

State Space Representation of Gaussian Processes

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January 16, 2014



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Contents

- 1 From Linear Regression to Kalman Filter and Beyond
- 2 Bayesian Filtering and Smoothing
- 3 State Space Representation of Gaussian Process Regression
- 4 Spatio-Temporal Systems, Latent Force Models and Other Extensions
- 5 Application examples
- 6 Summary

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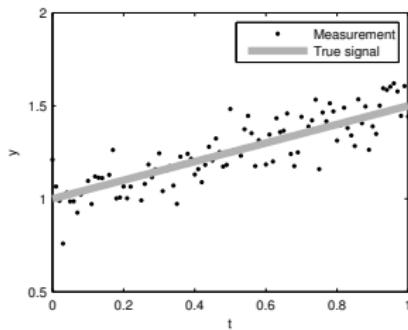
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Batch Linear Regression [1/2]



- Consider the **linear regression model**

$$y_k = \theta_1 + \theta_2 t_k + \varepsilon_k, \quad k = 1, \dots, T,$$

with $\varepsilon_k \sim N(0, \sigma^2)$ and $\boldsymbol{\theta} = (\theta_1, \theta_2) \sim N(\mathbf{m}_0, \mathbf{P}_0)$.

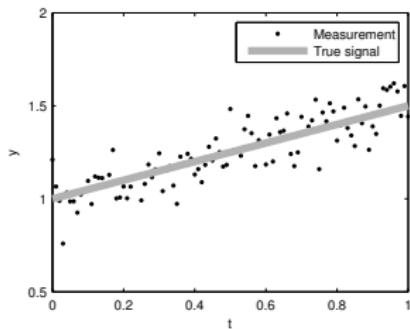
- In **probabilistic notation** this is:

$$p(y_k | \boldsymbol{\theta}) = N(y_k | \mathbf{H}_k \boldsymbol{\theta}, \sigma^2)$$

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where $\mathbf{H}_k = (1 \ t_k)$.

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Batch Linear Regression [2/2]

- The Bayesian batch solution by the Bayes' rule:

$$\begin{aligned} p(\boldsymbol{\theta} | y_{1:T}) &\propto p(\boldsymbol{\theta}) \prod_{k=1}^T p(y_k | \boldsymbol{\theta}) \\ &= N(\boldsymbol{\theta} | \mathbf{m}_0, \mathbf{P}_0) \prod_{k=1}^T N(y_k | \mathbf{H}_k \boldsymbol{\theta}, \sigma^2). \end{aligned}$$

- The posterior is Gaussian

$$p(\boldsymbol{\theta} | y_{1:T}) = N(\boldsymbol{\theta} | \mathbf{m}_T, \mathbf{P}_T).$$

- The mean and covariance are given as

$$\begin{aligned} \mathbf{m}_T &= \left[\mathbf{P}_0^{-1} + \frac{1}{\sigma^2} \mathbf{H}^T \mathbf{H} \right]^{-1} \left[\frac{1}{\sigma^2} \mathbf{H}^T \mathbf{y} + \mathbf{P}_0^{-1} \mathbf{m}_0 \right] \\ \mathbf{P}_T &= \left[\mathbf{P}_0^{-1} + \frac{1}{\sigma^2} \mathbf{H}^T \mathbf{H} \right]^{-1}, \end{aligned}$$

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Recursive Linear Regression [1/3]

- Assume that we have already computed the posterior distribution, which is **conditioned on the measurements up to $k - 1$** :

$$p(\boldsymbol{\theta} | y_{1:k-1}) = N(\boldsymbol{\theta} | \mathbf{m}_{k-1}, \mathbf{P}_{k-1}).$$

- Assume that we get the **k th measurement y_k** . Using the equations from the previous slide we get

$$\begin{aligned} p(\boldsymbol{\theta} | y_{1:k}) &\propto p(y_k | \boldsymbol{\theta}) p(\boldsymbol{\theta} | y_{1:k-1}) \\ &\propto N(\boldsymbol{\theta} | \mathbf{m}_k, \mathbf{P}_k). \end{aligned}$$

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Recursive Linear Regression [2/3]

- By the **matrix inversion lemma** (or Woodbury identity):

$$\mathbf{P}_k = \mathbf{P}_{k-1} - \mathbf{P}_{k-1} \mathbf{H}_k^T \left[\mathbf{H}_k \mathbf{P}_{k-1} \mathbf{H}_k^T + \sigma^2 \right]^{-1} \mathbf{H}_k \mathbf{P}_{k-1}.$$

- Now the equations for the **mean and covariance** reduce to

$$S_k = \mathbf{H}_k \mathbf{P}_{k-1} \mathbf{H}_k^T + \sigma^2$$

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- Computing these for $k = 0, \dots, T$ gives **exactly the linear regression solution**.
- A special case of **Kalman filter**.

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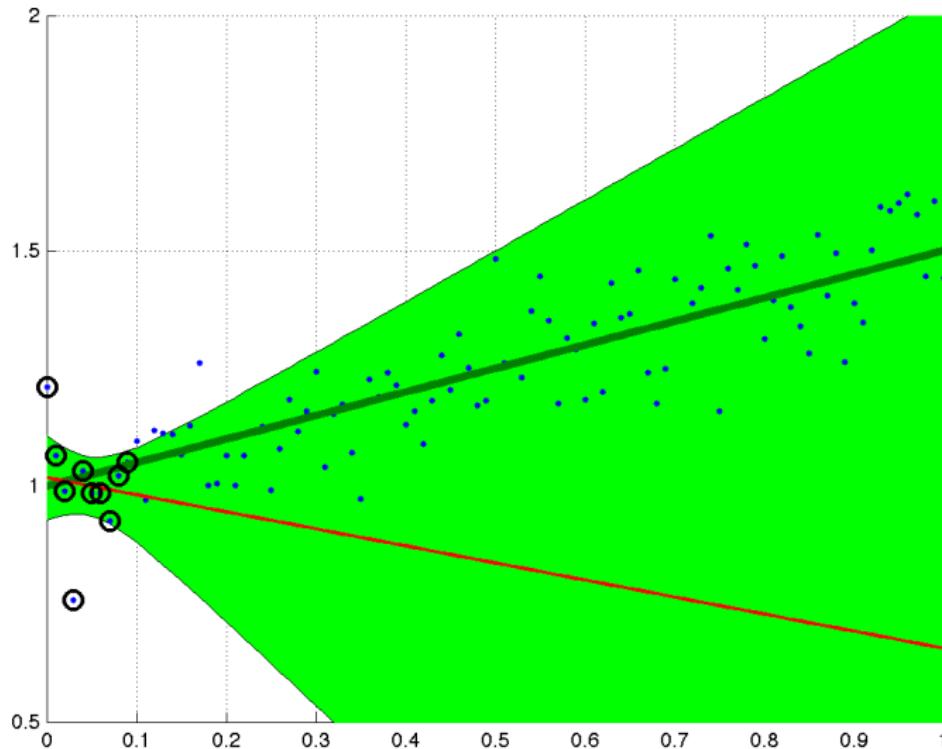
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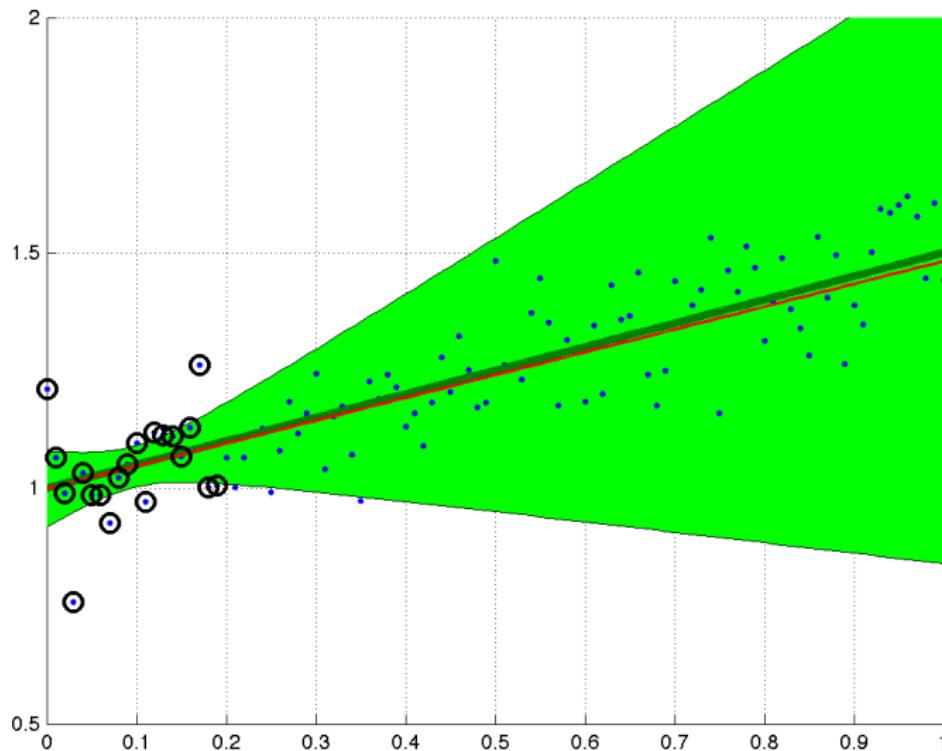
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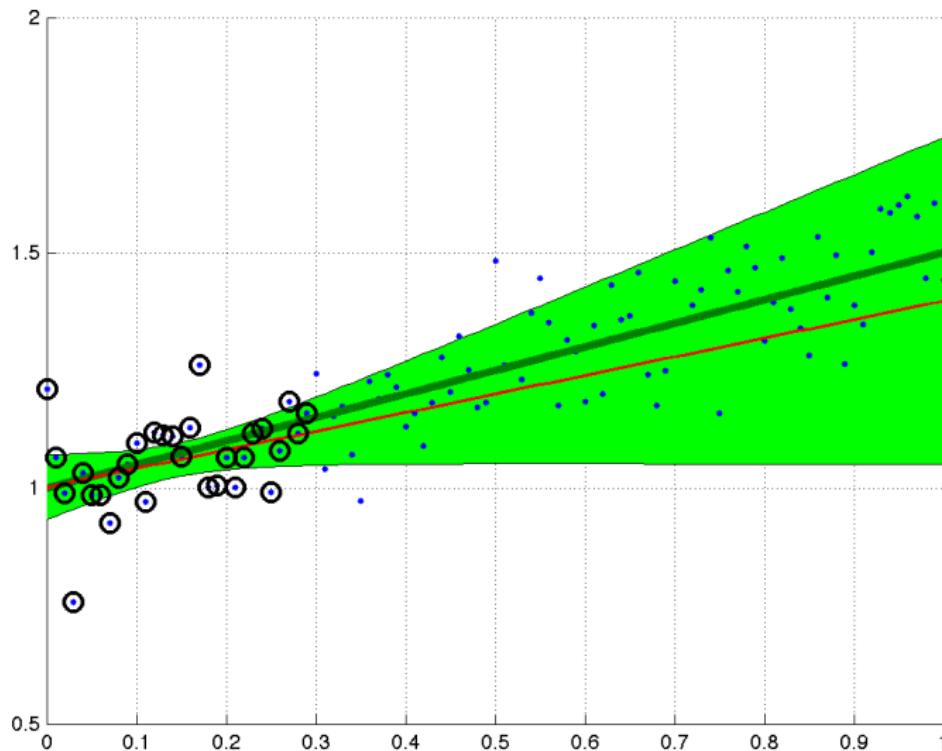
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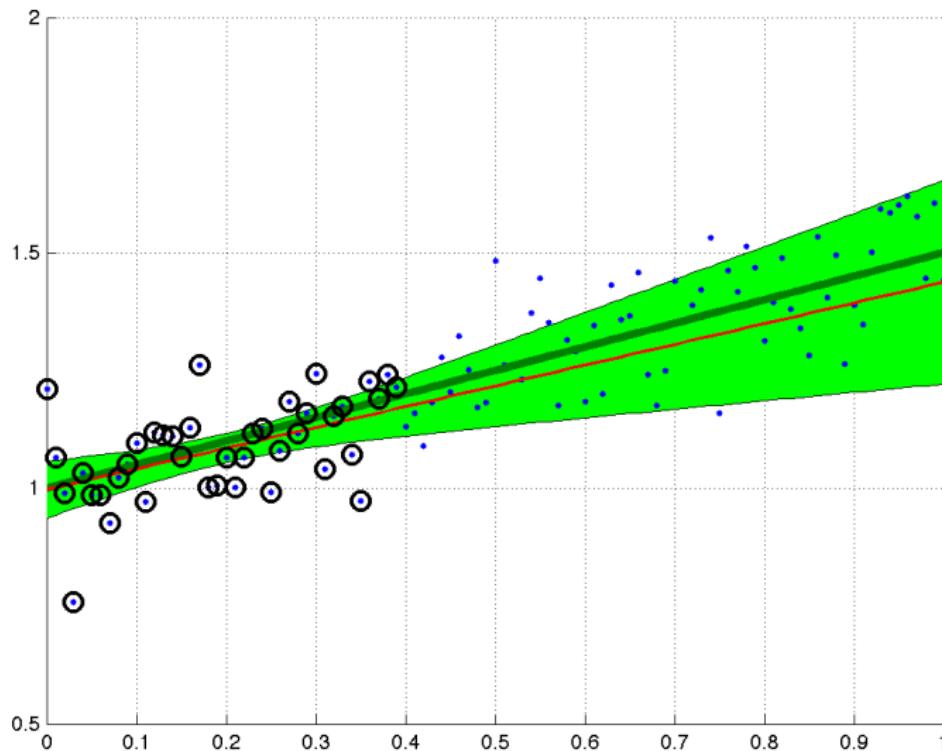
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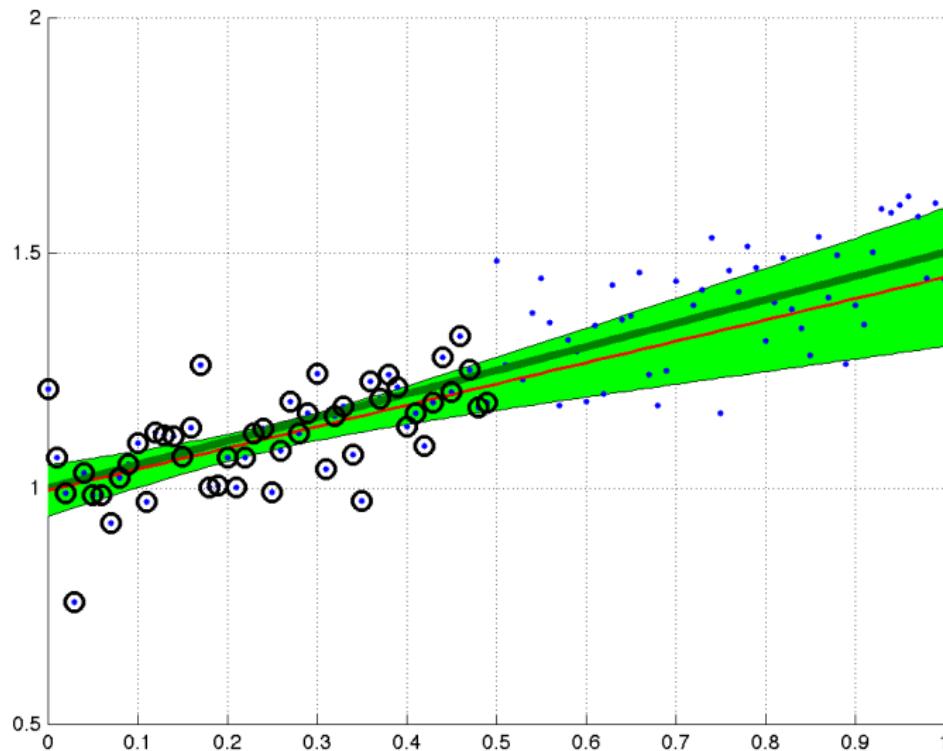
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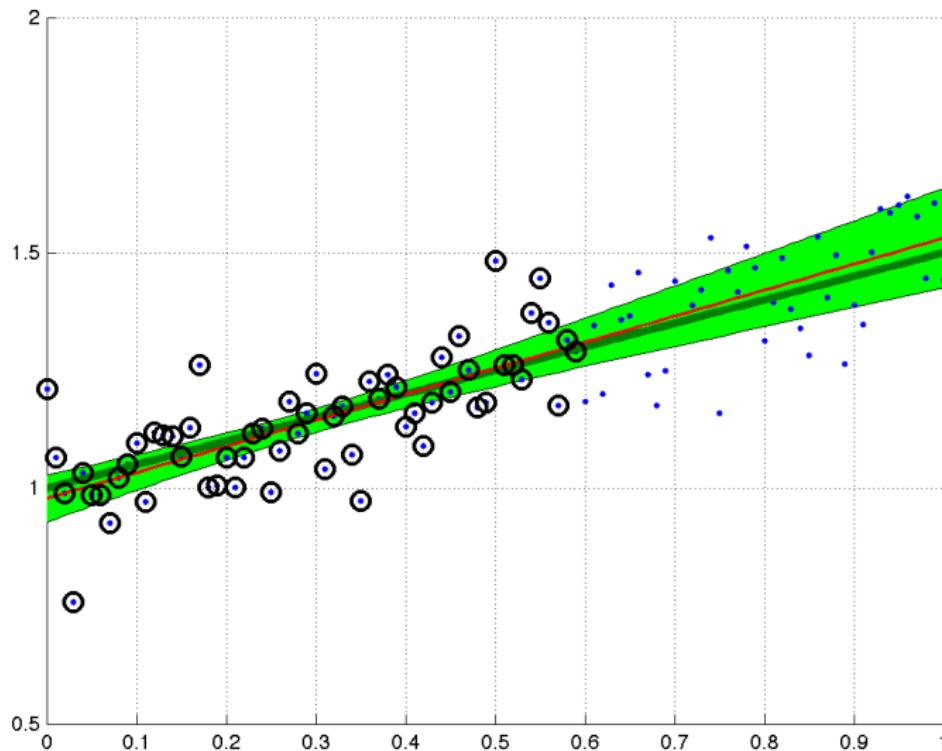
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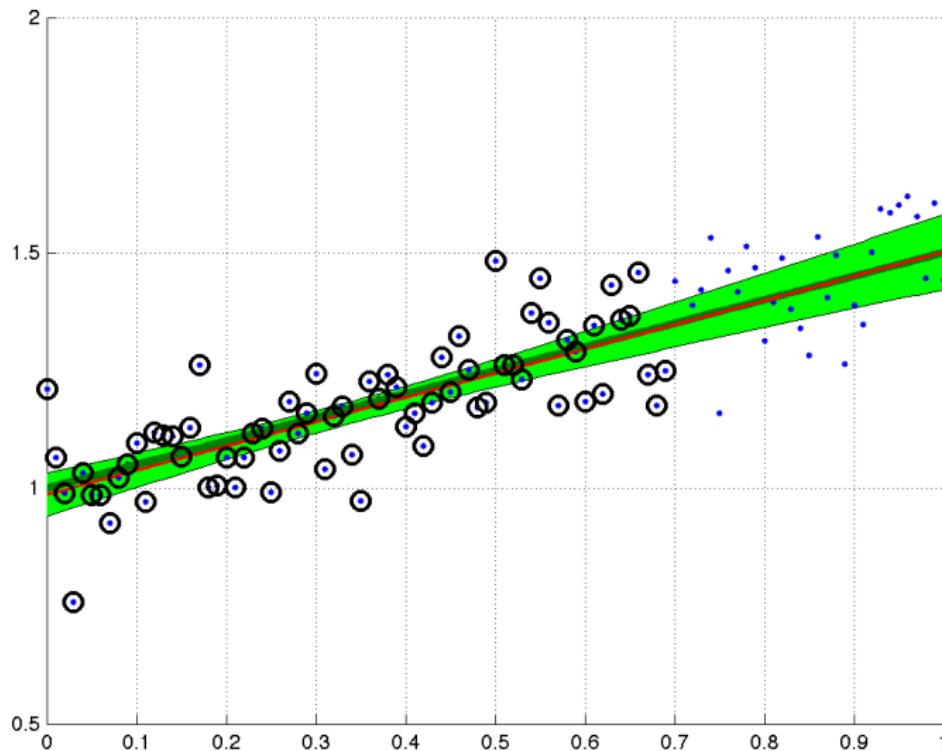
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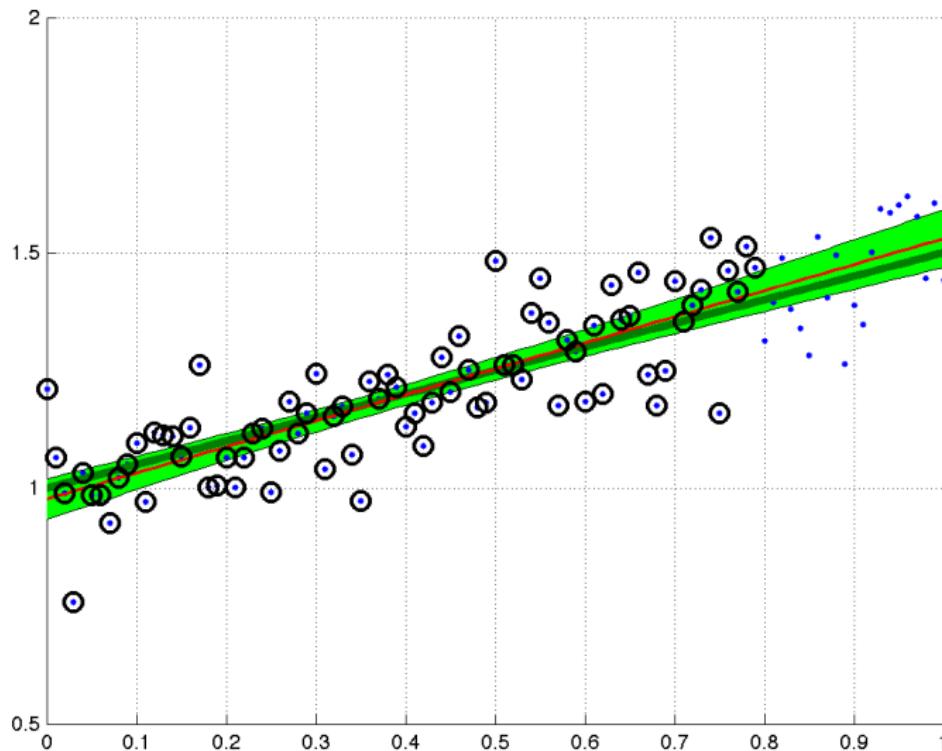
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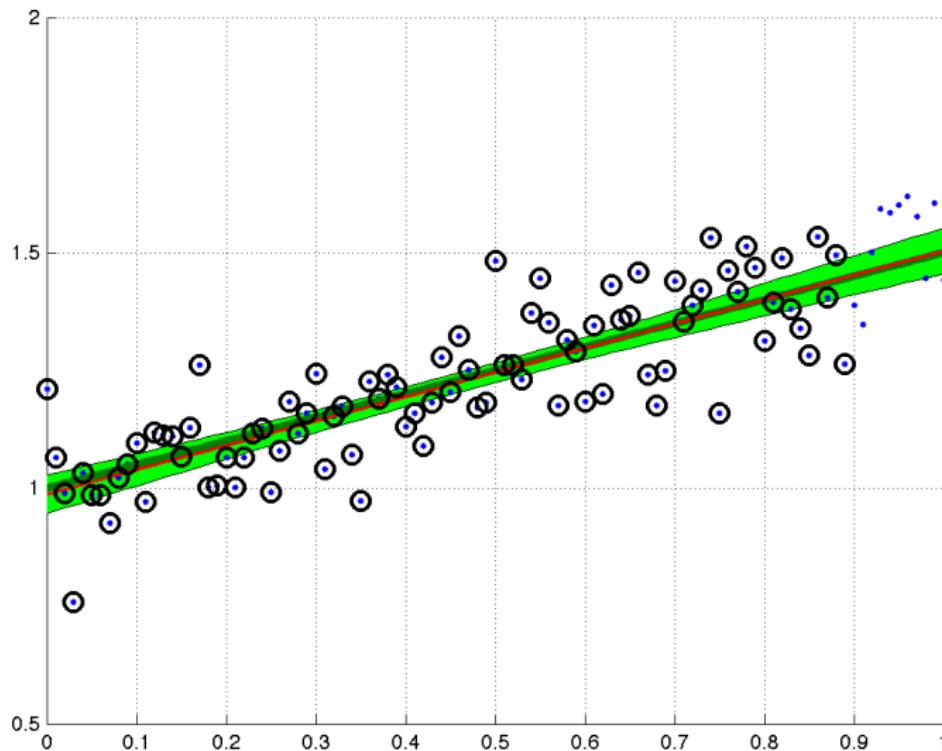
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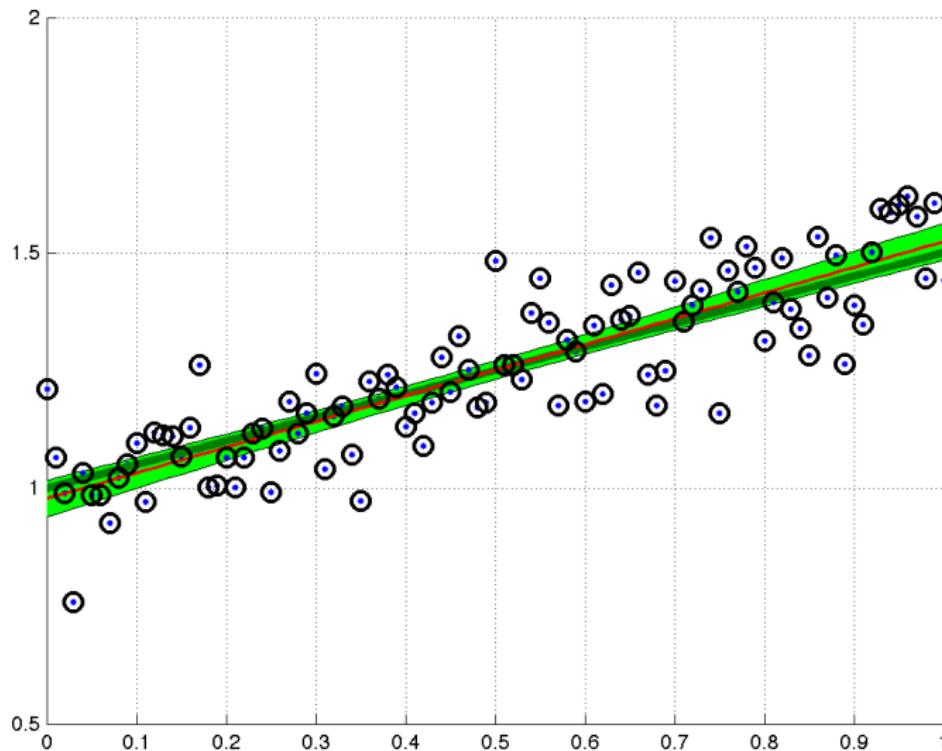
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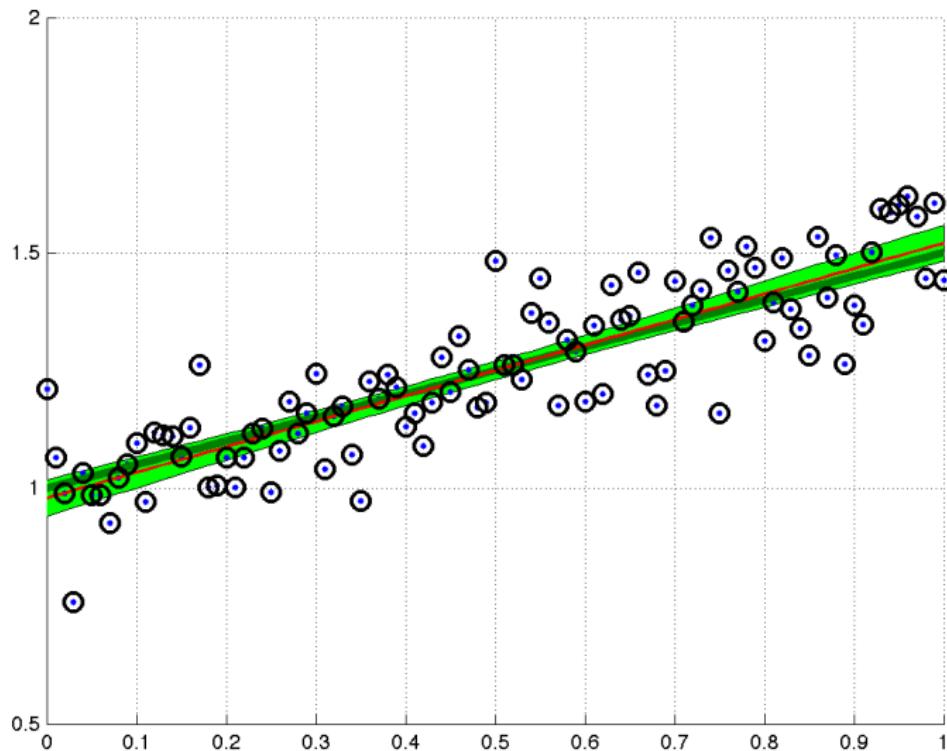
Recursive Linear Regression [3/3]



