$\mathbf{py}_{grama}$

Release 0.3.3

Jul 15, 2023

Contents:

CHAPTER 1

Overview

The `py_grama` package is an implementation of a *grammar of model analysis* (*grama*)—a language for describing and analyzing models.

1.1 What Models?

Statisticians often use "model" to refer to random variable models. Scientists and engineers often use "model" to refer to simplified physics resulting in function models. In *grama* we refer to a collection of random variables and functions *together* as a model.

1.2 Why *grama*?

Considering both the functional mapping between variables and the uncertainties in those variables is of critical importance to a full understanding of a given problem. Given the "split" perspective between statisticians and engineers, unifying the perspectives is a conceptual challenge.

While much effort in the uncertainty quantification (UQ) community has been made on merging the two perspectives on the *algorithmic* side, relatively little work has been done to merge the two perspectives *conceptually*. The aforementioned understanding of "models"—functions plus random variables—is a step towards conceptually unifying these two perspectives.

1.3 Why `py_grama`?

Furthermore, virtually *no* work has been done to make UQ techniques easily learnable and accessible. The `py_grama` package is heavily inspired by the Tidyverse, partly in terms of functional programming patterns, but primarily in terms of its *user-first perspective*. `py_grama` is designed to help users learn and use UQ tools to analyze models.

1.4 Why quantify uncertainty?

Uncertainty quantification is a relatively new scientific discipline, so the motivation for doing UQ may not be immediately obvious. The following example notebooks demonstrate UQ in a number of settings:

- structural safety: cable design example—failing to account for uncertainty can lead to unsafe structures. UQ enables safer design.

1.5 What does it look like?

For a quick demonstration of `py_grama`, see the following demo notebooks:

- The model building demo shows how to build a *grama* model in a scientifically-reproducible way.
- The model analysis demo shows how *grama* can be used to analyze an existing model, using compact syntax to probe how both functions and randomness affect model outputs.

CHAPTER 2

Language Details

The following is a fairly extensive introduction to the *grama* language. This is (admittedly) not a great place to start learning how to *use* `py_grama`, but is instead provided as a reference.

grama is a conceptual language, and `py_grama` is a code implementation of that concept. This page is a description of both the concept and its implementation.

2.1 Running example

We'll use a running example throughout this page; the built-in `py_grama` Cantilever Beam model.

```
import grama as gr
from grama.models import make_cantilever_beam

md_beam = make_cantilever_beam()
md_beam.printpretty()
```

```
model: Cantilever Beam

  inputs:
    var_det:
      w: [2, 4]
      t: [2, 4]
    var_rand:
      H: (+1) norm, {'loc': 500.0, 'scale': 100.0}
      V: (+1) norm, {'loc': 1000.0, 'scale': 100.0}
      E: (+0) norm, {'loc': 29000000.0, 'scale': 1450000.0}
      Y: (-1) norm, {'loc': 40000.0, 'scale': 2000.0}
  functions:
    cross-sectional area: ['w', 't'] -> ['c_area']
    limit state: stress: ['w', 't', 'H', 'V', 'E', 'Y'] -> ['g_stress']
    limit state: displacement: ['w', 't', 'H', 'V', 'E', 'Y'] -> ['g_disp']
```

2.2 Objects

grama focuses on two categories of objects:

- **data** (`df`): observations on various quantities, implemented by the Python package Pandas
- **models** (`md`): functions and a complete description of their inputs, implemented by py_grama

For readability, we suggest using prefixes `df_` and `md_` when naming DataFrames and models.

2.2.1 Data

Data are observations on some quantities. Data often come from the real world, but data are also used to inform models, and models can be used to generate new data. `py_grama` uses the Pandas `DataFrame` implementation to represent data. Since data operations are already well-handled by Pandas, `py_grama` uses the existing Pandas infrastructure and focuses on providing tools to handle models and their interface with data.

2.2.2 Models

Models in *grama* have both functions and inputs. `py_grama` implements models in the `Model` class, which in turn have three primary objects:

- `Domain`: Defines bounds on variables
- `Density`: Defines a joint density for variables
- List of`Functions`: Maps variables to outputs

Domain

The domain of the model defines bounds for all the variables. If a variable is not included in the domain object, it is assumed to be unbounded. The model above has bounds on `t, w`, both of which are `[2, 4]`.

Density

The density of the model defines a joint density for the *random* variables. If a variable is included in the density it is random, otherwise it is *deterministic*. The model above has a joint density on `H, V, E, Y`. The model summary gives details on each marginal distribution.

Functions

A function has a set of variables, which map to a set of outputs; for instance, the `cross-sectional area` function above maps `['w', 't'] -> ['c_area']`. The other functions take more variables, all of which map to their respective outputs.

Inputs

The full set of model inputs are organized into:

- **Variables** are inputs to the model's functions
  - **Deterministic** variables are chosen by the user; the model above has `w, t`

  - **Random** variables are not controlled; the model above has `H, V, E, Y`

- **Parameters** are inputs to the model's density
  - **Deterministic** parameters are currently implemented; these are listed under `var_rand` with their associated random variable
  - **Random** parameters* are not yet implemented

The full set of *variables* is determined by the domain, density, and functions. Formally, the full set of variables is given (in pseudocode) by `domain.var + [f.var for f in functions]`. The set of random variables is then given by `domain.var + [f.var for f in functions] - density.marginals.keys()`, while the deterministic variables are the remainder `var_det = var_full - var_rand`.

2.3 Verbs

Verbs are used to take action on different *grama* objects. We use verbs to generate data from models, build new models from data, and ultimately make sense of the two.

The following table summarizes the categories of `py_grama` verbs. Verbs take either data (`df`) or a model (`md`), and may return either object type. The prefix of a verb immediately tells one both the input and output types. The short prefix is used to denote the *pipe-enabled version* of a verb.

Since `py_grama` is focused on models, the majority of functions lie in the Evaluate, Fit, and Compose categories, with only a few original Transform utilities provided. Some shortcut plotting utilities are also provided for covenience.

`py_grama` verbs are used to both *build* and *analyze* models.

2.3.1 Model Building

The *recommended* way to build `py_grama` models is with *composition calls*. Calling `Model()` creates an "empty" model, to which one can add.

```
md = gr.Model()
md.printpretty()
```

```
model: None

  inputs:
    var_det:
    var_rand:
  functions:
```

We can then use Compose functions to build up a complete model step-by step. We recommend starting with the functions, as those highlight the required variables.

```
md = gr.Model("Test") >> \
     gr.cp_function(
          fun=lambda x: [x[0], x[1]],
          var=["x0", "x1"],
          out=2,
          name="Identity"
     )
md.printpretty()
```

```
model: Test

  inputs:
    var_det:
      x0: (unbounded)
      x1: (unbounded)
    var_rand:
  functions:
    Identity: ['x0', 'x1'] -> ['y0', 'y1']
```

Note that by default all of the variables are assumed to be deterministic. We can override this by adding marginal distributions for one or more of the variables.

```
md = gr.Model("Test") >> \
     gr.cp_function(
         fun=lambda x: [x[0], x[1]],
         var=["x0", "x1"],
         out=2,
         name="Identity"
     ) >> \
     gr.cp_marginals(
         x1=dict(dist="norm", loc=0, scale=1)
     )
md.printpretty()
```

```
model: Test

  inputs:
    var_det:
      x0: (unbounded)
    var_rand:
      x1: (+0) norm, {'loc': 0, 'scale': 1}
  functions:
    Identity: ['x0', 'x1'] -> ['y0', 'y1']
```

The marginals are implemented in terms of the Scipy continuous distributions; see the variable `gr.valid_dist.keys()` for a list of implemented marginals. When calling `gr.comp_marginals()`, we provide the target variable name as a keyword argument, and the marginal information via dictionary. The marginal shape is specified with the "dist" keyword; all distributions require the `loc, scale` parameters, but some require additional keywords. See `gr.param_dist` for a dictionary mapping between distributions and parameters.

Once we have constructed our model, we can analyze it with a number of tools.

2.3.2 Model Analysis

One question in model analysis is to what degree the random variables affect the outputs. A way to quantify this is with *Sobol' indices* (Sobol', 1999). We can estimate Sobol' indices in `py_grama` with the following code.

```
df_sobol = \
    md_beam >> \
    gr.ev_hybrid(n=1e3, df_det="nom", seed=101) >> \
    gr.tf_sobol()
print(df_sobol)
```

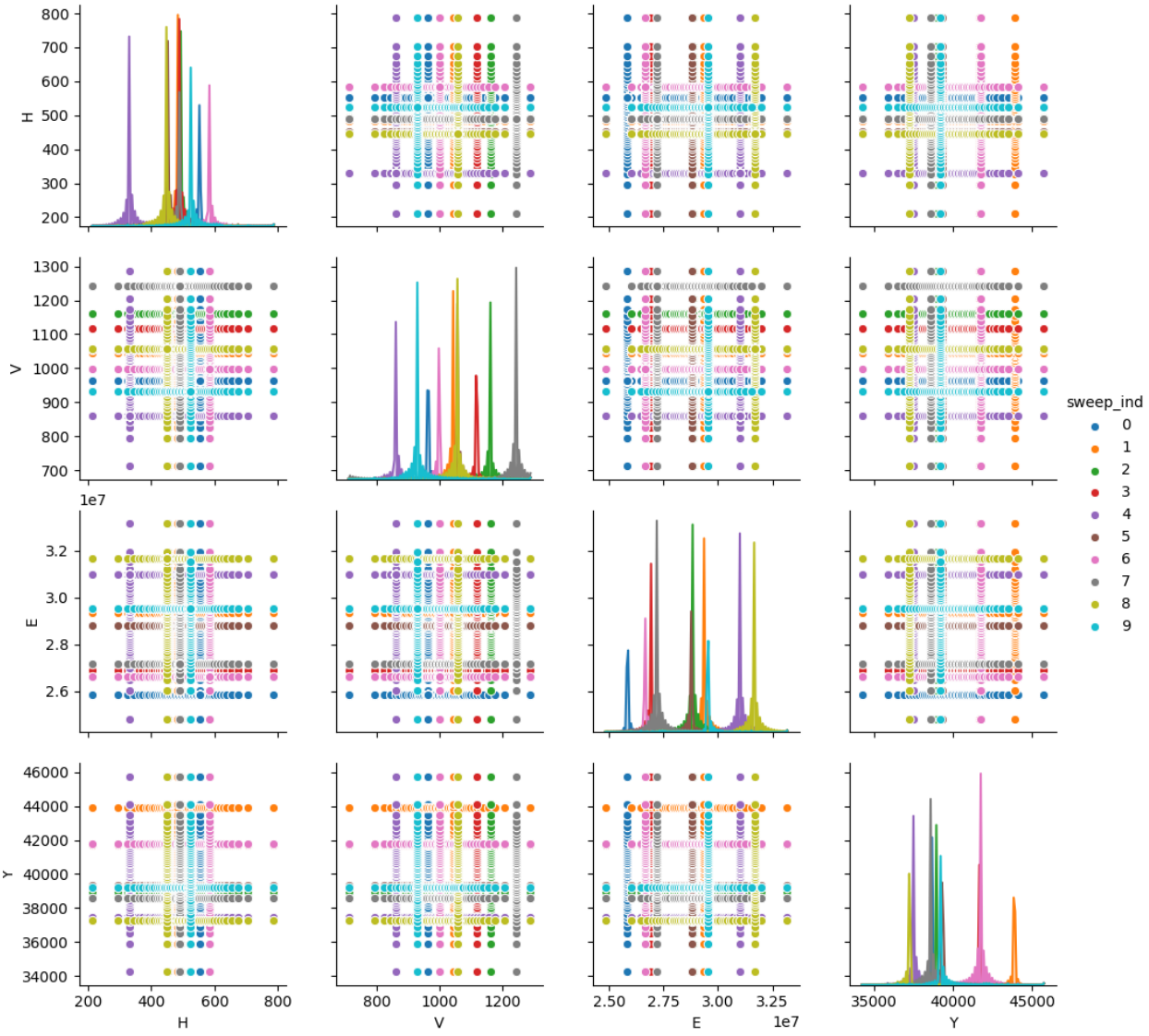
```
eval_hybrid() is rounding n...
     w    t  c_area     g_stress  g_disp  ind
0  NaN  NaN     NaN        -0.03    0.28  S_E
0  NaN  NaN     NaN         0.35    0.21  S_H
0  NaN  NaN     NaN         0.33    0.64  S_V
0  NaN  NaN     NaN         0.31    0.02  S_Y
0  0.0  0.0     0.0   -345263.39    0.01  T_E
0  0.0  0.0     0.0    4867712.30    0.01  T_H
0  0.0  0.0     0.0    4577175.85    0.02  T_V
0  0.0  0.0     0.0    4224965.01    0.00  T_Y
0  0.0  0.0     0.0  13758547.04    0.04  var
```

The normalized Sobol' indices are reported with `S_[var]` labels; they indicate that `g_stress` is affected roughly equally by the inputs `H,V,Y`, while `g_disp` is affected about twice as much by `V` as by `E` or `H`. Note that the Sobol' indices are *only* defined for the random variables—since Sobol' indices are defined in terms of fractional variances, they are only formally valid for quantifying contributions from sources of randomness.

Under the hood `gr.eval_hybrid()` attaches metadata to its resulting DataFrame, which `gr.tran_sobol()` detects and uses in post-processing the data.

`py_grama` also provides tools for constructing visual summaries of models. We can construct a *sinew plot* with a couple lines of code. First we inspect the design:

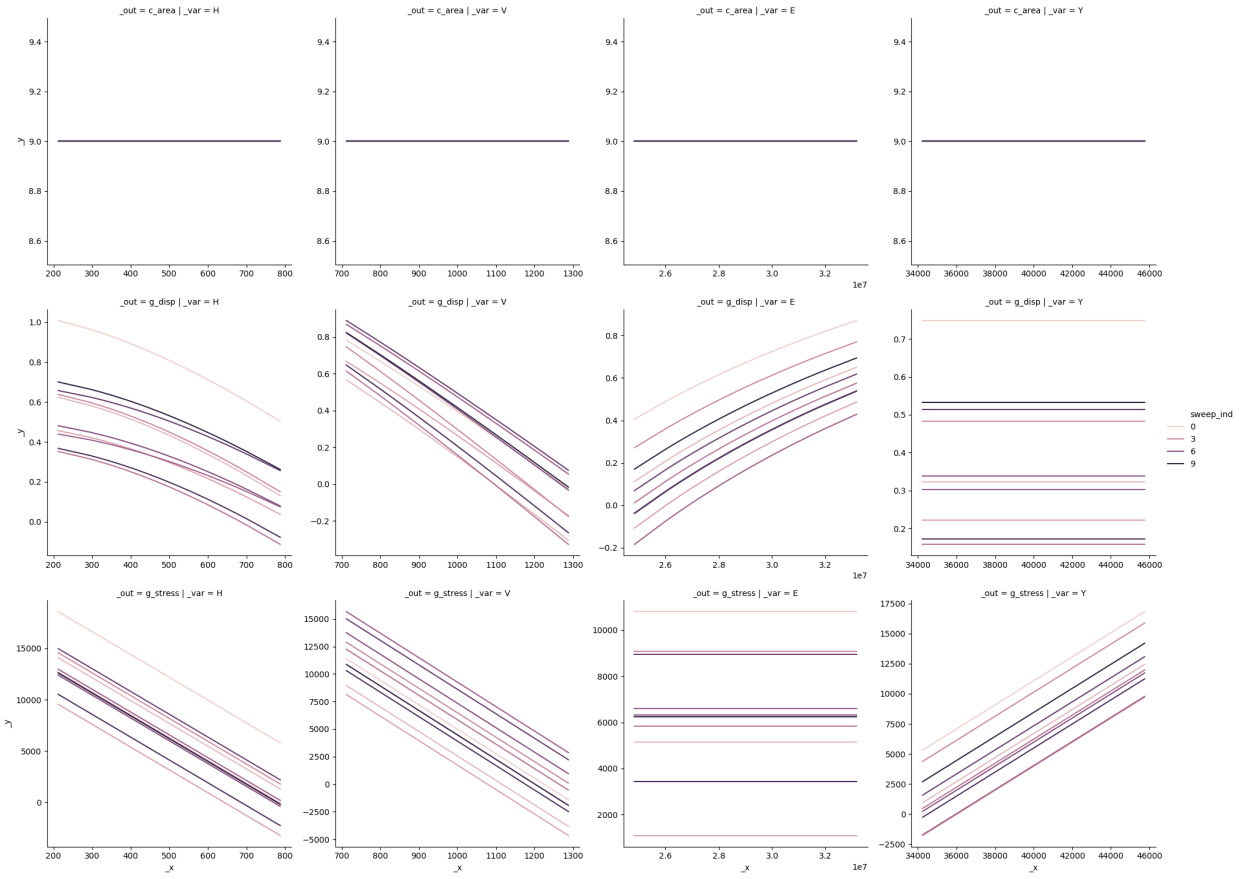
```
md_beam >> \
    gr.ev_sinews(n_density=50, n_sweeps=10, df_det="nom", skip=True) >> \
    gr.pt_auto()
```



beam sinew results

The "sinews" are sweeps across random variable space which start at random locations, and continue parallel to the variable axes. Evaluating these samples allows us to construct a sinew plot:

```
md_beam >> \
    gr.ev_sinews(n_density=50, n_sweeps=10, df_det="nom", skip=False) >> \
    gr.pt_auto()
```



beam sinew results

Here we can see that inputs `H,E` tend to saturate in their effects on `g_disp`, while `V` is linear over its domain. This may explain the difference in contributed variance seen above via Sobol' indices.

By providing tools to quickly perform different analyses, one can quickly get a sense of model behavior using `py_grama`.

2.4 Layers and Defaults

`py_grama` is built around *layers and defaults*. As much as is possible `py_grama` is designed to provide sensible defaults "out-of-the-box". We saw the concept of *layers* above in the model building example. The following example shows defaults in action.

2.4.1 Example Defaults: `gr.eval_monte_carlo()`

Attempting to provide no arguments to `gr.eval_monte_carlo()` yields the following error:

```
df_res = md_beam >> gr.ev_monte_carlo()
```

```
...
ValueError: df_det must be DataFrame or 'nom'
```

One can sample over the random variables given their joint density, but this tells us nothing about how to treat the deterministic variables. The error message above tells us that we have to define the deterministic variable levels

through `df_det`. To perform simple studies, we can explicitly limit attention to the nominal conditions.

```
df_res = md_beam >> gr.ev_monte_carlo(df_det="nom")
print(df_res.describe())
```

```
                H           V             E  ...  c_area    g_stress    g_disp
count    1.000000    1.000000  1.000000e+00  ...     1.0     1.00000  1.000000
mean   505.743982  906.946892  2.824652e+07  ...     9.0  9758.06826  0.438044
std           NaN         NaN           NaN  ...     NaN         NaN       NaN
min    505.743982  906.946892  2.824652e+07  ...     9.0  9758.06826  0.438044
25%    505.743982  906.946892  2.824652e+07  ...     9.0  9758.06826  0.438044
50%    505.743982  906.946892  2.824652e+07  ...     9.0  9758.06826  0.438044
75%    505.743982  906.946892  2.824652e+07  ...     9.0  9758.06826  0.438044
max    505.743982  906.946892  2.824652e+07  ...     9.0  9758.06826  0.438044

[8 rows x 9 columns]
```

By default `gr.eval_monte_carlo()` will draw a single sample; this leads to the `NaN` standard deviation (`std`) results. We can override this default behavior by providing the `n` keyword.

```
df_res = md_beam >> gr.ev_monte_carlo(df_det="nom", n=1e3)
print(df_res.describe())
```

```
eval_monte_carlo() is rounding n...
                H            V             E  ...  c_area      g_stress       g_disp
count  1000.000000  1000.000000  1.000000e+03  ...  1000.0   1000.000000  1000.000000
mean    499.776481  1001.908814  2.899238e+07  ...     9.0   6589.731053     0.333387
std     100.878972   102.929434  1.523033e+06  ...     0.0   3807.292688     0.199576
min     168.466610   635.220875  2.427615e+07  ...     9.0  -5830.363269    -0.339594
25%     433.466349   933.698938  2.799035e+07  ...     9.0   3921.581411     0.200657
50%     500.201964  1002.514072  2.896188e+07  ...     9.0   6633.083925     0.339702
75%     569.159912  1065.489928  2.993924e+07  ...     9.0   9161.066426     0.465231
max     798.543698  1327.618914  3.378264e+07  ...     9.0  18682.531892     1.045742

[8 rows x 9 columns]
```

Formally `1e3` is a float, which is not a valid iteration count. The routine `gr.eval_monte_carlo()` informs us that it first rounds the given value before proceeding. Here we can see some variation in the inputs and outputs, though `c_area` is clearly unaffected by the randomness.

We can also provide an explicit DataFrame to the `df_det` argument. The `gr.eval_monte_carlo()` routine will automatically take an *outer product* of the deterministic settings with the random samples; this will lead to a multiplication in sample size of `df_det.shape[0] * n`. Since this can get quite large, we should reduce `n` before proceeding. We can also *delay evaluation* first with the `skip` keyword, and inspect the design first before evaluating it.

```
df_det = pd.DataFrame(dict(
    w=[3] * 10,
    t=[2.5 + i/10 for i in range(10)]
))

df_design = md_beam >> gr.ev_monte_carlo(df_det=df_det, n=1e2, skip=True)
print(df_design.describe())
```

```
eval_monte_carlo() is rounding n...
                H            V             E             Y       w            t
```

(continues on next page)

(continued from previous page)

```
count  1000.000000  1000.000000  1.000000e+03   1000.000000  1000.0  1000.000000
mean    485.021539   989.376268  2.890355e+07  40135.172902     3.0     2.950000
std     112.546373    92.381768  1.462286e+06   2135.788506     0.0     0.287372
min     137.606474   764.764234  2.586955e+07  33320.789307     3.0     2.500000
25%     411.652958   927.448139  2.763002e+07  39104.255172     3.0     2.700000
50%     490.765903  1002.513232  2.903287e+07  40121.853496     3.0     2.950000
75%     561.317283  1046.038620  2.994359e+07  41279.345157     3.0     3.200000
max     726.351812  1239.473097  3.176696e+07  45753.627265     3.0     3.400000
```

If we are happy with the design (possibly after visual inspection), we can pass the input DataFrame to the straight evaluation routine

```
df_res = md_beam >> gr.ev_df(df=df_design)
print(df_res.describe())
```

```
                H            V             E  ...       c_area      g_stress       g_
disp
count  1000.000000  1000.000000  1.000000e+03  ...  1000.000000   1000.000000  1000.00
0000
mean    510.457048  1003.972079  2.887534e+07  ...     8.850000   4555.508097     0.12
0805
std     105.566743    91.443354  1.486829e+06  ...     0.862116   7027.137049     0.59
9538
min     269.102628   830.234813  2.553299e+07  ...     7.500000 -18370.732185    -1.84
8058
25%     437.342719   939.490354  2.794973e+07  ...     8.100000   -385.620306    -0.29
7274
50%     515.387982   995.468715  2.868415e+07  ...     8.850000   5347.337598     0.23
2133
75%     584.899669  1054.815972  2.982724e+07  ...     9.600000   9824.615141     0.60
9096
max     775.221819  1257.095025  3.369872e+07  ...    10.200000  21238.954122     1.23
6387

[8 rows x 9 columns]
```

2.5 Functional Programming (Pipes)

Functional programming touches both the practical and conceptual aspects of the language. `py_grama` provides tools to use functional programming patterns. Short-stem versions of `py_grama` functions are *pipe-enabled*, meaning they can be used in functional programming form with the pipe operator `>>`. These pipe-enabled functions are simply aliases for the base functions, as demonstrated below:

```
df_base = gr.eval_nominal(md_beam, df_det="nom")
df_functional = md_beam >> gr.ev_nominal(df_det="nom")

df_base.equals(df_functional)
```

```
True
```

Functional patterns enable chaining multiple commands, as demonstrated in the following Sobol' index analysis. In nested form using base functions, this would be:

```
df_sobol = gr.tran_sobol(gr.eval_hybrid(md_beam, n=1e3, df_det="nom", seed=101))
```

From the code above, it is difficult to see that we first consider `md_beam`, perform a hybrid-point evaluation, then use those data to estimate Sobol' indices. With more chained functions, this only becomes more difficult. One could make the code significantly more readable by introducing intermediate variables:

```
df_samples = gr.eval_hybrid(md_beam, n=1e3, df_det="nom", seed=101)
df_sobol = gr.tran_sobol(df_samples)
```

Conceptually, using *pipe-enabled* functions allows one to skip assigning intermediate variables, and instead pass results along to the next function. The pipe operator >> inserts the results of one function as the first argument of the next function. A pipe-enabled version of the code above would be:

```
df_sobol = \
    md_beam >> \
    gr.ev_hybrid(n=1e3, df_det="nom", seed=101) >> \
    gr.tf_sobol()
```

2.6 References

- I.M. Sobol', "Sensitivity Estimates for Nonlinear Mathematical Models" (1999) MMCE, Vol 1.

