Probabilistic Machine Learning

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

Exercise 6

Summer Term 2023

Full Name	Matriculation No
Batuhan Özcömlekci	6300476

Eberhards Karls University of Tübingen, June 12, 2023

Exercise Sheet 6

a) Given $X = [x_1, \dots, x_n]$ and targets $y \in \mathbb{R}^n$

$$p(y \mid f) = \mathcal{N}(y; f(X), \Lambda)$$
$$p(f) = GP(\mu, k)$$

Then, $p(y \mid X) = \int p(y \mid f(X))\, p(f)\, df$

$$= \int \mathcal{N}(y; f(X), \Lambda)\, \mathcal{N}(f_X; \mu_X, K_{XX})\, df_X$$

$\star$ The property of "multiplication of gaussians", i.e.

with $C = (A^{-1} + B^{-1})^{-1}$

$$\mathcal{N}(x; a, A)\, \mathcal{N}(x, b, B) = \mathcal{N}(x; C(A^{-1}a + B^{-1}b), C)\, \mathcal{N}(a; b, A + B)$$

---

where $C = (\Lambda^{-1} + K_{XX}^{-1})^{-1}$

$$\mathcal{N}(y; f(x), \Lambda)\, \mathcal{N}(f_X; \mu_X, K_{XX}) = \mathcal{N}(y; C(\Lambda^{-1} f(x) + K_{XX}^{-1}\mu_X), C) \cdot \mathcal{N}(f(X); \mu_X, \Lambda + K_{XX})$$

We can swap mean ($f(X)$) and the parameter (y) w.l.o.g.

$$\mathcal{N}(f(x); y, \Lambda)\, \mathcal{N}(f_X; \mu_X, K_{XX}) = \mathcal{N}(f(x); \underbrace{C(\Lambda^{-1} y + K_{XX}^{-1}\mu_X)}_{\text{call } \mu'}, \underbrace{C}_{\text{call } \Lambda'}) \cdot \mathcal{N}(y; \mu_X, \Lambda + K_{XX})$$

Then $p(y \mid X) = \underbrace{\left(\int \mathcal{N}(f(x); \mu', \Lambda')\, df\right)}_{1} \mathcal{N}(y; \mu_X, \Lambda + K_{XX})$

$$= \mathcal{N}(y; \mu_X, \Lambda + K_{XX}) \quad \text{Q.E.D.}$$

where μ_X and K_{XX} are as defined in the question.

b) $-\log p(y|x) = +\frac{1}{2}(y-\mu_x)^T(K_{xx}+\Lambda)^{-1}(y-\mu_x)$ → Square Error Term

$+\frac{1}{2}\log\det(K_{xx}+\Lambda)$ → Model complexity/Occam factor Term

$+\frac{n}{2}\log(2\pi)$ → Constant term

c) A perfect model match would be $y=\mu_x$ so that square error term in the negative log probabilty expression is eliminated and the remaining terms are minimal. The occam factor term is dependent on the model complexity and can be decreased by decreasing the model complexity induced by Λ.

For a perfect model match, $\log p(y|x) = -\frac{1}{2}\log\det(K_{xx}) - \frac{n}{2}\log(2\pi)$

→ Expected value of $\log p(y|x)$ under $y=f(x)+\varepsilon$ with $\varepsilon \sim \mathcal{N}(0,\Lambda)$

is
$$\begin{aligned} E(\log p(y|x)) = -\frac{1}{2}\Big[& E[(y-\mu_x)^T(K_{xx}+\Lambda)^{-1}(y-\mu_x)] \\ & + E[\log\det(K_{xx}+\Lambda)] \\ & + E[n\log 2\pi]\Big] \end{aligned}$$

By the linearity of expectation

mean $f(x)$ with $\varepsilon\sim\mathcal{N}(0,\Lambda)$ leads to

$$\to E_{y\sim\mathcal{N}(f(x),\Lambda)}[(y-\mu_x)^T(K_{xx}+\Lambda)^{-1}(y-\mu_x)] = tr((K_{xx}+\Lambda)^{-1}\Lambda)$$
$$+(f(x)-\mu_x)^T(K_{xx}+\Lambda)^{-1}(f(x)-\mu_x)$$

using the given property

And the expectation of the rest of the terms are same since they don't have y involved, thus:

$$\begin{aligned} E(\log p(y|x)) = -\frac{1}{2}\Big[& tr((K_{xx}+\Lambda)^{-1}\Lambda) + (f(x)-\mu_x)^T(K_{xx}+\Lambda)^{-1}(f(x)-\mu_x)^T \\ & + \log\det(K_{xx}+\Lambda) \\ & + n\log 2\pi\Big] \end{aligned}$$

Maybe further simplified with Woodbury matrix identities but left in this form.

Note
Since it is not explicity stated to simplify the final equation, the equation is left in the form seen.
From the question I understand that the property is taken for granted, not something we should prove explicitly.

ii) $$\frac{\partial \log p(y|x)}{\partial \theta} = -\frac{1}{2}\left[\frac{\partial}{\partial \theta}\left[(y-\mu_x)^T(\Lambda + K_{xx})^{-1}(y-\mu_x)\right] + \frac{\partial}{\partial \theta}\left\{\log(\det(K_{xx}+\Lambda))\right\} + \underbrace{\frac{\partial}{\partial \theta}\left[n \log 2\pi\right]}_{0}\right]$$

=

For a symmetric positive definite matrix $K_{xx} = UDU^T$ invertible with its inverse $A^{-1} = A^T$

and $K_{xx}^T K_{xx} = 1 = \underbrace{K_{xx}^{-1}K_{xx}}_{\text{Take derivative wrt } \theta} = UD^TU^TUDU^T$

$$\frac{\partial K_{xx}^{-1}}{\partial \theta} K_{xx} + K_{xx}^{-1}\frac{\partial K_{xx}}{\partial \theta} = 0$$

$$\frac{\partial K_{xx}^{-1}}{\partial \theta} K_{xx} = -K_{xx}^{-1}\frac{\partial K_{xx}}{\partial \theta} \Rightarrow \boxed{\frac{\partial K_{xx}^{-1}}{\partial \theta} = -K_{xx}^{-1}\frac{\partial K_{xx}}{\partial \theta}K_{xx}^{-1}} \star$$

$\star\star$

$$\boxed{\frac{\partial}{\partial \theta}\left[\log(\det(K_{xx}))\right] = \frac{\frac{\partial(\det(K_{xx}))}{\partial \theta}}{\det(K_{xx})} = \mathrm{tr}\left[K_{xx}^{-1}\frac{\partial K_{xx}}{\partial \theta}\right]}$$

Insert

$\star$ Jacobi's formula for invertible K_{xx} is:

$$\frac{\partial(\det(K_{xx}))}{\partial \theta} = \det(K_{xx})\,\mathrm{tr}\left[K_{xx}^{-1}\frac{\partial K_{xx}}{\partial \theta}\right]$$

Finally using a transformation $K'_{xx} = K_{xx} + \Lambda \Rightarrow \frac{\partial K'_{xx}}{\partial \theta} = \frac{\partial K_{xx}}{\partial \theta}$ or just simply taking $\Lambda = 0$ w.l.o.g., the identities above ($\star$ and $\star\star$) yield:

$$\underbrace{\frac{\partial \log p(y|x)}{\partial \theta} = -\frac{1}{2}\left[(y-\mu_x)^T\left(-K_{xx}^{-1}\frac{\partial K_{xx}}{\partial \theta}K_{xx}^{-1}\right)(y-\mu_x) + \mathrm{tr}\left[K_{xx}^{-1}\frac{\partial K_{xx}}{\partial \theta}\right]\right]}_{\text{Analytic form for the gradient of log prob. expressed in terms of } K_{xx} \text{ whose elements are single ks.}}$$

Note that, to be more precise $K_{xx} := K_{xx} + \Lambda$ assignment can be made.

