# gvar Documentation

Release 7.3.1

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**CHAPTER** 

ONE

### **OVERVIEW AND TUTORIAL**

### 1.1 Introduction

This module provides tools for representing, manipulating, and simulating Gaussian random variables numerically. It can deal with individual variables or arbitrarily large sets of variables, correlated or uncorrelated. It also supports complicated (Python) functions of Gaussian variables, automatically propagating uncertainties and correlations through the functions.

A Gaussian variable x represents a Gaussian probability distribution, and is therefore completely characterized by its mean x.mean and standard deviation x.sdev. They are used to represent quantities whose values are uncertain: for example, the mass,  $125.7\pm0.4$  GeV, of the recently discovered Higgs boson from particle physics. The following code illustrates a (very) simple application of gvar; it calculates the Higgs boson's energy when it carries momentum  $50\pm0.15$  GeV.

```
>>> import gvar as gv

>>> m = gv.gvar(125.7, 0.4)  # Higgs boson mass

>>> p = gv.gvar(50, 0.15)  # Higgs boson momentum

>>> E = (p ** 2 + m ** 2) ** 0.5  # Higgs boson energy

>>> print(m, E)

125.70(40) 135.28(38)

>>> print(E.mean, '+-', E.sdev)

135.279303665 +- 0.375787639425
```

Here method gvar.gvar() creates objects m and p of type gvar.GVar that represent Gaussian random variables for the Higgs mass and momentum, respectively. The energy E computed from the mass and momentum must, like them, be uncertain and so is also an object of type gvar.GVar — with mean E.mean=135.28 and standard deviation E.sdev=0.38. (Note that gvar uses the compact notation 135.28(38) to represent a Gaussian variable, where the number in parentheses is the uncertainty in the corresponding rightmost digits of the quoted mean value.)

A highly nontrivial feature of gvar. GVars is that they automatically track statistical correlations between different Gaussian variables. In the Higgs boson code above, for example, the uncertainty in the energy is due mostly to the initial uncertainty in the boson's mass. Consequently statistical fluctuations in the energy are strongly correlated with those in the mass, and largely cancel, for example, in the ratio:

```
>>> print (E / m)
1.07621(64)
```

The ratio is 4–5 times more accurate than the either the mass or energy separately.

The correlation between m and E is obvious from their covariance and correlation matrices, both of which have large off-diagonal elements:

The correlation matrix shows that there is a 98.9% statistical correlation between the mass and energy.

A extreme example of correlation arises if we reconstruct the Higgs boson's mass from its energy and momentum:

```
>>> print((E ** 2 - p ** 2) / m ** 2)
1 +- 1.4e-18
```

The numerator and denominator are completely correlated, indeed identical to machine precision, as they should be. This works only because *gvar.GVar* object E knows that its uncertainty comes from the uncertainties associated with variables m and p.

We can verify that the uncertainty in the Higgs boson's energy comes mostly from its mass by creating an *error budget* for the Higgs energy (and for its energy to mass ratio):

For each output (E and E/m), the error budget lists the contribution to the total uncertainty coming from each of the inputs (m and p). The total uncertainty in the energy is  $\pm 0.28\%$ , and almost all of that comes from the mass — only  $\pm 0.04\%$  comes from the uncertainty in the momentum. The two sources of uncertainty contribute equally, however, to the ratio E/m, which has a total uncertainty of only 0.06%.

This example is relatively simple. Module gvar, however, can easily handle thousands of Gaussian random variables and all of their correlations. These can be combined in arbitrary arithmetic expressions and/or fed through complicated (pure) Python functions, while the gvar. GVars automatically track uncertainties and correlations for and between all of these variables. The code for tracking correlations is the most complex part of the module's design, particularly since this is done automatically, behind the scenes.

What follows is a tutorial showing how to create gvar. GVars and manipulate them to solve common problems in error propagation. Another way to learn about gvar is to look at the case studies later in the documentation. Each focuses on a single problem, and includes the full code and data, to allow for further experimentation.

gvar was originally written for use by the lsqfit module, which does multidimensional (Bayesian) least-squares fitting. It used to be distributed as part of lsqfit, but is now distributed separately because it is used by other modules (e.g., vegas for multidimensional Monte Carlo integration).

About Printing: The examples in this tutorial use the print function as it is used in Python 3. Drop the outermost parenthesis in each print statement if using Python 2; or add

```
from __future__ import print_function
```

at the start of your file.

### 1.2 Gaussian Random Variables

The Higgs boson mass ( $125.7\pm0.4~GeV$ ) from the previous section is an example of a Gaussian random variable. As discussed above, such variables x represent Gaussian probability distributions, and therefore are completely characterized by their mean x.mean and standard deviation x.sdev. A mathematical function f(x) of a Gaussian variable is defined as the probability distribution of function values obtained by evaluating the function for random numbers drawn from the original distribution. The distribution of function values is itself approximately Gaussian provided the standard deviation x.sdev of the Gaussian variable is sufficiently small. Thus we can define a function f of a Gaussian variable x to be a Gaussian variable itself, with

```
f(x).mean = f(x.mean)

f(x).sdev = x.sdev | f'(x.mean) |,
```

which follows from linearizing the x dependence of f(x) about point x.mean. This formula, together with its multidimensional generalization, lead to a full calculus for Gaussian random variables that assigns Gaussian-variable values to arbitrary arithmetic expressions and functions involving Gaussian variables. This calculus, which is built into gvar, provides the rules for standard error propagation — an important application of Gaussian random variables and of the gvar module.

A multidimensional collection x[i] of Gaussian variables is characterized by the means x[i] .mean for each variable, together with a covariance matrix cov[i, j]. Diagonal elements of cov specify the standard deviations of different variables: x[i].sdev = cov[i, i]\*\*0.5. Nonzero off-diagonal elements imply correlations (or anti-correlations) between different variables:

```
cov[i, j] = \langle x[i] * x[j] \rangle - \langle x[i] \rangle * \langle x[j] \rangle
```

where <y> denotes the expectation value or mean for a random variable y.

# 1.3 Creating Gaussian Variables

Objects of type gvar.GVar are of two types: 1) primary gvar.GVars that are created from means and covariances using gvar.gvar(); and 2) derived gvar.GVars that result from arithmetic expressions or functions involving gvar.GVars. The primary gvar.GVars are the primordial sources of all uncertainties in a gvar code. A single (primary) gvar.GVar is created from its mean xmean and standard deviation xsdev using:

```
x = gvar.gvar(xmean, xsdev).
```

This function can also be used to convert strings like "-72.374 (22)" or "511.2 +- 0.3" into gvar. GVars: for example,

```
>>> import gvar
>>> x = gvar.gvar(3.1415, 0.0002)
>>> print(x)
3.14150(20)
>>> x = gvar.gvar("3.1415(2)")
>>> print(x)
3.14150(20)
>>> x = gvar.gvar("3.1415 +- 0.0002")
>>> print(x)
3.14150(20)
```

Note that x = gvar.gvar(x) is useful when you are unsure whether x is initially a gvar.GVar or a string representing a gvar.GVar.

gvar. GVars are usually more interesting when used to describe multidimensional distributions, especially if there are correlations between different variables. Such distributions are represented by collections of gvar. GVars in

one of two standard formats: 1) numpy arrays of gvar. GVars (any shape); or, more flexibly, 2) Python dictionaries whose values are gvar. GVars or arrays of gvar. GVars. Most functions in gvar that handle multiple gvar. GVars work with either format, and if they return multidimensional results do so in the same format as the inputs (that is, arrays or dictionaries). Any dictionary is converted internally into a specialized (ordered) dictionary of type gvar. BufferDict, and dictionary-valued results are also gvar. BufferDicts.

To create an array of gvar. GVars with mean values specified by array xmean and covariance matrix xcov, use

```
x = gvar.gvar(xmean, xcov)
```

where array x has the same shape as xmean (and xcov.shape = xmean.shape+xmean.shape). Then each element x[i] of a one-dimensional array, for example, is a gvar.GVar where:

```
x[i].mean = xmean[i]  # mean of x[i]
x[i].val = xmean[i]  # same as x[i].mean
x[i].sdev = xcov[i, i]**0.5  # std deviation of x[i]
x[i].var = xcov[i, i]  # variance of x[i]
```

As an example,

makes x and y gvar.GVars with standard deviations  $sigma_x=0.125$  and  $sigma_y=2$ , and a fairly strong statistical correlation:

Here functions gvar.evalcov() and gvar.evalcorr() compute the covariance and correlation matrices, respectively, of the list of gvar.GVars in their arguments.

gvar.gvar() can also be used to convert strings or tuples stored in arrays or dictionaries into gvar.GVars: for example,

```
>>> garray = gvar.gvar(['2(1)', '10+-5', (99, 3), gvar.gvar(0, 2)])
>>> print(garray)
[2.0(1.0) 10.0(5.0) 99.0(3.0) 0.0(2.0)]
>>> gdict = gvar.gvar(dict(a='2(1)', b=['10+-5', (99, 3), gvar.gvar(0, 2)]))
>>> print(gdict)
{'a': 2.0(1.0),'b': array([10.0(5.0), 99.0(3.0), 0.0(2.0)], dtype=object)}
```

If the covariance matrix in gvar.gvar is diagonal, it can be replaced by an array of standard deviations (square roots of diagonal entries in cov). The example above without correlations, therefore, would be:

# 1.4 gvar. GVar Arithmetic and Functions

The gvar. GVars discussed in the previous section are all primary gvar. GVars since they were created by specifying their means and covariances explicitly, using gvar.gvar(). What makes gvar. GVars particularly useful is that they can be used in arithemtic expressions (and numeric pure-Python functions), just like Python floats. Such expressions result in new, derived gvar. GVars whose means, standard deviations, and correlations are determined from the covariance matrix of the primary gvar. GVars. The automatic propagation of correlations through arbitrarily complicated arithmetic is an especially useful feature of gvar. GVars.

As an example, again define

```
>>> x, y = gvar.gvar([0.1, 10.], [0.125, 2.])
```

and set

```
>>> f = x + y
>>> print('f =', f)
f = 10.1(2.0)
```

Then f is a (derived) gvar. GVar whose variance f.var equals

```
df/dx cov[0, 0] df/dx + 2 df/dx cov[0, 1] df/dy + ... = 2.0039**2
```

where cov is the original covariance matrix used to define x and y (in gvar.gvar). Note that while f and y separately have 20% uncertainties in this example, the ratio f/y has much smaller errors:

```
>>> print(f / y)
1.010(13)
```

This happens, of course, because the errors in f and g are highly correlated — the error in f comes mostly from g. gvar. gvars automatically track correlations even through complicated arithmetic expressions and functions: for example, the following more complicated ratio has a still smaller error, because of stronger correlations between numerator and denominator:

The *gvar* module defines versions of the standard Python mathematical functions that work with *gvar*. *GVar* arguments. These include: exp, log, sqrt, sin, cos, tan, arcsin, arccos, arctan, arctan2, sinh, cosh, tanh, arcsinh, arccosh, arctanh, erf. Numeric functions defined entirely in Python (*i.e.*, pure-Python functions) will likely also work with *gvar*. *GVars*.

Numeric functions implemented by modules using low-level languages like C will *not* work with *gvar.GVars*. Such functions must be replaced by equivalent code written directly in Python. In some cases it is possible to construct a *gvar.GVar*-capable function from low-level code for the function and its derivative. For example, the following code defines a new version of the standard Python error function that accepts either floats or *gvar.GVars* as its argument:

```
import math
import gvar

def erf(x):
    if isinstance(x, gvar.GVar):
```

```
f = math.erf(x.mean)
  dfdx = 2. * math.exp(- x.mean ** 2) / math.sqrt(math.pi)
  return gvar.gvar_function(x, f, dfdx)
else:
  return math.erf(x)
```

Here function  $gvar\_function()$  creates the  $gvar\_GVar$  for a function with mean value f and derivative dfdx at point x. A more complete version of erf is included in gvar.

Some sample numerical analysis codes, adapted for use with gvar. GVars, are described in Numerical Analysis Modules in gvar.

Arithmetic operators + - \* / \*\* == != <> += -= \*= /= are all defined for gvar.GVars. Comparison operators are also supported: == != >> = <=. They are applied to the mean values of gvar.GVars: for example, gvar.gvar(1,1) == gvar.var(1,2) is true, as is gvar.gvar(1,1) > 0. Logically x>y for gvar.GVars should evaluate to a boolean-valued random variable, but such variables are beyond the scope of this module. Comparison operators that act only on the mean values make it easier to implement pure-Python functions that work with either gvar.GVars or floats as arguments.

Implementation Notes: Each gvar. GVar keeps track of three pieces of information: 1) its mean value; 2) its derivatives with respect to the primary gvar. GVars (created by gvar. gvar()); and 3) the location of the covariance matrix for the primary gvar. GVars. The derivatives and covariance matrix allow one to compute the standard deviation of the gvar. GVar, as well as correlations between it and any other function of the primary gvar. GVars. The derivatives for derived gvar. GVars are computed automatically, using automatic differentiation.

The derivative of a gvar.GVar f with respect to a primary gvar.GVar x is obtained from f.deriv(x). A list of derivatives with respect to all primary gvar.GVars is given by f.der, where the order of derivatives is the same as the order in which the primary gvar.GVars were created.

A gvar. GVar can be constructed at a very low level by supplying all the three essential pieces of information — for example,

```
f = gvar.gvar(fmean, fder, cov)
```

where fmean is the mean, fder is an array where fder[i] is the derivative of f with respect to the i-th primary gvar. GVar (numbered in the order in which they were created using gvar.gvar()), and cov is the covariance matrix for the primary gvar. GVars (easily obtained from an existing gvar. GVar x using x.cov).

# 1.5 Error Budgets from gvar. GVars

It is sometimes useful to know how much of the uncertainty in a derived quantity is due to a particular input uncertainty. Continuing the example above, for example, we might want to know how much of fs standard deviation is due to the standard deviation of f and how much comes from f. This is easily computed:

```
>>> x, y = gvar.gvar([0.1, 10.], [0.125, 2.])
>>> f = x + y
>>> print(f.partialsdev(x))  # uncertainty in f due to x
0.125
>>> print(f.partialsdev(y))  # uncertainty in f due to y
2.0
>>> print(f.partialsdev(x, y))  # uncertainty in f due to x and y
2.00390244274
>>> print(f.sdev)  # should be the same
2.00390244274
```

This shows, for example, that most (2.0) of the uncertainty in £ (2.0039) is from y.

gvar provides a useful tool for compiling an "error budget" for derived gvar. GVars relative to the primary qvar. GVars from which they were constructed: continuing the example above,

```
>>> outputs = {'f':f, 'f/y':f/y}
>>> inputs = {'x':x, 'y':y}
>>> print (gvar.fmt_values(outputs))
Values:
                f/y: 1.010(13)
                  f: 10.1(2.0)
>>> print(gvar.fmt_errorbudget(outputs=outputs, inputs=inputs))
Partial % Errors:
                 f/y
                              f
                0.20
                         19.80
        у:
                          1.24
                1.24
        х:
                1.25
                          19.84
    total:
```

This shows y is responsible for 19.80% of the 19.84% uncertainty in f, but only 0.2% of the 1.25% uncertainty in f/y. The total uncertainty in each case is obtained by adding the x and y contributions in quadrature.

# 1.6 Storing gvar. GVars for Later Use; gvar. BufferDicts

Storing gvar. GVars in a file for later use is complicated by the need to capture the covariances between different gvar. GVars as well as their means. To pickle an array or dictionary g of gvar. GVars, for example, we might use

```
>>> gtuple = (gvar.mean(g), gvar.evalcov(g))
>>> import pickle
>>> pickle.dump(gtuple, open('outputfile.p', 'wb'))
```

to extract the means and covariance matrix into a tuple which then is saved in file 'output.p' using Python's standard pickle module. To reassemble the *qvar.GVars* we use:

```
>>> g = gvar.gvar(pickle.load('outputfile.p', 'rb'))
```

where pickle.load() reads gtuple back in, and <code>gvar.gvar()</code> converts it back into a collection of <code>gvar.GVars</code>. The correlations between different <code>gvar.GVars</code> in the original array/dictionary g are preserved here, but their correlations with other <code>gvar.GVars</code> are lost. So it is important to include all <code>gvar.GVars</code> of interest in a single array or dictionary before saving them.

This recipe works for gs that are: single gvar. GVars, arrays of gvar. GVars (any shape), or dictionaries whose values are gvar. GVars and/or arrays of gvar. GVars. For convenience, it is implemented in functions gvar.dump(), gvar.dumps(), gvar.load(), and gvar.loads().

Pickling is simplified if the *gvar.GVars* that need saving are all in a *gvar.BufferDict* since these can be serialized and saved to a file again using Python's pickle module. So if g is a *gvar.BufferDict* containing *gvar.GVars* (and/or arrays of *gvar.GVars*),

```
>>> import pickle
>>> pickle.dump(g, open('outputfile.p', 'wb'))
```

saves the contents of q to a file named outputfile.p. The qvar. GVars are retrieved using:

```
>>> g = pickle.load(open('outputfile.p', 'rb'))
```

gvar.BufferDicts also have methods that allow saving their contents using Python's json module rather than pickle.

