Probabilistic Machine Learning

Exercise Sheet #5

due on Tuesday, 1 June 2021, 10am sharp

1. **EXAMple: Kernels**
   Remember that a symmetric $N \times N$ matrix K is positive definite if and only if $\boldsymbol{v}^T K \boldsymbol{v} > 0$ for all vectors $\boldsymbol{v} \in \mathbb{R}^N \setminus \mathbf{0}$.

   (a) For $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^D$, prove or disprove that the function $k(\boldsymbol{a}, \boldsymbol{b}) = \boldsymbol{a}^\intercal \boldsymbol{b}$ is a Mercer (i.e. positive definite) kernel.

   (b) Suppose k is a Mercer kernel. Prove or disprove that $\alpha^2 k$ is also a Mercer kernel, for $\alpha \in \mathbb{R}$

   (c) Suppose k and h are Mercer kernels. Prove or disprove that $k + h$ is also a Mercer kernel.

2. **Theory Question: Parametric and nonparametric regression**
   Consider the random function $f : \mathbb{R} \rightarrow \mathbb{R}$ from the centered (i.e. zero-mean) GP prior $p(f) = \mathcal{GP}(f; 0, k)$ with the "square-exponential" kernel

   $$k(a, b) = \theta^2 \exp\left(-\frac{(a-b)^2}{2\lambda^2}\right) \quad \text{with parameters } \theta, \lambda \in \mathbb{R}_+,$$

   and, independently, the random parametric function $g(x) = \boldsymbol{\phi}_x^\intercal \boldsymbol{w}$ with $\boldsymbol{\phi}_x, \boldsymbol{w} \in \mathbb{R}^F$ induced by the prior $p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}, \Sigma)$.

   (a) What is the prior distribution over the function $h(x) = f(x) + g(x)$?

   (b) Consider observations $\boldsymbol{y} \in \mathbb{R}^N$ observed with the likelihood $p(\boldsymbol{y} \mid h) = \mathcal{N}(\boldsymbol{y}; h_X, \sigma^2 I)$ at locations $X = [x_1, \ldots, x_n]$. Given these observations, what is the posterior distribution over $\boldsymbol{w}$?

3. **Practical Question**

   This week you will get to collect some experience with Gaussian process regression. More information on Ilias.

1

a) k is a Mercer kernel iff $\forall N \in \mathbb{N}\ \forall X \in \mathbb{R}^{D\times N}$: k_{XX} is psd, where $[k_{XX}]_{ij} = k(\underbrace{x_i, x_j}_{\in \mathbb{R}^D}) = x_i^T x_j$. Clearly, k_{XX} is symmetric, because $[k_{XX}]_{ij} = x_i^T x_j = x_j^T x_i = [k_{XX}]_{ji}$. A symmetric $\overset{N\times N}{\text{matrix}}$ A is psd, if it is a Gram matrix: there is a list X of N vectors, s.t. $A_{ij} = x_i^T x_j$. This is exactly the form we have above, so k is a Mercer kernel.

b) We know that $\forall N \in \mathbb{N}\ \forall X \in \mathbb{X}^N$: k_{XX} is psd. Thus, for any $X \in \mathbb{X}^N$ and $v \in \mathbb{R}^N \setminus \{0\}$, we have:

$$v^T k_{XX} v \geq 0 \qquad \Big| \cdot \alpha^2 \leadsto \text{positive so} \geq \text{stays} \geq.$$

$$\Rightarrow \alpha^2 v^T k_{XX} v \geq 0 \qquad (\alpha^2 \text{ is a scalar})$$

$$\Rightarrow v^T \underbrace{(\alpha^2 k_{XX})}_{} v \geq 0$$

Multiplying a matrix by a constant is just multiplying each component, but these are the (evaluated) kernel functions. Thus, $\alpha^2 k_{XX} = (\alpha^2 k)_{XX} =: k'_{XX}$

$$\Rightarrow v^T \underbrace{k'_{XX}}_{} v \geq 0$$

Kernel matrix with kernel function $k' := \alpha^2 k$.

$\Rightarrow k' = \alpha^2 k$ is a Mercer kernel.

c) For any $X \in \mathbb{X}^N$ $(N \in \mathbb{N})$ and $v \in \mathbb{R}^N \setminus 0$, we know that

$$v^T k_{XX} v \geq 0 \quad \wedge \quad v^T h_{XX} v \geq 0$$

$$\Rightarrow v^T k_{XX} v + v^T h_{XX} v \geq 0 \qquad (\text{addition of positive real numbers} \to \text{positive})$$

$$\Rightarrow v^T \underbrace{(k_{XX} + h_{XX})}_{} v \geq 0 \qquad (\text{distributivity, twice}).$$

Matrix addition = elementwise addition.

$$\Rightarrow v^T (k+h)_{XX} v \geq 0$$

$\Rightarrow k+h$ is a Mercer kernel.

2/

a) $p(h_x) = p(f_x + g_x)$ Luckily, f_x and g_x are Gaussian.