Exercise 06

June 12, 2023

1 Probabilistic Machine Learning

University of Tübingen, Summer Term 2023 © 2023 P. Hennig

1.1 Exercise Sheet No. 6 — Source Separation

Submission by:

- Batuhan, Oezcoemlekci, Matrikelnummer: 6300476

[ ]:
```
import functools

import jax
import jax.numpy as jnp
import numpy as np


jax.config.update("jax_enable_x64", True)
```

[ ]:
```
from matplotlib import pyplot as plt
from tueplots import bundles
from tueplots.constants.color import rgb


plt.rcParams.update(bundles.beamer_moml())
plt.rcParams.update({'figure.dpi': 200})
```

1.2 Exercise 6.2 (Coding Exercise)

The lecture covered an extended example, in which a GP was used to model the Keeling curve, i.e. the temporal evolution of the atmospheric CO_2 concentration at Mauna Loa Observatory in Hawaii. This model is useful for separating certain effects in the data like long- and mid-term trends as well as periodicity.

However, since all kernels used for modelling the data are in fact so-called stationary (or translation-invariant) kernels, i.e. $k(t_0, t_1) = k(|t_0 - t_1|)$, the model will not extrapolate well. Rather, its prediction will at some point return to the prior mean, which is just set to a constant.

In this exercise, we will attempt to fix this problem by injecting more prior knowledge into the model. Specifically, we will add a covariate, which we hypothesize to have causal influence on the atmospheric CO_2 concentration. By scrutinizing the behavior of the model on the dataset, we can gain insights into the predictive power of the covariate.

Disclaimer: This is a very crude data analysis, which is merely meant to illustrate how GPs can be augmented with additional input data. It should not be used to make any scientific statement about the dynamics of atmospheric CO_2 concentration.

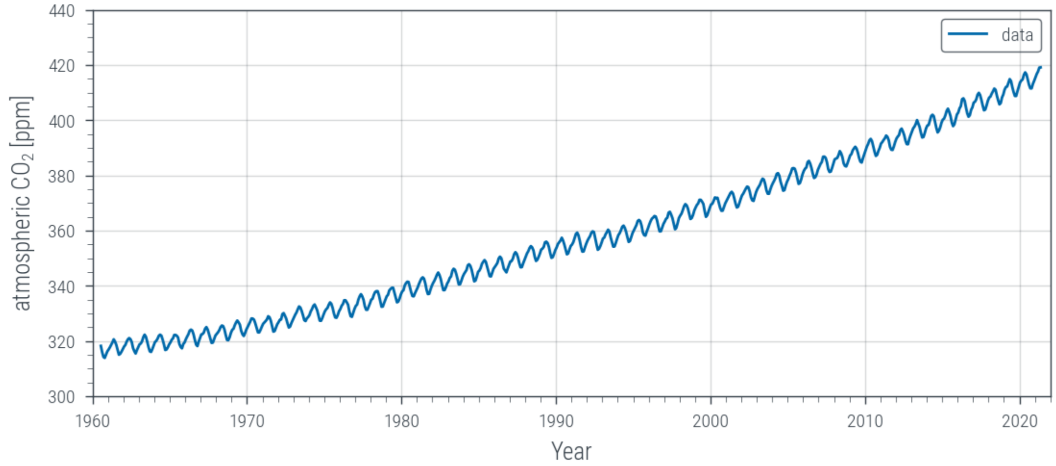
1.2.1 Data

First, let's load and plot the data.

[ ]:
```
data = np.load("Ex06_data.npz")
```

[ ]:
```
from matplotlib import ticker


def setup_plot(ax):
    ax.set_xlabel("Year")
    ax.xaxis.set_major_locator(ticker.MultipleLocator(10))
    ax.xaxis.set_minor_locator(ticker.MultipleLocator(1))
    ax.set_xlim([1960, 2022])
    ax.grid(which="major", axis="both")


def plot_data(ax):
    ax.plot(
        data["date"],
        data["atmospheric_co2"],
        label="data",
        color=rgb.tue_blue,
    )
    ax.yaxis.set_major_locator(ticker.MultipleLocator(20))
    ax.yaxis.set_minor_locator(ticker.MultipleLocator(5))
    ax.set_ylabel("atmospheric CO$_2$ [ppm]")
    ax.set_ylim([300, 440])


setup_plot(plt.gca())
plot_data(plt.gca())

plt.legend()
```

[ ]:
```
<matplotlib.legend.Legend at 0x7fb6e0ae13d0>
```

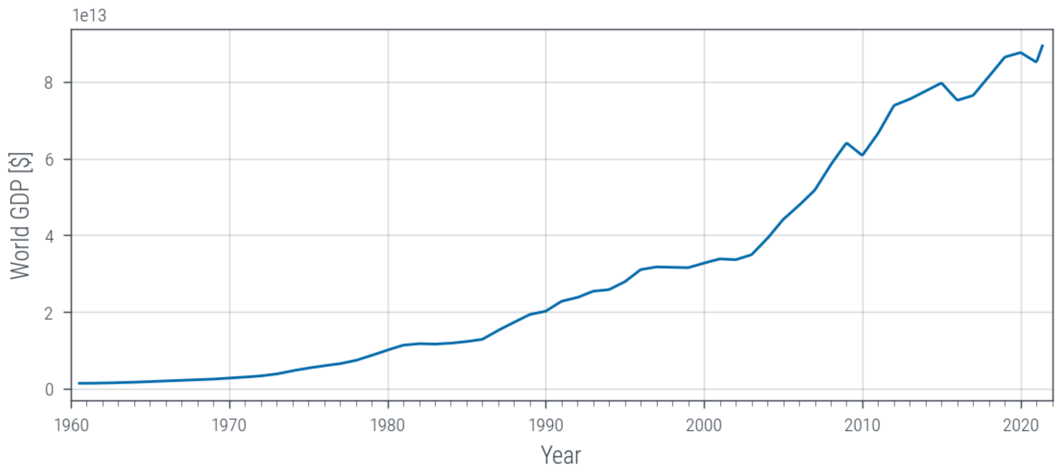


We will work under the hypothesis that the total gross domestic product (GDP) of the world economy has a causal effect on the atmospheric CO2 concentration.