# 1.7 Non-Gaussian Expectation Values

By default functions of *gvar.GVars* are also *gvar.GVars*, but there are cases where such functions cannot be represented accurately by Gaussian distributions. The product of 0.1(4) and 0.2(5), for example, is not very Gaussian because the standard deviations are large compared to the scale over which the product changes appreciably. In such cases one may want to use the true distribution of the function, instead of its Gaussian approximation, in an analysis.

Class gvar.PDFIntegrator evaluates integrals over multi-dimensional Gaussian probability density functions (PDFs) using the vegas module, which does adaptive multi-dimensional integration. This permits us, for example, to calculate the true mean and standard deviation of a function of Gaussian variables, or to test the extent to which the true distribution of the function is Gaussian. The following code analyzes the distribution of sin(p[0] \* p[1]) where p = [0.1(4), 0.2(5)]:

```
import numpy as np
import gvar as gv
p = gv.gvar(['0.1(4)', '0.2(5)'])
# function of interest
def f(p):
   return np.sin(p[0] * p[1])
# histogram for values of f(p)
fhist = gv.PDFHistogram(f(p), nbin=16)
# want expectation value of fstats(p)
def fstats(p):
    fp = f(p)
    return dict(
        moments=[fp, fp ** 2, fp ** 3, fp ** 4],
        histogram=fhist.count(fp),
        )
# evaluate expectation value of fstats in 3 steps
# 1 - create an integrator to evaluate expectation values of functions of p
p_expval = gv.PDFIntegrator(p)
\# 2 - adapt p_expval to the p's PDF (N.B., no function specified)
p_expval(neval=5000, nitn=10)
# 3 - evaluate expectation value of function(s) fhist(p)
results = p_expval(fstats, neval=5000, nitn=10, adapt=False)
# results from expectation value integration
print (results.summary())
print('moments:', results['moments'])
stats = qv.PDFStatistics(
   moments=results['moments'],
   histogram=(fhist.bins, results['histogram']),
print('Statistics from Bayesian integrals:')
print(stats)
print('Gaussian approx:', f(p))
# plot histogram from integration (plt = matplotlib.pyplot)
plt = fhist.make_plot(results['histogram'])
plt.xlabel(r'$\sin(p_0 p_1)$')
plt.xlim(-1, 1)
# add extra curve corresponding to Gaussian with "correct" mean and sdev
correct_fp = gv.gvar(stats.mean.mean, stats.sdev.mean)
```

```
x = np.linspace(-1.,1.,50)
pdf = gv.PDF(correct_fp)
y = [pdf(xi) * fhist.widths[0] for xi in x]
plt.plot(x, y, 'k:')
plt.show()
```

The key construct here is p\_expval which is a vegas integrator designed so that p\_expval(f) returns the expectation value of any function f(p) with respect to the probability distribution specified by p = gv.gvar(['0.1(4)', '0.2(5)']). The integrator is adaptive so it is called once without a function, to allow it to adapt to the probability density function (PDF). It is then applied to function fstats(p), which calculates various moments of f(p) as well as information for histogramming values of f(p) (using gvar.PDFHistogram). Parameters nitn and neval control the multidimensional integrator, telling it how many iterations of its adaptive algorithm to use and the maximum number of integrand evaluations to use in each iteration.

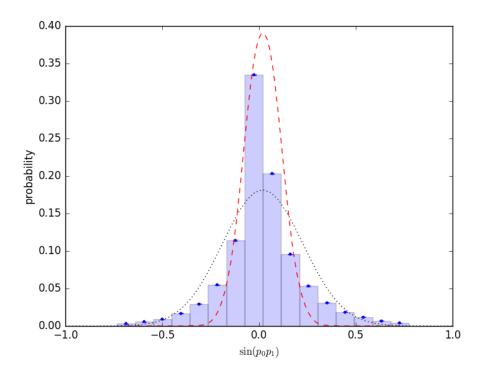
The output from this code is:

```
itn
      integral
                                       chi2/dof
                                                         Q
                       average
  1
      1.00032(90)
                                            0.00
                       1.00032(90)
                                                     1.00
  2.
      0.9992(10)
                       0.99976(69)
                                            1.10
                                                     0.33
  3
      0.9987(10)
                       0.99942 (57)
                                            0.97
                                                     0.53
      1.00058(92)
                       0.99971(49)
                                            0.89
                                                     0.74
  5
      0.99992(99)
                       0.99975(44)
                                            0.91
                                                     0.73
                                            0.92
                                                     0.71
  6
      1.00059(99)
                       0.99989(40)
  7
      0.99830(96)
                       0.99966(37)
                                            0.90
                                                     0.80
  8
      1.00201(88)
                       0.99996(34)
                                            0.91
                                                     0.77
  9
      0.9977(12)
                       0.99971(33)
                                            0.89
                                                     0.86
10
      0.9996(10)
                       0.99970(32)
                                            0.84
                                                     0.95
moments: [0.01862(13) 0.043161(90) 0.004672(80) 0.011470(72)]
Statistics from Bayesian integrals:
   mean = 0.01862(13) sdev = 0.20692(21)
                                               skew = 0.2567(75)
                                                                    ex_kurt = 3.116(20)
   median = 0.00017(14)
                           plus = 0.17397(49)
                                                 minus = 0.11705(43)
Gaussian approx: 0.020(94)
```

The table summarizes the integrator's performance over the nitn=10 iterations it performed to obtain the final results; see the vegas documentation for further information. The expectation values for moments of f(p) are then listed, followed by the mean and standard deviation computed from these moments, as well as the skewness and excess kurtosis of the f(p) distribution. The median value for the distribution is estimated from the histogram, as are the intervals on either side of the median ((median-minus, median) and (median, median+plus)) containing 34% of the probability. Finally the mean and standard deviation in the Gaussian approximate are listed.

The exact mean of the f(p) distribution is 0.0186(1), which is somewhat lower than Gaussian approximation of 0.020. A more important difference is in the standard deviation which is 0.2072(3) for the real distribution, but less than half that size (0.094) in the Gaussian approximation. The real distribution is significantly broader than the Gaussian approximation suggests, though its mean is close. The real distribution also has nonzero skewness (0.28(1)) and excess kurtosis (3.11(2)), which suggest that it is not well described by any Gaussian. (Skewness and excess kurtosis vanish for Gaussian distributions.)

The code also displays a histogram showing the probability distribution for values of f (p):



This shows the actual probability associated with each f(p) bin, together with the shape (red dashed line) expected from the Gaussian approximation (0.020(94)). It also shows the Gaussian distribution corresponding to correct mean and standard deviation (0.186(207)) of the distribution (black dotted line).

Neither Gaussian in this plot is quite right: the first is more accurate close to the maximimum, while the second does better further out. From the histogram we can estimate that 68% of the probability lies within  $\pm 0.14$  of 0.03, which is probably the best succinct characterization of the uncertainty (0.03 (14)).

This example is relatively simple since the underlying Gaussian distribution is only two dimensional. The vegas integrator used here is adaptive and so can function effectively even for high dimensions (10, 20, 50 ... Gaussian variables). High dimensions usually cost more, requiring many more function evaluations (neval).

### 1.8 Random Number Generators and Simulations

gvar. GVars represent probability distributions. It is possible to use them to generate random numbers from those distributions. For example, in

```
>>> z = gvar.gvar(2.0, 0.5)
>>> print(z())
2.29895701465
>>> print(z())
3.00633184275
>>> print(z())
1.92649199321
```

calls to z () generate random numbers from a Gaussian random number generator with mean z.mean=2.0 and standard deviation z.sdev=0.5.

To obtain random arrays from an array g of gvar. GVars use giter=gvar.raniter(g) (see gvar.raniter()) to create a random array generator giter. Each call to next(giter) generates a new

array of random numbers. The random number arrays have the same shape as the array g of gvar. GVars and have the distribution implied by those random variables (including correlations). For example,

```
>>> a = gvar.gvar(1.0, 1.0)

>>> da = gvar.gvar(0.0, 0.1)

>>> g = [a, a+da]

>>> giter = gvar.raniter(g)

>>> print(next(giter))

[ 1.51874589    1.59987422]

>>> print(next(giter))

[-1.39755111 -1.24780937]

>>> print(next(giter))

[ 0.49840244    0.50643312]
```

Note how the two random numbers separately vary over the region  $1\pm1$  (approximately), but the separation between the two is rarely more than  $0\pm0.1$ . This is as expected given the strong correlation between a and a+da.

gvar.raniter(g) also works when g is a dictionary (or gvar.BufferDict) whose entries g[k] are gvar.GVars or arrays of gvar.GVars. In such cases the iterator returns a dictionary with the same layout:

```
>>> g = dict(a=gvar.gvar(0, 1), b=[gvar.gvar(0, 100), gvar.gvar(10, 1e-3)])
>>> print(g)
{'a': 0.0(1.0), 'b': [0(100), 10.0000(10)]}
>>> giter = gvar.raniter(g)
>>> print(next(giter))
{'a': -0.88986130981173306, 'b': array([-67.02994213, 9.99973707])}
>>> print(next(giter))
{'a': 0.21289976681277872, 'b': array([ 29.9351328 , 10.00008606])}
```

One use for such random number generators is dealing with situations where the standard deviations are too large to justify the linearization assumed in defining functions of Gaussian variables. Consider, for example,

```
>>> x = gvar.gvar(1., 3.)
>>> print(cos(x))
0.5(2.5)
```

The standard deviation for  $\cos(x)$  is obviously wrong since  $\cos(x)$  can never be larger than one. We can estimate the the real mean and standard deviation using a simulation. To do this, we: 1) generate a large number of random numbers xi from x; 2) compute  $\cos(xi)$  for each; and 3) compute the mean and standard deviation for the resulting distribution (or any other statistical quantity, particularly if the resulting distribution is not Gaussian):

This procedure generalizes trivially for multidimensional analyses, using arrays or dictionaries with gvar.raniter().

Note finally that *bootstrap* copies of gvar.GVars are easily created. A bootstrap copy of  $gvar.GVar \times \pm dx$  is another gvar.GVar with the same width but where the mean value is replaced by a random number drawn from the original distribution. Bootstrap copies of a data set, described by a collection of gvar.GVars, can be used as new (fake) data sets having the same statistical errors and correlations:

```
>>> g = gvar.gvar([1.1, 0.8], [[0.01, 0.005], [0.005, 0.01]])
>>> print(g)
[1.10(10) 0.80(10)]
>>> print (gvar.evalcov(g))
                                             # print covariance matrix
[[ 0.01
        0.005]
[ 0.005 0.01 ]]
>>> gbs_iter = gvar.bootstrap_iter(g)
>>> gbs = next(gbs_iter)
                                             # bootstrap copy of f
>>> print (gbs)
[1.14(10) 0.90(10)]
                                             # different means
>>> print (gvar.evalcov(gbs))
[[ 0.01 0.005]
                                             # same covariance matrix
[ 0.005 0.01 ]]
```

Such fake data sets are useful for analyzing non-Gaussian behavior, for example, in nonlinear fits.

### 1.9 Limitations

The most fundamental limitation of this module is that the calculus of Gaussian variables that it assumes is only valid when standard deviations are small (compared to the distances over which the functions of interest change appreciably). One way of dealing with this limitation is to use simulations, as discussed in *Random Number Generators and Simulations*.

Another potential issue is roundoff error, which can become problematic if there is a wide range of standard deviations among correlated modes. For example, the following code works as expected:

```
>>> from gvar import gvar, evalcov
>>> tiny = 1e-4
>>> a = gvar(0., 1.)
>>> da = gvar(tiny, tiny)
>>> a, ada = gvar([a.mean, (a+da).mean], evalcov([a, a+da])) # = a,a+da
>>> print(ada-a) # should be da again
0.00010(10)
```

Reducing tiny, however, leads to problems:

```
>>> from gvar import gvar, evalcov
>>> tiny = 1e-8
>>> a = gvar(0., 1.)
>>> da = gvar(tiny, tiny)
>>> a, ada = gvar([a.mean, (a+da).mean], evalcov([a, a+da])) # = a, a+da
>>> print(ada-a) # should be da again
1(0)e-08
```

Here the call to <code>gvar.evalcov()</code> creates a new covariance matrix for a and <code>ada = a+da</code>, but the matrix does not have enough numerical precision to encode the size of <code>da</code>'s variance, which gets set, in effect, to zero. The problem arises here for values of <code>tiny</code> less than about 2e-8 (with 64-bit floating point numbers — <code>tiny\*\*2</code> is what appears in the covariance matrix).

# 1.10 Optimizations

When there are lots of primary gvar. GVars, the number of derivatives stored for each derived gvar. GVar can become rather large, potentially (though not necessarily) leading to slower calculations. One way to alleviate this problem, should it arise, is to separate the primary variables into groups that are never mixed in calculations and to

use different gvar.gvar()s when generating the variables in different groups. New versions of gvar.gvar() are obtained using  $gvar.switch\_gvar()$ : for example,

```
import gvar
...
x = gvar.gvar(...)
y = gvar.gvar(...)
z = f(x, y)
... other manipulations involving x and y ...
gvar.switch_gvar()
a = gvar(...)
b = gvar(...)
c = g(a, b)
... other manipulations involving a and b (but not x and y) ...
```

Here the <code>gvar.gvar()</code> used to create a and <code>b</code> is a different function than the one used to create <code>x</code> and <code>y</code>. A derived quantity, like <code>c</code>, knows about its derivatives with respect to <code>a</code> and <code>b</code>, and about their covariance matrix; but it carries no derivative information about <code>x</code> and <code>y</code>. Absent the <code>switch\_gvar</code> line, <code>c</code> would have information about its derivatives with respect to <code>x</code> and <code>y</code> (zero derivative in both cases) and this would make calculations involving <code>c</code> slightly slower than with the <code>switch\_gvar</code> line. Usually the difference is negligible — it used to be more important, in earlier implementations of <code>gvar.GVar</code> before sparse matrices were introduced to keep track of covariances. Note that the previous <code>gvar.gvar()</code> can be restored using <code>gvar.restore\_gvar()</code>.

### **GVAR - GAUSSIAN RANDOM VARIABLES**

### 2.1 Introduction

Objects of type gvar. GVar represent gaussian random variables, which are specified by a mean and standard deviation. They are created using gvar. gvar(): for example,

```
>>> x = gvar.gvar(10,3) # 0 +- 3

>>> y = gvar.gvar(12,4) # 2 +- 4

>>> z = x + y # 2 +- 5

>>> print(z)

22.0(5.0)

>>> print(z.mean)

22.0

>>> print(z.sdev)

5.0
```

This module contains a variety of tools for creating and manipulating gaussian random variables, including:

- mean (g) extract means.
- sdev (g) extract standard deviations.
- var (g) extract variances.
- fmt (g) replace all gvar. GVars in array/dictionary by string representations.
- tabulate(g) tabulate entries in array/dictionary of gvar. GVars.
- correlate(g, corr) add correlations to gvar. GVars in array/dictionary g.
- chi2(g1, g2) chi\*\*2 of g1-g2.
- equivalent (q1, q2) gvar. GVars the same in q1 and q2?
- evalcov (g) compute covariance matrix.
- evalcorr(g) compute correlation matrix.
- fmt\_values(g) list values for printing.
- fmt\_errorbudget (g) create error-budget table for printing.
- fmt\_chi2 (f) format chi\*\*2 information in f as string for printing.
- class <code>BufferDict</code> ordered dictionary with data buffer.
- class *PDF* probability density function.
- class PDFIntegrator integrator for probability density functions.
- $\bullet \ class \ {\it PDFStatistics} -- statistical \ analysis \ of \ moments \ of \ a \ random \ variable. \\$

- class PDFHistogram tool for building PDF histograms.
- dump (g, outputfile) pickle a collection of gvar. GVars in file.
- dumps (g) pickle a collection of gvar. GVars in a string.
- load (inputfile) reconstitute a collection of gvar. GVars from a file.
- loads (inputstr) reconstitute a collection of gvar. GVars from a string.
- raniter (g, N) iterator for random numbers.
- bootstrap\_iter(g, N) bootstrap iterator.
- svd (q) SVD modification of correlation matrix.
- dataset.bin\_data(data) bin random sample data.
- dataset.avg\_data(data) estimate means of random sample data.
- dataset.bootstrap\_iter(data, N) bootstrap random sample data.
- class dataset. Dataset class for collecting random sample data.

### 2.2 Functions

The function used to create Gaussian variable objects is:

```
gvar.gvar(...)
```

Create one or more new gvar. GVars.

