Kernel Guide

In this guide, we introduce the kernels available in GPJax and demonstrate how to create custom kernels.

```python
# Enable Float64 for more stable matrix inversions.
from jax import config
import jax.numpy as jnp
import jax.random as jr
from jaxtyping import (
    Array,
    Float,
    install_import_hook,
)
import matplotlib.pyplot as plt
import tensorflow_probability.substrates.jax as tfp

from examples.utils import use_mpl_style
from gpjax.kernels.computations import DenseKernelComputation
from gpjax.parameters import (
    DEFAULT_BIJECTION,
    PositiveReal,
    Static,
)

config.update("jax_enable_x64", True)


with install_import_hook("gpjax", "beartype.beartype"):
    import gpjax as gpx


tfb = tfp.bijectors

# set the default style for plotting
use_mpl_style()

key = jr.key(42)

cols = plt.rcParams["axes.prop_cycle"].by_key()["color"]
```

Supported Kernels

The following kernels are natively supported in GPJax.

- Matérn 1/2, 3/2 and 5/2.
- RBF (or squared exponential).
- Rational quadratic.
- Powered exponential.
- Polynomial.
- White noise
- Linear.
- Polynomial.
- Graph kernels.

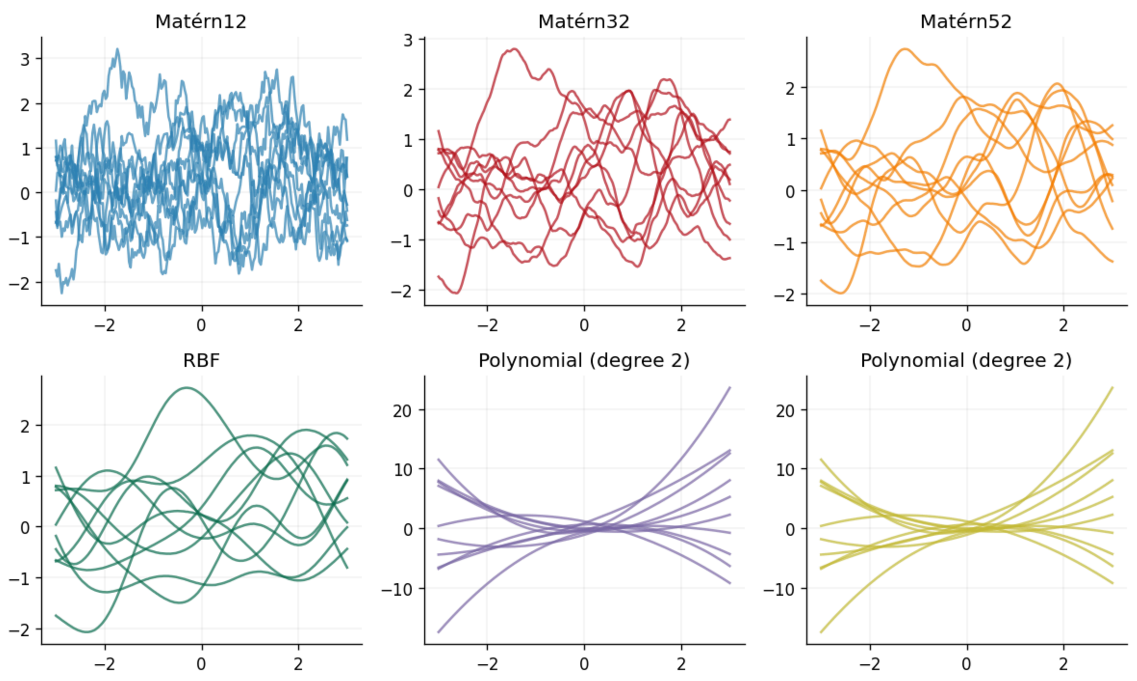
While the syntax is consistent, each kernel's type influences the characteristics of the sample paths drawn. We visualise this below with 10 function draws per kernel.

```
kernels = [
    gpx.kernels.Matern12(),
    gpx.kernels.Matern32(),
    gpx.kernels.Matern52(),
    gpx.kernels.RBF(),
    gpx.kernels.Polynomial(),
    gpx.kernels.Polynomial(degree=2),
]
fig, axes = plt.subplots(ncols=3, nrows=2, figsize=(10, 6),
tight_layout=True)

x = jnp.linspace(-3.0, 3.0, num=200).reshape(-1, 1)

meanf = gpx.mean_functions.Zero()

for k, ax, c in zip(kernels, axes.ravel(), cols, strict=False):
    prior = gpx.gps.Prior(mean_function=meanf, kernel=k)
    rv = prior(x)
    y = rv.sample(seed=key, sample_shape=(10,))
    ax.plot(x, y.T, alpha=0.7, color=c)
    ax.set_title(k.name)
```



Active dimensions

By default, kernels operate over every dimension of the supplied inputs. In some use cases, it is desirable to restrict kernels to specific dimensions of the input data. We can achieve this by the `active dims` argument, which determines which input index values the kernel evaluates.