The `data["world_gdp"]` array contains estimates of the world GDP over time. The raw data is made available by the World Bank and has been linearly interpolated to match the temporal resolution of the atmospheric CO_2 data.

[ ]:
```
setup_plot(plt.gca())

plt.plot(
    data["date"],
    data["world_gdp"],
    label="World GDP",
    color=rgb.tue_blue,
)

plt.ylabel("World GDP [$]")
```

[ ]:
```
Text(0, 0.5, 'World GDP [$]')
```

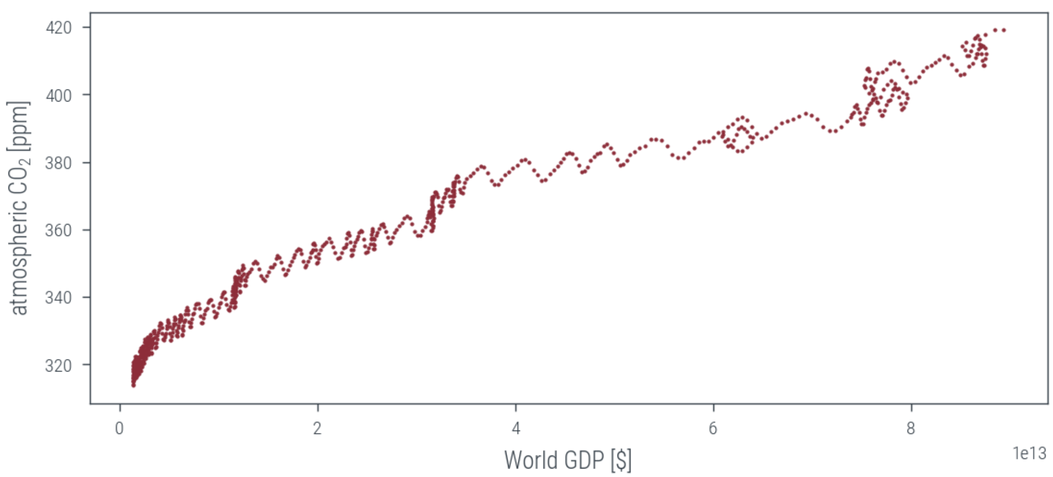


Comparing the plots of the atmospheric CO_2 concentration and the world GDP over time, there seems to be a relationship between the two.

To emphasize this, we plot the two against one another.

[ ]:
```
plt.plot(
    data["world_gdp"],
    data["atmospheric_co2"],
    ".",
    markersize=1,
)

plt.xlabel("World GDP [$]")
plt.ylabel("atmospheric CO$_2$ [ppm]")
```

[ ]:
```
Text(0, 0.5, 'atmospheric CO$_2$ [ppm]')
```



This plot suggests that a globally linear relationship between the world GDP and the atmospheric CO_2 concentration with some local deviations might explain the data reasonably well.

1.2.2 Building a Prior

We will now build a non-stationary GP prior f for explaining this phenomenon.