Each of the following creates new gvar. GVars:

```
gvar.gvar(x, xsdev)
```

Returns a gvar.GVar with mean x and standard deviation xsdev. Returns an array of gvar.GVars if x and xsdev are arrays with the same shape; the shape of the result is the same as the shape of x. Returns a gvar.BufferDict if x and xsdev are dictionaries with the same keys and layout; the result has the same keys and layout as x.

```
gvar.gvar(x, xcov)
```

Returns an array of gvar.GVars with means given by array x and a covariance matrix given by array xcov, where xcov.shape =  $2 \times x.shape$ ; the result has the same shape as x. Returns a gvar.BufferDict if x and xcov are dictionaries, where the keys in xcov are (k1,k2) for any keys k1 and k2 in x. Returns a single gvar.GVar if x is a number and xcov is a one-by-one matrix. The layout for xcov is compatible with that produced by gvar.evalcov() for a single gvar.GVar, an array of gvar.GVars, or a dictionary whose values are gvar.GVars and/or arrays of gvar.GVars. Therefore gvar.gvar(gvar.mean(g), gvar.evalcov(g)) creates gvar.GVars with the same means and covariance matrix as the gvar.GVars in g provided g is a single gvar.GVar, or an array or dictionary of gvar.GVars.

```
gvar.gvar((x, xsdev))
```

Returns a gvar. GVar with mean x and standard deviation xsdev.

```
gvar.gvar(xstr)
```

Returns a *gvar.GVar* corresponding to string xstr which is either of the form "xmean +- xsdev" or "x (xerr) " (see *GVar.fmt* ()).

```
gvar.gvar (xgvar)
```

Returns gvar. GVar xgvar unchanged.

```
gvar.gvar(xdict)
```

Returns a dictionary (BufferDict) b where b[k] = gvar(xdict[k]) for every key in dictionary xdict. The values in xdict, therefore, can be strings, tuples or gvar.GVars (see above), or arrays of these.

```
gvar.gvar(xarray)
```

Returns an array a having the same shape as xarray where every element a[i...] = gvar(xarray[i...]). The values in xarray, therefore, can be strings, tuples or gvar.GVars (see above).

gvar.gvar is actually an object of type gvar.GVarFactory.

The following function is useful for constructing new functions that can accept gvar. GVars as arguments:

```
gvar.gvar_function (x, f, dfdx)
```

Create a gvar.GVar for function f(x) given f and df/dx at x.

This function creates a <code>gvar.GVar</code> corresponding to a function of <code>gvar.GVars</code> x whose value is f and whose derivatives with respect to each x are given by <code>dfdx</code>. Here x can be a single <code>gvar.GVars</code>, an array of <code>gvar.GVars</code> (for a multidimensional function), or a dictionary whose values are <code>gvar.GVars</code> or arrays of <code>gvar.GVars</code>, while <code>dfdx</code> must be a float, an array of floats, or a dictionary whose values are floats or arrays of floats, respectively.

This function is useful for creating functions that can accept gvar. GVars as arguments. For example,

```
import math
import gvar as gv

def sin(x):
    if isinstance(x, gv.GVar):
        f = math.sin(x.mean)
        dfdx = math.cos(x.mean)
        return gv.gvar_function(x, f, dfdx)
    else:
        return math.sin(x)
```

creates a version of sin(x) that works with either floats or gvar.GVars as its argument. This particular function is unnecessary since it is already provided by gvar.

#### **Parameters**

- **x** (*gvar. GVar*, array of *gvar. GVars*, or a dictionary of *gvar. GVars*) Point at which the function is evaluated.
- **f** (*float*) Value of function at point gvar.mean(x).
- **dfdx** (*float*, *array of floats*, *or a dictionary of floats*) Derivatives of function with respect to x at point gvar.mean(x).

**Returns** A gvar. GVar representing the function's value at x.

Means, standard deviations, variances, formatted strings, covariance matrices and correlation/comparison information can be extracted from arrays (or dictionaries) of gvar. GVars using:

```
gvar.mean(g)
```

Extract means from gvar. GVars in g.

g can be a gvar. GVar, an array of gvar. GVars, or a dictionary containing gvar. GVars or arrays of gvar. GVars. Result has the same layout as g.

Elements of g that are not gvar. GVars are left unchanged.

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#### qvar.sdev(g)

Extract standard deviations from gvar. GVars in g.

g can be a gvar. GVar, an array of gvar. GVars, or a dictionary containing gvar. GVars or arrays of gvar. GVars. Result has the same layout as g.

The deviation is set to 0.0 for elements of g that are not gvar. GVars.

#### gvar.var(g)

Extract variances from gvar. GVars in q.

g can be a gvar. GVar, an array of gvar. GVars, or a dictionary containing gvar. GVars or arrays of gvar. GVars. Result has the same layout as q.

The variance is set to 0.0 for elements of g that are not gvar. GVars.

```
gvar.fmt (g, ndecimal=None, sep='')
```

Format gvar. GVars in g.

g can be a gvar.GVar, an array of gvar.GVars, or a dictionary containing gvar.GVars or arrays of gvar.GVars. Each gvar.GVargi in g is replaced by the string generated by gi.fmt (ndecimal, sep). Result has same structure as g.

#### gvar.tabulate(g, ncol=1, headers=True, offset='', ndecimal=None)

Tabulate contents of an array or dictionary of gvar. GVars.

Given an array g of gvar. GVars or a dictionary whose values are gvar. GVars or arrays of gvar. GVars, gvar.tabulate(g) returns a string containing a table of the values of g's entries. For example, the code

```
import collections
import gvar as gv

g = collections.OrderedDict()
g['scalar'] = gv.gvar('10.3(1)')
g['vector'] = gv.gvar(['0.52(3)', '0.09(10)', '1.2(1)'])
g['tensor'] = gv.gvar([
        ['0.01(50)', '0.001(20)', '0.033(15)'],
        ['0.001(20)', '2.00(5)', '0.12(52)'],
        ['0.007(45)', '0.237(4)', '10.23(75)'],
        ])
print(gv.tabulate(g, ncol=2))
```

prints the following table:

key/index	V	value	key/index	7	7alue
scalar	10 20	(10)	1 0	0.001	(20)
	10.30		1,0		
vector 0	0.520	(30)	1,1	2.000	(50)
1	0.09	(10)	1,2	0.12	(52)
2	1.20	(10)	2,0	0.007	(45)
tensor 0,0	0.01	(50)	2,1	0.2370	(40)
0,1	0.001	(20)	2,2	10.23	(75)
0,2	0.033	(15)			

#### **Parameters**

- **g** Array of *gvar.GVars* (any shape) or dictionary whose values are *gvar.GVars* or arrays of *gvar.GVars* (any shape).
- ncol The table is split over ncol columns of key/index values plus gvar. GVar values. Default value is 1.

- headers Prints standard header on table if True; omits the header if False. If headers is a 2-tuple, then headers [0] is used in the header over the indices/keys and headers [1] over the *qvar.GVar* values. (Default is True.)
- offset (str) String inserted at the beginning of each line in the table. Default is ''.
- ndecimal Number of digits displayed after the decimal point. Default is ndecimal=None which adjusts table entries to show 2 digits of error.

#### gvar.correlate(g, corr)

Add correlations to uncorrelated gvar. GVars in g.

This method creates correlated gvar. GVars from uncorrelated gvar. GVars g, using the correlations specified in corr.

Note that correlations initially present in g, if any, are ignored.

#### **Examples**

A typical application involves the construction of correlated gvar. GVars give the means and standard deviations, together with a correlation matrix:

This also works when g and corr are dictionaries:

```
>>> g = gv.gvar(dict(a='1(1)', b='2(10)'))
>>> print(gv.evalcorr(g))
{('a', 'a'): array([[ 1.]]),('a', 'b'): array([[ 0.]]),('b', 'a'): array([[ 0.]]),('b', 'b'): ar
>>> corr = {}
>>> corr['a', 'a'] = 1.0
>>> corr['a', 'b'] = 0.1
>>> corr['b', 'a'] = 0.1
>>> corr['b', 'b'] = 1.0
>>> g = correlate(g, corr)
>>> print(gv.evalcorr(g))
{('a', 'a'): array([[ 1.]]),('a', 'b'): array([[ 0.1]]),('b', 'a'): array([[ 0.1]]),('b', 'b'):
```

#### **Parameters**

- **g** An array of *gvar*. *GVars* or a dictionary whose values are *gvar*. *GVars* or arrays of *gvar*. *GVars*.
- **corr** Correlations between *gvar.GVars*: corr[i, j] is the correlation between g[i] and g[j].

#### gvar.evalcov(g)

Compute covariance matrix for elements of array/dictionary g.

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If g is an array of gvar.GVars, evalcov returns the covariance matrix as an array with shape g.shape+g.shape. If g is a dictionary whose values are gvar.GVars or arrays of gvar.GVars, the result is a doubly-indexed dictionary where cov[k1,k2] is the covariance for g[k1] and g[k2].

#### gvar.evalcorr(g)

Compute correlation matrix for elements of array/dictionary g.

If g is an array of gvar.GVars, evalcorr returns the correlation matrix as an array with shape g.shape+g.shape. If g is a dictionary whose values are gvar.GVars or arrays of gvar.GVars, the result is a doubly-indexed dictionary where corr[k1, k2] is the correlation for g[k1] and g[k2].

The correlation matrix is related to the covariance matrix by:

```
corr[i,j] = cov[i,j] / (cov[i,i] * cov[j,j]) ** 0.5
```

```
gvar.uncorrelated(g1, g2)
```

Return True if *qvar*. *GVar*s in q1 uncorrelated with those in q2.

g1 and g2 can be gvar. GVars, arrays of gvar. GVars, or dictionaries containing gvar. GVars or arrays of gvar. GVars. Returns True if either of g1 or g2 is None.

```
gvar.chi2 (g1, g2, svdcut=1e-15, fmt=False)
Compute chi**2 of g1-g2.
```

chi\*\*2 is a measure of whether the multi-dimensional Gaussian distributions g1 and g2 (dictionaries or arrays) agree with each other — that is, do their means agree within errors for corresponding elements. The probability is high if chi2(g1,g2)/chi2.dof is of order 1 or smaller.

Usually g1 and g2 are dictionaries with the same keys, where g1 [k] and g2 [k] are gvar. GVars or arrays of gvar. GVars having the same shape. Alternatively g1 and g2 can be gvar. GVars, or arrays of gvar. GVars having the same shape.

One of g1 or g2 can contain numbers instead of gvar.GVars, in which case chi\*\*2 is a measure of the likelihood that the numbers came from the distribution specified by the other argument.

One or the other of g1 or g2 can be missing keys, or missing elements from arrays. Only the parts of g1 and g2 that overlap are used. Also setting g2=None is equivalent to replacing its elements by zeros.

chi\*\*2 is computed from the inverse of the covariance matrix of g1-g2. The matrix inversion can be sensitive to roundoff errors. In such cases, SVD cuts can be applied by setting parameters svdcut; see the documentation for gvar.svd(), which is used to apply the cut.

The return value is the chi\*\*2. Extra attributes attached to this value give additional information:

- •dof Number of degrees of freedom (that is, the number of variables compared).
- •Q The probability that the chi\*\*2 could have been larger, by chance, even if g1 and g2 agree. Values smaller than 0.1 or so suggest that they do not agree. Also called the *p-value*.

```
gvar.fmt_chi2(f)
```

Return string containing chi\*\*2/dof, dof and Q from f.

Assumes f has attributes chi2, dof and Q. The logarithm of the Bayes factor will also be printed if f has attribute logGBF.

```
gvar. GVars are compared by:
```

```
gvar.equivalent (g1, g2, rtol=1e-10, atol=1e-10)
```

Determine whether g1 and g2 contain equivalent gvar. GVars.

Compares sums and differences of gvar. GVars stored in g1 and g2 to see if they agree with tolerances. Operationally, agreement means that:

```
abs(diff) < abs(summ) / 2 * rtol + atol
```

where diff and summ are the difference and sum of the mean values (g.mean) or derivatives (g.der) associated with each pair of gvar. GVars.

gvar. GVars that are equivalent are effectively interchangeable with respect to both their means and also their covariances with any other gvar. GVar (including ones not in g1 and g2).

g1 and g2 can be individual *gvar.GVars* or arrays of *gvar.GVars* or dictionaries whose values are *gvar.GVars* and/or arrays of *gvar.GVars*. Comparisons are made only for shared keys when they are dictionaries. Array dimensions must match between g1 and g2, but the shapes can be different; comparisons are made for the parts of the arrays that overlap in shape.

#### **Parameters**

- g1 A gvar. GVar or an array of gvar. GVars or a dictionary of gvar. GVars and/or arrays of gvar. GVars.
- **g2** A gvar. GVar or an array of gvar. GVars or a dictionary of gvar. GVars and/or arrays of gvar. GVars.
- rtol Relative tolerance with which mean values and derivatives must agree with each other. Default is 1e-10.
- atol Absolute tolerance within which mean values and derivatives must agree with each other. Default is 1e-10.

gvar. GVars can be stored (pickled) and retrieved from files (or strings) using:

```
gvar.dump (g, outputfile)
```

pickle a collection g of gvar. GVars in file outputfile.

The gvar. GVars are recovered using gvar.load().

#### **Parameters**

- **g** A gvar. GVar, array of gvar. GVars, or dictionary whose values are gvar. GVars and/or arrays of gvar. GVars.
- **outputfile** (*string or file-like object*) The name of a file or a file object in which the pickled *gvar. GVars* are stored.

```
gvar.dumps(g)
```

pickle a collection g of gvar. GVars and return as a string.

The gvar. GVars are recovered using gvar.loads().

Parameters g - A gvar. GVar, array of gvar. GVars, or dictionary whose values are gvar. GVars and/or arrays of gvar. GVars.

### $\verb"gvar.load" (\textit{inputfile})$

Load and return pickled gvar. GVars from file inputfile.

This function recovers gvar. GVars pickled with gvar. dump ().

**Parameters outputfile** (*string or file-like object*) – The name of the file or a file object in which the pickled *gvar. GVars* are stored.

**Returns** The reconstructed gvar. GVar, or array or dictionary of gvar. GVars.

#### gvar.loads (inputstring)

Load and return pickled *gvar*. *GVars* from string inputstring.

This function recovers gvar. GVars pickled with gvar. dumps ().

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**Parameters** inputstring – A string containing gvar. GVars pickled using gvar. dumps ().

**Returns** The reconstructed *qvar.GVar*, or array or dictionary of *qvar.GVars*.

gvar. GVars contain information about derivatives with respect to the *independent gvar. GVars* from which they were constructed. This information can be extracted using:

```
qvar.deriv(g,x)
```

Compute first derivatives wrt x of gvar. GVars in q.

g can be a gvar. GVar, an array of gvar. GVars, or a dictionary containing gvar. GVars or arrays of gvar. GVars. Result has the same layout as g.

x must be an *primary gvar.GVar*, which is a *gvar.GVar* created by a call to gvar.gvar() (e.g., x = gvar.gvar(xmean, xsdev)) or a function f(x) of such a *gvar.GVar*. (More precisely, x.der must have only one nonzero entry.)

The following function creates an iterator that generates random arrays from the distribution defined by array (or dictionary) q of *qvar. GVars*. The random numbers incorporate any correlations implied by the qs.

```
gvar.raniter(g, n=None, svdcut=None)
```

Return iterator for random samples from distribution q

The gaussian variables (<code>gvar.GVar</code> objects) in array (or dictionary) g collectively define a multidimensional gaussian distribution. The iterator defined by <code>raniter()</code> generates an array (or dictionary) containing random numbers drawn from that distribution, with correlations intact.

The layout for the result is the same as for g. So an array of the same shape is returned if g is an array. When g is a dictionary, individual entries g [k] may be gvar. GVars or arrays of gvar. GVars, with arbitrary shapes.

raniter() also works when g is a single gvar. GVar, in which case the resulting iterator returns random numbers drawn from the distribution specified by g.

#### **Parameters**

- **g** (array or dictionary or BufferDict or GVar) An array (or dictionary) of objects of type gvar. GVar; or a gvar. GVar.
- n Maximum number of random iterations. Setting n=None (the default) implies there is no maximum number.
- **svdcut** (None or number) If positive, replace eigenvalues eig of g's correlation matrix with max (eig, svdcut \* max\_eig) where max\_eig is the largest eigenvalue; if negative, discard eigenmodes with eigenvalues smaller than |svdcut| \* max\_eig.

  Default is None.

**Returns** An iterator that returns random arrays or dictionaries with the same shape as g drawn from the gaussian distribution defined by g.

```
gvar.bootstrap_iter(g, n=None, svdcut=None)
```

Return iterator for bootstrap copies of g.

The gaussian variables (<code>gvar.GVar</code> objects) in array (or dictionary) g collectively define a multidimensional gaussian distribution. The iterator created by <code>bootstrap\_iter()</code> generates an array (or dictionary) of new <code>gvar.GVars</code> whose covariance matrix is the same as g's but whose means are drawn at random from the original g distribution. This is a <code>bootstrap copy</code> of the original distribution. Each iteration of the iterator has different means (but the same covariance matrix).

bootstrap\_iter() also works when g is a single gvar. GVar, in which case the resulting iterator returns bootstrap copies of the g.

#### **Parameters**

- g (array or dictionary or BufferDict) An array (or dictionary) of objects of type gvar. GVar.
- n Maximum number of random iterations. Setting n=None (the default) implies there is no maximum number.
- svdcut (None or number) If positive, replace eigenvalues eig of g's correlation matrix with max (eig, svdcut \* max\_eig) where max\_eig is the largest eigenvalue; if negative, discard eigenmodes with eigenvalues smaller than |svdcut| \* max\_eig. Default is None.

**Returns** An iterator that returns bootstrap copies of q.

#### gvar.ranseed(a)

Seed random number generators with tuple seed.

Argument seed is a tuple of integers that is used to seed the random number generators used by numpy and random (and therefore by gvar). Reusing the same seed results in the same set of random numbers.

ranseed generates its own seed when called without an argument or with seed=None. This seed is stored in ranseed. seed and also returned by the function. The seed can be used to regenerate the same set of random numbers at a later time.

Parameters seed (tuple or None) - A tuple of integers. Generates a random tuple if None.

