TUM-DI-LAB Documentation

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SIMPLE EXAMPLE OF A GAUSSIAN PROCESS

The following example illustrates how we move from process to distribution and also shows that the Gaussian process defines a distribution over functions.

$f \sim \mathcal{GP}(m, k)$

$m(x) = \frac{x^2}{4}$

$k(x, x') = exp(-\frac{1}{2}(x - x')^2)$

$y = f + \epsilon$

$\epsilon \sim \mathcal{N}(0, \sigma^2)$

```
import numpy as np
import scipy as sp
import matplotlib.pyplot as plt
```

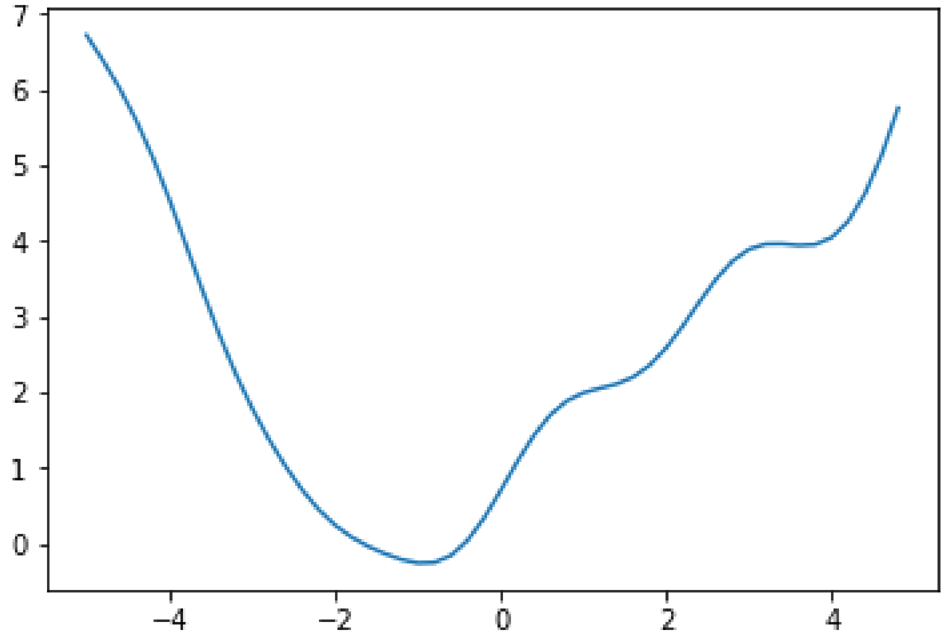
```
x = np.arange(-5,5,0.2)
n = x.size
s = 1e-9
```

```
m = np.square(x) * 0.25
```

```
a = np.repeat(x, n).reshape(n, n)
k = np.exp(-0.5*np.square(a - a.transpose())) + s*np.identity(n)
```

```
r = np.random.multivariate_normal(m, k, 1)
y = np.reshape(r, n)
```

```
plt.plot(x,y)
plt.show()
```


7
6
5
4
3
2
1
0
−4
−2
0
2
4

CHAPTER

FOUR

PARAMETER ESTIMATION FOR A LINEAR OPERATOR USING GAUSSIAN PROCESSES

Assumptions about the linear operator:

$\mathcal{L}_x^{\phi} u(x) = f(x)$

$u(x) \sim \mathcal{GP}(0, k_{uu}(x, x', \theta))$

$f(x) \sim \mathcal{GP}(0, k_{ff}(x, x', \theta, \phi))$

$y_u = u(X_u) + \epsilon_u; \epsilon_u \sim \mathcal{N}(0, \sigma_u^2 I)$

$y_f = f(X_f) + \epsilon_f; \epsilon_f \sim \mathcal{N}(0, \sigma_f^2 I)$

Taking a simple operator as example:

$\mathcal{L}_x^{\phi} := \phi \cdot + \frac{d}{dx} \cdot$

$u(x) = sin(x)$

$f(x) = \phi sin(x) + cos(x)$

Problem at hand:

Given $\{X_u, y_u\}$ and $\{X_f, y_f\}$, estimate ϕ.