$p(f_x) = \mathcal{N}(f_x \mid 0, k(x,x))$

$p(g_x) = \mathcal{N}(g_x \mid \phi_x^T \mu, \phi_x^T \Sigma \phi_x)$

$\Rightarrow p(h_x) = \mathcal{N}(h_x \mid \phi_x^T \mu, \phi_x^T \Sigma \phi_x + k(x,x))$ (Sum of Gaussian RVs).

b) $p(w \mid y, X) \propto p(y \mid w, X)\, p(w)$

$= \mathcal{N}(y \mid h_x, \sigma^2 I)\, \mathcal{N}(w \mid \mu, \Sigma)$

Exercise_05

May 31, 2021

1 Probabilistic Machine Learning

University of Tübingen, Summer Term 2021

1.1 Exercise Sheet 5

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This sheet is **due on Tuesday June 1, 2021 at 10am sharp.**

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2 Kernels and Gaussian Processes

In this homework sheet you will implement Gaussian process regression. The first goal is to get a feel for kernels and the properties they encode about the corresponding functions. The second goal is to understand Gaussian processes by implementing a `GaussianProcess` class, which we will use to predict the daily number of reported COVID-19 cases in Germany as reported by the Robert Koch Institut.

[1]:
```
# Plotting setup
import matplotlib.pyplot as plt
import datetime

# Make inline plots vector graphics
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats("pdf", "svg")
# %config InlineBackend.figure_format='svg'

# Package imports
from functools import partial
import numpy as np
import pandas as pd
from scipy.spatial.distance import cdist
from scipy.linalg import det, solve
```

[2]:
```
# Seeded random number generator
rng = np.random.default_rng(42)
```

2.1 Kernels

Kernels are symmetric positive definite functions, which can be thought of as measuring the similarity between two points in the input space. As covariance functions of random processes they are often used to encode properties of a function which we are trying to model. Classic examples are its smoothness or periodicity.

Task: Implement the kernels below based on the given definitions. If only X_0 is given the kernel evaluated pairwise $k(X_0, X_0)$ should be returned.

Hint: The function `scipy.spatial.distance` may be helpful.

Polynomial Kernel

$$k(x_0, x_1) = (x_0^\top x_1 + c)^d$$

where $c \geq 0$ is a constant and $d \in \mathbb{N}$ the degree of the polynomial.

[3]:
```
def polynomial(x0, x1=None, constant=0, exponent=1):
    """x0, x1 \in R^{D \times N}"""
    if x1 is None:
        x1 = x0

    return (x0.T@x1 + constant)**exponent
```

Exponentiated Quadratic Kernel Also known as radial basis function (RBF) or squared exponential kernel.

$$k(x_0, x_1) = \exp\left(-\frac{\|x_0 - x_1\|^2}{2\ell^2}\right)$$

with lengthscale $\ell \in \mathbb{R}$.

[4]:
```
def expquad(x0, x1=None, lengthscale=1.0):
    """x0, x1 \in R^{D \times N}"""
    if x1 is None:
        x1 = x0

    d = cdist(x0.T, x1.T)**2
    return np.exp(-d / (2 * lengthscale**2))
```

Rational Quadratic Kernel

$$k(x_0, x_1) = \exp\left(-\frac{\|x_0 - x_1\|^2}{2\ell^2}\right)$$

with lengthscale $\ell \in \mathbb{R}$ and scale mixture $\alpha > 0$.

[5]:
```
def ratquad(x0, x1=None, lengthscale=1.0, alpha=0.01):
    """x0, x1 \in R^{D \times N}"""
```

```
    if x1 is None:
        x1 = x0

    d = cdist(x0.T, x1.T)**2
    return (1 + d/(2 * alpha * lengthscale**2)) ** (-alpha)
```

Periodic Kernel

$$k(x_0, x_1) = \exp\left(-\frac{2\sin^2(\pi\|x_0 - x_1\|/p)}{\ell^2}\right)$$

with lengthscale $\ell \in \mathbb{R}$ and period $p > 0$.

[6]:
```
def periodic(x0, x1=None, lengthscale=1.0, period=2 * np.pi):
    """x0, x1 \in R^{D \times N}"""
    if x1 is None:
        x1 = x0

    d = cdist(x0.T, x1.T)
    return np.exp(-2 * np.sin(np.pi * d / period)**2 / lengthscale**2)
```

Custom kernel Define a custom kernel

$$k(x_0, x_1) = \langle \varphi(x_0), \varphi(x_1) \rangle$$

for a given feature transformation φ.

[7]:
```
def feature_trafo(X):
    """X \in R^{1 \times N}, returns R^{11 \times N}"""
    return (X > np.linspace(-5, 5, 11)[:, None]).astype(float)
```