[ ]:
```
import dataclasses
from collections.abc import Callable


@dataclasses.dataclass
class Gaussian:
    # Gaussian distribution with mean mu and covariance Sigma
    mu: jnp.ndarray  # shape (D,)
    Sigma: jnp.ndarray  # shape (D,D)

    @functools.cached_property
    def L(self):
        """Cholesky decomposition of the covariance matrix"""
        return jnp.linalg.cholesky(self.Sigma)

    @functools.cached_property
    def L_factor(self):
        """Cholesky factorization of the covariance matrix
        (for use in jax.scipy.linalg.cho_solve)"""
        return jax.scipy.linalg.cho_factor(self.Sigma, lower=True)

    @functools.cached_property
    def logdet(self):
        """log-determinant of the covariance matrix
        e.g. for computing the log-pdf
        """
        return 2 * jnp.sum(jnp.log(jnp.diag(self.L)))

    @functools.cached_property
    def prec(self):
        """precision matrix.
        you probably don't want to use this directly, but rather prec_mult
        """
        return jnp.linalg.inv(self.Sigma)

    def prec_mult(self, x):
        """precision matrix multiplication
        implements Sigma^{-1} @ x. For numerical stability, we use the Cholesky␣
 ↪factorization
        """
        return jax.scipy.linalg.cho_solve(self.L_factor, x)
```

```
    @functools.cached_property
    def mp(self):
        """precision-adjusted mean"""
        return self.prec_mult(self.mu)

    def log_pdf(self, x):
        """log N(x;mu,Sigma)"""
        return (
            -0.5 * (x - self.mu) @ self.prec_mult(x - self.mu)
            - 0.5 * self.logdet
            - 0.5 * len(self.mu) * jnp.log(2 * jnp.pi)
        )

    def __mult__(self, other):
        """
        Products of Gaussian pdfs are Gaussian pdfs!
        Multiplication of two Gaussian PDFs  (not RVs!)
        other: Gaussian RV
        """
        Sigma = jnp.linalg.inv(self.prec + other.prec)
        mu = Sigma @ (self.mp + other.mp)
        return Gaussian(mu=mu, Sigma=Sigma)

    def __rmatmul__(self, A):
        """Linear maps of Gaussian RVs are Gaussian RVs
        A: linear map, shape (N,D)
        """
        return Gaussian(mu=A @ self.mu, Sigma=A @ self.Sigma @ A.T)

    @functools.singledispatchmethod
    def __add__(self, other):
        """Affine maps of Gaussian RVs are Gaussian RVs
        shift of a Gaussian RV by a constant.
        We implement this as a singledispatchmethod, because jnp.ndarrays can␣
↪not be dispatched on,
        and register the addition of two RVs below
        """
        other = jnp.asarray(other)
        return Gaussian(mu=self.mu + other, Sigma=self.Sigma)

    def condition(self, A, y, Lambda):
        """Linear conditionals of Gaussian RVs are Gaussian RVs
        Conditioning of a Gaussian RV on a linear observation
        A: observation matrix, shape (N,D)
        y: observation, shape (N,)
        Lambda: observation noise covariance, shape (N,N)
```

```
        """
        Gram = A @ self.Sigma @ A.T + Lambda
        L = jax.scipy.linalg.cho_factor(Gram, lower=True)
        mu = self.mu + self.Sigma @ A.T @ jax.scipy.linalg.cho_solve(L, y - A @␣
↪self.mu)
        Sigma = self.Sigma - self.Sigma @ A.T @ jax.scipy.linalg.cho_solve(
            L, A @ self.Sigma
        )
        return Gaussian(mu=mu, Sigma=Sigma)

    @functools.cached_property
    def std(self):
        # standard deviation
        return jnp.sqrt(jnp.diag(self.Sigma))

    def sample(self, key, num_samples=1):
        """
         sample from the Gaussian
        # alternative implementation: works because the @ operator contracts on␣
↪the second-to-last axis on the right
        # return (self.L @ jax.random.normal(key, shape=(num_samples, self.mu.
↪shape[0], 1)))[...,0] + self.mu
        # or like this, more explicit, but not as easy to read
        # return jnp.einsum("ij,kj->ki", self.L, jax.random.normal(key,␣
↪shape=(num_samples, self.mu.shape[0]))) + self.mu
        # or the scipy version:
        """
        return jax.random.multivariate_normal(
            key, mean=self.mu, cov=self.Sigma, shape=(num_samples,),␣
↪method="svd"
        )


@Gaussian.__add__.register
def _add_gaussians(self, other: Gaussian):
    # sum of two Gaussian RVs
    return Gaussian(mu=self.mu + other.mu, Sigma=self.Sigma + other.Sigma)


@dataclasses.dataclass
class GaussianProcess:
    # mean function
    m: Callable[[jnp.ndarray], jnp.ndarray]
    # covariance function
    k: Callable[[jnp.ndarray, jnp.ndarray], jnp.ndarray]

    def __call__(self, x):
```

```
        return Gaussian(mu=self.m(x), Sigma=self.k(x[:, None, :], x[None, :, :
↪]))

    def condition(self, y, X, sigma):
        return ConditionalGaussianProcess(
            self, y, X, Gaussian(mu=jnp.zeros_like(y), Sigma=sigma * jnp.
↪eye(len(y)))
        )

    def plot(
        self,
        ax,
        x,
        color=rgb.tue_gray,
        mean_kwargs={},
        std_kwargs={},
        num_samples=0,
        rng_key=None,
    ):
        gp_x = self(x)
        ax.plot(x[:, 0], gp_x.mu, color=color, **mean_kwargs)
        ax.fill_between(
            x[:, 0],
            gp_x.mu - 2 * gp_x.std,
            gp_x.mu + 2 * gp_x.std,
            color=color,
            **std_kwargs
        )
        if num_samples > 0:
            ax.plot(
                x[:, 0],
                gp_x.sample(rng_key, num_samples=num_samples).T,
                color=color,
                alpha=0.2,
            )

    def plot_shaded(
        self,
        ax,
        x,
        color=rgb.tue_gray,
        yrange=None,
        yres=1000,
        mean_kwargs={},
        std_kwargs={},
        num_samples=0,
        rng_key=None,
```

```python
    ):
        if yrange is None:
            yrange = ax.get_ylim()

        gp_x = self(x)
        ax.plot(x[:, 0], gp_x.mu, color=color, **mean_kwargs)

        yy = jnp.linspace(*yrange, yres)[:, None]
        ax.imshow(
            gp_shading(yy, gp_x.mu, gp_x.std),
            extent=[x[0, 0], x[-1, 0], *yrange],
            **std_kwargs,
            aspect="auto",
            origin="lower"
        )

        ax.plot(x[:, 0], gp_x.mu - 2 * gp_x.std, color=color, lw=0.25)
        ax.plot(x[:, 0], gp_x.mu + 2 * gp_x.std, color=color, lw=0.25)
        if num_samples > 0:
            ax.plot(
                x[:, 0],
                gp_x.sample(rng_key, num_samples=num_samples).T,
                color=color,
                alpha=0.2,
            )

def gp_shading(yy, mu, std):
        return jnp.exp(-((yy - mu) ** 2) / (2 * std**2)) # / (std * jnp.sqrt(2␣
 ↪* jnp.pi))

class ConditionalGaussianProcess(GaussianProcess):
    """
    A Gaussian process conditioned on data.
    Implented as a proper python class, which allows inheritance from the␣
 ↪GaussianProcess superclass:
    A conditional Gaussian process contains a Gaussian process prior, provided␣
 ↪at instantiation.
    """

    def __init__(self, prior, y, X, epsilon: Gaussian):
        self.prior = prior
        self.y = jnp.atleast_1d(y)  # shape: (n_samples,)
        self.X = jnp.atleast_2d(X)  # shape: (n_samples, n_features)
        self.epsilon = epsilon
        # initialize the super class
        super().__init__(self._mean, self._covariance)
```

```
    @functools.cached_property
    def predictive_covariance(self):
        return self.prior.k(self.X[:, None, :], self.X[None, :, :]) + self.
↪epsilon.Sigma

    @functools.cached_property
    def predictive_mean(self):
        return self.prior.m(self.X) + self.epsilon.mu

    @functools.cached_property
    def predictive_covariance_cho(self):
        return jax.scipy.linalg.cho_factor(self.predictive_covariance)

    @functools.cached_property
    def representer_weights(self):
        return jax.scipy.linalg.cho_solve(
            self.predictive_covariance_cho,
            self.y - self.predictive_mean,
        )

    def _mean(self, x):
        x = jnp.asarray(x)
        return (
            self.prior.m(x)
            + self.prior.k(x[..., None, :], self.X[None, :, :])
            @ self.representer_weights
        )

    @functools.partial(jnp.vectorize, signature="(d),(d)->()", excluded={0})
    def _covariance(self, a, b):
        return self.prior.k(a, b) - self.prior.k(
            a, self.X
        ) @ jax.scipy.linalg.cho_solve(
            self.predictive_covariance_cho,
            self.prior.k(self.X, b),
        )

    def _m_proj(self, x, projection, projection_mean):
        x = jnp.asarray(x)

        if projection_mean is None:
            projection_mean = self.prior.m

        return (
            projection_mean(x)
            + projection(x[..., None, :], self.X[None, :, :]) @ self.
↪representer_weights
```

```
        )

    @functools.partial(jnp.vectorize, signature="(d),(d)->()", excluded={0, 3})
    def _cov_proj(self, a, b, projection):
        return projection(a, b) - projection(a, self.X) @ jax.scipy.linalg.
↪cho_solve(
            self.predictive_covariance_cho,
            projection(b, self.X),
        )

    def project(self, k_proj, m_proj=None):
        return GaussianProcess(
            lambda x: self._m_proj(x, k_proj, m_proj),
            lambda x0, x1: self._cov_proj(x0, x1, k_proj),
        )
```

[ ]:
```
# Let's define some commonly used building blocks for GP models
def zero_mean(x):
    return jnp.zeros_like(x[..., 0])

def gaussian_kernel(x0, x1, ell=1.0, theta=1.0):
    return theta**2 * jnp.exp(-jnp.sum((x0 - x1)**2, axis=-1) / (2. * ell**2))

def rational_quadratic_kernel(x0, x1, alpha=1.0, ell=1.0, theta=1.0):
    return theta**2 * (
        1 + jnp.sum((x0 - x1) ** 2, axis=-1) / (2 * alpha * ell**2)
    ) ** (-alpha)

def matern_1_2_kernel(x0, x1, ell=1.0, theta=1.0):
    return theta**2 * jnp.exp(
        -jnp.linalg.norm(x0 - x1, 2, axis=-1) / ell
    )
```

