Aalto University
School of Science

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:**

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

  $$y_k = f(t_k) + \varepsilon_k, \quad \varepsilon_k \sim \mathcal{N}(0, \sigma_\mathrm{n}^2),$$

  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 $\mathcal{O}(n^3)$.

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- **State space approach:**

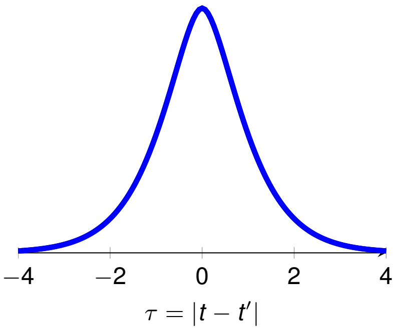
$$\frac{\mathrm{d}\mathbf{f}(t)}{\mathrm{d}t} = \mathbf{F}\mathbf{f}(t) + \mathbf{L}\mathbf{w}(t)$$
$$y_k = \mathbf{H}\mathbf{f}(t_k) + \varepsilon_k, \quad \varepsilon_k \sim \mathcal{N}(0, \sigma_\mathrm{n}^2),$$

  where $\mathbf{w}(t)$ is a white noise process with spectral density $\mathbf{Q}_\mathrm{c}$.

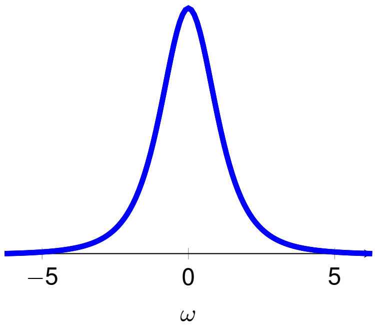
- Model defined by $\mathbf{F}$, $\mathbf{L}$, $\mathbf{Q}_\mathrm{c}$, the stationary covariance $\mathbf{P}_\infty$, and the observation model $\mathbf{H}$.
- Solved using Kalman filtering and Rauch–Tung–Striebel smoothing in $\mathcal{O}(n)$ time complexity.

