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import numpy as np

from matplotlib import pyplot as plt
from sklearn.datasets import fetch_openml
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels \
    import RBF, WhiteKernel, RationalQuadratic, ExpSineSquared

print(__doc__)

def load_mauna_loa_atmospheric_co2():
    ml_data = fetch_openml(data_id=41187, as_frame=False)
    months = []
    ppmv_sums = []
    counts = []

    y = ml_data.data[:, 0]
    m = ml_data.data[:, 1]
    month_float = y + (m - 1) / 12
    ppmvs = ml_data.target

    for month, ppmv in zip(month_float, ppmvs):
        if not months or month != months[-1]:
            months.append(month)
            ppmv_sums.append(ppmv)
            counts.append(1)
        else:
            # aggregate monthly sum to produce average
            ppmv_sums[-1] += ppmv
            counts[-1] += 1

    months = np.asarray(months).reshape(-1, 1)
    avg_ppmvs = np.asarray(ppmv_sums) / counts
    return months, avg_ppmvs

X, y = load_mauna_loa_atmospheric_co2()

# Kernel with parameters given in GPML book
k1 = 66.0**2 * RBF(length_scale=67.0) # long term smooth rising trend
k2 = 2.4**2 * RBF(length_scale=90.0) \
    * ExpSineSquared(length_scale=1.3, periodicity=1.0) # seasonal component
# medium term irregularity
k3 = 0.66**2 \
    * RationalQuadratic(length_scale=1.2, alpha=0.78)
k4 = 0.18**2 * RBF(length_scale=0.134) \
    + WhiteKernel(noise_level=0.19**2) # noise terms
kernel_gpml = k1 + k2 + k3 + k4

gp = GaussianProcessRegressor(kernel=kernel_gpml, alpha=0,
                              optimizer=None, normalize_y=True)

gp.fit(X, y)

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print("GPML kernel: %s" % gp.kernel_)
print("Log-marginal-likelihood: %.3f"
      % gp.log_marginal_likelihood(gp.kernel_.theta))

# Kernel with optimized parameters
k1 = 50.0**2 * RBF(length_scale=50.0) # long term smooth rising trend
k2 = 2.0**2 * RBF(length_scale=100.0) \
    * ExpSineSquared(length_scale=1.0, periodicity=1.0,
                      periodicity_bounds="fixed") # seasonal component
# medium term irregularities
k3 = 0.5**2 * RationalQuadratic(length_scale=1.0, alpha=1.0)
k4 = 0.1**2 * RBF(length_scale=0.1) \
    + WhiteKernel(noise_level=0.1**2,
                  noise_level_bounds=(1e-5, np.inf)) # noise terms
kernel = k1 + k2 + k3 + k4

gp = GaussianProcessRegressor(kernel=kernel, alpha=0,
                              normalize_y=True)
gp.fit(X, y)

print("\nLearned kernel: %s" % gp.kernel_)
print("Log-marginal-likelihood: %.3f"
      % gp.log_marginal_likelihood(gp.kernel_.theta))

X_ = np.linspace(X.min(), X.max() + 30, 1000)[: , np.newaxis]
y_pred, y_std = gp.predict(X_, return_std=True)

# Illustration
plt.scatter(X, y, c='k')
plt.plot(X_, y_pred)
plt.fill_between(X_[ :, 0], y_pred - y_std, y_pred + y_std,
                 alpha=0.5, color='k')
plt.xlim(X_.min(), X_.max())
plt.xlabel("Year")
plt.ylabel(r"CO$_2$ in ppm")
plt.title(r"Atmospheric CO$_2$ concentration at Mauna Loa")
plt.tight_layout()
plt.show()

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Automatically created module for IPython interactive environment

GPML kernel: 66**2 * RBF(length_scale=67) + 2.4**2 * RBF(length_scale=90) * ExpSineS
 Log-marginal-likelihood: -117.023

Learned kernel: 44.8**2 * RBF(length_scale=51.6) + 2.64**2 * RBF(length_scale=91.5)

Log-marginal-likelihood: -115.050

