
paragami Documentation

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Contributors

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Parameter folding and flattening, parameter origami¹: paragami!

This is a library (very much still in development) intended to make sensitivity analysis easier for optimization problems. The core functionality consists of tools for “folding” and “flattening” collections of parameters – i.e., for converting data structures of constrained parameters to and from vectors of unconstrained parameters.

The purpose is to automate much of the boilerplate required to perform optimization and sensitivity analysis for statistical problems that employ optimization or estimating equations.

The functionality of paragami can be divided into three mutually supportive pieces:

- Tools for converting structured parameters to and from “flattened” representations,
- Tools for wrapping functions to accept flattened parameters as arguments, and
- Tools for using functions that accept flattened parameters to perform sensitivity analysis.

A good place to get started is the *Examples*.

For additional background and motivation, see the following papers:

Covariances, Robustness, and Variational Bayes

Ryan Giordano, Tamara Broderick, Michael I. Jordan

<https://arxiv.org/abs/1709.02536>

A Swiss Army Infinitesimal Jackknife

Ryan Giordano, Will Stephenson, Runjing Liu, Michael I. Jordan, Tamara Broderick

<https://arxiv.org/abs/1806.00550>

Evaluating Sensitivity to the Stick Breaking Prior in Bayesian Nonparametrics

Runjing Liu, Ryan Giordano, Michael I. Jordan, Tamara Broderick

<https://arxiv.org/abs/1810.06587>

¹ Thanks to Stéfan van der Walt for the suggesting the package name.

CHAPTER 1

Installation and Testing

To get the latest released version, just use pip:

```
$ pip install paragami
```

However, paragami is under active development, and you may want to install the latest version from github:

```
$ pip install git+git://github.com/rgiordan/paragami
```

To run the tests, in the root of the repository, run:

```
$ python3 -m pytest
```

To see code coverage, in the root of the repository, run:

```
$ coverage run --include='paragami/[A-Za-z]*.py' -m pytest
$ coverage html
```

Then view the `htmlcov/index.html` in your web browser.

CHAPTER 2

Examples

2.1 Flattening and Folding With Covariance Matrices.

```
[35]: import numpy as np
import paragami
```

In this example, we will consider flattening and folding a simple symmetric positive semi-definite matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}.$$

Of course, symmetry and positive semi-definiteness impose constraints on the entries a_{ij} of A .

2.1.1 Flattening and Folding.

In the Original Space.

Let us first consider how to represent A as a vector, which we call simply *flattening*, and then as an unconstrained vector, which we call *free flattening*.

When a parameter is flattened, it is simply re-shaped as a vector. Every number that was in the original parameter will occur exactly once in the flattened shape. (In the present case of a matrix, this is exactly the same as `np.flatten()`.)

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \xrightarrow{\text{flatten}} A_{\text{flat}} = \begin{bmatrix} a_{\text{flat},1} \\ a_{\text{flat},2} \\ a_{\text{flat},3} \\ a_{\text{flat},4} \\ a_{\text{flat},5} \\ a_{\text{flat},6} \\ a_{\text{flat},7} \\ a_{\text{flat},8} \\ a_{\text{flat},9} \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{12} \\ a_{13} \\ a_{21} \\ a_{22} \\ a_{23} \\ a_{31} \\ a_{32} \\ a_{33} \end{bmatrix}$$

Converting to and from A and A_{flat} can be done with the `flatten` method of a `paragami.PSDSymmetricMatrixPattern` pattern.

For the moment, because we are flattening, not free flattening, we use the option `free=False`. We will discuss the `free=True` option shortly.

```
[2]: # A sample positive semi-definite matrix.
a = np.eye(3) + np.random.random((3, 3))
a = 0.5 * (a + a.T)

# Define a pattern and fold.
a_pattern = paragami.PSDSymmetricMatrixPattern(size=3)
a_flat = a_pattern.flatten(a, free=False)

print('Now, a_flat contains the elements of a exactly as shown in the formula above.\n'
      '→')
print('a:\n{}\n'.format(a))
print('a_flat:\n{}\n'.format(a_flat))

Now, a_flat contains the elements of a exactly as shown in the formula above.

a:
[[1.46982005 0.44700975 0.635101]
 [0.44700975 1.54334054 0.60507272]
 [0.635101    0.60507272 1.34595469]]

a_flat:
[1.46982005 0.44700975 0.635101    0.44700975 1.54334054 0.60507272
 0.635101    0.60507272 1.34595469]
```

We can also convert from A_{flat} back to A by ‘folding’.

```
[3]: print('Folding the flattened value recovers the original matrix.\n')
a_fold = a_pattern.fold(a_flat, free=False)
print('a:\n{}\n'.format(a))
print('a_fold:\n{}\n'.format(a_fold))

Folding the flattened value recovers the original matrix.

a:
[[1.46982005 0.44700975 0.635101]
 [0.44700975 1.54334054 0.60507272]
 [0.635101    0.60507272 1.34595469]]

a_fold:
[[1.46982005 0.44700975 0.635101]
 [0.44700975 1.54334054 0.60507272]
 [0.635101    0.60507272 1.34595469]]
```

By default, flattening and folding perform checks to make sure the result is a valid instance of the parameter type – in this case, a symmetric positive definite matrix.

The diagonal of a positive semi-definite matrix must not be less than 0, and folding checks this when `validate=True`, which it is by default.

```
[19]: a_flat_bad = np.array([-1, 0, 0, 0, 0, 0, 0, 0])
print('A bad folded value: {}'.format(a_flat_bad))
```

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```
try:
    a_fold_bad = a_pattern.fold(a_flat_bad, free=False)
except ValueError as err:
    print('Folding with a_pattern raised the following ValueError:\n{}'.format(err))

A bad folded value: [-1  0  0  0  0  0  0  0  0]
Folding with a_pattern raised the following ValueError:
Diagonal is less than the lower bound 0.0.
```

If `validate_value` is `False`, folding will produce an invalid matrix without an error.

```
[22]: a_fold_bad = a_pattern.fold(a_flat_bad, free=False, validate_value=False)
print('Folding a non-pd matrix with validate=False:\n{}'.format(a_fold_bad))

Folding a non-pd matrix with validate=False:
[[-1  0  0]
 [ 0  0  0]
 [ 0  0  0]]
```

However, it will not produce a matrix of the wrong shape even when `validate` is `False`.

```
[24]: a_flat_very_bad = np.array([1, 0, 0])
print('A very bad folded value: {}'.format(a_flat_very_bad))
try:
    a_fold_very_bad = a_pattern.fold(a_flat_very_bad, free=False, validate_
                                     value=False)
except ValueError as err:
    print('Folding with a_pattern raised the following ValueError:\n{}'.format(err))

A very bad folded value: [1 0 0].
Folding with a_pattern raised the following ValueError:
Wrong length for PSDSymmetricMatrix flat value.
```

You can always check validity of a folded value with the `validate_folded` method of a pattern, which returns a boolean and an error message.

```
[30]: valid, msg = a_pattern.validate_folded(a_fold)
print('Valid: {}.\nMessage: {}'.format(valid, msg))

valid, msg = a_pattern.validate_folded(a_fold - 10 * np.eye(3))
print('Valid: {}.\nMessage: {}'.format(valid, msg))

Valid: True.    Message:
Valid: False.   Message: Diagonal is less than the lower bound 0.0.
```

In an Unconstrained Space: “Free” Flattening and Folding.

Ordinary flattening converts a 3×3 symmetric PSD matrix into a 9-d vector. However, as seen above, not every 9-d vector is a valid 3×3 symmetric positive definite matrix. It is useful to have an “free” flattened representation of a parameter, where every finite value of the free flattened vector corresponds is guaranteed valid.

To accomplish this for a symmetric positive definite matrix, we consider the Cholesky decomposition A_{chol} . This is an lower-triangular matrix with positive diagonal entries such that $A = A_{chol}A_{chol}^T$. By taking the log of the diagonal of A_{chol} and stacking the non-zero entries, we can construct a 6-d vector, every value of which corresponds to a

symmetric PSD matrix.

$$A \rightarrow A_{chol} = \begin{bmatrix} \alpha_{11} & 0 & 0 \\ \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \rightarrow A_{freeflat} = \begin{bmatrix} \log(\alpha_{11}) \\ \alpha_{21} \\ \alpha_{31} \\ \log(\alpha_{22}) \\ \alpha_{32} \\ \log(\alpha_{33}) \end{bmatrix}.$$

The details of the freeing transform aren't important to the end user, as paragami takes care of the transformation behind the scenes with the option `free=True`. We denote the flattened A in the free parameterization as $A_{freeflat}$.

The free flat value `a_freeflat` is not immediately recognizable as `a`.

```
[33]: a_freeflat = a_pattern.flatten(a, free=True)
print('a:\n{}\n'.format(a))
print('a_freeflat:\n{}\n'.format(a_freeflat))

a:
[[1.46982005 0.44700975 0.635101]
 [0.44700975 1.54334054 0.60507272]
 [0.635101 0.60507272 1.34595469]]

a_freeflat:
[ 0.19256999  0.36870999  0.1708697   0.52385454  0.34722226 -0.02513753]
```

However, it transforms correctly back to `a` when folded.