Covariance and Spectral Density

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

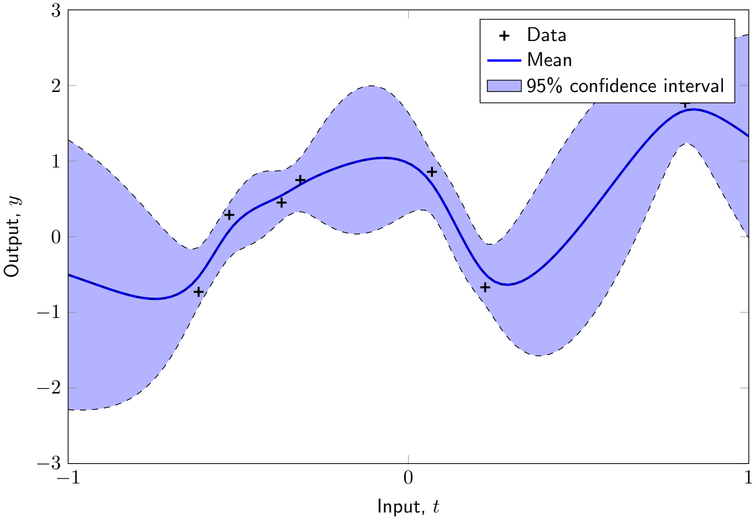


Covariance function $k(\tau)$

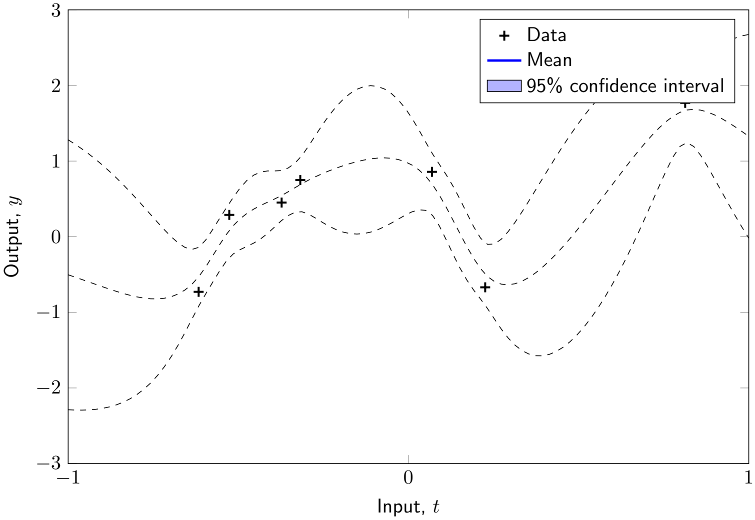


Spectral density $S(\omega)$

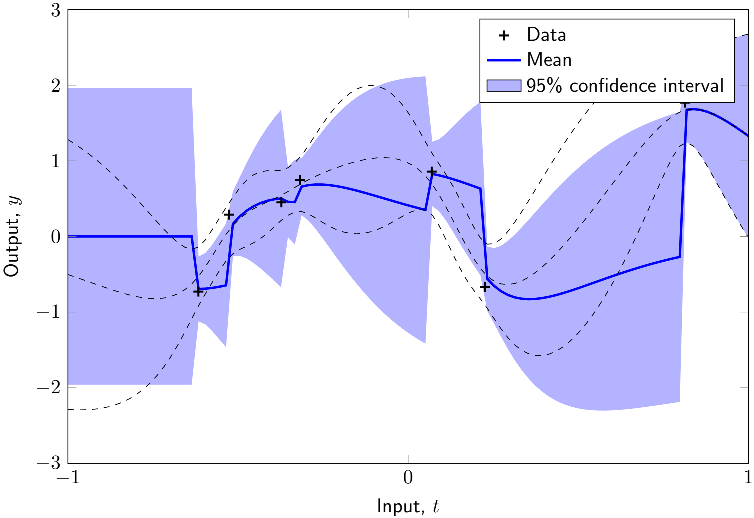
GP Regression (naive solution)



GP Regression (filtering)



GP Regression (smoothing)



Periodic Covariance Functions

Canonical Periodic Covariance Function

Start off with the squared exponential:

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

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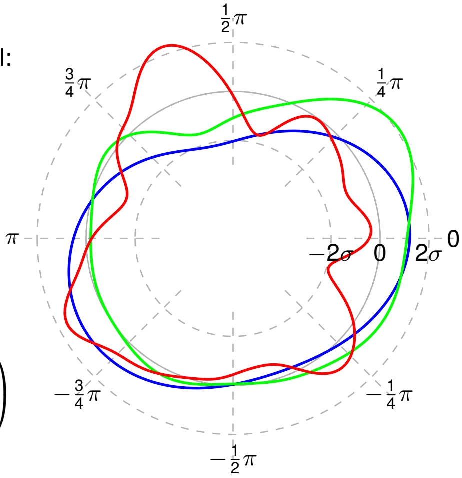
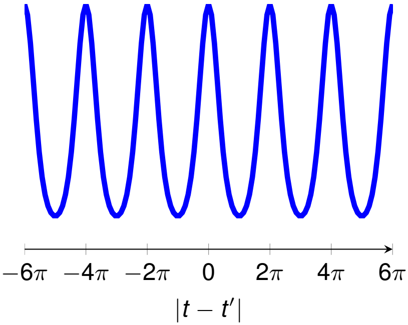
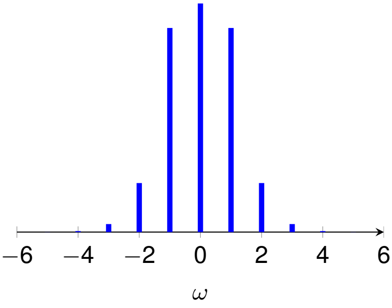
The *canonical* periodic covariance:

$$k_{\mathrm{p}}(t, t') = \sigma^2 \exp\left(-\frac{2\sin^2\left(\omega_0 \frac{t-t'}{2}\right)}{\ell^2}\right)$$