To see this, consider the following 5-dimensional dataset for which we would like our RBF kernel to act on the first, second and fourth dimensions.

```
slice_kernel = gpx.kernels.RBF(active_dims=[0, 1, 3],
lengthscale=jnp.ones((3,)))
```

The resulting kernel has one length-scale parameter per input dimension --- an ARD kernel.

```
print(f"Lengthscales: {slice_kernel.lengthscale}")
```

```
Lengthscales:
 [38;2;79;201;177mPositiveReal [0m [38;2;255;213;3m( [0m [38;2;105;105;105m
# 3 (24 B) [0m
   [38;2;156;220;254mvalue [0m [38;2;212;212;212m= [0mArray([1., 1., 1.],
dtype=float64),

 [38;2;156;220;254m_tag [0m [38;2;212;212;212m= [0m [38;2;207;144;120m"'pos
```

```
itive'" [0m
 [38;2;255;213;3m) [0m
```

We'll now simulate some data and evaluate the kernel on the previously selected input dimensions.

```
# Inputs
x_matrix = jr.normal(key, shape=(50, 5))

# Compute the Gram matrix
K = slice_kernel.gram(x_matrix)
print(K.shape)
```

```
(50, 50)
```

Kernel combinations

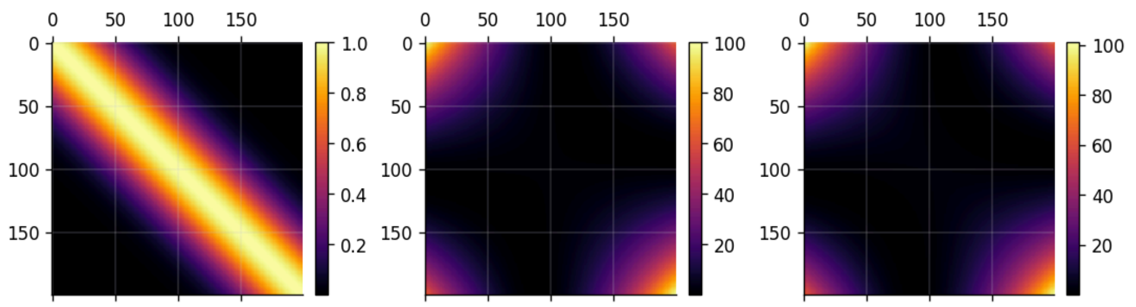
The product or sum of two positive definite matrices yields a positive definite matrix. Consequently, summing or multiplying sets of kernels is a valid operation that can give rich kernel functions. In GPJax, functionality for a sum kernel is provided by the `SumKernel` class.

```
k1 = gpx.kernels.RBF()
k2 = gpx.kernels.Polynomial()
sum_k = gpx.kernels.SumKernel(kernels=[k1, k2])

fig, ax = plt.subplots(ncols=3, figsize=(9, 3))
im0 = ax[0].matshow(k1.gram(x).to_dense())
im1 = ax[1].matshow(k2.gram(x).to_dense())
im2 = ax[2].matshow(sum_k.gram(x).to_dense())

fig.colorbar(im0, ax=ax[0], fraction=0.05)
fig.colorbar(im1, ax=ax[1], fraction=0.05)
fig.colorbar(im2, ax=ax[2], fraction=0.05)
```

```
<matplotlib.colorbar.Colorbar at 0x7f05e038bfd0>
```



Similarly, products of kernels can be created through the `ProductKernel` class.