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Recursive Linear Regression [3/3]



Batch vs. Recursive Estimation [1/2]

General batch solution:

- Specify the **measurement model**:

$$p(\mathbf{y}_{1:T} | \boldsymbol{\theta}) = \prod_k p(\mathbf{y}_k | \boldsymbol{\theta}).$$

- Specify the **prior distribution** $p(\boldsymbol{\theta})$.
- Compute **posterior distribution** by the Bayes' rule:

$$p(\boldsymbol{\theta} | \mathbf{y}_{1:T}) = \frac{1}{Z} p(\boldsymbol{\theta}) \prod_k p(\mathbf{y}_k | \boldsymbol{\theta}).$$

- Compute point estimates, moments, predictive quantities etc. from the posterior distribution.

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Batch vs. Recursive Estimation [2/2]

General recursive solution:

- Specify the **measurement likelihood** $p(\mathbf{y}_k | \boldsymbol{\theta})$.
- Specify the **prior distribution** $p(\boldsymbol{\theta})$.
- Process measurements $\mathbf{y}_1, \dots, \mathbf{y}_T$ with the Bayes' rule **one at a time**, starting from the prior:

$$p(\boldsymbol{\theta} | \mathbf{y}_1) = \frac{1}{Z_1} p(\mathbf{y}_1 | \boldsymbol{\theta}) p(\boldsymbol{\theta})$$

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- The posterior at the last step is the **same as the batch solution**.

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Drift Model for Linear Regression [1/4]

- Let assume **Gaussian random walk** between the measurements in the linear regression model:

$$\begin{aligned} p(y_k | \boldsymbol{\theta}_k) &= N(y_k | \mathbf{H}_k \boldsymbol{\theta}_k, \sigma^2) \\ p(\boldsymbol{\theta}_k | \boldsymbol{\theta}_{k-1}) &= N(\boldsymbol{\theta}_k | \boldsymbol{\theta}_{k-1}, \mathbf{Q}) \\ p(\boldsymbol{\theta}_0) &= N(\boldsymbol{\theta}_0 | \mathbf{m}_0, \mathbf{P}_0). \end{aligned}$$

- Again, assume that we already know

$$p(\boldsymbol{\theta}_{k-1} | y_{1:k-1}) = N(\boldsymbol{\theta}_{k-1} | \mathbf{m}_{k-1}, \mathbf{P}_{k-1}).$$

- The **joint distribution** of $\boldsymbol{\theta}_k$ and $\boldsymbol{\theta}_{k-1}$ is (due to Markovianity of dynamics!):

$$p(\boldsymbol{\theta}_k, \boldsymbol{\theta}_{k-1} | y_{1:k-1}) = p(\boldsymbol{\theta}_k | \boldsymbol{\theta}_{k-1}) p(\boldsymbol{\theta}_{k-1} | y_{1:k-1}).$$

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Drift Model for Linear Regression [1/4]

- Let assume **Gaussian random walk** between the measurements in the linear regression model:

$$\begin{aligned} p(y_k | \boldsymbol{\theta}_k) &= N(y_k | \mathbf{H}_k \boldsymbol{\theta}_k, \sigma^2) \\ p(\boldsymbol{\theta}_k | \boldsymbol{\theta}_{k-1}) &= N(\boldsymbol{\theta}_k | \boldsymbol{\theta}_{k-1}, \mathbf{Q}) \\ p(\boldsymbol{\theta}_0) &= N(\boldsymbol{\theta}_0 | \mathbf{m}_0, \mathbf{P}_0). \end{aligned}$$

- Again, assume that we already know

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Drift Model for Linear Regression [2/4]

- Integrating over θ_{k-1} gives:

$$p(\theta_k | y_{1:k-1}) = \int p(\theta_k | \theta_{k-1}) p(\theta_{k-1} | y_{1:k-1}) d\theta_{k-1}.$$

- This equation for **Markov processes** is called the **Chapman-Kolmogorov equation**.
- Because the distributions are Gaussian, the **result is Gaussian**

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Drift Model for Linear Regression [3/4]

- As in the pure recursive estimation, we get

$$\begin{aligned} p(\boldsymbol{\theta}_k \mid y_{1:k}) &\propto p(y_k \mid \boldsymbol{\theta}_k) p(\boldsymbol{\theta}_k \mid y_{1:k-1}) \\ &\propto N(\boldsymbol{\theta}_k \mid \mathbf{m}_k, \mathbf{P}_k). \end{aligned}$$

- After applying the matrix inversion lemma, mean and covariance can be written as

$$\begin{aligned} S_k &= \mathbf{H}_k \mathbf{P}_k^{-} \mathbf{H}_k^T + \sigma^2 \\ \mathbf{K}_k &= \mathbf{P}_k^{-} \mathbf{H}_k^T S_k^{-1} \\ \mathbf{m}_k &= \mathbf{m}_k^{-} + \mathbf{K}_k [y_k - \mathbf{H}_k \mathbf{m}_k^{-}] \\ \mathbf{P}_k &= \mathbf{P}_k^{-} - \mathbf{K}_k S_k \mathbf{K}_k^T. \end{aligned}$$