Canonical Periodic Covariance Function





Covariance function | **Spectral density**

State Space Formulation (1/2)

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

$$k_{\mathrm{p}}(\tau) = \sum_{j=0}^{\infty} q_j^2 \cos(j\, \omega_0\, \tau)$$

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$$k_{\mathrm{p}}(\tau) = \sum_{j=0}^{\infty} q_j^2 \cos(j\,\omega_0\,\tau)$$

- 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:

$$\mathbf{F}_j^{\mathrm{p}} = \begin{pmatrix} 0 & -\omega_0\, j \\ \omega_0\, j & 0 \end{pmatrix}, \quad \mathbf{H}_j^{\mathrm{p}} = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad \mathbf{P}_{\infty,j}^{\mathrm{p}} = q_j^2 \mathbf{I}_2$$

The diffusion part is zero (*i.e.* the model is deterministic).

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- The spectral (variance) coefficients are

$$q_j^2 = \frac{2\,\mathrm{I}_j(\ell^{-2})}{\exp(\ell^{-2})}, \text{ for } j = 1, 2, \ldots,$$

  and $q_0^2 = \mathrm{I}_0(\ell^{-2}) / \exp(\ell^{-2})$, where $\mathrm{I}_\alpha(z)$ is the modified Bessel function.

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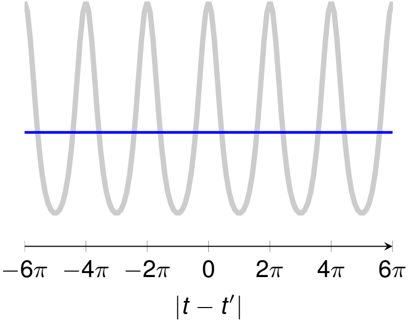
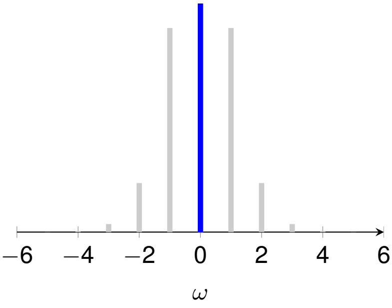
- Taking the J first terms in the series gives an approximation, and this approximation converges uniformly to the actual covariance as $J \to \infty$.

Approximative Covariance Function ($J = 0$)

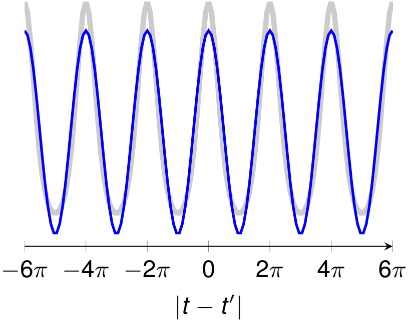


Covariance function

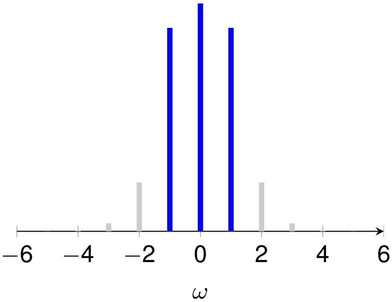


Spectral density

Approximative Covariance Function ($J = 1$)