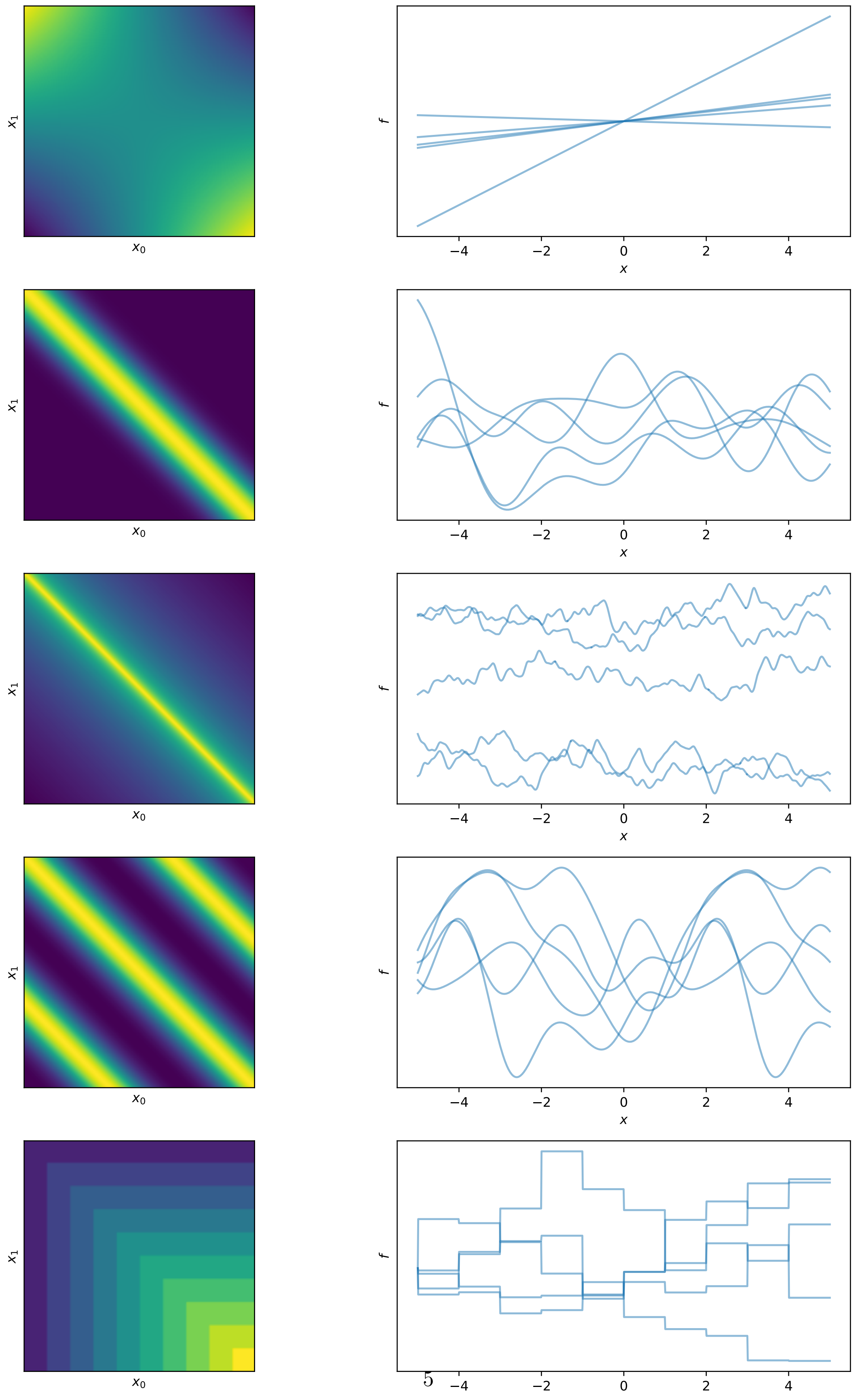
[8]:
```
def custom_kernel(x0, x1=None, phi=feature_trafo):
    """x0, x1 \in R^{D \times N}"""
    if x1 is None:
        x1 = x0

    y0, y1 = phi(x0), phi(x1)
    return y0.T @ y1
```

Task: Plot kernel matrices and samples for some synthetic 1D data for the kernels you just defined.

[9]:
```
def plot_kernel_matrix(ax, X, kernel, **kernkwargs):
    ax.imshow(kernel(X, **kernkwargs))
    ax.set_xticks([])
    ax.set_yticks([])
    ax.set_xlabel("$x_0$")
    ax.set_ylabel("$x_1$")
```

```python
def plot_prior_samples(ax, X, kernel, nsamples=5, rng=np.random.default_rng(),␣
↪**kernkwargs):
    n = len(X.T)
    mean = np.zeros(n)
    cov = kernel(X, **kernkwargs)
    f = rng.multivariate_normal(mean, cov, size=5)

    ax.set_yticks([])
    ax.plot(X.flatten(), f.T, color="C0", alpha=0.5)
    ax.set_xlabel("$x$")
    ax.set_ylabel("$f$")
```

[10]:
```python
# Generate synthetic data and plot
N = 1000
x = np.linspace(-5, 5, N)[None, :]

fig, ax = plt.subplots(5, 2, figsize=(10, 15), constrained_layout=True)
plot_kernel_matrix(ax[0, 0], x, polynomial)
plot_prior_samples(ax[0, 1], x, polynomial)
plot_kernel_matrix(ax[1, 0], x, expquad)
plot_prior_samples(ax[1, 1], x, expquad)
plot_kernel_matrix(ax[2, 0], x, ratquad)
plot_prior_samples(ax[2, 1], x, ratquad)
plot_kernel_matrix(ax[3, 0], x, periodic)
plot_prior_samples(ax[3, 1], x, periodic)
plot_kernel_matrix(ax[4, 0], x, custom_kernel)
plot_prior_samples(ax[4, 1], x, custom_kernel)
```



x_1
x_0
f
−4 −2 0 2 4
x

Notice that apart from the polynomial kernel, the above kernels all only depend on the distance between points, not their absolute position. Such kernels are called *stationary*.