```
[32]: a_freefold = a_pattern.fold(a_freeflat, free=True)
print('a:\n{}\n'.format(a))
print('a_fold:\n{}\n'.format(a_freefold))

a:
[[1.46982005 0.44700975 0.635101]
 [0.44700975 1.54334054 0.60507272]
 [0.635101 0.60507272 1.34595469]]

a_fold:
[[1.46982005 0.44700975 0.635101]
 [0.44700975 1.54334054 0.60507272]
 [0.635101 0.60507272 1.34595469]]
```

Any length-six vector will free fold back to a valid PSD matrix up to floating point error. Let's draw 100 random vectors, fold them, and check that this is true.

```
[34]: # Draw random free vectors and confirm that they are positive semi definite.
def assert_is_pd(mat):
    eigvals = np.linalg.eigvals(mat)
    assert np.min(eigvals) >= -1e-8

for draw in range(100):
    a_rand_freeflat = np.random.normal(scale=2, size=(6, ))
    a_rand_fold = a_pattern.fold(a_rand_freeflat, free=True)
    assert_is_pd(a_rand_fold)
```

Default values for `free`.

You can set a default value for whether or not a parameter is free.

```
[49]: a_free_pattern = paragami.PSDSymmetricMatrixPattern(size=3, free_default=True)

a_freeflat = a_free_pattern.flatten(a)
print('a_freeflat:\n{}\n'.format(a_freeflat))
print('a:\n{}\n'.format(a_free_pattern.fold(a_freeflat)))
```



```
a_freeflat:
[ 0.19256999  0.36870999  0.1708697   0.52385454  0.34722226 -0.02513753]

a:
[[1.46982005 0.44700975 0.635101]
 [0.44700975 1.54334054 0.60507272]
 [0.635101   0.60507272 1.34595469]]
```



```
a_flat:
[1.46982005 0.44700975 0.635101   0.44700975 1.54334054 0.60507272
 0.635101   0.60507272 1.34595469]
```



```
a_flat:
[1.46982005 0.44700975 0.635101   0.44700975 1.54334054 0.60507272
 0.635101   0.60507272 1.34595469]
```

The default is be overridden by setting the argument `free`.

```
[51]: a_flat = a_free_pattern.flatten(a, free=False)
print('a_flat:\n{}\n'.format(a_flat))
print('a:\n{}\n'.format(a_free_pattern.fold(a_flat, free=False)))
```



```
a_flat:
[1.46982005 0.44700975 0.635101   0.44700975 1.54334054 0.60507272
 0.635101   0.60507272 1.34595469]

a:
[[1.46982005 0.44700975 0.635101]
 [0.44700975 1.54334054 0.60507272]
 [0.635101   0.60507272 1.34595469]]
```

You can change the default by setting the attribute `free_default`.

```
[53]: # Now this pattern is misnamed!
a_free_pattern.free_default = False
print('a_flat:\n{}\n'.format(a_free_pattern.flatten(a)))

a_flat:
[1.46982005 0.44700975 0.635101   0.44700975 1.54334054 0.60507272
 0.635101   0.60507272 1.34595469]
```

An error is raised if `free_default` is `None` and `free` is not specified.

```
[55]: a_free_pattern.free_default = None
try:
    a_free_pattern.flatten(a)
except ValueError as err:
    print('Folding with a_free_pattern raised the following ValueError:\n{}'.
          format(err))
```

```
Folding with a_free_pattern raised the following ValueError:
If ``free_default`` is ``None``, ``free`` must be specified.
```

2.2 Flattening and Folding for Optimization and Frequentist Covariances.

```
[1]: import autograd
from autograd import numpy as np

import matplotlib.pyplot as plt
%matplotlib inline
import paragami

# Use the original scipy ("osp") for functions we don't need to differentiate.
# When using scipy functions in functions that are passed to autograd,
# use autograd.scipy instead.
import scipy as osp
```

2.2.1 Using Flattening and Folding for Optimization.

An Example Model.

Suppose we are interested in optimizing some function of A , say, a normal model in which the data $x_n \sim \mathcal{N}(0, A)$. Specifically, Let the data be $X = (x_1, \dots, x_N)$, where $x_n \in \mathbb{R}^3$, and write a loss function as

$$\ell(X, A) = - \sum_{n=1}^N \log P(x_n|A) = \frac{1}{2} \sum_{n=1}^N (x_n^T A^{-1} x_n - \log |A|)$$

Let's simulate some data under this model.

```
[13]: np.random.seed(42)

num_obs = 100

# True value of A
true_a = np.eye(3) * np.diag(np.array([1, 2, 3])) + np.random.random((3, 3)) * 0.1
true_a = 0.5 * (true_a + true_a.T)

# Data
def draw_data(num_obs, true_a):
    return np.random.multivariate_normal(
        mean=np.zeros(3), cov=true_a, size=(num_obs,))

x = draw_data(num_obs, true_a)
print('X shape: {}'.format(x.shape))
```

```
x shape: (100, 3)
```

We can estimate the covariance matrix using the negative log likelihood as a loss function.

```
[14]: def get_loss(x, a):
    num_obs = x.shape[0]
    a_inv = np.linalg.inv(a)
    a_det_sign, a_log_det = np.linalg.slogdet(a)
    assert a_det_sign > 0
    return 0.5 * (np.einsum('ni,ij,nj', x, a_inv, x) + num_obs * a_log_det)

print('Loss at true parameter: {}'.format(get_loss(x, true_a)))
Loss at true parameter: 242.28536625488033
```

Using autograd and scipy.optimize with paragami.

We would like to minimize the function `loss` using tools like `scipy.optimize.minimize`. Standard optimization functions take vectors, not matrices, as input, and often require the vector to take valid values in the entire domain.

As-written, our loss function takes a positive definite matrix as an input. We can wrap the loss as a function of the free flattened value using the `paragami.FlattenFunctionInput` class. That is, we want to define a function $\ell_{freeflat}$ so that

$$\ell_{freeflat}(X, A_{freeflat}) = \ell(X, A).$$

```
[17]: a_pattern = paragami.PSDSymmetricMatrixPattern(size=3)

# The arguments mean we're flattening the function get_loss, using
# the pattern a_pattern, with free parameterization, and the parameter
# is the second one (argnums uses 0-indexing like autograd).
get_freeflat_loss = paragami.FlattenFunctionInput(
    original_fun=get_loss, patterns=a_pattern, free=True, argnums=1)

print('The two losses are the same when evaluated on the folded and flat values:\n')
print('Original loss: \t{}\t'.format(get_loss(x, true_a)))
true_a_freeflat = a_pattern.flatten(true_a, free=True)
print('Free-flattened loss: \t{}\t'.format(
    get_freeflat_loss(x, true_a_freeflat)))

The two losses are the same when evaluated on the folded and flat values:

Original loss:      242.28536625488033
Free-flattened loss: 242.28536625488036
```

The resulting function can be passed directly to `autograd` and `scipy.optimize`, and we can estimate

$$\hat{A}_{freeflat} := \operatorname{argmin}_{A_{freeflat}} \ell_{freeflat}(X, A_{freeflat}).$$

Note that (as of writing) A bad approximation caused failure to predict improvement errors are common with second order methods even when optimization was successful. This is because `osp.optimize.minimize` only uses the norm of the gradient before multiplication by the inverse Hessian as a convergence criterion.

```
[26]: get_freeflat_loss_grad = autograd.grad(get_freeflat_loss, argnum=1)
get_freeflat_loss_hessian = autograd.hessian(get_freeflat_loss, argnum=1)

def get_optimum(x, init_val):
    loss_opt = osp.optimize.minimize(
        method='trust-ncg',
        x0=init_val,
        fun=lambda par: get_freeflat_loss(x, par),
        jac=lambda par: get_freeflat_loss_grad(x, par),
        hess=lambda par: get_freeflat_loss_hessian(x, par),
        options={'gtol': 1e-8, 'disp': False})
    return loss_opt

init_val = np.zeros(a_pattern.flat_length(free=True))
loss_opt = get_optimum(x, init_val)

print('Optimization status: {}\nOptimal value: {}'.format(
    loss_opt.message, loss_opt.fun))
```

Optimization status: A bad approximation caused failure to predict improvement.
Optimal value: 239.37556057055355

The optimization was in the free flattened space, so to get the optimal value of A we must fold it. We can see that the optimal value is close to the true value of A , though it differs due to randomness in X .