CHAPTER 3

Random Variable Modeling

Random variable modeling is a *huge* topic, but there are some key ideas that are important to know. This short chapter is a brief introduction to random variable modeling.

```
import grama as gr
DF = gr.Intention()
```

3.1 Random Variables in Grama

Random variables in grama are defined as part of a model. For instance, the following syntax defines a joint distribution for two inputs `x` and `y`.

```
(
    gr.Model("An example")
    # ... Function definitions
    >> gr.cp_marginals(
        x=gr.marg_mom("norm", mean=0, sd=1),
        y=gr.marg_mom("lognorm", mean=0, sd=1, floc=0),
    )
    >> gr.cp_copula_gaussian(
        df_corr=gr.df_make(var1="x", var2="y", corr=0.5)
    )
)
```

Grama defines joint distributions in terms of *marginals* and a *copula*. This definition is justified by Skylar's Theorem, which states that an arbitrary joint distribution can be expressed in terms of its marginals and a copula. Practically, this modeling approach decomposes random variable modeling into two stages: Modeling the individual uncertainties with marginals, then modeling their dependency with a copula.

3.2 Running Example

As a running example, we will study the built-in die cast aluminum dataset.

```
from grama.data import df_shewhart
```

3.3 Marginals

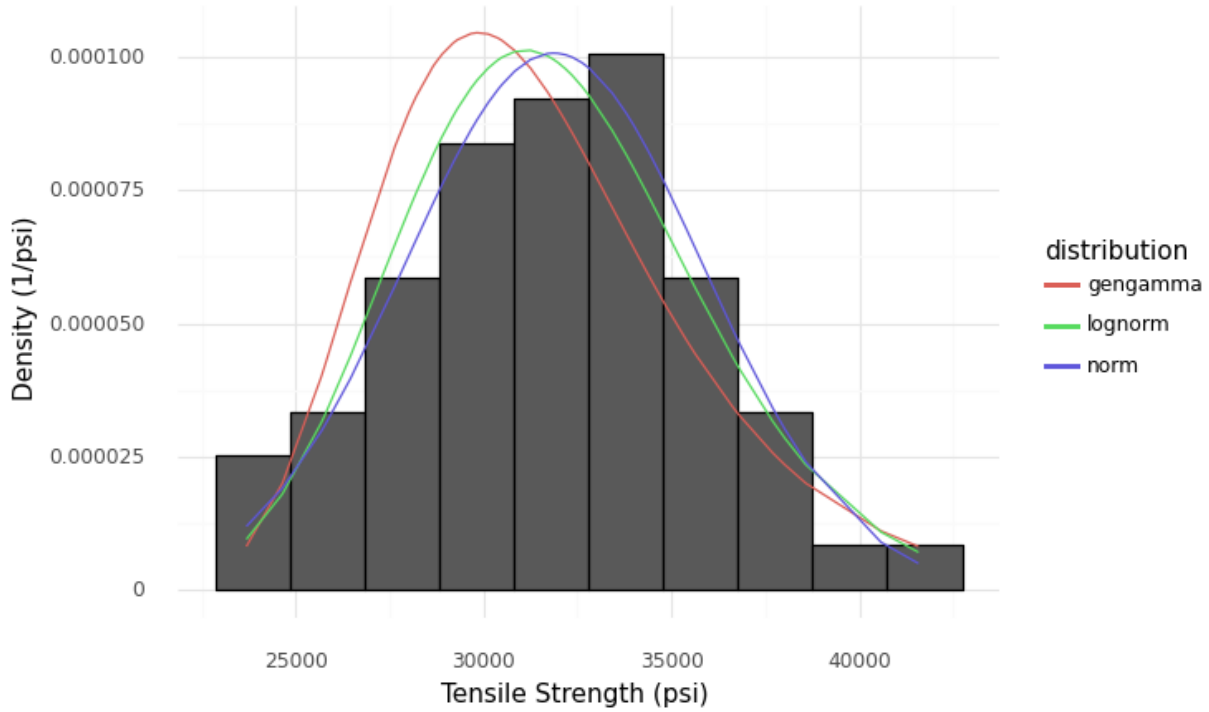
Marginal distributions provide a quantitative description of uncertainty for a single quantity. Perhaps the most important factor in modeling a marginal is the shape of the distribution used to describe that quantity; there are often multiple competing distribution shapes that we could pick to fit the same dataset. For instance, the following code fits three different shapes to the `tensile_strength` in the example dataset.

```
mg_ts_norm = gr.marg_named(
    df_shewhart.tensile_strength,
    "norm", # Normal distribution
)

mg_ts_lognorm = gr.marg_named(
    df_shewhart.tensile_strength,
    "lognorm", # Lognormal distribution
    floc=0, # 2-parameter lognormal
)

mg_ts_gengamma = gr.marg_named(
    df_shewhart.tensile_strength,
    "gengamma", # Generalized gamma distribution
    floc=0, # 3-parameter generalized gamma
)
```

Visualizing the distributions gives three fairly plausible fits to the data:

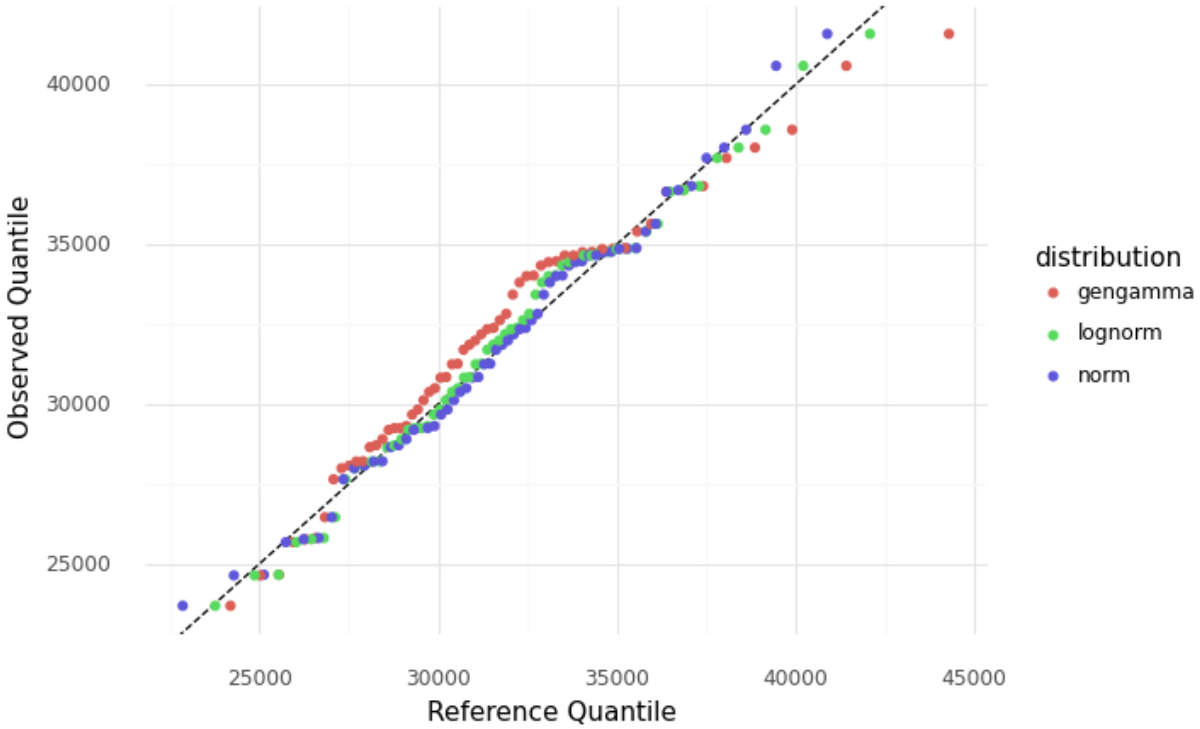


Comparison of three fitted distributions with a histogram of the tensile strength data

A more sensitive way to make this comparison is with a QQ plot.

```
(
    df_shewhart
    >> gr.tf_mutate(
        q_norm=gr.qqvals(DF.tensile_strength, marg=mg_ts_norm),
        q_lognorm=gr.qqvals(DF.tensile_strength, marg=mg_ts_lognorm),
        q_gengamma=gr.qqvals(DF.tensile_strength, marg=mg_ts_gengamma),
    )
    >> gr.tf_pivot_longer(
        columns=["q_norm", "q_lognorm", "q_gengamma"],
        names_to=[".value", "distribution"],
        names_sep="_",
    )

    >> gr.ggplot(gr.aes("q", "tensile_strength"))
    + gr.geom_abline(intercept=0, slope=1, linetype="dashed")
    + gr.geom_point(gr.aes(color="distribution"))
    + gr.theme_minimal()
    + gr.theme(plot_background=gr.element_rect(color="white", fill="white"))
    + gr.labs(x="Reference Quantile", y="Observed Quantile")
)
```



Comparison of three fitted distributions with a qq plot

This comparison reveals that the gamma distribution is shifted in its center, while the normal and lognormal fits are both fairly plausible.

3.4 Dependency

Marginals alone do not define a random variable. Dependency describes how values from different variables are related. Independent random variables are specified with an independence copula with `gr.cp_copula_independence()`. This is a common assumption, but it is frequently violated in practice.

Experimental and simulated observations, independent marginals

A simple way to represent dependency is with a gaussian copula, accessed with `gr.cp_copula_gaussian()`.

Experimental and simulated observations, gaussian copula

Note that it is *critically important* to state your assumptions when modeling random variables! You may have been

sent to this page by an error message: That's because grama *requires* you to make your assumptions about dependency explicit.

CHAPTER 4

grama

4.1 grama package

4.1.1 Subpackages

grama.data package

Submodules

grama.data.datasets module

Module contents

Datasets

Built-in datasets.

Datasets:

df_diamonds: Diamond characteristics and prices. Columns: carat:

cut:

color:

clarity:

depth:

table:

price:

x:

y:

z:

df_stang: Aluminum alloy data from Stang et al. (1946). Columns: thick (inches): Nominal thickness

alloy: Alloy designation

E (Kips/inch^2): Young's modulus

mu (-): Poisson's ratio

ang (degrees): Angle of test to alloy roll direction

df_ruff: Metal data from Ruff (1984). Columns: part: Part identifier

TYS: Tensile Yield Stress (ksi)

TUS: Tensile Ultimate Stress (ksi)

thickness: Part thickness (in)

df_trajectory_full: Simulated trajectory data. Columns:

t: Time since projectile launch (seconds)

x: Projectile range (meters)

y: Projectile height (meters)

df_shewhart: Aluminum die cast data from Table 3 in Shewhart (1931)

specimen: Specimen identifier

tensile_strength: Specimen tensile strength (psi). The original reference does not specify if this is the yield or ultimate strength.

hardness: Specimen hardness (Rockwell's "E")

density: Specimen density (gm/cm^3)

References

Stang, Greenspan, and Newman, "Poisson's ratio of some structural alloys for large strains" (1946) U.S. Department of Commerce National Bureau of Standards

Ruff, Paul E. An Overview of the MIL-HDBK-5 Program. BATTELLE COLUMBUS DIV OH, 1984.

Shewhart *Economic Control of Quality of Manufactured Product* (1931) D. Van Nostrand Company, Inc.

grama.dfply package

Submodules

grama.dfply.base module

class grama.dfply.base.**Intention**(*function=<function Intention.<lambda>>*, *invert=False*)

Bases: object

evaluate(*context*)

grama.dfply.base.**dfdelegate**(*f*)

grama.dfply.base.**make_symbolic**(*f*)

grama.dfply.base.**symbolic_evaluation**(*function=None*, *eval_symbols=True*, *eval_as_label=[]*, *eval_as_selector=[]*)

class grama.dfply.base.**group_delegation**(*function*)
Bases: object

grama.dfply.base.**flatten**(*l*)

grama.dfply.count module

grama.dfply.group module

grama.dfply.group.**tran_ungroup**(*df*)

grama.dfply.join module

grama.dfply.mask_helpers module

grama.dfply.mask_helpers.**var_in**(**args*, ***kwargs*)
Determine if value is in collection

Returns a boolean series where each entry denotes inclusion in the provided collection. Intended for use in tran_filter() calls.

Parameters

- **series** – column to compute inclusion bools
- **collection** – set for inclusion calcs

grama.dfply.mask_helpers.**is_nan**(**args*, ***kwargs*)
Determine if nan

Returns a boolean series where each entry denotes NaN or not. Intended for use in tran_filter() calls.

Parameters

- **series** (*Pandas series*) – column to compute NaN bools
- **inv** (*bool*) – Invert logic

grama.dfply.mask_helpers.**not_nan**(**args*, ***kwargs*)
Determine if NOT nan

Returns a boolean series where each entry denotes NOT NaN or yes. Intended for use in tran_filter() calls.

Parameters

- **series** (*Pandas series*) – column to compute NOT NaN bools
- **inv** (*bool*) – Invert logic

grama.dfply.reshape module

grama.dfply.reshape.**convert_type**(*df*, *columns*)
Helper function that attempts to convert columns into their appropriate data type.

grama.dfply.select module

grama.dfply.select.**is_numeric**(**args*, ***kwargs*)

Determine if column is numeric

Returns True if the provided column is numeric, False otherwise. Intended for calls to select_if() or mutate_if().

Parameters **bool** – Boolean corresponding to the datatype of the given column

Examples:: import grama as gr from grama.data import df_diamonds

(df_diamonds gr.tf_select_if(gr.is_numeric)

)

grama.dfply.select.**starts_with**(**args*, ***kwargs*)

grama.dfply.select.**ends_with**(**args*, ***kwargs*)

grama.dfply.select.**contains**(**args*, ***kwargs*)

grama.dfply.select.**matches**(**args*, ***kwargs*)

grama.dfply.select.**everything**(**args*, ***kwargs*)

grama.dfply.select.**num_range**(**args*, ***kwargs*)

grama.dfply.select.**one_of**(**args*, ***kwargs*)

grama.dfply.select.**columns_between**(**args*, ***kwargs*)

grama.dfply.select.**columns_from**(**args*, ***kwargs*)

grama.dfply.select.**columns_to**(**args*, ***kwargs*)

grama.dfply.select.**resolve_selection**(*df*, **args*, *drop=False*)

grama.dfply.set_ops module

grama.dfply.string_helpers module

grama.dfply.subset module

grama.dfply.summarize module

grama.dfply.summary_functions module

grama.dfply.summary_functions.**binomial_ci**(**args*, ***kwargs*)

Returns a binomial confidence interval

Computes a binomial confidence interval based on boolean data. Uses Wilson interval

Parameters

- **series** (*pandas.Series*) – Column to summarize; must be boolean or 0/1.
- **alpha** (*float*) – Confidence level; value in (0, 1)
- **side** (*string*) – Chosen side of interval - “both”: Return a 2-tuple of series - “lo”: Return the lower interval bound - “up”: Return the upper interval bound

grama.dfply.summary_functions.**corr**(**args*, ***kwargs*)
Computes a correlation coefficient

Computes a correlation coefficient using either the pearson or spearman formulation.

Parameters

- **series1** (*pandas.Series*) – Column 1 to study
- **series2** (*pandas.Series*) – Column 2 to study
- **method** (*str*) – Method to use; either "pearson" or "spearman"
- **res** (*str*) – Quantities to return; either "corr" or "both"
- **na_drop** (*bool*) – Drop NaN values before computation?

Returns correlation coefficient

Return type pandas.Series

grama.dfply.summary_functions.**mean**(**args*, ***kwargs*)
Returns the mean of a series.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**mean_lo**(**args*, ***kwargs*)
Return a confidence interval (lower bound) for the mean

Uses a central limit approximation for a lower confidence bound of an estimated mean. That is:

m - q(alpha) * s / sqrt(n)

where

m = sample mean s = sample standard deviation n = sample size q(alpha) = alpha-level lower-quantile of standard normal

= (-norm.ppf(alpha))

For a two-sided interval at a confidence level of `C`, set `alpha = 1 - C` and use `[gr.mean_lo(X, alpha=alpha/2), gr.mean_up(X, alpha=alpha/2)`. Note that the default `alpha` level for both helpers is calibrated for a two-sided interval with `C = 0.99`.

Parameters

- **series** (*pandas.Series*) – column to summarize
- **alpha** (*float*) – alpha-level for calculation. Note that the confidence level C is given by `C = 1 - alpha`.

Returns Lower confidence interval for the mean

Return type float

grama.dfply.summary_functions.**mean_up**(**args*, ***kwargs*)
Return a confidence interval (upper bound) for the mean

Uses a central limit approximation for a upper confidence bound of an estimated mean. That is:

m + q(alpha) * s / sqrt(n)

where

m = sample mean s = sample standard deviation n = sample size q(alpha) = alpha-level lower-quantile of standard normal

= (-norm.ppf(alpha))

For a two-sided interval at a confidence level of `C`, set `alpha = 1 - C` and use `[gr.mean_lo(X, alpha=alpha/2), gr.mean_up(X, alpha=alpha/2)]`. Note that the default `alpha` level for both helpers is calibrated for a two-sided interval with `C = 0.99`.

Parameters

- **series** (*pandas.Series*) – column to summarize
- **alpha** (*float*) – alpha-level for calculation. Note that the confidence level C is given by `C = 1 - alpha`.

Returns Upper confidence interval for the mean

Return type float

grama.dfply.summary_functions.**IQR**(**args*, ***kwargs*)

Returns the inter-quartile range (IQR) of a series.

The IRQ is defined as the 75th quantile minus the 25th quantile values.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**quant**(**args*, ***kwargs*)

Returns the specified quantile value.

Parameters

- **series** (*pandas.Series*) – Column to summarize
- **p** (*float*) – Fraction for desired quantile, 0 <= p <= 1

Returns Desired quantile

Return type float

grama.dfply.summary_functions.**pint_lo**(**args*, ***kwargs*)

Lower prediction interval

Compute a one-sided lower prediction interval using a distribution-free approach.

For a two-sided interval at a confidence level of `C`, set `alpha = 1 - C` and use `[gr.pint_lo(X, alpha=alpha/2), gr.pint_up(X, alpha=alpha/2)]`. Note that the default `alpha` level for both helpers is calibrated for a two-sided interval with `C = 0.99`.

Parameters **series** (*pd.Series*) – Dataset to analyze

Kwargs: m (int): Number of observations in future dataset (Default m=1) j (int): Order statistic to target; 1 <= j <= m (Default j=1) alpha (float): alpha-level for calculation, in (0, 1). Note that the confidence level C is given by `C = 1 - alpha`.

References

Hahn, Gerald J., and William Q. Meeker. Statistical intervals: a guide for practitioners. Vol. 92. John Wiley & Sons, 2011.

grama.dfply.summary_functions.**pint_lo_index**(*n*, *m*, *j*, *alpha*)

PI lower bound index

Compute the order statistic index for the lower bound of a distribution-free prediction interval.

grama.dfply.summary_functions.**pint_up**(**args*, ***kwargs*)

Upper prediction interval

Compute a one-sided upper prediction interval using a distribution-free approach.

For a two-sided interval at a confidence level of `C`, set `alpha = 1 - C` and use `[gr.pint_lo(X, alpha=alpha/2), gr.pint_up(X, alpha=alpha/2)]`. Note that the default `alpha` level for both helpers is calibrated for a two-sided interval with `C = 0.99`.

Parameters **series** (*pd.Series*) – Dataset to analyze

Kwargs: m (int): Number of observations in future dataset (Default m=1) j (int): Order statistic to target; 1 <= j <= m (Default j=1) alpha (float): alpha-level for calculation, in (0, 1). Note that the confidence level C is given by `C = 1 - alpha`.

References

Hahn, Gerald J., and William Q. Meeker. Statistical intervals: a guide for practitioners. Vol. 92. John Wiley & Sons, 2011.

grama.dfply.summary_functions.**pint_up_index**(*n*, *m*, *j*, *alpha*)

PI upper bound index

Compute the order statistic index for the upper bound of a distribution-free prediction interval.

grama.dfply.summary_functions.**pr**(**args*, ***kwargs*)

Estimate a probability

Estimate a probability from a random sample. Provided series must be boolean, with 1 corresponding to the event of interest.

Use logical statements together with column values to construct a boolean indicator for the event you're interested in. Remember that you can chain multiple statements with logical and *&* and or *|* operators. See the examples below for more details.

Parameters **series** (*pandas.Series*) – Column to summarize; must be boolean or 0/1.

Examples:

```
import grama as gr
DF = gr.Intention()
## Cantilever beam examples
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()

## Estimate probabilities
(
    md_beam
    # Generate large
    >> gr.ev_sample(n=1e5, df_det="nom")
    # Estimate probabilities of failure
    >> gr.tf_summarize(
        pof_stress=gr.pr(DF.g_stress <= 0),
        pof_disp=gr.pr(DF.g_disp <= 0),
        pof_joint=gr.pr( (DF.g_stress <= 0) & (DF.g_disp) ),
        pof_either=gr.pr( (DF.g_stress <= 0) | (DF.g_disp) ),
    )
)
```

grama.dfply.summary_functions.**pr_lo**(**args*, ***kwargs*)

Estimate a confidence interval for a probability

Estimate the lower side of a confidence interval for a probability from a random sample. Provided series must be boolean, with 1 corresponding to the event of interest.

Uses Wilson interval method.

Use logical statements together with column values to construct a boolean indicator for the event you're interested in. Remember that you can chain multiple statements with logical and *&* and or *|* operators. See the documentation for *gr.pr()* for more details and examples.

For a two-sided interval at a confidence level of `C`, set `alpha = 1 - C` and use `[gr.mean_lo(X, alpha=alpha/2), gr.mean_up(X, alpha=alpha/2)]`. Note that the default `alpha` level for both helpers is calibrated for a two-sided interval with `C = 0.99`.

Parameters

- **series** (*pandas.Series*) – Column to summarize; must be boolean or 0/1.
- **alpha** (*float*) – alpha-level for calculation, in (0, 1) Note that the confidence level C is given by C = 1 - alpha

Returns Lower confidence interval

Return type float

Examples:

```
import grama as gr
DF = gr.Intention()
## Cantilever beam examples
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()

## Estimate probabilities
(
    md_beam
    # Generate large
    >> gr.ev_sample(n=1e5, df_det="nom")
    # Estimate probabilities with a confidence interval
    >> gr.tf_summarize(
        pof_lo=gr.pr_lo(DF.g_stress <= 0),
        pof=gr.pr(DF.g_stress <= 0),
        pof_up=gr.pr_up(DF.g_stress <= 0),
    )
)
```

grama.dfply.summary_functions.**pr_up**(**args*, ***kwargs*)

Estimate the upper side of a confidence interval for a probability from a random sample. Provided series must be boolean, with 1 corresponding to the event of interest.

Uses Wilson interval method.