2.1.1 Combining Kernels

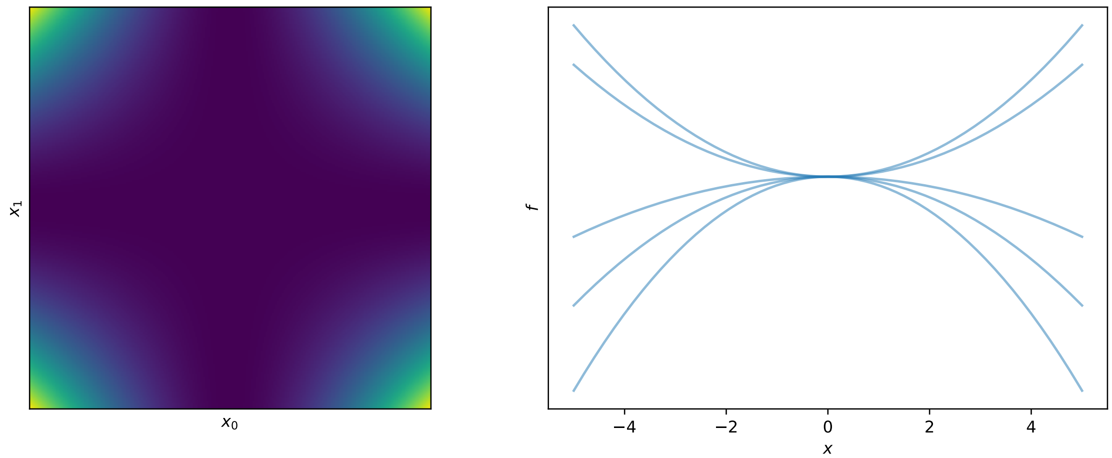
Kernels can be combined to represent a richer class of functions. In particular, kernels can be multiplied and added together.

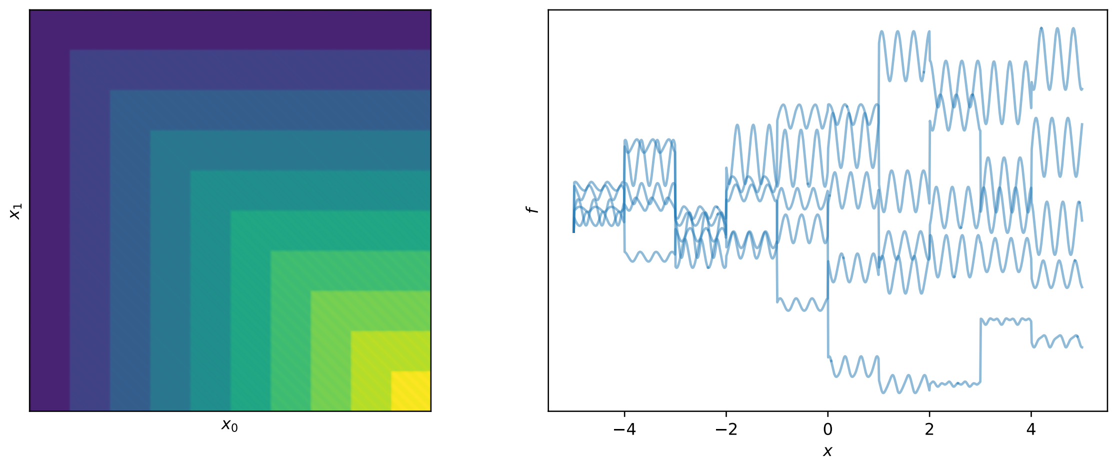
Multiplying Kernels **Task:** Define a quadratic kernel and a locally periodic kernel using a product of exactly two kernels you defined above.

[11]:
```
def quadratic(x0, x1=None):
    k1 = k2 = polynomial(x0, x1)
    return k1 * k2
```

[12]:
```
def locally_periodic(x0, x1=None):
    k1 = custom_kernel(x0, x1)
    k2 = periodic(x0, x1, lengthscale=10, period=0.1*np.pi)
    return k1 * k2
```

[13]:
```
# Generate synthetic data and plot
N = 1000
x = np.linspace(-5, 5, N)[None, :]

fig, ax = plt.subplots(2, 2, figsize=(10, 8), constrained_layout=True)
plot_kernel_matrix(ax[0, 0], x, quadratic)
plot_prior_samples(ax[0, 1], x, quadratic)
plot_kernel_matrix(ax[1, 0], x, locally_periodic)
plot_prior_samples(ax[1, 1], x, locally_periodic)
```