[ ]:
```
from matplotlib.colors import LinearSegmentedColormap

cmap_rw = LinearSegmentedColormap.from_list(
    "rw", [(1, 1, 1), rgb.tue_red], N=1024)
cmap_dw = LinearSegmentedColormap.from_list(
    "dw", [(1, 1, 1), rgb.tue_dark], N=1024)
cmap_bw = LinearSegmentedColormap.from_list(
    "bw", [(1, 1, 1), rgb.tue_blue], N=1024)
cmap_gw = LinearSegmentedColormap.from_list(
    "gw", [(1, 1, 1), rgb.tue_green], N=1024)
cmap_bwr = LinearSegmentedColormap.from_list(
    "bwr", [rgb.tue_blue, (1, 1, 1), rgb.tue_red], N=1024
)
```

Our prior will be a modification of the model from the lecture, which replaces the long-term trend by a GDP-based additive component. To inform the GP about the current value of the GDP, we will construct a bivariate model with inputs

$$f(t, \mathrm{GDP}(t)). \tag{1}$$

This way, we can still interpret our GP as a univariate function of time if we know the (approximate) GPD at every evaluation point t.

[ ]:
```
X = jnp.stack(
    (data["date"], data["world_gdp"]),
    axis=-1,
)
y = jnp.asarray(data["atmospheric_co2"])

X_train = X[:-200, :]
y_train = y[:-200]
```

```
No GPU/TPU found, falling back to CPU. (Set TF_CPP_MIN_LOG_LEVEL=0 and rerun for
more info.)
```

[ ]:
```
def decompose_t_gdp(t_gdp):
    """This function will come in handy when implementing mean functions and␣
↪kernels for the GP."""
    t_gdp = jnp.asarray(t_gdp)
    return t_gdp[..., 0], t_gdp[..., 1]
```

Like the model in the lecture, our GP prior will be an additive combination of simpler GP priors with different responsibilities:

$$f(t, \mathrm{GDP}(t)) = f_{\mathrm{const}}(t) + f_{\mathrm{GDP}}(t, \mathrm{GDP}(t)) + f_{\mathrm{period}}(t) + f_{\text{mid-term}}(t) + f_{\mathrm{weather}}(t). \tag{2}$$

First, we extend the model from the lecture by allowing the GP to learn the constant component f_{const} of the posterior. We can achieve this this by constructing a parametric GP with one constant feature function $\phi(t) = 1$, i.e.

$$f_{\mathrm{const}}(t) = \phi(t) w_{\mathrm{const}}, \tag{3}$$

where $w_{\mathrm{const}} \sim \mathcal{N}(\mu_{\mathrm{const}}, \theta^2_{\mathrm{const}})$. The constant mean function in the model from the lecture was a limiting case of this component with $\theta^2_{\mathrm{const}} = 0$.

Task: Implement the mean and kernel of f_{const}.

[ ]:
```
# we set the mean to a constant function at the data minimum
mu_const = np.min(y_train)
theta_const = jnp.std(y_train)


def constant_mean(t_gdp, mu=mu_const):
    t, _ = decompose_t_gdp(t_gdp)
    const_mean = mu * jnp.ones_like(t)
```

```
    return const_mean


def constant_kernel(t_gdp0, t_gdp1, theta=theta_const):
    t0, _ = decompose_t_gdp(t_gdp0)
    t1, _ = decompose_t_gdp(t_gdp1)
    const_kernel = gaussian_kernel(jnp.ones_like(t0[..., None]), jnp.
 ↪ones_like(t1[..., None]), theta=theta)
    return const_kernel
```

As noted above, the data suggests a globally linear relationship with some local deviations between atmospheric CO_2 concentration and world GDP. The component f_{GDP} models this assumption using a GP:

$$f_{\mathrm{GDP}}(t, \mathrm{GDP}(t)) := \mathrm{GDP}(t) \cdot (c_{\mathrm{GDP}} + g_{\mathrm{GDP}}(t)), \tag{4}$$

with

$$\begin{aligned} c_{\mathrm{GDP}} &\sim \mathcal{N}(\mu_{\mathrm{GDP,c}}, \theta^2_{\mathrm{GDP,c}}), \qquad \text{and} \\ g_{\mathrm{GDP}} &\sim \mathcal{GP}(0, \theta^2_{\mathrm{GDP,g}} \cdot k_{\mathrm{RQ}}), \end{aligned}$$

where k_{RQ} is a rational quadratic kernel with lengthscale $\ell_{\mathrm{GDP,g}}$ and shape parameter $\alpha_{\mathrm{GDP,g}}$.

Task: Implement the mean and kernel of f_{GDP}.

[ ]:
```
# Parameters for the GDP mean function
mu_c_gdp = np.mean((y_train - mu_const) / X_train[..., 1])  # ppm / dollar
theta_c_gdp = np.std((y_train - mu_const) / X_train[..., 1])  # ppm / dollar

# Parameters for the GDP kernel
alpha_g_gdp = 1.  # unitless
ell_g_gdp = 10.  # years
theta_g_gdp = mu_c_gdp / 2. - theta_c_gdp  # ppm / dollar

def gdp_mean(t_gdp, mu_c=mu_c_gdp):
    _, gdp = decompose_t_gdp(t_gdp)
    f_gdp_mean = gdp * mu_c
    return f_gdp_mean

def gdp_kernel(
    t_gdp0,
    t_gdp1,
    theta_c=theta_c_gdp,
    alpha_g=alpha_g_gdp,
    ell_g=ell_g_gdp,
    theta_g=theta_g_gdp,
```

```
):
    t0, gdp0 = decompose_t_gdp(t_gdp0)
    t1, gdp1 = decompose_t_gdp(t_gdp1)
    c_gdp = gaussian_kernel(jnp.ones_like(t0[..., None]), jnp.ones_like(t1[...,␣
↪None]), theta=theta_c)
    g_gdp_kernel = rational_quadratic_kernel(t0[..., None],  t1[..., None],␣
↪alpha=alpha_g, ell=ell_g, theta=theta_g)
    f_gdp_kernel = gdp0 * gdp1 * (c_gdp + g_gdp_kernel)

    # Alternative implementation:
    # kernel = rational_quadratic_kernel(t0[..., None],  t1[..., None],␣
↪alpha=alpha_g, ell=ell_g, theta=theta_g) * theta_g**2
    # f_gdp_kernel = gdp0 * gdp1 * (kernel + theta_c**2)
    return f_gdp_kernel
```

The periodic and mid-term components are identical to those in the model from the lecture.