```
[27]: optimal_freeflat_a = loss_opt.x
optimal_a = a_pattern.fold(optimal_freeflat_a, free=True)
print('True a:\n{}\n\nOptimal a:\n{}'.format(true_a, optimal_a))

True a:
[[1.03745401 0.07746864 0.03950388]
 [0.07746864 2.01560186 0.05110853]
 [0.03950388 0.05110853 3.0601115]]

Optimal a:
[[ 1.13076002 -0.16382566  0.18449819]
 [-0.16382566  1.97854146  0.3020592 ]
 [ 0.18449819  0.3020592   2.78831733]]
```

2.2.2 Using Flattening and Folding with the Fisher Information for Frequentist Uncertainty.

Fisher Information and the Delta Method.

Suppose we wanted to use the Hessian of the objective (the observed Fisher information) to estimate a frequentist confidence region for A . In standard notation, covariance is of a vector, so we can write what we want in terms of A_{flat} as $\text{Cov}(A_{flat})$. The covariance between two elements of A_{flat} corresponds to that between two elements of A . For example, using the notation given above,

$$\begin{aligned}\text{Cov}(a_{flat,1}, a_{flat,2}) &= \text{Cov}(a_{11}, a_{12}) = \text{Cov}(a_{11}, a_{21}) \\ \text{Var}(a_{flat,4}) &= \text{Var}(a_{21}) = \text{Var}(a_{12}), \\ &\quad \text{etc.}\end{aligned}$$

Here, we will use the observed Fisher information of $\ell_{freeflat}$ and the Delta method to estimate $\text{Cov}(A_{flat})$.

$$\text{Cov}(A_{freeflat}) \approx - \left(\frac{\partial^2 \ell_{freeflat}}{\partial A_{freeflat} \partial A_{freeflat}^T} \Big|_{\hat{A}_{freeflat}} \right)^{-1} \quad (\text{Fisher information})$$

$$\text{Cov}(A_{free}) \approx \left(\frac{dA_{free}}{dA_{freeflat}^T} \right) \text{Cov}(A_{freeflat}) \left(\frac{dA_{free}}{dA_{freeflat}^T} \right)^T \quad (\text{Delta method})$$

The Hessian required for the covariance can be calculated directly using `autograd`. (Note that the loss is the negative of the log likelihood.) The shape is, of course, the size of $A_{freeflat}$.

```
[5]: fisher_info = -1 * get_freeflat_loss_hessian(x, loss_opt.x)
print("The shape of the Fisher information amtrix is {}.".format(fisher_info.shape))
The shape of the Fisher information amtrix is (6, 6).
```

The Jacobian matrix $\frac{dA_{free}}{dA_{freeflat}^T}$ of the “unfreeing transform” $A_{free} = A_{free}(A_{freeflat})$ is provided by `paragami` as a function of the `folded` parameter. Following standard notation for Jacobian matrices, the rows correspond to A_{flat} , the output of the unfreeing transform, and the columns correspond to $A_{freeflat}$, the input to the unfreeing transform.

By default this Jacobian matrix is sparse (in large problems, most flat parameters are independent of most free flat parameters), but a dense matrix is fine in this small problem, so we use `sparse=False`.

```
[6]: freeing_jac = a_pattern.unfreeing_jacobian(optimal_a, sparse=False)
print("The shape of the Jacobian matrix is {}.".format(freeing_jac.shape))
The shape of the Jacobian matrix is (9, 6).
```

We can now plug in to estimate the covariance.

```
[7]: # Estimate the covariance of the flattened value using the Hessian at the optimum.
a_flattened_cov = -1 * freeing_jac @ np.linalg.solve(fisher_info, freeing_jac.T)
```

A Cautionary Note on Using the Fisher Information With Constrained Variables.

Note that the estimated covariance is rank-deficient. This is expected, since, for example, A_{12} and A_{21} cannot vary independently.

```
[8]: print('The shape of the covariance matrix is {}.'.format(a_flattened_cov.shape))
print('The rank of the covariance matrix is {}.'.format(np.linalg.matrix_rank(a_
    ↪flattened_cov)))
The shape of the covariance matrix is (9, 9).
The rank of the covariance matrix is 6.
```

Suppose we had erroneously defined the function $\ell_{flat}(A_{flat})$ and tried to estimate the covariance of A using the Hessian of ℓ_{flat} . Then the resulting Hessian would have been *full rank*, because the loss function `get_loss` does not enforce the constraint that A be symmetric.

```
[9]: print('An example of an erroneous use of Fisher information!')
get_flat_loss = paragami.FlattenFunctionInput(
    original_fun=get_loss, patterns=a_pattern, free=False, argnums=1)
get_flat_loss_hessian = autograd.hessian(get_flat_loss, argnum=1)
a_flat_opt = a_pattern.flatten(optimal_a, free=False)
bad_fisher_info = get_flat_loss_hessian(x, a_flat_opt)
```

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```
bad_a_flattened_cov = -1 * np.linalg.inv(bad_fisher_info)

print('The shape of the erroneous covariance matrix is {}'.format(bad_a_flattened_
    ↴cov.shape))
print('The rank of the erroneous covariance matrix is {}'.format(np.linalg.matrix_
    ↴rank(bad_a_flattened_cov)))

An example of an erroneous use of Fisher information!
The shape of the erroneous covariance matrix is (9, 9).
The rank of the erroneous covariance matrix is 9.
```

Theoretically, we are not justified using the Hessian of ℓ_{flat} to estimate the covariance of its optimizer because the optimum is not “interior” – that is, the argument A_{flat} cannot take legal values in a neighborhood of the optimum, since such values may not be valid covariance matrices. Overcoming this difficulty is a key advantage of using unconstrained parameterizations.

Inspecting and Checking the Result.

This shape of $\text{Cov}(A_{flat})$ is inconvenient because it’s not obvious visually which entry of the flattened vector corresponds to which element of A . Again, we can use folding to put the estimated marginal standard deviations in a readable shape.

Because the result is not a valid covariance matrix, and we are just using the pattern for its shape, we set `validate` to `False`.

```
[10]: a_pattern.verify = False
a_sd = a_pattern.fold(np.sqrt(np.diag(a_flattened_cov)), free=False, validate_
    ↴value=False)
print('The marginal standard deviations of the elements of A:\n{}'.format(a_sd))

The marginal standard deviations of the elements of A:
[[0.15991362 0.15046908 0.17852051]
 [0.15046908 0.27980802 0.23681303]
 [0.17852051 0.23681303 0.39432762]]
```

As a sanity check, we can compare this estimated covariance with the variability incurred by drawing new datasets and re-optimizing.

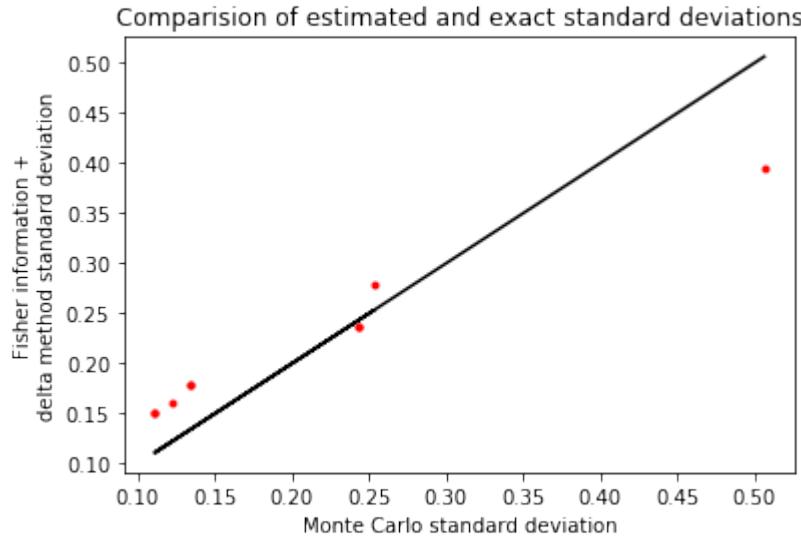
```
[11]: num_sims = 20
optimal_a_draws = np.empty((num_sims, ) + true_a.shape)
for sim in range(num_sims):
    new_x = draw_data(num_obs, true_a)
    new_loss_opt = get_optimum(new_x)
    optimal_a_draws[sim] = a_pattern.fold(new_loss_opt.x, free=True)
```

```
[12]: a_sd_monte_carlo = np.std(optimal_a_draws, axis=0)

plt.plot(a_sd_monte_carlo.flatten(), a_sd.flatten(), 'r.')
plt.plot(a_sd_monte_carlo.flatten(), a_sd_monte_carlo.flatten(), 'k')
plt.xlabel('Monte Carlo standard deviation')
plt.ylabel('Fisher information +\ndelta method standard deviation')
plt.title('Comparision of estimated and exact standard deviations')

print('Actual standard deviation:\n{}'.format(a_sd_monte_carlo))
print('Estimated standard deviation:\n{}'.format(a_sd))
```

```
Actual standard deviation:
[[0.12203849 0.11104834 0.13347622]
 [0.11104834 0.25363392 0.24355346]
 [0.13347622 0.24355346 0.50647563]]
Estimated standard deviation:
[[0.15991362 0.15046908 0.17852051]
 [0.15046908 0.27980802 0.23681303]
 [0.17852051 0.23681303 0.39432762]]
```