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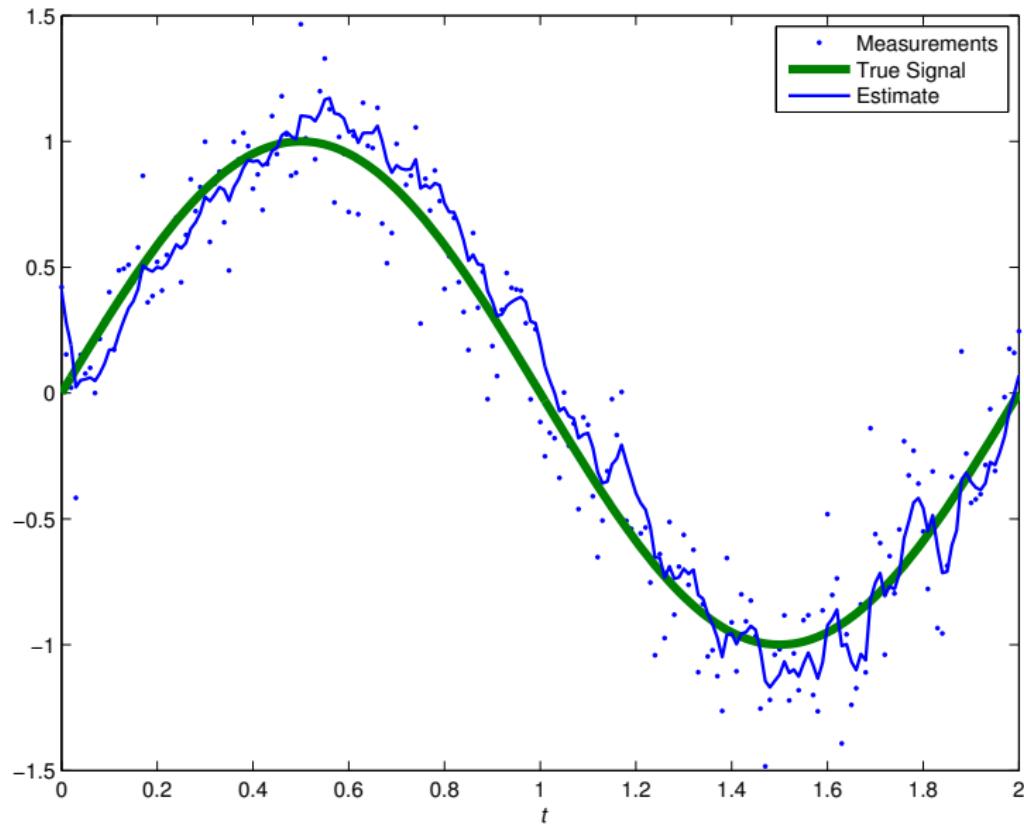
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- But in *Kalman filtering and control theory* the vector of parameters $\boldsymbol{\theta}_k$ is usually called “state” and denoted as \mathbf{x}_k .
- More standard state space notation:

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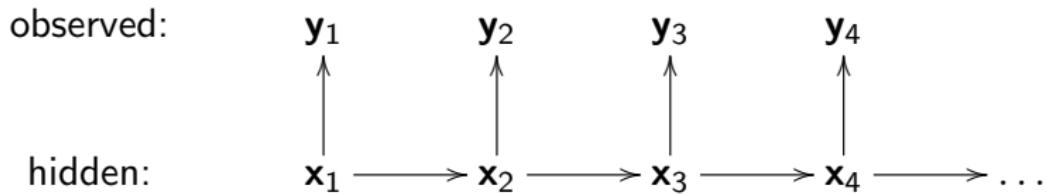
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Probabilistic State Space Models: Example

Example (Gaussian random walk)

Gaussian random walk model can be written as

$$x_k = x_{k-1} + w_{k-1}, \quad w_{k-1} \sim N(0, q)$$
$$y_k = x_k + e_k, \quad e_k \sim N(0, r),$$

where x_k is the hidden state and y_k is the measurement. In terms of probability densities the model can be written as

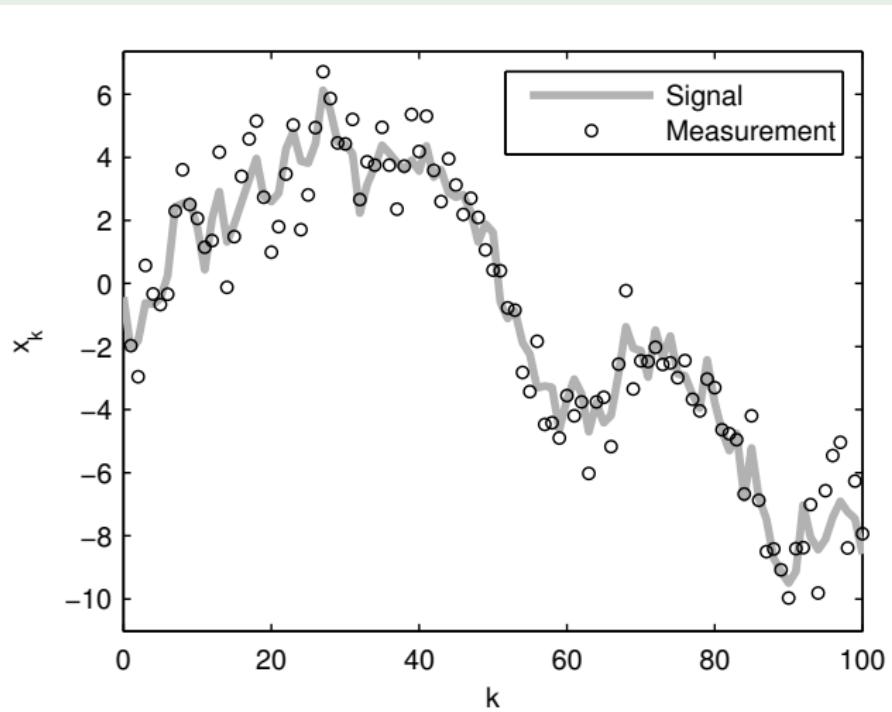
$$p(x_k | x_{k-1}) = \frac{1}{\sqrt{2\pi q}} \exp\left(-\frac{1}{2q}(x_k - x_{k-1})^2\right)$$

$$p(y_k | x_k) = \frac{1}{\sqrt{2\pi r}} \exp\left(-\frac{1}{2r}(y_k - x_k)^2\right)$$

which is a discrete-time state space model.

Probabilistic State Space Models: Example (cont.)

Example (Gaussian random walk (cont.))



Probabilistic State Space Models: Further Examples

- Linear Gauss-Markov model – which defines a Gaussian process:

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

- Gaussian driven non-linear model – a non-Gaussian process:

$$\begin{aligned}\mathbf{x}_k &= \mathbf{f}(\mathbf{x}_{k-1}, \mathbf{q}_{k-1}) \\ \mathbf{y}_k &= \mathbf{h}(\mathbf{x}_k, \mathbf{r}_k).\end{aligned}$$

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Bayesian Filtering, Prediction and Smoothing

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- Curse of computational complexity: complexity grows more than linearly with number of measurements (typically we have $O(T^3)$).
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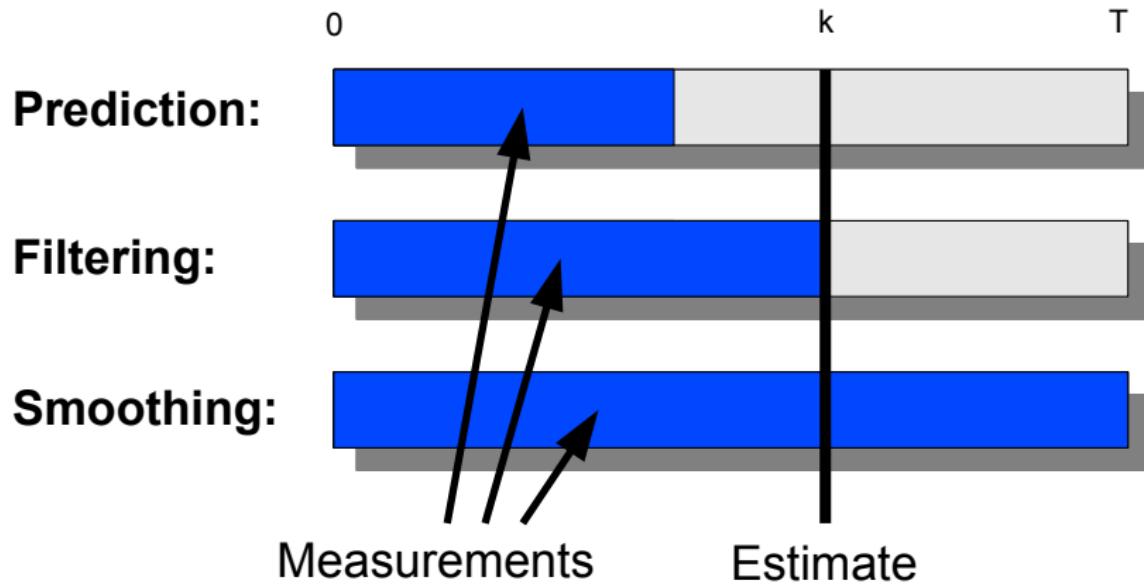
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Contents

- 1 From Linear Regression to Kalman Filter and Beyond
- 2 Bayesian Filtering and Smoothing
- 3 State Space Representation of Gaussian Process Regression
- 4 Spatio-Temporal Systems, Latent Force Models and Other Extensions
- 5 Application examples
- 6 Summary

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- Bayesian optimal filter computes the distribution

$$p(\mathbf{x}_k | \mathbf{y}_{1:k})$$

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- ➌ Measurement sequence $\mathbf{y}_{1:k} = \mathbf{y}_1, \dots, \mathbf{y}_k$.
- Computation is based on recursion rule for incorporation of the new measurement \mathbf{y}_k into the posterior:

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Bayesian Optimal Filter: Formal Equations

Optimal filter

- **Initialization:** The recursion starts from the prior distribution $p(\mathbf{x}_0)$.
- **Prediction:** by the Chapman-Kolmogorov equation

$$p(\mathbf{x}_k | \mathbf{y}_{1:k-1}) = \int p(\mathbf{x}_k | \mathbf{x}_{k-1}) p(\mathbf{x}_{k-1} | \mathbf{y}_{1:k-1}) d\mathbf{x}_{k-1}.$$

- **Update:** by the Bayes' rule

$$p(\mathbf{x}_k | \mathbf{y}_{1:k}) = \frac{1}{Z_k} p(\mathbf{y}_k | \mathbf{x}_k) p(\mathbf{x}_k | \mathbf{y}_{1:k-1}).$$

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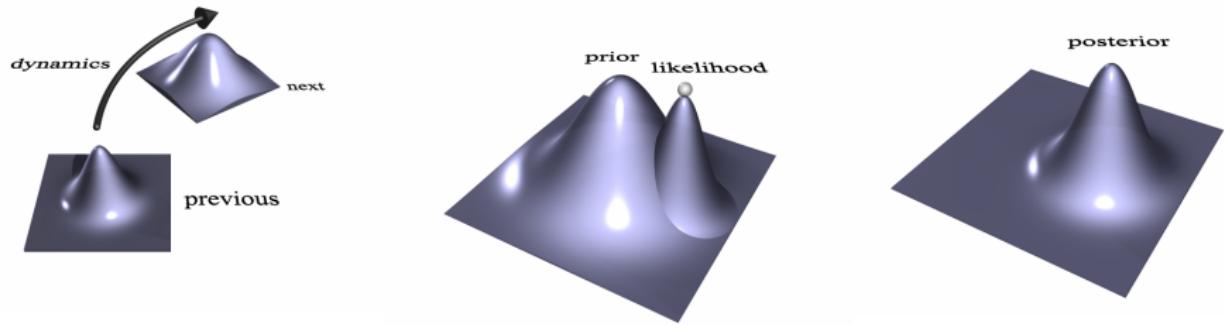
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Bayesian Optimal Filter: Graphical Explanation



On prediction step the distribution of previous step is propagated through the dynamics.

Prior distribution from prediction and the likelihood of measurement.

The posterior distribution after combining the prior and likelihood by Bayes' rule.

Filtering Algorithms

- **Kalman filter** is the classical optimal filter for linear-Gaussian models.
- **Extended Kalman filter (EKF)** is linearization based extension of Kalman filter to non-linear models.
- **Unscented Kalman filter (UKF)** is sigma-point transformation based extension of Kalman filter.
- **Gauss-Hermite and Cubature Kalman filters (GHKF/CKF)** are numerical integration based extensions of Kalman filter.
- **Particle filter** forms a **Monte Carlo representation** (particle set) to the distribution of the state estimate.
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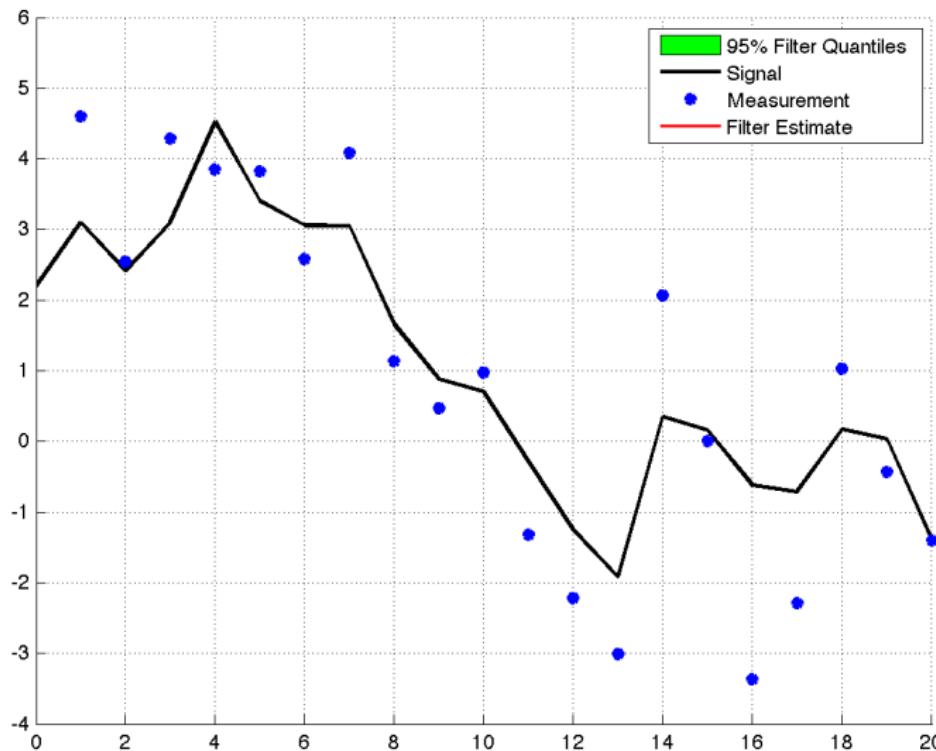
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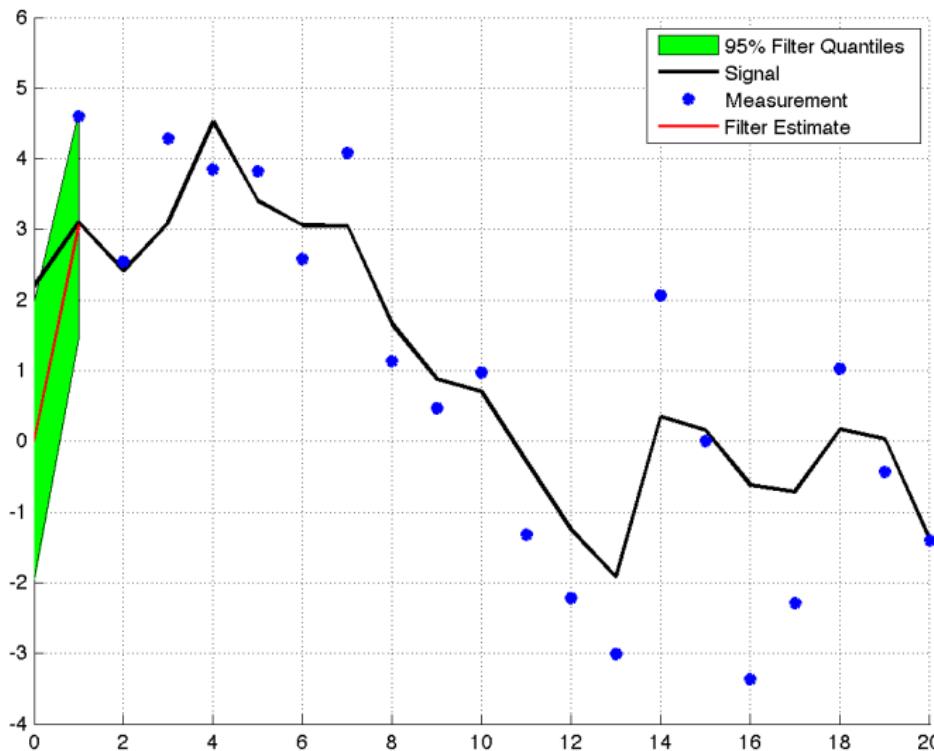
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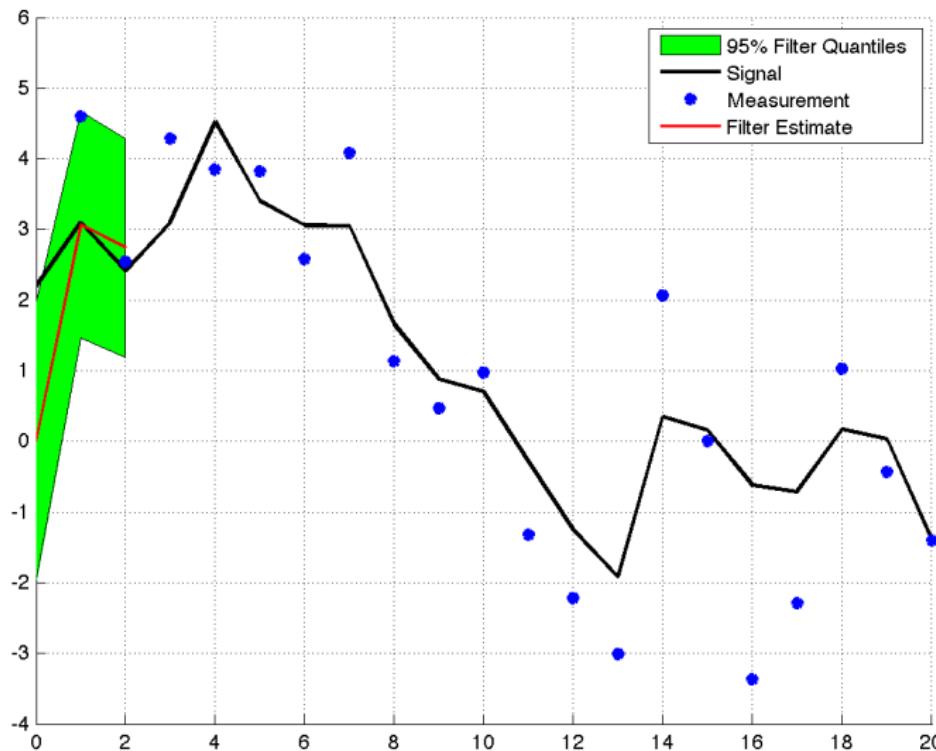
Kalman Filter Example