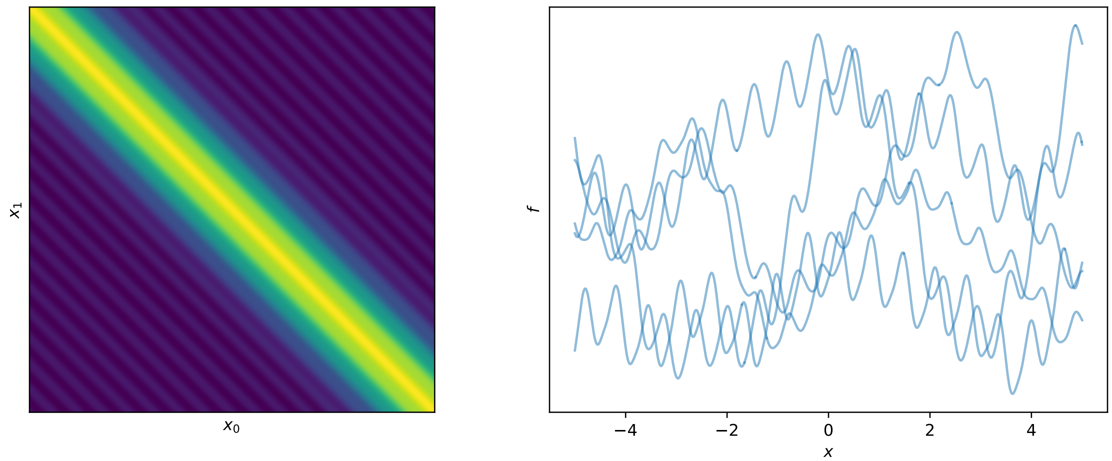




Adding Kernels **Task:** Define a kernel representing a global pattern which has periodic local structure using a sum of two (scaled) kernels.

[14]:
```
def sum_kernel(x0, x1=None, lengthscale1=1, lengthscale2=5, period=0.2*np.pi):
    k1 = expquad(x0, x1, lengthscale=lengthscale1)
    k2 = periodic(x0, x1, lengthscale=lengthscale2, period=period)
    return k1 + k2
```

[15]:
```
# Generate synthetic data and plot
N = 1000
x = np.linspace(-5, 5, N)[None, :]

fig, ax = plt.subplots(1, 2, figsize=(10, 4), constrained_layout=True)
plot_kernel_matrix(ax[0], x, sum_kernel)
plot_prior_samples(ax[1], x, sum_kernel)
```



Task: Plot kernel matrices and samples for the same synthetic 1D data.

(see above)

2.2 Implementing Gaussian Processes

Task: Implement Gaussian process regression by completing the class implementation below.

Hint: One way to implement the solution of linear systems $(K + \sigma^2 I)^{-1} y$ arising in GP inference is via a Cholesky decomposition $K + \sigma^2 I = LL^\top$. See also `cho_factor` and `cho_solve`.

[16]:
```
from scipy.linalg import cho_factor, cho_solve
```

[17]:
```
class GaussianProcess:
    """Gaussian process regression.

    Parameters
    ----------
    mean :
        Mean function.
    cov :
        Covariance function / kernel.
    sigma :
        Scalar observation noise.
    """

    def __init__(self, mean, cov, sigma=10 ** -6):
        self.m = mean      # Prior mean
        self.k = cov       # Prior kernel
        self.mp = mean     # Posterior mean
        self.kp = cov      # Posterior kernel
        self.sigma = sigma
```

```python
        self.X = None
        self.y = None

    def fit(self, X, y):
        self.X = X
        self.y = y
        gram = self.k(X) + (self.sigma**2 * np.eye(len(y)))
        gain = lambda x: cho_solve(cho_factor(gram.T), self.k(x, X).T).T
        self.mp = lambda x: self.m(x) + gain(x)@(y - self.m(X))
        self.kp = lambda x: self.k(x, x) - gain(x)@self.k(X, x)

    def predict(self, Xnew):
        return self.mp(Xnew), self.kp(Xnew)

    def sample(self, Xnew, size, rng=None):
        if rng is None:
            rng = np.random.default_rng()
        return rng.multivariate_normal(self.mp(Xnew), self.kp(Xnew), size=size)

    def log_marginal_likelihood(self, **hyperparams):
        X = self.X
        y = self.y
        G = (np.eye(len(y)) * self.sigma**2) + self.k(X, **hyperparams)
        E = (y - self.m(X)).T @ cho_solve(cho_factor(G), y - self.m(X))
        return -1/2 * (len(y)*np.log(2*np.pi) + E) #  - 1/2 * np.log(det(G)) (Taken out because det(G) is 0 in RKI data)
```

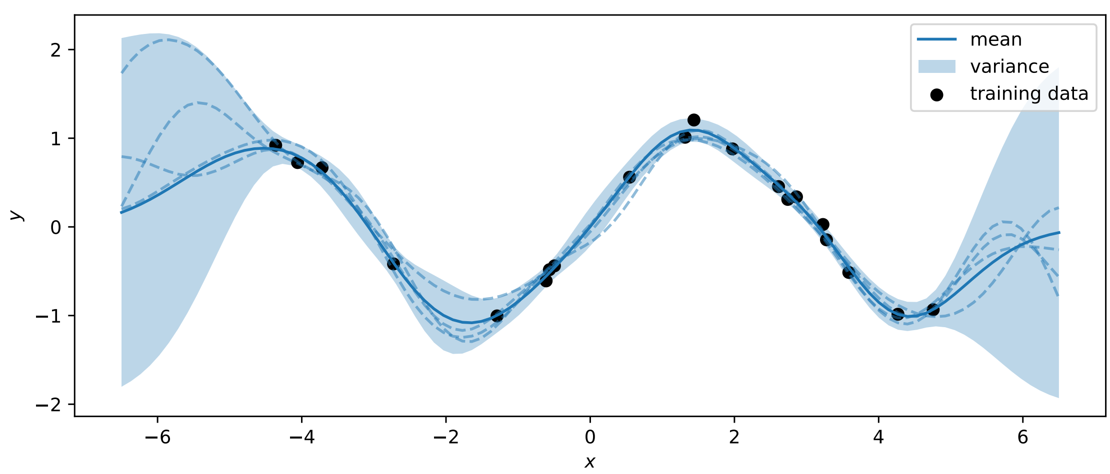
Task: Test your implementation by fitting a Gaussian process to the synthetically generated test data.