2.3 Default values for free.

```
[1]: import numpy as np
import paragami
```

You can set a default value for whether or not a parameter is free.

```
[4]: a = np.eye(3) + np.random.random((3, 3))
a = 0.5 * (a + a.T)

a_free_pattern = paragami.PSDSymmetricMatrixPattern(size=3, free_default=True)

a_freeflat = a_free_pattern.flatten(a)
print('a_freeflat:\n{}\n'.format(a_freeflat))
print('a:\n{}\n'.format(a_free_pattern.fold(a_freeflat)))

a_freeflat:
[ 0.13919912  0.41973416  0.12037979  0.7396427   0.44432253 -0.06185827]

a:
[[1.32101217 0.48242269 0.85011051]
 [0.48242269 1.4483919 0.81161586]
 [0.85011051 0.81161586 1.6281241 ]]
```

The default is be overridden by setting the argument `free`.

```
[5]: a_flat = a_free_pattern.flatten(a, free=False)
print('a_flat:\n{}\n'.format(a_flat))
print('a:\n{}\n'.format(a_free_pattern.fold(a_flat, free=False)))

a_flat:
[1.32101217 0.48242269 0.85011051 0.48242269 1.4483919 0.81161586
 0.85011051 0.81161586 1.6281241 ]

a:
[[1.32101217 0.48242269 0.85011051]
 [0.48242269 1.4483919 0.81161586]
 [0.85011051 0.81161586 1.6281241 ]]
```

You can change the default by setting the attribute `free_default`.

```
[6]: # Now this pattern is misnamed!
a_free_pattern.free_default = False
print('a_flat:\n{}\n'.format(a_free_pattern.flatten(a)))

a_flat:
[1.32101217 0.48242269 0.85011051 0.48242269 1.4483919 0.81161586
 0.85011051 0.81161586 1.6281241 ]
```

An error is raised if `free_default` is `None` and `free` is not specified.

```
[7]: a_free_pattern.free_default = None
try:
    a_free_pattern.flatten(a)
except ValueError as err:
    print('Folding with a_free_pattern raised the following ValueError:\n{}'.
          format(err))
```

Folding with `a_free_pattern` raised the following `ValueError`:
If ```free_default``` is ```None```, ```free``` must be specified.

Pattern containers override the default values of their contents so you don't accidentally mix free and non-free flattened values.

```
[19]: dict_pattern = paragami.PatternDict(free_default=True)

dict_pattern['a1'] = paragami.PSDSymmetricMatrixPattern(size=3, free_default=False)
dict_pattern['a2'] = paragami.PSDSymmetricMatrixPattern(size=3, free_default=True)

print('\nThis pattern alone is non-free by default:')
print(dict_pattern['a1'].flatten(a))

print('\nThis pattern alone is free by default:')
print(dict_pattern['a2'].flatten(a))

print('\nBut the dictionary pattern overrides the default:')
param_dict = { 'a1': a, 'a2': a}
print(dict_pattern.flatten(param_dict))

print('\nIf no default is specified, an error is raised ' +
```

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```
'so that you do not accidentally mix free and non-free flat values.')
dict_pattern_nodefault = paragami.PatternDict()
try:
    dict_pattern_nodefault.flatten(param_dict)
except ValueError as err:
    print('Folding a container with no default raised the follding ValueError:\n{}'.
        format(err))
```

This pattern alone is non-free by default:

```
[1.32101217 0.48242269 0.85011051 0.48242269 1.4483919 0.81161586
 0.85011051 0.81161586 1.6281241 ]
```

This pattern alone is free by default:

```
[ 0.13919912  0.41973416  0.12037979  0.7396427   0.44432253 -0.06185827]
```

But the dictionary pattern overrides the default:

```
[ 0.13919912  0.41973416  0.12037979  0.7396427   0.44432253 -0.06185827
 0.13919912  0.41973416  0.12037979  0.7396427   0.44432253 -0.06185827]
```

If no default is specified, an error is raised so that you do not accidentally mix
free and non-free flat values.

Folding a container with no default raised the follding ValueError:

If ``free_default`` is ``None``, ``free`` must be specified.

CHAPTER 3

API

3.1 Pattern Parent Class

Every pattern described herein inherits from the parent *Pattern* class and implements its methods.

class paragami.base_patterns.**Pattern** (*flat_length*, *free_flat_length*, *free_default*=*None*)
A abstract class for a parameter pattern.

See derived classes for examples.

__init__ (*flat_length*, *free_flat_length*, *free_default*=*None*)

Parameters

flat_length [*int*] The length of a non-free flattened vector.

free_flat_length [*int*] The length of a free flattened vector.

as_dict()

Return a dictionary of attributes describing the pattern.

The dictionary should completely describe the pattern in the sense that if the contents of two patterns' dictionaries are identical the patterns should be considered identical.

If the keys of the returned dictionary match the arguments to **__init__**, then the default methods for **to_json** and **from_json** will work with no additional modification.

empty (*valid*)

Return an empty parameter in its folded shape.

Parameters

valid [*bool*] Whether or folded shape should be filled with valid values.

Returns

folded_val [Folded value] A parameter value in its original folded shape.

empty_bool (*value*)

Return folded shape containing booleans.

Parameters

value [bool] The value with which to fill the folded shape.

Returns

folded_bool [Folded value] A boolean value in its original folded shape.

flat_indices (folded_bool, free=None)

Get which flattened indices correspond to which folded values.

Parameters

folded_bool [Folded booleans] A variable in the folded shape but containing booleans. The elements that are True are the ones for which we will return the flat indices.

free [bool] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute free_default is used.

Returns

indices [numpy.ndarray (N,)] A list of indices into the flattened value corresponding to the True members of folded_bool.

flat_length (free=None)

Return the length of the pattern's flattened value.

Parameters

free [bool, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, free_default is used.

Returns

length [int] The length of the pattern's flattened value.

flatten (folded_val, free=None, validate_value=None)

Flatten a folded value into a flat vector.

Parameters

folded_val [Folded value] The parameter in its original folded shape.

free [bool, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute free_default is used.

validate_value [bool] Whether to check that the folded value is valid. If None, the pattern will employ a default behavior.

Returns

flat_val [numpy.ndarray, (N,)] The flattened value.

fold (flat_val, free=None, validate_value=None)

Fold a flat value into a parameter.

Parameters

flat_val [numpy.ndarray, (N,)] The flattened value.

free [bool, optional.] Whether or not the flattened value is a free parameterization. If not specified, the attribute free_default is used.

validate_value [bool, optional.] Whether to check that the folded value is valid. If None, the pattern will employ a default behavior.

Returns

folded_val [Folded value] The parameter value in its original folded shape.

freeing_jacobian (*folded_val*, *sparse=True*)

The Jacobian of the map from a flat free value to a flat value.

If the folded value of the parameter is *val*, *val_flat* = `flatten(val, free=False)`, and *val_freeflat* = `flatten(val, free=True)`, then this calculates the Jacobian matrix $\frac{d \text{val_free}}{d \text{val_freeflat}}$. For entries with no dependence between them, the Jacobian is taken to be zero.

Parameters

folded_val [Folded value] The folded value at which the Jacobian is to be evaluated.

sparse [*bool*, optional] Whether to return a sparse or a dense matrix.

Returns

“numpy.ndarray”, (*N*, *M*) The Jacobian matrix $\frac{d \text{val_free}}{d \text{val_freeflat}}$.

Consistent with standard Jacobian notation, the elements of *val_free* correspond to the rows of the Jacobian matrix and the elements of *val_freeflat* correspond to the columns.

See also:

Pattern.unfreeing_jacobian

classmethod from_json (*json_string*)

Return a pattern from *json_string* created by `to_json`.

See also:

Pattern.to_json

random()

Return an random, valid parameter in its folded shape.

Note: There is no reason this provides a meaningful distribution over folded values. This function is intended to be used as a convenience for testing.

Returns

folded_val [Folded value] A random parameter value in its original folded shape.

to_json()

Return a JSON representation of the pattern.

See also:

Pattern.from_json

unfreeing_jacobian (*folded_val*, *sparse=True*)

The Jacobian of the map from a flat value to a flat free value.

If the folded value of the parameter is *val*, *val_flat* = `flatten(val, free=False)`, and *val_freeflat* = `flatten(val, free=True)`, then this calculates the Jacobian matrix $\frac{d \text{val_freeflat}}{d \text{val_free}}$. For entries with no dependence between them, the Jacobian is taken to be zero.

Parameters

folded_val [Folded value] The folded value at which the Jacobian is to be evaluated.

sparse [bool, optional] If True, return a sparse matrix. Otherwise, return a dense numpy 2d array.

Returns

“numpy.ndarray”, (N, N) The Jacobian matrix d val_freeflat / d val_free. Consistent with standard Jacobian notation, the elements of val_freeflat correspond to the rows of the Jacobian matrix and the elements of val_free correspond to the columns.

See also:

Pattern.freeing_jacobian

validate_folded (folded_val, validate_value=None)

Check whether a folded value is valid.

Parameters

folded_val [Folded value] A parameter value in its original folded shape.

validate_value [bool] Whether to validate the value in addition to the shape. The shape is always validated.

Returns

is_valid [bool] Whether folded_val is an allowable shape and value.

err_msg [str]

3.2 Numeric patterns

3.2.1 Numeric Arrays

