EXPLICIT LINK
BETWEEN PERIODIC COVARIANCE FUNCTIONS AND STATE SPACE MODELS

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Gaussian processes and state space models
Periodic covariance functions
Quasi-periodic covariance functions
Example studies
Gaussian Process Regression in 1D

- The kernel approach:

\[ f(t) \sim \mathcal{GP}(0, k(t, t')) \]

\[ y_k = f(t_k) + \varepsilon_k, \quad \varepsilon_k \sim \mathcal{N}(0, \sigma_n^2), \]

where the observed data is \( \{(t_k, y_k), k = 1, 2, \ldots, n\} \).

- Prior assumptions of the process encoded into the covariance function \( k(t, t') \).

- Can be solved in closed-form, but the naive solution scales as \( \mathcal{O}(n^3) \).
Gaussian Process Regression in 1D

- **The kernel approach:**

  \[ f(t) \sim \mathcal{GP}(0, k(t, t')) \]

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  where the observed data is \( \{(t_k, y_k), k = 1, 2, \ldots, n\} \).

- **State space approach:**

  \[ \frac{df(t)}{dt} = Ff(t) + Lw(t) \]

  \[ y_k = Hf(t_k) + \varepsilon_k, \quad \varepsilon_k \sim \mathcal{N}(0, \sigma_n^2), \]

  where \( w(t) \) is a white noise process with spectral density \( Q_c \).

- Prior assumptions of the process encoded into the covariance function \( k(t, t') \).
- Can be solved in closed-form, but the naive solution scales as \( O(n^3) \).
- Model defined by \( F, L, Q_c \), the stationary covariance \( P_\infty \), and the observation model \( H \).
- Solved using Kalman filtering and Rauch–Tung–Striebel smoothing in \( O(n) \) time complexity.
Covariance and Spectral Density

\[ k(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} S(\omega) \exp(-i\omega\tau) \, d\omega. \]

\( \tau = |t - t'| \)

Covariance function \( k(\tau) \)  
Spectral density \( S(\omega) \)
GP Regression (naive solution)
GP Regression (filtering)
GP Regression (smoothing)
Periodic Covariance Functions
Canonical Periodic Covariance Function

Start off with the squared exponential:

\[
k(x, x') = \sigma^2 \exp\left(-\frac{\|x - x'\|^2}{2\ell^2}\right)
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Canonical Periodic Covariance Function

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Polar coordinates:

\[ x(t) = \begin{pmatrix} \cos(\omega_0 t) \\ \sin(\omega_0 t) \end{pmatrix} \]
Canonical Periodic Covariance Function

Start off with the squared exponential:

\[ k(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left( -\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell^2} \right) \]

Polar coordinates:

\[ \mathbf{x}(t) = \begin{pmatrix} \cos(\omega_0 t) \\ \sin(\omega_0 t) \end{pmatrix} \]

The canonical periodic covariance:

\[ k_p(t, t') = \sigma^2 \exp\left( -\frac{2 \sin^2(\omega_0 \frac{t-t'}{2})}{\ell^2} \right) \]
Canonical Periodic Covariance Function

Covariance function

Spectral density
State Space Formulation (1/2)

▷ Fourier series representation ($\tau = |t - t'|$)

$$k_p(\tau) = \sum_{j=0}^{\infty} q_j^2 \cos(j \omega_0 \tau)$$
State Space Formulation (1/2)

- Fourier series representation ($\tau = |t - t'|$)

$$k_p(\tau) = \sum_{j=0}^{\infty} q_j^2 \cos(j \omega_0 \tau)$$

- The model can be constructed as solutions to second-order ODEs:

$$
\begin{pmatrix}
\dot{x}_j(t) \\
\dot{y}_j(t)
\end{pmatrix} =
\begin{pmatrix}
0 & -\omega_0 j \\
\omega_0 j & 0
\end{pmatrix}
\begin{pmatrix}
x_j(t) \\
y_j(t)
\end{pmatrix}
$$
State Space Formulation (2/2)

The state space model can be given as a superposition the following kind of models:

\[ F_j^p = \begin{pmatrix} 0 & -\omega_0 j \\ \omega_0 j & 0 \end{pmatrix}, \quad H_j^p = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad P_{\infty,j}^p = q_j^2 I_2 \]

The diffusion part is zero (i.e. the model is deterministic).
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The spectral (variance) coefficients are

\[
q_j^2 = \frac{2 I_j(\ell^{-2})}{\exp(\ell^{-2})}, \text{ for } j = 1, 2, \ldots,
\]

and \(q_0^2 = I_0(\ell^{-2}) / \exp(\ell^{-2})\), where \(I_\alpha(z)\) is the modified Bessel function.
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The diffusion part is zero (i.e. the model is deterministic).