Returns The seed.

The following two functions that are useful for tabulating results and for analyzing where the errors in a *gvar.GVar* constructed from other *gvar.GVar*s come from:

gvar.fmt\_errorbudget (outputs, inputs, ndecimal=2, percent=True, verify=False, colwidth=10)
Tabulate error budget for outputs [ko] due to inputs [ki].

For each output outputs [ko], fmt\_errorbudget computes the contributions to outputs [ko] 's standard deviation coming from the <code>gvar.GVars</code> collected in inputs [ki]. This is done for each key combination (ko, ki) and the results are tabulated with columns and rows labeled by ko and ki, respectively. If a <code>gvar.GVar</code> in inputs [ki] is correlated with other <code>gvar.GVars</code>, the contribution from the others is included in the ki contribution as well (since contributions from correlated <code>gvar.GVars</code> cannot be distinguished). The table is returned as a string.

### **Parameters**

- outputs Dictionary of gvar. GVars for which an error budget is computed.
- inputs Dictionary of: gvar. GVars, arrays/dictionaries of gvar. GVars, or lists of gvar. GVars and/or arrays/dictionaries of gvar. GVars. fmt\_errorbudget tabulates the parts of the standard deviations of each outputs [ko] due to each inputs [ki].
- **ndecimal** (int) Number of decimal places displayed in table.
- **percent** (*boolean*) Tabulate % errors if percent is True; otherwise tabulate the errors themselves.
- **colwidth** (*positive integer or None*) Width of each column. This is set automatically, to accommodate label widths, if colwidth=None (default).
- **verify** (boolean) If True, a warning is issued if: 1) different inputs are correlated (and therefore double count errors); or 2) the sum (in quadrature) of partial errors is not equal to the total error to within 0.1% of the error (and the error budget is incomplete or overcomplete). No checking is done if verify==False (default).

**Returns** A table (str) containing the error budget. Output variables are labeled by the keys in outputs (columns); sources of uncertainty are labeled by the keys in inputs (rows).

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```
gvar.fmt_values (outputs, ndecimal=None)
```

Tabulate gvar. GVars in outputs.

#### **Parameters**

- outputs A dictionary of gvar. GVar objects.
- ndecimal (int or None) Format values v using v.fmt (ndecimal).

**Returns** A table (str) containing values and standard deviations for variables in outputs, labeled by the keys in outputs.

The following function applies an SVD cut to the correlation matrix of a set of qvar. GVars:

```
gvar.svd(g, svdcut=1e-15, wgts=False)
```

Apply svd cuts to collection of gvar. GVars in g.

Standard usage is, for example,

```
svdcut = ...
gmod = svd(g, svdcut=svdcut)
```

where g is an array of <code>gvar.GVars</code> or a dictionary containing <code>gvar.GVars</code> and/or arrays of <code>gvar.GVars</code>. When <code>svdcut>0</code>, <code>gmod</code> is a copy of g whose <code>gvar.GVars</code> have been modified to make their correlation matrix less singular than that of the original g: each eigenvalue <code>eig</code> of the correlation matrix is replaced by <code>max(eig, svdcut \* max\_eig)</code> where <code>max\_eig</code> is the largest eigenvalue. This SVD cut, which is applied separately to each block-diagonal sub-matrix of the correlation matrix, increases the variance of the eigenmodes with eigenvalues smaller than <code>svdcut \* max\_eig</code>.

When svdcut is negative, eigenmodes of the correlation matrix whose eigenvalues are smaller than  $| \text{svdcut} | * \text{max\_eig}$  are dropped from the new matrix and the corresponding components of g are zeroed out (that is, replaced by 0(0)) in gmod.

There is an additional parameter wgts in gvar.svd() whose default value is False. Setting wgts=1 or wgts=-1 instead causes gvar.svd() to return a tuple (gmod, i\_wgts) where gmod is the modified copy of g, and i\_wgts contains a spectral decomposition of the covariance matrix corresponding to the modified correlation matrix if wgts=1, or a decomposition of its inverse if wgts=-1. The first entry i, wgts = i\_wgts[0] specifies the diagonal part of the matrix: i is a list of the indices in gmod.flat corresponding to diagonal elements, and wgts \*\* 2 gives the corresponding matrix elements. The second and subsequent entries, i, wgts = i\_wgts[n] for n > 0, each correspond to block-diagonal sub-matrices, where i is the list of indices corresponding to the block, and wgts[j] are eigenvectors of the sub-matrix rescaled so that

```
numpy.sum(numpy.outer(wi, wi) for wi in wgts[j]
```

is the sub-matrix (wgts=1) or its inverse (wgts=-1).

To compute the inverse of the covariance matrix from i\_wgts, for example, one could use code like:

```
gmod, i_wgts = svd(g, svdcut=svdcut, wgts=-1)

inv_cov = numpy.zeros((n, n), float)
i, wgts = i_wgts[0]  # 1x1 sub-matrices

if len(i) > 0:
    inv_cov[i, i] = numpy.array(wgts) ** 2

for i, wgts in i_wgts[1:]:  # nxn sub-matrices (n>1)
    for w in wgts:
        inv_cov[i, i[:, None]] += numpy.outer(w, w)
```

This sets  $inv\_cov$  equal to the inverse of the covariance matrix of the gmods. Similarly, we can compute the expectation value, u.dot  $(inv\_cov.dot(v))$ , between two vectors (numpy arrays) using:

where result is the desired expectation value.

The input parameters are:

#### **Parameters**

- **g** An array of gvar. GVars or a dicitionary whose values are gvar. GVars and/or arrays of gvar. GVars.
- svdcut (None or number (|svdcut|<=1).) If positive, replace eigenvalues eig of the correlation matrix with max(eig, svdcut \* max\_eig) where max\_eig is the largest eigenvalue; if negative, discard eigenmodes with eigenvalues smaller than |svdcut| \* max\_eig. Default is 1e-15.
- wgts Setting wgts=1 causes gvar.svd() to compute and return a spectral decomposition of the covariance matrix of the modified gvar.GVars, gmod. Setting wgts=-1 results in a decomposition of the inverse of the covariance matrix. The default value is False, in which case only gmod is returned.

**Returns** A copy gmod of g whose correlation matrix is modified by *svd* cuts. If wgts is not False, a tuple (g, i\_wgts) is returned where i\_wgts contains a spectral decomposition of gmod's covariance matrix or its inverse.

Data from the *svd* analysis of g's covariance matrix is stored in svd itself:

#### svd.dof

Number of independent degrees of freedom left after the svd cut. This is the same as the number initially unless svdcut < 0 in which case it may be smaller.

#### svd.nmod

Number of modes whose eignevalue was modified by the svd cut.

#### svd.nblocks

A dictionary where svd.nblocks[s] contains the number of block-diagonal s-by-s sub-matrices in the correlation matrix.

#### svd.eigen range

Ratio of the smallest to largest eigenvalue before svd cuts are applied (but after rescaling).

#### svd.logdet

Logarithm of the determinant of the covariance matrix after svd cuts are applied (excluding any omitted modes when svdcut < 0).

#### svd.correction

Array containing the svd corrections that were added to q.flat to create the modified qs.

This function is useful when the correlation matrix is singular or almost singular, and its inverse is needed (as in curve fitting).

The following function can be used to rebuild collections of gvar. GVars, ignoring all correlations with other variables. It can also be used to introduce correlations between uncorrelated variables.

```
gvar.rebuild(g, gvar=gvar, corr=0.0)
```

Rebuild q stripping correlations with variables not in q.

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g is either an array of gvar. GVars or a dictionary containing gvar. GVars and/or arrays of gvar. GVars. rebuild(g) creates a new collection gvar. GVars with the same layout, means and covariance matrix as those in g, but discarding all correlations with variables not in g.

If corr is nonzero, rebuild will introduce correlations wherever there aren't any using

```
cov[i,j] -> corr * sqrt(cov[i,i]*cov[j,j])
```

wherever cov[i,j] == 0.0 initially. Positive values for corr introduce positive correlations, negative values anti-correlations.

Parameter gvar specifies a function for creating new gvar. GVars that replaces gvar. gvar () (the default).

#### **Parameters**

- **g** (*array or dictionary*) *gvar. GVars* to be rebuilt.
- **gvar** (gvar. GVarFactory or None) Replacement for gvar.gvar() to use in rebuilding. Default is gvar.gvar().
- **corr** (*number*) Size of correlations to introduce where none exist initially.

**Returns** Array or dictionary (gvar.BufferDict) of gvar. GVars (same layout as g) where all correlations with variables other than those in g are erased.

The following functions creates new functions that generate gvar. GVars (to replace gvar.gvar()):

```
gvar.switch_gvar()
    Switch gvar.gvar() to new gvar.GVarFactory.
    Returns New gvar.gvar().

gvar.restore_gvar()
    Restore previous gvar.gvar().

    Returns Previous gvar.gvar().

gvar.gvar_factory(cov=None)
    Return new function for creating gvar.GVars (to replace gvar.gvar()).
```

If cov is specified, it is used as the covariance matrix for new *gvar.GVars* created by the function returned by gvar\_factory (cov). Otherwise a new covariance matrix is created internally.

gvar. GVars created by different functions cannot be combined in arithmetic expressions (the error message "Incompatible GVars." results).

# 2.3 gvar. GVar Objects

The fundamental class for representing Gaussian variables is:

```
class gvar. GVar
The basic attributes are:

mean
Mean value.

sdev
Standard deviation.

var
Variance.
```

Two methods allow one to isolate the contributions to the variance or standard deviation coming from other quar. GVars:

#### partialvar(\*args)

Compute partial variance due to gvar. GVars in args.

This method computes the part of self.var due to the *gvar.GVars* in args. If args[i] is correlated with other *gvar.GVars*, the variance coming from these is included in the result as well. (This last convention is necessary because variances associated with correlated *gvar.GVars* cannot be disentangled into contributions corresponding to each variable separately.)

**Parameters args[i]** (gvar. GVar or array/dictionary of gvar. GVars) – Variables contributing to the partial variance.

Returns Partial variance due to all of args.

#### partialsdev(\*args)

Compute partial standard deviation due to gvar. GVars in args.

This method computes the part of self.sdev due to the *gvar.GVars* in args. If args[i] is correlated with other *gvar.GVars*, the standard deviation coming from these is included in the result as well. (This last convention is necessary because variances associated with correlated *gvar.GVars* cannot be disentangled into contributions corresponding to each variable separately.)

**Parameters args[i]** (*gvar.GVar* or array/dictionary of *gvar.GVars*) – Variables contributing to the partial standard deviation.

**Returns** Partial standard deviation due to args.

Partial derivatives of the gvar. GVar with respect to the independent gvar. GVars from which it was constructed are given by:

#### deriv(x)

Derivative of self with respest to *primary gvar.GVar* x.

All gvar. GVars are constructed from primary gvar. GVars. self.deriv(x) returns the partial derivative of self with respect to primary gvar. GVarx, holding all of the other primary gvar. GVars constant.

**Parameters x** – A primary *gvar*. *GVar* (or a function of a single primary *gvar*. *GVar*).

**Returns** The derivative of self with respect to x.

There are two methods for converting self into a string, for printing:

```
__str__()
```

Return string representation of self.

The representation is designed to show at least one digit of the mean and two digits of the standard deviation. For cases where mean and standard deviation are not too different in magnitude, the representation is of the form 'mean (sdev)'. When this is not possible, the string has the form 'mean +- sdev'.

```
fmt (ndecimal=None, sep='')
```

Convert to string with format: mean (sdev).

Leading zeros in the standard deviation are omitted: for example, 25.67 +- 0.02 becomes 25.67(2). Parameter ndecimal specifies how many digits follow the decimal point in the mean. Parameter sep is a string that is inserted between the mean and the (sdev). If ndecimal is None (default), it is set automatically to the larger of int (2-log10(self.sdev)) or 0; this will display at least two digits of error. Very large or very small numbers are written with exponential notation when ndecimal is None.

Setting ndecimal < 0 returns mean +- sdev.

Two attributes and a method make reference to the original variables from which self is derived:

COV

Underlying covariance matrix (type gvar.smat) shared by all gvar. GVars.

der

Array of derivatives with respect to underlying (original) gvar. GVars.

```
dotder(v)
```

Return the dot product of self.der and v.

# 2.4 gvar.BufferDict Objects

The following class is a specialized form of an ordered dictionary for holding gvar. GVars (or other scalars) and arrays of gvar. GVars (or other scalars) that supports Python pickling:

```
class gvar.BufferDict
```

Ordered dictionary whose data are packed into a 1-d buffer (numpy.array).

A gvar.BufferDict object is an ordered dictionary whose values must either be scalars or arrays (like numpy arrays, with arbitrary shapes). The scalars and arrays are assembled into different parts of a single one-dimensional buffer. The various scalars and arrays are retrieved using keys: e.g.,

```
>>> a = BufferDict()
>>> a['scalar'] = 0.0
>>> a['vector'] = [1.,2.]
>>> a['tensor'] = [[3.,4.],[5.,6.]]
>>> print(a.flatten())
                                   # print a's buffer
[ 0. 1. 2. 3. 4. 5. 6.]
>>> for k in a:
                                   # iterate over keys in a
       print(k,a[k])
scalar 0.0
vector [ 1. 2.]
tensor [[ 3. 4.]
[ 5. 6.]]
>>> a['vector'] = a['vector']*10  # change the 'vector' part of a
>>> print(a.flatten())
[ 0. 10. 20.
                           5.
                                6.]
                      4.
```

The first four lines here could have been collapsed to one statement:

```
a = BufferDict(scalar=0.0, vector=[1.,2.], tensor=[[3.,4.],[5.,6.]])
```

or

where in the second case the order of the keys is preserved in a (since BufferDict is an ordered dictionary).

The keys and associated shapes in a *gvar.BufferDict* can be transferred to a different buffer, creating a new *gvar.BufferDict*: *e.g.*, using a from above,

```
>>> buf = numpy.array([0.,10.,20.,30.,40.,50.,60.])
>>> b = BufferDict(a, buf=buf) # clone a but with new buffer
>>> print(b['tensor'])
[[ 30. 40.]
  [ 50. 60.]]
>>> b['scalar'] += 1
```

```
>>> print(buf)
[ 1. 10. 20. 30. 40. 50. 60.]
```

Note how b references buf and can modify it. One can also replace the buffer in the original gvar.BufferDict using, for example, a.buf = buf:

```
>>> a.buf = buf
>>> print(a['tensor'])
[[ 30. 40.]
  [ 50. 60.]]
>>> a['tensor'] *= 10.
>>> print(buf)
[ 1. 10. 20. 300. 400. 500. 600.]
```

a.buf is the numpy array used for a's buffer. It can be used to access and change the buffer directly. In a.buf = buf, the new buffer buf must be a numpy array of the correct shape. The buffer can also be accessed through iterator a.flat (in analogy with numpy arrays), and through a.flatten() which returns a copy of the buffer.

When creating a gvar.BufferDict from a dictionary (or another gvar.BufferDict), the keys included and their order can be specified using a list of keys: for example,

```
>>> d = dict(a=0.0,b=[1.,2.],c=[[3.,4.],[5.,6.]],d=None)
>>> print(d)
{'a': 0.0, 'c': [[3.0, 4.0], [5.0, 6.0]], 'b': [1.0, 2.0], 'd': None}
>>> a = BufferDict(d, keys=['d', 'b', 'a'])
>>> for k in a:
...     print(k, a[k])
d None
b [1.0 2.0]
a 0.0
```

A gvar.BufferDict functions like a dictionary except: a) items cannot be deleted once inserted; b) all values must be either scalars or arrays of scalars, where the scalars can be any noniterable type that works with numpy arrays; and c) any new value assigned to an existing key must have the same size and shape as the original value.

Note that gvar.BufferDicts can be pickled and unpickled even when they store gvar.GVars (which themselves cannot be pickled separately).

The main attributes are:

#### size

Size of buffer array.

#### flat

Buffer array iterator.

#### dtype

Data type of buffer array elements.

#### buf

The (1d) buffer array. Allows direct access to the buffer: for example, self.buf[i] = new\_val sets the value of the i-th element in the buffer to value new\_val. Setting self.buf = nbuf replaces the old buffer by new buffer nbuf. This only works if nbuf is a one-dimensional numpy array having the same length as the old buffer, since nbuf itself is used as the new buffer (not a copy).

#### shape

Always equal to None. This attribute is included since gvar. BufferDicts share several attributes

with numpy arrays to simplify coding that might support either type. Being dictionaries they do not have shapes in the sense of numpy arrays (hence the shape is None).

The main methods are:

#### flatten()

Copy of buffer array.

#### slice(k)

Return slice/index in self.flat corresponding to key k.

#### $slice\_shape(k)$

Return tuple (slice/index, shape) corresponding to key k.

#### isscalar(k)

Return True if self[k] is scalar else False.

#### update(d)

Add contents of dictionary d to self.

#### static load (fobj, use\_json=False)

Load serialized *gvar.BufferDict* from file object fobj. Uses pickle unless use\_json is True, in which case it uses json (obvioulsy).

#### static loads (s, use\_json=False)

Load serialized *gvar.BufferDict* from string object s. Uses pickle unless use\_json is True, in which case it uses json (obvioulsy).

#### dump (fobj, use\_json=False)

Serialize gvar. BufferDict in file object fobj.

Uses pickle unless use\_json is True, in which case it uses json (obviously). json does not handle non-string valued keys very well. This attempts a workaround, but it will only work in simpler cases. Serialization only works when pickle (or json) knows how to serialize the data type stored in the gvar.BufferDict's buffer (or for gvar.GVars).

#### dumps (use\_json=False)

Serialize gvar. BufferDict into string.

Uses pickle unless use\_json is True, in which case it uses json (obviously). json does not handle non-string valued keys very well. This attempts a workaround, but it will only work in simpler cases (e.g., integers, tuples of integers, etc.). Serialization only works when pickle (or json) knows how to serialize the data type stored in the <code>gvar.BufferDict</code>'s buffer (or for <code>gvar.GVars</code>).

# 2.5 gvar. SVD Objects

SVD analysis is handled by the following class:

```
class gvar . SVD (mat, svdcut=None, svdnum=None, compute_delta=False, rescale=False) SVD decomposition of a pos. sym. matrix.
```

SVD is a function-class that computes the eigenvalues and eigenvectors of a positive symmetric matrix mat. Eigenvalues that are small (or negative, because of roundoff) can be eliminated or modified using svd cuts. Typical usage is:

```
[ 0.97324899 -0.22975292]
>>> print(s.vec[1])
                             # 2nd eigenvector (for s.val[1])
[ 0.22975292  0.97324899]
>>> s = SVD(mat,svdcut=0.6)  # force s.val[i]>=s.val[-1]*0.6
>>> print(s.val)
[ 1.2354102
            2.05901699]
>>> print(s.vec[0])
                             # eigenvector unchanged
[ 0.97324899 -0.22975292]
>>> s = SVD (mat)
>>> w = s.decomp(-1)
                             # decomposition of inverse of mat
>>> invmat = sum(numpy.outer(wj,wj) for wj in w)
>>> print (numpy.dot(mat,invmat))
                                    # should be unit matrix
[[ 1.00000000e+00 2.77555756e-17]
[ 1.66533454e-16 1.00000000e+00]]
```

Input parameters are:

#### **Parameters**

- mat (2-d sequence (numpy.array or list or ...)) Positive, symmetric matrix.
- **svdcut** (None or number (|svdcut|<=1).) If positive, replace eigenvalues of mat with svdcut\* (max eigenvalue); if negative, discard eigenmodes with eigenvalues smaller than svdcut times the maximum eigenvalue.
- **svdnum** (None or int) If positive, keep only the modes with the largest svdnum eigenvalues; ignore if set to None.
- compute\_delta (boolean) Compute delta (see below) if True; set delta=None otherwise.
- **rescale** Rescale the input matrix to make its diagonal elements equal to 1.0 before diagonalizing.

The results are accessed using:

#### val

An ordered array containing the eigenvalues or mat. Note that  $val[i] \le val[i+1]$ .

#### vec

Eigenvectors vec[i] corresponding to the eigenvalues val[i].

D

The diagonal matrix used to precondition the input matrix if rescale == True. The matrix diagonalized is D M D where M is the input matrix. D is stored as a one-dimensional vector of diagonal elements. D is None if rescale == False.

#### nmod

The first nmod eigenvalues in self.val were modified by the SVD cut (equals 0 unless svdcut > 0).

#### eigen\_range

Ratio of the smallest to the largest eigenvector in the unconditioned matrix (after rescaling if rescale=True)

#### delta

A vector of gvars whose means are zero and whose covariance matrix is what was added to mat to condition its eigenvalues. Is None if svdcut<0 or compute\_delta==False.

#### decomp(n)

Vector decomposition of input matrix raised to power n.

Computes vectors w [i] such that

```
mat**n = sum_i numpy.outer(w[i],w[i])
```

where mat is the original input matrix to svd. This decomposition cannot be computed if the input matrix was rescaled (rescale=True) except for n=1 and n=-1.

**Parameters n** (*number*) – Power of input matrix.

**Returns** Array w of vectors.

## 2.6 gvar.PDFIntegrator and other PDF-related Objects

Expectation values using probability density functions defined by collections of gvar. GVars can be evaluated using the vegas module (for multi-dimensional integration) and the following class:

```
class gvar.PDFIntegrator (g, limit=1e15, scale=1., svdcut=1e-15) vegas integrator for PDF expectation values.
```

PDFIntegrator (g) is a vegas integrator that evaluates expectation values for the multi-dimensional Gaussian distribution specified by with g, which is a *gvar.GVar* or an array of *gvar.GVar*s or a dictionary whose values are *gvar.GVars* or arrays of *gvar.GVars*.

PDFIntegrator integrates over the entire parameter space of the distribution but reexpresses integrals in terms of variables that diagonalize g's covariance matrix and are centered at its mean value. This greatly facilitates integration over these variables using the vegas module, making integrals over 10s or more of parameters feasible. (The vegas module must be installed separately in order to use PDFIntegrator.)

A simple illustration of PDFIntegrator is given by the following code:

```
import gvar as gv
# multi-dimensional Gaussian distribution
g = gv.BufferDict()
g['a'] = gv.gvar([0., 1.], [[1., 0.9], [0.9, 1.]])
g['b'] = gv.gvar('1(1)')
# integrator for expectation values in distribution g
g_expval = gv.PDFIntegrator(g)
# adapt integrator to PDF
warmup = g_expval(neval=1000, nitn=5)
# want expectation value of [fp, fp**2]
def f_f2(p):
   fp = p['a'][0] * p['a'][1] + p['b']
    return [fp, fp ** 2]
\# results = \langle f_f 2 \rangle in distribution g
results = g_expval(f_f2, neval=1000, nitn=5, adapt=False)
print (results.summary())
print ('results =', results, '\n')
# mean and standard deviation of f(p)'s distribution
fmean = results[0]
fsdev = gv.sqrt(results[1] - results[0] ** 2)
```

```
print ('f.mean =', fmean, ' f.sdev =', fsdev)
print ("Gaussian approx'n for f(g) =", f_f2(g)[0])
```

where the warmup calls to the integrator are used to adapt it to the PDF, and the final results are in results. Here neval is the (approximate) number of function calls per iteration of the vegas algorithm and nitn is the number of iterations. We use the integrator to calculated the expectation value of fp and fp\*\*2, so we can compute the standard deviation for the distribution of fps. The output from this code shows that the Gaussian approximation (1.0(1.4)) for the mean and standard deviation of the fp distribution is not particularly accurate here (correct value is 1.9(2.0)), because of the large uncertainties in q:

```
itn
                                         chi2/dof
                                                          Q
      integral
                       average
  1
      0.995(12)
                       0.995(12)
                                             0.00
                                                       1.00
  2.
      1.014(11)
                       1.0043(79)
                                             1.39
                                                       0.24
  3
      1.005(11)
                       1.0046(65)
                                             1.75
                                                       0.10
      0.977(13)
                       0.9978(58)
                                             2.40
                                                       0.01
  4
                                                       0.03
  5
      1.004(12)
                       0.9990(52)
                                             1.94
results = [1.904(17) 7.57(17)]
f.mean = 1.904(17)
                       f.sdev = 1.986(31)
Gaussian approx'n for f(g) = 1.0(1.4)
```

In general functions being integrated can return a number, or an array of numbers, or a dictionary whose values are numbers or arrays of numbers. This allows multiple expectation values to be evaluated simultaneously.

See the documentation with the vegas module for more details on its use, and on the attributes and methods associated with integrators. The example above sets adapt=False when computing final results. This gives more reliable error estimates when neval is small. Note that neval may need to be much larger (tens or hundreds of thousands) for more difficult high-dimension integrals.

#### **Parameters**

- g gvar. GVar, array of gvar. GVars, or dictionary whose values are gvar. GVars or arrays of gvar. GVars that specifies the multi-dimensional Gaussian distribution used to construct the probability density function.
- limit (positive float) Limits the integrations to a finite region of size limit times the standard deviation on either side of the mean. This can be useful if the functions being integrated misbehave for large parameter values (e.g., numpy.exp overflows for a large range of arguments). Default is 1e15.
- **scale** (*positive float*) The integration variables are rescaled to emphasize parameter values of order scale times the standard deviation. The rescaling does not change the value of the integral but it can reduce uncertainties in the vegas estimate. Default is 1.0.
- svdcut (non-negative float or None) If not None, replace covariance matrix of g with a new matrix whose small eigenvalues are modified: eigenvalues smaller than svdcut times the maximum eigenvalue eig\_max are replaced by svdcut\*eig\_max. This can ameliorate problems caused by roundoff errors when inverting the covariance matrix. It increases the uncertainty associated with the modified eigenvalues and so is conservative. Setting svdcut=None or svdcut=0 leaves the covariance matrix unchanged. Default is 1e-15.

```
__call__(f, nopdf=False, mpi=False, **kargs)

Estimate expectation value of function f (p).
```

Uses module vegas to estimate the integral of f(p) multiplied by the probability density function associated with g(i.e., pdf(p)). The probability density function is omitted if nopdf=True (default setting

is False). Setting mpi=True configures vegas for multi-processor running using MPI.

#### **Parameters**

- **f** (*function*) Function f (p) to integrate. Integral is the expectation value of the function with respect to the distribution. The function can return a number, an array of numbers, or a dictionary whose values are numbers or arrays of numbers.
- **nopdf** (*bool*) If True drop the probability density function from the integrand (so no longer an expectation value). This is useful if one wants to use the optimized integrator for something other than a standard expectation value. Default is False.
- mpi (bool) If True configure for use with multiple processors and MPI. This option requires module mpi4py. A script xxx.py using an MPI integrator is run with mpirun: e.g.,

```
mpirun -np 4 -output-filename xxx.out python xxx.py
```

runs on 4 processors. Setting mpi=False (default) does not support multiple processors. The MPI processor rank can be obtained from the mpi\_rank attribute of the integrator.

All other keyword arguments are passed on to a vegas integrator; see the vegas documentation for further information.

Related classes are:

```
class gvar.PDF (g, svdcut=1e-15)
```

Probability density function (PDF) for q.

Given an array or dictionary g of gvar. GVars, pdf=PDF (g) is the probability density function for the (usually correlated) multi-dimensional Gaussian distribution defined by g. That is pdf (p) is the probability density for random sample p drawn from q. The logarithm of the PDF is obtained using pdf.logpdf (p).

#### **Parameters**

- **g** *gvar.GVar* or array of *gvar.GVars*, or dictionary of *gvar.GVars* or arrays of *gvar.GVars*.
- **svdcut** (*non-negative float or None*) If not None, replace covariance matrix of g with a new matrix whose small eigenvalues are modified: eigenvalues smaller than svdcut times the maximum eigenvalue eig\_max are replaced by svdcut\*eig\_max. This can ameliorate problems caused by roundoff errors when inverting the covariance matrix. It increases the uncertainty associated with the modified eigenvalues and so is conservative. Setting svdcut=None or svdcut=0 leaves the covariance matrix unchanged. Default is 1e-15.

class gvar.PDFStatistics (moments=None, histogram=None)

Compute statistical information about a distribution.

Given moments m[i] of a random variable, computes mean, standard deviation, skewness, and excess kurtosis.

### Parameters

- moments (array of floats) moments[i] is the (i+1)-th moment. Optional argument unless histgram=None.
- histogram (tuple) Tuple (bins, prob) where prob[i] is the probability in the bin between bins[i-1] and bins[i]. prob[0] is the probability below bins[0] and prob[-1] is the probability above bins[-1]. Array bins is ordered. The format for prob is what is returned by accumulating calls to gvar.PDFHistogram.count(). Optional argument unless moments=None.

The attributes are as follows:

```
mean
```

mean value

#### sdev

standard deviation

#### skew

skewness coefficient

#### ex kurt

excess kurtosis

#### mediar

median (if histogram provided)

#### plus

interval (median, median+plus) contains 34.1% of probability

#### minus

interval (median-minus, median) contains 34.1% of probability

#### gvar

```
gvar.gvar(mean, sdev)
```

class gvar.PDFHistogram(g, nbin=None, binwidth=None, bins=None)

Utility class for creating PDF histograms.

This class is designed to facilitate studies of probability density functions associated with *gvar.GVars*. The following code, for example, makes a histogram of probabilities for the Gaussian distribution corresponding to *gvar.GVar* 1.0(5):

```
g = gv.gvar('1.0(5)')
data = [g() for i in range(10000)]

hist = gv.PDFHistogram(g)
count = hist.count(data)
a = hist.analyze(count)
print('probabilities:', a.prob)
print('statistics:\n', a.stats)
```

Here hist defines a histogram with 8 bins, centered on g.mean, and each with width equal to g.sdev. The data in array data is a random sampling from g's distribution. The number of data elements in each bin is determined by hist.count (data) and turned into probabilities by hist.analyze(count). The probabilities (a.prob) and a statistical analysis of the probability distribution based on the histogram (a.stats) are then printed out:

```
probabilities: [ 0.0017
                         0.0213
                                 0.1358
                                         0.3401
                                                  0.3418
                                                          0.1351
                                                                  0.0222
                                                                          0.0018]
statistics:
      mean = 1.001
                     sdev = 0.52334
                                       skew = 0.0069999
                                                          ex_kurt = 0.034105
   median = 1.00141666398
                            plus = 0.499891542549
                                                     minus = 0.501710986504
```

A plot of the histogram can be created and displayed using, for example:

```
plt = hist.make_plot(count)
plt.xlabel('g')
plt.ylabel('probabilities')
plt.show()
```

PDFIntegrator can be used to create histograms for more complicated, multi-dimensional distributions: the expectation value of hist.count(f(p)) over values of p drawn from a multi-dimensional distribution gives the the probability distribution for function f(p).

#### **Parameters**

- g (gvar. GVar or None) The mean and standard deviation of g are used to design the histogram bins, which are centered on g.mean. Ignored if None (in which case bins must be specified).
- **nbin** (*int*) The number of histogram bins. Set equal to PDFHistogram.default\_nbin'' (=8 initially) if 'None.
- binwidth (float) The width of each bin is binwidth \* g.sdev. Set equal to PDFHistogram.default\_binwidth'' (=1. initially) if 'None.
- bins (array or None) Ignored if None (default). Otherwise specifies the histogram's bin edges, overriding the default bin design specified by g. len (bins) is one larger than the number of bins. If specified it overrides the default bin design indicated by g. One of g or bins must be specified.

The main attributes are:

g

gvar. GVar used to design the histogram.

#### bins

Bin edges for the histogram (see above).

#### midpoints

Bin midpoints.

#### widths

Bin widths.

The main methods are:

#### count (data)

Compute histogram of data.

Counts the number of elements from array data in each bin of the histogram. Results are returned in an array, call it h, of length nbin+2 where h[0] is the number of data elements that fall below the range of the histogram, h[-1] (i.e., h[nbin+1]) is the number that fall above the range, and h[i] is the number in the i-th bin for i=1...nbin.

Argument data can also be a float, in which case the result is the same as from histogram ([data]). Note that the expectation value of count (f(p)) over parameter values p drawn from a random distribution gives the probabilities for values of f(p) to fall in each histogram bin. Dividing by the bin widths gives the average probability density for random variable f(p) in each bin.

Bin intervals are closed on the left and open on the right, except for the last interval which is closed on both ends.

#### analyze(count)

Analyze count data from PDFHistogram.count().

Turns an array of counts (see *PDFHistogram.count()*) into a histogram of probabilities, and estimates the mean, standard deviation, and other statistical characteristics of the corresponding probability distribution.

**Parameters count** (*array*) – Array of length nbin+2 containing histogram data where count [0] is the count for values that are below the range of the histogram, count [-1]

is the count for values above the range, and count[i] is the count for the i-th bin where i=1...nbin.

Returns a named tuple containing the following information (in order):

```
bins: Array of bin edges for histogram (length nbin+1)
```

prob: Array of probabilities for each bin.

stats: Statistical data about histogram. See PDFStatistics.

norm: Convert counts into probabilities by dividing by norm.

#### **Parameters**

- count (array) Array of histogram counts (see PDFHistogram.count()).
- plot (plotter) matplotlib plotting window. If None uses the default window. Default is None.
- show (boolean) Displayes plot if True; otherwise returns the plot. Default is False.
- plottype (str) The probabilities in each bin are plotted if plottype='probability' (default). The average probability density is plot if plottype='density'. The cumulative probability is plotted if plottype=cumulative.
- **bar** (*dictionary*) Additional plotting arguments for the bar graph showing the histogram. This part of the plot is omitted if bar=None.
- **errorbar** (*dictionary*) Additional plotting arguments for the errorbar graph, showing error bars on the histogram. This part of the plot is omitted if errorbar=None.
- **gaussian** (*dictionary*) Additional plotting arguments for the plot of the Gaussian probability for the *gvar.GVar* (g) specified in the initialization. This part of the plot is omitted if gaussian=None or if no g was specified.

## 2.7 Requirements

*gvar* makes heavy use of numpy for array manipulations. It also uses the numpy code for implementing elementary functions (*e.g.*, sin, exp...) in terms of member functions.

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**CHAPTER** 

THREE

## GVAR. DATASET - RANDOM DATA SETS

## 3.1 Introduction

gvar. dataset contains a several tools for collecting and analyzing random samples from arbitrary distributions. The random samples are represented by lists of numbers or arrays, where each number/array is a new sample from the underlying distribution. For example, six samples from a one-dimensional gaussian distribution,  $1\pm 1$ , might look like