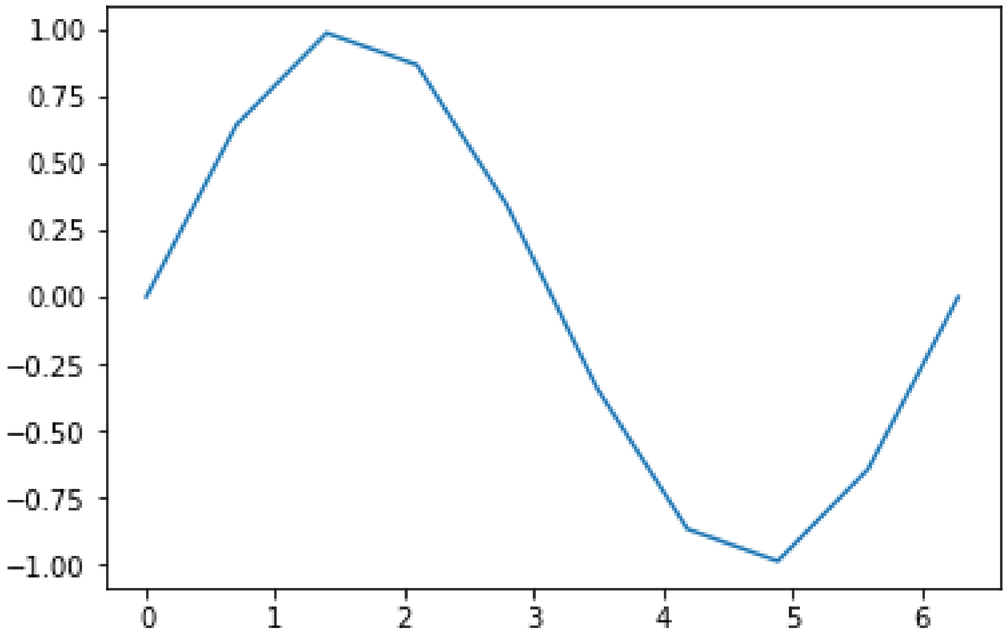
4.1 step 1: simulate data

Use $\phi = 2$

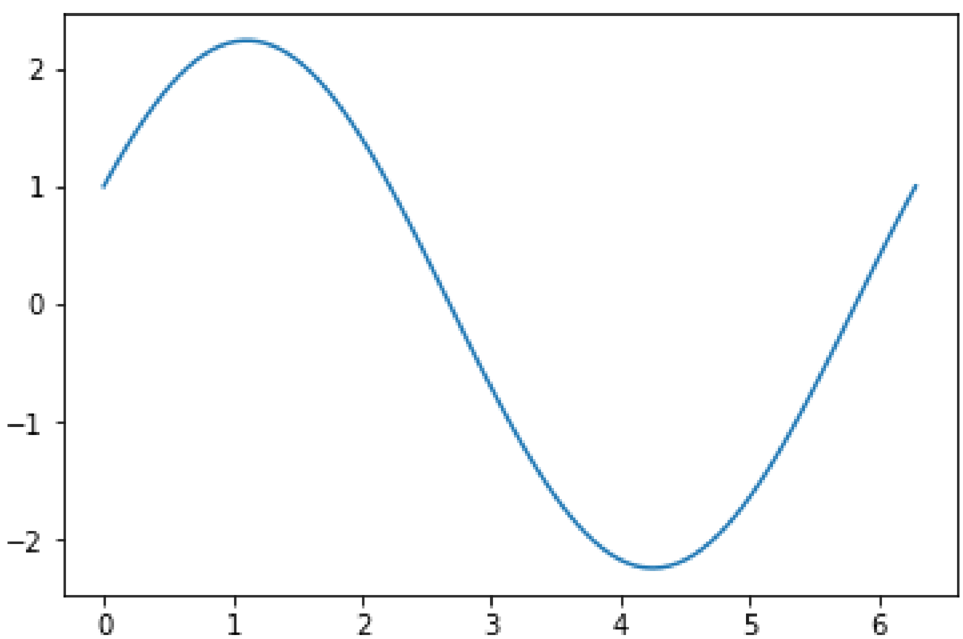
```
import numpy as np
import sympy as sp
from scipy.optimize import minimize
import matplotlib.pyplot as plt
```

```
x_u = np.linspace(0,2*np.pi,10)
y_u = np.sin(x_u)
x_f = np.linspace(0,2*np.pi, 10)
y_f = 2.0*np.sin(x_f) + np.cos(x_f)
```

```
plt.plot(x_u,y_u)
plt.show()
```




```
x1 = np.linspace(0,2*np.pi,100)
y1 = 2.0*np.sin(x1) + np.cos(x1)
plt.plot(x1,y1)
plt.show()
```