Use logical statements together with column values to construct a boolean indicator for the event you're interested in. Remember that you can chain multiple statements with logical and *&* and or *|* operators. See the documentation for *gr.pr()* for more details and examples.

For a two-sided interval at a confidence level of `C`, set `alpha = 1 - C` and use `[gr.mean_lo(X, alpha=alpha/2), gr.mean_up(X, alpha=alpha/2)]`. Note that the default `alpha` level for both helpers is calibrated for a two-sided interval with `C = 0.99`.

Parameters

- **series** (*pandas.Series*) – Column to summarize; must be boolean or 0/1.
- **alpha** (*float*) – alpha-level for calculation, in (0, 1) Note that the confidence level C is given by C = 1 - alpha

Returns Upper confidence interval

Return type float

Examples:

```
import grama as gr
DF = gr.Intention()
## Cantilever beam examples
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()

## Estimate probabilities
(
    md_beam
    # Generate large
    >> gr.ev_sample(n=1e5, df_det="nom")
    # Estimate probabilities with a confidence interval
    >> gr.tf_summarize(
        pof_lo=gr.pr_lo(DF.g_stress <= 0),
        pof=gr.pr(DF.g_stress <= 0),
        pof_up=gr.pr_up(DF.g_stress <= 0),
    )
)
```

grama.dfply.summary_functions.**var**(**args*, ***kwargs*)
Returns the variance of values in a series.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**sd**(**args*, ***kwargs*)
Returns the standard deviation of values in a series.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**skew**(**args*, ***kwargs*)
Returns the skewness of a series.

Parameters

- **series** (*pandas.Series*) – column to summarize.
- **bias** (*bool*) – Correct for bias?
- **nan_policy** (*str*) – How to handle NaN values: - “propagate”: return NaN - “raise”: throws an error - “omit”: remove NaN before calculating skew

grama.dfply.summary_functions.**kurt**(**args*, ***kwargs*)
Returns the kurtosis of a series.

A distribution with kurtosis greater than three is called *leptokurtic*; such a distribution has “fatter” tails and will tend to exhibit more outliers. A distribution with kurtosis less than three is called *platykurtic*; such a distribution has less-fat tails and will tend to exhibit fewer outliers.

Parameters

- **series** (*pandas.Series*) – column to summarize.
- **bias** (*bool*) – Correct for bias?
- **excess** (*bool*) – Return excess kurtosis (excess = kurtosis - 3). Note that a normal distribution has kurtosis == 3, which informs the excess kurtosis definition.

- **nan_policy** (*str*) – How to handle NaN values: - "propagate": return NaN - "raise": throws an error - "omit": remove NaN before calculating skew

grama.dfply.summary_functions.**min**(**args*, ***kwargs*)
Returns the minimum value of a series.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**max**(**args*, ***kwargs*)
Returns the maximum value of a series.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**sum**(**args*, ***kwargs*)
Returns the sum of values in a series.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**median**(**args*, ***kwargs*)
Returns the median value of a series.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**first**(**args*, ***kwargs*)
Returns the first value of a series.

Parameters **series** (*pandas.Series*) – column to summarize.

Kwargs:

order_by: a pandas.Series or list of series (can be symbolic) to order the input series by before summarization.

grama.dfply.summary_functions.**last**(**args*, ***kwargs*)
Returns the last value of a series.

Parameters **series** (*pandas.Series*) – column to summarize.

Kwargs: order_by: a pandas.Series or list of series (can be symbolic) to order the input series by before summarization.

grama.dfply.summary_functions.**n**(**args*, ***kwargs*)
Returns the length of a series.

Parameters **series** (*pandas.Series*) – column to summarize. Default is the size of the parent DataFrame.

Examples:

```
import grama as gr
from grama.data import df_diamonds
DF = gr.Intention()

## Count entries in series
gr.n(df_diamonds.cut)
## Use implicit mode to get size of current DataFrame
(
    df_diamonds
    >> gr.tf_mutate(n_total=gr.n())
)
## Use implicit mode in groups
```

(continues on next page)

(continued from previous page)

```
(
    df_diamonds
    >> gr.tf_group_by(DF.cut)
    >> gr.tf_mutate(n_cut=gr.n())
)
```

grama.dfply.summary_functions.**nth**(**args*, ***kwargs*)
Returns the nth value of a series.

Parameters

- **series** (*pandas.Series*) – column to summarize.
- **n** (*integer*) – position of desired value. Returns *NaN* if out of range.

Kwargs: order_by: a pandas.Series or list of series (can be symbolic) to order the input series by before summarization.

grama.dfply.summary_functions.**n_distinct**(**args*, ***kwargs*)
Returns the number of distinct values in a series.

Parameters **series** (*pandas.Series*) – column to summarize.

grama.dfply.summary_functions.**neff_is**(**args*, ***kwargs*)
Importance sampling n_eff

Computes the effective sample size based on importance sampling weights. See Equation 9.13 of Owen (2013) for details. See `gr.tran_reweight()` for more details.

Parameters **series** (*pandas.Series*) – column of importance sampling weights.

References

A.B. Owen, "Monte Carlo theory, methods and examples" (2013)

grama.dfply.summary_functions.**mad**(**args*, ***kwargs*)
Compute MAD

Returns the mean absolute deviation (MAD) between predicted and measured values.

Parameters

- **series_pred** (*pandas.Series*) – column of predicted values
- **series_meas** (*pandas.Series*) – column of measured values

Returns Mean absolute deviation (MAD)

Return type float

grama.dfply.summary_functions.**mead**(**args*, ***kwargs*)
Compute median absolute deviation

Returns the median absolute deviation (MEAD) between predicted and measured values.

Parameters

- **series_pred** (*pandas.Series*) – column of predicted values
- **series_meas** (*pandas.Series*) – column of measured values

Returns Median absolute deviation (MEAD)

Return type float

grama.dfply.summary_functions.**mse**(**args*, ***kwargs*)
Compute MSE

Returns the mean-square-error (MSE) between predicted and measured values.

Parameters

- **series_pred** (*pandas.Series*) – column of predicted values
- **series_meas** (*pandas.Series*) – column of measured values

Returns Mean squared error (MSE)

Return type float

grama.dfply.summary_functions.**rmse**(**args*, ***kwargs*)
Compute RMSE

Returns the root-mean-square-error (RMSE) between predicted and measured values.

Parameters

- **series_pred** (*pandas.Series*) – column of predicted values
- **series_meas** (*pandas.Series*) – column of measured values

Returns Root-mean squared error (RMSE)

Return type float

grama.dfply.summary_functions.**ndme**(**args*, ***kwargs*)
Compute non-dimensional model error

Returns the non-dimensional model error (NDME) between predicted and measured values. The NDME is related to the coefficient of determination (aka R^2) via

NDME = sqrt(1 - R^2)

Parameters

- **series_pred** (*pandas.Series*) – column of predicted values
- **series_meas** (*pandas.Series*) – column of measured values

grama.dfply.summary_functions.**rsq**(**args*, ***kwargs*)
Compute coefficient of determination

Returns the coefficient of determination (aka R^2) between predicted and measured values. Theoretically 0 <= R^2 <= 1, with R^2 == 0 corresponding to a model no more predictive than guessing the mean of observed values, and R^2 == 1 corresponding to a perfect model. Note that sampling variability can lead to R^2 < 0 or R^2 > 1.

Parameters

- **series_pred** (*pandas.Series*) – column of predicted values
- **series_meas** (*pandas.Series*) – column of measured values

grama.dfply.transform module

grama.dfply.vector module

grama.dfply.vector.**order_series_by**(**args*, ***kwargs*)

Orders one series according to another series, or a list of other series. If a list of other series are specified, ordering is done hierarchically like when a list of columns is supplied to *.sort_values()*.

Parameters

- **series** (pandas.Series) – the pandas Series object to be reordered.
- **order_series** – either a pandas Series object or a list of pandas Series objects. These will be sorted using *.sort_values()* with *ascending=True*, and the new order will be used to reorder the Series supplied in the first argument.

Returns reordered *pandas.Series* object

grama.dfply.vector.**desc**(**args*, ***kwargs*)

Mimics the functionality of the R desc function. Essentially inverts a series object to make ascending sort act like descending sort.

Parameters **series** (pandas.Series) – pandas series to be inverted prior to ordering/sorting.

Returns

inverted *pandas.Series*. The returned series will be numeric (integers), regardless of the type of the original series.

Examples:

```
First group by cut, then find the first value of price when ordering by
price ascending, and ordering by price descending using the `desc` function.

diamonds >> group_by(X.cut) >> summarize(carat_low=first(X.price, order_by=X.
↪price),
                                         carat_high=first(X.price, order_
↪by=desc(X.price)))

         cut  carat_high  carat_low
0       Fair       18574        337
1       Good       18788        327
2      Ideal       18806        326
3    Premium       18823        326
4  Very Good       18818        336
```

grama.dfply.vector.**coalesce**(**args*, ***kwargs*)

Takes the first non-NaN value in order across the specified series, returning a new series. Mimics the coalesce function in dplyr and SQL.

Parameters ***series** – Series objects, typically represented in their symbolic form (like X.series).

Examples:

```
df = pd.DataFrame({
    'a':[1,np.nan,np.nan,np.nan,np.nan],
    'b':[2,3,np.nan,np.nan,np.nan],
    'c':[np.nan,np.nan,4,5,np.nan],
    'd':[6,7,8,9,np.nan]
})
df >> transmute(coal=coalesce(X.a, X.b, X.c, X.d))

     coal
```

(continues on next page)

(continued from previous page)

```
0       1
1       3
2       4
3       5
4  np.nan
```

grama.dfply.vector.**case_when**(**args*, ***kwargs*)

Functions as a switch statement, creating a new series out of logical conditions specified by 2-item lists where the left-hand item is the logical condition and the right-hand item is the value where that condition is true.

Conditions should go from the most specific to the most general. A conditional that appears earlier in the series will "overwrite" one that appears later. Think of it like a series of if-else statements.

The logicals and values of the condition pairs must be all the same length, or length 1. Logicals can be vectors of booleans or a single boolean (*True*, for example, can be the logical statement for the final conditional to catch all remaining.).

Parameters ***conditions** – Each condition should be a list with two values. The first value is a boolean or vector of booleans that specify indices in which the condition is met. The second value is a vector of values or single value specifying the outcome where that condition is met.

Example:

```
df = pd.DataFrame({
    'num':np.arange(16)
})
df >> mutate(strnum=case_when([X.num % 15 == 0, 'fizzbuzz'],
                              [X.num % 3 == 0, 'fizz'],
                              [X.num % 5 == 0, 'buzz'],
                              [True, X.num.astype(str)]))

    num    strnum
0     0  fizzbuzz
1     1         1
2     2         2
3     3      fizz
4     4         4
5     5      buzz
6     6      fizz
7     7         7
8     8         8
9     9      fizz
10   10      buzz
11   11        11
12   12      fizz
13   13        13
14   14        14
15   15  fizzbuzz
```

grama.dfply.vector.**if_else**(**args*, ***kwargs*)

Wraps creation of a series based on if-else conditional logic into a function call.

Provide a boolean vector condition, value(s) when true, and value(s) when false, and a vector will be returned the same length as the conditional vector according to the logical statement.

Parameters

- **condition** – A boolean vector representing the condition. This is often a logical statement with a symbolic series.

- **when_true** – A vector the same length as the condition vector or a single value to apply when the condition is *True*.
- **otherwise** – A vector the same length as the condition vector or a single value to apply when the condition is *False*.

Example:

```
import grama as gr
from grama.data import df_diamonds
DF = gr.Intention()
(
    df_diamonds
    >> gr.tf_mutate(
        # Recode nonsensical x values
        x=gr.if_else(
            DF.x == 0
            gr.NaN,
            DF.x,
        )
    )
)
```

grama.dfply.vector.**na_if**(**args*, ***kwargs*)

If values in a series match a specified value, change them to *np.nan*.

Parameters

- **series** – Series or vector, often symbolic.
- ***values** – Value(s) to convert to *np.nan* in the series.

grama.dfply.window_functions module

grama.dfply.window_functions.**lead**(**args*, ***kwargs*)

Returns a series shifted forward by a value. *NaN* values will be filled in the end.

Same as a call to *series.shift(i)*

Parameters

- **series** – column to shift forward.
- **i** (*int*) – number of positions to shift forward.

grama.dfply.window_functions.**lag**(**args*, ***kwargs*)

Returns a series shifted backwards by a value. *NaN* values will be filled in the beginning.

Same as a call to *series.shift(-i)*

Parameters

- **series** – column to shift backward.
- **i** (*int*) – number of positions to shift backward.

grama.dfply.window_functions.**between**(**args*, ***kwargs*)

Returns a boolean series specifying whether rows of the input series are between values *a* and *b*.

Parameters

- **series** – column to compare, typically symbolic.

- **a** – value series must be greater than (or equal to if *inclusive=True*) for the output series to be *True* at that position.
- **b** – value series must be less than (or equal to if *inclusive=True*) for the output series to be *True* at that position.

Kwargs:

inclusive (bool): If *True*, comparison is done with >= and <=. If *False* (the default), comparison uses > and <.

grama.dfply.window_functions.**dense_rank**(**args*, ***kwargs*)
Equivalent to *series.rank(method='dense', ascending=ascending)*.

Parameters **series** – column to rank.

Kwargs: ascending (bool): whether to rank in ascending order (default is *True*).

grama.dfply.window_functions.**min_rank**(**args*, ***kwargs*)
Equivalent to *series.rank(method='min', ascending=ascending)*.

Parameters **series** – column to rank.

Kwargs: ascending (bool): whether to rank in ascending order (default is *True*).

grama.dfply.window_functions.**cumsum**(**args*, ***kwargs*)
Calculates cumulative sum of values. Equivalent to *series.cumsum()*.

Parameters **series** – column to compute cumulative sum for.

grama.dfply.window_functions.**cummean**(**args*, ***kwargs*)
Calculates cumulative mean of values. Equivalent to *series.expanding().mean()*.

Parameters **series** – column to compute cumulative mean for.

grama.dfply.window_functions.**cumsd**(**args*, ***kwargs*)
Calculates cumulative standard deviation of values. Equivalent to *series.expanding().sd()*.

Parameters **series** – column to compute cumulative sd for.

grama.dfply.window_functions.**cummax**(**args*, ***kwargs*)
Calculates cumulative maximum of values. Equivalent to *series.expanding().max()*.

Parameters **series** – column to compute cumulative maximum for.

grama.dfply.window_functions.**cummin**(**args*, ***kwargs*)
Calculates cumulative minimum of values. Equivalent to *series.expanding().min()*.

Parameters **series** – column to compute cumulative minimum for.

grama.dfply.window_functions.**cumprod**(**args*, ***kwargs*)
Calculates cumulative product of values. Equivalent to *series.cumprod()*.

Parameters **series** – column to compute cumulative product for.

grama.dfply.window_functions.**cumany**(**args*, ***kwargs*)
Calculates cumulative any of values. Equivalent to *series.expanding().apply(np.any).astype(bool)*.

Parameters **series** – column to compute cumulative any for.

grama.dfply.window_functions.**cumall**(**args*, ***kwargs*)
Calculates cumulative all of values. Equivalent to *series.expanding().apply(np.all).astype(bool)*.

Parameters **series** – column to compute cumulative all for.

grama.dfply.window_functions.**percent_rank**(**args*, ***kwargs*)

grama.dfply.window_functions.**row_number**(**args*, ***kwargs*)

Returns row number based on column rank Equivalent to *series.rank(method='first', ascending=ascending)*.

Parameters **series** – column to rank.

Kwargs: ascending (bool): whether to rank in ascending order (default is *True*).

Usage: diamonds >> head() >> mutate(rn=row_number(X.x))

carat cut color clarity depth table price x y z rn

0 0.23 Ideal E SI2 61.5 55.0 326 3.95 3.98 2.43 2.0 1 0.21 Premium E SI1 59.8 61.0 326 3.89 3.84 2.31 1.0 2 0.23 Good E VS1 56.9 65.0 327 4.05 4.07 2.31 3.0 3 0.29 Premium I VS2 62.4 58.0 334 4.20 4.23 2.63 4.0 4 0.31 Good J SI2 63.3 58.0 335 4.34 4.35 2.75 5.0

Module contents

grama.eval package

Submodules

grama.eval.eval_pyDOE module

grama.eval.eval_pyDOE.**eval_lhs**

Latin Hypercube evaluation Evaluates a given model on a latin hypercube sample (LHS) using the model's density. :param model: Model to evaluate :type model: gr.Model :param n: Number of LHS samples to draw :type n: numeric :param df_det: Deterministic levels for evaluation; use "nom"

for nominal deterministic levels.

Parameters

- **seed** (*int*) – Random seed to use
- **append** (*bool*) – Append results to conservative inputs?
- **skip** (*bool*) – Skip evaluation of the functions?
- **criterion** (*str*) – flag for LHS sample criterion allowable values: None, "center" ("c"), "maxmin" ("m"), "centermaxmin" ("cm"), "correlation" ("corr")

Returns Results of evaluation or unevaluated design

Return type DataFrame

Notes

- Wrapper on pyDOE.lhs

Module contents

grama.fit package

Submodules

grama.fit.fit_lolo module

grama.fit.fit_lolo.**fit_lolo**

Fit a random forest

DEPRECATED DO NOT USE

Fit a random forest to given data. Specify inputs and outputs, or inherit from an existing model.

Parameters

- **df** (*DataFrame*) – Data for function fitting
- **md** (*gr.Model*) – Model from which to inherit metadata
- **var** (*list(str) or None*) – List of features or None for all except outputs
- **out** (*list(str)*) – List of outputs to fit
- **domain** (*gr.Domain*) – Domain for new model
- **density** (*gr.Density*) – Density for new model
- **seed** (*int or None*) – Random seed for fitting process
- **return_std** (*bool*) – Return predictive standard deviations?
- **suppress_warnings** (*bool*) – Suppress warnings when fitting?

Keyword Arguments

- **num_trees** (*int*) –
- **use_jackknife** (*bool*) –
- **()** (*leaf_learner*) –
- **()** –
- **subset_strategy** (*str*) –
- **min_leaf_instances** (*int*) –
- **max_depth** (*int*) –
- **uncertainty_calibration** (*bool*) –
- **randomize_pivot_location** (*bool*) –
- **randomly_rotate_features** (*bool*) –

Returns A grama model with fitted function(s)

Return type gr.Model

Notes

- Wrapper for lolopy.learners.RandomForestRegressor

grama.fit.fit_scikitlearn module

grama.fit.fit_scikitlearn.**fit_gp**
Fit a gaussian process

Fit a gaussian process to given data. Specify var and out, or inherit from an existing model.

Note that the new model will have two outputs *y_mean, y_sd* for each original output *y*. The quantity *y_mean* is the best-fit value, while *y_sd* is a measure of predictive uncertainty.

Parameters

- **df** (*DataFrame*) – Data for function fitting
- **md** (*gr.Model*) – Model from which to inherit metadata
- **var** (*list(str) or None*) – List of features or None for all except outputs
- **out** (*list(str)*) – List of outputs to fit
- **domain** (*gr.Domain*) – Domain for new model
- **density** (*gr.Density*) – Density for new model
- **seed** (*int or None*) – Random seed for fitting process
- **kernels** (*sklearn.gaussian_process.kernels.Kernel or dict or None*) – Kernel for GP
- **n_restart** (*int*) – Restarts for optimization
- **alpha** (*float or iterable*) – Value added to diagonal of kernel matrix
- **suppress_warnings** (*bool*) – Suppress warnings when fitting?

Returns A grama model with fitted function(s)

Return type gr.Model

Notes

- Wrapper for sklearn.gaussian_process.GaussianProcessRegressor

grama.fit.fit_scikitlearn.**fit_lm**
Fit a linear model

Fit a linear model to given data. Specify inputs and outputs, or inherit from an existing model.

Parameters

- **df** (*DataFrame*) – Data for function fitting
- **md** (*gr.Model*) – Model from which to inherit metadata
- **var** (*list(str) or None*) – List of features or None for all except outputs
- **out** (*list(str)*) – List of outputs to fit
- **domain** (*gr.Domain*) – Domain for new model
- **density** (*gr.Density*) – Density for new model
- **seed** (*int or None*) – Random seed for fitting process
- **suppress_warnings** (*bool*) – Suppress warnings when fitting?

Returns A grama model with fitted function(s)

Return type gr.Model

Notes

- Wrapper for sklearn.ensemble.RandomForestRegressor

grama.fit.fit_scikitlearn.**fit_rf**

Fit a random forest

Fit a random forest to given data. Specify inputs and outputs, or inherit from an existing model.

Parameters

- **df** (*DataFrame*) – Data for function fitting
- **md** (*gr.Model*) – Model from which to inherit metadata
- **var** (*list(str) or None*) – List of features or None for all except outputs
- **out** (*list(str)*) – List of outputs to fit
- **domain** (*gr.Domain*) – Domain for new model
- **density** (*gr.Density*) – Density for new model
- **seed** (*int or None*) – Random seed for fitting process
- **suppress_warnings** (*bool*) – Suppress warnings when fitting?

Keyword Arguments

- **n_estimators** (*int*) –
- **criterion** (*int*) –
- **max_depth** (*int or None*) –
- **min_samples_split** (*int, float*) –
- **min_samples_leaf** (*int, float*) –
- **min_weight_fraction_leaf** (*float*) –
- **max_features** (*int, float, string*) –
- **max_leaf_nodes** (*int or None*) –
- **min_impurity_decrease** (*float*) –
- **min_impurity_split** (*float*) –
- **bootstrap** (*bool*) –
- **oob_score** (*bool*) –
- **n_jobs** (*int or None*) –
- **random_state** (*int*) –

Returns A grama model with fitted function(s)

Return type gr.Model

Notes

- Wrapper for sklearn.ensemble.RandomForestRegressor

grama.fit.fit_scikitlearn.**fit_kmeans**

K-means cluster a dataset

Create a cluster-labeling model on a dataset using the K-means algorithm.

Parameters

- **df** (*DataFrame*) – Hybrid point results from gr.eval_hybrid()
- **var** (*list or None*) – Variables in df on which to cluster. Use None to cluster on all variables.
- **colname** (*string*) – Name of cluster id; will be output in cluster model.
- **seed** (*int*) – Random seed for kmeans clustering

Kwargs: n_clusters (int): Number of clusters to fit random_state (int or None):

Returns Model that labels input data

Return type gr.Model

Notes

- A wrapper for sklearn.cluster.KMeans

References

Scikit-learn: Machine Learning in Python, Pedregosa et al. JMLR 12, pp. 2825-2830, 2011.

Examples:

```
import grama as gr
from grama.data import df_stang
from grama.fit import ft_kmeans
DF = gr.Intention()
md_cluster = (
    df_stang
    >> ft_kmeans(var=["E", "mu"], n_clusters=2)
)
(
    md_cluster
    >> gr.ev_df(df_stang)
    >> gr.tf_group_by(DF.cluster_id)
    >> gr.tf_summarize(
        thick_mean=gr.mean(DF.thick),
        thick_sd=gr.sd(DF.thick),
        n=gr.n(),
    )
)
```

grama.fit.fit_statsmodels module

grama.fit.fit_statsmodels.**fit_ols**
Fit a function via Ordinary Least Squares

Fit a function via ordinary least squares. Specify features via statsmodels formula.

Parameters

- **df** (*DataFrame*) – Data for function fitting
- **formulae** (*list(str)*) – List of statsmodels formulae
- **domain** (*gr.Domain*) – Domain for new model
- **density** (*gr.Density*) – Density for new model

Returns A grama model with fitted function(s)

Return type gr.Model

@pre domain is not None @pre len(formulae) == len(domain.inputs)

Notes

- Wrapper for statsmodels.formula.api.ols

Module contents

grama.models package

Submodules

grama.models.cantilever_beam module

grama.models.cantilever_beam.**make_cantilever_beam**()
Cantilever beam

A standard reliability test-case, often used for benchmarking reliability analysis and design algorithms.