```
class paragami.numeric_array_patterns.NumericArrayPattern(shape, lb=-inf, ub=inf,
                                                          default_validate=True,
                                                          free_default=None)
```

A pattern for (optionally bounded) arrays of numbers.

Attributes

default_validate: ‘bool’, optional Whether or not the array is checked by default to lie within the specified bounds.

__init__ (shape, lb=-inf, ub=inf, default_validate=True, free_default=None)

Parameters

shape: ‘tuple’ of ‘int’ The shape of the array.

lb: ‘float’ The (inclusive) lower bound for the entries of the array.

ub: ‘float’ The (inclusive) upper bound for the entries of the array.

default_validate: ‘bool’, optional Whether or not the array is checked by default to lie within the specified bounds.

free_default: ‘bool’, optional Whether the pattern is free by default.

as_dict()

Return a dictionary of attributes describing the pattern.

The dictionary should completely describe the pattern in the sense that if the contents of two patterns' dictionaries are identical the patterns should be considered identical.

If the keys of the returned dictionary match the arguments to `__init__`, then the default methods for `to_json` and `from_json` will work with no additional modification.

`empty(valid)`

Return an empty parameter in its folded shape.

Parameters

valid [bool] Whether or folded shape should be filled with valid values.

Returns

folded_val [Folded value] A parameter value in its original folded shape.

`flat_indices(folded_bool, free=None)`

Get which flattened indices correspond to which folded values.

Parameters

folded_bool [Folded booleans] A variable in the folded shape but containing booleans. The elements that are `True` are the ones for which we will return the flat indices.

free [bool] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

Returns

indices [numpy.ndarray (N,)] A list of indices into the flattened value corresponding to the `True` members of `folded_bool`.

`flat_length(free=None)`

Return the length of the pattern's flattened value.

Parameters

free [bool, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, `free_default` is used.

Returns

length [int] The length of the pattern's flattened value.

`flatten(folded_val, free=None, validate_value=None)`

Flatten a folded value into a flat vector.

Parameters

folded_val [Folded value] The parameter in its original folded shape.

free [bool, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [bool] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

flat_val [numpy.ndarray, (N,)] The flattened value.

`fold(flat_val, free=None, validate_value=None)`

Fold a flat value into a parameter.

Parameters

flat_val [numpy.ndarray, (N,)] The flattened value.
free [bool, optional.] Whether or not the flattened value is a free parameterization. If not specified, the attribute `free_default` is used.
validate_value [bool, optional.] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

folded_val [Folded value] The parameter value in its original folded shape.

validate_folded (`folded_val`, `validate_value=None`)
Check whether a folded value is valid.

Parameters

folded_val [Folded value] A parameter value in its original folded shape.
validate_value [bool] Whether to validate the value in addition to the shape. The shape is always validated.

Returns

is_valid [bool] Whether `folded_val` is an allowable shape and value.
err_msg [str]

3.2.2 Symmetric Positive Definite Matrices

```
class paragami.psdmatrix_patterns.PSDSymmetricMatrixPattern(size,  
                                                               diag_lb=0.0,      de-  
                                                               default_validate=True,  
                                                               free_default=None)
```

A pattern for a symmetric, positive-definite matrix parameter.

Attributes

validate: Bool Whether or not the matrix is automatically checked for symmetry positive-definiteness, and the diagonal lower bound.

__init__ (`size`, `diag_lb=0.0`, `default_validate=True`, `free_default=None`)

Parameters

size: ‘int’ The length of one side of the square matrix.

diag_lb: ‘float’ A lower bound for the diagonal entries. Must be ≥ 0 .

default_validate: ‘bool’, optional Whether or not to check for legal (i.e., symmetric positive-definite) folded values by default.

free_default: ‘bool’, optional Default setting for free.

as_dict()

Return a dictionary of attributes describing the pattern.

The dictionary should completely describe the pattern in the sense that if the contents of two patterns' dictionaries are identical the patterns should be considered identical.

If the keys of the returned dictionary match the arguments to `__init__`, then the default methods for `to_json` and `from_json` will work with no additional modification.

diag_lb()

Returns the diagonal lower bound.

empty (*valid*)

Return an empty parameter in its folded shape.

Parameters

valid [*bool*] Whether or folded shape should be filled with valid values.

Returns

folded_val [Folded value] A parameter value in its original folded shape.

flat_indices (*folded_bool*, *free=None*)

Get which flattened indices correspond to which folded values.

Parameters

folded_bool [Folded booleans] A variable in the folded shape but containing booleans. The elements that are `True` are the ones for which we will return the flat indices.

free [*bool*] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

Returns

indices [*numpy.ndarray* (N,)] A list of indices into the flattened value corresponding to the `True` members of `folded_bool`.

flatten (*folded_val*, *free=None*, *validate_value=None*)

Flatten a folded value into a flat vector.

Parameters

folded_val [Folded value] The parameter in its original folded shape.

free [*bool*, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [*bool*] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

flat_val [*numpy.ndarray*, (N,)] The flattened value.

fold (*flat_val*, *free=None*, *validate_value=None*)

Fold a flat value into a parameter.

Parameters

flat_val [*numpy.ndarray*, (N,)] The flattened value.

free [*bool*, optional.] Whether or not the flattened value is a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [*bool*, optional.] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

folded_val [Folded value] The parameter value in its original folded shape.

shape ()

Returns the matrix shape, i.e., (size, size).

size ()

Returns the matrix size.

validate_folded(*folded_val*, *validate_value=None*)

Check that the folded value is valid.

If *validate_value = True*, checks that *folded_val* is a symmetric, matrix of the correct shape with diagonal entries greater than the specified lower bound. Otherwise, only the shape is checked.

Note: This method does not currently check for positive-definiteness.

Parameters

folded_val [Folded value] A candidate value for a positive definite matrix.

validate_value: ‘bool’, optional Whether to check the matrix for attributes other than shape. If *None*, the value of *self.default_validate* is used.

Returns

is_valid [bool] Whether *folded_val* is a valid positive semi-definite matrix.

err_msg [str] A message describing the reason the value is invalid or an empty string if the value is valid.

3.2.3 Simplexes

```
class paragami.simplex_patterns.SimplexArrayPattern(simplex_size, array_shape,
                                                    default_validate=True,
                                                    free_default=None)
```

A pattern for an array of simplex parameters.

The last index represents entries of the simplex. For example, if *array_shape=(2, 3)* and *simplex_size=4*, then the pattern is for a 2x3 array of 4d simplexes. If such value of the simplex array is given by *val*, then *val.shape = (2, 3, 4)* and *val[i, j, :]* is the *i,j'th of the six simplicial vectors*, i.e., *‘np.sum(val[i, j, :]’* equals 1 for each *i* and *j*.

Attributes

default_validate: Bool Whether or not the simplex is checked by default to be non-negative and to sum to one.

Methods

array_shape: tuple of ints	The shape of the array of simplexes, not including the simplex dimension.
simplex_size: int	The length of each simplex.
shape: tuple of ints	The shape of the entire array including the simplex dimension.

__init__(*simplex_size*, *array_shape*, *default_validate=True*, *free_default=None*)**Parameters**

simplex_size: ‘int’ The length of the simplexes.

array_shape: ‘tuple’ of ‘int’ The size of the array of simplexes (not including the simplexes themselves).

default_validate: ‘bool’, optional Whether or not to check for legal (i.e., positive and normalized) folded values by default.

free_default: ‘bool’, optional The default value for free.

as_dict()

Return a dictionary of attributes describing the pattern.

The dictionary should completely describe the pattern in the sense that if the contents of two patterns’ dictionaries are identical the patterns should be considered identical.

If the keys of the returned dictionary match the arguments to `__init__`, then the default methods for `to_json` and `from_json` will work with no additional modification.

empty(valid)

Return an empty parameter in its folded shape.

Parameters

valid [bool] Whether or folded shape should be filled with valid values.

Returns

folded_val [Folded value] A parameter value in its original folded shape.

flat_indices(folded_bool, free=None)

Get which flattened indices correspond to which folded values.

Parameters

folded_bool [Folded booleans] A variable in the folded shape but containing booleans. The elements that are True are the ones for which we will return the flat indices.

free [bool] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

Returns

indices [numpy.ndarray (N,)] A list of indices into the flattened value corresponding to the True members of `folded_bool`.

flatten(folded_val, free=None, validate_value=None)

Flatten a folded value into a flat vector.

Parameters

folded_val [Folded value] The parameter in its original folded shape.

free [bool, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [bool] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

flat_val [numpy.ndarray, (N,)] The flattened value.

fold(flat_val, free=None, validate_value=None)

Fold a flat value into a parameter.

Parameters

flat_val [numpy.ndarray, (N,)] The flattened value.

free [bool, optional.] Whether or not the flattened value is a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [bool, optional.] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

folded_val [Folded value] The parameter value in its original folded shape.

classmethod from_json(json_string)

Return a pattern instance from json_string created by to_json.

validate_folded(folded_val, validate_value=None)

Check whether a folded value is valid.

Parameters

folded_val [Folded value] A parameter value in its original folded shape.

validate_value [bool] Whether to validate the value in addition to the shape. The shape is always validated.

Returns

is_valid [bool] Whether folded_val is an allowable shape and value.

err_msg [str]

3.3 Containers of Patterns

Containers of patterns are themselves patterns, and so can contain instantiations of themselves.

3.3.1 Dictionaries of Patterns

class paragami.pattern_containers.PatternDict (free_default=None)

A dictionary of patterns (which is itself a pattern).

Examples

