A Python package for simulating Gaussian random fields

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We introduce the python package `GaussRF`, a package concerned primarily with simulating Gaussian random fields. The package implements two sampling methods, one exact and one approximate, on rectangular domains in one- and two dimensions. The approximate method is the Karhunen-Loéve expansion and the exact sampling procedure is the circulant embedding method. In section 1 we outline the key functions in the package and their use. In section 2, we give some examples

1 Package overview

The package simulates random fields via the Karhunen-Loève expansion through two primary classes. The first class is `GaussF_KL1D`, which simulates Gaussian processes. Input parameters are the expansion order `N`, the number of points `M`, the Covaraince function `Cov`, a method `method`, and a sample size `samples`. The method defaults to `"KL_EOLE"`, utilising the KL expansion with EOLE weights, and `samples = 1` so that only one realization is returned. The random field object is then acted on by its various methods to do various things, such as produce its values as an array or produce the grid of points used in the simulation. For example, Brownian motion is simulated and then outputted as an array using the method `Gfield()`:

```
# Define Brownian motion
def Bm_cov(s, t):
    return np.minimum(s, t)
# Generate a Brownian motion simulation object

X_sim = GaussF_KL1D(N = 20, M = 100, a = 0., b = 1.,
                 Cov = Bm_cov, method = "KL_EOLE", samples = 1)

# Get the Brownian motion simulation as an array
X = X_sim.Gfield()
```

Or, omitting explicit references to the argument variables

```
def Bm_cov(s, t):
    return np.minimum(s, t)
X_sim = GaussF_KL1D(20, 100, 0., 1., Bm_cov)
X = X_sim.Gfield()
t = X_sim.grid()
```

2 examples

Here we present some examples of random fields calculated using `GaussRF`. The examples include convergence tests with random fields whose Karhunen-Loève expansions are known analytically, and realisations of other random fields.

2.1 Convergence of the Nyström method

As a first example, we test the convergence of the Karhunen-Loéve expansion. For a random field $H(\boldsymbol{x}, \omega)$, approximated by the truncated series $\hat{H}(\boldsymbol{x}, \omega)$, the error measure[1] is

$$\varepsilon(\boldsymbol{x}) = \frac{\mathrm{Var}\left(H(\boldsymbol{x}, \omega) - \hat{H}(\boldsymbol{x}, \omega)\right)}{\mathrm{Var}(H(\boldsymbol{x}, \omega))}. \tag{1}$$

Since a Gaussian RF is determined by its covariance and mean, and we are presuming the mean has been removed, this error should converge pointwise as the approximation $\hat{H}$ becomes better. A global measure of the error variance is

$$\varepsilon = \int_{\Omega} \varepsilon(\boldsymbol{x})\, dV \tag{2}$$

If the variance of the function is a constant, the global square integrated error variance is

$$\varepsilon = 1 - \frac{1}{\Omega \sigma^2} \sum_{i=1}^{N} \lambda_i \tag{3}$$

For $d = 1, 2$, consider the Gaussian RF on the domain $D = [0, 1]^d$ with covariance function

$$\exp\left(-||\boldsymbol{x} - \boldsymbol{y}||_1\right). \tag{4}$$

This is one of the rare cases where the eigenvalues and eigenfunctions of the Karhunen-Loève expansion are known analytically [**?**]. In one dimension, the eigenvalues are

