# Lecture 6: State-Space Inference in Gaussian Process Regression

## GP Regression via Kalman Filtering and RTS Smoothing

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# Contents

# Definition and Notation of Gaussian Processes in Regression

- **Gaussian process regression**:
  - GPs are used as non-parametric prior models for "learning" input-output $\mathbb{R}^d \mapsto \mathbb{R}^m$ mappings in form $\mathbf{y} = \mathbf{f}(\mathbf{x})$.
  - A set of noisy training samples $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_n, \mathbf{y}_n)\}$ given.
  - The values of function $\mathbf{f}(\mathbf{x})$ at measurement points and test points are of interest.
- Gaussian process (GP) or Gaussian field is a random function $\mathbf{f}(\mathbf{x})$, such that all finite-dimensional distributions $p(\mathbf{f}(\mathbf{x}_1), \ldots, \mathbf{f}(\mathbf{x}_n))$ are Gaussian.
- Note that $\mathbf{x}$ is the input – not the state! And $\mathbf{f}(\bullet)$ is not the drift! – BEWARE of the notation!
- GP can be defined in terms of mean and covariance functions:

$$\mathbf{m}(\mathbf{x}) = \mathrm{E}[\mathbf{f}(\mathbf{x})]$$
$$\mathbf{K}(\mathbf{x}, \mathbf{x}') = \mathrm{E}[(\mathbf{f}(\mathbf{x}) - \mathbf{m}(\mathbf{x}))\,(\mathbf{f}(\mathbf{x}') - \mathbf{m}(\mathbf{x}'))^{\mathsf{T}}].$$

# Definition and Notation of Gaussian Processes in Regression (cont.)

- The joint distribution of an arbitrary collection of random variables $\mathbf{f}(\mathbf{x}_1), \ldots, \mathbf{f}(\mathbf{x}_n)$ is then given as

$$\begin{pmatrix} \mathbf{f}(\mathbf{x}_1) \\ \vdots \\ \mathbf{f}(\mathbf{x}_n) \end{pmatrix} \sim \mathrm{N}\left( \begin{pmatrix} \mathbf{m}(\mathbf{x}_1) \\ \vdots \\ \mathbf{m}(\mathbf{x}_n) \end{pmatrix}, \begin{pmatrix} \mathbf{K}(\mathbf{x}_1, \mathbf{x}_1) & \ldots & \mathbf{K}(\mathbf{x}_1, \mathbf{x}_n) \\ \vdots & \ddots & \\ \mathbf{K}(\mathbf{x}_n, \mathbf{x}_1) & & \mathbf{K}(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \right)$$

- **Temporal** Gaussian process (GP) is a temporal random function $\mathbf{f}(t)$, such that joint distribution of $\mathbf{f}(t_1), \ldots, \mathbf{f}(t_n)$ is always Gaussian
- Note that on this course we have denoted these as $\mathbf{x}(t)$!
- In this case the input is the time $t$ and thus our regressor functions have the form $\mathbf{y} = \mathbf{f}(t)$.
- Mean and covariance functions have the form:

$$\begin{aligned} \mathbf{m}(t) &= \mathrm{E}[\mathbf{f}(t)] \\ \mathbf{K}(t, t') &= \mathrm{E}[(\mathbf{f}(t) - \mathbf{m}(t))\,(\mathbf{f}(t') - \mathbf{m}(t'))^\mathsf{T}]. \end{aligned}$$

# Gaussian Process Regression [1/5]

- Gaussian process regression considers predicting the value of an unknown function ($y$ and $x$ are scalar for illustration)

$$y = f(x)$$

  at a certain test point $(y^*, x^*)$ based on a finite number of training samples $(y_j, x_j)$ observed from it.
- To keep the notation less confusing, let's replace $x$ with $t$:

$$y = f(t).$$

- In classic regression, we postulates parametric form of $f(t; \boldsymbol{\theta})$ and estimate the parameters $\boldsymbol{\theta}$.
- In GP regression, we instead assume that $f(t)$ is a sample from a Gaussian process with a given covariance function $K(t, t')$, e.g.,

$$K(t, t') = s^2 \exp\left(-\frac{1}{2\ell^2} ||t - t'||^2\right),$$

# Gaussian Process Regression [2/5]

- Let's denote the vector of observed points as $\mathbf{y} = (y_1, \ldots, y_n)$, and test point as $y^*$.
- Gaussian process assumption implies that their joint distribution is

$$\begin{pmatrix} \mathbf{y} \\ y^* \end{pmatrix} = \mathrm{N}\left( \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}, \begin{pmatrix} \mathbf{K}(t_{1:m}, t_{1:m}) & \mathbf{K}^T(t^*, t_{1:m}) \\ \mathbf{K}(t^*, t_{1:m}) & K(t^*, t^*) \end{pmatrix} \right)$$

  where
  - $\mathbf{K}(t_{1:m}, t_{1:m}) = [K(t_i, t_j)]$ is the joint covariance of observed points,
  - $K(t^*, t^*)$ is the (co)variance of the test point,
  - $\mathbf{K}(t^*, t_{1:m}) = [K(t^*, t_j)]$ is the cross covariance.
- By using the computation rules of Gaussian distributions we get

$$\begin{aligned} \mathrm{E}[y^* \mid \mathbf{y}] &= \mathbf{K}(t^*, t_{1:m})\, \mathbf{K}^{-1}(t_{1:m}, t_{1:m})\, \mathbf{y} \\ \mathrm{Var}[y^* \mid \mathbf{y}] &= K(t^*, t^*) - \mathbf{K}(t^*, t_{1:m})\, \mathbf{K}^{-1}(t_{1:m}, t_{1:m})\, \mathbf{K}^T(t^*, t_{1:m}). \end{aligned}$$

- These equations can be used for interpolating the value of $y^* = f(t^*)$ at any test point $t^*$.