[ ]:
```
theta_periodic = 5.0  # ppm
ell_decay_periodic = 50.0  # years
ell_periodic = 1.0  # years

periodic_mean = zero_mean

def periodic_kernel(
    t_gdp0,
    t_gdp1,
    period=1.0,
    ell_periodic=ell_periodic,
    ell_decay=ell_decay_periodic,
    theta=theta_periodic,
):
    t0, _ = decompose_t_gdp(t_gdp0)
    t1, _ = decompose_t_gdp(t_gdp1)

    return (
        theta**2
        * jnp.exp(
            -2
            * jnp.sin(jnp.pi * (t0 - t1) / period) ** 2
            / ell_periodic**2
        )
        * gaussian_kernel(
            t0[..., None],
            t1[..., None],
            ell=ell_decay,
        )
    )
```

```
[ ]: theta_mid_term = 1.0  # ppm
ell_mid_term = 1.0  # years
alpha_mid_term = 1.0  # unitless

mid_term_trend_mean = zero_mean

def mid_term_trend_kernel(t_gdp0, t_gdp1, ell=ell_mid_term,␣
 ↪alpha=alpha_mid_term, theta=theta_mid_term):
    t0, _ = decompose_t_gdp(t_gdp0)
    t1, _ = decompose_t_gdp(t_gdp1)

    return rational_quadratic_kernel(
        t0[..., None],
        t1[..., None],
        alpha=alpha,
        ell=ell,
        theta=theta,
    )
```

The local weather component is a slight modification of the corresponding term in the model from the lecture. Instead of the Gaussian kernel, we use a Matérn-$\frac{1}{2}$ kernel here and we also drop the white-noise kernel, since we model measurement noise explicitly.

```
[ ]: theta_weather = 0.1  # ppm
ell_weather = 0.1  # years

weather_mean = zero_mean

def weather_kernel(t_gdp0, t_gdp1, ell=ell_weather, theta=theta_weather):
    t0, _ = decompose_t_gdp(t_gdp0)
    t1, _ = decompose_t_gdp(t_gdp1)

    return matern_1_2_kernel(
        t0[..., None],
        t1[..., None],
        ell=ell,
        theta=theta,
    )
```

We now combine these building blocks into a common model.

```
[ ]: def model_mean(t_gdp, parameters):
    return (
        constant_mean(t_gdp, mu=parameters["mu_const"])
        + gdp_mean(t_gdp, mu_c=parameters["mu_c_gdp"])
        + periodic_mean(t_gdp)
        + mid_term_trend_mean(t_gdp)
        + weather_mean(t_gdp)
```

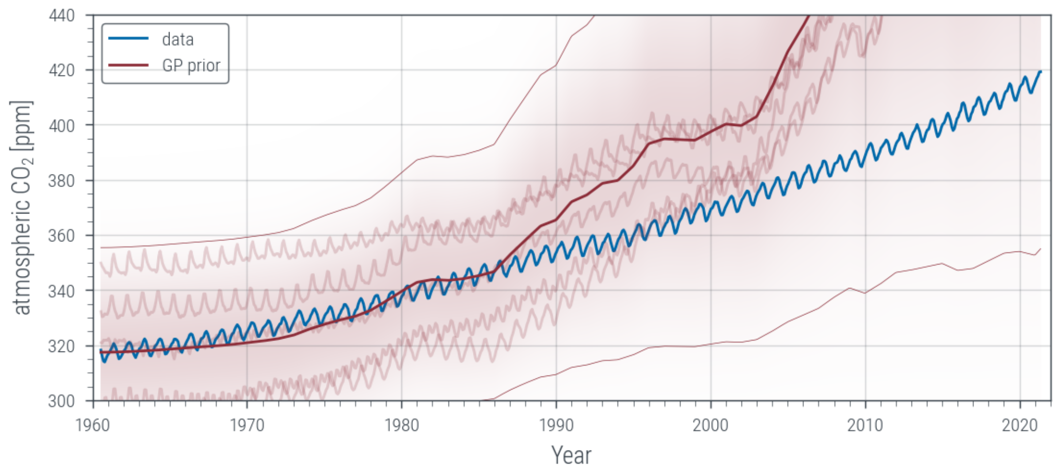
```
    )


def model_kernel(t_gdp0, t_gdp1, parameters):
    return (
        constant_kernel(
            t_gdp0,
            t_gdp1,
            theta=parameters["theta_const"],
        )
        + gdp_kernel(
            t_gdp0,
            t_gdp1,
            theta_c=theta_c_gdp,  # parameters["theta_c_gdp"],
            alpha_g=parameters["alpha_g_gdp"],
            ell_g=parameters["ell_g_gdp"],
            theta_g=theta_g_gdp,  # parameters["theta_g_gdp"],
        )
        + periodic_kernel(
            t_gdp0,
            t_gdp1,
            ell_periodic=parameters["ell_periodic"],
            ell_decay=parameters["ell_decay_periodic"],
            theta=parameters["theta_periodic"],
        )
        + mid_term_trend_kernel(
            t_gdp0,
            t_gdp1,
            ell=parameters["ell_mid_term"],
            alpha=parameters["alpha_mid_term"],
            theta=parameters["theta_mid_term"],
        )
        + weather_kernel(
            t_gdp0,
            t_gdp1,
            ell=parameters["ell_weather"],
            theta=parameters["theta_weather"],
        )
    )


# initial guesses for the parameters:
init_params = {
    "mu_const": mu_const,
    "theta_const": theta_const,
    "mu_c_gdp": mu_c_gdp,
    "theta_c_gdp": theta_c_gdp,
```

```python
    "alpha_g_gdp": alpha_g_gdp,
    "ell_g_gdp": ell_g_gdp,
    "theta_g_gdp": theta_g_gdp,
    "ell_periodic": ell_periodic,
    "ell_decay_periodic": ell_decay_periodic,
    "theta_periodic": theta_periodic,
    "ell_mid_term": ell_mid_term,
    "alpha_mid_term": alpha_mid_term,
    "theta_mid_term": theta_mid_term,
    "ell_weather": ell_weather,
    "theta_weather": theta_weather,
    "sigma": 0.2,
}


gp = GaussianProcess(
    functools.partial(model_mean, parameters=init_params),
    functools.partial(model_kernel, parameters=init_params),
)
```

Let's visualize the prior.