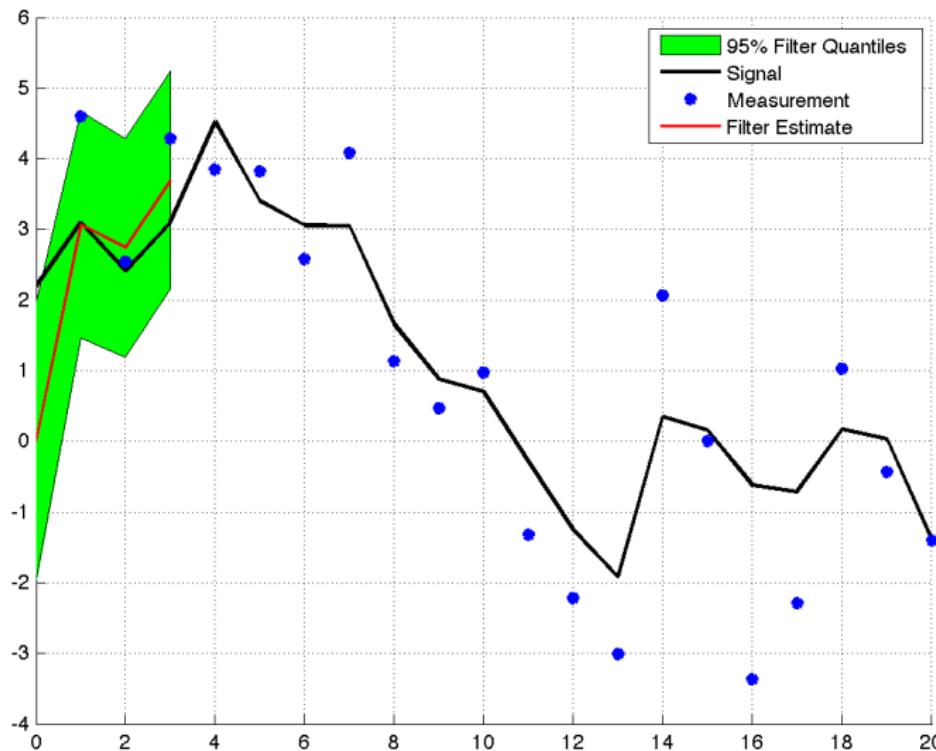
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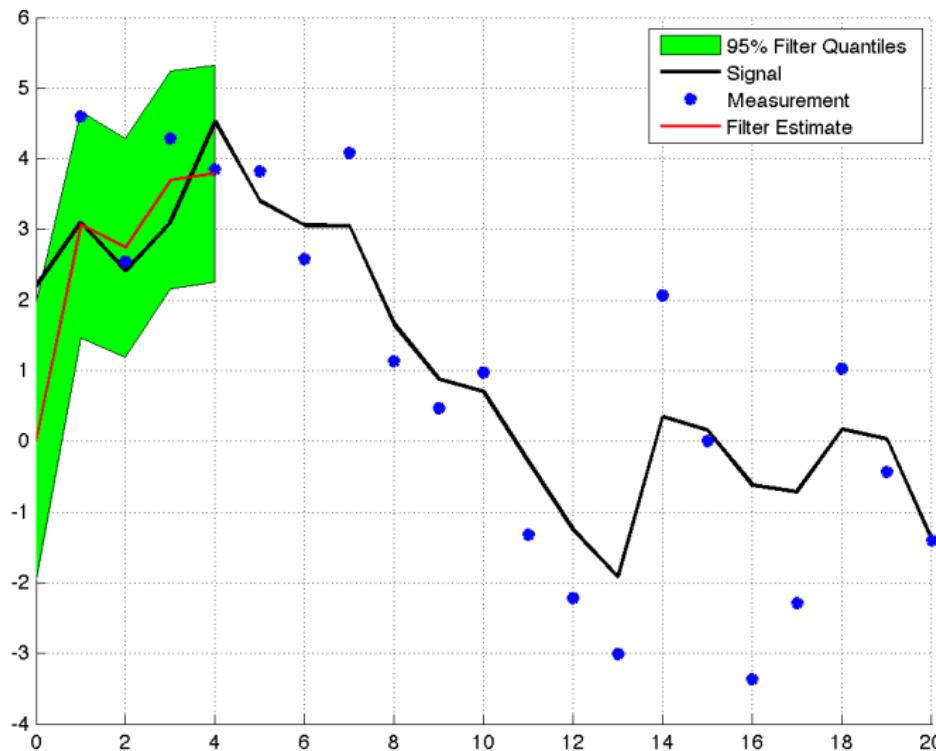
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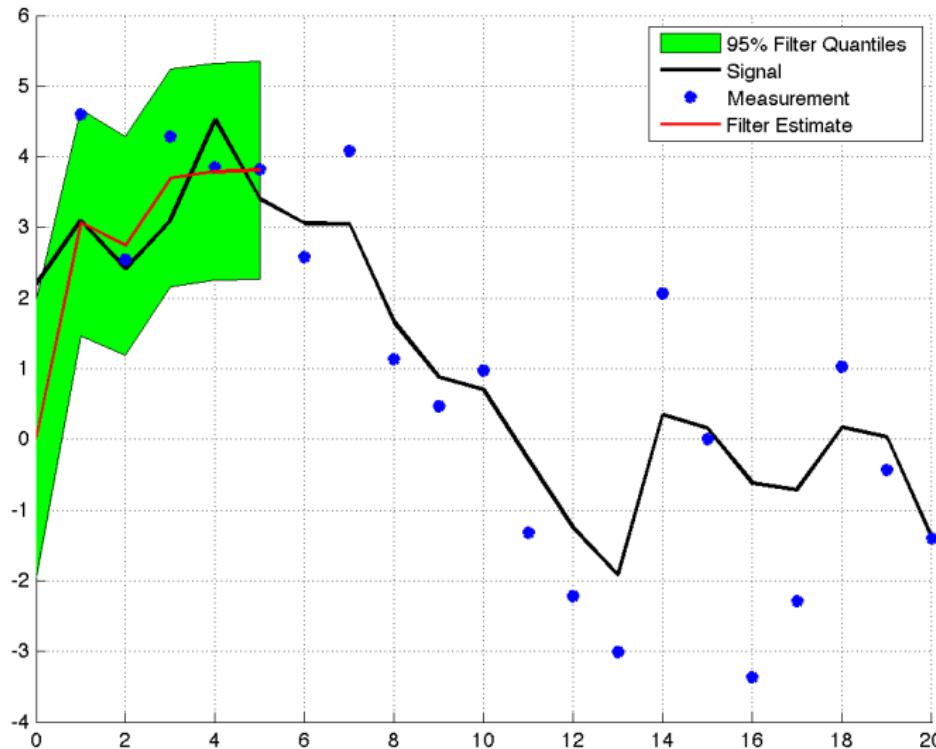
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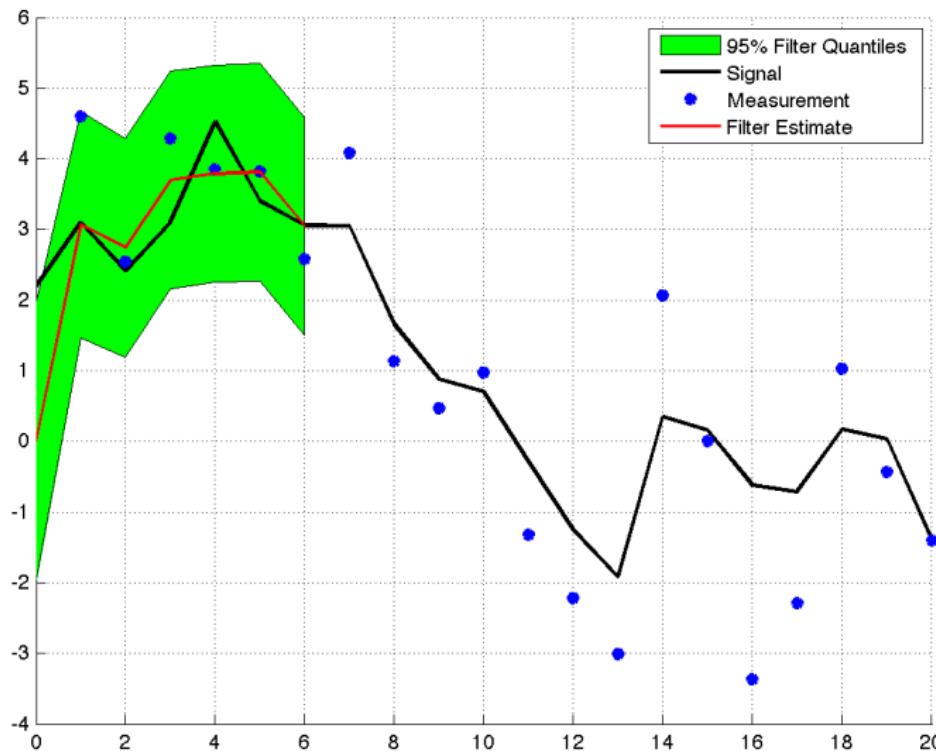
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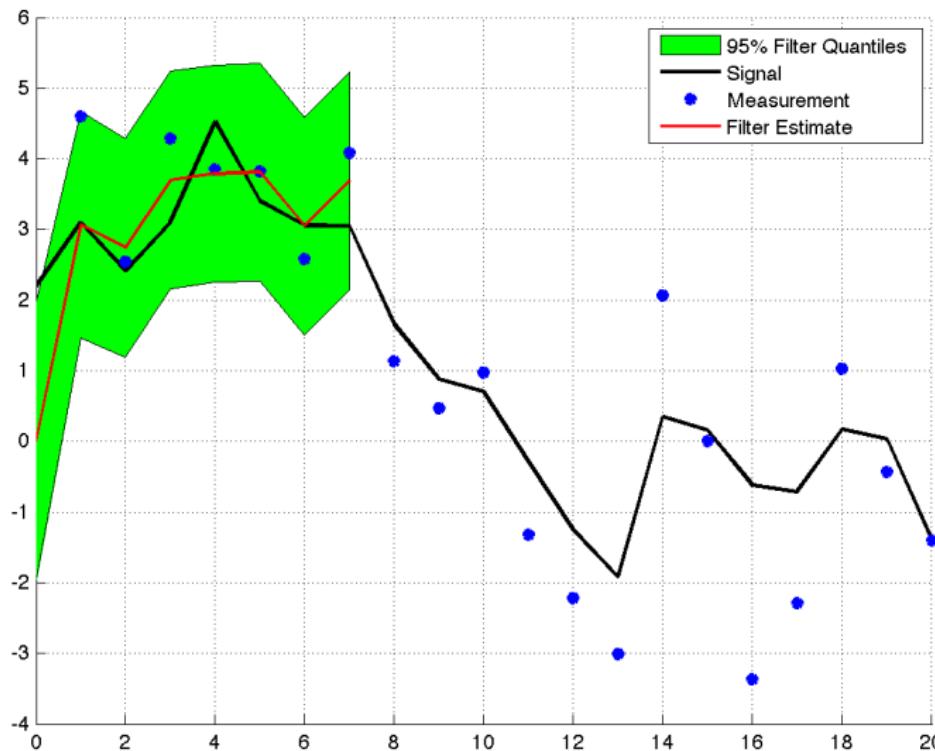
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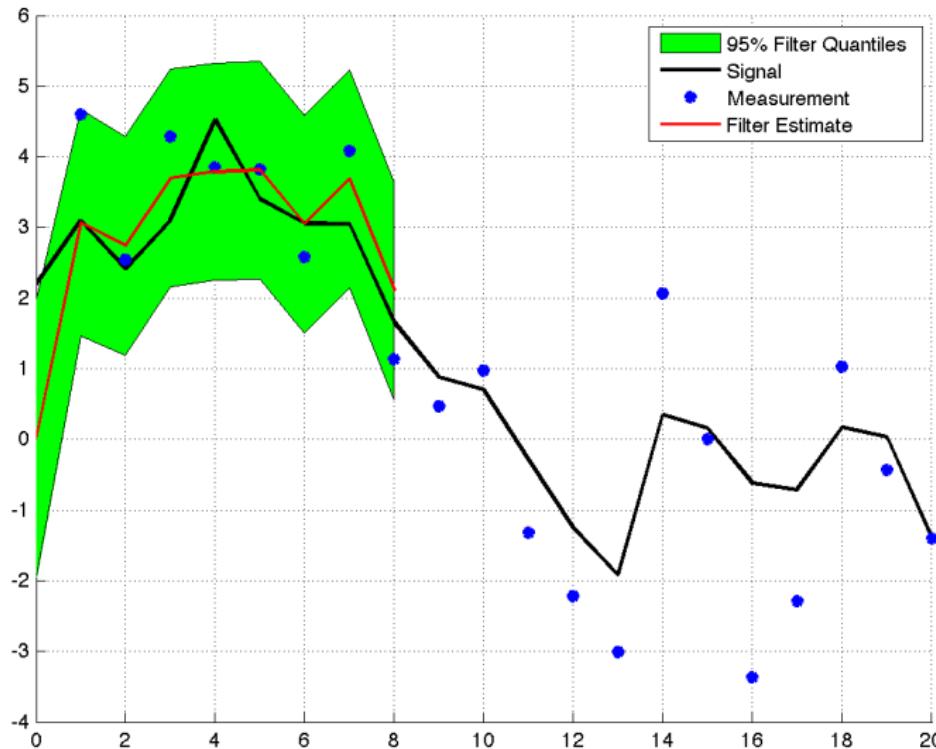
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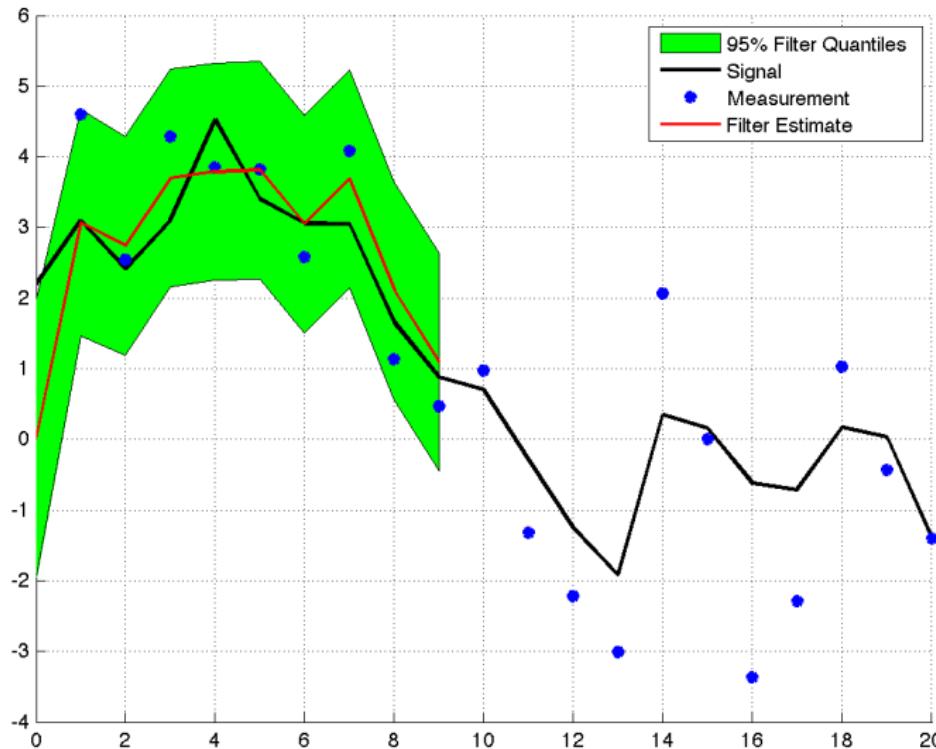
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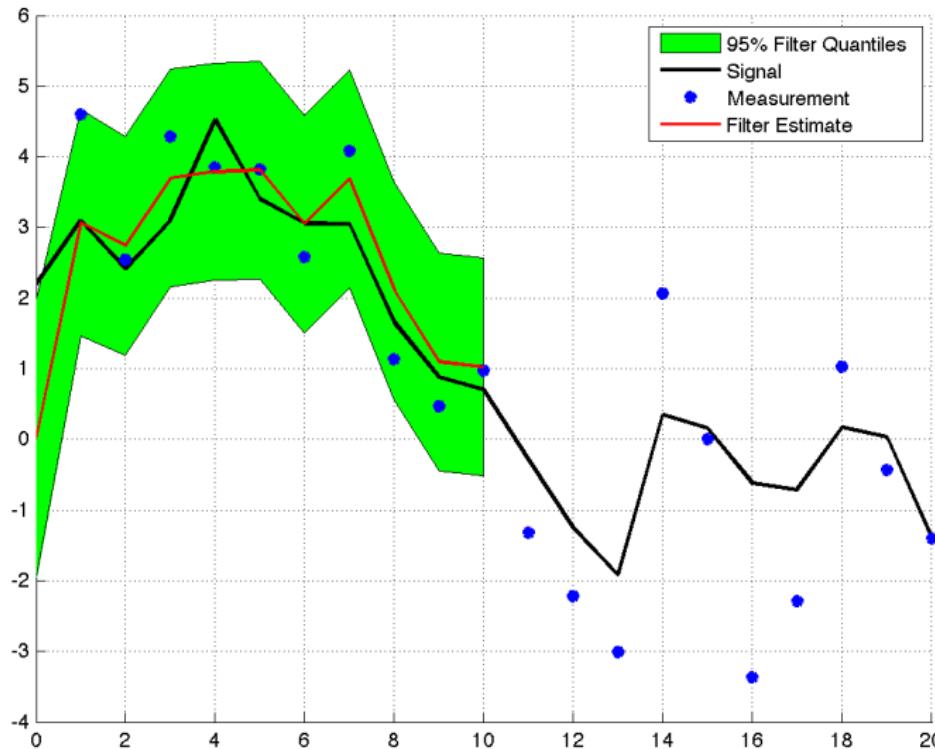
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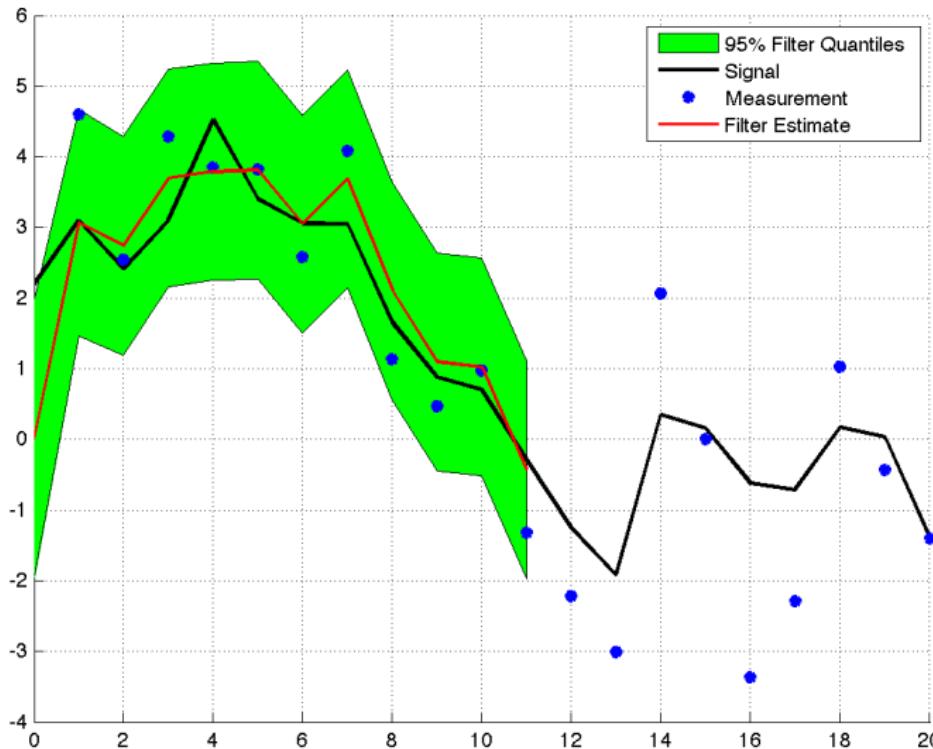
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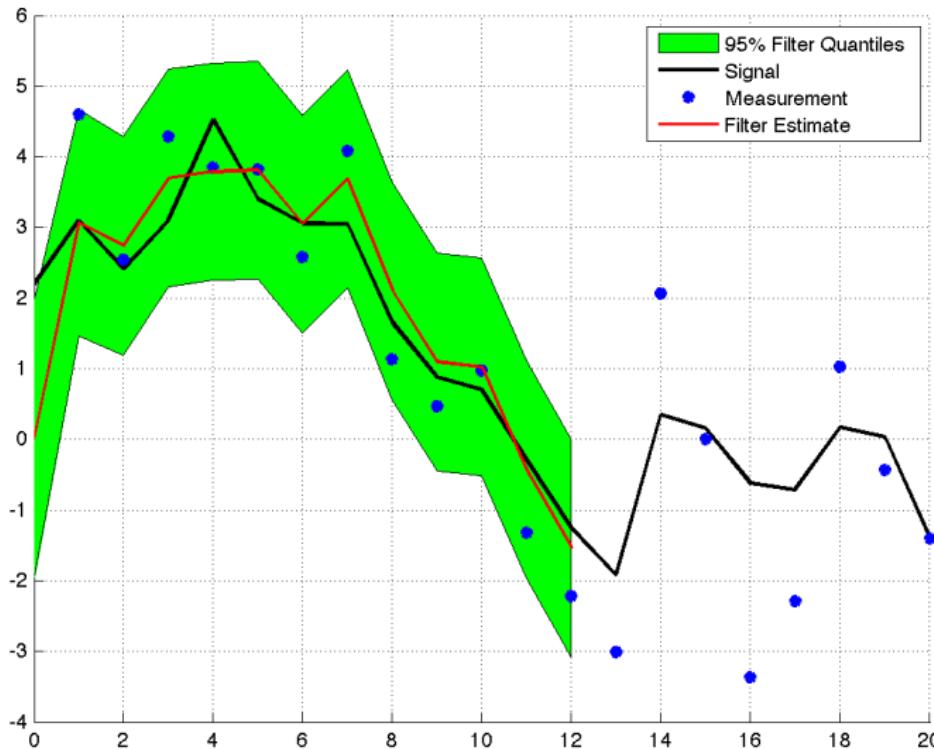