- In practice, the measurements usually have noise:

$$y_k = f(t_k) + e_k, \qquad e_k \sim \mathrm{N}(0, \sigma^2).$$

- We want to estimate the value of the "clean" function $f(t^*)$ at a test point $t^*$.
- Due to the Gaussian process assumption we now get

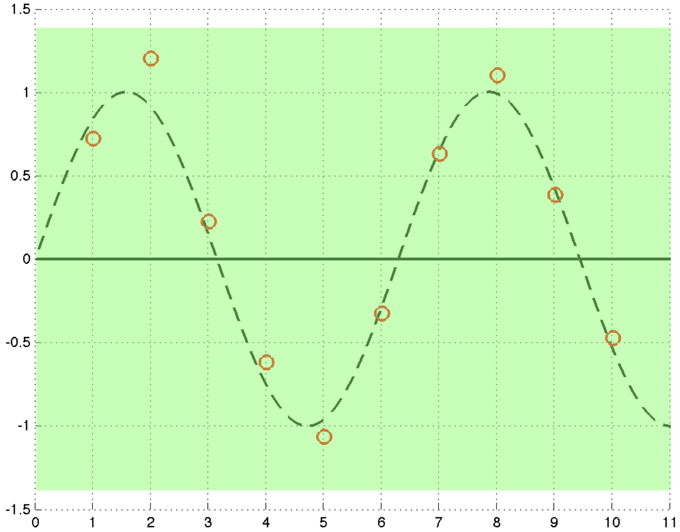
$$\begin{pmatrix} \mathbf{y} \\ f(t^*) \end{pmatrix} = \mathrm{N}\left( \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}, \begin{pmatrix} \mathbf{K}(t_{1:m}, t_{1:m}) + \sigma^2 \mathbf{I} & \mathbf{K}^T(t^*, t_{1:m}) \\ \mathbf{K}(t^*, t_{1:m}) & K(t^*, t^*) \end{pmatrix} \right)$$

- The conditional mean and variance are given as

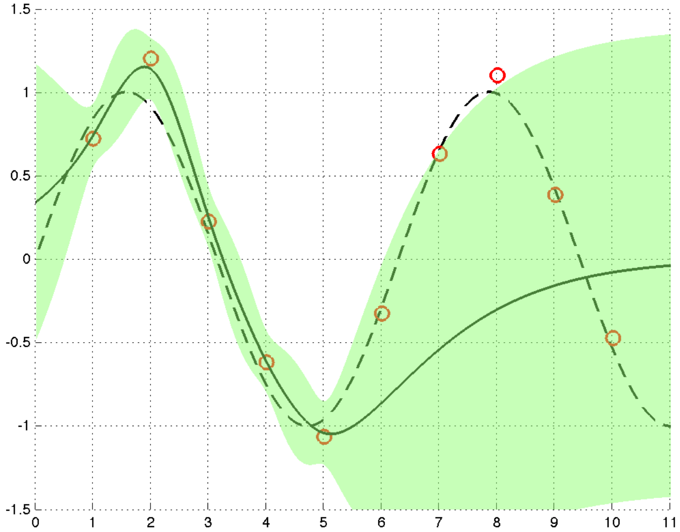
$$\begin{aligned} \mathrm{E}[f(t^*) \mid \mathbf{y}] &= \mathbf{K}(t^*, t_{1:m}) \, (\mathbf{K}(t_{1:m}, t_{1:m}) + \sigma^2 \mathbf{I})^{-1} \, \mathbf{y} \\ \mathrm{Var}[f(t^*) \mid \mathbf{y}] &= K(t^*, t^*) \\ &\quad - \mathbf{K}(t^*, t_{1:m}) \, (\mathbf{K}(t_{1:m}, t_{1:m}) + \sigma^2 \mathbf{I})^{-1} \, \mathbf{K}^T(t^*, t_{1:m}). \end{aligned}$$

- These are the Gaussian process regression equations in their typical form - scalar special cases though.

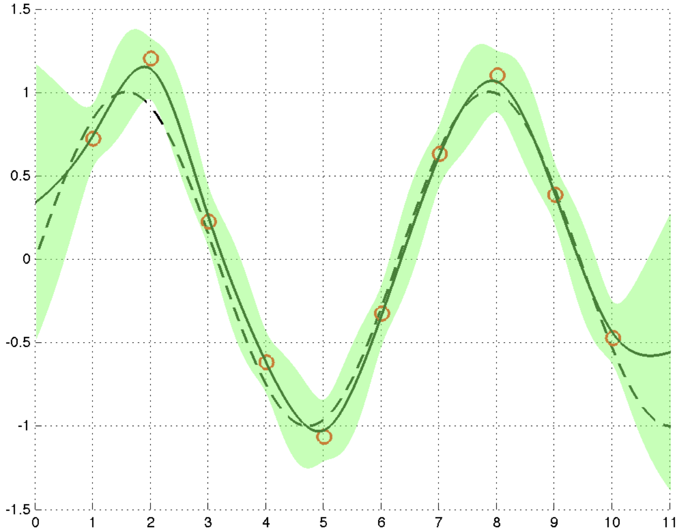
# Gaussian Process Regression [4/5]



