of the orbital-elements and DT2 is the frequency

(in days) of the ephemerides. Positive values for DT1 and DT2 indicate going forwards in time from the epoch, whereas negative values indicate going backwards. The ephemeris prediction based on the sampled PDF is a discrete set of predicted positions on the sky and their individual weights, and the ephemeris prediction based on the single-point estimate is the nominal position with a 3- σ uncertainty ellipse. Note that the non-Gaussian uncertainty region equivalent to the Gaussian 3- σ region can also be obtained for the sampled prediction by normalizing the sum of the weights to unity and requiring that 99.73002% of the total weight (probability mass) is within the boundaries. The ephemerides are written to standard out.

3.5 Dynamical classification

For cases where the orbital-element PDF has been sampled, it is possible to classify the object in a dynamical sense by using the relative weight of sample orbits. The classification

```
oorb --task=classification --orb-in=INFILE
```

The results are written to standard output. The classification criteria can be changed by modifying the <code>getGroupProbabilities</code> subroutine in <code>StochastiOrbit_class.f90</code>. Note that the current implementation of the dynamical classification is only done in the osculating (a, e, i, q, Q) space, which means that, e.g., the classification of Jupiter Trojans is not carried out rigorously.

3.6 Conversion between file types

Use

```
oorb --task=mpctompc3 --obs-in=FILE1 [ --obs-out=FILE2]
```

to convert an observation file (FILE1) formatted according to the current MPC format to a file (FILE2) formatted according to the proposed new MPC format. Observational uncertainties are taken from the configuration file. If they are not defined, the default uncertainty is zero. Use

```
oorb --task=mpc3tompc --obs-in=FILE1 [ --obs-out=FILE2]
```

to convert an observation file (FILE1) formatted according to the proposed new MPC format to a file (FILE2) formatted according to the current MPC format. Note that information regarding observational uncertainties is lost during the conversion. Use

```
oorb --task=astorbtoorb --astorb=FILE1 [ --orb-out=FILE2]
```

to convert the orbital elements and the (H,G) values in Ted Bowell's astorb.dat file to the .orb format. Here FILE1 is the astorb.dat file and FILE2 is the output .orb file. Again, if FILE2 is omitted the output is sent to standard out.

3.7 Example

In the <code>OpenOrb/test/</code> directory you can find two almost identical observation files in the MPC format, <code>KO8K42V_ranging.mpc</code> and <code>KO8K42V_lsl.mpc</code>. The difference between these files is that in the previous file all but the three first observations have been commented out, whereas in the latter none are commented out.

First, compute a Ranging solution for observation set #1:

```
oorb --task=ranging --obs-in=K08K42V_ranging.mpc \
    --orb-out=K08K42V_ranging.orb
```

The output is written both in the form of an orbital-element PDF file called K08K42V_ranging.orb and a more general output file called K08K42V_ranging.sor. Moreover, two separate plots were also produced: K08K0042V_0.08_sor_keplerian_results.eps.gz shows the orbital-element PDF and K08K0042V_0.08_sor_residual_stamps.eps.gz shows stamps of the O-C residual distributions corresponding to each observation included in the inversion.

Then, use the orbits produced by Ranging to initiate the differential correction (LSL) using observation set #2:

```
oorb --task=lsl --obs-in=K08K42V_lsl.mpc \
    --orb-in=K08K42V_ranging.orb --orb-out=K08K42V_lsl.orb
```

Again, the output is written in the form of an orbital-element file called K08K42V_lsl.orb which contains the nominal orbit and the standard deviations and correlations for the elements, and a general output file called

K08K42V_lsl.1s. The nominal orbit and the 1- σ and the 3- σ uncertainty ellipsoids are shown in plot K08K0042V_37.80_ls_keplerian_results.eps.gz.

To make a dynamical classification of the object, do

```
oorb --task=classification --orb-in=KO8K42V_ranging.orb
```

The result strongly suggests that the object is something unknown to the current classification scheme and, in fact, the object is the first retrograde TNO discovered.

To propagate the orbital-element PDF to the current date (2008-08-12) epoch, do

```
oorb --task=propagation --orb-in=K08K42V_ranging.orb \
    --epoch-mjd-tt=54690 --orb-out=K08K42V_ranging_54690.orb
```

The file K08K42V_ranging_54690.orb contains the orbital-element PDF at the new epoch.

To compute follow-up ephemerides (topocentric distance, R.A., Dec., and their corresponding time derivatives) for 10 dates with one-day intervals starting at 2008-08-12.0 TT, use

```
oorb --task=ephemeris --orb-in=K08K42V_ranging_54690.orb \
    --timespan=10.0 --step=1.0
```

The ephemerides are written to standard out.

Developing your own applications based on OpenOrb

It is reasonably straightforward to develop your own applications in the OpenOrb framework due to the object-oriented approach. Although Fortran 90/95 is not a pure object-oriented language, we have mimicked object-oriented concepts in the software by using the guidelines by Decyk et al. (1997).

More to be added later if there is interest...

Communication

5.1 Getting help

Due to manpower limitations, we cannot promise to give personal assistance in all situations. It is assumed that the user is familiar with state-of-the-art orbit computation methods and Bayesian inversion theory through published literature (for reviews, see Virtanen 2005, Bowell et al. 2002, Virtanen et al. 2008). However, if you intend to publish results obtained with OpenOrb and have doubt regarding the interpretation of the results, we encourage you to contact either Mikael Granvik (mgranvik@iki.fi) or Jenni Virtanen (jenni.virtanen@fgi.fi) for assistance.

If needed, there may be help available for developing source code based on OpenOrb to solve more complicated orbit-computation-related problems. However, the help has a price, which is typically to be paid in the currency which our funding agencies understand and accept, that is, as a co-authorship in the resulting publication(s).

5.2 Reporting bugs

OpenOrb has been tested during the years by comparing the results to the results obtained with either our older software or by software by colleagues. If you nevertheless find a bug, please report it to us so that we can fix the problem. The report should be concise and contain everything needed for reproducing the erroneous result. Send the report to MG (mgranvik@iki.fi) with the text "OpenOrb bug" in the subject line.

5.3 Acknowledging the use of OpenOrb

If you find OpenOrb useful in your work, please acknowledge our efforts by citing, in addition to the relevant original papers, the following abstract (which will hopefully evolve into an ACM 2008 conference proceedings manuscript) on the OpenOrb software package:

Granvik, M., Virtanen, J., and Muinonen, K. (2008), 'OpenOrb: Open-source asteroid-orbit-computation software including statistical orbital ranging', Asteroids, Comets, Meteors 2008, Abstract #8206, CD-ROM, LPI Contribution No. 1405.

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