[ ]:
```python
setup_plot(plt.gca())
plot_data(plt.gca())
gp.plot_shaded(
    plt.gca(),
    X,
    yres=1000,
    color=rgb.tue_red,
    mean_kwargs={"label": "GP prior"},
    std_kwargs={"alpha": 0.2, "cmap": cmap_rw},
    num_samples=5,
    rng_key=jax.random.PRNGKey(3),
)
plt.legend()
```

[ ]:
```
<matplotlib.legend.Legend at 0x7fb6e0a361d0>
```

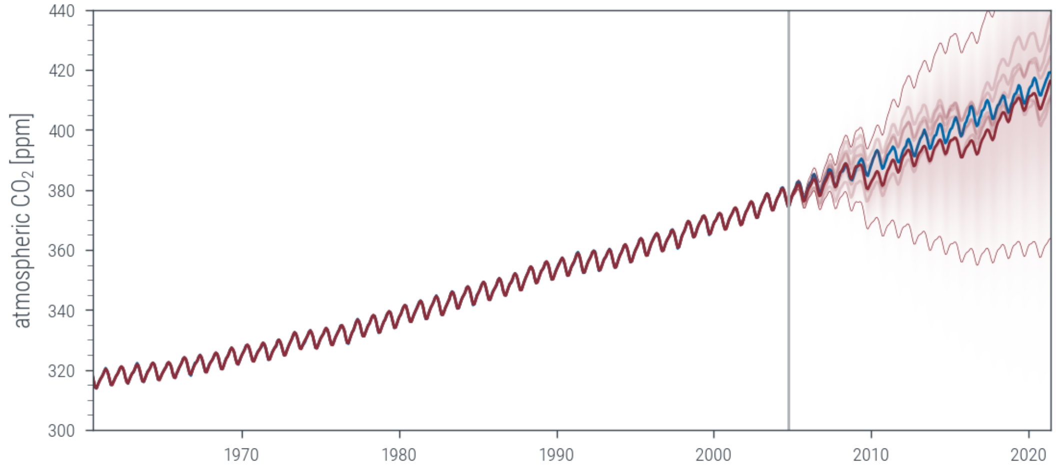


Compared to the model from the lecture, it is arguably much more plausible that the data was generated by this model.

1.2.3 Posterior

[ ]:
```
gp_posterior = gp.condition(y_train, X_train, sigma=init_params["sigma"]**2)

plot_data(plt.gca())
gp_posterior.plot_shaded(
    plt.gca(),
    X,
    yres=1000,
    color=rgb.tue_red,
    mean_kwargs={"label": "GP posterior mean"},
    std_kwargs={"alpha": 0.2, "cmap": cmap_rw},
    num_samples=5,
    rng_key=jax.random.PRNGKey(3),
)
plt.axvline(X_train[-1, 0], color=rgb.tue_gray)
```

[ ]:
```
<matplotlib.lines.Line2D at 0x7fb6a82e6b50>
```



The posterior belief also seems to extrapolate reasonably well.

1.2.4 Hyperparameter Optimization

[ ]:
```
import jaxopt


def NegEvidence(parameters):
    gp = GaussianProcess(
        functools.partial(model_mean, parameters=parameters),
        functools.partial(model_kernel, parameters=parameters),
    )

    noise = Gaussian(
        jnp.zeros_like(y_train),
        parameters["sigma"]**2 * jnp.eye(y_train.size),
    )

    predictive = gp(X_train) + noise

    return -predictive.log_pdf(y_train)

print(NegEvidence(init_params))

optim = jaxopt.ScipyMinimize(
    fun=jax.value_and_grad(NegEvidence),
    method="CG",
    value_and_grad=True,
    maxiter=100,
    jit=True,
    options={"disp": True},
```

```python
)

opt_params, _ = optim.run(init_params)
```

```
200.27384305112673
Warning: Desired error not necessarily achieved due to precision loss.
         Current function value: 200.273843
         Iterations: 0
         Function evaluations: 15
         Gradient evaluations: 3
```

[ ]:
```python
init_params
```

[ ]:
```
{'mu_const': Array(313.83, dtype=float64),
 'theta_const': Array(18.2290585, dtype=float64),
 'mu_c_gdp': Array(2.55110483e-12, dtype=float64),
 'theta_c_gdp': Array(9.80674419e-13, dtype=float64),
 'alpha_g_gdp': 1.0,
 'ell_g_gdp': 10.0,
 'theta_g_gdp': Array(2.94877997e-13, dtype=float64),
 'ell_periodic': 1.0,
 'ell_decay_periodic': 50.0,
 'theta_periodic': 5.0,
 'ell_mid_term': 1.0,
 'alpha_mid_term': 1.0,
 'theta_mid_term': 1.0,
 'ell_weather': 0.1,
 'theta_weather': 0.1,
 'sigma': 0.2}
```

[ ]:
```python
opt_params
```

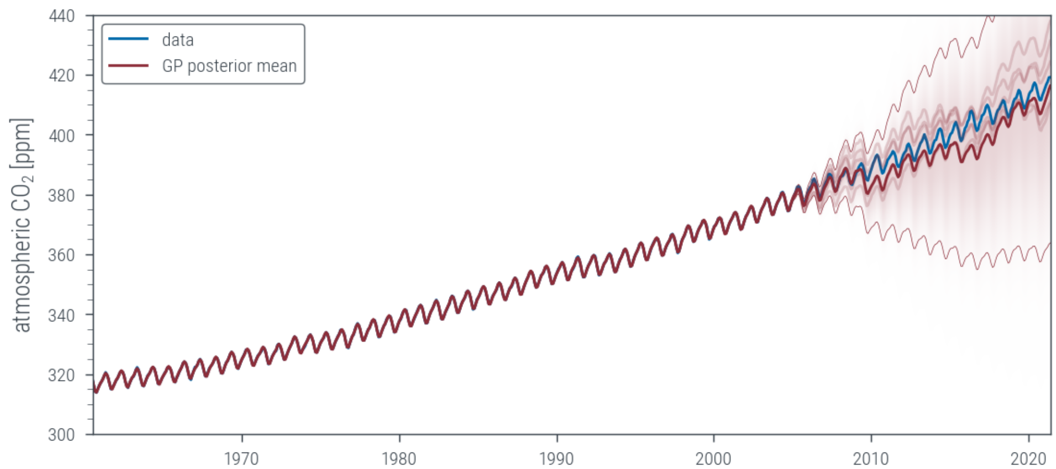
[ ]:
```
{'alpha_g_gdp': Array(1., dtype=float64),
 'alpha_mid_term': Array(1., dtype=float64),
 'ell_decay_periodic': Array(50., dtype=float64),
 'ell_g_gdp': Array(10., dtype=float64),
 'ell_mid_term': Array(1., dtype=float64),
 'ell_periodic': Array(1., dtype=float64),
 'ell_weather': Array(0.1, dtype=float64),
 'mu_c_gdp': Array(2.55110483e-12, dtype=float64),
 'mu_const': Array(313.83, dtype=float64),
 'sigma': Array(0.2, dtype=float64),
 'theta_c_gdp': Array(9.80674419e-13, dtype=float64),
 'theta_const': Array(18.2290585, dtype=float64),
 'theta_g_gdp': Array(2.94877997e-13, dtype=float64),
 'theta_mid_term': Array(1., dtype=float64),
 'theta_periodic': Array(5., dtype=float64),
```

```
 'theta_weather': Array(0.1, dtype=float64)}
```

[ ]:
```
gp = GaussianProcess(
    functools.partial(model_mean, parameters=opt_params),
    functools.partial(model_kernel, parameters=opt_params),
)
```