# Gaussian Process Regression [4/5]



# Gaussian Process Regression [4/5]



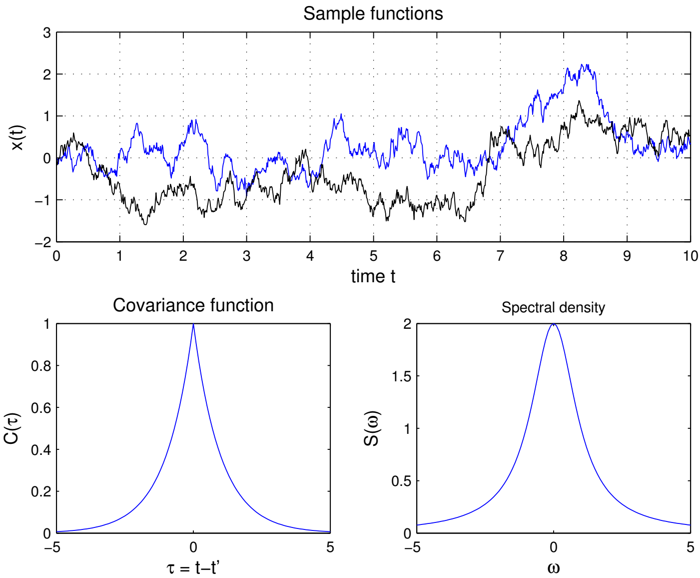
# Gaussian Process Regression [5/5]

- The GP-regression has cubic computational complexity $O(m^3)$ in the number of measurements.
- This results from the inversion of the $m \times m$ matrix:

$$
\begin{aligned}
\mathrm{E}[f(t^*) \mid \mathbf{y}] &= \mathbf{K}(t^*, t_{1:m}) \left(\mathbf{K}(t_{1:m}, t_{1:m}) + \sigma^2 \mathbf{I}\right)^{-1} \mathbf{y} \\
\mathrm{Var}[f(t^*) \mid \mathbf{y}] &= K(t^*, t^*) \\
&\quad - \mathbf{K}(t^*, t_{1:m}) \left(\mathbf{K}(t_{1:m}, t_{1:m}) + \sigma^2 \mathbf{I}\right)^{-1} \mathbf{K}^T(t^*, t_{1:m}).
\end{aligned}
$$

- In practice, we use Cholesky factorization and do not invert explicitly – but still the $O(m^3)$ problem remains.
- Various sparse, reduced-rank, and related approximations have been developed for this purpose.
- Here we study another method – we reduce GP regression into Kalman filtering/smoothing problem which has linear $O(m)$ complexity – in time direction.

# Representations of Temporal Gaussian Processes



# Representations of Temporal Gaussian Processes

- Example: Ornstein-Uhlenbeck process – path representation as a stochastic differential equation (SDE):

$$\frac{df(t)}{dt} = -\lambda\, f(t) + w(t).$$

  where $w(t)$ is a white noise process.
- The mean and covariance functions:

$$m(t) = 0$$
$$k(t, t') = \exp(-\lambda |t - t'|)$$

- Spectral density:

$$S(\omega) = \frac{2\lambda}{\omega^2 + \lambda^2}$$

- Ornstein-Uhlenbeck process $f(t)$ is Markovian in the sense that given $f(t)$ the past $\{f(s), s < t\}$ does not affect the distribution of the future $\{f(s'), s' > t\}$.

# State Space Form of Linear Time-Invariant SDEs

- Consider a *N*th order LTI SDE of the form

$$\frac{d^N f}{dt^N} + a_{N-1} \frac{d^{N-1} f}{dt^{N-1}} + \cdots + a_0 f = w(t).$$

- If we define $\mathbf{f} = (f, \ldots, d^{N-1} f / dt^{N-1})$, we get a state space model:

$$\frac{d\mathbf{f}}{dt} = \underbrace{\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ -a_0 & -a_1 & \ldots & -a_{N-1} \end{pmatrix}}_{\mathbf{F}} \mathbf{f} + \underbrace{\begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}}_{\mathbf{L}} w(t)$$

$$f(t) = \underbrace{\begin{pmatrix} 1 & 0 & \cdots & 0 \end{pmatrix}}_{\mathbf{H}} \mathbf{f}.$$

- The vector process $\mathbf{f}(t)$ is now time-Markovian although $f(t)$ is not.

# Spectra of Linear Time-Invariant SDEs

- By taking the Fourier transform of the LTI SDE, we can derive the spectral density which has the form:

$$S(\omega) = \frac{\text{(constant)}}{\text{(polynomial in } \omega^2\text{)}}$$

- It turns out that we can also do this conversion to the other direction:
  - With certain parameter values, the Matérn has the form:

$$S(\omega) \propto (\lambda^2 + \omega^2)^{-(p+1)}.$$

  - Many non-rational spectral densities can be approximated, e.g.:

$$S(\omega) = \sigma^2 \sqrt{\frac{\pi}{\kappa}} \exp\left(-\frac{\omega^2}{4\kappa}\right) \approx \frac{\text{(const)}}{N!/0!(4\kappa)^N + \cdots + \omega^{2N}}$$

- For the conversion of a rational spectral density to a Markovian (state-space) model, we can use the classical spectral factorization –