Generally used in the following optimization problem:

min_{w,t} c_area

s.t. P[g_stress <= 0] <= 1.35e-3

P[g_disp <= 0] <= 1.35e-3

1 <= w, t <= 4

Deterministic Variables: w: Beam width t: Beam thickness

Random Variables: H: Horizontal applied force V: Vertical applied force E: Elastic modulus Y: Yield stress

Outputs: c_area: Cost; beam cross-sectional area g_stress: Limit state; stress g_disp: Limit state; tip displacement

References

Wu, Y.-T., Shin, Y., Sues, R., and Cesare, M., "Safety-factor based approach for probability-based design optimization," American Institute of Aeronautics and Astronautics, Seattle, Washington, April 2001. Sues, R., Aminpour, M., and Shin, Y., "Reliability-based Multi-Disciplinary Optimiation for Aerospace Systems," American Institute of Aeronautics and Astronautics, Seattle, Washington, April 2001.

grama.models.channel1d module

grama.models.channel1d.**make_channel_nondim**()
Make 1d channel model; dimensionless form

Instantiates a model for particle and fluid temperature rise; particles are suspended in a fluid with bulk velocity along a square cross-section channel. The walls of said channel are transparent, and radiation heats the particles as they travel down the channel.

References

Banko, A.J. "RADIATION ABSORPTION BY INERTIAL PARTICLES IN A TURBULENT SQUARE DUCT FLOW" (2018) PhD Thesis, Stanford University, Chapter 2

grama.models.channel1d.**make_channel**()
Make 1d channel model; dimensional form

Instantiates a model for particle and fluid temperature rise; particles are suspended in a fluid with bulk velocity along a square cross-section channel. The walls of said channel are transparent, and radiation heats the particles as they travel down the channel.

Note that this takes the same inputs as the builtin dataset *df_channel*.

References

Banko, A.J. "RADIATION ABSORPTION BY INERTIAL PARTICLES IN A TURBULENT SQUARE DUCT FLOW" (2018) PhD Thesis, Stanford University, Chapter 2

Examples:

```
>>> import grama as gr
>>> from grama.data import df_channel
>>> from grama.models import make_channel
>>> md_channel = make_channel()
```

```
>>> (
>>>     df_channel
>>>     >> gr.tf_md(md_channel)
```

```
>>>     >> gr.ggplot(gr.aes("T_f", "T_norm"))
>>>     + gr.geom_abline(slope=1, intercept=0, linetype="dashed")
>>>     + gr.geom_point()
>>>     + gr.labs(x="1D Model", y="3D DNS")
>>> )
```

grama.models.circuit_RLC module

grama.models.circuit_RLC.**make_prlc**()

grama.models.circuit_RLC.**make_prlc_rand**()

grama.models.ishigami module

grama.models.ishigami.**make_ishigami**()

Ishigami function

The Ishigami function is commonly used as a test case for estimating Sobol' indices.

Model definition:

y0 = sin(x1) + a sin(x2)^2 + b x3^4 sin(x1)

x1 ~ U[-pi, +pi]

x2 ~ U[-pi, +pi]

x3 ~ U[-pi, +pi]

Sobol' index data:

V[y0] = a^2/8 + b pi^4/5 + b^2 pi^8/18 + 0.5

T1 = 0.5(1 + b pi^4/5)^2

T2 = a^2/8

T3 = 0

Tt1 = 0.5(1 + b pi^4/5)^2 + 8 b^2 pi^8/225

Tt2 = a^2/8

Tt3 = 8 b^2 pi^8/225

References

T. Ishigami and T. Homma, "An importance quantification technique in uncertainty analysis for computer models," In the First International Symposium on Uncertainty Modeling and Analysis, Maryland, USA, Dec. 3–5, 1990. DOI:10.1109/SUMA.1990.151285

grama.models.linear_normal module

grama.models.linear_normal.**make_linear_normal**()

grama.models.pareto_random module

grama.models.pareto_random.**make_pareto_random**(*twoDim=True*)

Create a model of random points for a pareto frontier evaluation :param twoDim: determines whether to create a 2D or 3D model :type twoDim: bool

grama.models.plane_laminate module

class grama.models.plane_laminate.**make_composite_plate_tension**(*Theta_nom*, *T_nom=0.001*)

Bases: *grama.core.Model*

grama.models.plate_buckling module

grama.models.plate_buckling.**make_plate_buckle**()

Initialize a buckling plate model

Variables (deterministic): w (in): Plate width h (in): Plate height t (in): Plate thickness m (-): Wavenumber L (kips): Applied (compressive) load;

uniformly applied along top and bottom edges

Variables (random): E (kips/in^2): Elasticity mu (-): Poisson's ratio

Outputs: k_cr (-): Prefactor for buckling stress g_buckle (kips/in^2): Buckling limit state:

critical stress - applied stress

grama.models.poly module

grama.models.poly.**make_poly**()

grama.models.test module

grama.models.test.**make_test**()

grama.models.time_cantilever module

grama.models.trajectory_linear_drag module

grama.models.trajectory_linear_drag.**make_trajectory_linear**()

Module contents

grama.tran package

Submodules

grama.tran.tran_matminer module

grama.tran.tran_matminer.**tran_feat_composition**

Featurize a dataset using matminer

Featurize chemical composition using matminer package.

Parameters

- **df** (*DataFrame*) – Data to featurize

- **var_formula** (*string*) – Column in df with chemical formula; formula given as string
- **append** (*bool*) – Append results to original columns?
- **preset_name** (*string*) – Matminer featurization preset

Kwargs:

ignore_errors (bool): Do not throw an error while parsing formulae; set to True to return NaN's for invalid formulae.

Notes

- A pre-processor and wrapper for matminer.featurizers.composition

References

Ward, L., Dunn, A., Faghaninia, A., Zimmermann, N. E. R., Bajaj, S., Wang, Q., Montoya, J. H., Chen, J., Bystrom, K., Dylla, M., Chard, K., Asta, M., Persson, K., Snyder, G. J., Foster, I., Jain, A., Matminer: An open source toolkit for materials data mining. Comput. Mater. Sci. 152, 60-69 (2018).

Examples:

```
import grama as gr
from grama.tran import tf_feat_composition
(
    gr.df_make(FORMULA=["C6H12O6"])
    >> gr.tf_feat_composition()
)
```

grama.tran.tran_scikitlearn module

grama.tran.tran_scikitlearn.**tran_tsne**

t-SNE dimension reduction of a dataset

Apply the t-SNE algorithm to reduce the dimensionality of a dataset.

Parameters

- **df** (*DataFrame*) – Hybrid point results from gr.eval_hybrid()
- **var** (*list or None*) – Variables in df on which to perform dimension reduction. Use None to compute with all variables.
- **out** (*string*) – Name of reduced-dimensionality output; indexed from 0 .. n_dim-1
- **keep** (*bool*) – Keep unused columns (outside *var*) in new DataFrame?
- **append** (*bool*) – Append results to original columns?
- **n_dim** (*int*) – Target dimensionality

Kwargs: n_iter (int): Maximum number of iterations for optimization. As Wattenberg et al. note, this is the most important parameter in using t-SNE. If you see strange "pinched" shapes, increase n_iter. perplexity (int): Usually between 5 and 50. Low perplexity means local variations dominate; High perplexity tends to merge clusters. early_exaggeration (float): learning_rate (float):

Notes

- A wrapper for sklearn.manifold.TSNE

References

Scikit-learn: Machine Learning in Python, Pedregosa et al. JMLR 12, pp. 2825-2830, 2011.

Wattenberg, Viegas, and Johnson, "How to use t-SNE effectively" (2016) Distil.pub

Examples:

grama.tran.tran_umap module

grama.tran.tran_umap.**tran_umap**

UMAP dimension reduction of a dataset

Apply the UMAP algorithm to reduce the dimensionality of a dataset.

Parameters

- **df** (*DataFrame*) – Data to summarize
- **var** (*list or None*) – Variables in df on which to perform dimension reduction. Use None to compute with all variables.
- **out** (*string*) – Name of reduced-dimensionality output; indexed from 0 .. n_dim-1
- **keep** (*bool*) – Keep unused columns (outside *var*) in new DataFrame?
- **append** (*bool*) – Append results to original columns?
- **n_dim** (*int*) – Target dimensionality

Kwargs: n_neighbors (int): A smaller value emphasizes local structure, larger value emphasizes global structure. Assumed number of nearest-neighbors in clusters. Coenen and Pearce claim this is the most important hyperparameter for UMAP. default=15 min_dist (float): Minimum distance between mapped points. default=0.1 metric (str or function): Metric used for distance computations. See url: https://umap-learn.readthedocs.io/en/latest/parameters.html#metric

Notes

A wrapper for umap.UMAP

References

McInnes, L, Healy, J, UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction, ArXiv e-prints 1802.03426, 2018 Andy Coenen, Adam Pearce "Understanding UMAP" url: https://pair-code.github.io/understanding-umap/

Examples

import grama as gr from grama.data import df_diamonds (

df_diamonds >> gr.tf_sample(1000) # For speed >> gr.tf_umap(var=["x", "y", "z", "carat"]) >> gr.ggplot(gr.aes("xi0", "xi1")) + gr.geom_point()

)

Module contents

4.1.2 Submodules

4.1.3 grama.comp_building module

grama.comp_building.**comp_freeze**
Freeze inputs to a model

Composition. Remove inputs from a model by "freezing" them to fixed values.

Parameters

- **model** (*gr.Model*) – Model to compose
- **df** (*pd.DataFrame*) – DataFrame of values for freeze
- **var** (*dict*) – Dictionary of inputs to freeze (keys) to specific values (value) Provide each key/value pair as a keyword argument

Returns New model with frozen inputs

Return type gr.Model

Examples:: import grama as gr

grama.comp_building.**comp_function**
Add a function to a model

Composition. Add a (non-vectorized) function to an existing model. See `gr.comp_vec_function()` to add a function that is vectorized over DataFrames.

Parameters

- **model** (*gr.Model*) – Model to compose
- **fun** (*function*) – Function taking at least one real input and returns at least one real output (fun: R^d -> R^r). Each input to *fun* must be a scalar (See examples below).
- **var** (*list (string)*) – List of variable names or number of inputs
- **out** (*list (string)*) – List of output names or number of outputs
- **runtime** (*numeric*) – Estimated single-eval runtime (in seconds)

Returns New model with added function

Return type gr.Model

@pre (len(var) == d) | (var == d) @pre (len(out) == r) | (var == r)

Examples:

```
import grama as gr
## Simple example
md = (
    gr.Model("test")
    >> gr.cp_function(
        fun=lambda x: x,
```

(continues on next page)

(continued from previous page)

```
        var=["x"],
        out=["y"],
        name="identity"
    )
)

## Providing a function with multiple inputs
md2 = (
    gr.Model("test 2")
    >> gr.cp_function(
        fun=lambda x, y: x + y,
        var=["x", "y"],
        out=["f"],
    )
)

## Providing a function with multiple inputs and multiple outputs
md3 = (
    gr.Model("test 3")
    >> gr.cp_function(
        fun=lambda x, y: [x + y, x - y],
        var=["x", "y"],
        out=["f", "g"],
    )
)
```

grama.comp_building.**comp_vec_function**

Add a vectorized function to a model

Composition. Add a function to an existing model. Function must be vectorized over DataFrames, and must add new columns matching its *out* set. See `gr.cp_function()` to add a non-vectorized function.

Notes

The helper function `gr.df_make()` is useful for constructing a vectorized lambda function (see Examples below).

Parameters

- **model** (*gr.model*) – Model to compose
- **fun** (*function*) – Function taking R^d -> R^r; must be *vectorized* over DataFrames; it must take a DataFrame as input and return a new DataFrame
- **var** (*list (string)*) – List of variable names or number of inputs
- **out** (*list (string)*) – List of output names or number of outputs
- **runtime** (*numeric*) – Estimated single-eval runtime (in seconds)

Returns New model with added function

Return type gr.model

@pre (len(var) == d) | (var == d) @pre (len(out) == r) | (var == r)

Examples:

```
import grama as gr
## Simple example
md = (
    gr.Model("Test")
    >> gr.cp_vec_function(
        fun=lambda df: gr.df_make(y=1 + 0.5 * df.x),
        var=["x"],
        out=["y"],
        name="Simple linear function",
    )
)
```

grama.comp_building.**comp_md_det**

Add a Model with deterministic evaluation

Composition. Add a model as function to an existing model. Evaluate the model deterministically (ignore any random variables).

Parameters

- **model** (*gr.model*) – Model to compose
- **md** (*gr.model*) – Model to add as function

Returns New model with added function

Return type gr.model

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
## Use functions from beam model, but introduce new marginals
md_plate = (
    gr.Model("New beam model")
    >> gr.cp_md_det(md=make_cantilever_beam())
    >> gr.cp_marginals(
        H=gr.marg_mom("norm", mean=1000, cov=0.1),
        V=gr.marg_mom("norm", mean=500, cov=0.1),
    )
    >> gr.cp_copula_independence()
)
```

grama.comp_building.**comp_md_sample**

Add a Model with sampled evaluation

Composition. Add a model as function to an existing model. Evaluate the model via sampling (one sample per evaluation). Use *param* to turn model parameters into variables of new model. Random variables of composed model are turned into outputs of new model.

Parameters

- **model** (*gr.model*) – Model to compose
- **md** (*gr.model*) – Model to add as function
- **param** (*dict*) – Parameters in md to treat as var; entries must be of the form "var": ("param1", "param2", ...)
- **rand2out** (*bool*) – Add model's var_rand to outputs (to track values)

Returns New model with added function

Return type gr.model

Examples:

grama.comp_building.**comp_bounds**

Add variable bounds to a model

Composition. Add variable bounds to an existing model. Bounds are specified by iterable; the model variable name is specified by the keyword argument name.

Parameters **model** (*gr.model*) – Model to modify

Kwargs: var (iterable): Bound information; keyword argument name is targeted variable, value should be a length 2 iterable of the form (lower_bound, upper_bound)

Returns Model with new marginals

Return type gr.model

@pre len(var) >= 2

Examples:

```
import grama as gr
md = (
    gr.Model("Simple Model")
    >> gr.cp_function(
        lambda x: x[0] + x[1],
        var=["x0", "x1"],
        out=1
    )
    >> gr.cp_bounds(
        x0=(-1, 1),     # Finite bounds
        x1=(0, np.inf)  # Semi-infinite bounds
    )
)
```

grama.comp_building.**comp_copula_independence**

Add an independence copula to model

Composition. Add an independence copula to an existing model.

NOTE: Independence of random variables is a *very* strong assumption! Recommend using comp_copula_gaussian instead.

Parameters **model** (*gr.model*) – Model to modify

Returns Model with independence copula

Return type gr.model

Examples:

```
import grama as gr
md = (
    gr.Model()
    >> gr.cp_marginals(
        x0=gr.marg_mom("norm", mean=0, sd=1),
        x1=gr.marg_mom("beta", mean=0, sd=1, skew=0, kurt=2),
    )
    >> gr.cp_copula_independence()
)
```

grama.comp_building.**comp_copula_gaussian**

Add a Gaussian copula to model

Composition. Add a gaussian copula to an existing model.

Parameters

- **model** (*gr.model*) – Model to modify
- **df_corr** (*DataFrame*) – Correlation information
- **df_data** (*DataFrame*) – Data for automated fitting

Returns Model with Gaussian copula

Return type gr.model

Examples:

```
import grama as gr
## Manual assignment
md_manual = (gr.Model()
    >> gr.cp_marginals(
        x0=gr.marg_mom("norm", mean=0, sd=1),
        x1=gr.marg_mom("uniform", mean=0, sd=1),
    )
    >> gr.cp_copula_gaussian(
        # Specify correlation structure explicitly
        df_corr=gr.df_make(var1="x0", var2="x1", corr=0.5)
    )
)
## Automated fitting
from grama.data import df_stang
md_auto = (
    gr.Model()
    >> gr.cp_marginals(
        E=gr.marg_fit("norm", df_stang.E),
        mu=gr.marg_fit("beta", df_stang.mu),
        thick=gr.marg_fit("norm", df_stang.thick)
    )
    >> gr.cp_copula_gaussian(df_data=df_stang)
)
```

grama.comp_building.**comp_marginals**

Add marginals to a model

Composition. Add marginals to an existing model. Marginals are specified either by dictionary entries or by gr.Marginal() object. The model variable name is specified by the keyword argument name.

Notes

Several helper functions are available to fit marginal distributions

- `gr.marg_fit()` fits a distribution using a dataset (via maximum likelihood estimation)
- `gr.marg_mom()` fits a distribution using moments (via the method of moments)
- `gr.marg_gkde()` fits a gaussian kernel density using a dataset

Parameters

- **model** (*gr.model*) – Model to modify

- **var** (*dict OR gr.Marginal*) – Marginal information

Returns Model with new marginals

Return type gr.model

Examples:

```
import grama as gr
## Print all of the grama-supported distributions
print(gr.valid_dist.keys())
## Construct a simple example model
md = (
    gr.Model()
    >> gr.cp_function(
        lambda x: x[0] + x[1],
        var=["x0", "x1"],
        out=["y"],
    )
    >> gr.cp_marginals(
        x0=gr.marg_mom("norm", mean=0, sd=1),
    )
)
```

grama.comp_building.**getvars**(*f*)

Get a function's variable names

Convenience function for extracting a function's variable names. Intended for use with gr.cp_function().

Parameters **f** (*function*) – Function whose variable names are desired

Returns Variable names

Return type tuple

Examples:: import grama as gr

def fun(x, y, z): return x + y + z

md = (gr.Model("Test model") >> gr.cp_function(

fun=fun, var=gr.getvars(fun), out=["w"],

)

)

4.1.4 grama.comp_metamodels module

grama.comp_metamodels.**comp_metamodel**

Create a metamodel

Composition: Create a metamodel from an existing model. This convenience function essentially applies a recipe of Evaluation followed by Fitting. Default methods are Latin Hypercube Evaluation and Ordinary Least Squares Fitting with linear features.

Parameters

- **model** (*gr.model*) – Original model, to be evaluated and fit
- **n** (*numeric*) – Number of samples to draw

- **ev** (**gr.eval_**) – Evaluation strategy, default eval_lhs
- **ft** (**gr.fit_**) – Fitting strategy, default fit_ols w/ linear features
- **seed** (*int*) – Random seed, default None

Returns Metamodel

Return type gr.model

4.1.5 grama.core module

class grama.core.**CopulaIndependence**(*var_rand*)

Bases: grama.core.Copula

copy()

Copy

Returns Copy of present copula

Return type gr.CopulaIndependence

d(*u*)

Density function

Parameters **u** (*array-like*) –

Returns Copula density values

Return type array

dudz(*z*)

Jacobian

Parameters **z** (*array-like*) –

Returns

Return type array

sample(*n=1*, *seed=None*)

Draw samples from copula

Parameters

- **n** (*int*) – Number of samples
- **seed** (*int*) – Random seed

Returns Independent samples

Return type DataFrame

summary()

u2z(*u*)

Transform to standard-normal space

Parameters **u** (*array-like*) –

Returns

Return type array

z2u(*z*)

Transform to uniform-marginal space

Parameters **z** (*array-like*) –

Returns

Return type array

class grama.core.**CopulaGaussian**(*var_rand*, *df_corr*)

Bases: grama.core.Copula

copy()

Copy

Parameters **self** (*gr.CopulaGaussian*) –

Returns

Return type gr.CopulaGaussian

d(*u*)

Copula density function

Parameters **u** (*array-like*) –

Returns

Return type array

dudz(*z*)

Jacobian

Parameters **z** (*array-like*) –

Returns

Return type array

sample(*n=1*, *seed=None*)

Draw samples from copula

Draw samples according to gaussian copula dependence structure.

Parameters

- **self** (*gr.CopulaGaussian*) –
- **n** (*int*) – Number of samples to draw

Returns Copula samples

Return type array

summary()

u2z(*u*)

Transform to standard-normal space

Parameters **u** (*array-like*) –

Returns

Return type array

z2u(*z*)

Transform to uniform-marginal space

Parameters **z** (*array-like*) –

Returns

Return type array

class grama.core.**Domain**(*bounds=None*, *feasible=None*)
Bases: object

Parent class for input domains

The domain defines constraints on the variables. Together with a model's functions, it defines the mathematical domain of a model.

bound_summary(*var*)

copy()

get_bound(*var*)

get_nominal(*var*)

get_width(*var*)

update()

class grama.core.**Density**(*marginals=None*, *copula=None*)
Bases: object

Parent class for joint densities

The density is defined for all the random variables; therefore it explicitly defines the list of random variables, and together implicitly defines the deterministic variables via

domain.var + [functions.var] - density.marginals.keys()

copy()

d(*df*)
Evaluate PDF

Evaluate the PDF of the density.

Parameters **df** (*DataFrame*) – Values

pr2sample(*df_prval*)
Convert CDF probabilities to samples

Convert random variable CDF probabilities to random variable samples. Ignores dependence structure.

Parameters **df_prval** (*DataFrame*) – Values in [0,1]

Returns Variable samples (quantiles)

Return type DataFrame

@pre df_prval.shape[1] == len(self.var_rand) @post result.shape[1] == len(self.var_rand)

sample(*n=1*, *seed=None*)
Draw samples from joint density

Draw samples according to joint density using marginal and copula information.

Parameters

- **n** (*int*) – Number of samples to draw
- **seed** (*int*) – random seed to use

Returns Joint density samples

Return type DataFrame

sample2pr(*df_sample*)
Convert samples to CDF probabilities

Convert random variable samples to CDF probabilities. Ignores dependence structure.

Parameters **df_sample** (*DataFrame*) – Values in [0,1]

Returns Variable samples (quantiles)

Return type DataFrame

@pre df_sample.shape[1] == len(self.var_rand) @post result.shape[1] == len(self.var_rand)

summary_copula()

summary_marginal(*var*)

class grama.core.**Function**(*func*, *var*, *out*, *name*, *runtime*)
Bases: object

Parent class for functions.

A function specifies its own inputs and outputs; these are subsets of the full model's inputs and outputs.

copy()
Make a copy

eval(*df*)
Evaluate function

Evaluate a grama function; loops over dataframe rows. Intended for internal use.

Args: df (DataFrame): Input values to evaluate

Returns Result values

Return type DataFrame

summary()
Returns a summary string

class grama.core.**FunctionModel**(*md*, *ev=None*, *var=None*, *out=None*)
Bases: *grama.core.Function*

gr.Model as gr.Function

copy()
Make a copy

eval(*df*)
Evaluate function; DataFrame vectorized

Evaluate grama model as a function. Modify the parameters before

Parameters **df** (*DataFrame*) – Input values to evaluate

Returns Result values

Return type DataFrame

class grama.core.**FunctionVectorized**(*func*, *var*, *out*, *name*, *runtime*)
Bases: *grama.core.Function*

copy()
Make a copy

eval(*df*)
Evaluate function; DataFrame vectorized

Evaluate grama function. Assumes function is vectorized over dataframes.

Parameters **df** (*DataFrame*) – Input values to evaluate

Returns Result values

Return type DataFrame

class grama.core.**Model**(*name=None*, *functions=None*, *domain=None*, *density=None*)
Bases: object

Parent class for grama models.

copy()
Make a copy of this model

det_nom()
Return nominal conditions for deterministic variables

Returns Nominal values for deterministic variables

Return type DataFrame

dxdz(*z*)
Inverse transform jacobian

Compute jacobian of the inverse transform X = phi^{-1}(Z)

Parameters **z** (*array*) – Single vector of standard normal values. Order of entries must match self.var_rand

Returns Jacobian of inverse transform

Return type 2d array

evaluate_df(*df*)
Evaluate function using an input dataframe

Parameters **df** (*DataFrame*) – Variable values at which to evaluate model functions

Returns Output results

Return type DataFrame

make_dag(*expand={}*)
Generate a DAG for the model

name_corr()
Name the correlation elements

norm2rand(*df*)
Transform standard normal samples to model random variable space

Transform a DataFrame of standard normal samples to model random variable space.

Parameters **df** (*DataFrame*) – Random variable samples; must have columns for all of self.var_rand.

Returns Samples in standard-normal space

Return type DataFrame

printpretty()
Formatted print of model attributes

rand2norm(*df*)
Transform random samples to standard normal space

Transform a DataFrame of random variable samples to standard normal space

Parameters **df** (*DataFrame*) – Random variable samples; must have columns for all of self.var_rand.

Returns Samples in standard-normal space

Return type DataFrame

runtime(*n*)
Estimate runtime

Estimate the total runtime to evaluate n observations.

Parameters

- **self** (*gr.Model*) –
- **n** (*int*) – Number of observations

Returns Estimated runtime, in seconds

Return type float

runtime_message(*df*)
Runtime message

Estimate total runtime based on proposed DataFrame, prepare a message for console print.

Parameters

- **self** (*gr.Model*) –
- **df** (*DataFrame*) – Data to evaluate

Returns Runtime message

Return type str

show_dag(*expand={}*)
Generate and show a DAG for the model

string_rep()

update()
Update model public attributes based on functions, domain, and density.

The variables and parameters are implicitly defined by the model attributes. For internal use.

- self.functions defines the full list of inputs
- self.domain defines the constraints on the model's domain
- self.density defines the random variables

var_outer(*df_rand*, *df_det=None*)
Outer product of random and deterministic samples

Parameters

- **df_rand** (*DataFrame*) –
- **df_det** (*DataFrame*) – set to "nom" for nominal evaluation

Returns Outer product of samples

Return type DataFrame

x2z (x)
Transform to standard normal space

Transform a single vector of random variable values to standard normal space.

Parameters **x** (*array*) – Single vector of values in var_rand. Order of entries must match self.var_rand

Returns Single vector of values transformed to standard normal space

Return type array

z2x (z)
Transform to random variable space

Transform a single vector of normal values to the model's random variable space.

Parameters **z** (*array*) – Single vector of standard normal values. Order of entries must match self.var_rand

Returns Single vector of values transformed to model random variable space

Return type array

4.1.6 grama.dataframe module

grama.dataframe.**df_equal** (*df1*, *df2*, *close=False*, *precision=3*)
Check DataFrame equality

Check that two dataframes have the same columns and values. Allows column order to differ.

Parameters

- **df1** (*DataFrame*) – Comparison input 1
- **df2** (*DataFrame*) – Comparison input 2

Returns Result of comparison

Return type bool

grama.dataframe.**df_make** (***kwargs*)
Construct a DataFrame

Helper function to construct a DataFrame. A common use-case is to use df_make() to pass values to the df (and related) keyword arguments succinctly.

Kwargs: varname (iterable): Column for constructed dataframe; column name inferred from variable name.

Returns Constructed DataFrame

Return type DataFrame

Preconditions: All provided iterables must have identical length or be of length one. All provided variable names (keyword arguments) must be distinct.

Examples:

```
import grama as gr
from models import make_test
md = make_test()
(
    md
    >> gr.ev_sample(
        n=1e3,
        df_det=gr.df_make(x2=[1, 2])
    )
)
```

grama.dataframe.**df_grid**(***kwargs*)

Construct a DataFrame as outer-product

Helper function to construct a DataFrame as an outer-product of the given columns.

Kwargs: varname (iterable): Column for constructed dataframe; column name inferred from variable name.

Returns Constructed DataFrame

Return type DataFrame

Preconditions: All provided variable names (keyword arguments) must be distinct.

Examples:

```
import grama as gr
## Make an empty DataFrame
gr.df_grid()
## Create a row for every pair of values (6 rows total)
gr.df_grid(x=["A", "B"], y=[1, 2, 3])
```

4.1.7 grama.eval_contour module

grama.eval_contour.**eval_contour**

Generate contours from a model

Generates contours from a model. Evaluates the model on a dense grid, then runs marching squares to generate contours. Supports targeting multiple outputs and handling auxiliary inputs not included in the contour map.

Parameters

- **model** (*gr.Model*) – Model to evaluate.
- **var** (*list of str*) – Model inputs to target; must provide exactly two inputs, and both must have finite domain width.
- **out** (*list of str*) – Model output(s) for contour generation.
- **df** (*DataFrame or None*) – Levels for model variables not included in var (auxiliary inputs). If provided var and model.var contain the same values, then df may equal None.
- **levels** (*dict*) – Specific output levels for contour generation; overrides n_levels.
- **n_side** (*int*) – Side resolution for grid; n_side**2 total evaluations.
- **n_levels** (*int*) – Number of contour levels.

Returns Points along contours, organized by output and auxiliary variable levels.

Return type DataFrame

Examples:

```
import grama as gr
## Multiple outputs
(
    gr.Model()
    >> gr.cp_vec_function(
        fun=lambda df: gr.df_make(
            f=df.x**2 + df.y**2,
            g=df.x + df.y,
        ),
        var=["x", "y"],
        out=["f", "g"],
    )
    >> gr.cp_bounds(
        x=(-1, +1),
        y=(-1, +1),
    )
    >> gr.ev_contour(
        var=["x", "y"],
        out=["f", "g"],
    )
    # Contours with no auxiliary variables can autoplot
    >> gr.pt_auto()
)

## Auxiliary inputs
(
    gr.Model()
    >> gr.cp_vec_function(
        fun=lambda df: gr.df_make(
            f=df.c * df.x + (1 - df.c) * df.y,
        ),
        var=["x", "y"],
        out=["f", "g"],
    )
    >> gr.cp_bounds(
        x=(-1, +1),
        y=(-1, +1),
    )
    >> gr.ev_contour(
        var=["x", "y"],
        out=["f"],
        df=gr.df_make(c=[0, 1])
    )

    # Contours with auxiliary variables should be manually plotted
    >> gr.ggplot(gr.aes("x", "y"))
    + gr.geom_segment(gr.aes(xend="x_end", yend="y_end", group="level", color="c
↪"))
)
```

4.1.8 grama.eval_defaults module

grama.eval_defaults.**eval_df**

Evaluate model at given values

Evaluates a given model at a given dataframe.

Parameters

- **model** (*gr.Model*) – Model to evaluate
- **df** (*DataFrame*) – Input dataframe to evaluate
- **append** (*bool*) – Append results to original dataframe?

Returns Results of model evaluation

Return type DataFrame

Examples:

```
import grama as gr
from grama.models import make_test
md = make_test()
df = gr.df_make(x0=0, x1=1, x2=2)
md >> gr.ev_df(df=df)
```

grama.eval_defaults.**eval_linup**

Linear uncertainty propagation

Approximates the variance of output models using a linearization of functions—linear uncertainty propagation. Optionally decomposes the output variance according to additive factors from each input.

Parameters

- **model** (*gr.Model*) – Model to evaluate
- **df_base** (*DataFrame or None*) – Base levels for evaluation; use "nom" for nominal levels.
- **append** (*bool*) – Append results to nominal inputs?
- **decomp** (*bool*) – Decompose the fractional variances according to each input?
- **decimals** (*int*) – Decimals to report for fractional variances
- **n** (*float*) – Monte Carlo sample size, for estimating covariance matrix
- **seed** (*int or None*) – Monte Carlo seed

Returns Output variances at each deterministic level

Return type DataFrame

Examples:

```
import grama as gr
from grama.models import make_test
md = make_test()
## Set manual levels for deterministic inputs; nominal levels for random inputs
md >> gr.ev_linup(df_det=gr.df_make(x2=[0, 1, 2])
## Use nominal deterministic levels
md >> gr.ev_linup(df_base="nom")
```

grama.eval_defaults.**eval_nominal**

Evaluate model at nominal values

Evaluates a given model at a model nominal conditions (median) of random inputs. Optionally set nominal values for the deterministic inputs.

Parameters

- **model** (*gr.Model*) – Model to evaluate
- **df_det** (*DataFrame or None*) – Deterministic levels for evaluation; use "nom" for nominal deterministic levels. If provided model has no deterministic variables (model.n_var_det == 0), then df_det may equal None.
- **append** (*bool*) – Append results to nominal inputs?
- **skip** (*bool*) – Skip evaluation of the functions?

Returns Results of nominal model evaluation or unevaluated design

Return type DataFrame

Examples:

```
import grama as gr
from grama.models import make_test
md = make_test()
## Set manual levels for deterministic inputs; nominal levels for random inputs
md >> gr.ev_nominal(df_det=gr.df_make(x2=[0, 1, 2])
## Use nominal deterministic levels
md >> gr.ev_nominal(df_det="nom")
```

grama.eval_defaults.**eval_grad_fd**

Finite-difference gradient approximation

Evaluates a given model with a central-difference stencil to approximate the gradient.

Parameters

- **model** (*gr.Model*) – Model to differentiate
- **h** (*numeric*) – finite difference stepsize, single (scalar): or per-input (array)
- **df_base** (*DataFrame*) – Base-points for gradient calculations
- **var** (*list(str) or string*) – list of variables to differentiate, or flag; "rand" for var_rand, "det" for var_det
- **append** (*bool*) – Append results to base point inputs?
- **skip** (*bool*) – Skip evaluation of the functions?

Returns Gradient approximation or unevaluated design

Return type DataFrame

@pre (not isinstance(h, collections.Sequence)) | (h.shape[0] == df_base.shape[1])

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md = make_cantilever_beam()
# Select base point(s)
```

(continues on next page)

(continued from previous page)

```
df_nom = md >> gr.ev_nominal(df_det="nom")
# Approximate the gradient
df_grad = md >> gr.ev_grad_fd(df_base=df_nom)
```

grama.eval_defaults.**eval_sample**

Draw a random sample

Evaluates a model with a random sample of the random model inputs. Generates outer product with deterministic levels (common random numbers) OR generates a sample fully-independent of deterministic levels (non-common random numbers).

For more expensive models, it can be helpful to tune n to achieve a reasonable runtime. An even more effective approach is to use skip evaluation along with tran_sp() to evaluate a small, representative sample. (See examples below.)

Parameters

- **model** (*gr.Model*) – Model to evaluate
- **n** (*numeric*) – number of observations to draw
- **df_det** (*DataFrame or None*) – Deterministic levels for evaluation; use "nom" for nominal deterministic levels. If provided model has no deterministic variables (model.n_var_det == 0), then df_det may equal None.
- **seed** (*int*) – random seed to use
- **append** (*bool*) – Append results to input values?
- **skip** (*bool*) – Skip evaluation of the functions?
- **comm** (*bool*) – Use common random numbers (CRN) across deterministic levels? CRN will tend to aid in the comparison of statistics across deterministic levels and enhance the convergence of stochastic optimization.
- **ind_comm** (*str or None*) – Name of realization index column; not added if None

Returns Results of evaluation or unevaluated design

Return type DataFrame

Examples:

```
import grama as gr
from grama.models import make_test
DF = gr.Intention()

# Simple random sample evaluation
md = make_test()
df = md >> gr.ev_sample(n=1e2, df_det="nom")
df.describe()

## Use autoplot to visualize results
(
    md
    >> gr.ev_sample(n=1e2, df_det="nom")
    >> gr.pt_auto()
)

## Cantilever beam examples
from grama.models import make_cantilever_beam
```

(continues on next page)

(continued from previous page)

```
md_beam = make_cantilever_beam()

## Use the realization index to facilitate plotting
# Try running this without the `group` aesthetic in `geom_line()`;
# without the group the plot will not have multiple lines.
(
    md_beam
    >> gr.ev_sample(
        n=20,
        df_det=gr.df_make(w=3, t=gr.linspace(2, 4, 100)),
        ind_comm="idx",
    )

    >> gr.ggplot(gr.aes("t", "g_stress"))
    + gr.geom_line(gr.aes(color="w", group="idx"))
)

## Use iocorr to generate input/output correlation tile plot
(
    md_beam
    >> gr.ev_sample(n=1e3, df_det="nom", skip=True)
    # Generate input/output correlation summary
    >> gr.tf_iocorr()
    # Visualize
    >> gr.pt_auto()
)

## Use support points to reduce model runtime
(
    md_beam
    # Generate large input sample but don't evaluate outputs
    >> gr.ev_sample(n=1e5, df_det="nom", skip=True)
    # Reduce to a smaller---but representative---sample
    >> gr.tf_sp(n=50)
    # Evaluate the outputs
    >> gr.tf_md(md_beam)
)

## Estimate probabilities
(
    md_beam
    # Generate large
    >> gr.ev_sample(n=1e5, df_det="nom")
    # Estimate probabilities of failure
    >> gr.tf_summarize(
        pof_stress=gr.mean(DF.g_stress <= 0),
        pof_disp=gr.mean(DF.g_disp <= 0),
    )
)
```

grama.eval_defaults.**eval_conservative**

Evaluates a given model at conservative input quantiles

Uses model specifications to determine the "conservative" direction for each input, and evaluates the model at the desired quantile. Provided primarily for comparing UQ against pseudo-deterministic design criteria (del Rosario et al.; 2021).

Note that if there is no conservative direction for the given input, the given quantile will be ignored and the

median will automatically be selected.

Parameters

- **model** (*gr.Model*) – Model to evaluate
- **quantiles** (*numeric*) – lower quantile value(s) for conservative evaluation; can be single value for all inputs, array of values for each random variable, or None for default 0.01. values in [0, 0.5]
- **df_det** (*DataFrame or None*) – Deterministic levels for evaluation; use "nom" for nominal deterministic levels. If provided model has no deterministic variables (model.n_var_det == 0), then df_det may equal None.
- **append** (*bool*) – Append results to conservative inputs?
- **skip** (*bool*) – Skip evaluation of the functions?

Returns Conservative evaluation or unevaluated design

Return type DataFrame

References

del Rosario, Zachary, Richard W. Fenrich, and Gianluca Iaccarino. "When Are Allowables Conservative?." AIAA Journal 59.5 (2021): 1760-1772.

Examples:

```
import grama as gr
from grama.models import make_plate_buckle
md = make_plate_buckle()
# Evaluate at conservative input values
md >> gr.ev_conservative(df_det="nom")
```

4.1.9 grama.eval_opt module

grama.eval_opt.**eval_nls**

Estimate with Nonlinear Least Squares (NLS)

Estimate best-fit variable levels with nonlinear least squares (NLS).

Parameters

- **model** (*gr.Model*) – Model to analyze. All model variables selected for fitting must be bounded or random. Deterministic variables may have semi-infinite bounds.
- **df_data** (*DataFrame*) – Data for estimating parameters. Variables not found in df_data optimized in fitting.
- **out** (*list or None*) – Output contributions to consider in computing MSE. Assumed to be model.out if left as None.
- **var_fix** (*list or None*) – Variables to fix to nominal levels. Note that variables with domain width zero will automatically be fixed.
- **df_init** (*DataFrame or None*) – Initial guesses for parameters; overrides
- **n_restart** (*int*) –
- **append** (*bool*) – Append metadata? (Initial guess, MSE, optimizer status)

- **tol** (*float*) – Optimizer convergence tolerance
- **n_maxiter** (*int*) – Optimizer maximum iterations
- **n_restart** – Number of restarts; beyond n_restart=1 random restarts are used.
- **seed** (*int OR None*) – Random seed for restarts
- **verbose** (*bool*) – Print messages to console?

Returns Results of estimation

Return type DataFrame

Examples:

```
import grama as gr
from grama.data import df_trajectory_full
from grama.models import make_trajectory_linear

md_trajectory = make_trajectory_linear()

df_fit = (
    md_trajectory
    >> gr.ev_nls(df_data=df_trajectory_full)
)

print(df_fit)
```

grama.eval_opt.**eval_min**

Constrained minimization using functions from a model

Perform constrained minimization using functions from a model. Model must have deterministic variables only.

Wrapper for scipy.optimize.minimize

Parameters

- **model** (*gr.Model*) – Model to analyze. All model variables must be deterministic.
- **out_min** (*str*) – Output to use as minimization objective.
- **out_geq** (*None OR list of str*) – Outputs to use as geq constraints; out >= 0
- **out_leq** (*None OR list of str*) – Outputs to use as leq constraints; out <= 0
- **out_eq** (*None OR list of str*) – Outputs to use as equality constraints; out == 0
- **method** (*str*) – Optimization method; see the documentation for scipy.optimize.minimize for options.
- **tol** (*float*) – Optimization objective convergence tolerance
- **n_restart** (*int*) – Number of restarts; beyond n_restart=1 random restarts are used.
- **df_start** (*None or DataFrame*) – Specific starting values to use; overrides n_restart if non None provided.

Returns Results of optimization

Return type DataFrame

Examples:

```
import grama as gr
## Define a model with objective and constraints
md = (
    gr.Model("Constrained Rosenbrock")
    >> gr.cp_function(
        fun=lambda x: (1 - x[0])**2 + 100*(x[1] - x[0]**2)**2,
        var=["x", "y"],
        out=["c"],
    )
    >> gr.cp_function(
        fun=lambda x: (x[0] - 1)**3 - x[1] + 1,
        var=["x", "y"],
        out=["g1"],
    )
    >> gr.cp_function(
        fun=lambda x: x[0] + x[1] - 2,
        var=["x", "y"],
        out=["g2"],
    )
    >> gr.cp_bounds(
        x=(-1.5, +1.5),
        y=(-0.5, +2.5),
    )
)

## Run the optimizer
md >> gr.ev_min(
    out_min="c",
    out_leq=["g1", "g2"]
)
```

4.1.10 grama.eval_pnd module

grama.eval_pnd.**approx_pnd**(*X_pred*, *X_cov*, *X_train*, *signs*, *n=10000*, *seed=None*)

Approximate the PND via mixture importance sampling

Approximate the probability non-dominated (PND) for a set of predictive points using a mixture importance sampling approach. Predictive points are assumed to have predictive gaussian distributions (with specified mean and covariance matrix).

Parameters

- **X_pred** (*2d numpy array*) – Predictive values
- **X_cov** (*iterable of 2d numpy arrays*) – Predictive covariance matrices
- **X_train** (*2d numpy array*) – Training values, used to determine existing Pareto frontier
- **signs** (*numpy array of +/-1 values*) – Array of optimization signs: {-1: Minimize, +1 Maximize}

Kwargs: n (int): Number of draws for importance sampler seed (int): Seed for random state

Returns Estimated PND values var_values (array): Estimated variance values

Return type pr_scores (array)

References

Owen *Monte Carlo theory, methods and examples* (2013)

grama.eval_pnd.**choice**(*a*, *size=None*, *replace=True*, *p=None*)
Generates a random sample from a given 1-D array

New in version 1.7.0.

Note: New code should use the `choice` method of a `default_rng()` instance instead; please see the random-quick-start.

Parameters

- **a** (*1-D array-like or int*) – If an ndarray, a random sample is generated from its elements. If an int, the random sample is generated as if it were `np.arange(a)`
- **size** (*int or tuple of ints, optional*) – Output shape. If the given shape is, e.g., `(m, n, k)`, then `m * n * k` samples are drawn. Default is None, in which case a single value is returned.
- **replace** (*boolean, optional*) – Whether the sample is with or without replacement. Default is True, meaning that a value of `a` can be selected multiple times.
- **p** (*1-D array-like, optional*) – The probabilities associated with each entry in a. If not given, the sample assumes a uniform distribution over all entries in `a`.

Returns **samples** – The generated random samples

Return type single item or ndarray

Raises `ValueError` – If a is an int and less than zero, if a or p are not 1-dimensional, if a is an array-like of size 0, if p is not a vector of probabilities, if a and p have different lengths, or if replace=False and the sample size is greater than the population size

See also:

`randint()`, `shuffle()`, `permutation()`

`Generator.choice()` which should be used in new code

Notes

Setting user-specified probabilities through `p` uses a more general but less efficient sampler than the default. The general sampler produces a different sample than the optimized sampler even if each element of `p` is 1 / len(a).

Sampling random rows from a 2-D array is not possible with this function, but is possible with *Generator.choice* through its `axis` keyword.

Examples

Generate a uniform random sample from np.arange(5) of size 3:

```
>>> np.random.choice(5, 3)
array([0, 3, 4]) # random
>>> #This is equivalent to np.random.randint(0,5,3)
```

Generate a non-uniform random sample from np.arange(5) of size 3:

```
>>> np.random.choice(5, 3, p=[0.1, 0, 0.3, 0.6, 0])
array([3, 3, 0]) # random
```

Generate a uniform random sample from np.arange(5) of size 3 without replacement:

```
>>> np.random.choice(5, 3, replace=False)
array([3,1,0]) # random
>>> #This is equivalent to np.random.permutation(np.arange(5))[:3]
```

Generate a non-uniform random sample from np.arange(5) of size 3 without replacement:

```
>>> np.random.choice(5, 3, replace=False, p=[0.1, 0, 0.3, 0.6, 0])
array([2, 3, 0]) # random
```

Any of the above can be repeated with an arbitrary array-like instead of just integers. For instance:

```
>>> aa_milne_arr = ['pooh', 'rabbit', 'piglet', 'Christopher']
>>> np.random.choice(aa_milne_arr, 5, p=[0.5, 0.1, 0.1, 0.3])
array(['pooh', 'pooh', 'pooh', 'Christopher', 'piglet'], # random
      dtype='<U11')
```

grama.eval_pnd.**dprop**(*X*, *Sigma*, *X_means*)

Evaluate the PDF of a mixture proposal distribution

Evaluate the PDF of a gaussian mixture distribution with a common covariance matrix and different means.

Parameters

- **X** (*2d numpy array*) – Observations for which to evaluate the density
- **Sigma** (*2d numpy array*) – Common covariance matrix for mixture distribution
- **X_means** (*2d numpy array*) – Means for mixture distribution

Preconditions: X.shape[1] == X_means.shape[1] Sigma.shape[0] == X_means.shape[1] Sigma.shape[1] == X_means.shape[1]

Returns Density values

Return type numpy array

grama.eval_pnd.**eval_pnd**

Approximate the probability non-dominated (PND)

Approximates the probability non-dominated (PND) for a set of training points given a fitted probabilistic model. Used to rank a set of candidates in the context of multiobjective optimization.

Parameters

- **model** (*gr.model*) – predictive model to evaluate
- **df_train** (*DataFrame*) – dataframe with training data
- **df_test** (*DataFrame*) – dataframe with test data
- **signs** (*dict*) – dict with the variables you would like to use and minimization or maximization parameter for each
- **append** (*bool*) – Append df_test to pnd algorithm outputs

Kwargs: n (int): Number of draws for importance sampler seed (int): declarble seed value for reproducibility

Returns Results of predictive model going through a PND algorithm. Conatians both values and their scores.

Return type DataFrame

References

del Rosario, Zachary, et al. "Assessing the frontier: Active learning, model accuracy, and multi-objective candidate discovery and optimization." The Journal of Chemical Physics 153.2 (2020): 024112.

Examples:

```
import grama as gr

## Define a ground-truth model
md_true = gr.make_pareto_random()
df_data = (
    md_true
    >> gr.ev_sample(n=2e3, seed=101, df_det="nom")
)
## Generate test/train data
df_train = (
    df_data
    >> gr.tf_sample(n=10)
)

df_test = (
    df_data
    >> gr.anti_join(
        df_train,
        by = ["x1","x2"]
    )
    >> gr.tf_sample(n=200)
)
## Fit a model to training data
md_fit = (
    df_train
    >> gr.ft_gp(
        var=["x1","x2"]
        out=["y1","y2"]
    )
)
## Rank training points by PND algorithm
df_pnd = (
    md_fit
    >> gr.ev_pnd(
        df_train,
        df_test,
        signs = {"y1":1, "y2":1},
        seed = 101
    )
    >> gr.tf_arrange(gr.desc(DF.pr_scores))
)
```

grama.eval_pnd.**floor_sig**(*sig*, *sig_min=1e-08*)

Floor an array of variances

grama.eval_pnd.**make_proposal_sigma**(*X*, *idx_pareto*, *X_cov*)
Estimate parameters for PND importance distribution

Parameters

- **X** (*2d numpy array*) – Full set of response values
- **idx_pareto** (*boolean array*) – Whether each response value is a Pareto point
- **X_cov** (*iterable of 2d numpy array*) – Predictive covariance matrices

Preconditions: X.shape[0] == len(idx_pareto) X_cov[i].shape[0] == X.shape[1] for all valid i X_cov[i].shape[1] == X.shape[1] for all valid i

Returns Common covariance matrix for PND importance distribution

Return type 2d numpy array

grama.eval_pnd.**multivariate_normal**(*mean*, *cov*, *size=None*, *check_valid='warn'*, *tol=1e-8*)
Draw random samples from a multivariate normal distribution.