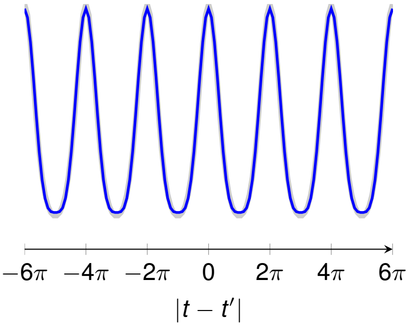


Covariance function

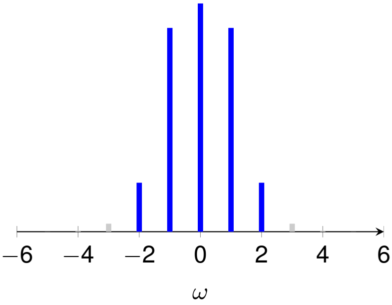


Spectral density

Approximative Covariance Function ($J = 2$)

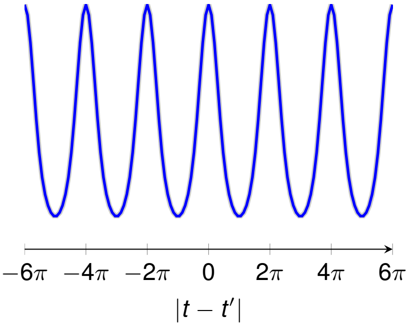


Covariance function

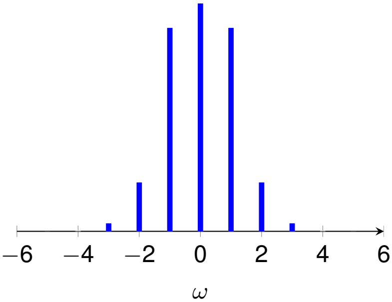


Spectral density

Approximative Covariance Function ($J = 3$)



Covariance function



Spectral density

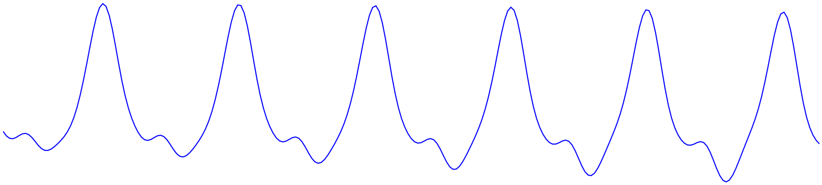
Quasi-Periodic Covariance Functions

Quasi-Periodic Covariance

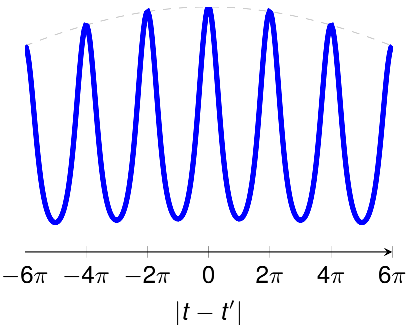
- Allow the shape of the periodic effect to change over time.
- Take the product of a periodic covariance function $k_\mathrm{p}(t, t')$ with a covariance function $k_\mathrm{q}(t, t')$ with rather long characteristic length-scale,

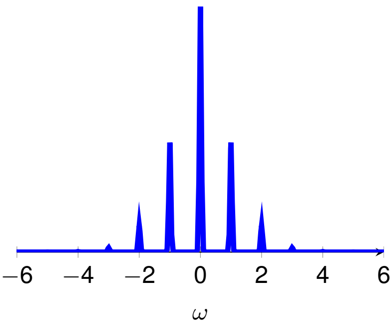
$$k(t, t') = k_\mathrm{p}(t, t')\, k_\mathrm{q}(t, t'),$$

allowing the covariance to decay away from exact periodicity.



Quasi-Periodic Covariance Function





Covariance function

Spectral density

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 ($\mathbf{F}_\mathrm{p}\mathbf{F}_\mathrm{q} = \mathbf{F}_\mathrm{q}\mathbf{F}_\mathrm{p}$.).
- This can be accomplished by using the special features of the Kronecker product.