# Converting Covariance Functions to State Space Models

- Spectral factorization finds rational stable transfer function

$$G(i\,\omega) = \frac{b_m\,(i\,\omega)^M + \cdots + b_1\,(i\,\omega) + b_0}{(i\,\omega)^N + \cdots + a_1\,(i\,\omega) + a_0}$$

  such that

$$S(\omega) = G(i\,\omega)\,q_c\,G(-i\,\omega).$$

- The procedure practice:
  - Compute the roots of the numerator and denominator polynomials.
  - Construct the numerator and denominator polynomials of the transfer function $G(i\,\omega)$ from the positive-imaginary-part roots only.
- The SDE is then the inverse Fourier transform of

$$F(i\,\omega) = G(i\,\omega)\,W(i\,\omega).$$

- Can be further converted into a state space model –

# Converting Covariance Functions to State Space Models (cont.)

- We have a Fourier-domain system with white noise input:

$$F(i\,\omega) = \left( \frac{b_M\,(i\,\omega)^M + \cdots + b_1\,(i\,\omega) + b_0}{(i\,\omega)^N + \cdots + a_1\,(i\,\omega) + a_0} \right) W(i\,\omega).$$

- A standard conversion from transfer function form into state-space form (see control engineering literature), e.g.,

$$\frac{d\mathbf{f}}{dt} = \underbrace{\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ -a_0 & -a_1 & \ldots & -a_{N-1} \end{pmatrix}}_{\mathbf{F}} \mathbf{f} + \underbrace{\begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}}_{\mathbf{L}} w(t)$$

$$f(t) = \underbrace{\begin{pmatrix} b_0 & b_1 & \cdots & b_M & 0 & \cdots & 0 \end{pmatrix}}_{\mathbf{H}} \mathbf{f}.$$

# Application to Gaussian Process Regression

- Consider a Gaussian process regression problem of the form

$$f(x) \sim \mathcal{GP}(0, k(x, x'))$$
$$y_i = f(x_i) + e_i, \qquad e_i \sim \mathrm{N}(0, \sigma^2_{\text{noise}}).$$

- Renaming $x$ into time $t$ gives:

$$f(t) \sim \mathcal{GP}(0, k(t, t'))$$
$$y_i = f(t_i) + e_i, \qquad e_i \sim \mathrm{N}(0, \sigma^2_{\text{noise}}).$$

- We can can now convert this to state estimation problem:

$$\frac{d\mathbf{f}(t)}{dt} = \mathbf{F}\,\mathbf{f}(t) + \mathbf{L}\,w(t)$$
$$y_i = \mathbf{H}\,\mathbf{f}(t_i) + e_i.$$

- The GP-regression solution $p(f(t^*) \mid y_1, \ldots, y_m)$ can now be computed with Kalman filter and RTS smoother!

# Example: Matérn Covariance Function

## Example (1D Matérn covariance function)

- 1D Matérn family is ($\tau = |t - t'|$):

$$k(\tau) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \sqrt{2\nu} \, \frac{\tau}{l} \right)^{\nu} K_{\nu} \left( \sqrt{2\nu} \, \frac{\tau}{l} \right),$$

  where $\nu, \sigma, l > 0$ are the smoothness, magnitude and length scale parameters, and $K_{\nu}(\cdot)$ the modified Bessel function.

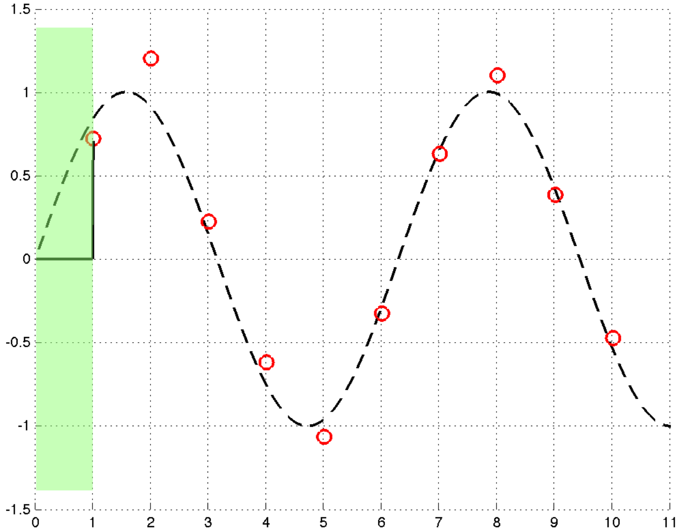
- For example, when $\nu = 5/2$, we get

$$\frac{\mathrm{d}\mathbf{f}(t)}{dt} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -\lambda^3 & -3\lambda^2 & -3\lambda \end{pmatrix} \mathbf{f}(t) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} w(t).$$