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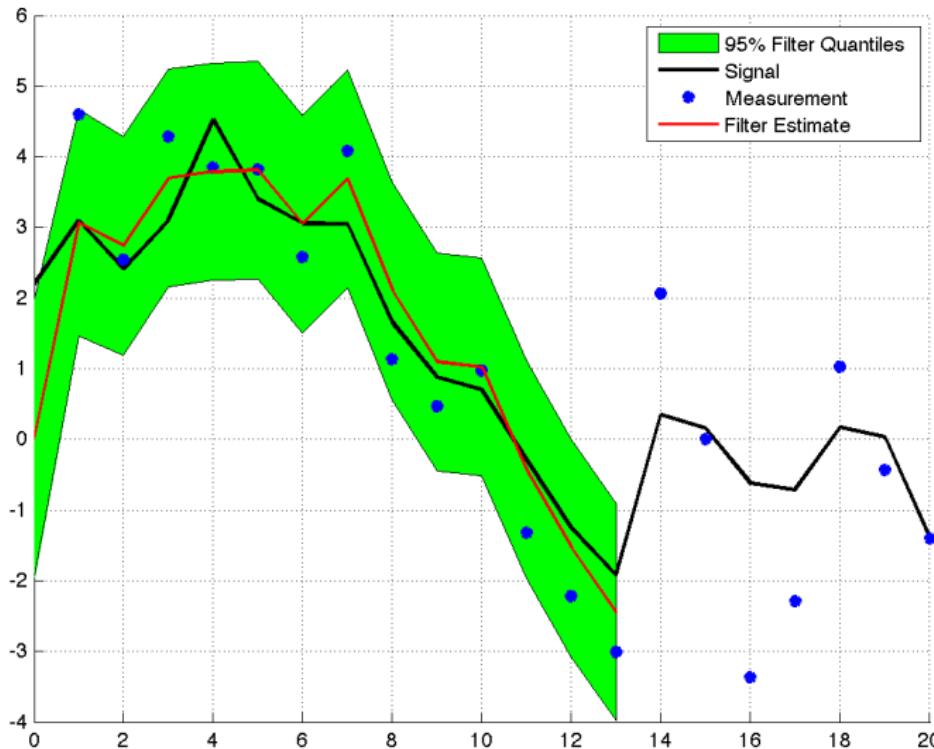
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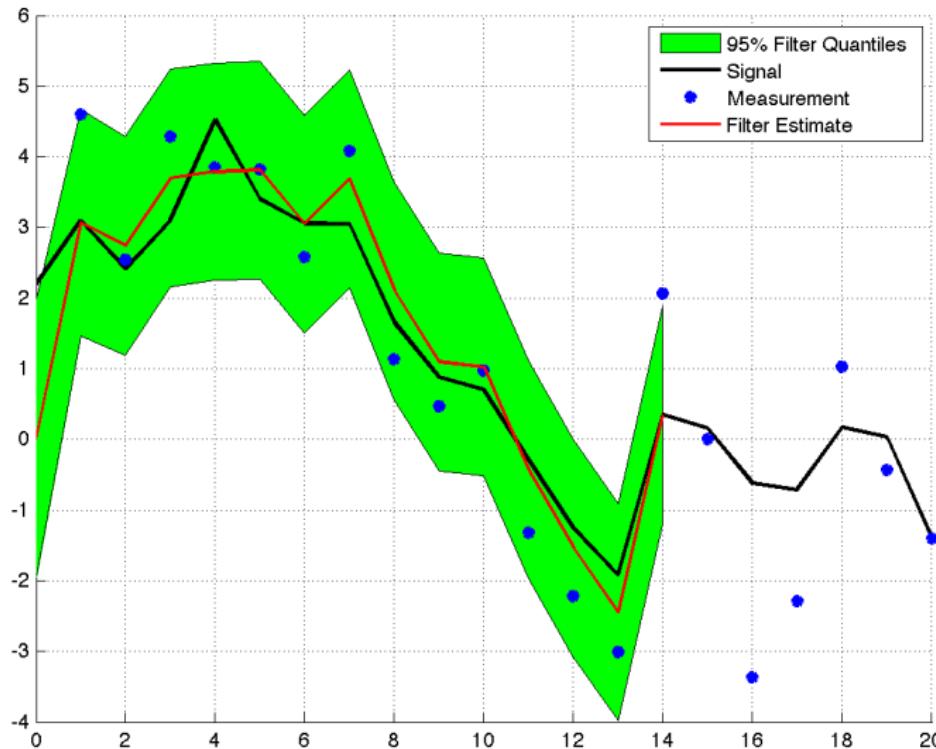
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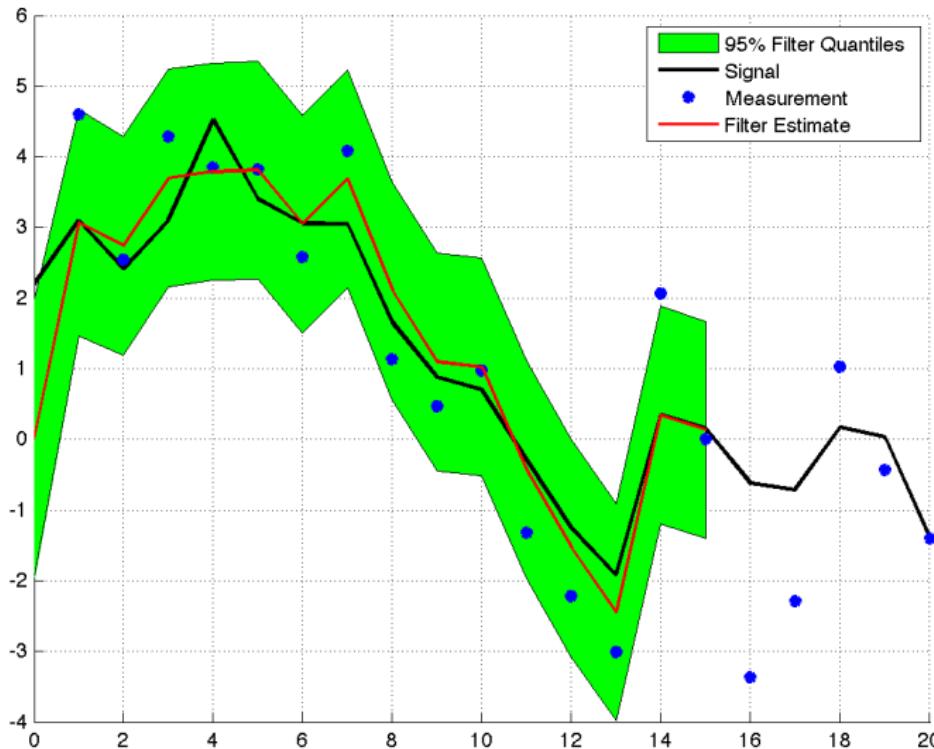
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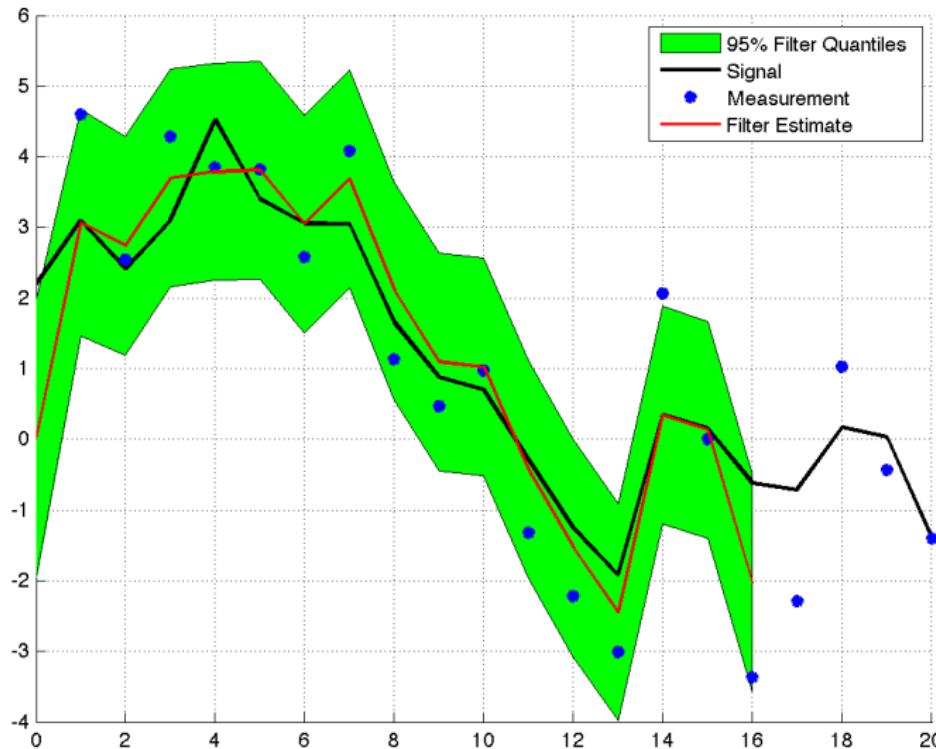
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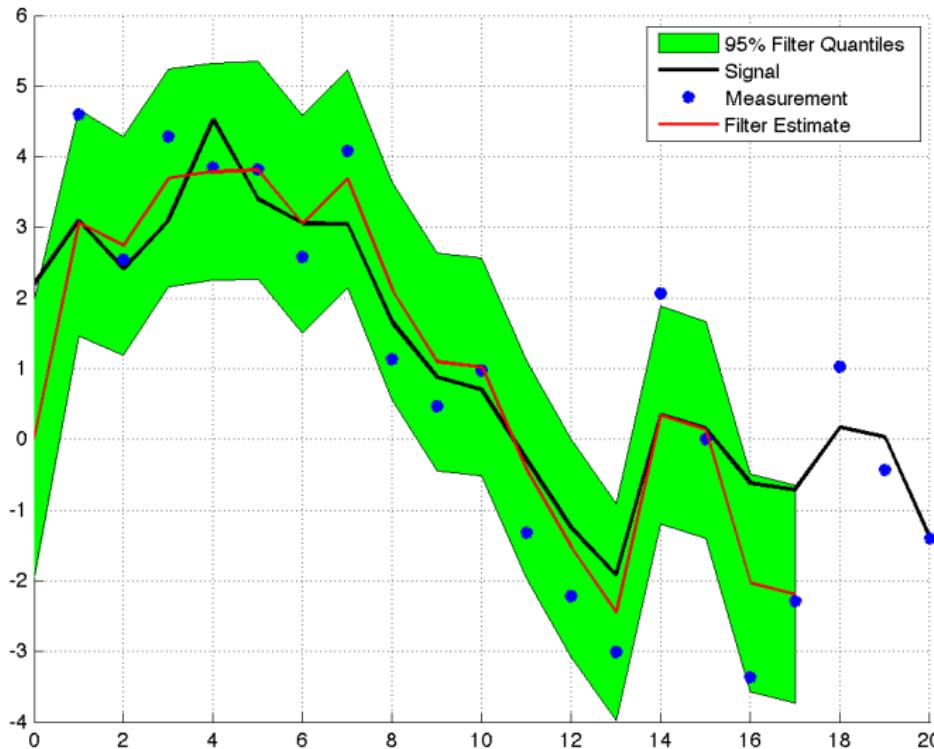
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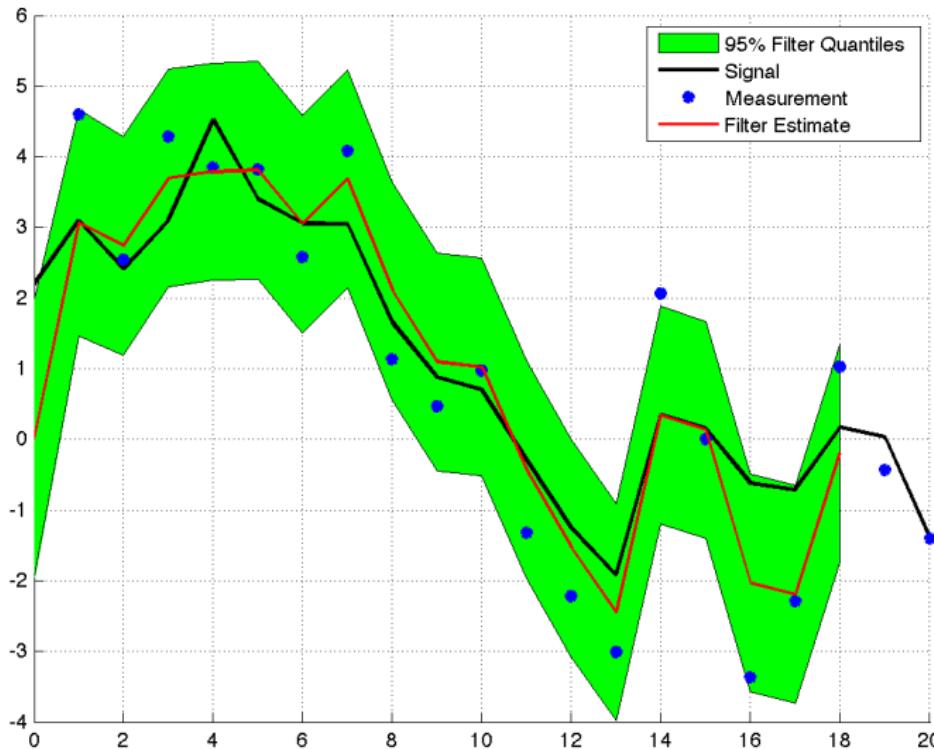
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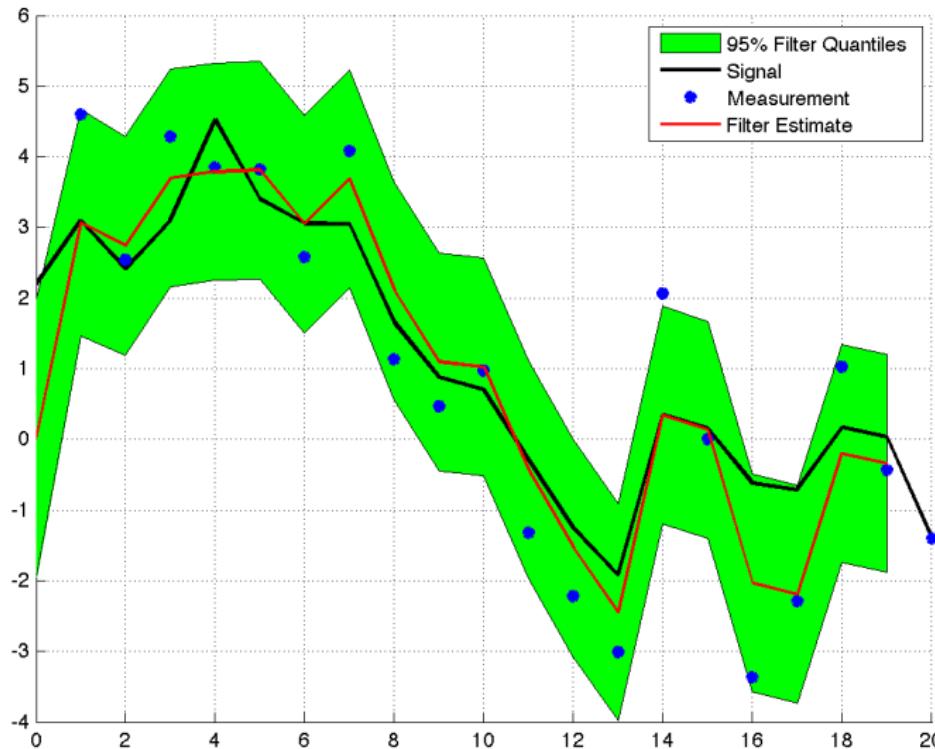
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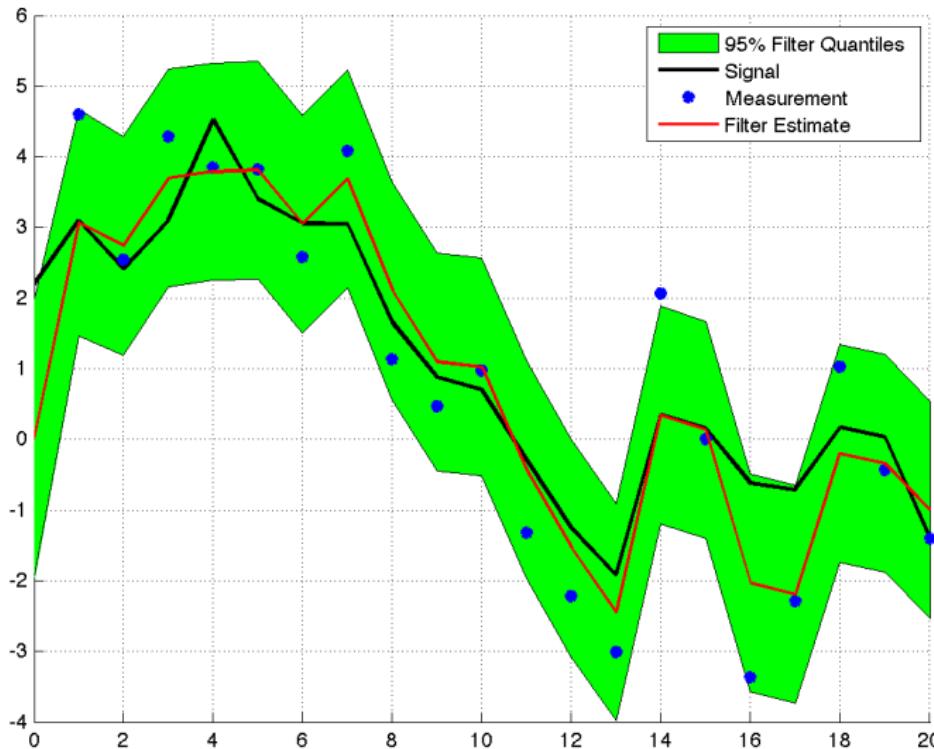
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Bayesian Smoothing Problem