4.2 step 2: create covariance matrix

This step uses information about $\mathcal{L}_x^\phi$ but not about $u(x)$ or $f(x)$.

$k_{uu}(x_i, x_j; \theta) = \theta exp(-\frac{1}{2}(x_i - x_j)^2)$

```
x_i, x_j, theta, phi = sp.symbols('x_i x_j theta phi')
kuu_sym = theta*sp.exp(-1/(2)*((x_i - x_j)**2))
kuu_fn = sp.lambdify((x_i, x_j, theta), kuu_sym, "numpy")
def kuu(x, theta):
    k = np.zeros((x.size, x.size))
    for i in range(x.size):
        for j in range(x.size):
            k[i,j] = kuu_fn(x[i], x[j], theta)
    return k
```

$k_{ff}(x_i,x_j;:raw-latex:*theta*,:raw-latex:*phi*) \ = **:raw-latex:‘\mathcal{L}‘***{x_i}^:raw-latex:‘phi ‘:raw-latex:‘mathcal{L}‘*{x_j}^:raw-latex:*phi ‘k_{uu}(x_i, x_j; :raw-latex:*theta‘) \ = **:raw-latex:‘\mathcal{L}‘***{x_i}^:raw-latex:‘phi ‘:raw-latex:‘left‘(:raw-latex:‘phi ‘k*{uu} + **:raw-latex:‘\frac{\partial}{\partial x_j}‘k_{uu} :raw-latex:‘**right‘) \ = **:raw-latex:‘\phi‘^2 k_{uu} + :raw-latex:‘**phi *:raw-latex:*frac{partial}{partial x_j}‘k_{uu} + **:raw-latex:‘\phi ‘:raw-latex:‘**frac{partial}{partial x_i}‘k_{uu} + **:raw-latex:‘\frac{\partial}{\partial x_i}‘**:raw-latex:**‘**frac{partial}{partial x_j}‘k_{uu}\ $

More explicit calculations follow:

$$
\begin{aligned}
&= \mathcal{L}_{x_i}^{\phi} \mathcal{L}_{x_j}^{\phi} \left(\theta exp(-\tfrac{1}{2}(x_i - x_j)^2)\right] \\
&= \mathcal{L}_{x_i}^{\phi} \left[\theta exp(-\tfrac{1}{2}(x_i - x_j)^2) \left(\phi + (-\tfrac{1}{2})2(x_i - x_j)(-1)\right)\right] \\
&= \mathcal{L}_{x_i}^{\phi} \left[\theta exp(-\tfrac{1}{2}(x_i - x_j)^2)(\phi + x_i - x_j)\right] \\
&= \phi\theta exp(-\tfrac{1}{2}(x_i - x_j)^2)(\phi + x_i - x_j) + \theta exp(-\tfrac{1}{2}(x_i - x_j)^2) \left[-\tfrac{1}{2}2(x_i - x_j)(\phi + x_i - x_j) + 1\right] \\
&= \theta exp(-\tfrac{1}{2}(x_i - x_j)^2) \left[\phi^2 - (x_i - x_j)^2 + 1\right]
\end{aligned}
$$

```
kff_sym = phi**2*kuu_sym + phi*sp.diff(kuu_sym, x_j) + phi*sp.diff(kuu_sym, x_i) + sp.
↪diff(kuu_sym, x_j, x_i)
kff_fn = sp.lambdify((x_i, x_j, theta, phi), kff_sym, "numpy")
def kff(x, theta, phi):
    k = np.zeros((x.size, x.size))
    for i in range(x.size):
        for j in range(x.size):
            k[i,j] = kff_fn(x[i], x[j], theta, phi)
    return k
```