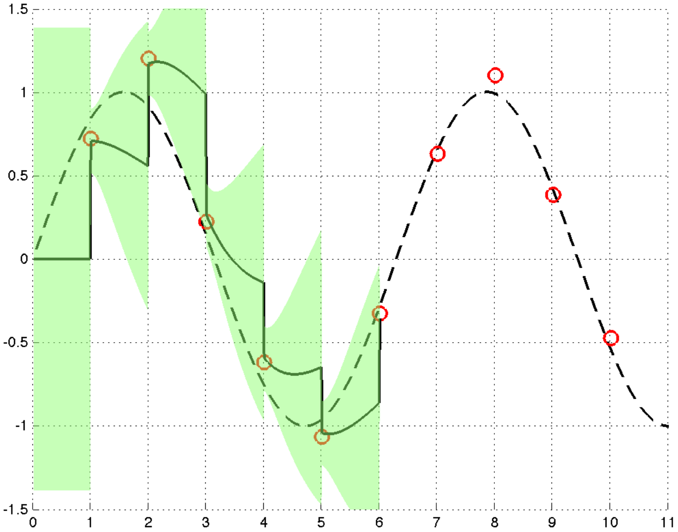
# Inference in Practice

- Conventional GP regression:
  1. Evaluate the covariance function at the training and test set points.
  2. Use GP regression formulas to compute the posterior process statistics.
  3. Use the mean function as the prediction.
- State-space GP regression:
  1. Form the state space model.
  2. Run Kalman filter through the measurement sequence.
  3. Run RTS smoother through the filter results.
  4. Use the smoother mean function as the prediction.
- With both GP regression and state-space formulation we have the corresponding parameter estimation methods – see, e.g., Rasmussen & Williams (2006) and Särkkä (2013), respectively.