The multivariate normal, multinormal or Gaussian distribution is a generalization of the one-dimensional normal distribution to higher dimensions. Such a distribution is specified by its mean and covariance matrix. These parameters are analogous to the mean (average or "center") and variance (standard deviation, or "width," squared) of the one-dimensional normal distribution.

Note: New code should use the `multivariate_normal` method of a `default_rng()` instance instead; please see the random-quick-start.

Parameters

- **mean** (*1-D array_like, of length N*) – Mean of the N-dimensional distribution.
- **cov** (*2-D array_like, of shape (N, N)*) – Covariance matrix of the distribution. It must be symmetric and positive-semidefinite for proper sampling.
- **size** (*int or tuple of ints, optional*) – Given a shape of, for example, `(m,n,k)`, `m*n*k` samples are generated, and packed in an *m*-by-*n*-by-*k* arrangement. Because each sample is *N*-dimensional, the output shape is `(m,n,k,N)`. If no shape is specified, a single (*N*-D) sample is returned.
- **check_valid** (*{ 'warn', 'raise', 'ignore' }, optional*) – Behavior when the covariance matrix is not positive semidefinite.
- **tol** (*float, optional*) – Tolerance when checking the singular values in covariance matrix. cov is cast to double before the check.

Returns

out – The drawn samples, of shape *size*, if that was provided. If not, the shape is `(N,)`.

In other words, each entry `out[i,j,...,:]` is an N-dimensional value drawn from the distribution.

Return type ndarray

See also:

Generator.multivariate_normal() which should be used for new code.

Notes

The mean is a coordinate in N-dimensional space, which represents the location where samples are most likely to be generated. This is analogous to the peak of the bell curve for the one-dimensional or univariate normal distribution.

Covariance indicates the level to which two variables vary together. From the multivariate normal distribution, we draw N-dimensional samples, $X = [x_1, x_2, ...x_N]$. The covariance matrix element C_{ij} is the covariance of x_i and x_j. The element C_{ii} is the variance of x_i (i.e. its "spread").

Instead of specifying the full covariance matrix, popular approximations include:

- Spherical covariance (*cov* is a multiple of the identity matrix)
- Diagonal covariance (*cov* has non-negative elements, and only on the diagonal)

This geometrical property can be seen in two dimensions by plotting generated data-points:

```
>>> mean = [0, 0]
>>> cov = [[1, 0], [0, 100]]  # diagonal covariance
```

Diagonal covariance means that points are oriented along x or y-axis:

```
>>> import matplotlib.pyplot as plt
>>> x, y = np.random.multivariate_normal(mean, cov, 5000).T
>>> plt.plot(x, y, 'x')
>>> plt.axis('equal')
>>> plt.show()
```

Note that the covariance matrix must be positive semidefinite (a.k.a. nonnegative-definite). Otherwise, the behavior of this method is undefined and backwards compatibility is not guaranteed.

References

Examples

```
>>> mean = (1, 2)
>>> cov = [[1, 0], [0, 1]]
>>> x = np.random.multivariate_normal(mean, cov, (3, 3))
>>> x.shape
(3, 3, 2)
```

The following is probably true, given that 0.6 is roughly twice the standard deviation:

```
>>> list((x[0,0,:] - mean) < 0.6)
[True, True] # random
```

grama.eval_pnd.**pareto_min_rel**(*X_test*, *X_base=None*)

Determine if rows in X_test are optimal, compared to X_base

Finds the Pareto-efficient test-points that minimize the column values, relative to a given set of base-points.

Parameters

- **X_test** (*2d numpy array*) – Test point observations; rows are observations, columns are features
- **X_base** (*2d numpy array*) – Base point observations; rows are observations, columns are features

Returns Indicates if test observation is Pareto-efficient, relative to base points

Return type array of boolean values

References

Owen *Monte Carlo theory, methods and examples* (2013)

grama.eval_pnd.**rprop**(*n*, *Sigma*, *X_means*, *seed=None*)
Draw a sample from gaussian mixture distribution

Draw a sample from a gaussian mixture distribution with a common covariance matrix and different means.

Parameters

- **n** (*int*) – Number of observations in sample
- **Sigma** (*2d numpy array*) – Common covariance matrix for mixture distribution
- **X_means** (*2d numpy array*) – Means for mixture distribution

Preconditions: Sigma.shape[0] == X_means.shape[1] Sigma.shape[1] == X_means.shape[1]

Returns Sample of observations

Return type 2d numpy array

grama.eval_pnd.**set_seed**()
seed(self, seed=None)

Reseed a legacy MT19937 BitGenerator

Notes

This is a convenience, legacy function.

The best practice is to **not** reseed a BitGenerator, rather to recreate a new one. This method is here for legacy reasons. This example demonstrates best practice.

```
>>> from numpy.random import MT19937
>>> from numpy.random import RandomState, SeedSequence
>>> rs = RandomState(MT19937(SeedSequence(123456789)))
# Later, you want to restart the stream
>>> rs = RandomState(MT19937(SeedSequence(987654321)))
```

4.1.11 grama.eval_random module

grama.eval_random.**eval_sinews**
Sweep study

Perform coordinate sweeps over each model random variable ("sinew" design). Use random starting points drawn from the joint density. Optionally sweep the deterministic variables.

For more expensive models, it can be helpful to tune n_density and n_sweeps to achieve a reasonable runtime.

Use gr.plot_auto() to construct a quick visualization of the output dataframe. Use *skip* version to visualize the design, and non-skipped version to visualize the results.

Parameters

- **model** (*gr.Model*) – Model to evaluate
- **n_density** (*numeric*) – Number of points along each sweep
- **n_sweeps** (*numeric*) – Number of sweeps per-random variable
- **seed** (*int*) – Random seed to use
- **df_det** (*DataFrame*) – Deterministic levels for evaluation; use "nom" for nominal deterministic levels, use "swp" to sweep deterministic variables
- **varname** (*str*) – Column name to give for sweep variable; default="sweep_var"
- **indname** (*str*) – Column name to give for sweep index; default="sweep_ind"
- **append** (*bool*) – Append results to conservative inputs?
- **skip** (*bool*) – Skip evaluation of the functions?

Returns Results of evaluation or unevaluated design

Return type DataFrame

Examples:

```
import grama as gr
md = gr.make_cantilever_beam()
# Skip evaluation, used to visualize the design (input points)
df_design = md >> gr.ev_sinews(df_det="nom", skip=True)
df_design >> gr.pt_auto()
# Visualize the input-to-output relationships of the model
df_sinew = md >> gr.ev_sinews(df_det="nom")
df_sinew >> gr.pt_auto()
```

grama.eval_random.**eval_hybrid**

Hybrid points for Sobol' indices

Use the "hybrid point" design (Sobol', 1999) to support estimating Sobol' indices. Use gr.tran_sobol() to post-process the results and compute estimates.

Parameters

- **model** (*gr.Model*) – Model to evaluate; must have CopulaIndependence
- **n** (*numeric*) – Number of points along each sweep
- **plan** (*str*) – Sobol' index to compute; plan={"first", "total"}
- **seed** (*int*) – Random seed to use
- **df_det** (*DataFrame*) – Deterministic levels for evaluation; use "nom" for nominal deterministic levels.
- **varname** (*str*) – Column name to give for sweep variable; default="hybrid_var"
- **append** (*bool*) – Append results to conservative inputs?
- **skip** (*bool*) – Skip evaluation of the functions?

Returns Results of evaluation or unevaluated design

Return type DataFrame

References

I.M. Sobol', "Sensitivity Estimates for Nonlinear Mathematical Models" (1999) MMCE, Vol 1.

Examples:

```
import grama as gr
md = gr.make_cantilever_beam()
## Compute the first-order indices
df_first = md >> gr.ev_hybrid(df_det="nom", plan="first")
df_first >> gr.tf_sobol()
## Compute the total-order indices
df_total = md >> gr.ev_hybrid(df_det="nom", plan="total")
df_total >> gr.tf_sobol()
```

4.1.12 grama.eval_tail module

grama.eval_tail.**eval_form_pma**

Tail quantile via FORM PMA

Approximate the desired tail quantiles using the performance measure approach (PMA) of the first-order reliability method (FORM) [1]. Select limit states to minimize at desired quantile with one of: *betas* (reliability indices), *rels* (reliability values), or *pofs* (probabilities of failure). Provide confidence levels *cons* and estimator covariance *df_corr* to compute with margin in beta [2].

Note that under the performance measure approach, the optimized limit state value g is sought to be non-negative $g geq 0$. This is usually included as a constraint in optimization, which can be accomplished in by using ‘‘gr.eval_form_pnd()‘ *within* a model definition—see the Examples below for more details.

Parameters

- **model** (*gr.Model*) – Model to analyze
- **df_det** (*DataFrame*) – Deterministic levels for evaluation; use "nom" for nominal deterministic levels.
- **betas** (*dict*) – Target reliability indices; key = limit state name; must be in model.out value = reliability index; beta = Phi^{-1}(reliability)
- **rels** (*dict*) – Target reliability values; key = limit state name; must be in model.out value = reliability
- **pofs** (*dict*) – Target probabilities of failure (POFs); key = limit state name; must be in model.out value = probability of failure; pof = 1 - reliability
- **cons** (*dict or None*) – Target confidence levels; key = limit state name; must be in model.out value = confidence level, in (0, 1)
- **df_corr** (*DataFrame or None*) – Sampling distribution covariance entries; parameters with no information assumed to be known exactly.
- **n_maxiter** (*int*) – Maximum iterations for each optimization run
- **n_restart** (*int*) – Number of restarts (== number of optimization runs)
- **append** (*bool*) – Append MPP results for random values?
- **verbose** (*bool*) – Print optimization results?

Returns Results of MPP search

Return type DataFrame

Notes

Since FORM PMA relies on optimization over the limit state, it is often beneficial to scale your limit state to keep values near unity.

References

Tu, Choi, and Park, "A new study on reliability-based design optimization," Journal of Mechanical Design, 1999 del Rosario, Fenrich, and Iaccarino, "Fast precision margin with the first-order reliability method," AIAA Journal, 2019

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
## Evaluate the reliability of specified designs
(
    md_beam
    >> gr.ev_form_pma(
        # Specify target reliability
        betas=dict(g_stress=3, g_disp=3),
        # Analyze three different thicknesses
        df_det=gr.df_make(t=[2, 3, 4], w=3)
    )
)

## Specify reliability in POF form
(
    md_beam
    >> gr.ev_form_pma(
        # Specify target reliability
        pofs=dict(g_stress=1e-3, g_disp=1e-3),
        # Analyze three different thicknesses
        df_det=gr.df_make(t=[2, 3, 4], w=3)
    )
)

## Build a nested model for optimization under uncertainty
md_opt = (
    gr.Model("Beam Optimization")
    >> gr.cp_vec_function(
        fun=lambda df: gr.df_make(c_area=df.w * df.t),
        var=["w", "t"],
        out=["c_area"],
        name="Area objective",
    )
    >> gr.cp_vec_function(
        fun=lambda df: gr.eval_form_pma(
            md_beam,
            betas=dict(g_stress=3, g_disp=3),
            df_det=df,
            append=False,
        )
        var=["w", "t"],
        out=["g_stress", "g_disp"],
        name="Reliability constraints",
```

(continues on next page)

(continued from previous page)

```
    )
    >> gr.cp_bounds(w=(2, 4), t=(2, 4))
)
# Run the optimization
(
    md_opt
    >> gr.ev_min(
        out_min="c_area",
        out_geq=["g_stress", "g_disp"],
    )
)
```

grama.eval_tail.**eval_form_ria**

Tail reliability via FORM RIA

Approximate the desired tail probability using the reliability index approach (RIA) of the first-order reliability method (FORM) [1]. Select limit states to analyze with list input *limits*. Choose output type using *format* argument (*betas* for reliability indices, *rels* for realibility values, *pofs* for probabilify of failure values). Provide confidence levels *cons* and estimator covariance *df_corr* to compute with margin in beta [2].

Note that the reliability index approach (RIA) is generally less stable than the performance measure approach (PMA). Consider using `gr.eval_form_pma()` instead, particularly when using FORM to optimize a design.

Parameters

- **model** (*gr.Model*) – Model to analyze
- **limits** (*list*) – Target limit states; must be in model.out; limit state assumed to be critical at g == 0.
- **format** (*str*) – One of ("betas", "rels", "pofs"). Format for computed reliability information
- **cons** (*dict or None*) – Target confidence levels; key = limit state name; must be in model.out value = confidence level, in (0, 1)
- **df_corr** (*DataFrame or None*) – Sampling distribution covariance entries; parameters with no information assumed to be known exactly.
- **df_det** (*DataFrame*) – Deterministic levels for evaluation; use "nom" for nominal deterministic levels.
- **n_maxiter** (*int*) – Maximum iterations for each optimization run
- **n_restart** (*int*) – Number of restarts (== number of optimization runs)
- **append** (*bool*) – Append MPP results for random values?
- **verbose** (*bool*) – Print optimization results?

Returns Results of MPP search

Return type DataFrame

Notes

Since FORM RIA relies on optimization over the limit state, it is often beneficial to scale your limit state to keep values near unity.

References

[1] Tu, Choi, and Park, "A new study on reliability-based design optimization," Journal of Mechanical Design, 1999 [2] del Rosario, Fenrich, and Iaccarino, "Fast precision margin with the first-order reliability method," AIAA Journal, 2019

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
## Evaluate the reliability of specified designs
(
    md_beam
    >> gr.ev_form_ria(
        # Specify limit states to analyze
        limits=("g_stress", "g_disp"),
        # Analyze three different thicknesses
        df_det=gr.df_make(t=[2, 3, 4], w=3)
    )
)
```

4.1.13 grama.fit_synonyms module

grama.fit_synonyms.**fit_nls**

Fit a model with Nonlinear Least Squares (NLS)

Estimate best-fit variable levels with nonlinear least squares (NLS), and return an executable model with those frozen best-fit levels. Optionally, fit a distribution on the parameters to quantify parametric uncertainty.

Note that it is **highly likely** you will need to adjust either the bounds of your model or the initial guess of the optimizer (via *df_init*). Use these to guide the optimizer towards *reasonable* input values, otherwise you are likely to get nonsensical results.

Note: This is a *synonym* for eval_nls(); see the documentation for eval_nls() for keyword argument options available beyond those listed here.

Parameters

- **df_data** (*DataFrame*) – Data for estimating best-fit variable levels. Variables not found in df_data optimized for fitting.
- **md** (*gr.Model*) – Model to analyze. All model variables selected for fitting must be bounded or random. Deterministic variables may have semi-infinite bounds.
- **var_fix** (*list or None*) – Variables to fix to nominal levels. Note that variables with domain width zero will automatically be fixed.
- **df_init** (*DataFrame*) – Initial guesses for parameters; overrides n_restart
- **n_restart** (*int*) – Number of restarts to try; the first try is at the nominal conditions of the model. Returned model will use the least-error parameter set among restarts tested.
- **n_maxiter** (*int*) – Optimizer maximum iterations
- **verbose** (*bool*) – Print best-fit parameters to console?
- **uq_method** (*str OR None*) – If string, select method to quantify parameter uncertainties. If None, provide best-fit values only. Methods: uq_method = "linpool": assume normal

errors; linearly approximate parameter effects; equally pool variance matrices for each output

Returns

Model for evaluation with best-fit variables frozen to optimized levels.

Return type gr.Model

Examples:

```
import grama as gr
from grama.data import df_trajectory_windowed
from grama.models import make_trajectory_linear
DF = gr.Intention()

md_trajectory = make_trajectory_linear()

## Fit
md_fitted = (
    df_trajectory_windowed
    >> gr.ft_nls(md=md_trajectory)
)

## Fit, stabilize with initial guess
md_fitted = (
    df_trajectory_windowed
    >> gr.ft_nls(
        md=md_trajectory,
        df_init=gr.df_make(u0=18, v0=18, tau=16),
    )
)

## Fit, and return input uncertainties
md_fitted_uq = (
    df_trajectory_windowed
    >> gr.ft_nls(
        md=md_trajectory,
        df_init=gr.df_make(u0=18, v0=18, tau=16),
        uq_method="linpool",
    )
)
```

4.1.14 grama.marginals module

grama.marginals.**marg_gkde**(*data*, *sign=None*)

Fit a gaussian KDE to data

Fits a gaussian kernel density estimate (KDE) to data.

Parameters

- **data** (*iterable*) – Data for fit
- **sign** (*bool*) – Include sign? (Optional)

Returns Marginal distribution

Return type gr.MarginalGKDE

Examples:

```
import grama as gr
from grama.data import df_stang
md = (
    gr.Model("Marginal Example")
    >> gr.cp_marginals(
        E=gr.marg_gkde(df_stang.E),
        mu=gr.marg_gkde(df_stang.mu),
    )
)
md
```

grama.marginals.**marg_fit**(*dist*, *data*, *name=True*, *sign=None*, ***kwargs*)

Fit scipy.stats continuous distirbution

Fits a scipy.stats continuous distribution. Intended to be used to define a marginal distribution from data.

Parameters

- **dist** (*str*) – Distribution to fit
- **data** (*iterable*) – Data for fit
- **name** (*bool*) – Include distribution name?
- **sign** (*bool*) – Include sign? (Optional)
- **loc** (*float*) – Initial guess for location *loc* parameter (Optional)
- **scale** (*float*) – Initial guess for scale *scale* parameter (Optional)
- **floc** (*float*) – Value to fix the location *loc* parameter (Optional) Note that for distributions such as "lognorm" or "weibull_min", setting floc=0 selects the 2-parameter version of the distribution.
- **fscale** (*float*) – Value to fix the location *scale* parameter (Optional)
- **f*** (*float*) – Value to fix the specified shape parameter (Optional) e.g. give fc to fix the *c* parameter

Returns Distribution

Return type gr.MarginalNamed

Examples:

```
import grama as gr
from grama.data import df_shewhart
# Fit normal distribution
mg_normal = gr.marg_named(
    "norm",
    df_shewhart.tensile_strength,
)
# Fit two-parameter Weibull distribution
mg_weibull2 = gr.marg_named(
    "weibull_min",
    df_shewhart.tensile_strength,
    floc=0,         # 2-parameter has frozen loc == 0
)
# Fit three-parameter Weibull distribution
mg_weibull3 = gr.marg_named(
    "weibull_min",
    df_shewhart.tensile_strength,
```

(continues on next page)

(continued from previous page)

```
    loc=0,          # 3-parameter fit tends to be unstable;
                    # an inital guess helps stabilize fit
)
# Inspect fits with QQ plot
(
    df_shewhart
    >> gr.tf_mutate(
        q_normal=gr.qqvals(DF.tensile_strength, marg=mg_normal),
        q_weibull2=gr.qqvals(DF.tensile_strength, marg=mg_weibull2),
    )
    >> gr.tf_pivot_longer(
        columns=[
            "q_normal",
            "q_weibull2",
        ],
        names_to=[".value", "Distribution"],
        names_sep="_"
    )

    >> gr.ggplot(gr.aes("q", "tensile_strength"))
    + gr.geom_abline(intercept=0, slope=1, linetype="dashed")
    + gr.geom_point(gr.aes(color="Distribution"))
)
```

grama.marginals.**marg_mom**(*dist*, *mean=None*, *sd=None*, *cov=None*, *var=None*, *skew=None*, *kurt=None*, *kurt_excess=None*, *floc=None*, *sign=0*, *dict_x0=None*)

Fit scipy.stats continuous distribution via moments

Fit a continuous distribution using the method of moments. Select a distribution shape and provide numerical values for a convenient set of common moments.

This routine uses a vector-output root finding routine to match the moments. You may set an optional initial guess for the distribution parameters using the dict_x0 argument.

Parameters **dist** (*str*) – Name of distribution to fit

Kwargs: mean (float): Mean of distribution sd (float): Standard deviation of distribution cov (float): Coefficient of Variation of distribution (sd / mean) var (float): Variance of distribution; only one of *sd* and *var* can be provided. skew (float): Skewness of distribution kurt (float): Kurtosis of distribution kurt_excess (float): Excess kurtosis of distribution; kurt_excess = kurt - 3.

Only one of *kurt* and *kurt_excess* can be provided.

floc (float or None): Frozen value for location parameter Note that for distributions such as "lognorm" or "weibull_min", setting floc=0 selects the 2-parameter version of the distribution.

sign (-1, 0, +1): Sign dict_x0 (dict): Dictionary of initial parameter guesses

Returns Distribution

Return type gr.MarginalNamed

Examples:

```
import grama as gr
## Fit a normal distribution
mg_norm = gr.marg_mom("norm", mean=0, sd=1)
```

(continues on next page)

(continued from previous page)

```
## Fit a (3-parameter) lognormal distribution
mg_lognorm = gr.marg_mom("lognorm", mean=1, sd=1, skew=1)
## Fit a lognormal, controlling kurtosis instead
mg_lognorm = gr.marg_mom("lognorm", mean=1, sd=1, kurt=1)
## Fit a 2-parameter lognormal; no skewness or kurtosis needed
mg_lognorm = gr.marg_mom("lognorm", mean=1, sd=1, floc=0)

## Not all moment combinations are feasible; this will fail
gr.marg_mom("beta", mean=1, sd=1, skew=0, kurt=4)
## Skewness and kurtosis are related for the beta distribution;
## a different combination is feasible
gr.marg_mom("beta", mean=1, sd=1, skew=0, kurt=2)
```

class grama.marginals.**Marginal**(*sign=0*)

Bases: abc.ABC

Parent class for marginal distributions

copy()

d(*x*)

fit(*data*)

p(*x*)

q(*p*)

r(*n*)

summary()

class grama.marginals.**MarginalNamed**(*d_name=None*, *d_param=None*, ***kw*)

Bases: *grama.marginals.Marginal*

Marginal using a named distribution from gr.valid_dist

copy()

d(***kwargs*)

fit(*data*, ***kwargs*)

p(***kwargs*)

q(***kwargs*)

summary(*dig=2*)

class grama.marginals.**MarginalGKDE**(*kde*, *atol=1e-06*, ***kw*)

Bases: *grama.marginals.Marginal*

Marginal using scipy.stats.gaussian_kde

copy()

d(***kwargs*)

fit(*data*)

p(***kwargs*)

q(***kwargs*)

summary()

4.1.15 grama.mutate_helpers module

grama.mutate_helpers.**abs**(**args*, ***kwargs*)
Absolute value

grama.mutate_helpers.**sin**(**args*, ***kwargs*)
Sine

grama.mutate_helpers.**cos**(**args*, ***kwargs*)
Cosine

grama.mutate_helpers.**tan**(**args*, ***kwargs*)
Tangent

grama.mutate_helpers.**log**(**args*, ***kwargs*)
(Natural) log

grama.mutate_helpers.**exp**(**args*, ***kwargs*)
Exponential (e-base)

grama.mutate_helpers.**sqrt**(**args*, ***kwargs*)
Square-root

grama.mutate_helpers.**pow**(**args*, ***kwargs*)
Power

Usage: q = pow(x, p) := x ^ p

Parameters

- **= base** (*x*) –
- **= exponent** (*p*) –

grama.mutate_helpers.**floor**(**args*, ***kwargs*)
Round downwards to nearest integer

grama.mutate_helpers.**ceil**(**args*, ***kwargs*)
Round upwards to nearest integer

grama.mutate_helpers.**round**(**args*, ***kwargs*)
Round value to desired precision

Parameters

- **x** (*float or iterable of floats*) – Value(s) to round
- **decimals** (*int*) – Number of decimal places for rounding; decimals=0 rounds to integers

grama.mutate_helpers.**as_int**(**args*, ***kwargs*)
Cast to integer

grama.mutate_helpers.**as_float**(**args*, ***kwargs*)
Cast to float

grama.mutate_helpers.**as_str**(**args*, ***kwargs*)
Cast to string

grama.mutate_helpers.**as_factor**(**args*, ***kwargs*)
Cast to factor

Parameters

- **x** (*pd.Series*) – Column to convert

- **categories** (*list*) – Categories (levels) of factor (Optional)
- **ordered** (*boolean*) – Order the factor?

grama.mutate_helpers.**as_numeric**(**args*, ***kwargs*)
Cast to numeric

grama.mutate_helpers.**fct_reorder**(**args*, ***kwargs*)
Reorder a factor on another variable

Parameters

- **f** (*iterable OR DataFrame column*) – factor to reorder
- **x** (*iterable OR DataFrame column*) – variable on which to reorder; specify aggregation method with fun
- **fun** (*function*) – aggregation function for reordering, default=median

Returns Iterable with levels sorted according to x

Return type Categorical

Examples:

```
import grama as gr
from grama.data import df_diamonds
DF = gr.Intention()
(
    df_diamonds
    >> gr.tf_mutate(cut=gr.fct_reorder(DF.cut, DF.price))
    >> gr.tf_group_by(DF.cut)
    >> gr.tf_summarize(max=gr.colmax(DF.price), mean=gr.mean(DF.price))
)
```

grama.mutate_helpers.**fillna**(**args*, ***kwargs*)
Wrapper for pandas Series.fillna

(See below for Pandas documentation)

Examples:

```
import grama as gr
X = gr.Intention()
df = gr.df_make(x=[1, gr.NaN], y=[2, 3])
df_filled = (
    df
    >> gr.tf_mutate(x=gr.fillna(X.x, 0))
)
```

Fill NA/NaN values using the specified method.