```
>>> random_numbers = [1.739, 2.682, 2.493, -0.460, 0.603, 0.800]
```

while six samples from a two-dimensional distribution, [1 $\pm$ 1, 2 $\pm$ 1], might be

```
>>> random_arrays = [[ 0.494, 2.734], [ 0.172, 1.400], [ 1.571, 1.304], ... [ 1.532, 1.510], [ 0.669, 0.873], [ 1.242, 2.188]]
```

Samples from more complicated multidimensional distributions are represented by dictionaries whose values are lists of numbers or arrays: for example,

```
>>> random_dict = dict(n=random_numbers, a=random_arrays)
```

where list elements random\_dict['n'][i] and random\_dict['a'][i] are part of the same multidimensional sample for every i — that is, the lists for different keys in the dictionary are synchronized one with the other.

With large samples, we typically want to estimate the mean value of the underlying distribution. This is done using <code>gvar.dataset.avg\_data()</code>: for example,

```
>>> print(avg_data(random_numbers))
1.31(45)
```

indicates that 1.31 (45) is our best guess, based only upon the samples in random\_numbers, for the mean of the distribution from which those samples were drawn. Similarly

```
>>> print(avg_data(random_arrays))
[0.95(22) 1.67(25)]
```

indicates that the means for the two-dimensional distribution behind random\_arrays are [0.95(22), 1.67(25)]. avg\_data() can also be applied to a dictionary whose values are lists of numbers/arrays: for example,

```
>>> print(avg_data(random_dict))
{'a': array([0.95(22), 1.67(25)], dtype=object),'n': 1.31(45)}
```

Class gvar.dataset.Dataset can be used to assemble dictionaries containing random samples. For example, imagine that the random samples above were originally written into a file, as they were generated:

```
# file: datafile
n 1.739
a [ 0.494, 2.734]
n 2.682
a [ 0.172, 1.400]
n 2.493
a [ 1.571, 1.304]
n -0.460
a [ 1.532, 1.510]
n 0.603
a [ 0.669, 0.873]
n 0.800
a [ 1.242, 2.188]
```

Here each line is a different random sample, either from the one-dimensional distribution (labeled n) or from the two-dimensional distribution (labeled a). Assuming the file is called datafile, this data can be read into a dictionary, essentially identical to the data dictionary above, using:

```
>>> data = Dataset("datafile")
>>> print(data['a'])
[array([ 0.494, 2.734]), array([ 0.172, 1.400]), array([ 1.571, 1.304]) ... ]
>>> print(avg_data(data['n']))
1.31(45)
```

The brackets and commas can be omitted in the input file for one-dimensional arrays: for example, datafile (above) could equivalently be written

```
# file: datafile
n 1.739
a 0.494 2.734
n 2.682
a 0.172 1.400
...
```

Other data formats may also be easy to use. For example, a data file written using yaml would look like

```
# file: datafile
---
n: 1.739
a: [ 0.494, 2.734]
---
n: 2.682
a: [ 0.172, 1.400]
.
.
```

and could be read into a gvar.dataset.Dataset using:

```
import yaml

data = Dataset()
with open("datafile", "r") as dfile:
    for d in yaml.load_all(dfile.read()): # iterate over yaml records
        data.append(d) # d is a dictionary
```

Finally note that data can be binned, into bins of size binsize, using <code>gvar.dataset.bin\_data()</code>. For example, <code>gvar.dataset.bin\_data(data, binsize=3)</code> replaces every three samples in data by the average of those samples. This creates a dataset that is 1/3 the size of the original but has the same mean. Binning is use-

ful for making large datasets more manageable, and also for removing sample-to-sample correlations. Over-binning, however, erases statistical information.

Class gvar. dataset. Dataset can also be used to build a dataset sample by sample in code: for example,

```
>>> a = Dataset()
>>> a.append(n=1.739, a=[ 0.494, 2.734])
>>> a.append(n=2.682, a=[ 0.172, 1.400])
...
```

creates the same dataset as above.

### 3.2 Functions

The functions defined in the module are:

```
gvar.dataset.avg_data(data, spread=False, median=False, bstrap=False, noerror=False, warn=True)

Average random data to estimate mean.
```

data is a list of random numbers, a list of random arrays, or a dictionary of lists of random numbers and/or arrays: for example,

```
>>> random_numbers = [1.60, 0.99, 1.28, 1.30, 0.54, 2.15]
>>> random_arrays = [[12.2,121.3],[13.4,149.2],[11.7,135.3],
... [7.2,64.6],[15.2,69.0],[8.3,108.3]]
>>> random_dict = dict(n=random_numbers,a=random_arrays)
```

where in each case there are six random numbers/arrays. avg\_data estimates the means of the distributions from which the random numbers/arrays are drawn, together with the uncertainties in those estimates. The results are returned as a <code>gvar.GVar</code> or an array of <code>gvar.GVars</code>, or a dictionary of <code>gvar.GVars</code> and/or arrays of <code>gvar.GVars</code>:

```
>>> print (avg_data(random_numbers))
1.31(20)
>>> print (avg_data(random_arrays))
[11.3(1.1) 108(13)]
>>> print (avg_data(random_dict))
{'a': array([11.3(1.1), 108(13)], dtype=object),'n': 1.31(20)}
```

The arrays in random\_arrays are one dimensional; in general, they can have any shape.

avg\_data (data) also estimates any correlations between different quantities in data. When data is a dictionary, it does this by assuming that the lists of random numbers/arrays for the different data[k]s are synchronized, with the first element in one list corresponding to the first elements in all other lists, and so on. If some lists are shorter than others, the longer lists are truncated to the same length as the shortest list (discarding data samples).

There are four optional arguments. If argument spread=True each standard deviation in the results refers to the spread in the data, not the uncertainty in the estimate of the mean. The former is sqrt (N) larger where N is the number of random numbers (or arrays) being averaged:

```
>>> print(avg_data(random_numbers, spread=True))
1.31(50)
>>> print(avg_data(random_numbers))
1.31(20)
>>> print((0.50 / 0.20) ** 2) # should be (about) 6
6.25
```

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This is useful, for example, when averaging bootstrap data. The default value is spread=False.

The second option is triggered by setting median=True. This replaces the means in the results by medians, while the standard deviations are approximated by the half-width of the interval, centered around the median, that contains 68% of the data. These estimates are more robust than the mean and standard deviation when averaging over small amounts of data; in particular, they are unaffected by extreme outliers in the data. The default is median=False.

The third option is triggered by setting bstrap=True. This is shorthand for setting median=True and spread=True, and overrides any explicit setting for these keyword arguments. This is the typical choice for analyzing bootstrap data — hence its name. The default value is bstrap=False.

The fourth option is to omit the error estimates on the averages, which is triggered by setting noerror=True. Just the mean values are returned. The default value is noerror=False.

The final option warn determines whether or not a warning is issued when different components of a dictionary data set have different sample sizes.

```
gvar.dataset.autocorr(data)
```

Compute autocorrelation in random data.

data is a list of random numbers or random arrays, or a dictionary of lists of random numbers/arrays.

When data is a list of random numbers, autocorr (data) returns an array where autocorr (data) [i] is the correlation between elements in data that are separated by distance i in the list: for example,

shows perfect correlation between elements separated by an even interval in the list, and perfect anticorrelation between elements by an odd interval.

autocorr (data) returns a list of arrays of autocorrelation coefficients when data is a list of random arrays. Again autocorr (data) [i] gives the autocorrelations for data elements separated by distance i in the list. Similarly autocorr (data) returns a dictionary when data is a dictionary.

autocorr (data) uses FFTs to compute the autocorrelations; the cost of computing the autocorrelations should grow roughly linearly with the number of random samples in data (up to logarithms).

```
gvar.dataset.bin_data(data, binsize=2)
```

Bin random data.

data is a list of random numbers or random arrays, or a dictionary of lists of random numbers/arrays. bin\_data(data,binsize) replaces consecutive groups of binsize numbers/arrays by the average of those numbers/arrays. The result is new data list (or dictionary) with 1/binsize times as much random data: for example,

```
>>> print (bin_data([1,2,3,4,5,6,7],binsize=2))
[1.5, 3.5, 5.5]
>>> print (bin_data(dict(s=[1,2,3,4,5],v=[[1,2],[3,4],[5,6],[7,8]]),binsize=2))
{'s': [1.5, 3.5], 'v': [array([ 2., 3.]), array([ 6., 7.])]}
```

Data is dropped at the end if there is insufficient data to from complete bins. Binning is used to make calculations faster and to reduce measurement-to-measurement correlations, if they exist. Over-binning erases useful information.

```
gvar.dataset.bootstrap_iter(data, n=None)
```

Create iterator that returns bootstrap copies of data.

data is a list of random numbers or random arrays, or a dictionary of lists of random numbers/arrays. bootstrap\_iter(data,n) is an iterator that returns n bootstrap copies of data. The random num-

bers/arrays in a bootstrap copy are drawn at random (with repetition allowed) from among the samples in data: for example,

```
>>> data = [1.1, 2.3, 0.5, 1.9]
>>> data_iter = bootstrap_iter(data)
>>> print (next (data_iter))
[ 1.1 1.1 0.5 1.9]
>>> print (next (data_iter))
[ 0.5 2.3 1.9 0.5]
>>> data = dict(a=[1,2,3,4],b=[1,2,3,4])
>>> data_iter = bootstrap_iter(data)
>>> print (next (data_iter))
{'a': array([3, 3, 1, 2]), 'b': array([3, 3, 1, 2])}
>>> print (next (data_iter))
{'a': array([1, 3, 3, 2]), 'b': array([1, 3, 3, 2])}
>>> data = [[1,2],[3,4],[5,6],[7,8]]
>>> data_iter = bootstrap_iter(data)
>>> print (next (data_iter))
[[7. 8.]
 [ 1.
      2.1
 [ 1. 2.]
 [ 7. 8.]]
>>> print (next (data_iter))
[[ 3. 4.]
 [ 7. 8.]
 [ 3.
      4.]
 [ 1.
       2.11
```

The distribution of bootstrap copies is an approximation to the distribution from which data was drawn. Consequently means, variances and correlations for bootstrap copies should be similar to those in data. Analyzing variations from bootstrap copy to copy is often useful when dealing with non-gaussian behavior or complicated correlations between different quantities.

Parameter n specifies the maximum number of copies; there is no maximum if n is None.

### 3.3 Classes

gvar.dataset.Dataset is used to assemble random samples from multidimensional distributions:

class gvar.dataset.Dataset

Dictionary for collecting random data.

This dictionary class simplifies the collection of random data. The random data are stored in a dictionary, with each piece of random data being a number or a numpy array of numbers. For example, consider a situation where there are four random values for a scalar s and four random values for vector v. These can be collected as follows:

```
>>> data = Dataset()
>>> data.append(s=1.1,v=[12.2,20.6])
>>> data.append(s=0.8,v=[14.1,19.2])
>>> data.append(s=0.95,v=[10.3,19.7])
>>> data.append(s=0.91,v=[8.2,21.0])
>>> print(data['s']) # 4 random values of s
[ 1.1, 0.8, 0.95, 0.91]
```

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```
>>> print(data['v']) # 4 random vector-values of v
[array([ 12.2, 20.6]), array([ 14.1, 19.2]), array([ 10.3, 19.7]), array([ 8.2, 21. ])]
```

The argument to data.append() could be a dictionary: for example, dd = dict(s=1.1, v=[12.2, 20.6]); data.append(dd) is equivalent to the first append statement above. This is useful, for example, if the data comes from a function (that returns a dictionary).

One can also append data key-by-key: for example, data.append('s',1.1); data.append('v',[12.2,20.6]) is equivalent to the first append in the example above. One could also achieve this with, for example, data['s'].append(1.1); data['v'].append([12.2,20.6]), since each dictionary value is a list, but gvar.Dataset's append checks for consistency between the new data and data already collected and so is preferable.

Use extend in place of append to add data in batches: for example,

```
>>> data = Dataset()
>>> data.extend(s=[1.1,0.8],v=[[12.2,20.6],[14.1,19.2]])
>>> data.extend(s=[0.95,0.91],v=[[10.3,19.7],[8.2,21.0]])
>>> print(data['s']) # 4 random values of s
[ 1.1, 0.8, 0.95, 0.91]
```

gives the same dataset as the first example above.

A *Dataset* can also be created from a file where every line is a new random sample. The data in the first example above could have been stored in a file with the following content:

```
# file: datafile
s 1.1
v [12.2,20.6]
s 0.8
v [14.1,19.2]
s 0.95
v [10.3,19.7]
s 0.91
v [8.2,21.0]
```

Lines that begin with # are ignored. Assuming the file is called datafile, we create a dataset identical to that above using the code:

```
>>> data = Dataset('datafile')
>>> print(data['s'])
[ 1.1, 0.8, 0.95, 0.91]
```

Data can be binned while reading it in, which might be useful if the data set is huge. To bin the data contained in file datafile in bins of binsize 2 we use:

```
>>> data = Dataset('datafile',binsize=2)
>>> print(data['s'])
[0.95, 0.93]
```

The keys read from a data file are restricted to those listed in keyword keys and those that are matched (or partially matched) by regular expression grep if one or other of these is specified: for example,

```
>>> data = Dataset('datafile')
>>> print([k for k in a])
['s', 'v']
>>> data = Dataset('datafile', keys=['v'])
>>> print([k for k in a])
['v']
>>> data = Dataset('datafile', grep='[^v]')
```

```
>>> print([k for k in a])
['s']
>>> data = Dataset('datafile', keys=['v'], grep='[^v]')
>>> print([k for k in a])
[]
```

Datasets can also be constructed from dictionaries, other Datasets, or lists of key-data tuples. For example,

```
>>> data = Dataset('datafile')
>>> data_binned = Dataset(data, binsize=2)
>>> data_v = Dataset(data, keys=['v'])
```

reads data from file 'datafile' into Dataset data, and then creates a new Dataset with the data binned (data\_binned), and another that only containes the data with key 'v' (data\_v).

The main attributes and methods are:

#### samplesize

Smallest number of samples for any key.

```
append (*args, **kargs)
```

Append data to dataset.

There are three equivalent ways of adding data to a dataset data: for example, each of

```
data.append(n=1.739, a=[0.494,2.734]) # method 1

data.append(n,1.739) # method 2

data.append(a,[0.494,2.734])

dd = dict(n=1.739, a=[0.494,2.734]) # method 3

data.append(dd)
```

adds one new random number to data ['n'], and a new vector to data ['a'].

```
extend(*args, **kargs)
```

Add batched data to dataset.

There are three equivalent ways of adding batched data, containing multiple samples for each quantity, to a dataset data: for example, each of

adds two new random numbers to data ['n'], and two new random vectors to data ['a'].

This method can be used to merge two datasets, whether or not they share keys: for example,

```
data = Dataset("file1")
  data_extra = Dataset("file2")
  data.extend(data_extra) # data now contains all of data_extra
```

#### grep (rexp)

Create new dataset containing items whose keys match rexp.

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Returns a new gwar.dataset.Dataset 'containing only the items self[k] whose keys k match regular expression rexp (a string) according to Python module re:

```
>>> a = Dataset()
>>> a.append(xx=1.,xy=[10.,100.])
>>> a.append(xx=2.,xy=[20.,200.])
>>> print(a.grep('y'))
{'yy': [array([ 10., 100.]), array([ 20., 200.])]}
>>> print(a.grep('x'))
{'xx': [1.0, 2.0], 'xy': [array([ 10., 100.]), array([ 20., 200.])]}
>>> print(a.grep('x|y'))
{'xx': [1.0, 2.0], 'xy': [array([ 10., 100.]), array([ 20., 200.])]}
>>> print a.grep('[^y][^x]')
{'xy': [array([ 10., 100.]), array([ 20., 200.])]}
```

Items are retained even if rexp matches only part of the item's key.

#### slice(sl)

Create new dataset with self[k] -> self[k][sl].

Parameter sl is a slice object that is applied to every item in the dataset to produce a new gvar. Dataset. Setting sl = slice(0, None, 2), for example, discards every other sample for each quantity in the dataset. Setting sl = slice(100, None) discards the first 100 samples for each quantity.

If parameter sl is a tuple of slice objects, these are applied to successive indices of self[k]. An exception is called if the number of slice objects exceeds the number of dimensions for any self[k].

#### arrayzip (template)

Merge lists of random data according to template.

template is an array of keys in the dataset, where the shapes of self[k] are the same for all keys k in template. self.arrayzip(template) merges the lists of random numbers/arrays associated with these keys to create a new list of (merged) random arrays whose layout is specified by template: for example,

```
>>> d = Dataset()
>>> d.append(a=1,b=10)
>>> d.append(a=2,b=20)
>>> d.append(a=3,b=30)
>>> print(d)
                        # three random samples each for a and b
{'a': [1.0, 2.0, 3.0], 'b': [10.0, 20.0, 30.0]}
>>> # merge into list of 2-vectors:
>>> print(d.arrayzip(['a','b']))
[[ 1. 10.]
[ 2. 20.]
[ 3. 30.]]
>>> # merge into list of (symmetric) 2x2 matrices:
>>> print(d.arrayzip([['b','a'],['a','b']]))
[[[ 10.
        1.]
  Γ
   1. 10.]]
 [[ 20.
         2.1
    2.
        20.]]
 [[ 30.
         30.]]
```

The number of samples in each merged result is the same as the number samples for each key (here 3). The keys used in this example represent scalar quantities; in general, they could be either scalars or arrays

(of any shape, so long as all have the same shape).