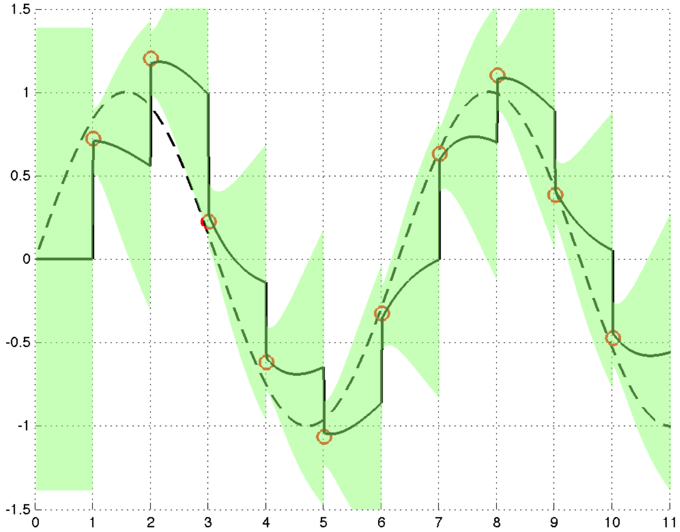
# State-Space GP Regression Demo



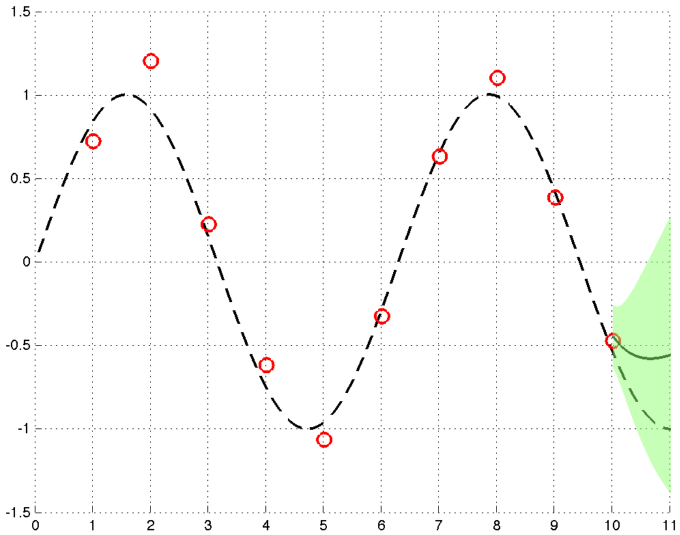
# State-Space GP Regression Demo



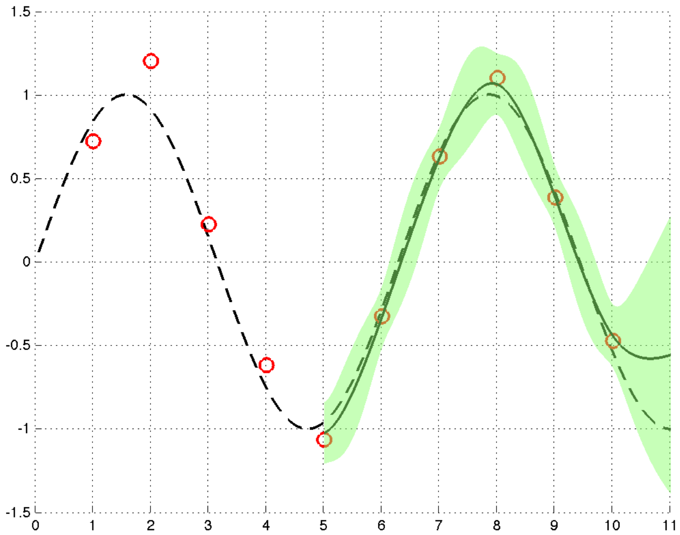
# State-Space GP Regression Demo



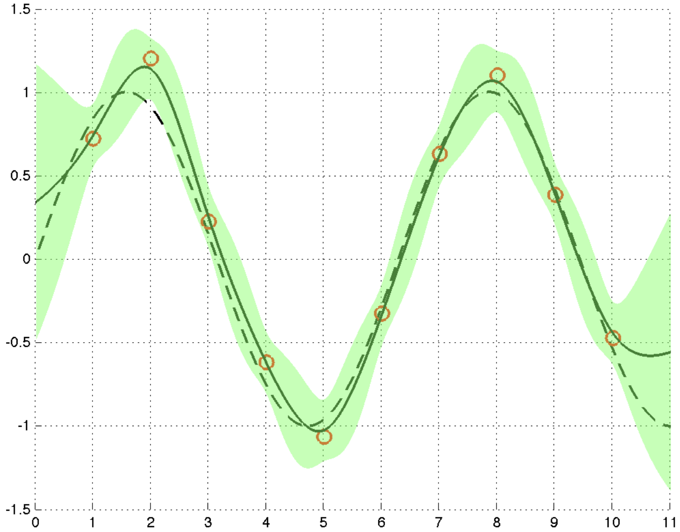
# State-Space GP Regression Demo



# State-Space GP Regression Demo

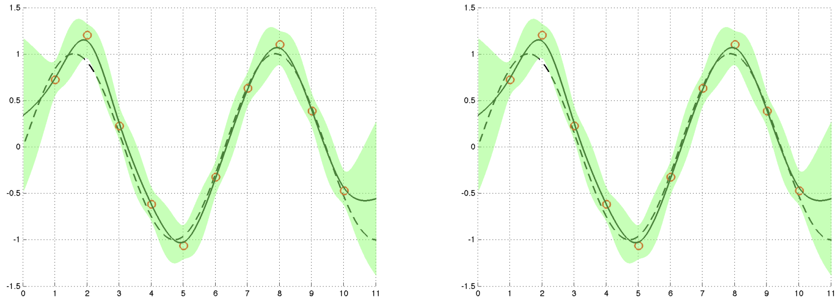


# State-Space GP Regression Demo



# State-Space GP Regression Demo (cont.)

## Comparison of GP regression (L) and RTS smoother (R) results



# The Basic Idea of State-Space Representation of LFMs

- A latent force model (LFM) is of the form

$$\frac{dx_f(t)}{dt} = g(x_f(t)) + u(t),$$

  where $u(t)$ is the latent force.
- We measure the system at discrete instants of time:

$$y_k = x_f(t_k) + r_k$$

- Let's now model $u(t)$ as a Gaussian process of Matern type

$$K(\tau) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\,\frac{\tau}{l}\right)^{\nu} K_\nu \left(\sqrt{2\nu}\,\frac{\tau}{l}\right)$$

- Recall that if, for example, $\nu = 1/2$ then the GP can be expressed as the solution of the stochastic differential equation (SDE)

$$\frac{\mathrm{d}u(t)}{\mathrm{d}t} = -\lambda\, u(t) + w(t)$$

# The Basic Idea of State-Space Representation (cont.)

- If we define $\mathbf{x} = (x_f, u)$, we get a two-dimensional SDE

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \underbrace{\begin{pmatrix} g(x_1(t)) + x_2(t) \\ -\lambda\, x_2(t) \end{pmatrix}}_{\mathbf{a}(\mathbf{x})} + \underbrace{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}_{\mathbf{L}} w(t)$$

- We can now rewrite the measurement model as

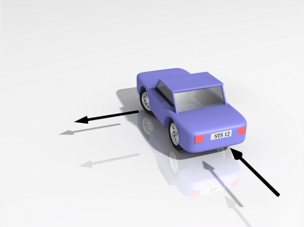
$$y_k = \underbrace{\begin{pmatrix} 1 & 0 \end{pmatrix}}_{\mathbf{H}} \mathbf{x}(t_k) + r_k$$

- Thus the result is a model of the generic form

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \mathbf{a}(\mathbf{x}) + \mathbf{L}\,\mathbf{w}(t) \\ \mathbf{y}_k &= \mathbf{H}\,\mathbf{x}(t_k) + \mathbf{r}_k. \end{aligned}$$

- This model can now be efficiently tackled with non-linear Kalman filtering and smoothing.

# Recall: State Space Model for a Car [1/2]




- The dynamics of the car in 2d $(x_1, x_2)$ are given by Newton's law:

$$\mathbf{F}(t) = m\,\mathbf{a}(t),$$

where $\mathbf{a}(t)$ is the acceleration, $m$ is the mass of the car, and $\mathbf{F}(t)$ is a vector of (unknown) forces acting the car.

- We model $\mathbf{F}(t)/m$ as a 2-dimensional white noise process:

$$d^2 x_1 / dt^2 = w_1(t)$$
$$d^2 x_2 / dt^2 = w_2(t).$$

# Recall: State Space Model for a Car [2/2]

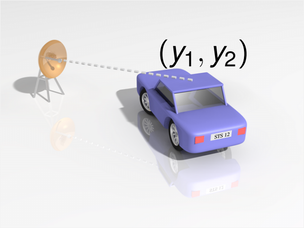
- If we define $x_3(t) = dx_1/dt$, $x_4(t) = dx_2/dt$, then the model can be written as a first order system of differential equations:

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{\mathbf{F}} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} + \underbrace{\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}}_{\mathbf{L}} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}.$$

- In shorter matrix form:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}\,\mathbf{x} + \mathbf{L}\,\mathbf{w}.$$

# Measurement Model for a Car




- Assume that the position of the car $(x_1, x_2)$ is measured and the measurements are corrupted by Gaussian measurement noise $e_{1,k}, e_{2,k}$:

$$
\begin{aligned}
y_{1,k} &= x_1(t_k) + e_{1,k} \\
y_{2,k} &= x_2(t_k) + e_{2,k}.
\end{aligned}
$$

- The measurement model can be now written as

$$
\mathbf{y}_k = \mathbf{H}\,\mathbf{x}(t_k) + \mathbf{e}_k, \qquad \mathbf{H} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}
$$