[18]:
```python
# Test function (changed shapes to those used in lecture)
X = np.sort(rng.uniform(-5,5,20))[None, :]
y = (np.sin(X) + 0.1 * rng.normal(size=X.shape[1])[None, :]).flatten()
```

[19]:
```python
# Gaussian process (changed shapes to those used in lecture)
mu = lambda x: np.zeros(shape=(x.shape[1]))
cov = expquad
g = GaussianProcess(mu, cov, sigma=10 ** -1)
g.fit(X, y)

Xnew = np.linspace(-6.5, 6.5, 100)[None, :]
ypred = g.predict(Xnew)
g.log_marginal_likelihood()
```

[19]: -23.507255008581204

[20]:
```python
# Plot

def plot_gp(Xnew, ypred, samples=None, traindata=None):
    fig, ax = plt.subplots(ncols=1, nrows=1, figsize=(10, 4))

    ax.plot(Xnew.flatten(), ypred[0], label="mean")
    ax.fill_between(
        x=Xnew.flatten(),
        y1=ypred[0].flatten() - 2 * np.sqrt(np.diag(ypred[1])),
        y2=ypred[0].flatten() + 2 * np.sqrt(np.diag(ypred[1])),
        alpha=0.3,
        label="variance"
    )

    if samples is not None:
        ax.plot(Xnew.flatten(), samples.T, linestyle="--", color="C0", alpha=0.
↪5)

    if traindata is not None:
        ax.scatter(traindata[0], traindata[1], color="k", label="training data")

    ax.set_xlabel("$x$")
    ax.set_ylabel("$y$")
    ax.legend()

    plt.show()

plot_gp(Xnew, ypred, samples=g.sample(Xnew, 4), traindata=(X,y))
```



2.3 German COVID-19 Data

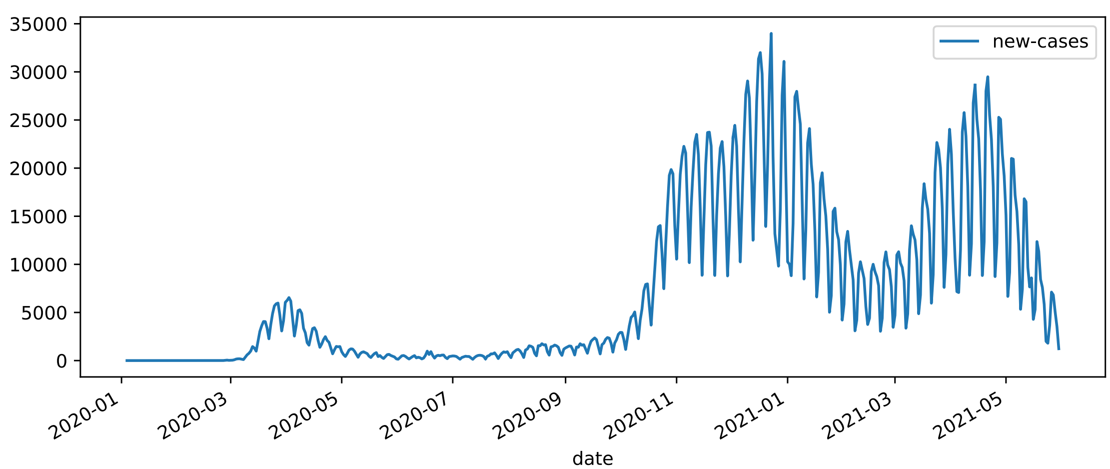
We will now use the Gaussian process class you just implemented to predict the future development of COVID-19 numbers in Germany.

Disclaimer: *Although the exercise uses real data, it does not aspire to satisfy the standards of epidemiology or public policy making. It is deliberately simple and designed to be feasible within the scope of this lecture course. Do not mistake it for a thorough scientific analysis, and do not draw overly confident conclusions from it.*

Task: Download the COVID-19 data for Germany from the Robert Koch Institute.

[23]:
```python
import ssl
ssl._create_default_https_context = ssl._create_unverified_context

# Link to current data of the RKI
url = "https://www.arcgis.com/sharing/rest/content/items/
↪f10774f1c63e40168479a1feb6c7ca74/data"

# Read CSV data from URL
data_rki = pd.read_csv(url)

# Create dataframe of number of new cases
data_rki_cases = pd.DataFrame(
    data_rki[data_rki.NeuerFall > -1].groupby(["Meldedatum"]).AnzahlFall.sum()
)
data_rki_cases = data_rki_cases.rename(columns={"AnzahlFall": "new-cases"})
data_rki_cases.index.name = "date"

# Reset index and parse dates
data_rki_cases = data_rki_cases.reset_index()
data_rki_cases["date"] = pd.to_datetime(data_rki_cases.date, format="%Y-%m-%d")
```

[24]:
```python
data_rki_cases.plot(x="date", y="new-cases", figsize=(10, 4))
plt.show()
```



2.3.1 Data Transformation

In order to satisfy the assumptions a GP model makes implicitly we will transform the non-negative count data with a log-transform.