### trim()

Create new dataset where all entries have same sample size.

### toarray()

Create dictionary d where d[k]=numpy.array(self[k]) for all k.

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## **NUMERICAL ANALYSIS MODULES IN GVAR**

gvar. GVars can be used in many numerical algorithms, to propagates errors through the algorithm. A code that is written in pure Python is likely to work well with gvar. GVars, perhaps with minor modifications. Here we describe some sample numerical codes, included in gvar, that have been adapted to work with gvar. GVars, as well as with floats. More examples will follow with time.

The sub-modules included here are:

- qvar.cspline cubic splines for 1-d data.
- gvar.linalg basic linear algebra.
- qvar. ode integration of systems of ordinary differential equations; one-dimensional integrals.
- gvar.powerseries power series representation of functions.
- *gvar.root* root-finding for one-dimensional functions.

## 4.1 Cubic Splines

Module gvar.cspline implements a class for smoothing and/or interpolating one-dimensional data using cubic splines:

**class** gvar.cspline.**CSpline** (*xknots*, *yknots*, *deriv*=(*None*, *None*), *extrap\_order*=3, *warn*=*True*) Cubic spline approximation to a function.

Given N values of a function yknot[i] at N points xknot[i] for i=0..N-1 (the 'knots' of the spline), the code

```
from gvar.cspline import CSpline

f = CSpline(xknot, yknot)
```

defines a function f such that: a) f(xknot[i]) = yknot[i] for all i; and b) f(x) is continuous, as are its first and second derivatives. Function f(x) is a cubic polynomial between the knots xknot[i].

CSpline (xknot, yknot) creates a *natural spline*, which has zero second derivative at the end points, xknot[0] and xknot[-1] (assuming the knots are sorted). More generally one can specify the derivatives of f(x) at one or both of the endpoints:

```
f = CSpline(xknot, yknot, deriv=[dydx_i, dydx_f])
```

where dydx\_i is the derivative at xknot [0] and dydx\_f is the derivative at xknot [-1]. Replacing either (or both) of these with None results in a derivative corresponding to zero second derivative at that boundary (i.e., a *natural* boundary).

Derivatives and integrals of the spline function can also be evaluated:

```
f.D(x) — first derivative at x;
f.D2(x) — second derivative at x;
f.integ(x) — integral from xknot[0] to x.
```

Splines can be used outside the range covered by the defining xknot values. As this is often a bad idea, the CSpline methods issue a warning when called with out-of-range points. The warning can be suppressed by setting parameter warn=False. The spline value for an out-of-range point is calculated using a polynomial whose value and derivatives match those of the spline at the knot closest to the out-of-range point. The extrapolation polynomial is cubic by default, but lower orders can be specified by setting parameter extrap\_order to a (non-negative) integer less than 3; this is often a good idea.

#### **Examples**

Typical usage is:

```
>>> import math
>>> import gvar as gv
>>> xknot = [0., 0.78539816, 1.57079633, 2.35619449, 3.14159265]
>>> yknot = [0., 0.70710678, 1.0, 0.70710678, 0.]
>>> f = gv.cspline.CSpline(xknot, yknot)
>>> print(f(0.7), f.D(0.7), f.D2(0.7), f.integ(0.7))
0.644243383101 0.765592448296 -0.663236750777 0.234963942648
```

Here the yknot values were obtained by taking sin(xknot). Tabulating results from the spline together with the exact results shows that this 5-knot spline gives a pretty good approximation of the function sin(x), as well as its derivatives and integral:

```
f(x)
            f.D(x) f.D2(x) f.inteq(x) | sin(x) cos(x) 1-cos(x)
0.3 0.2951 0.9551 -0.2842 0.04458
                                    1 0.2955 0.9553 0.04466
0.5 0.4791 0.8793 -0.4737 0.1222
                                    | 0.4794 0.8776 0.1224
0.7 0.6442 0.7656 -0.6632 0.235
                                    0.6442
                                              0.7648 0.2352
0.9 0.783
           0.6176 -0.7891 0.3782
                                    0.7833
                                              0.6216 0.3784
    0.8902 0.452
                   -0.8676 \ 0.5461
                                    0.8912
                                             0.4536 0.5464
1.3
    0.9627
           0.2706 -0.9461 0.7319
                                    1 0.9636 0.2675 0.7325
    0.9974
           0.07352 -1.025 0.9286
                                    1 0.9975 0.07074 0.9293
```

Using the spline outside the range covered by the knots is less good:

```
>>> print(f(2 * math.pi))
gvar/cspline.py:164: UserWarning: x outside of spline range: [ 6.28318531]
1.7618635470106501
```

The correct answer is 0.0, of course. This is why the spline function issues a warning. Working just outside the knot region is often fine, although it is usually a good idea to limit the order of the polynomial used in such regions: for example, setting

```
>>> f = gv.cspline.CSpline(xknot, yknot, extrap_order=2)
```

implies that quadratic polynomials are used outside the spline range. Finally one can specify the values of the first derivatives of the function at one or the other endpoints of the spline region, if they are known. Continuing from above, for example, one would take

```
>>> f = gv.cspline.CSpline(xknot, yknot, deriv=[1., -1.])
```

since the derivatives of sin(x) at x=0 and x=3.14159265 are 1 and -1, respectively.

#### **Parameters**

- **xknot** (*1-d sequence of number*) The knots of the spline, where the function values are specified. The knots are sorted (from small to large) if necessary.
- **yknot** (*1-d sequence of number*) Function values at the locations specified by xknot[i].
- **deriv** (2-component sequence) Derivatives at initial and final boundaries of the region specified by xknot [i]. Default value is None for each boundary.
- **extrap\_order** (*int*) Order of polynomial used for extrapolations outside of the spline range. The polynomial is constructed from the spline's value and derivatives at the (nearest) knot of the spline. The allowed range is 0 <= extrap\_order <= 3. The default value is 3 although it is common practice to use smaller values.
- warn (bool) If True, warnings are generated when the spline function is called for x values that fall outside of the original range of xknots used to define the spline. Default value is True; out-of-range warnings are suppressed if set to False.

## 4.2 Linear Algebra

Module gvar.linalg implements several methods for doing basic linear algebra with matrices whose elements can be either numbers or gvar.GVars:

```
linalg.det(a)
```

Determinant of matrix a.

**Parameters a** – Two-dimensional, square matrix/array of numbers and/or gvar. GVars.

Returns Deterimant of the matrix.

**Raises** ValueError – If matrix is not square and two-dimensional.

```
linalg.slogdet(a)
```

Sign and logarithm of determinant of matrix a.

**Parameters a** – Two-dimensional, square matrix/array of numbers and/or gvar. GVars.

**Returns** Tuple (s, logdet) where the determinant of matrix a is s \* exp(logdet).

Raises ValueError – If matrix is not square and two-dimensional.

```
linalg.inv(a)
```

Inverse of matrix a.

**Parameters a** – Two-dimensional, square matrix/array of numbers and/or gvar. GVars.

**Returns** The inverse of matrix a.

**Raises** ValueError – If matrix is not square and two-dimensional.

```
\texttt{linalg.solve}\left(a,b\right)
```

Find x such that a.dot (x) = b for matrix a.

#### **Parameters**

- a Two-dimensional, square matrix/array of numbers and/or gvar. GVars.
- **b** One-dimensional vector/array of numbers and/or *gvar.GVars*, or an array of such vectors. Requires b.shape[0] == a.shape[1].

**Returns** The solution x of a.dot (x) = b, which is equivalent to inv (a).dot (b).

**Raises** 

- ValueError If a is not square and two-dimensional.
- ValueError If shape of b does not match that of a (that is b.shape[0] != a.shape[1]).

linalg.eigvalsh(a, eigvec=False)

Eigenvalues of Hermitian matrix a.

#### **Parameters**

- a Two-dimensional, square matrix/array of numbers and/or gvar. GVars.
- eigvec (bool) If True, method returns a tuple of arrays (val, vec) where the val[i] are the eigenvalues. Arrays vec[:, i] are the corresponding eigenvectors of a when one ignores uncertainties (that is, they are eigenvectors of gvar.mean(a)). Only val is returned if eigvec=False (default).

Returns Array of eigenvalues of matrix a if parameter eigvec==False (default). where the val[i] are the eigenvalues; otherwise it returns a tuple of arrays (val, vec) where the val[i] are the eigenvalues. Arrays vec[:, i] are the corresponding eigenvectors of a when one ignores uncertainties (that is, they are eigenvectors of qvar.mean(a)).

**Raises** ValueError – If matrix is not square and two-dimensional.

## 4.3 Ordinary Differential Equations

Module *gvar.ode* implements two classes for integrating systems of first-order differential equations using an adaptive Runge-Kutta algorithm. One integrates scalar- or array-valued equations, while the other integrates dictionary-valued equations:

```
class gvar.ode.Integrator(deriv, tol=1e-05, h=None, hmin=None, analyzer=None)
Integrate dy/dx = deriv(x,y).
```

An Integrator object odeint integrates dy/dx = f(x,y) to obtain y(x1) from y0 = y(x0). y and f(x,y) can be scalars or numpy arrays. Typical usage is illustrated by the following code for integrating dy/dx = y:

```
from gvar.ode import Integrator

def f(x, y):
    return y

odeint = Integrator(deriv=f, tol=1e-8)
y0 = 1.
y1 = odeint(y0, interval=(0, 1.))
y2 = odeint(y1, interval=(1., 2.))
...
```

Here the first call to odeint integrates the differential equation from x=0 to x=1 starting with y=y0 at x=0; the result is y1=exp(1), of course. Similarly the second call to odeint continues the integration from x=1 to x=2, giving y2=exp(2).

If the interval is a list with more than two entries, then odeint (y0, interval=[x0, x1, x2 ...]) in the example above returns an array of solutions for points x1, x2 .... So the example above could have been written equivalently as

```
odeint = Integrator(deriv=f, tol=1e-8)
```

```
y0 = 1.
y1, y2 ... = odeint(y0, interval=[0, 1., 2. ...])
```

An alternative interface creates a new function which is the solution of the differential equation for specific initial conditions. The code above could be rewritten:

```
x0 = 0.  # initial conditions
y0 = 1.
y = Integrator(deriv=f, tol=1e-8).solution(x0, y0)
y1 = y(1)
y2 = y(2)
...
```

Here method Integrator.solution() returns a function y(x) where: a) y(x0) = y0; and b) y(x) uses the integrator to integrate the differential equation to point x starting from the last point at which y was evaluated (or from x0 for the first call to y(x)). The function can also be called with an array of x values, in which case an array containing the corresponding y values is returned.

The integrator uses an adaptive Runge-Kutta algorithm that adjusts the integrator's step size to obtain relative accuracy tol in the solution. An initial step size can be set in the *Integrator* by specifying parameter h. A minimum step size hmin can also be specified; the *Integrator* raises an exception if the step size becomes smaller than hmin. The *Integrator* keeps track of the number of good steps, where h is increased, and the number of bad steps, where h is decreased and the step is repeated: odeint.ngood and odeint.nbad, respectively.

A custom criterion for step-size changes can be implemented by specifying a function for parameter delta. This is a function delta(yerr, y, delta\_y) — of the estimated error yerr after a given step, the proposed value for y, and the proposed change delta\_y in y — that returns a number to compare with tolerance tol. The step size is decreased and the step repeated if delta(yerr, y, delta\_y) > tol; otherwise the step is accepted and the step size increased. The default definition of delta is roughly equivalent to:

A custom definition can be used to allow an Integrator to work with data types other than floats or numpy arrays of floats. All that is required of the data type is that it support ordinary arithmetic. Therefore, for example, defining delta(yerr, y, delta\_y) with np.abs() instead of np.fabs() allows y to be complex valued. (Actually the default delta allows this as well.)

An analyzer analyzer (x, y) can be specified using parameter analyzer. This function is called after every full step of the integration, with the current values of x and y. Objects of type gvar.ode.Solution are examples of (simple) analyzers.

#### **Parameters**

- deriv Function of x and y that returns dy/dx. The return value should have the same shape as y if arrays are used.
- tol (*float*) Relative accuracy in y relative to |y| + h|dy/dx| for each step in the integration. Any integration step that achieves less precision is repeated with a smaller step size. The step size is increased if precision is higher than needed. Default is 1e-5.
- h (*float or None*) Absolute value of initial step size. The default value equals the entire width of the integration interval.

- **hmin** (*float or None*) Smallest step size allowed. A warning is raised if a smaller step size is requested, and the step size is not decreased. This prevents infinite loops at singular points, but the solution may not be reliable when a warning has been issued. The default value is None (which does *not* prevent infinite loops).
- delta-Function delta(yerr, y, delta\_y) that returns a number to be compared with tol at each integration step: if it is larger than tol, the step is repeated with a smaller step size; if it is smaller the step is accepted and a larger step size used for the subsequent step. Here yerr is an estimate of the error in y on the last step; y is the proposed value; and delta\_y is the change in y over the last step.
- analyzer Function of x and y that is called after each step of the integration. This can be used to analyze intermediate results.

class gvar.ode.DictIntegrator (deriv, tol=1e-05, h=None, hmin=None, analyzer=None)

Integrate dy/dx = deriv(x,y) where y is a dictionary.

An DictIntegrator object odeint integrates dy/dx = f(x,y) to obtain y(x1) from y0 = y(x0). y and f(x,y) are dictionary types having the same keys, and containing scalars and/or numpy arrays as values. Typical usage is:

The first call to odeint integrates from x=x0 to x=x1, returning y1=y(x1). The second call continues the integration to x=x2, returning y2=y(x2). Multiple integration points can be specified in interval, in which case a list of the corresponding y values is returned: for example,

```
odeint = DictIntegrator(deriv=f, tol=1e-8)
y1, y2 ... = odeint(y0, interval=[x0, x1, x2 ...])
```

The integrator uses an adaptive Runge-Kutta algorithm that adjusts the integrator's step size to obtain relative accuracy tol in the solution. An initial step size can be set in the <code>DictIntegrator</code> by specifying parameter h. A minimum step size hmin can also be specified; the <code>Integrator</code> raises an exception if the step size becomes smaller than hmin. The <code>DictIntegrator</code> keeps track of the number of good steps, where h is increased, and the number of bad steps, where h is decreases and the step is repeated: odeint.ngood and odeint.nbad, respectively.

An analyzer analyzer (x, y) can be specified using parameter analyzer. This function is called after every full step of the integration with the current values of x and y. Objects of type gvar.ode.Solution are examples of (simple) analyzers.

### **Parameters**

- deriv Function of x and y that returns dy/dx. The return value should be a dictionary
  with the same keys as y, and values that have the same shape as the corresponding values in
  y.
- tol (float) Relative accuracy in y relative to |y| + h|dy/dx| for each step in the integration. Any integration step that achieves less precision is repeated with a smaller step size. The step size is increased if precision is higher than needed.
- **h** (*float*) Absolute value of initial step size. The default value equals the entire width of the integration interval.

- hmin (float) Smallest step size allowed. A warning is raised if a smaller step size is requested, and the step size is not decreased. This prevents infinite loops at singular points, but the solution may not be reliable when a warning has been issued. The default value is None (which does not prevent infinite loops).
- analyzer Function of x and y that is called after each step of the integration. This can be used to analyze intermediate results.

A simple analyzer class is:

```
class gvar.ode.Solution
```

ODE analyzer for storing intermediate values.

Usage: eg, given

```
odeint = Integrator(...)
soln = Solution()
y0 = ...
y = odeint(y0, interval=(x0, x), analyzer=soln)
```

then the soln.x[i] are the points at which the integrator evaluated the solution, and soln.y[i] is the solution of the differential equation at that point.

## 4.4 One-Dimensional Integration

Module gvar.ode also provides a method for evaluating one-dimensional integrals (using its adaptive Runge-Kutta algorithm):

ode.integral (fcn, interval, fcnshape=None, tol=1e-08, hmin=None) Compute integral of fcn(x) on interval.

Given a function fcn(x) the call

```
result = integral(fcn, interval=(x0, x1))
```

calculates the integral of fcn(x) from x0 to x1. For example:

```
>>> def fcn(x):
...    return math.sin(x) ** 2 / math.pi
>>> result = integral(fcn, (0, math.pi))
>>> print(result)
0.500000002834
```

Function fcn(x) can return a scalar or an array (any shape): for example,

```
>>> def fcn(x):
...    return np.array([1., x, x**3])

>>> result = integral(fcn, (0,1))
>>> print(result)
[1. 0.5 0.25]
```

The function can also return dictionaries whose values are scalars or arrays: for example,

```
>>> def fcn(x):
...    return dict(x=x, x3=x**3)
>>> result = integral(fcn, (0,1))
>>> print(result)
{'x': 0.5,'x3': 0.25}
```

#### **Parameters**

- fcn Function of scalar variable x that returns the integrand. The return value should be either a scalar or an array, or a dictionary whose values are scalars and/or arrays.
- **interval** Contains the interval (x0, x1) over which the integral is computed.
- fcnshape Contains the shape of the array returned by f(x) or () if the function returns a scalar. Setting fshape=None (the default) results in an extra function evaluation to determine the shape.
- tol Relative accuracy of result.
- hmin Smallest step size allowed in adaptive integral. A warning is raised if a smaller step size is requested, and the step size is not decreased. This prevents infinite loops at singular points, but the integral may not be accurate when a warning has been issued. The default value is None (which does *not* prevent infinite loops).