[ ]:
```
gp_posterior = gp.condition(y_train, X_train, sigma=opt_params["sigma"]**2)

plot_data(plt.gca())
gp_posterior.plot_shaded(
    plt.gca(),
    X,
    yres=1000,
    color=rgb.tue_red,
    mean_kwargs={"label": "GP posterior mean"},
    std_kwargs={"alpha": 0.2, "cmap": cmap_rw},
    num_samples=5,
    rng_key=jax.random.PRNGKey(3),
)
plt.legend()
```

[ ]:
```
<matplotlib.legend.Legend at 0x7fb628681a50>
```



1.2.5 Source Separation

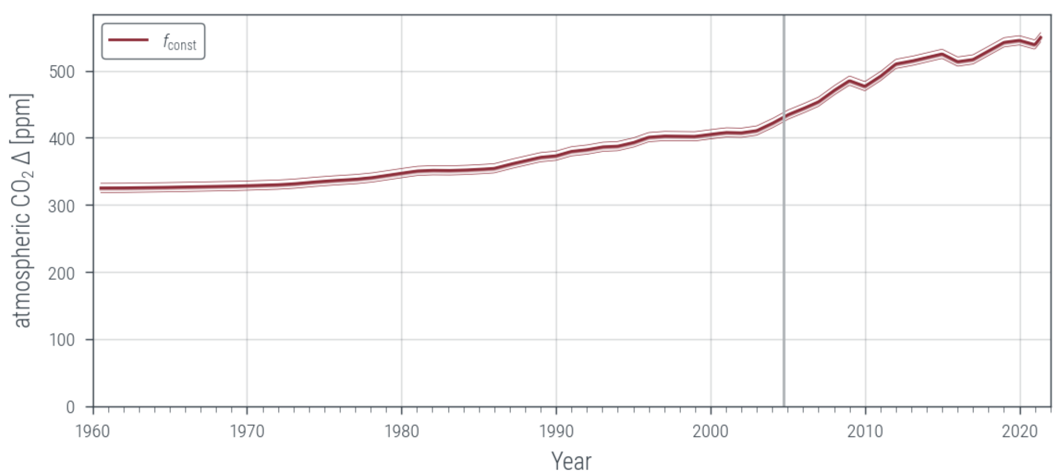
Task: Visualize the individual posterior belief over all additive components (f_{const}, f_{GDP}, f_{periodic}, $f_{\text{mid-term}}$, f_{weather}) using source separation.

[ ]:
```
def plot_component(ax, gp_component: GaussianProcess, component_label: str):
    setup_plot(ax)
```

```
    ax.set_ylabel("atmospheric CO$_2$ $\Delta$ [ppm]")
    gp_component.plot_shaded(
        ax,
        X,
        yres=1000,
        color=rgb.tue_red,
        mean_kwargs={"label": component_label},
        std_kwargs={"alpha": 0.2, "cmap": cmap_rw},
        num_samples=5,
        rng_key=jax.random.PRNGKey(3),
    )
    ax.axvline(X_train[-1, 0], color=rgb.tue_gray)
```

[ ]:
```
# Use this instead to view the constant component contribution
# gp_constant = GaussianProcess(
#     functools.partial(constant_mean, mu=opt_params["mu_const"]),
#     functools.partial(constant_kernel, theta=opt_params["theta_const"]),
# )

# Similar to lecture examples
const_comp = functools.partial(constant_kernel, theta=opt_params["theta_const"])
gp_constant = gp_posterior.project(const_comp)

plot_component(plt.gca(), gp_constant, "$f_\mathrm{const}$")
plt.legend()
```

[ ]:
```
<matplotlib.legend.Legend at 0x7fb6286c5d90>
```



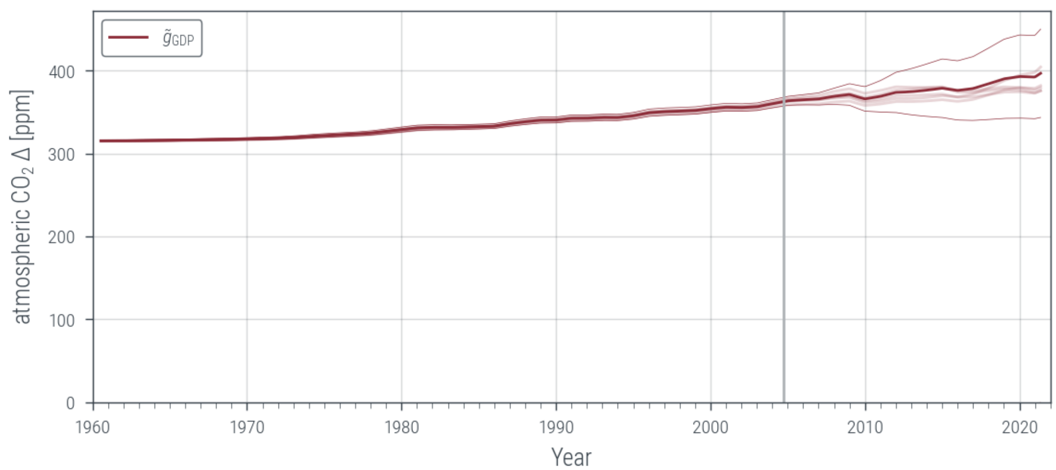
Task: Plot the posterior belief over

$$\tilde{g}_{\mathrm{GDP}}(t, \mathrm{GDP}(t)) := \mathrm{GDP}(t) \cdot g_{\mathrm{GDP}}(t)$$

using source separation.

[ ]:
```
# Use this instead to view the contribution
# gp_g_tilde =  GaussianProcess(
#     functools.partial(gdp_mean, mu_c=opt_params["mu_c_gdp"]),
#     functools.partial(gdp_kernel, theta_c=opt_params["theta_c_gdp"],␣
↪alpha_g=opt_params["alpha_g_gdp"], ell_g=opt_params["ell_g_gdp"],␣
↪theta_g=opt_params["theta_g_gdp"]),
# )

# Similar to Lecture Examples
gp_g_comp = functools.partial(gdp_kernel, alpha_g=opt_params["alpha_g_gdp"],␣
↪ell_g=opt_params["ell_g_gdp"], theta_g=opt_params["theta_g_gdp"])
gp_g_tilde = gp_posterior.project(gp_g_comp)

plot_component(plt.gca(), gp_g_tilde, r"$\tilde{g}_\mathrm{GDP}$")
plt.legend()
```

[ ]:
```
<matplotlib.legend.Legend at 0x7fb6285a8a90>
```



1.2.6 Discussion

Interpret the results. Is this a good model of the data? What could be improved and how?

If there is enough time in the tutorial, we'll discuss your thoughts.

In its current state, the model is able to represent big portion of the data. To improve the model, more terms/parameters can be added to increase capacity of the model for the cost of computation and memory.