- We have a **probabilistic state space model**:

$$\begin{aligned}\mathbf{y}_k &\sim p(\mathbf{y}_k \mid \mathbf{x}_k) \\ \mathbf{x}_k &\sim p(\mathbf{x}_k \mid \mathbf{x}_{k-1})\end{aligned}$$

- Assume that the filtering distributions $p(\mathbf{x}_k \mid \mathbf{y}_{1:k})$ have already been computed for all $k = 0, \dots, T$.
- We want **recursive equations** of computing the smoothing distribution for all $k < T$:

$$p(\mathbf{x}_k \mid \mathbf{y}_{1:T}).$$

- The **recursion** will go **backwards in time**, because on the last step, the filtering and smoothing distributions coincide:

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Bayesian Smoothing Equations

The Bayesian smoothing equations consist of prediction step and backward update step:

$$p(\mathbf{x}_{k+1} | \mathbf{y}_{1:k}) = \int p(\mathbf{x}_{k+1} | \mathbf{x}_k) p(\mathbf{x}_k | \mathbf{y}_{1:k}) d\mathbf{x}_k$$

$$p(\mathbf{x}_k | \mathbf{y}_{1:T}) = p(\mathbf{x}_k | \mathbf{y}_{1:k}) \int \left[\frac{p(\mathbf{x}_{k+1} | \mathbf{x}_k) p(\mathbf{x}_{k+1} | \mathbf{y}_{1:T})}{p(\mathbf{x}_{k+1} | \mathbf{y}_{1:k})} \right] d\mathbf{x}_{k+1}$$

The recursion is started from the filtering (and smoothing) distribution of the last time step $p(\mathbf{x}_T | \mathbf{y}_{1:T})$.

Smoothing Algorithms

- **Rauch-Tung-Striebel (RTS) smoother** is the closed form smoother for linear Gaussian models.
- Extended, statistically linearized and unscented RTS smoothers are the approximate nonlinear smoothers corresponding to EKF, SLF and UKF.
- Gaussian RTS smoothers: cubature RTS smoother, Gauss-Hermite RTS smoothers and various others
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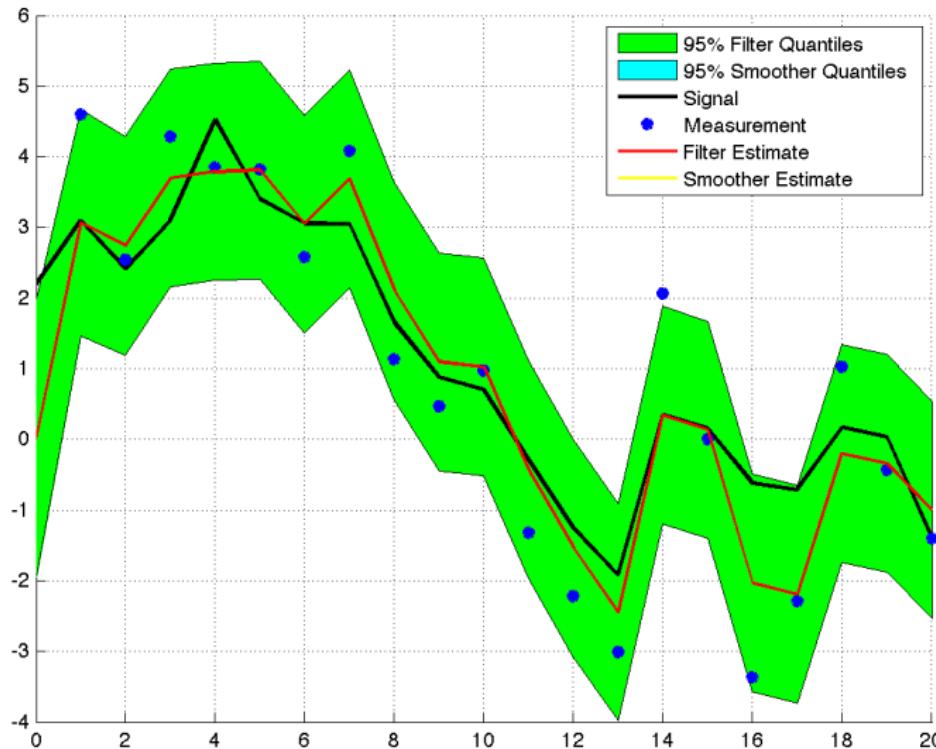
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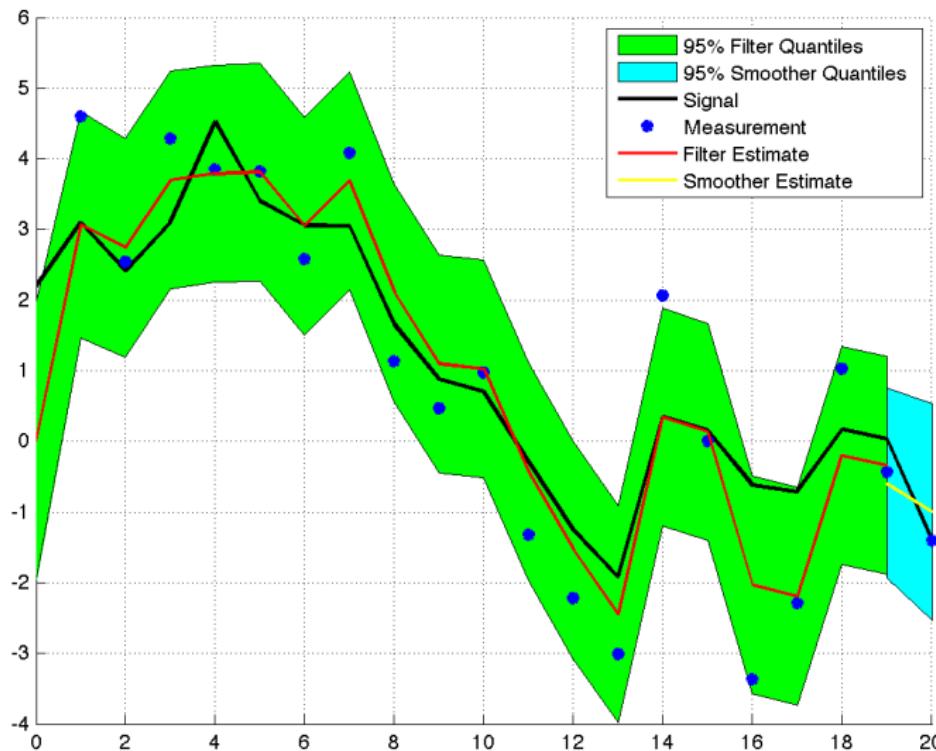
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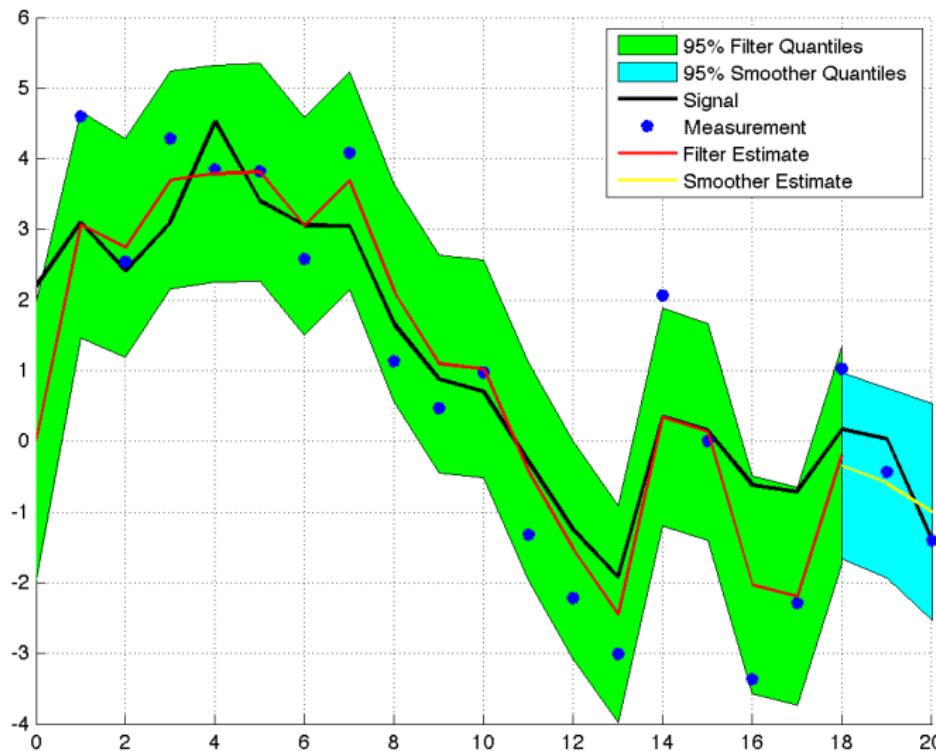
Rauch-Tung-Striebel Smoother Example