Task: Implement a transformation (and its inverse) using the logarithm, shifting and scaling such that your data has range $\subset (-\infty, \infty)$, is centered and has variance one.

[25]:
```
def transform_data(X):
    """Log-transform and standardize data."""
    return ((Z := np.log(X)) - (m := Z.mean())) / (s := Z.std()), (m, s)

def retransform_data(Z, mu, sigma):
    """Transform back to original data range."""
    return np.exp(Z*sigma + mu)
```

[26]:
```
data_trafo, (Z_mean, Z_sigma) = transform_data(data_rki_cases["new-cases"])
data_rki_cases["new-cases-transformed"] = data_trafo
data_rki_cases["days"] = (data_rki_cases["date"] - data_rki_cases["date"][0]).
↪dt.days
data_rki_cases.describe()
```

[26]:

	new-cases	new-cases-transformed	days
count	480.000000	4.800000e+02	480.000000
mean	7669.012500	-5.921189e-17	271.991667
std	8412.951814	1.000000e+00	139.596211
min	1.000000	-3.529234e+00	0.000000
25%	748.750000	-5.279212e-01	152.750000
50%	3738.500000	2.013481e-01	272.500000
75%	12719.500000	7.565408e-01	392.250000
max	33999.000000	1.202489e+00	512.000000

[35]:
```
# Data (changed shapes to those used in lecture)
X = data_rki_cases["days"].to_numpy()[None, :]
y = data_rki_cases["new-cases-transformed"].to_numpy().flatten()
```

2.3.2 Prior Choice

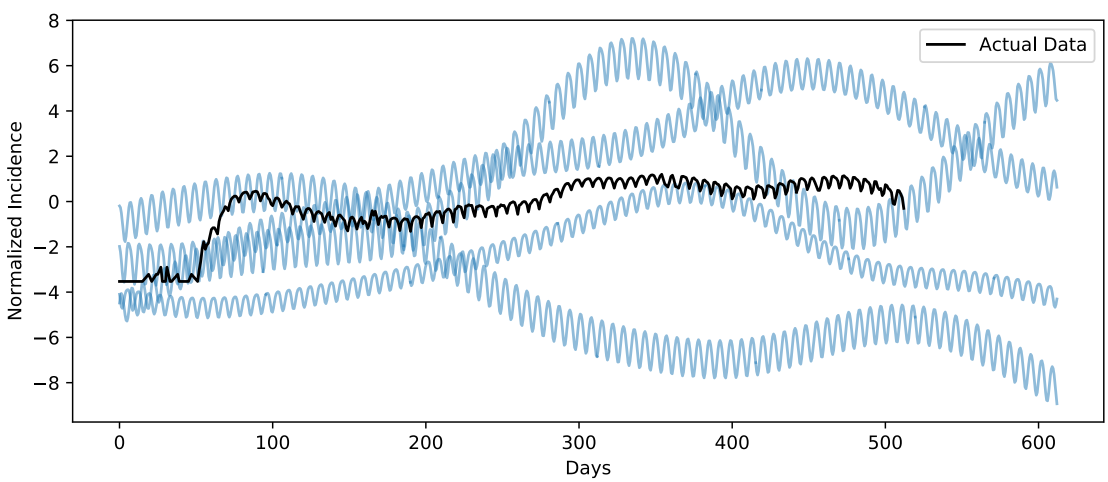
Task: Implement a custom kernel (e.g. by combining kernels you previously defined) which encodes any prior assumptions you might have about the COVID numbers. You can check how your prior assumptions translate into the functions your GP represents by drawing samples from the prior and comparing them to the transformed data.

[36]:
```
# Custom kernel
def custom_kernel(x0, x1=None, l1=100, l2=5, p=7):
```

```
    return 10*sum_kernel(x0, x1, l1, l2, p)
```

[37]:
```
# Gaussian process (changed shapes to those used in lecture)
cov = custom_kernel
g = GaussianProcess(mu, cov, sigma=10 ** -1)

Xnew = np.linspace(0, np.max(X) + 100, 1000)[None, :]
ypred = g.predict(Xnew)
```

[38]:
```
fig, ax = plt.subplots(ncols=1, nrows=1, figsize=(10, 4))

# Samples
ax.plot(Xnew.flatten(), g.sample(Xnew, size=4).T, linestyle="-", color="C0",␣
↪alpha=0.5)

# Data
ax.plot(X.flatten(), y, color="k", label="Actual Data")

ax.set_xlabel("Days")
ax.set_ylabel("Normalized Incidence")
ax.legend()

plt.show()
```