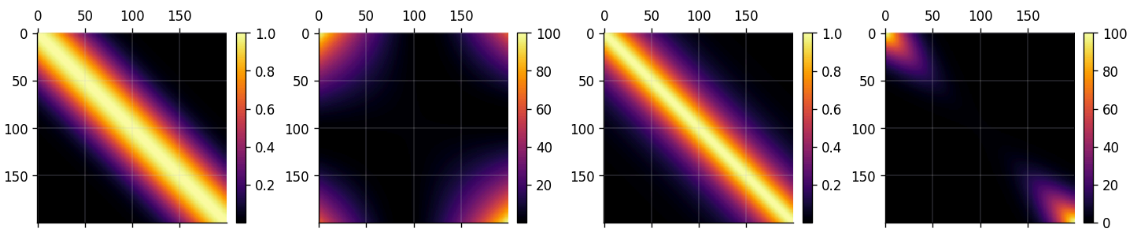
```
k3 = gpx.kernels.Matern32()

prod_k = gpx.kernels.ProductKernel(kernels=[k1, k2, k3])

fig, ax = plt.subplots(ncols=4, figsize=(12, 3))
im0 = ax[0].matshow(k1.gram(x).to_dense())
im1 = ax[1].matshow(k2.gram(x).to_dense())
im2 = ax[2].matshow(k3.gram(x).to_dense())
im3 = ax[3].matshow(prod_k.gram(x).to_dense())

fig.colorbar(im0, ax=ax[0], fraction=0.05)
fig.colorbar(im1, ax=ax[1], fraction=0.05)
fig.colorbar(im2, ax=ax[2], fraction=0.05)
fig.colorbar(im3, ax=ax[3], fraction=0.05)
```

```
<matplotlib.colorbar.Colorbar at 0x7f05e2373b50>
```



Custom kernel

GPJax makes the process of implementing kernels of your choice straightforward with two key steps:

1. Listing the kernel's parameters.
2. Defining the kernel's pairwise operation.

We'll demonstrate this process now for a circular kernel --- an adaption of the excellent guide given in the PYMC3 documentation. We encourage curious readers to visit their notebook here.

Circular kernel

When the underlying space is polar, typical Euclidean kernels such as Matérn kernels are insufficient at the boundary where discontinuities will present themselves. This is due to the fact that for a polar space $|0, 2\pi| = 0$ i.e., the space wraps. Euclidean kernels have no mechanism in them to represent this logic and will instead treat 0 and 2π and elements far apart. Circular kernels do not exhibit this behaviour and instead *wrap* around the boundary points to create a smooth function. Such a kernel was given in Padonou & Roustant (2015) where any two angles θ and θ' are written as

$$W_c(\theta, \theta') = \left| \left(1 + \tau \frac{d(\theta, \theta')}{c}\right) \left(1 - \frac{d(\theta, \theta')}{c}\right)^\tau \right| \quad \tau \geq 4. \tag{1}$$

Here the hyperparameter τ is analogous to a lengthscale for Euclidean stationary kernels, controlling the correlation between pairs of observations. While d is an angular distance metric

$$d(\theta, \theta') = |(\theta - \theta' + c) \bmod 2c - c|.$$

To implement this, one must write the following class.

```python
def angular_distance(x, y, c):
    return jnp.abs((x - y + c) % (c * 2) - c)


bij = tfb.SoftClip(low=jnp.array(4.0, dtype=jnp.float64))

DEFAULT_BIJECTION["polar"] = bij


class Polar(gpx.kernels.AbstractKernel):
    period: Static
    tau: PositiveReal
    def __init__(
        self,
        tau: float = 5.0,
        period: float = 2 * jnp.pi,
        active_dims: list[int] | slice | None = None,
        n_dims: int | None = None,
    ):
        super().__init__(active_dims, n_dims, DenseKernelComputation())
        self.period = Static(jnp.array(period))
        self.tau = PositiveReal(jnp.array(tau), tag="polar")

    def __call__(
        self, x: Float[Array, "1 D"], y: Float[Array, "1 D"]
    ) -> Float[Array, "1"]:
        c = self.period.value / 2.0
        t = angular_distance(x, y, c)
        K = (1 + self.tau.value * t / c) * jnp.clip(
            1 - t / c, 0, jnp.inf
        ) ** self.tau.value
        return K.squeeze()
```

We unpack this now to make better sense of it. In the kernel's initialiser we specify the length of a single period. As the underlying domain is a circle, this is 2π. We then define the kernel's `__call__` function which is a direct implementation of Equation (1) where we define `c` as half the value of `period`.

To constrain τ to be greater than 4, we use a `Softplus` bijector with a clipped lower bound of 4.0. This is done by specifying the `bijector` argument when we define the parameter field.