```
import paragami

# Add some patterns.
dict_pattern = paragami.PatternDict()
dict_pattern['vec'] = paragami.NumericArrayPattern(shape=(2, ))
dict_pattern['mat'] = paragami.PSDSymmetricMatrixPattern(size=3)

# Dictionaries can also contain dictionaries (but they have to
# be populated /before/ being added to the parent).
sub_dict_pattern = paragami.PatternDict()
sub_dict_pattern['vec1'] = paragami.NumericArrayPattern(shape=(2, ))
sub_dict_pattern['vec2'] = paragami.NumericArrayPattern(shape=(2, ))
dict_pattern['sub_dict'] = sub_dict_pattern

# We're done adding patterns, so lock the dictionary.
dict_pattern.lock()

# Get a random intial value for the whole dictionary.
dict_val = dict_pattern.random()
print(dict_val['mat']) # Prints a 3x3 positive definite numpy matrix.

# Get a flattened value of the whole dictionary.
```

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```
dict_val_flat = dict_pattern.flatten(dict_val, free=True)

# Get a new random folded value of the dictionary.
new_dict_val_flat = np.random.random(len(dict_val_flat))
new_dict_val = dict_pattern.fold(new_dict_val_flat, free=True)
```

Methods

lock:	Prevent additional patterns from being added or removed.
--------------	--

__init__ (*free_default=None*)

Parameters

flat_length [*int*] The length of a non-free flattened vector.

free_flat_length [*int*] The length of a free flattened vector.

as_dict()

Return a dictionary of attributes describing the pattern.

The dictionary should completely describe the pattern in the sense that if the contents of two patterns' dictionaries are identical the patterns should be considered identical.

If the keys of the returned dictionary match the arguments to `__init__`, then the default methods for `to_json` and `from_json` will work with no additional modification.

empty (*valid*)

Return an empty parameter in its folded shape.

Parameters

valid [*bool*] Whether or folded shape should be filled with valid values.

Returns

folded_val [Folded value] A parameter value in its original folded shape.

flat_indices (*folded_bool, free=None*)

Get which flattened indices correspond to which folded values.

Parameters

folded_bool [Folded booleans] A variable in the folded shape but containing booleans. The elements that are `True` are the ones for which we will return the flat indices.

free [*bool*] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

Returns

indices [`numpy.ndarray` (*N_i*)] A list of indices into the flattened value corresponding to the `True` members of `folded_bool`.

flatten (*folded_val, free=None, validate_value=None*)

Flatten a folded value into a flat vector.

Parameters

folded_val [Folded value] The parameter in its original folded shape.

free [bool, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [bool] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

flat_val [numpy.ndarray, (N,)] The flattened value.

fold(*flat_val*, *free=None*, *validate_value=None*)

Fold a flat value into a parameter.

Parameters

flat_val [numpy.ndarray, (N,)] The flattened value.

free [bool, optional.] Whether or not the flattened value is a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [bool, optional.] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

folded_val [Folded value] The parameter value in its original folded shape.

freeing_jacobian(*folded_val*, *sparse=True*)

The Jacobian of the map from a flat free value to a flat value.

If the folded value of the parameter is `val`, `val_flat = flatten(val, free=False)`, and `val_freeflat = flatten(val, free=True)`, then this calculates the Jacobian matrix $\frac{d \ val_free}{d \ val_freeflat}$. For entries with no dependence between them, the Jacobian is taken to be zero.

Parameters

folded_val [Folded value] The folded value at which the Jacobian is to be evaluated.

sparse [bool, optional] Whether to return a sparse or a dense matrix.

Returns

“numpy.ndarray”, (N, M) The Jacobian matrix $\frac{d \ val_free}{d \ val_freeflat}$.

Consistent with standard Jacobian notation, the elements of `val_free` correspond to the rows of the Jacobian matrix and the elements of `val_freeflat` correspond to the columns.

See also:

`Pattern.unfreeing_jacobian`

classmethod from_json(*json_string*)

Return a pattern from `json_string` created by `to_json`.

See also:

`Pattern.to_json`

unfreeing_jacobian(*folded_val*, *sparse=True*)

The Jacobian of the map from a flat value to a flat free value.

If the folded value of the parameter is `val`, `val_flat = flatten(val, free=False)`, and `val_freeflat = flatten(val, free=True)`, then this calculates the Jacobian matrix $\frac{d \ val_freeflat}{d \ val_free}$. For entries with no dependence between them, the Jacobian is taken to be zero.

Parameters

folded_val [Folded value] The folded value at which the Jacobian is to be evaluated.
sparse [bool, optional] If True, return a sparse matrix. Otherwise, return a dense numpy 2d array.

Returns

“numpy.ndarray”, (N, N) The Jacobian matrix d val_freeflat / d val_free. Consistent with standard Jacobian notation, the elements of val_freeflat correspond to the rows of the Jacobian matrix and the elements of val_free correspond to the columns.

See also:

`Pattern.freeing_jacobian`

validate_folded (`folded_val, validate_value=None`)

Check whether a folded value is valid.

Parameters

folded_val [Folded value] A parameter value in its original folded shape.
validate_value [bool] Whether to validate the value in addition to the shape. The shape is always validated.

Returns

is_valid [bool] Whether `folded_val` is an allowable shape and value.
err_msg [str]

3.3.2 Arrays of Patterns

```
class paragami.pattern_containers.PatternArray(array_shape, base_pattern,
free_default=None)
```

An array of a pattern (which is also itself a pattern).

The first indices of the folded pattern are the array and the final indices are of the base pattern. For example, if `shape=(3, 4)` and `base_pattern = PSDSymmetricMatrixPattern(size=5)`, then the folded value of the array will have shape (3, 4, 5, 5), where the entry `folded_val[i, j, :, :]` is a 5x5 positive definite matrix.

Currently this can only contain patterns whose folded values are numeric arrays (i.e., `NumericArrayPattern`, `SimplexArrayPattern`, and `PSDSymmetricMatrixPattern`).

__init__ (`array_shape, base_pattern, free_default=None`)

Parameters

array_shape: tuple of int The shape of the array (not including the base parameter)
base_pattern: The base pattern.

array_shape()

The shape of the array of parameters.

This does not include the dimension of the folded parameters.

as_dict()

Return a dictionary of attributes describing the pattern.

The dictionary should completely describe the pattern in the sense that if the contents of two patterns' dictionaries are identical the patterns should be considered identical.

If the keys of the returned dictionary match the arguments to `__init__`, then the default methods for `to_json` and `from_json` will work with no additional modification.

empty (*valid*)

Return an empty parameter in its folded shape.

Parameters

valid [*bool*] Whether or folded shape should be filled with valid values.

Returns

folded_val [Folded value] A parameter value in its original folded shape.

flat_indices (*folded_bool*, *free=None*)

Get which flattened indices correspond to which folded values.

Parameters

folded_bool [Folded booleans] A variable in the folded shape but containing booleans. The elements that are `True` are the ones for which we will return the flat indices.

free [*bool*] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

Returns

indices [*numpy.ndarray* (*N*,)] A list of indices into the flattened value corresponding to the `True` members of `folded_bool`.

flat_length (*free=None*)

Return the length of the pattern's flattened value.

Parameters

free [*bool*, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, `free_default` is used.

Returns

length [*int*] The length of the pattern's flattened value.

flatten (*folded_val*, *free=None*, *validate_value=None*)

Flatten a folded value into a flat vector.

Parameters

folded_val [Folded value] The parameter in its original folded shape.

free [*bool*, optional] Whether or not the flattened value is to be in a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [*bool*] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

flat_val [*numpy.ndarray*, (*N*,)] The flattened value.

fold (*flat_val*, *free=None*, *validate_value=None*)

Fold a flat value into a parameter.

Parameters

flat_val [*numpy.ndarray*, (*N*,)] The flattened value.

free [*bool*, optional.] Whether or not the flattened value is a free parameterization. If not specified, the attribute `free_default` is used.

validate_value [*bool*, optional.] Whether to check that the folded value is valid. If `None`, the pattern will employ a default behavior.