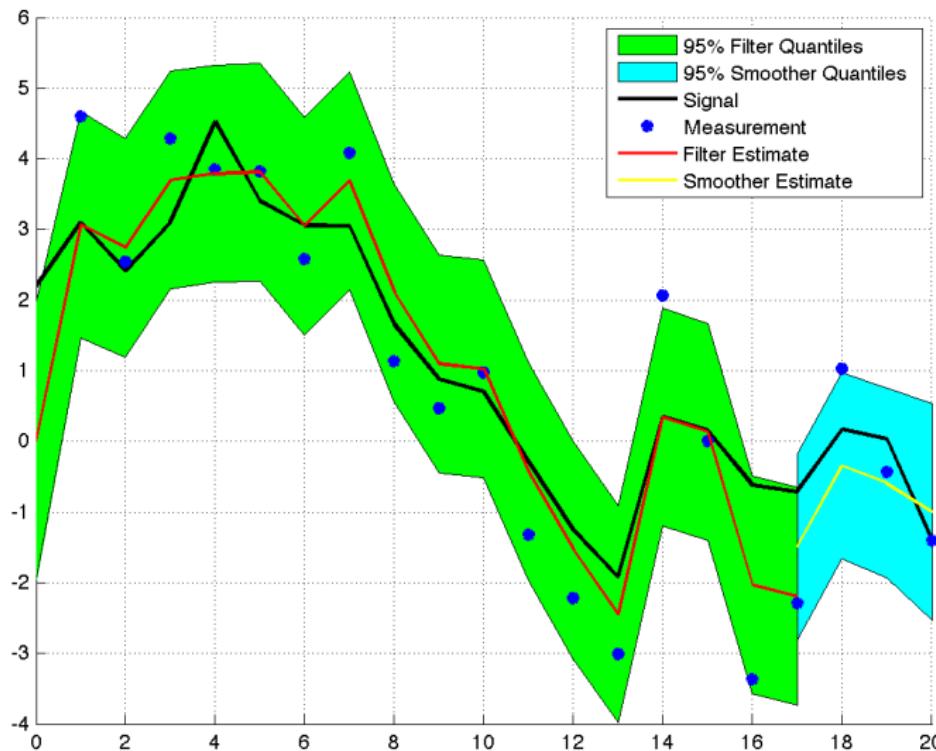
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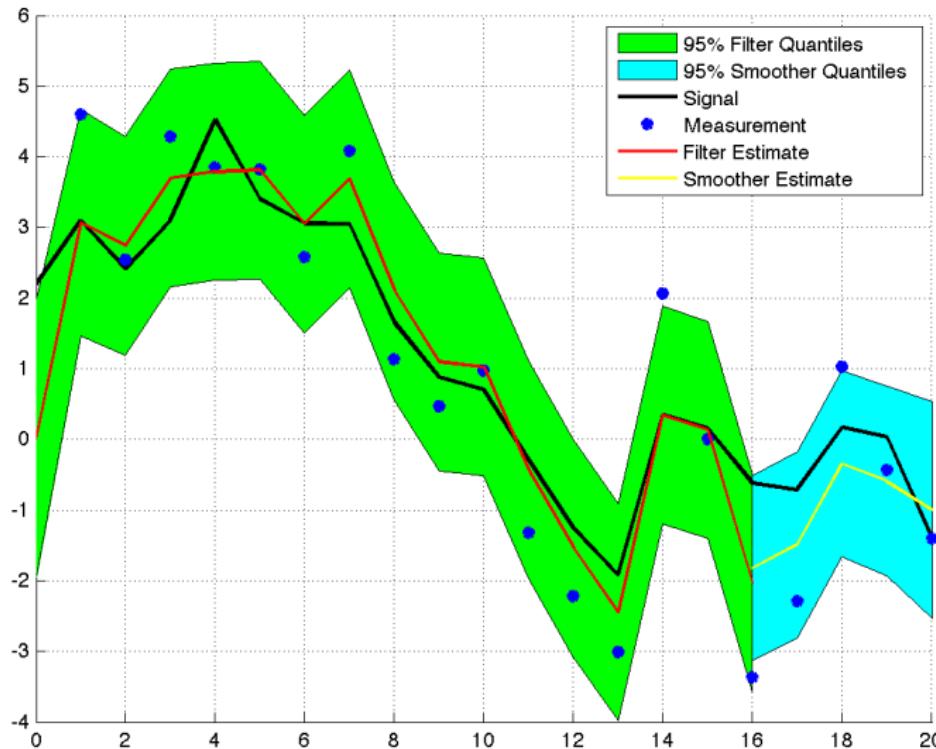
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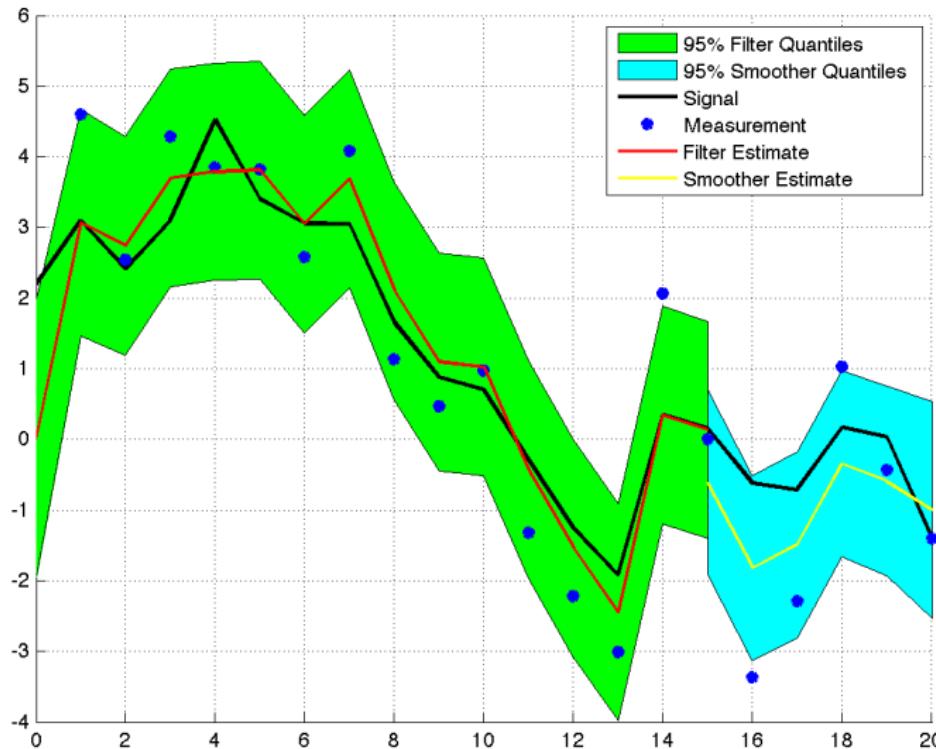
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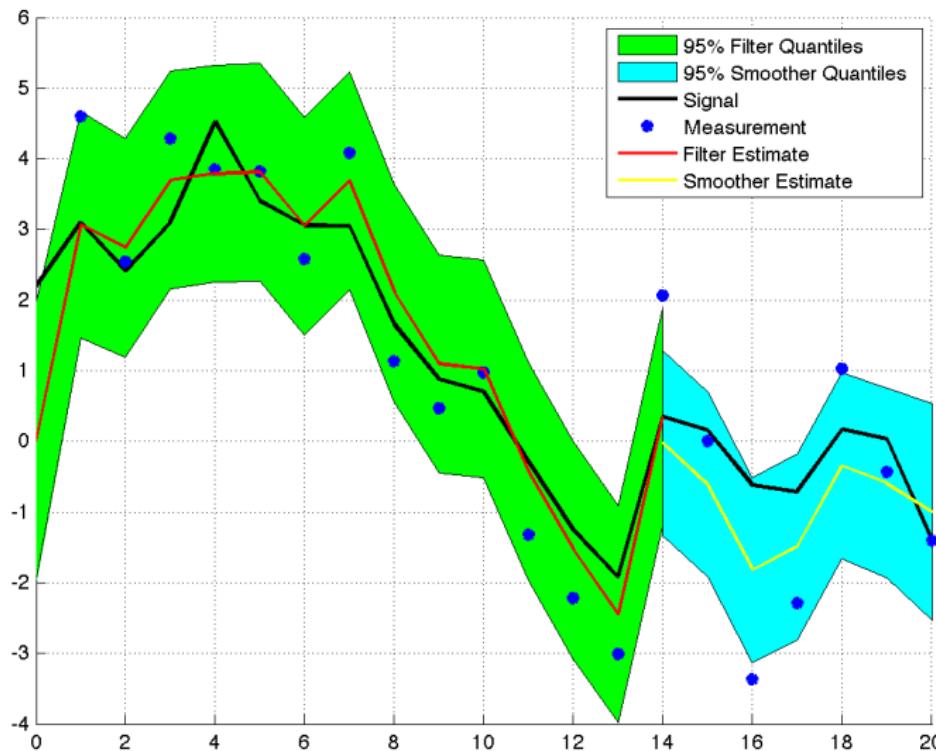
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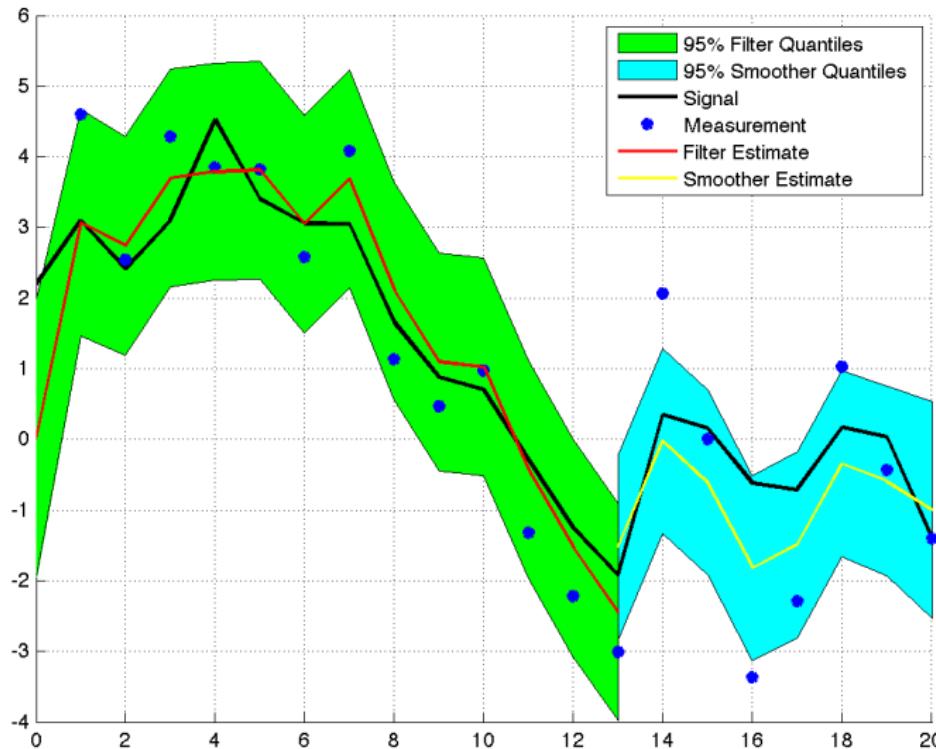
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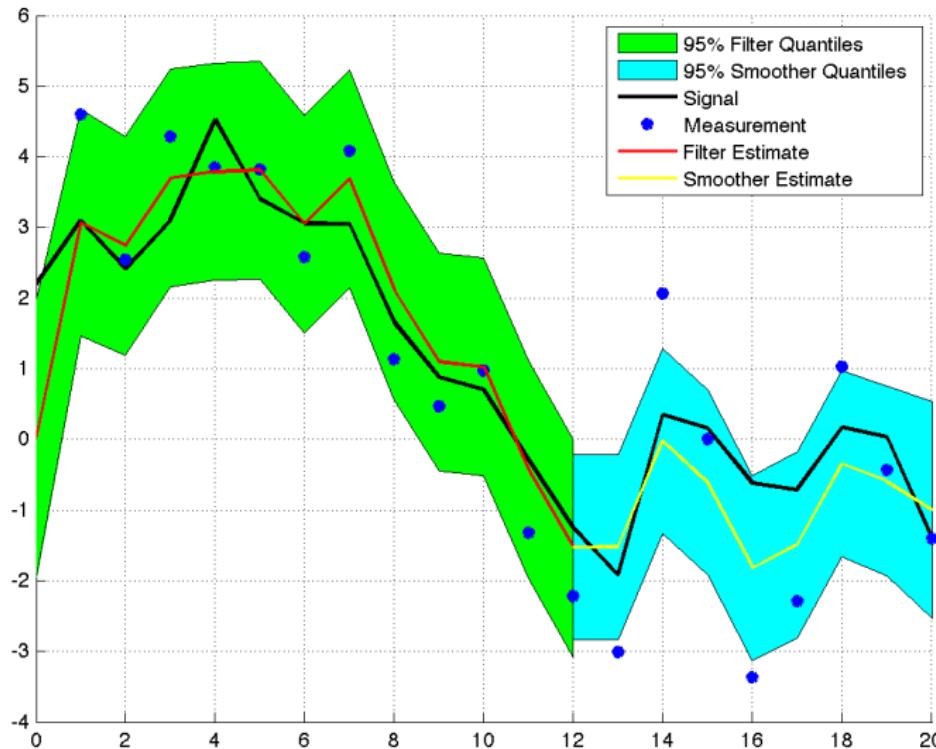
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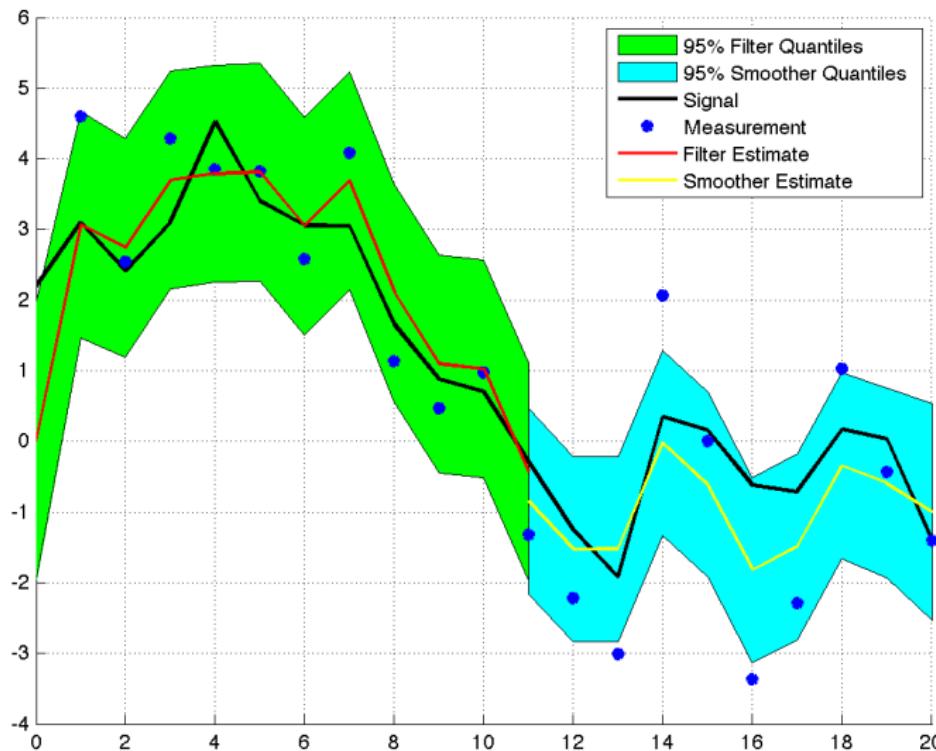
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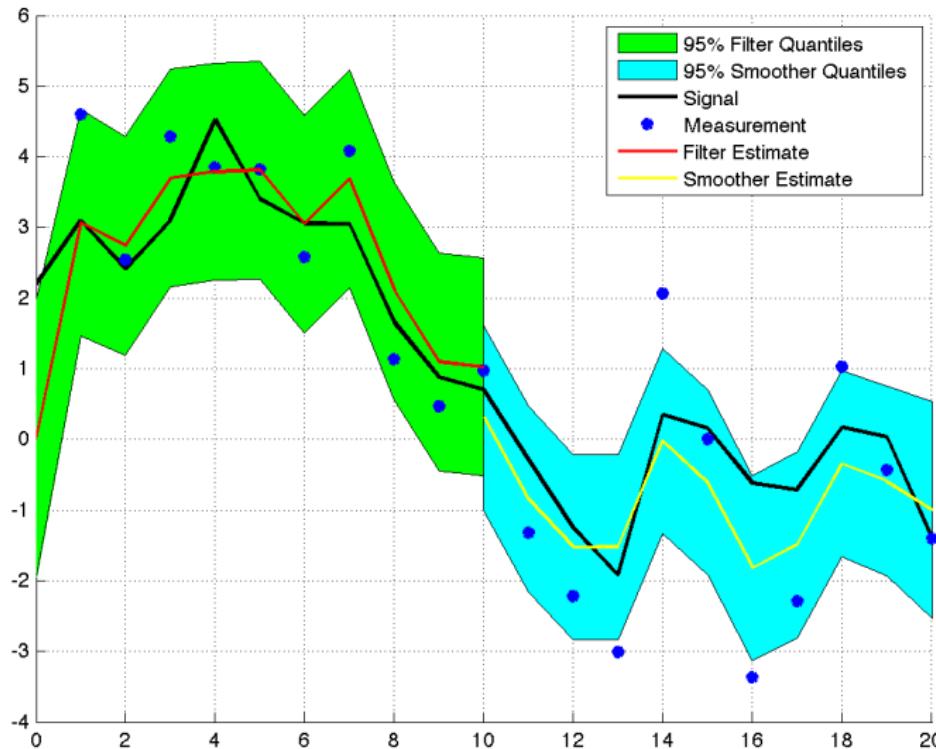