# Model for Car Tracking

- The dynamic and measurement models of the car now form a linear Gaussian state-space model:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}\,\mathbf{x} + \mathbf{L}\,\mathbf{w}$$
$$\mathbf{y}_k = \mathbf{H}\,\mathbf{x}(t_k) + \mathbf{r}_k,$$

- In this case it is possible to solve the transition density explicitly:

$$p(\mathbf{x}(t_k) \mid \mathbf{x}(t_{k-1})) = \mathrm{N}(\mathbf{x}(t_k) \mid \mathbf{A}_{k-1}\,\mathbf{x}(t_{k-1}), \mathbf{Q}_{k-1})$$

  where $\mathbf{A}_{k-1}$ and $\mathbf{Q}_{k-1}$ can be expressed in terms of the matrix exponential function (see yesterday's lecture).
- Thus we can actually write this as a discrete-time model:

$$\mathbf{x}_k = \mathbf{A}_{k-1}\,\mathbf{x}_{k-1} + \mathbf{q}_{k-1}$$
$$\mathbf{y}_k = \mathbf{H}\,\mathbf{x}_k + \mathbf{r}_k,$$

  where $\mathbf{q}_{k-1} \sim \mathrm{N}(\mathbf{0}, \mathbf{Q}_{k-1})$.

# Latent Force Model for a Car

- We can also start from a latent force model

$$
\begin{aligned}
d^2 x_1 / dt^2 &= u(t) \\
d^2 x_2 / dt^2 &= v(t),
\end{aligned}
$$

  where $u$ and $v$ are, say, Matern 3/2 processes.
- In state-space form this leads to

$$
\frac{\mathrm{d}\mathbf{u}(t)}{\mathrm{d}t} = \begin{pmatrix} 0 & 1 \\ -\lambda^2 & -2\lambda \end{pmatrix} \mathbf{u}(t) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} w_u(t), \quad j = 1, 2
$$

  where $\mathbf{u}(t) = (u(t), \mathrm{d}u(t)/\,\mathrm{d}t)$.
- We can also have both white noises and latent forces:

$$
\begin{aligned}
d^2 x_1 / dt^2 &= u(t) + w_1(t) \\
d^2 x_2 / dt^2 &= v(t) + w_2(t).
\end{aligned}
$$

# Latent Force Model for a Car (cont.)

- Now we get

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ u_1 \\ v_1 \\ u_2 \\ v_2 \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -\lambda^2 & 0 & -2\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & -\lambda^2 & 0 & -2\lambda \end{pmatrix}}_{\mathbf{F}} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ u_1 \\ v_1 \\ u_2 \\ v_2 \end{pmatrix} + \underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{\mathbf{L}} \begin{pmatrix} w_1 \\ w_2 \\ w_u \\ w_v \end{pmatrix}$$

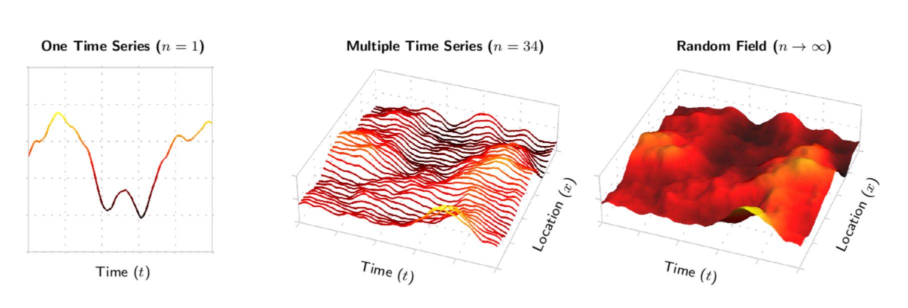
$$\mathbf{y}_k = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ u_1 \\ u_2 \\ v_1 \\ v_2 \end{pmatrix} + \mathbf{e}_k,$$

- But this is just a linear Gaussian state-space model:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}\,\mathbf{x} + \mathbf{L}\,\mathbf{w}$$

$$\mathbf{y}_k = \mathbf{H}\,\mathbf{x}(t_k) + \mathbf{r}_k,$$

# From Temporal to Spatio-Temporal Processes




The temporal vector-valued process becomes an infinite-dimensional function (Hilbert space) -valued process:

$$\mathbf{f}(t) = \begin{pmatrix} f_1(t) \\ \vdots \\ f_n(t) \end{pmatrix} \to \begin{pmatrix} f(\mathbf{x}_1, t) \\ \vdots \\ f(\mathbf{x}_n, t) \end{pmatrix} \to f(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^d.$$

# Representations of Spatio-Temporal Gaussian Processes

- Moment representation in terms of mean and covariance function

$$\begin{aligned}\mathbf{m}(\mathbf{x}, t) &= \mathrm{E}[\mathbf{f}(\mathbf{x}, t)] \\ \mathbf{K}(\mathbf{x}, \mathbf{x}'; t, t') &= \mathrm{E}[(\mathbf{f}(\mathbf{x}, t) - \mathbf{m}(\mathbf{x}, t))\,(\mathbf{f}(\mathbf{x}', t') - \mathbf{m}(\mathbf{x}', t'))^T].\end{aligned}$$

- Spectral representation in terms of spectral density function

$$\mathbf{S}(\omega_x, \omega_t) = \tilde{\mathbf{f}}(i\,\omega_x, i\,\omega_t)\,\tilde{\mathbf{f}}^T(-i\,\omega_x, -i\,\omega_t).$$