$$\lambda_k = \frac{2}{w_k^2 + 1}, \tag{5}$$

where w_k are the positive, increasing roots of the function

$$f(w) = (w^2 - 1)\tan w - 2w. \tag{6}$$

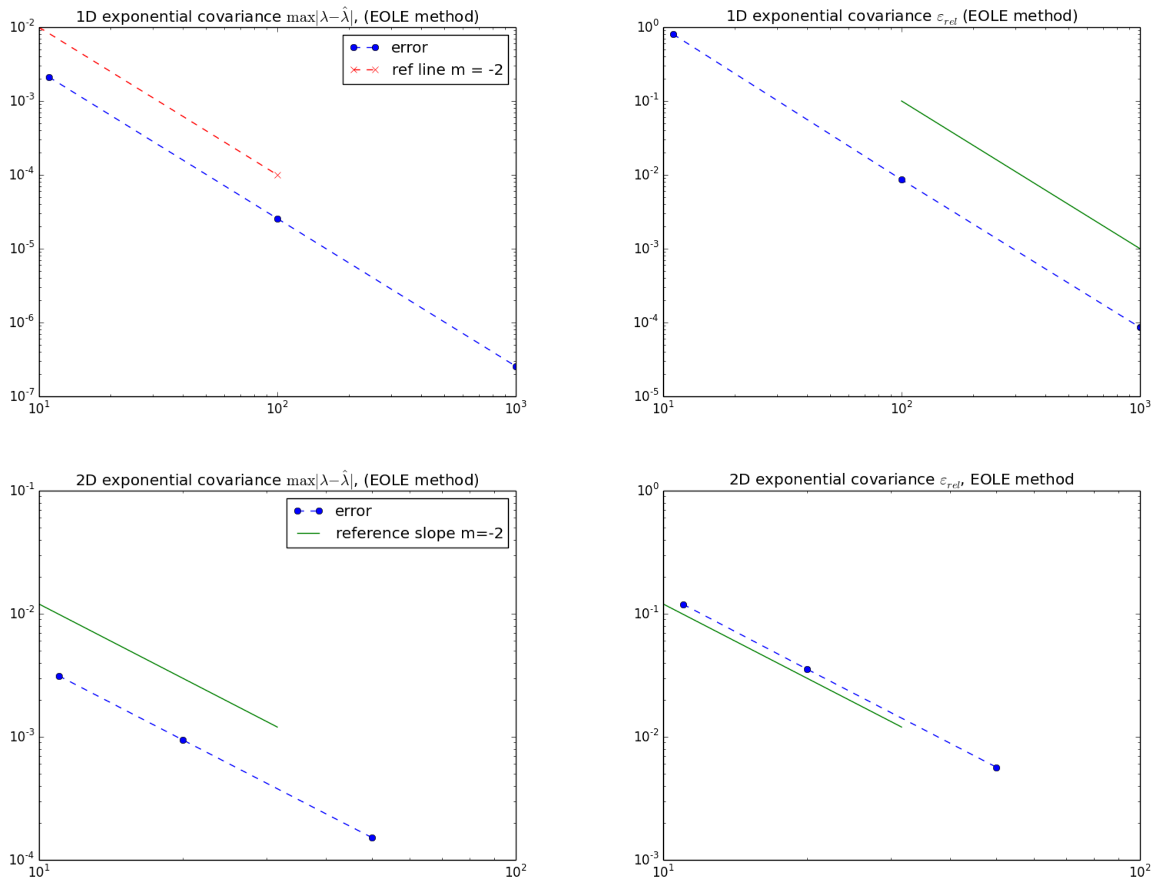

Figure 1: Top row: the maximum difference between the exact and numerical eigenvalues for the 1D exponential covariance on $[0, 1]$ (left) and the relative error variance between the approximate and exact truncated KL expansion (right). Bottom row: Similar to the top row, but in 2D rectangle $[0, 1]^2$.

In two dimensions, the eigenvalues and eigenfunctions are the simple tensor product of one-dimensional problem's spectral quantities. Thus the eigenvalues in two-dimensions can be indexed as

$$\lambda_{k_1\,k_2} = \lambda_{k_1}\lambda_{k_2} \tag{7}$$

for λ_{k_i} the k_ith eigenvalue of the one-dimensional exponential covariance. Using `GaussRF`, we can return the eigenvalues and -vectors from a simulation object using the method `eigens()`, and proceed to test convergence over a range of grid points. Supposing that we have an array `w_roots` of the roots $f(w)$, by using Newton's method for example, then a script for testing convergence would look like:

```
# 1- Dimensional convergence
def exp_cov(x, y):
    return np.exp(-np.abs(x - y))
N = 10
M_vals = [11, 100, 100] # 11 because M > N and N = 10
L_ref = 2. / ( 1 + w_roots**2)
errors = []
rel_evar = np.zeros(len(M_vals))
counter = 0
a, b = 0., 1.
err_var_ref = 1 - np.sum(L_ref) / (b - a)
for M in M_vals:
    phi, L = GaussF_KL1D(N, M, a, b, exp_cov).eigens()
    err_var_comp = 1 - np.sum(L_comp) / (b - a)
    rel_evar[counter] = np.abs( evar_comp - evar_ref) / evar_ref
    error.append(np.abs(L_ref - L_comp).max())
    counter += 1
```

Figure 1 shows log-log plots of the maximum eigenvalue error

$$\max|\lambda - \hat{\lambda}| \tag{8}$$

and the relative error variance, defined by

$$\varepsilon_{\text{rel}} = \frac{|\varepsilon - \varepsilon_{\text{ref}}|}{\varepsilon_{\text{ref}}}, \tag{9}$$

where ε_{ref} is (3) as calculated using the exact eigenvalues (5) and (7), against the mesh size h. The plots suggest that the convergence of the numerically computed eigenvalues $\hat{\lambda}$ is quadratic in the mesh size, i.e

$$\max|\lambda - \hat{\lambda}| \leq Ch^2 \tag{10}$$

where h is the mesh size. This quadratic convergence is consistent with [6], giving us confidence that the implemented Nyström method works.

2.2 2D exponential covariance

2.3 2D anisotropic field

References

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