$$
\begin{aligned}
&k_{fu}(x_i, x_j; \theta, \phi) \\
&= \mathcal{L}_{x_i}^{\phi} k_{uu}(x_i, x_j; \theta) \\
&= \phi k_{uu} + \tfrac{\partial}{\partial x_i} k_{uu} \\
&= \mathcal{L}_{x_i}^{\phi} \left[\theta exp(-\tfrac{1}{2}(x_i - x_j)^2)\right] \\
&= \theta exp(-\tfrac{1}{2}(x_i - x_j)^2) \left[(-\tfrac{1}{2})2(x_i - x_j) + \phi\right] \\
&= \theta exp(-\tfrac{1}{2}(x_i - x_j)^2)(\phi - x_i + x_j)
\end{aligned}
$$

```
kfu_sym = phi*kuu_sym + sp.diff(kuu_sym, x_i)
kfu_fn = sp.lambdify((x_i, x_j, theta, phi), kfu_sym, "numpy")
def kfu(x1, x2, theta, phi):
    k = np.zeros((x1.size, x2.size))
    for i in range(x1.size):
        for j in range(x2.size):
            k[i,j] = kfu_fn(x1[i], x2[j], theta, phi)
    return k
```

$$
\begin{aligned}
&k_{uf}(x_i, x_j; \theta, \phi) \\
&= \mathcal{L}_{x_j}^{\phi} k_{uu}(x_i, x_j; \theta) \\
&= \mathcal{L}_{x_j}^{\phi} \left[\theta exp(-\tfrac{1}{2}(x_i - x_j)^2)\right]
\end{aligned}
$$

$= \theta exp(-\frac{1}{2}(x_i - x_j)^2) \left[(-\frac{1}{2})2(x_i - x_j)(-1) + \phi\right]$
$= \theta exp(-\frac{1}{2}(x_i - x_j)^2)(\phi + x_i - x_j)$

```
def kuf(x1, x2, theta, phi):
    return kfu(x1,x2,theta,phi).T
```

4.3 step 3: define negative log marginal likelihood

$$K = \begin{bmatrix} k_{uu}(X_u, X_u; \theta) + \sigma_u^2 I & k_{uf}(X_u, X_f; \theta, \phi) \\ k_{fu}(X_f, X_u; \theta, \phi) & k_{ff}(X_f, X_f; \theta, \phi) + \sigma_f^2 I \end{bmatrix}$$

For simplicity, assume $\sigma_u = \sigma_f$.

$\mathcal{NLML} = \frac{1}{2}\left[log|K| + y^T K^{-1} y + N log(2\pi)\right]$

where $y = \begin{bmatrix} y_u \\ y_f \end{bmatrix}$

```
def nlml(params, x1, x2, y1, y2, s):
    K = np.block([
        [kuu(x1, params[0]) + s*np.identity(x1.size), kuf(x1, x2, params[0],␣
↪params[1])],
        [kfu(x1, x2, params[0], params[1]), kff(x2, params[0], params[1]) + s*np.
↪identity(x2.size)]
    ])
    y = np.concatenate((y1, y2))
    val = 0.5*(np.log(abs(np.linalg.det(K))) + np.mat(y) * np.linalg.inv(K) * np.
↪mat(y).T)
    return val.item(0)
```

```
nlml((1, 2), x_u, x_f, y_u, y_f, 1e-6)
```

```
-49.506869382523455
```