2.3.3 GP Regression and Extrapolation

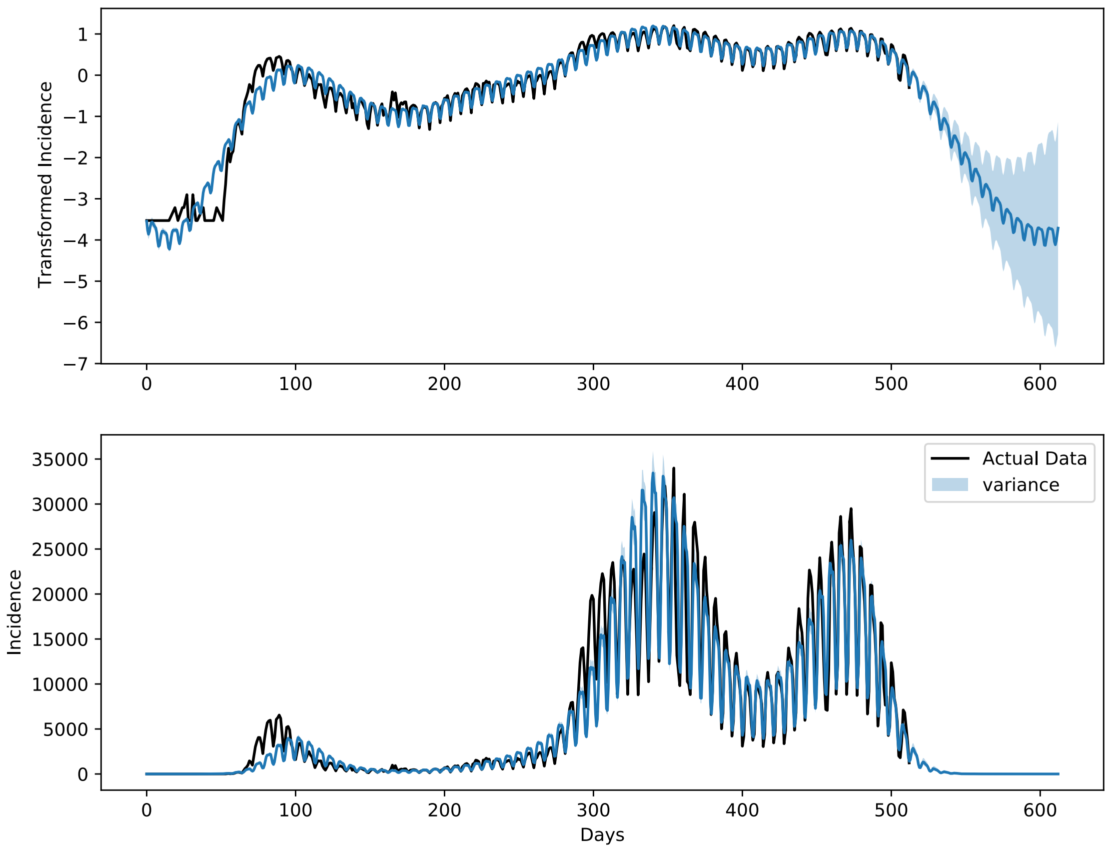
Task: Apply your GP model to the transformed incidence data from the RKI. What can you say about the prediction of your model for the next 100 days?

[31]:
```
g.fit(X, y)
ypred = g.predict(Xnew)
g.log_marginal_likelihood()
```

[31]: -1926.6899973092218

[32]:
```
# Retransform incidence
mean_retrafo = retransform_data(ypred[0], Z_mean, Z_sigma).flatten()
quantile_retrafo = np.quantile(
    retransform_data(g.sample(Xnew, size=10000), Z_mean, Z_sigma), q=(0.025, 0.
 ↪975), axis=0
)
```

[33]:
```
fig, axs = plt.subplots(ncols=1, nrows=2, figsize=(10, 8))

# Transformed incidence
axs[0].plot(X.flatten(), y, color="k", label="Actual Data")
axs[0].plot(Xnew.flatten(), ypred[0], label="mean")
axs[0].fill_between(
    x=Xnew.flatten(),
    y1=ypred[0].flatten() - 2 * np.sqrt(np.diag(ypred[1])),
    y2=ypred[0].flatten() + 2 * np.sqrt(np.diag(ypred[1])),
    alpha=0.3,
    label="variance"
)

# Incidence
axs[1].plot(X.flatten(), data_rki_cases["new-cases"], color="k", label="Actual␣
 ↪Data")
axs[1].plot(Xnew.flatten(), mean_retrafo)
axs[1].fill_between(
    x=Xnew.flatten(),
    y1=quantile_retrafo[0, :],
    y2=quantile_retrafo[1, :],
    alpha=0.3,
    label="variance"
)

axs[0].set_ylabel("Transformed Incidence")
axs[1].set_ylabel("Incidence")
axs[1].set_xlabel("Days")
axs[1].legend()
plt.show()
```



Question: What observations does your prior choice encode? How good is the fit? How could it be improved *automatically*?

It encodes the periodicity of 1 week (p=7) and the observed lengthscales of the periodic and non-periodic components. The kernel parameters (like the periodicity) can be automatically optimized by hierarchical Bayesian inference (Maximum Likelihood on the marginal log likelihood). The fit is surprisingly confident that cases will not rise again (in the near future); it definitely fails in the beginning, where the transformed data also visibly does not follow the Gaussian / smooth shape that it has elsewhere.