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and \( q^2_0 = I_0(\ell^2) / \exp(\ell^2) \), where \( I_\alpha(z) \) is the modified Bessel function.

Taking the \( J \) first terms in the series gives an approximation, and this approximation converges uniformly to the actual covariance as \( J \to \infty \).
Approximative Covariance Function \((J = 0)\)

\[
\begin{align*}
-6\pi & \quad -4\pi & \quad -2\pi & \quad 0 & \quad 2\pi & \quad 4\pi & \quad 6\pi \\
|t - t'| & \\
\omega & \quad -6 & \quad -4 & \quad -2 & \quad 0 & \quad 2 & \quad 4 & \quad 6
\end{align*}
\]

Covariance function

Spectral density
Approximative Covariance Function ($J = 1$)

Covariance function

Spectral density
Explicit link between periodic covariance functions and state space models

Approximative Covariance Function ($J = 2$)

Covariance function

Spectral density
Approximative Covariance Function ($J = 3$)

Covariance function

Spectral density
Quasi-Periodic Covariance Functions
Quasi-Periodic Covariance

- Allow the shape of the periodic effect to change over time.
- Take the product of a periodic covariance function $k_p(t, t')$ with a covariance function $k_q(t, t')$ with rather long characteristic length-scale,

$$k(t, t') = k_p(t, t') k_q(t, t'),$$

allowing the covariance to decay away from exact periodicity.
Quasi-Periodic Covariance Function

Covariance function

Spectral density
State space representation of both the ‘quasi’ and ‘periodic’ part.

The quasi-periodic state space model needs to be set up so that the feedback matrices commute ($F_p F_q = F_q F_p$).

This can be accomplished by using the special features of the Kronecker product.
Quasi-Periodic Covariances in State Space Form

- State space representation of both the ‘quasi’ and ‘periodic’ part.
- The quasi-periodic state space model needs to be set up so that the feedback matrices commute \((F_p F_q = F_q F_p)\).
- This can be accomplished by using the special features of the Kronecker product.

- The joint model corresponding to the quasi-periodic product of the two covariance functions can then be given in a block-form:

\[
\begin{align*}
F_j &= F_q \otimes I_2 + I_q \otimes F_p, \\
L_j &= L_q \otimes L_p, \\
Q_{c,j} &= Q_c^q \otimes q_j^2 I_2, \\
P_{\infty,j} &= P_{\infty}^q \otimes P_{\infty,j}^p, \\
H_j &= H_q \otimes H_p,
\end{align*}
\]

where ‘\(\otimes\)’ denotes the Kronecker product of two matrices.
Example Studies
Example: Computational Complexity

- Full GP solution
- State space solution

![Graph showing computational time vs. number of data points](image)

- Computation time (seconds)
  - Full GP solution
  - State space solution

- Number of data points, \( n \)
Example: Mauna Loa CO₂ Concentration

- CO₂ concentration observations ($n = 2227$, years 1958–2000 not shown in figure).
- The GP covariance function is as follows:
  
  $$k(t, t') = k_{SE}(t, t')$$
  $$+ k_p(t, t') \frac{3}{2}(t, t')$$
  $$+ k_{\nu=3/2}(t, t')$$

- Converted to state space and hyperparameters optimized with respect to marginal likelihood.
Example: Daily Births in 1969–1988

- Relative number of births in the US based on daily data between 1969–1988 ($n = 7305$).
- The model is as follows:
  - Matern ($\nu = 7/2$) for the slow trend
  - Matern ($\nu = 3/2$) for faster variation
  - Quasi-periodic (yearly) with Matern ($\nu = 3/2$) damping
  - Quasi-periodic (weekly) with Matern ($\nu = 3/2$) damping
- Converted to state space and hyperparameters optimized with respect to marginal likelihood
Conclusion

- We have established the explicit connection between periodic covariance functions and state space models.

- This link enables the use of efficient sequential inference methods to solve periodic GP regression problems in $\mathcal{O}(n)$ time complexity.

- The approximation converges uniformly and a rough upper bound for the error can be given in closed-form.

- This is a ‘best of both worlds’ approach; it brings together the convenient model specification and hyperparametrization of GPs with the computational efficiency of state space models.
Explicit Link Between Periodic Covariance Functions and State Space Models

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Codes for the examples available at: http://arno.solin.fi

The methods also implemented into the GPSTUFF toolbox for Matlab/Octave.