Using our polar kernel

We proceed to fit a GP with our custom circular kernel to a random sequence of points on a circle (see the Regression notebook for further details on this process).

```
# Simulate data
angles = jnp.linspace(0, 2 * jnp.pi, num=200).reshape(-1, 1)
n = 20
noise = 0.2

X = jnp.sort(jr.uniform(key, minval=0.0, maxval=jnp.pi * 2, shape=(n, 1)),
axis=0)
y = 4 + jnp.cos(2 * X) + jr.normal(key, shape=X.shape) * noise

D = gpx.Dataset(X=X, y=y)

# Define polar Gaussian process
```

```
PKern = Polar()
meanf = gpx.mean_functions.Zero()
likelihood = gpx.likelihoods.Gaussian(num_datapoints=n)
circular_posterior = gpx.gps.Prior(mean_function=meanf, kernel=PKern) *
likelihood

# Optimise GP's marginal log-likelihood using BFGS
opt_posterior, history = gpx.fit_scipy(
    model=circular_posterior,
    objective=lambda p, d: -gpx.objectives.conjugate_mll(p, d),
    train_data=D,
)
```

```
Optimization terminated successfully.
         Current function value: 31.146389
         Iterations: 18
         Function evaluations: 23
         Gradient evaluations: 23
```

Prediction

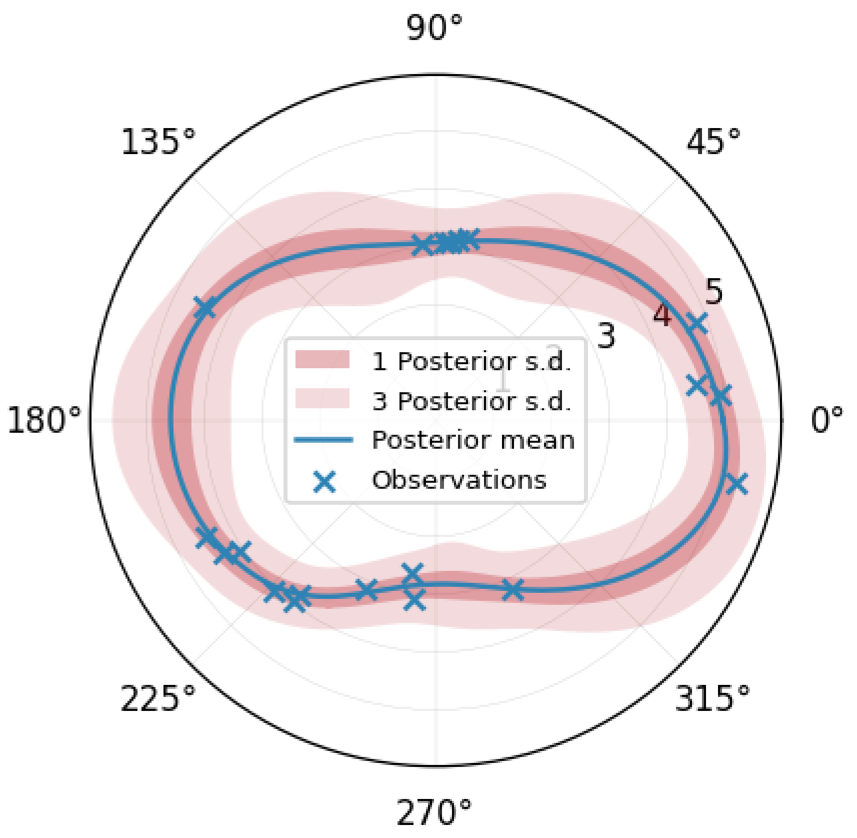
We'll now query the GP's predictive posterior at linearly spaced novel inputs and illustrate the results.

```
posterior_rv = opt_posterior.likelihood(opt_posterior.predict(angles,
train_data=D))
mu = posterior_rv.mean()
one_sigma = posterior_rv.stddev()
```

```
fig = plt.figure(figsize=(7, 3.5))
gridspec = fig.add_gridspec(1, 1)
ax = plt.subplot(gridspec[0], polar=True)

ax.fill_between(
    angles.squeeze(),
    mu - one_sigma,
    mu + one_sigma,
    alpha=0.3,
    label=r"1 Posterior s.d.",
    color=cols[1],
    lw=0,
)
ax.fill_between(
    angles.squeeze(),
    mu - 3 * one_sigma,
    mu + 3 * one_sigma,
    alpha=0.15,
    label=r"3 Posterior s.d.",
    color=cols[1],
    lw=0,
)
ax.plot(angles, mu, label="Posterior mean")
ax.scatter(D.X, D.y, alpha=1, label="Observations")
ax.legend()
```

```
<matplotlib.legend.Legend at 0x7f05cffd5570>
```



System configuration

```
%reload_ext watermark
%watermark -n -u -v -iv -w -a 'Thomas Pinder'
```

```
Author: Thomas Pinder

Last updated: Fri Apr 11 2025

Python implementation: CPython
Python version       : 3.10.16
IPython version      : 8.35.0
```

```
tensorflow_probability: 0.25.0
jax                   : 0.5.3
gpjax                 : 0.10.1
jaxtyping             : 0.3.1
matplotlib            : 3.10.1

Watermark: 2.5.0
```