Parameters

- **value** (*scalar, dict, Series, or DataFrame*) – Value to use to fill holes (e.g. 0), alternately a dict/Series/DataFrame of values specifying which value to use for each index (for a Series) or column (for a DataFrame). Values not in the dict/Series/DataFrame will not be filled. This value cannot be a list.
- **method** (*{'backfill', 'bfill', 'pad', 'ffill', None}, default None*) – Method to use for filling holes in reindexed Series pad / ffill: propagate last valid observation forward to next valid backfill / bfill: use next valid observation to fill gap.
- **axis** (*{0 or 'index'}*) – Axis along which to fill missing values.

- **inplace** (*bool, default False*) – If True, fill in-place. Note: this will modify any other views on this object (e.g., a no-copy slice for a column in a DataFrame).
- **limit** (*int, default None*) – If method is specified, this is the maximum number of consecutive NaN values to forward/backward fill. In other words, if there is a gap with more than this number of consecutive NaNs, it will only be partially filled. If method is not specified, this is the maximum number of entries along the entire axis where NaNs will be filled. Must be greater than 0 if not None.
- **downcast** (*dict, default is None*) – A dict of item->dtype of what to downcast if possible, or the string 'infer' which will try to downcast to an appropriate equal type (e.g. float64 to int64 if possible).

Returns Object with missing values filled or None if `inplace=True`.

Return type Series or None

See also:

interpolate() Fill NaN values using interpolation.

reindex() Conform object to new index.

asfreq() Convert TimeSeries to specified frequency.

Examples

```
>>> df = pd.DataFrame([[np.nan, 2, np.nan, 0],
...                    [3, 4, np.nan, 1],
...                    [np.nan, np.nan, np.nan, 5],
...                    [np.nan, 3, np.nan, 4]],
...                   columns=list("ABCD"))
>>> df
     A    B   C  D
0  NaN  2.0 NaN  0
1  3.0  4.0 NaN  1
2  NaN  NaN NaN  5
3  NaN  3.0 NaN  4
```

Replace all NaN elements with 0s.

```
>>> df.fillna(0)
    A   B   C   D
0   0.0 2.0 0.0 0
1   3.0 4.0 0.0 1
2   0.0 0.0 0.0 5
3   0.0 3.0 0.0 4
```

We can also propagate non-null values forward or backward.

```
>>> df.fillna(method="ffill")
    A   B   C   D
0   NaN 2.0 NaN 0
1   3.0 4.0 NaN 1
2   3.0 4.0 NaN 5
3   3.0 3.0 NaN 4
```

Replace all NaN elements in column 'A', 'B', 'C', and 'D', with 0, 1, 2, and 3 respectively.

```
>>> values = {"A": 0, "B": 1, "C": 2, "D": 3}
>>> df.fillna(value=values)
    A   B   C   D
0   0.0 2.0 2.0 0
1   3.0 4.0 2.0 1
2   0.0 1.0 2.0 5
3   0.0 3.0 2.0 4
```

Only replace the first NaN element.

```
>>> df.fillna(value=values, limit=1)
    A   B   C   D
0   0.0 2.0 2.0 0
1   3.0 4.0 NaN 1
2   NaN 1.0 NaN 5
3   NaN 3.0 NaN 4
```

When filling using a DataFrame, replacement happens along the same column names and same indices

```
>>> df2 = pd.DataFrame(np.zeros((4, 4)), columns=list("ABCE"))
>>> df.fillna(df2)
    A   B   C   D
0   0.0 2.0 0.0 0
1   3.0 4.0 0.0 1
2   0.0 0.0 0.0 5
3   0.0 3.0 0.0 4
```

grama.mutate_helpers.**qnorm**(**args*, ***kwargs*)
Normal quantile function (inverse CDF)

grama.mutate_helpers.**pnorm**(**args*, ***kwargs*)
Normal cumulative distribution function (CDF)

grama.mutate_helpers.**dnorm**(**args*, ***kwargs*)
Normal probability density function (PDF)

grama.mutate_helpers.**pareto_min**(**args*, ***kwargs*)
Determine if observation is a Pareto point

Find the Pareto-efficient points that minimize the provided features.

Parameters **xi** (*iterable OR gr.Intention()*) – Feature to minimize; use -X to maximize

Returns Indicates if observation is Pareto-efficient

Return type np.array of boolean

grama.mutate_helpers.**stratum_min**(**args*, ***kwargs*)
Compute Pareto stratum number

Compute the Pareto stratum number for a given dataset.

Parameters

- **xi** (*iterable OR gr.Intention()*) – Feature to minimize; use -X to maximize
- **max_depth** (*int*) – Maximum depth for recursive computation; stratum numbers exceeding this value will not be computed and will be flagged as NaN.

Returns Pareto stratum number

Return type np.array of floats

References

del Rosario, Rupp, Kim, Antono, and Ling "Assessing the frontier: Active learning, model accuracy, and multi-objective candidate discovery and optimization" (2020) J. Chem. Phys.

grama.mutate_helpers.**qqvals**(**args*, ***kwargs*)

Generate theoretical quantiles

Generate theoretical quantiles for a Q-Q plot. Can provide either a pre-defined Marginal object or the name of a distribution to fit.

Parameters **x** (*array-like or gr.Intention()*) – Target observations

Keyword Arguments

- **dist** (*str or None*) – Name of scipy distribution to fit; see gr.valid_dist for list of valid distributions
- **marg** (*gr.Marginal() or None*) – Pre-fitted marginal

Returns Theoretical quantiles, matched in order with target observations

Return type Series

References

Filliben, J. J., "The Probability Plot Correlation Coefficient Test for Normality" (1975) Technometrics. DOI: 10.1080/00401706.1975.10489279

Examples:

```
import grama as gr
from grama.data import df_shewhart
DF = gr.Intention()

## Make a Q-Q plot
(
    df_shewhart
    >> gr.tf_mutate(q=gr.qqvals(DF.tensile_strength, dist="norm"))
    >> gr.ggplot(gr.aes("q", "tensile_strength"))
    + gr.geom_abline(intercept=0, slope=1, linetype="dashed")
    + gr.geom_point()
)

## Fit a marginal, use in Q-Q plot
mg_tys = gr.marg_fit("lognorm", df_shewhart.tensile_strength, floc=0)
# Plot to assess the fit
(
    df_shewhart
    >> gr.tf_mutate(q=gr.qqvals(DF.tensile_strength, marg=mg_tys))
    >> gr.ggplot(gr.aes("q", "tensile_strength"))
    + gr.geom_abline(intercept=0, slope=1, linetype="dashed")
    + gr.geom_point()
)
```

grama.mutate_helpers.**linspace**(**args*, ***kwargs*)

Linearly-spaced values

Create an array of linearly-spaced values. Accepts keyword arguments for numpy.linspace.

Parameters

- **a** (*numeric*) – Smallest value
- **b** (*numeric*) – Largest value
- **n** (*int*) – Number of points

Returns Array of requested values

Return type numpy array

Notes

This is a symbolic alias for np.linspace(); you can use this in pipe-enabled functions.

Examples:

```
import grama as gr
from grama.data import df_stang
DF = gr.Intention()
(
    df_stang
    >> gr.tf_mutate(c=gr.linspace(0, 1, gr.n(DF.index)))
)
```

grama.mutate_helpers.**logspace**(**args*, ***kwargs*)

Logarithmically-spaced values

Create an array of logarithmically-spaced values. Accepts keyword arguments for numpy.logspace.

Parameters

- **a** (*numeric*) – Smallest value
- **b** (*numeric*) – Largest value
- **n** (*int*) – Number of points

Returns Array of requested values

Return type numpy array

Notes

This is a symbolic alias for np.logspace(); you can use this in pipe-enabled functions.

Examples:

```
import grama as gr
from grama.data import df_stang
DF = gr.Intention()
(
    df_stang
    >> gr.tf_mutate(c=gr.logspace(0, 1, gr.n(DF.index)))
)
```

grama.mutate_helpers.**consec**(**args*, ***kwargs*)

Flag consecutive runs of True values

Flag as True all entries associated with a "run" of True values. A "run" is defined as a user-defined count (given by i) of consecutive True values.

Parameters

- **series** (*pd.Series*) – Series of boolean values
- **i** (*int*) – User-defined count to define a run

Returns Boolean series flagging consecutive True values

Return type series

4.1.16 grama.plot_auto module

grama.plot_auto.**plot_contour**

Plot 2d contours

Plot contours. Usually called as a dispatch from plot_auto().

Parameters

- **var** (*array of str*) – Variables for plot axes
- **out** (*str*) – Name of output identifier column
- **level** (*str*) – Name of level identifier column
- **aux** (*bool*) – Auxillary variables present?
- **color** (*str*) – Color mode; options: "full", "bw"

Returns Contour image

Return type ggplot

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
(
    md_beam
    >> gr.ev_contour(
        var=["w", "t"],
        out=["g_stress"],
        # Set auxilliary inputs to nominal levels
        df=gr.eval_nominal(md_beam, df_det="nom"),
    )
    >> gr.pt_auto()
)
```

grama.plot_auto.**plot_corrtile**

grama.plot_auto.**plot_scattermat**

Create a scatterplot matrix

Create a scatterplot matrix. Often used to visualize a design (set of inputs points) before evaluating the functions.

Usually called as a dispatch from plot_auto().

Parameters

- **var** (*list of strings*) – Variables to plot
- **color** (*str*) – Color mode; value ignored as default vis is black & white

Returns Scatterplot matrix

Return type ggplot

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
## Dispatch from autoplotter
(
    md_beam
    >> gr.ev_sample(n=100, df_det="nom", skip=True)
    >> gr.pt_auto()
)
## Re-create plot without metadata
(
    md_beam
    >> gr.ev_sample(n=100, df_det="nom")
    >> gr.pt_scattermat(var=md.var)
)
```

grama.plot_auto.**plot_hists**

Construct histograms

Create a set of histograms. Often used to visualize the results of random sampling for multiple outputs.

Usually called as a dispatch from plot_auto().

Parameters

- **out** (*list of strings*) – Variables to plot
- **color** (*str*) – Color mode; value ignored as default vis is black & white

Returns Seaborn histogram plot

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
## Dispatch from autoplotter
(
    md_beam
    >> gr.ev_sample(n=100, df_det="nom")
    >> gr.pt_auto()
)
## Re-create without metadata
(
    md_beam
    >> gr.ev_sample(n=100, df_det="nom")
    >> gr.pt_hists(out=md.out)
)
```

grama.plot_auto.**plot_sinew_inputs**

Inspect a sinew design

Create a scatterplot matrix with hues. Often used to visualize a sinew design before evaluating the model functions.

Usually called as a dispatch from plot_auto().

Parameters

- **df** (*Pandas DataFrame*) – Input design data

- **var** (*list of strings*) – Variables to plot
- **sweep_ind** (*string*) – Sweep index column in df
- **color** (*str*) – Color mode; options: "full", "bw"

Returns Seaborn scatterplot matrix

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
## Dispatch from autoplotter
(
    md_beam
    >> gr.ev_sinews(df_det="swp", skip=True)
    >> gr.pt_auto()
)
## Re-create without metadata
(
    md_beam
    >> gr.ev_sinews(df_det="swp")
    >> gr.pt_sinew_inputs(var=md.var)
)
```

grama.plot_auto.**plot_sinew_outputs**

Construct sinew plot

Create a relational lineplot with hues for each sweep. Often used to visualize the outputs of a sinew design.

Usually called as a dispatch from plot_auto().

Parameters

- **df** (*Pandas DataFrame*) – Input design data with output results
- **var** (*list of strings*) – Variables to plot
- **out** (*list of strings*) – Outputs to plot
- **sweep_ind** (*string*) – Sweep index column in df
- **sweep_var** (*string*) – Swept variable column in df
- **color** (*str*) – Color mode; options: "full", "bw"

Returns Relational lineplot

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
## Dispatch from autoplotter
(
    md_beam
    >> gr.ev_sinews(df_det="swp")
    >> gr.pt_auto()
)
## Re-create without metadata
(
    md_beam
```

(continues on next page)

(continued from previous page)

```
    >> gr.ev_sinews(df_det="swp")
    >> gr.pt_sinew_inputs(var=md.var, out=md.out)
)
```

grama.plot_auto.**plot_auto**
Automagic plotting

Convenience tool for various grama outputs. Prints delegated plotting function, which can be called manually with different arguments for more tailored plotting.

Parameters

- **df** (*DataFrame*) – Data output from appropriate grama routine. See gr.plot_list.keys() for list of supported methods.
- **color** (*str*) – Color mode; options: "full", "bw"

Returns Plot results

4.1.17 grama.spc module

grama.spc.**c_sd**(*n*)
Anti-biasing constant for aggregate standard deviation

Returns the anti-biasing constant for aggregated standard deviation estimates. If the average of k samples each size n are averaged to produce $overline{S} = (1/k) sum_{i=1}^k S_i$, then the de-biased standard deviation is:

$$hat{sigma} = overline{S} / c(n)$$

Parameters **n** (*int*) – Sample (batch) size

Returns anti-biasing constant

Return type float

References

Kenett and Zacks, Modern Industrial Statistics (2014) 2nd Ed

grama.spc.**B3**(*n*)
Lower Control Limit constant for standard deviation

Returns the Lower Control Limit (LCL) constant for aggregated standard deviation estimates. If the average of k samples each size n are averaged to produce $overline{S} = (1/k) sum_{i=1}^k S_i$, then the LCL is:

$$LCL = B_3 overline{S}$$

Parameters **n** (*int*) – Sample (batch) size

Returns LCL constant

Return type float

References

Kenett and Zacks, Modern Industrial Statistics (2014) 2nd Ed, Equation (8.22)

grama.spc.**B4**(*n*)

Upper Control Limit constant for standard deviation

Returns the Upper Control Limit (UCL) constant for aggregated standard deviation estimates. If the average of k samples each size n are averaged to produce $overline{S} = (1/k) sum_{i=1}^k S_i$, then the UCL is:

$$UCL = B_4 overline{S}$$

Parameters **n** (*int*) – Sample (batch) size

Returns UCL constant

Return type float

References

Kenett and Zacks, Modern Industrial Statistics (2014) 2nd Ed, Equation (8.22)

grama.spc.**plot_xbs**(*df*, *group*, *var*, *n_side=9*, *n_delta=6*, *color='full'*)

Construct Xbar and S chart

Construct an Xbar and S chart to assess the state of statistical control of a dataset.

Parameters

- **df** (*DataFrame*) – Data to analyze
- **group** (*str*) – Variable for grouping
- **var** (*str*) – Variable to study

Keyword Arguments

- **n_side** (*int*) – Number of consecutive runs above/below centerline to flag
- **n_delta** (*int*) – Number of consecutive runs increasing/decreasing to flag
- **color** (*str*) – Color mode; "full" for full color, "bw" for greyscale

Returns Xbar and S chart

Return type plotnine object

Examples:

```
import grama as gr
DF = gr.Intention()

from grama.data import df_shewhart
(
    df_shewhart
    >> gr.tf_mutate(idx=DF.index // 10)
    >> gr.pt_xbs("idx", "tensile_strength")
)
```

4.1.18 grama.string_helpers module

grama.string_helpers.**str_c**(**args*, ***kwargs*)
Concatenate strings

grama.string_helpers.**str_count**(**args*, ***kwargs*)
Count the number of matches in a string.

grama.string_helpers.**str_detect**(**args*, ***kwargs*)
Detect the presence of a pattern match in a string.

grama.string_helpers.**str_extract**(**args*, ***kwargs*)
Extract the first regex pattern match

grama.string_helpers.**str_locate**(**args*, ***kwargs*)
Find the indices of all pattern matches.

grama.string_helpers.**str_replace**(**args*, ***kwargs*)
Replace the first matched pattern in each string.

grama.string_helpers.**str_replace_all**(**args*, ***kwargs*)
Replace all occurences of pattern in each string.

grama.string_helpers.**str_sub**(**args*, ***kwargs*)
Extract substrings

grama.string_helpers.**str_split**(**args*, ***kwargs*)
Split string into list on pattern

Parameters

- **string** (*str or iterable[str]*) – String(s) to split
- **pattern** (*str*) – Regex pattern on which to split

Kwargs: maxsplit (int): Maximum number of splits, or 0 for unlimited

Returns str or iterable[str]: List (of lists) of strings

grama.string_helpers.**str_which**(**args*, ***kwargs*)
Find the index of the first pattern match.

grama.string_helpers.**str_to_lower**(**args*, ***kwargs*)
Make string lower-case

Parameters **string** (*str or iterable[str]*) – String(s) to modify

Returns str or iterable[str]: List (of lists) of strings

grama.string_helpers.**str_to_upper**(**args*, ***kwargs*)
Make string upper-case

Parameters **string** (*str or iterable[str]*) – String(s) to modify

Returns str or iterable[str]: List (of lists) of strings

grama.string_helpers.**str_to_snake**(**args*, ***kwargs*)
Make string snake case

Parameters **string** (*str or iterable[str]*) – String(s) to modify

Returns str or iterable[str]: List (of lists) of strings

4.1.19 grama.support module

grama.support.**tran_sp**
Compact a dataset with support points

Parameters

- **df** (*DataFrame*) – dataset to compact
- **n** (*int*) – number of samples for compacted dataset
- **var** (*list of str*) – list of variables to compact, must all be numeric
- **n_maxiter** (*int*) – maximum number of iterations for support point algorithm
- **tol** (*float*) – convergence tolerance
- **verbose** (*bool*) – print messages to the console?
- **standardize** (*bool*) – standardize columns before running sp? (Restores after sp)

Returns dataset compacted with support points

Return type DataFrame

References

Mak and Joseph, "Support Points" (2018) *The Annals of Statistics*

Examples:

```
import grama as gr
# Compact an existing dataset
from grama.data import df_diamonds
df_sp = gr.tran_sp(df_diamonds, n=50, var=["price", "carat"])

# Use support points to reduce model runtime
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
(
    md_beam
    ## Generate input sample but don't evaluate outputs
    >> gr.ev_sample(n=1e4, df_det="nom", skip=True)
    ## Reduce to a smaller---but representative---sample
    >> gr.tf_sp(n=50)
    ## Evaluate the outputs
    >> gr.tf_md(md_beam)
)
```

4.1.20 grama.tools module

grama.tools.**add_pipe**(*fun*)

grama.tools.**copy_meta**(*df_source*, *df_target*)
Internal metadata copy tool

Parameters

- **df_source** (*DataFrame*) – Original dataframe
- **df_target** (*DataFrame*) – Target dataframe; receives metadata

Returns df_target with copied metadata

Return type DataFrame

grama.tools.**custom_formatwarning**(*msg*, **args*, ***kwargs*)

grama.tools.**lookup**(*df*, *row_labels*, *col_labels*)
2D lookup function for a dataframe (Old Pandas Lookup Method)

Parameters

- **df** (*DataFrame*) – DataFrame for lookup
- **row_labels** (*List*) – Row labels to use for lookup.
- **col_labels** (*List*) – Column labels to use for lookup.

Returns Found values

Return type numpy.ndarray

grama.tools.**hide_traceback**()
Configure Jupyter to hide error traceback

class grama.tools.**pipe**(*function*)
Bases: object

grama.tools.**tran_outer**
Outer merge

Perform an outer-merge on two dataframes.

Parameters

- **df** (*DataFrame*) – Data to merge
- **df_outer** (*DataFrame*) – Data to merge; outer

Returns Merged data

Return type DataFrame

Examples:

```
import grama as gr
import pandas as pd
df = pd.DataFrame(dict(x=[1,2]))
df_outer = pd.DataFrame(dict(y=[3,4]))
df_res = gr.tran_outer(df, df_outer)
df_res
     x  y
  0  1  3
  1  2  3
  2  1  4
  3  2  4
```

4.1.21 grama.tran_is module

grama.tran_is.**tran_reweight**
Reweight a sample using likelihood ratio

Reweight is a tool to facilitate "What If?" Monte Carlo simulation; specifically, to make testing a models with the same function(s) but different distributions more computationally efficient.

This tool automates calulation of the *likelihood ratio* between the distributions of two given models. Using the resulting weights to scale (elementwise multiply) output values and compute summaries is called *importance sampling*, enabling "What If?" testing. Use of this tool enables one to generate a single Monte Carlo sample, rather than multiple samples for each "What If?" scenario (avoiding extraneous function evaluations).

Let *y* be a generic output of the scenario. The importance sampling procedure is as follows:

1. Create a base scenario represented by *md_base*, and a desired number of alternative "What If?" scenarios represented my other models.
2. Use *gr.eval_monte_carlo* to generate a single sample *df_base* of size *n* using the base scenario *md_base*. Compute statistics of interest on the output *y* for this base scenario.
3. For each alternative scenario *md_new*, use *gr.tran_reweight* to generate weights *weight*, and use the tool *n_e = gr.neff_is(DF.weight)* to compute the effective sample size. If *n_e* << *n*, then importance sampling is unlikely to give an accurate estimate for this scenario.
4. For each alternative scenario *md_new*, use the relevant weights *weight* to scale the output value *y_new = y * weight*, and compute statistics of interest of the weighted output values.

Parameters

- **df_base** (*DataFrame*) – Monte Carlo results from *md_base*.
- **md_base** (Model) – Model used to generate *df_base*.
- **md_new** (Model) – Model defining a new "What If?" scenario.
- **var_weight** (*string*) – Name to give new column of weights.
- **append** (*bool*) – Append results to original DataFrame?

Returns Original df_base with added column of weights.

Return type DataFrame

Notes

- The base scenario *md_base* should have fatter tails than any of the scenarios considered as *df_new*. See Owen (2013) Chapter 9 for more details.

References

A.B. Owen, "Monte Carlo theory, methods and examples" (2013)

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
DF = gr.Intention()

md_base = make_cantilever_beam()
md_new = (
    md_base
    >> gr.cp_marginals(
        H=dict(dist="norm", loc=500.0, scale=50.0),
    )
)
```

(continues on next page)

(continued from previous page)

```
## Assess safety via simple Monte Carlo
df_base = gr.eval_monte_carlo(md_base, df_det="nom", n=1e3)
print(
    df_base
    >> gr.tf_summarize(
        pof_stress=gr.mean(DF.g_stress <= 0),
        pof_disp=gr.mean(DF.g_disp <= 0),
    )
)

## Re-use samples to test another scenario
print(
    df_base
    >> gr.tf_reweight(md_base=md_base, md_new=md_new)
    >> gr.tf_summarize(
        pof_stress=gr.mean((DF.g_stress <= 0) * DF.weight),
        pof_disp=gr.mean((DF.g_disp <= 0) * DF.weight),
        n_eff=gr.neff_is(DF.weight),
    )
)

## It is unsafe to study new scenarios with wider uncertainty than the base␣
↪scenario
md_poor = (
    md_base
    >> gr.cp_marginals(
        H=dict(dist="norm", loc=500.0, scale=400.0),
    )
)
## Note the tiny effective sample size in this case
print(
    md_base
    >> gr.ev_monte_carlo(n=1e3, df_det="nom")
    >> gr.tf_reweight(md_base=md_base, md_new=md_poor)
    >> gr.tf_summarize(
        pof_stress=gr.mean((DF.g_stress <= 0) * DF.weight),
        pof_disp=gr.mean((DF.g_disp <= 0) * DF.weight),
        n_eff=gr.neff_is(DF.weight),
    )
)
```

4.1.22 grama.tran_pivot module

grama.tran_pivot.**tran_pivot_longer**(*df*, *columns*, *index_to=None*, *names_to=None*, *names_sep=None*, *names_pattern=None*, *values_to=None*)

Lengthen a dataset

"Lengthens" data by increasing the number of rows and decreasing the number of columns.