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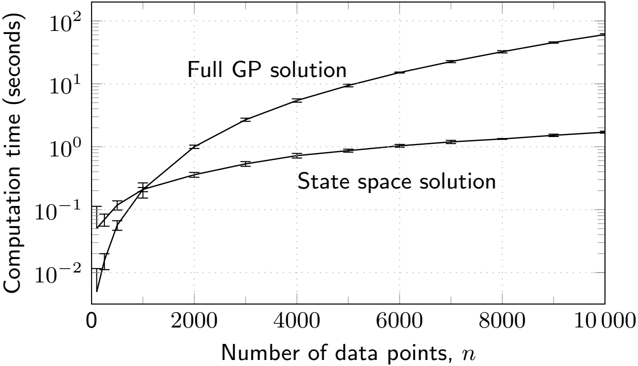
- This can be accomplished by using the special features of the Kronecker product.
- The joint model corresponding to the quasi-periodic product of the two covariance functions can then be given in a block-form:

$$
\begin{aligned}
\mathbf{F}_j &= \mathbf{F}^\mathrm{q} \otimes \mathbf{I}_2 + \mathbf{I}_q \otimes \mathbf{F}_j^\mathrm{p}, \\
\mathbf{L}_j &= \mathbf{L}^\mathrm{q} \otimes \mathbf{L}_j^\mathrm{p}, \\
\mathbf{Q}_{\mathrm{c},j} &= \mathbf{Q}_\mathrm{c}^\mathrm{q} \otimes q_j^2\, \mathbf{I}_2, \\
\mathbf{P}_{\infty,j} &= \mathbf{P}_\infty^\mathrm{q} \otimes \mathbf{P}_{\infty,j}^\mathrm{p}, \\
\mathbf{H}_j &= \mathbf{H}^\mathrm{q} \otimes \mathbf{H}_j^\mathrm{p},
\end{aligned}
$$

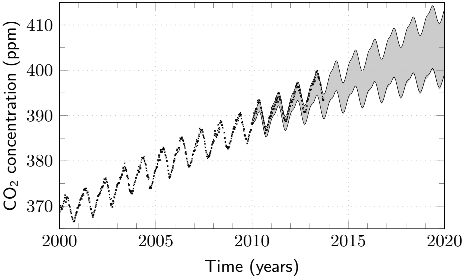
where '$\otimes$' denotes the Kronecker product of two matrices.

Example Studies

Example: Computational Complexity



Example: Mauna Loa CO_2 Concentration

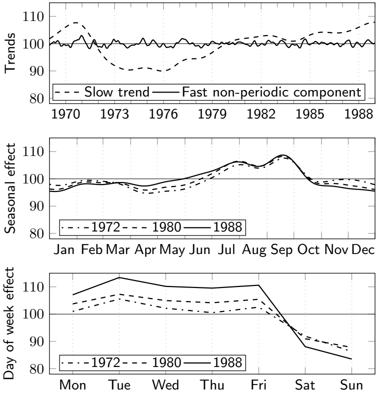


- CO_2 concentration observations ($n = 2227$, years 1958–2000 not shown in figure).
- The GP covariance function is as follows:

$$\begin{aligned} k(t,t') &= k_{\mathrm{SE}}(t,t') \\ &\quad + k_{\mathrm{p}}(t,t')\, k_{\nu=3/2}(t,t') \\ &\quad + k_{\nu=3/2}(t,t') \end{aligned}$$

- Converted to state space and hyperparameters optimized with respect to marginal likelihood.

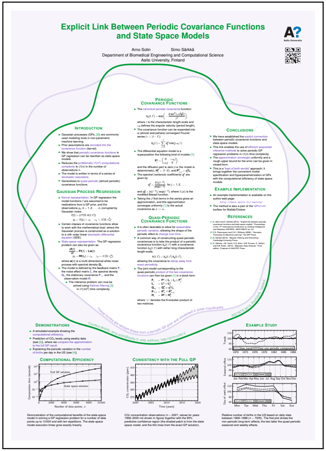
Example: Daily Births in 1969–1988



- 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.



- Codes for the examples available at:
  `http://arno.solin.fi`
- The methods also implemented into the GPstuff toolbox for Matlab/Octave.