4.4 step 4: optimise hyperparameters

```
minimize(nlml, np.random.rand(2), args=(x_u, x_f, y_u, y_f, 1e-6), method="Nelder-Mead
↪")
```

```
final_simplex: (array([[0.2339862 , 2.00000114],
      [0.23400558, 2.00000344],
      [0.23389067, 2.00000342]]), array([-54.80042016, -54.80042014, -54.80042004]))
          fun: -54.80042016441411
      message: 'Optimization terminated successfully.'
         nfev: 98
          nit: 52
       status: 0
      success: True
            x: array([0.2339862 , 2.00000114])
```

4.4.1 Using pyGPs (Arthur's Idea)

```
import pyGPs
model_u = pyGPs.GPR()
model_u.setData(x_u, y_u)
model_u.optimize(x_u, y_u)

model_f = pyGPs.GPR()
model_f.setData(x_f, y_f)
model_f.optimize(x_f, y_f)
```

```
Number of line searches 14
Number of line searches 40
```

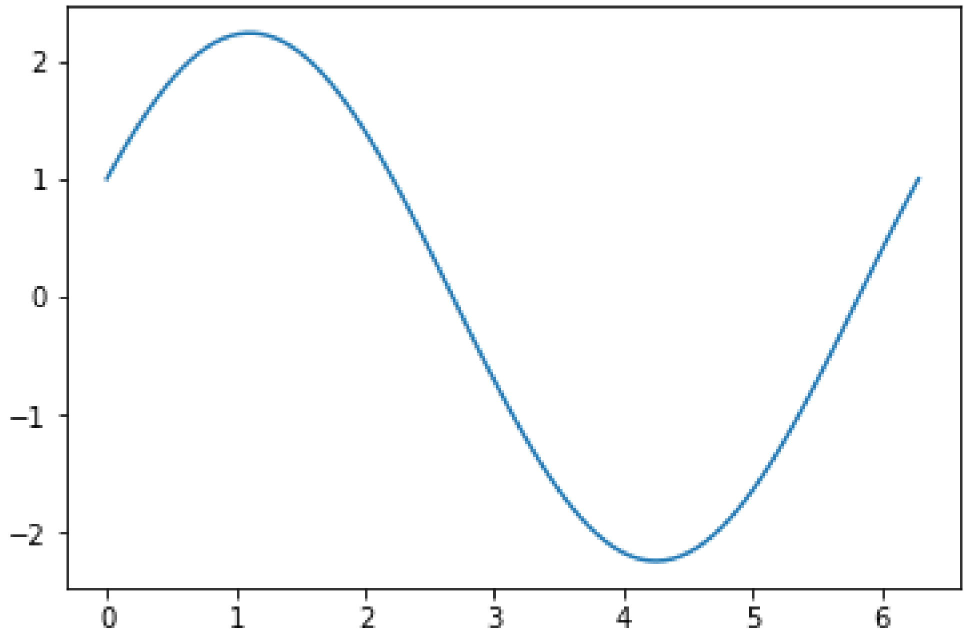
```
print(np.exp(model_f.covfunc.hyp))
print(np.exp(model_u.covfunc.hyp))
```

```
[3.01008812 7.20765418]
[3.05519677 3.43110287]
```

```
s_u = np.exp(model_u.covfunc.hyp[1])
l_u = np.exp(model_u.covfunc.hyp[0])
s_f = np.exp(model_f.covfunc.hyp[1])
phi = ((s_f/s_u)**2 - 1/l_u**2)**0.5
phi
```

```
2.075025301252897
```

```
x_p = np.linspace(0,2*np.pi,100)
y_p = model_f.predict(x_p)
# plot predictions
plt.plot(x_p,y_p[0])
plt.show()
```



Parameter estimation for PDEs

Limitations of available tools

Linear PDEs

Non-linear PDEs

PDEs without discretization

Results and Analysis

Conclusion