Parameters

- **df** (*DataFrame*) – DataFrame passed through
- **columns** (*str*) – Label of column(s) to pivot into longer format
- **index_to** (*str*) – str name to create a new representation index of observations; Optional.

- **names_to** (*str*) – name to use for the 'variable' column, if None frame.columns.name is used or 'variable'
  - .value indicates that component of the name defines the name of the column containing the cell values, overriding values_to
- **names_sep** (*str OR list of int*) – delimter to seperate the values of the argument(s) from the 'columns' parameter into 2 new columns with those values split by that delimeter
  - Regex expression is a valid input for names_sep
- **names_pattern** (*str*) – Regular expression with capture groups to define targets for names_to.
- **values_to** (*str*) – name to use for the 'value' column; overridden if ".value" is provided in names_to argument.

Notes

Only one of names_sep OR names_pattern may be given.

Returns result of being pivoted into a longer format

Return type DataFrame

Examples:

```
import grama as gr
## Simple example
(
    gr.df_make(
        A=[1, 2, 3],
        B=[4, 5, 6],
        C=[7, 8, 9],
    )
    >> gr.tf_pivot_longer(
        columns=["A", "B", "C"],
        names_to="variable",
        values_to="value",
    )
)

## Matching columns on patterns
(
    gr.df_make(
        x1=[1, 2, 3],
        x2=[4, 5, 6],
        x3=[7, 8, 9],
    )
    >> gr.tf_pivot_longer(
        columns=gr.matches("\d+"),
        names_to="variable",
        values_to="value",
    )
)

## Separating column names and data on a names_pattern
(
```

(continues on next page)

(continued from previous page)

```
    gr.df_make(
        E00=[1, 2, 3],
        E45=[4, 5, 6],
        E90=[7, 8, 9],
    )
    >> gr.tf_pivot_longer(
        columns=gr.matches("\d+"),
        names_to=[".value", "angle"],
        names_pattern="(E)(\d+)",
    )
)
```

grama.tran_pivot.**tran_pivot_wider**(*df*, *names_from*, *indexes_from=None*, *values_from=None*)

Widen a dataset

"Widens" data by increasing the number of columns and decreasing the number of rows.

Parameters

- **df** (*DataFrame*) – DataFrame passed through
- **names_from** (*str*) – Column(s) name(s) to use to make new columns
- **indexes_from** (*str*) – Column(s) to use to make new index, if None will preserve and use unspecified columns as index
- **values_from** (*str*) – Column(s) to use as new values column(s)

Returns result of being pivoted wider

Return type DataFrame

Examples:

```
import grama as gr
## Simple example
(
    gr.df_make(var=["x", "x", "y", "y"], value=[0, 1, 2, 3])
    >> gr.tf_pivot_wider(
        names_from="var",
        values_from="value",
    )
(
```

4.1.23 grama.tran_shapley module

grama.tran_shapley.**tran_shapley_cohort**

Compute cohort shapley values

Assess the impact of each variable on selected observations via cohort shapley [1]. Shapley values are a game-theoretic way to assess the importance of input variables (var) on each of a set of outputs (out). Since values are computed on each observation, cohort shapley can distinguish cases where a variable has a positive impact on one observation, and a negative impact on a different observation.

Note that cohort shapley is combinatorialy expensive in the number of variables, and this expense is multiplied by the number of observations. Use with caution in cases of high dimensionality. Consider using the *inds* argument to analyze a small subset of your observations.

Parameters

- **df** (*DataFrame*) – Variable and output data to analyze
- **var** (*list of strings*) – Input variables
- **out** (*list of strings*) – Outputs variables
- **bins** (*integer*) – Number of "bins" to define coordinate refinement distance
- **inds** (*iterable of indices or None*) – Indices of rows to analyze

References

[1] Mase, Owen, and Seiler, "Explaining black box decisions by Shapley cohort refinement" (2019) Arxiv

Examples:

```
import grama as gr
from grama.data import df_stang
DF = gr.Intention()
# Analyze all observations
(
    gr.tran_shapley_cohort(
        df_stang,
        var=["thick", "ang"],
        out=["E"],
    )
    >> gr.tf_bind_cols(df_stang)
    >> gr.tf_filter(DF.E_thick < 0)
)
# Compute subset of values
(
    gr.tran_shapley_cohort(
        df_stang,
        var=["thick", "ang"],
        out=["E"],
        inds=(
            df_stang
            >> gr.tf_filter(DF.thick > 0.08)
        ).index
    )
    >> gr.tf_bind_cols(df_stang)
)
```

4.1.24 grama.tran_summaries module

grama.tran_summaries.**tran_asub**

Active subspace estimator

Compute principal directions and eigenvalues for all outputs based on output of ev_grad_fd() to estimate the /active subspace/ (Constantine, 2015).

See also `gr.tran_polyridge()` for a gradient-free approach to approximating the active subspace.

Parameters

- **df** (*DataFrame*) – Gradient evaluations
- **prefix** (*str*) – Column name prefix; default="D"
- **outvar** (*str*) – Name to give output id column; default="output"

- **lambvar** (*str*) – Name to give eigenvalue column; default="lam"

Returns Active subspace directions and eigenvalues

Return type DataFrame

References

Constantine, "Active Subspaces" (2015) SIAM

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md = make_cantilever_beam()
df_base = md >> gr.ev_sample(n=1e2, df_det="nom", skip=True)
df_grad = md >> gr.ev_grad_fd(df_base=df_base)
df_as = df_grad >> gr.tf_asub()
```

grama.tran_summaries.**tran_describe**

Describe a dataframe

Synonym for Pandas df.describe()

Parameters **df** (*DataFrame*) – Data to describe

Returns Printed summary

grama.tran_summaries.**tran_inner**

Inner products

Compute inner product of target df with weights defined by df_weights.

Parameters

- **df** (*DataFrame*) – Data to compute inner products against
- **df_weights** (*DataFrame*) – Weights for inner prodcuts
- **prefix** (*str*) – Name prefix for resulting inner product columns; default="dot"
- **name** (*str*) – Name of identity column in df_weights or None
- **append** (*bool*) – Append new data to original DataFrame?

Returns Results of inner products

Return type DataFrame

Examples:

```
## Setup
import grama as gr
DF = gr.Intention()

## PCA example
from grama.data import df_diamonds
# Compute PCA weights
df_weights = gr.tran_pca(
    df_diamonds
    >> gr.tf_sample(1000),
    var=["x", "y", "z", "carat"],
)
```

(continues on next page)

(continued from previous page)

```
# Visualize
(
    df_diamonds
    >> gr.tf_inner(df_weights=df_weights)
    >> gr.ggplot(gr.aes("dot0", "dot1"))
    + gr.geom_point()
)

## Active subspace example
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
# Approximate the active subspace
df_data = gr.ev_sample(md_beam, n=1e2, df_det="nom")
df_weights = gr.tran_polyridge(
    df_data,
    var=md_beam.var_rand, # Use meaningful predictors only
    out="g_disp",         # Target g_disp for reduction
    n_degree=2,
    n_degree=1,
)
# Construct shadow plot; use tran_inner to calculate active variable
(
    df_data
    >> gr.tf_inner(df_weights=df_weights)
    >> gr.ggplot(gr.aes("dot", "g_disp"))
    + gr.geom_point()
)
```

grama.tran_summaries.**tran_pca**

Principal Component Analysis

Compute principal directions and eigenvalues for a dataset. Can specify columns to analyze, or just analyze all numerical columns.

Parameters

- **df** (*DataFrame*) – Data to analyze
- **var** (*list of str or None*) – List of columns to analyze
- **lambvar** (*str*) – Name to give eigenvalue column; default="lam"
- **standardize** (*bool*) – Standardize columns? default=False

Returns principal directions and eigenvalues

Return type DataFrame

References

TODO

Examples:

```
import grama as gr
from grama.data import df_stang
df_pca = df_stang >> gr.tf_pca()
```

grama.tran_summaries.**tran_sobol**

Post-process results from gr.eval_hybrid()

Estimate Sobol' indices based on hybrid point evaluations (Sobol', 1999). Intended as post-processor for gr.eval_hybrid().

Parameters

- **df** (*DataFrame*) – Hybrid point results from gr.eval_hybrid()
- **typename** (*str*) – Name to give index type column in results
- **digits** (*int*) – Number of digits for rounding reported results
- **full** (*bool*) – Return un-normalized indices and variance?

Returns Sobol' indices

Return type DataFrame

Notes

- Index type ["first", "total"] is inferred from input df._meta; this is assigned by gr.eval_hybrid().
- Index normalization coded in the "ind" column; S: Normalized index T: Un-normalized index var: Total variance

References

I.M. Sobol', "Sensitivity Estimates for Nonlinear Mathematical Models" (1999) MMCE, Vol 1.

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md = make_cantilever_beam()
df_first = md >> gr.ev_hybrid(df_det="nom", plan="first")
df_first >> gr.tf_sobol()

df_total = md >> gr.ev_hybrid(df_det="nom", plan="total")
df_total >> gr.tf_sobol()
```

grama.tran_summaries.**tran_iocorr**

Compute input-output correlations

Compute all correlations between input and output quantities.

Parameters

- **df** (*DataFrame*) – Data to summarize
- **var** (*iterable of strings*) – Column names for inputs
- **out** (*iterable of strings*) – Column names for outputs
- **method** (*str*) – Method for correlation; one of "pearson" or "spearman"

Returns Correlations between each input and output

Return type DataFrame

4.1.25 grama.tran_tools module

grama.tran_tools.**tran_angles**(*df*, *df2*)
Subspace angles

Compute the subspace angles between two matrices. A wrapper for scipy.linalg.subspace_angles that corrects for column ordering. Row ordering is assumed.

Parameters

- **df** (*DataFrame*) – First matrix to compare
- **df2** (*DataFrame*) – Second matrix to compare

Returns Array of angles (in radians)

Return type array

Examples:

```
import grama as gr
import pandas as pd
df = pd.DataFrame(dict(v=[+1, +1]))
df_v1 = pd.DataFrame(dict(w=[+1, -1]))
df_v2 = pd.DataFrame(dict(w=[+1, +1]))
theta1 = angles(df, df_v1)
theta2 = angles(df, df_v2)
```

grama.tran_tools.**tran_bootstrap**
Estimate bootstrap confidence intervals

Estimate bootstrap confidence intervals for a given transform. Uses the "bootstrap-t" procedure discussed in Efron and Tibshirani (1993).

Parameters

- **df** (*DataFrame*) – Data to bootstrap
- **tran** (grama **tran_** function) – Transform procedure which generates statistic
- **n_boot** (*numeric*) – Monte Carlo resamples for bootstrap
- **n_sub** (*numeric*) – Nested resamples to estimate SE
- **con** (*float*) – Confidence level
- **col_sel** (*list (string)*) – Columns to include in bootstrap calculation

Returns Results of tran(df), plus _lo and _up columns for numeric columns

Return type DataFrame

References and notes: Efron and Tibshirani (1993) "The bootstrap-t procedure... is particularly applicable to location statistics like the sample mean.... The bootstrap-t method, at least in its simple form, cannot be trusted for more general problems, like setting a confidence interval for a correlation coefficient."

Examples:

grama.tran_tools.**tran_copula_corr**(*df*, *model=None*, *density=None*)
Compute Gaussian copula correlations from data

Convenience function to fit a Gaussian copula (correlations) based on data and pre-fitted marginals. Intended for use with `gr.comp_copula_gaussian()`. Must provide either *model* or *density*.

Note: This is called automatically when you provide a dataset to `gr.comp_copula_gaussian()`.

Parameters

- **df** (*DataFrame*) – Matrix of data for correlation estimation
- **model** (*gr.Model*) – Model with defined marginals
- **density** (*gr.Density*) – Density with defined marginals

Returns Correlation data ready for use with `gr.comp_copula_gaussian()`

Return type DataFrame

Examples:

```
import grama as gr
from grama.data import df_stang
## Verbose, manual approach
md = (
    gr.Model()
    >> gr.cp_marginals(
        E=gr.marg_named(df_stang.E, "norm"),
        mu=gr.marg_named(df_stang.mu, "beta"),
        thick=gr.marg_named(df_stang.thick, "norm"),
    )
)
df_corr = gr.tran_copula_corr(df_stang, model=md)
md = gr.comp_copula_gaussian(md, df_corr=df_corr)

## Automatic approach
md = (
    gr.Model()
    >> gr.cp_marginals(
        E=gr.marg_named(df_stang.E, "norm"),
        mu=gr.marg_named(df_stang.mu, "beta"),
        thick=gr.marg_named(df_stang.thick, "norm"),
    )
    >> gr.cp_copula_gaussian(df_data=df_stang)
)
```

grama.tran_tools.**tran_kfolds**

Perform k-fold CV

Perform k-fold cross-validation (CV) using a given fitting procedure (ft). Optionally provide a fold identifier column, or (randomly) assign folds.

Parameters

- **df** (*DataFrame*) – Data to pass to given fitting procedure
- **ft** (gr.ft_) – Partially-evaluated grama fit function; defines model fitting procedure and outputs to aggregate
- **tf** (gr.tf_) – Partially-evaluated grama transform function; evaluation of fitted model will be passed to tf and provided with keyword arguments from summaries
- **out** (*list or None*) – Outputs for which to compute *summaries*; None uses ft.out
- **var_fold** (*str or None*) – Column to treat as fold identifier; overrides *k*
- **suffix** (*str*) – Suffix for predicted value; used to distinguish between predicted and actual

- **summaries** (*dict of functions*) – Summary functions to pass to tf; will be evaluated for outputs of ft. Each summary must have signature summary(f_pred, f_meas). Grama includes builtin options: gr.mse, gr.rmse, gr.rel_mse, gr.rsq, gr.ndme
- **k** (*int*) – Number of folds; k=5 to k=10 recommended [1]
- **shuffle** (*bool*) – Shuffle the data before CV? True recommended [1]

Notes

- Many grama functions support *partial evaluation*; this allows one to specify things like hyperparameters in fitting functions without providing data and executing the fit. You can take advantage of this functionality to easly do hyperparameter studies.

Returns

Aggregated results within each of k-folds using given model and summary transform

Return type DataFrame

References

[1] James, Witten, Hastie, and Tibshirani, "An introduction to statistical learning" (2017), Chapter 5. Resampling Methods

Examples:

```
import grama as gr
from grama.data import df_stang
df_kfolds = (
    df_stang
    >> gr.tf_kfolds(
        k=5,
        ft=gr.ft_rf(out=["thick"], var=["E", "mu"]),
    )
)
```

grama.tran_tools.**tran_md**

Model as transform

Use a model to transform data; useful when pre-processing data to evaluate a model.

Parameters

- **df** (*DataFrame*) – Data to merge
- **md** (*gr.Model*) – Model to use as transform

Returns Output of evaluated model

Return type DataFrame

Examples:

```
import grama as gr
from grama.models import make_cantilever_beam
md_beam = make_cantilever_beam()
## Use support points to generate a smaller---but representative---sample
df_res = (
```

(continues on next page)

(continued from previous page)

```
    md_beam
    >> gr.ev_sample(n=1e3, df_det="nom", skip=True, seed=101)
    >> gr.tf_sp(n=100)
    >> gr.tf_md(md=md_beam)
)
```

4.1.26 Module contents

grama.**choice**(*a*, *size=None*, *replace=True*, *p=None*)

Generates a random sample from a given 1-D array

New in version 1.7.0.

Note: New code should use the `choice` method of a `default_rng()` instance instead; please see the random-quick-start.

Parameters

- **a** (*1-D array-like or int*) – If an ndarray, a random sample is generated from its elements. If an int, the random sample is generated as if it were `np.arange(a)`
- **size** (*int or tuple of ints, optional*) – Output shape. If the given shape is, e.g., `(m, n, k)`, then `m * n * k` samples are drawn. Default is None, in which case a single value is returned.
- **replace** (*boolean, optional*) – Whether the sample is with or without replacement. Default is True, meaning that a value of `a` can be selected multiple times.
- **p** (*1-D array-like, optional*) – The probabilities associated with each entry in a. If not given, the sample assumes a uniform distribution over all entries in `a`.

Returns **samples** – The generated random samples

Return type single item or ndarray

Raises `ValueError` – If a is an int and less than zero, if a or p are not 1-dimensional, if a is an array-like of size 0, if p is not a vector of probabilities, if a and p have different lengths, or if replace=False and the sample size is greater than the population size

See also:

`randint()`, `shuffle()`, `permutation()`

`Generator.choice()` which should be used in new code

Notes

Setting user-specified probabilities through `p` uses a more general but less efficient sampler than the default. The general sampler produces a different sample than the optimized sampler even if each element of `p` is 1 / len(a).

Sampling random rows from a 2-D array is not possible with this function, but is possible with *Generator.choice* through its `axis` keyword.

Examples

Generate a uniform random sample from np.arange(5) of size 3:

```
>>> np.random.choice(5, 3)
array([0, 3, 4]) # random
>>> #This is equivalent to np.random.randint(0,5,3)
```

Generate a non-uniform random sample from np.arange(5) of size 3:

```
>>> np.random.choice(5, 3, p=[0.1, 0, 0.3, 0.6, 0])
array([3, 3, 0]) # random
```

Generate a uniform random sample from np.arange(5) of size 3 without replacement:

```
>>> np.random.choice(5, 3, replace=False)
array([3,1,0]) # random
>>> #This is equivalent to np.random.permutation(np.arange(5))[:3]
```

Generate a non-uniform random sample from np.arange(5) of size 3 without replacement:

```
>>> np.random.choice(5, 3, replace=False, p=[0.1, 0, 0.3, 0.6, 0])
array([2, 3, 0]) # random
```

Any of the above can be repeated with an arbitrary array-like instead of just integers. For instance:

```
>>> aa_milne_arr = ['pooh', 'rabbit', 'piglet', 'Christopher']
>>> np.random.choice(aa_milne_arr, 5, p=[0.5, 0.1, 0.1, 0.3])
array(['pooh', 'pooh', 'pooh', 'Christopher', 'piglet'], # random
      dtype='<U11')
```

grama.**multivariate_normal**(*mean*, *cov*, *size=None*, *check_valid='warn'*, *tol=1e-8*)

Draw random samples from a multivariate normal distribution.

The multivariate normal, multinormal or Gaussian distribution is a generalization of the one-dimensional normal distribution to higher dimensions. Such a distribution is specified by its mean and covariance matrix. These parameters are analogous to the mean (average or "center") and variance (standard deviation, or "width," squared) of the one-dimensional normal distribution.

Note: New code should use the `multivariate_normal` method of a `default_rng()` instance instead; please see the random-quick-start.

Parameters

- **mean** (*1-D array_like, of length N*) – Mean of the N-dimensional distribution.
- **cov** (*2-D array_like, of shape (N, N)*) – Covariance matrix of the distribution. It must be symmetric and positive-semidefinite for proper sampling.
- **size** (*int or tuple of ints, optional*) – Given a shape of, for example, `(m,n,k)`, `m*n*k` samples are generated, and packed in an *m*-by-*n*-by-*k* arrangement. Because each sample is *N*-dimensional, the output shape is `(m,n,k,N)`. If no shape is specified, a single (*N*-D) sample is returned.
- **check_valid** (*{ 'warn', 'raise', 'ignore' }, optional*) – Behavior when the covariance matrix is not positive semidefinite.

- **tol** (*float, optional*) – Tolerance when checking the singular values in covariance matrix. cov is cast to double before the check.

Returns

out – The drawn samples, of shape *size*, if that was provided. If not, the shape is `(N,)`.

In other words, each entry `out[i,j,...,:]` is an N-dimensional value drawn from the distribution.

Return type ndarray

See also:

`Generator.multivariate_normal()` which should be used for new code.

Notes

The mean is a coordinate in N-dimensional space, which represents the location where samples are most likely to be generated. This is analogous to the peak of the bell curve for the one-dimensional or univariate normal distribution.

Covariance indicates the level to which two variables vary together. From the multivariate normal distribution, we draw N-dimensional samples, $X = [x_1, x_2, ...x_N]$. The covariance matrix element C_{ij} is the covariance of x_i and x_j. The element C_{ii} is the variance of x_i (i.e. its "spread").

Instead of specifying the full covariance matrix, popular approximations include:

- Spherical covariance (*cov* is a multiple of the identity matrix)
- Diagonal covariance (*cov* has non-negative elements, and only on the diagonal)

This geometrical property can be seen in two dimensions by plotting generated data-points:

```
>>> mean = [0, 0]
>>> cov = [[1, 0], [0, 100]]  # diagonal covariance
```

Diagonal covariance means that points are oriented along x or y-axis:

```
>>> import matplotlib.pyplot as plt
>>> x, y = np.random.multivariate_normal(mean, cov, 5000).T
>>> plt.plot(x, y, 'x')
>>> plt.axis('equal')
>>> plt.show()
```

Note that the covariance matrix must be positive semidefinite (a.k.a. nonnegative-definite). Otherwise, the behavior of this method is undefined and backwards compatibility is not guaranteed.

References

Examples

```
>>> mean = (1, 2)
>>> cov = [[1, 0], [0, 1]]
>>> x = np.random.multivariate_normal(mean, cov, (3, 3))
>>> x.shape
(3, 3, 2)
```

The following is probably true, given that 0.6 is roughly twice the standard deviation:

```
>>> list((x[0,0,:] - mean) < 0.6)
[True, True] # random
```

grama.**set_seed**()
seed(self, seed=None)

Reseed a legacy MT19937 BitGenerator

Notes

This is a convenience, legacy function.

The best practice is to **not** reseed a BitGenerator, rather to recreate a new one. This method is here for legacy reasons. This example demonstrates best practice.

```
>>> from numpy.random import MT19937
>>> from numpy.random import RandomState, SeedSequence
>>> rs = RandomState(MT19937(SeedSequence(123456789)))
# Later, you want to restart the stream
>>> rs = RandomState(MT19937(SeedSequence(987654321)))
```

CHAPTER 5

Indices and tables

- genindex
- modindex
- search

Python Module Index

g

Index

D

E

F

G

H

I

K

L

M

N

O

P

Q

R

S

T

U

V

X

Z