### 4.5 Power Series

Module *gvar.powerseries* provides tools for manipulating power series approximations of functions. A function's power series is specified by the coefficients in its Taylor expansion with respect to an independent variable, say x:

```
f(x) = f(0) + f'(0)*x + (f''(0)/2)*x**2 + (f'''(0)/6)*x**3 + ...
= f0 + f1*x + f2*x**2 + f3*x**3 + ...
```

In practice a power series is different from a polynomial because power series, while infinite order in principle, are truncated at some finite order in numerical applications. The order of a power series is the highest power of x that is retained in the approximation; coefficients for still higher-order terms are assumed to be unknown (as opposed to zero).

Taylor's theorem can be used to generate power series for functions of power series:

```
g(f(x)) = g(f0) + g'(f0) * (f(x)-f0) + (g''(f0)/2) * (f(x)-f0) * * 2 + ...
= g0 + g1 * x + g2 * x * * 2 + ...
```

This allows us to define a full calculus for power series, where arithmetic expressions and (sufficiently differentiable) functions of power series return new power series.

#### 4.5.1 Power series arithmetic

Class *PowerSeries* provides a numerical implementation of the power series calculus. PowerSeries ([f0,f1,f2,f3...]) is a numerical representation of a power series with coefficients f0, f1, f2, f3... (as in f(x) above). Thus, for example, we can define a 4th-order power series approximation f to exp(x) = 1 + x + x + 2/2 + ... using

Arithmetic expressions involving instances of class *PowerSeries* are themselves *PowerSeries* as in, for example,

The standard arithmetic operators (+,-,\*,/,=,\*\*) are supported, as are the usual elementary functions (exp, log, sin, cos, tan ...). Different *PowerSeries* can be combined arithmetically to create new *PowerSeries*; the order of the result is that of the operand with the lowest order.

PowerSeries can be differentiated and integrated:

Each *PowerSeries* represents a function. The *PowerSeries* for a function of a function is easily obtained. For example, assume f represents function  $f(x) = \exp(x)$ , as above, and g represents  $g(x) = \log(1+x)$ :

```
>>> g = PowerSeries([0, 1, -1/2., 1/3., -1/4.])
```

Then f(g) gives the PowerSeries for exp(log(1+x)) = 1 + x:

```
>>> print f(g)
[ 1.0000e+00    1.0000e+00    0.0000e+00    -2.7755e-17    -7.6327e-17]
```

Individual coefficients from the powerseries can be accessed using array-element notation: for example,

## 4.5.2 Numerical evaluation of power series

The power series can also be evaluated for a particular numerical value of x: continuing the example,

```
>>> x = 0.01
>>> print f(x) # should be exp(0.01)-1 approximately
0.0100501670833
```

```
>>> print exp(x)-1  # verify that it is 0.0100501670842
```

The independent variable x could be of any arithmetic type (it need not be a float).

## 4.5.3 Taylor expansions of Python functions

PowerSeries can be used to compute Taylor series for more-or-less arbitrary pure-Python functions provided the functions are locally analytic (or at least sufficiently differentiable). To compute the N-th order expansion of a Python function g(x), first create a N-th order PowerSeries variable that represents the expansion parameter: say, x = PowerSeries([0.,1.],order=N). The Taylor series for function g(x) is then given by  $g_t(x)$  which is a PowerSeries instance. For example, consider:

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```
>>> from gvar.powerseries import *
>>> def g(x): # an example of a Python function
       return 0.5/sqrt(1+x) + 0.5/sqrt(1-x)
>>> x = PowerSeries([0.,1.],order=5)
                                   # Taylor series for x
>>> print x
[ 0. 1. 0. 0. 0. 0.]
>>> g_{taylor} = g(x) # Taylor series for g(x) about x=0
>>> print g_taylor
                      0.375 0.
           0.
                                         0.2734375 0.
                                                              ]
>>> exp_taylor = exp(x) # Taylor series for exp(x) about x=0
>>> print exp_taylor
                        0.5
             1.
                                    0.16666667 0.04166667 0.008333331
```

class gvar.powerseries.PowerSeries (c=None, order=None)

Power series representation of a function.

The power series created by PowerSeries (c) corresponds to:

```
c[0] + c[1]*x + c[2]*x**2 + ...
```

The order of the power series is normally determined by the length of the input list c. This can be overridden by specifying the order of the power series using the order parameter. The list of c[i]s is then padded with zeros if c is too short, or truncated if it is too long. Omitting c altogether results in a power series all of whose coefficients are zero. Individual series coefficients are accessed using array/list notation: for example, the 3rd-order coefficient of PowerSeries p is p[3]. The order of p is p.order. PowerSeries should work for coefficients of any data type that supports ordinary arithmetic.

Arithmetic expressions of *PowerSeries* variables yield new *PowerSeries* results that represent the power series expansion of the expression. Expressions can include the standard mathematical functions (log, exp, sqrt, sin, cos, tan...). *PowerSeries* can also be differentiated (p.deriv()) and integrated (p.integ()).

#### **Parameters**

- c (list or array) Power series coefficients (optional if parameter order specified).
- **order** (*integer*) Highest power in power series (optional if parameter *c* specified).

```
___iter__()
```

Iterate over coefficients of power series C{self}.

```
\_setitem\_(i, val)
```

Set C{i}th coefficient of power series equal to C{val}.

#### deriv(n=1)

Compute *n*-th derivative of self.

**Parameters n** (*positive integer*) – Number of derivatives.

**Returns** *n*-th derivative of self.

```
integ(n=1, x0=None)
```

Compute *n*-th indefinite integral of self.

If x0 is specified, then the definite integral, integrating from point x0, is returned.

#### **Parameters**

- **n** (*integer*) Number of integrations.
- **x0** Starting point for definite integral (optional).

**Returns** *n*-th integral of self.

order

Highest power in power series.

## 4.6 Root Finding

Module gvar.root contains methods for finding the roots of one-dimensional functions: that is, finding x such that fcn(x) = 0 for a given function fcn. Typical usage is:

```
>>> import math
>>> import gvar as gv
>>> interval = gv.root.search(math.sin, 1.)  # bracket root
>>> print(interval)
(3.1384283767210035, 3.4522712143931042)
>>> root = gv.root.refine(math.sin, interval)  # refine root
>>> print(root)
3.14159265359
```

This code finds the first root of sin(x) = 0 larger than 1. The first setp is a search to find an interval containing a root. Here gvar.root.search() examines sin(x) for a sequence of points 1. \* 1.1 \*\* n for n=0,1,2..., stopping when the function changes sign. The last two points in the sequence then bracket a root since sin(x) is continuous; they are returned as a tuple to interval. The final root is found by refining the interval, using gvar.root.refine. By default, the root is refined iteratively to machine precision, but this requires only a small number (4) of iterations:

```
>>> print(root.nit) # number of iterations
4
```

The most challenging situations are ones where the function is extremely flat in the vicinity of the root — that is, two or more of its leading derivatives vanish there. For example:

```
>>> import gvar as gv
>>> def f(x):
...    return (x + 1) ** 3 * (x - 0.5) ** 11
>>> root = gv.root.refine(f, (0, 2))
>>> print(root)
0.5
>>> print(root.nit)  # number of iterations
142
```

This routine also works with variables of type gvar. GVar: for example,

```
>>> import gvar as gv
>>> def f(x, w=gv.gvar(1, 0.1)):
... return gv.sin(w * x)
>>> root = gv.root.refine(f, (1, 4))
>>> print(root)
3.14(31)
```

returns a root with a 10% uncertainty, reflecting the uncertainty in parameter w.

Descriptions of the two methods follow.

```
root.search (fcn, x0, incr=0, fac=1.1, maxit=100, analyzer=None)
Search for and bracket root of one-dimensional function fcn (x).
```

This method searches for an interval in x that brackets a root of fcn (x) =0. It examines points

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```
x[j + 1] = fac * x[j] + incr
```

where x[0]=x0 and j=0...maxit-1, looking for a pair of successive points where fcn (x[j]) changes sign. These points bracket a root (assuming the function is continuous), providing a coarse estimate of the root. That estimate can be refined using root.refine().

#### **Example**

The following code seeks to bracket the first zero of sin(x) with x>0.1:

```
>>> import math
>>> import gvar as gv
>>> interval = gv.root.search(math.sin, 0.1)
>>> print(interval)
(3.0912680532870755, 3.4003948586157833)
```

The resulting interval correctly brackets the root at pi.

#### **Parameters**

- fcn One dimenionsal function whose root is sought.
- **x0** (*float*) Starting point for search.
- incr (float, optional) Increment used for linear searches. Default value is 0.
- fac (float, optional) Rescaling factor for exponential searches. Default value is 1.1.
- maxit (int, optional) Maximum number of steps allowed for search. An exception is raised if a root is not found in time. Default value is 100.
- analyzer Optional function f(x, fcn(x)) that is called for each point x that is examined. This can be used, for example, to monitor the search while debugging. Default is None.

#### Returns

Tuple (a, b) where fcn(a) \* fcn(b) <= 0, which implies that a root occurs between a and b (provided the function is continuous). The tuple has extra attributes that provide additional information about the search:

- **nit** Number of iterations used to find interval (a,b).
- fcnval Tuple containing the function values at (a,b).

Raises RuntimeError – If unable to find a root in maxit steps.

root.refine (fcn, interval, rtol=None, maxit=1000, analyzer=None)

Find root x of one-dimensional function fcn on an interval.

This method finds a root x of fcn(x) = 0 inside an interval = (a, b) that brackets the root, with fcn(a)  $\star$  fcn(b) <= 0.

This method is a pure Python adaptation of an algorithm from Richard Brent's book "Algorithms for Minimization without Derivatives" (1973). Being pure Python it works with *gvar.GVar*-valued functions and variables.

#### **Example**

The following code finds a root of sin(x) in the interval 1  $\leq$  x  $\leq$  4, using 7 iterative refinements of the initial interval:

```
>>> import math
>>> import gvar as gv
>>> root = gv.root.refine(math.sin, (1, 4))
>>> print(root)
3.14159265359
>>> print(root.nit)
7
```

#### **Parameters**

- fcn One-dimensional function whose zero/root is sought.
- interval Tuple (a,b) specifying an interval containing the root, with fcn(a) \* fcn(b) <= 0. The search for a root is confined to this interval.
- rtol (float, optional) Relative tolerance for the root. The default value is None, which sets rtol equal to machine precision (sys.float\_info.epsilon). A larger value usually leads to less precision but is faster.
- maxit (int, optional) Maximum number of iterations used to find a root with the given tolerance. A warning is issued if the algorithm does not converge in time. (Default value is 1000.)
- analyzer Optional function f(x, fcn(x)) that is called for each point x examined by the algorithm. This can be used, for example, to monitor convergence while debugging. Default is None.

#### Returns

The root, which is either a float or a gvar. GVar but with extra attributes that provide additional information about the root:

- **nit** Number of iterations used to find the root.
- **interval** Smallest interval (b, c) found containing the root, where b is the root returned by the method.
- fcnval Value of fcn(x) at the root.

#### Raises

- ValueError If fcn(a) \* fcn(b) > 0 for initial interval (a,b).
- UserWarning If the algorithm fails to converge after maxit iterations.

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**CHAPTER** 

**FIVE** 

### CASE STUDY: PENDULUM CLOCK

This case study illustrates how to mix gvar. GVars with numerical routines for integrating differential equations (gvar.ode) and for finding roots of functions (gvar.root). It also gives a simple example of a simulation that uses gvar. GVars.

### 5.1 The Problem

The precision of a particular pendulum clock is limited by two dominant factors: 1) the length of the pendulum (0.25m) can be adjusted with a precision of at best  $\pm 0.5\text{mm}$ ; and 2) irregularities in the drive mechanism mean that the maximum angle of swing  $(\pi/6)$  is uncertain by  $\pm 0.025$  radians. The challenge is to determine how these uncertainties affect time-keeping over a day.

The angle theta(t) of the pendulum satisfies a differential equation

```
d/dt \ d/dt \ theta(t) = -(g/l) \ sin(theta(t))
```

where g is the acceleration due to gravity and the 1 is the length of the pendulum.

## 5.2 Pendulum Dynamics; Finding the Period

We start by designing code to integrate the differential equation:

```
import numpy as np
import gvar as gv

def make_pendulum(theta0, 1):
    """ Create pendulum solution y(t) = [theta(t), d/dt theta(t)].

    Initial conditions are y(0) = [theta0, 0]. Parameter 1 is the length of the pendulum.
    """
    g_1 = 9.8 / 1
    def deriv(t, y):
        """ Calculate d/dt [theta(t), d/dt theta(t)]. """
        theta, dtheta_dt = y
        return np.array([dtheta_dt, - g_1 * gv.sin(theta)])
    y0 = np.array([theta0, 0.0])
    return gv.ode.Integrator(deriv=deriv).solution(0.0, y0)
```

Given a solution y(t) of the differential equation from this method, we find the period of oscillation using gvar.root: the period is the time at which the pendulum returns to its starting point and its velocity (y(t)[1]) vanishes:

```
def find_period(y, Tapprox):
    """ Find oscillation period of pendulum solution y(t).

Parameter Tapprox is the approximate period. The code finds the time between 0.7 * Tapprox and 1.3 * Tapprox where y(t)[1] = d/dt theta(t) vanishes. This is the period, provided Tapprox is correctly chosen.
    """
    def dtheta_dt(t):
        """ vanishes when dtheta/dt = 0 """
        return y(t)[1]
    return gv.root.refine(dtheta_dt, (0.7 * Tapprox, 1.3 * Tapprox))
```

## 5.3 Analysis

The last piece of the code does the analysis:

```
def main():
   1 = gv.gvar(0.25, 0.0005)
                                          # length of pendulum
   theta_max = gv.gvar(np.pi / 6, 0.025) # max angle of swing
                                          # y(t) = [theta(t), d/dt theta(t)]
   y = make_pendulum(theta_max, 1)
    # period in sec
   T = find_period(y, Tapprox=1.0)
   print('period T = {} sec'.format(T))
    # uncertainty in minutes per day
   fmt = 'uncertainty = {:.2f} min/day \n'
   print(fmt.format((T.sdev / T.mean) * 60. * 24.))
    # error budget for T
   inputs = dict(l=1, theta_max=theta_max)
   outputs = dict(T=T)
   print(gv.fmt_errorbudget(outputs=outputs, inputs=inputs))
if __name__ == '__main__':
    main()
```

Here both the length of the pendulum and the maximum angle of swing have uncertainties and are represented by gvar.GVar objects. These uncertainties work their way through both the integration and root finding to give a final result for the period that is also a gvar.GVar. Running the code results in the following output:

The period is T = 1.0210(20) sec, which has an uncertainty of about  $\pm 0.2\%$ . This corresponds to an uncertainty of  $\pm 2.8$  min/day for the clock.

The uncertainty in the period is caused by the uncertainties in the length 1 and the angle of maximum swing theta\_max. The error budget at the end of the output shows how much error comes from each source:

0.17% comes from the angle, and 0.10% comes from the length. (The two errors added in quadrature give the total.) We could have estimated the error due to the length from the standard formula  $2\pi$  sqrt(l/g) for the period, which is approximately true here. Estimating the uncertainty due to the angle is trickier, since it comes from nonlinearities in the differential equation.

The error budget tells us how to improve the clock. For example, we can reduce the error due to the angle by redesigning the clock so that the maximum angle of swing is  $\pi/36 \pm 0.025$  rather than  $\pi/6 \pm 0.025$ . The period becomes independent of the maximum angle as that angle vanishes, and so becomes less sensitive to uncertainties in it. Taking the smaller angle reduces that part of the period's error from 0.17% to 0.03%, thereby cutting the total error almost in half, to  $\pm 0.10\%$  or about  $\pm 1.5$  min/day. Further improvement requires tighter control over the length of the pendulum.

### 5.4 Simulation

We can check the error propagation analysis above using a simulation. Adding the following code at the end of main () above

```
# check errors in T using a simulation
Tlist = []
for i in range(100):
    y = make_pendulum(theta_max(), 1())
    T = find_period(y, Tapprox=1.0)
    Tlist.append(T)
print('period T = {:.4f} +- {:.4f}'.format(np.mean(Tlist), np.std(Tlist)))
```

gives the following additional output:

```
period T = 1.0209 +- 0.0020
```

The new code generates 100 different values for the period T, corresponding to randomly chosen values for the ta\_max and 1 drawn from the Gaussian distributions corresponding to their gvar.GVars. (In general, each call x () for gvar.GVar x is a new random number drawn from x's Gaussian distribution.) The mean and standard deviation of the list of periods give us our final result. Results fluctuate with only 100 samples; taking 10,000 samples shows that the result is 1.0210(20), as we obtained in the previous section above (using a tiny fraction of the computer time).

Note that the *gvar.GVars* in this simulation are uncorrelated and so their random values can be generated independently. *gvar.raniter()* should be used to generate random values from correlated *gvar.GVars*.

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## **CHAPTER**

# SIX

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