Returns

folded_val [Folded value] The parameter value in its original folded shape.

freeing_jacobian (*folded_val*, *sparse=True*)

The Jacobian of the map from a flat free value to a flat value.

If the folded value of the parameter is `val`, `val_flat = flatten(val, free=False)`, and `val_freeflat = flatten(val, free=True)`, then this calculates the Jacobian matrix $d \text{val_free} / d \text{val_freeflat}$. For entries with no dependence between them, the Jacobian is taken to be zero.

Parameters

folded_val [Folded value] The folded value at which the Jacobian is to be evaluated.

sparse [*bool*, optional] Whether to return a sparse or a dense matrix.

Returns

“numpy.ndarray”, (*N*, *M*) The Jacobian matrix $d \text{val_free} / d \text{val_freeflat}$.

Consistent with standard Jacobian notation, the elements of `val_free` correspond to the rows of the Jacobian matrix and the elements of `val_freeflat` correspond to the columns.

See also:

`Pattern.unfreeing_jacobian`

classmethod from_json (*json_string*)

Return a pattern from `json_string` created by `to_json`.

See also:

`Pattern.to_json`

shape()

The shape of a folded value.

unfreeing_jacobian (*folded_val*, *sparse=True*)

The Jacobian of the map from a flat value to a flat free value.

If the folded value of the parameter is `val`, `val_flat = flatten(val, free=False)`, and `val_freeflat = flatten(val, free=True)`, then this calculates the Jacobian matrix $d \text{val_freeflat} / d \text{val_free}$. For entries with no dependence between them, the Jacobian is taken to be zero.

Parameters

folded_val [Folded value] The folded value at which the Jacobian is to be evaluated.

sparse [*bool*, optional] If `True`, return a sparse matrix. Otherwise, return a dense numpy 2d array.

Returns

“numpy.ndarray”, (*N*, *N*) The Jacobian matrix $d \text{val_freeflat} / d \text{val_free}$.

Consistent with standard Jacobian notation, the elements of `val_freeflat` correspond

to the rows of the Jacobian matrix and the elements of `val_free` correspond to the columns.

See also:

`Pattern.freeing_jacobian`

validate_folded (`folded_val, validate_value=None`)

Check whether a folded value is valid.

Parameters

folded_val [Folded value] A parameter value in its original folded shape.

validate_value [bool] Whether to validate the value in addition to the shape. The shape is always validated.

Returns

is_valid [bool] Whether `folded_val` is an allowable shape and value.

err_msg [str]

3.4 Function Wrappers

3.4.1 Flattening and folding the input and outputs of a function

```
class paragami.function_patterns.TransformFunctionInput(original_fun,      patterns,
                                                       free,          original_is_flat,
                                                       argnums=None)
```

Convert a function of folded (or flattened) values into one that takes flattened (or folded) values.

Examples

```
mat_pattern = paragami.PSDSymmetricMatrixPattern(3)

def fun(offset, mat, kwoffset=3):
    return np.linalg.slogdet(mat + offset + kwoffset)[1]

flattened_fun = paragami.TransformFunctionInput(
    original_fun=fun, patterns=mat_pattern,
    free=True, argnums=1, original_is_flat=False)

# pd_mat is a matrix:
pd_mat = np.eye(3) + np.full((3, 3), 0.1)

# pd_mat_flat is an unconstrained vector:
pd_mat_flat = mat_pattern.flatten(pd_mat, free=True)

# These two functions return the same value:
print('Original: {}'.format(
    fun(2, pd_mat, kwoffset=3)))
print('Flat: {}'.format(
    flattened_fun(2, pd_mat_flat, kwoffset=3)))
```

__init__ (`original_fun, patterns, free, original_is_flat, argnums=None`)

Parameters

original_fun: callable A function that takes one or more values as input.

patterns: ‘paragami.Pattern’ or list of ‘paragami.PatternPattern’ A single pattern or array of patterns describing the input to *original_fun*.

free: ‘bool’ or list of ‘bool’ Whether or not the corresponding elements of *patterns* should use free or non-free flattened values.

original_is_flat: ‘bool’ If *True*, convert *original_fun* from taking flat arguments to one taking folded arguments. If *False*, convert *original_fun* from taking folded arguments to one taking flat arguments.

argnums: ‘int’ or list of ‘int’ The 0-indexed locations of the corresponding pattern in *patterns* in the order of the arguments fo *original_fun*.

```
class paragami.function_patterns.FlattenFunctionInput (original_fun, patterns, free,  
 argnums=None)
```

A convenience wrapper of *paragami.TransformFunctionInput*.

See also:

`paragami.TransformFunctionInput`
`__init__` (*original_fun*, *patterns*, *free*, *argnums=None*)

Parameters

original_fun: callable A function that takes one or more values as input.

patterns: ‘paragami.Pattern’ or list of ‘paragami.PatternPattern’ A single pattern or array of patterns describing the input to *original_fun*.

free: ‘bool’ or list of ‘bool’ Whether or not the corresponding elements of *patterns* should use free or non-free flattened values.

original_is_flat: ‘bool’ If *True*, convert *original_fun* from taking flat arguments to one taking folded arguments. If *False*, convert *original_fun* from taking folded arguments to one taking flat arguments.

argnums: ‘int’ or list of ‘int’ The 0-indexed locations of the corresponding pattern in *patterns* in the order of the arguments fo *original_fun*.

```
class paragami.function_patterns.FoldFunctionInput (original_fun, patterns, free,  
 argnums=None)
```

A convenience wrapper of *paragami.TransformFunctionInput*.

See also:

`paragami.TransformFunctionInput`
`__init__` (*original_fun*, *patterns*, *free*, *argnums=None*)

Parameters

original_fun: callable A function that takes one or more values as input.

patterns: ‘paragami.Pattern’ or list of ‘paragami.PatternPattern’ A single pattern or array of patterns describing the input to *original_fun*.

free: ‘bool’ or list of ‘bool’ Whether or not the corresponding elements of *patterns* should use free or non-free flattened values.

original_is_flat: ‘bool’ If *True*, convert *original_fun* from taking flat arguments to one taking folded arguments. If *False*, convert *original_fun* from taking folded arguments to one taking flat arguments.

argnums: ‘int’ or list of ‘int’ The 0-indexed locations of the corresponding pattern in *patterns* in the order of the arguments to *original_fun*.

class paragami.function_patterns.**FlattenFunctionOutput** (*original_fun*, *patterns*, *free*, *retnums=None*)

A convenience wrapper of *paragami.TransformFunctionOutput*.

See also:

paragami.TransformFunctionOutput

__init__ (*original_fun*, *patterns*, *free*, *retnums=None*)

Parameters

original_fun: callable A function that returns one or more values.

patterns: ‘paragami.Pattern’ or list of ‘paragami.PatternPattern’ A single pattern or array of patterns describing the return value of *original_fun*.

free: ‘bool’ or list of ‘bool’ Whether or not the corresponding elements of *patterns* should use free or non-free flattened values.

original_is_flat: ‘bool’ If *True*, convert *original_fun* from returning flat values to one returning folded values. If *False*, convert *original_fun* from returning folded values to one returning flat values.

retnums: ‘int’ or list of ‘int’ The 0-indexed locations of the corresponding pattern in *patterns* in the order of the return values of *original_fun*.

class paragami.function_patterns.**FoldFunctionOutput** (*original_fun*, *patterns*, *free*, *retnums=None*)

A convenience wrapper of *paragami.TransformFunctionOutput*.

See also:

paragami.TransformFunctionOutput

__init__ (*original_fun*, *patterns*, *free*, *retnums=None*)

Parameters

original_fun: callable A function that returns one or more values.

patterns: ‘paragami.Pattern’ or list of ‘paragami.PatternPattern’ A single pattern or array of patterns describing the return value of *original_fun*.

free: ‘bool’ or list of ‘bool’ Whether or not the corresponding elements of *patterns* should use free or non-free flattened values.

original_is_flat: ‘bool’ If *True*, convert *original_fun* from returning flat values to one returning folded values. If *False*, convert *original_fun* from returning folded values to one returning flat values.

retnums: ‘int’ or list of ‘int’ The 0-indexed locations of the corresponding pattern in *patterns* in the order of the return values of *original_fun*.

class paragami.function_patterns.**FoldFunctionInputAndOutput** (*original_fun*, *input_patterns*, *input_free*, *input_argnums*, *output_patterns*, *output_free*, *output_retnums=None*)

A convenience wrapper of *paragami.FoldFunctionInput* and *paragami.FoldFunctionOutput*.

See also:

`paragami.FoldFunctionInput`, `paragami.FoldFunctionOutput`

`__init__(original_fun, input_patterns, input_free, input_argnums, output_patterns, output_free, output_renums=None)`

Initialize self. See help(type(self)) for accurate signature.

A convenience wrapper of `paragami.FlattenFunctionInput` and `paragami.FlattenFunctionOutput`.

See also:

`paragami.FlattenFunctionInput`, `paragami.FlattenFunctionOutput`

`__init__(original_fun, input_patterns, input_free, input_argnums, output_patterns, output_free, output_renums=None)`

Initialize self. See help(type(self)) for accurate signature.