- As an infinite-dimensional state space model or stochastic evolution equation:

$$\frac{\partial \mathbf{f}(\mathbf{x}, t)}{\partial t} = \mathcal{F}\,\mathbf{f}(\mathbf{x}, t) + \mathbf{L}\,\mathbf{w}(\mathbf{x}, t).$$

# Infinite-Dimensional Kalman Filtering and Smoothing

- Infinite-dimensional state-space model with operators $\mathcal{F}$ and $\mathcal{H}_i$:

$$\frac{\partial \mathbf{f}(\mathbf{x}, t)}{\partial t} = \mathcal{F}\,\mathbf{f}(\mathbf{x}, t) + \mathbf{L}\,\mathbf{w}(\mathbf{x}, t)$$
$$\mathbf{y}_i = \mathcal{H}_i\,\mathbf{f}(\mathbf{x}, t_i) + \mathbf{e}_i$$

- We can use the infinite-dimensional Kalman filter and RTS smoother – scale linearly in time dimension.
- We can approximate with PDE methods such as basis function expansions, FEM, finite-differences, spectral methods, etc.
- If $\mathcal{F}$ and $\mathcal{H}_i$ are "diagonal" in the sense that they only involve point-wise evaluation in $\mathbf{x}$, we get a finite-dimensional algorithm.
  - Diagonal $\mathcal{F}$ corresponds to a separable model.
  - The evaluation operator $\mathcal{H}_i$ in GP regression and Kriging is diagonal.

# Conversion of Spatio-Temporal Covariance into Infinite-Dimensional State Space Model

- We can convert spatio-temporal covariance functions into state-space models as follows:
  1. First compute the spectral density $S(\boldsymbol{\omega}_x, \omega_t)$ by Fourier transforming the covariance function $K(\mathbf{x}, t)$.
  2. Form rational approximation in variable $i\omega_t$:

$$S(\boldsymbol{\omega}_x, \omega_t) = \frac{q(i\boldsymbol{\omega}_x)}{b_0(i\boldsymbol{\omega}_x) + b_1(i\boldsymbol{\omega}_x)\,(i\omega_t) + \cdots + (i\omega_t)^N}.$$

  3. Form the corresponding Fourier domain SDE (via the spectral factorization again):

$$\frac{\partial^N \tilde{f}(\boldsymbol{\omega}_x, t)}{\partial t^N} + a_{N-1}(i\boldsymbol{\omega}_x)\,\frac{\partial^{N-1} \tilde{f}(\boldsymbol{\omega}_x, t)}{\partial t^{N-1}} + \cdots$$
$$+ a_0(i\boldsymbol{\omega}_x)\,\tilde{f}(\boldsymbol{\omega}_x, t) = \tilde{w}(\boldsymbol{\omega}_x, t).$$

# Conversion of Spatio-Temporal Covariance into Infinite-Dimensional State Space Model (cont.)

- ... conversion method continues ...
  4. By converting this to state space form and by taking spatial inverse Fourier transform, we get the stochastic evolution equation

$$\frac{\partial \mathbf{f}(\mathbf{x}, t)}{\partial t} = \underbrace{\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ -\mathcal{A}_0 & -\mathcal{A}_1 & \dots & -\mathcal{A}_{N-1} \end{pmatrix}}_{\mathcal{F}} \mathbf{f}(\mathbf{x}, t) + \underbrace{\begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}}_{\mathbf{L}} w(\mathbf{x}, t)$$

  where $\mathcal{A}_j$ are pseudo-differential operators.

- We can now use infinite-dimensional Kalman filter and RTS smoother for efficient estimation of the "state" $\mathbf{f}(\cdot, t)$.

# Example: 2D Matérn Covariance Function

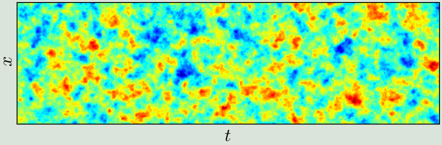
## Example (2D Matérn covariance function)

- The multidimensional Matérn covariance function is the following ($r = ||\xi - \xi'||$, for $\xi = (x_1, x_2, \ldots, x_{d-1}, t) \in \mathbb{R}^d$):

$$k(r) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\,\frac{r}{l}\right)^{\nu} K_{\nu}\left(\sqrt{2\nu}\,\frac{r}{l}\right).$$

- For example, if $\nu = 1$ and $d = 2$, we get the following:

$$\frac{\partial \mathbf{f}(x,t)}{\partial t} = \begin{pmatrix} 0 & 1 \\ \partial^2/\partial x^2 - \lambda^2 & -2\sqrt{\lambda^2 - \partial^2/\partial x^2} \end{pmatrix} \mathbf{f}(x,t) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} w(x,t).$$



# Summary

- In Gaussian process (GP) regression we put a Gaussian process prior on the regressor functions $f(t)$.
- The value of the function $f(t^*)$ at a test point $t^*$ is predicted by conditioning the process on the training set.
- GP regression has a problematic cubic $O(m^3)$ complexity in the number of measurements $m$.
- We can often convert a GP regression problem into a Kalman filtering/smoothing problem which has linear $O(m)$ time complexity.
- But – this is possible only in time-direction.
- Latent force models with GP forces can also be converted into Kalman filtering/smoothing problems.
- In space-time models we need to use infinite-dimensional Kalman filters and smoothers.