3.4.2 Preconditioning an objective function

```
class paragami.optimization_lib.PreconditionedFunction(original_fun, precondi-  
  tioner=None, precondi-  
  tioner_inv=None)
```

Get a function whose input has been preconditioned.

Throughout, the subscript $_c$ will denote quantities or functions in the preconditioned space. For example, x will refer to a variable in the original space and x_c to the same variable after preconditioning.

Preconditioning means transforming $x \rightarrow x_c = A^{-1}x$, where the matrix A is the “preconditioner”. If f operates on x , then the preconditioned function operates on x_c and is defined by $f_c(x_c) := f(Ax_c) = f(x)$. Gradients of the preconditioned function are defined with respect to its argument in the preconditioned space, e.g., $f'_c = \frac{df_c}{dx_c}$.

A typical value of the preconditioner is an inverse square root of the Hessian of f , because then the Hessian of f_C is the identity when the gradient is zero. This can help speed up the convergence of optimization algorithms.

Methods

set_preconditioner:	Set the preconditioner to a specified value.
set_preconditioner_with_hessian:	Set the preconditioner based on the Hessian of the objective at a point in the original domain.
get_preconditioner:	Return a copy of the current preconditioner.
get_preconditioner_inv:	Return a copy of the current inverse preconditioner.
precondition:	Convert from the original domain to the preconditioned domain.
unprecondition:	Convert from the preconditioned domain to the original domain.

`__init__(original_fun, preconditioner=None, preconditioner_inv=None)`

Parameters

original_fun: callable function of a single argument

preconditioner: The initial preconditioner.

preconditioner_inv: The inverse of the initial preconditioner.

precondition(*x*)

Multiply by the inverse of the preconditioner to convert *x* in the original domain to x_c in the preconditioned domain.

This function is provided for convenience, but it is more numerically stable to use `np.linalg.solve(preconditioner, x)`.

set_preconditioner_with_hessian(*x=None, hessian=None, ev_min=None, ev_max=None*)

Set the preconditioner to the inverse square root of the Hessian of the original objective (or an approximation thereof).

Parameters

x: Numeric vector The point at which to evaluate the Hessian of `original_fun`. If *x* is specified, the Hessian is evaluated with automatic differentiation. Specify either *x* or *hessian* but not both.

hessian: Numeric matrix The hessian of `original_fun` or an approximation of it. Specify either *x* or *hessian* but not both.

ev_min: float If not None, set eigenvalue of *hessian* that are less than *ev_min* to *ev_min* before taking the square root.

ev_maxs: float If not None, set eigenvalue of *hessian* that are greater than *ev_max* to *ev_max* before taking the square root.

Returns

Sets the preconditioner for the class and returns the Hessian with the eigenvalues thresholded by “*ev_min*“ and “*ev_max*“.

unprecondition(*x_c*)

Multiply by the preconditioner to convert x_c in the preconditioned domain to *x* in the original domain.

3.4.3 An optimization objective class

class `paragami.optimization_lib.OptimizationObjective`(*objective_fun, print_every=1, log_every=0*)

Derivatives and logging for an optimization objective function.

Attributes

optimization_log: Dictionary A record of the optimization progress as recorded by `log_value`.

Methods

f:	The objective function with logging.
grad:	The gradient of the objective function.
hessian:	The Hessian of the objective function.
hessian_vector_product:	The Hessian vector product of the objective function.
set_print_every:	Set how often to display optimization progress.
set_log_every:	Set how often to log optimization progress.
reset_iteration_count:	Reset the number of iterations for the purpose of printing and logging.
reset_log:	Clear the log.
reset:	Run <code>reset_iteration_count</code> and <code>reset_log</code> .
print_value:	Display a function evaluation.
log_value:	Log a function evaluation.

__init__ (*objective_fun*, *print_every*=1, *log_every*=0)

Parameters

obj_fun: Callable function of one argument The function to be minimized.

print_every: integer Print the optimization value every *print_every* iterations.

log_every: integer Log the optimization value every *log_every* iterations.

log_value (*num_f_evals*, *x*, *f_val*)

Log the optimization progress. To create a custom log, overload this function. By default, the log is a list of tuples (*iteration*, *x*, *f(x)*).

Parameters

num_f_vals: Integer The total number of function evaluations.

x: The current argument to the objective function.

f_val: The value of the objective at *x*.

num_iterations()

Return the number of times the optimization function has been called, not counting any derivative evaluations.

print_value (*num_f_evals*, *x*, *f_val*)

Display the optimization progress. To display a custom update, overload this function.

Parameters

num_f_vals: Integer The total number of function evaluations.

x: The current argument to the objective function.

f_val: The value of the objective at *x*.

reset()

Reset the iteration count and clear the log.

set_log_every (*n*)

Parameters

n: integer Log the objective function value every *n* iterations. If 0, do not log.

set_print_every (*n*)

Parameters

n: integer Print the objective function value every n iterations. If 0, do not print any output.

3.5 Sensitivity Functions

Warning: These functions are deprecated. Please use the vittles package instead.

3.6 Writing and reading patterns and values from disk

3.6.1 Saving Folded Values with Patterns

Flattening makes it easy to save and load structured data to and from disk.

```
pattern = paragami.PatternDict()
pattern['num'] = paragami.NumericArrayPattern((1, 2))
pattern['mat'] = paragami.PSDSymmetricMatrixPattern(5)

val_folded = pattern.random()
extra = np.random.random(5)

outfile = tempfile.NamedTemporaryFile()
outfile_name = outfile.name
outfile.close()

paragami.save_folded(outfile_name, val_folded, pattern, extra=extra)

val_folded_loaded, pattern_loaded, data = \
    paragami.load_folded(outfile_name + '.npz')

# The loaded values match the saved values.
assert pattern == pattern_loaded
assert np.all(val_folded['num'] == val_folded_loaded['num'])
assert np.all(val_folded['mat'] == val_folded_loaded['mat'])
assert np.all(data['extra'] == extra)
```

paragami.pattern_containers.**save_folded**(file, folded_val, pattern, **argk)

Save a folded value to a file with its pattern.

Flatten a folded value and save it with its pattern to a file using numpy . savez . Additional keyword arguments will also be saved to the file.

Parameters

file: String or file Follows the conventions of numpy . savez . Note that the npz extension will be added if it is not present.

folded_val: The folded value of a parameter.

pattern: A paragami pattern for the folded value.

paragami.pattern_containers.**load_folded**(file)

Load a folded value and its pattern from a file together with any additional data.

Note that pattern must be registered with register_pattern_json to use load_folded .

Parameters

file: String or file A file or filename of data saved with `save_folded`.

Returns

folded_val: The folded value of the saved parameter.

pattern: The paragami pattern of the saved parameter.

data: The data as returned from `np.load`. Additional saved values will exist as keys of `data`.

3.6.2 Saving patterns

You can convert a particular pattern class to and from JSON using the `to_json` and `from_json` methods.

```
>>> pattern = paragami.NumericArrayPattern(shape=(2, 3))
>>>
>>> # ``pattern_json_string`` is a JSON string that can be written to a file.
>>> pattern_json_string = pattern.to_json()
>>>
>>> # ``same_pattern`` is identical to ``pattern``.
>>> same_pattern = paragami.NumericArrayPattern.from_json(pattern_json_string)
```

However, in order to use `from_json`, you need to know which pattern the JSON string was generated from. In order to decode generic JSON strings, one can use `get_pattern_from_json`.

```
>>> pattern_json_string = pattern.to_json()
>>> # ``same_pattern`` is identical to ``pattern``.
>>> same_pattern = paragami.get_pattern_from_json(pattern_json_string)
```

Before a pattern can be used with `get_pattern_from_json`, it needs to be registered with `register_pattern_json`. All the patterns in paragami are automatically registered, but if you define your own patterns they will have to be registered before they can be used with `get_pattern_from_json`.

`paragami.pattern_containers.get_pattern_from_json(pattern_json)`

Return the appropriate pattern from `pattern_json`.

The pattern must have been registered using `register_pattern_json`.

Parameters

pattern_json: String A JSON string as created with a pattern's `to_json` method.

Returns

The pattern instance encoded in the “`pattern_json`“ string.

`paragami.pattern_containers.register_pattern_json(pattern, allow_overwrite=False)`

Register a pattern for automatic conversion from JSON.

Parameters

pattern: A Pattern class The pattern to register.

allow_overwrite: Boolean If true, allow overwriting already-registered patterns.

Examples

```
>>> class MyCustomPattern(paragami.Pattern):
>>>     ... definitions ...
>>>
>>> paragami.register_pattern_json(paragmi.MyCustomPattern)
>>>
>>> my_pattern = MyCustomPattern(...)
>>> my_pattern_json = my_pattern.to_json()
>>>
>>> # ``my_pattern_from_json`` should be identical to ``my_pattern``.
>>> my_pattern_from_json = paragami.get_pattern_from_json(my_pattern_json)
```

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