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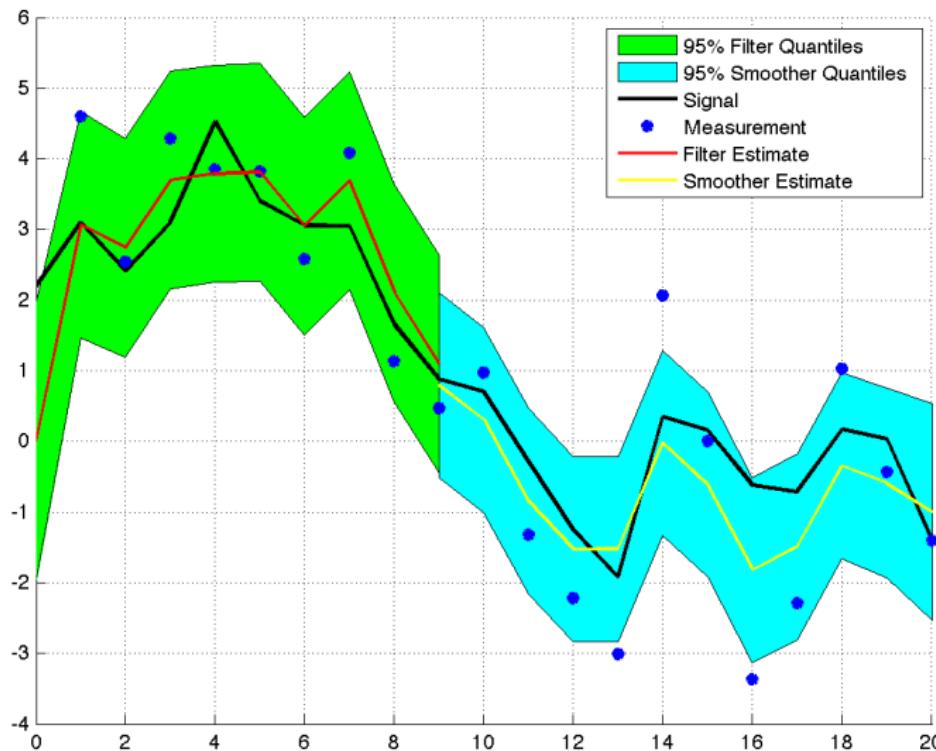
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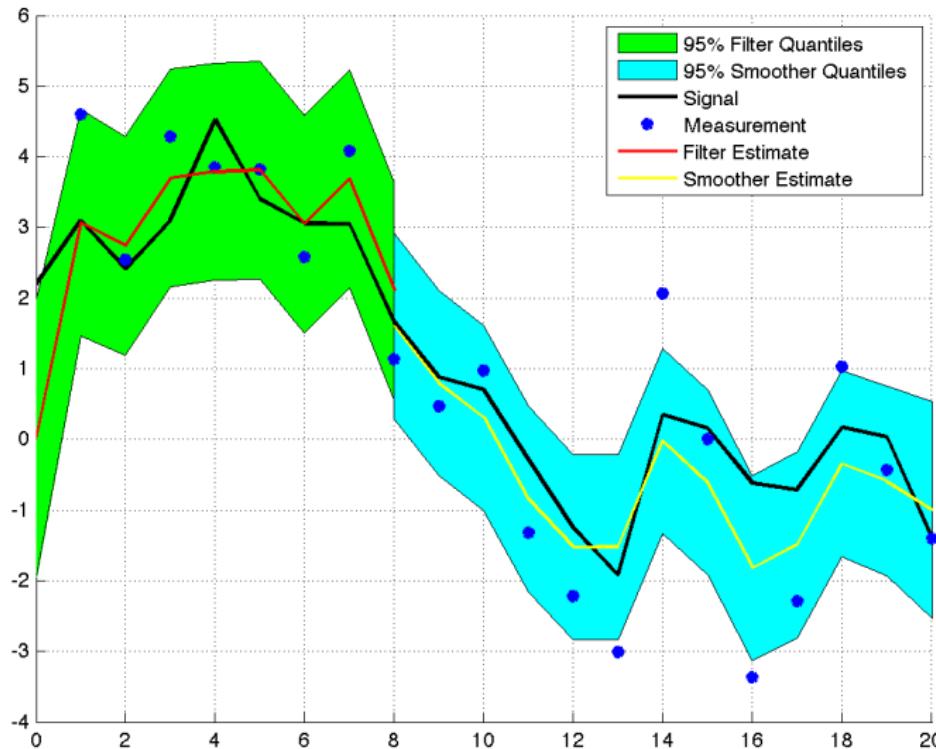
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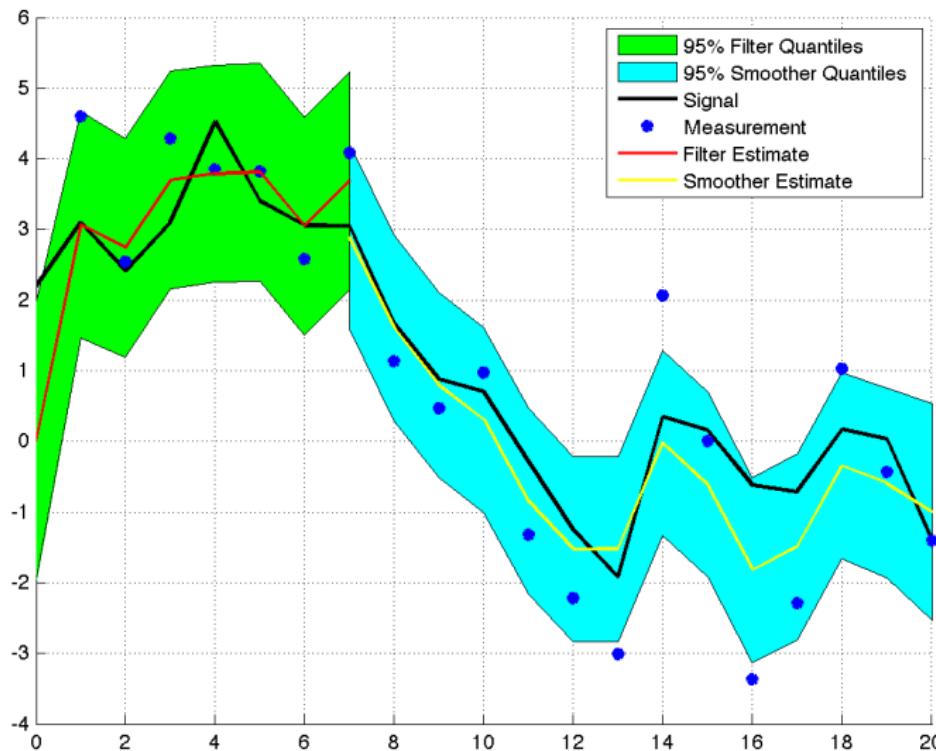
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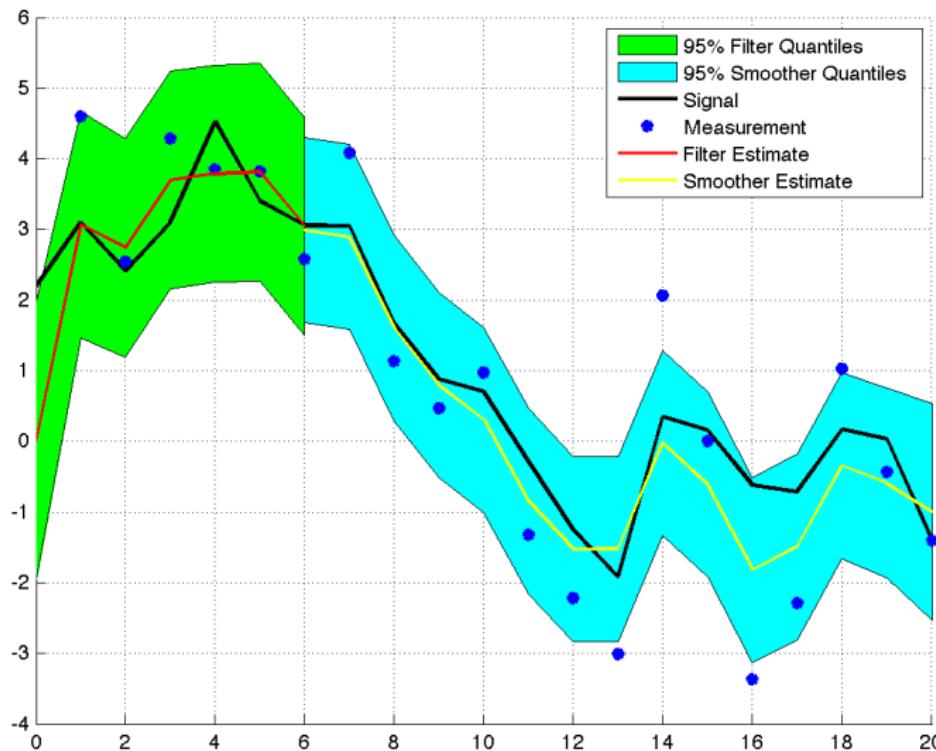
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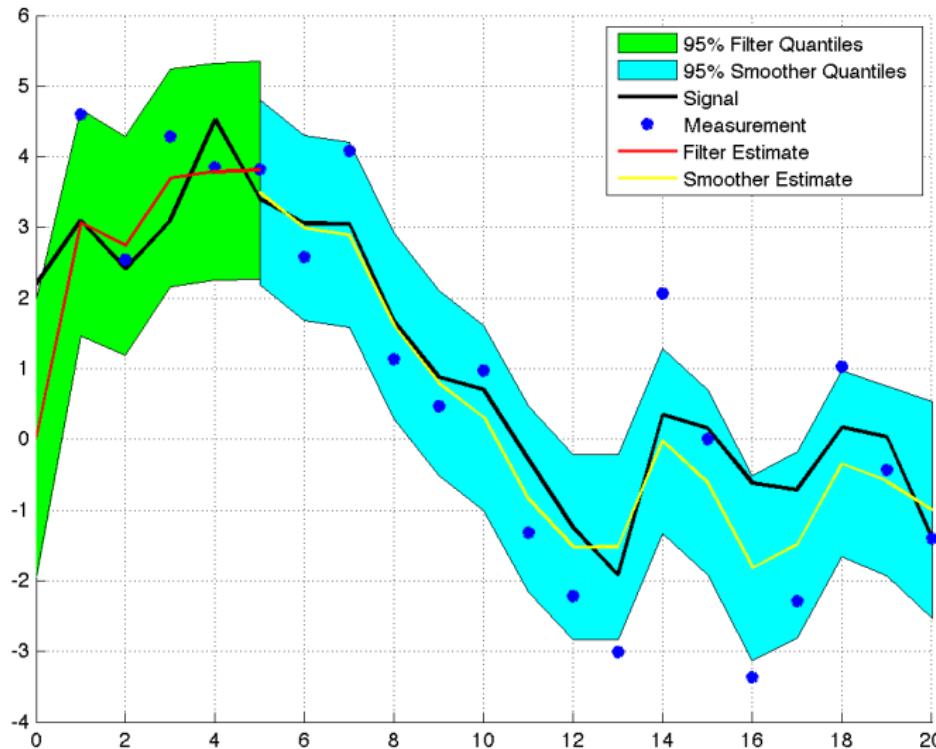
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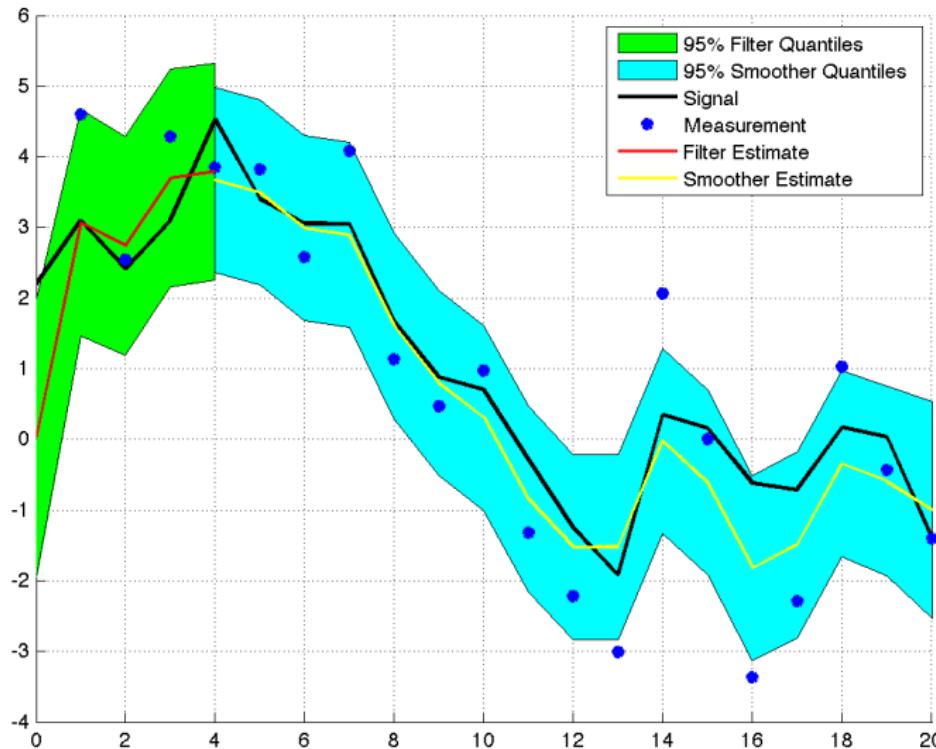
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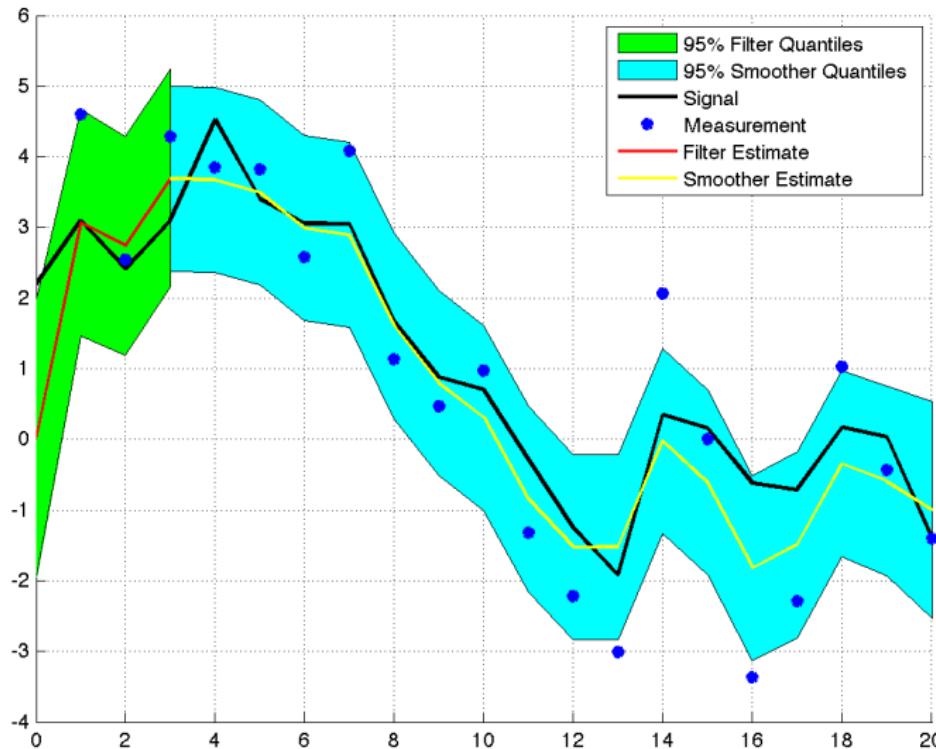
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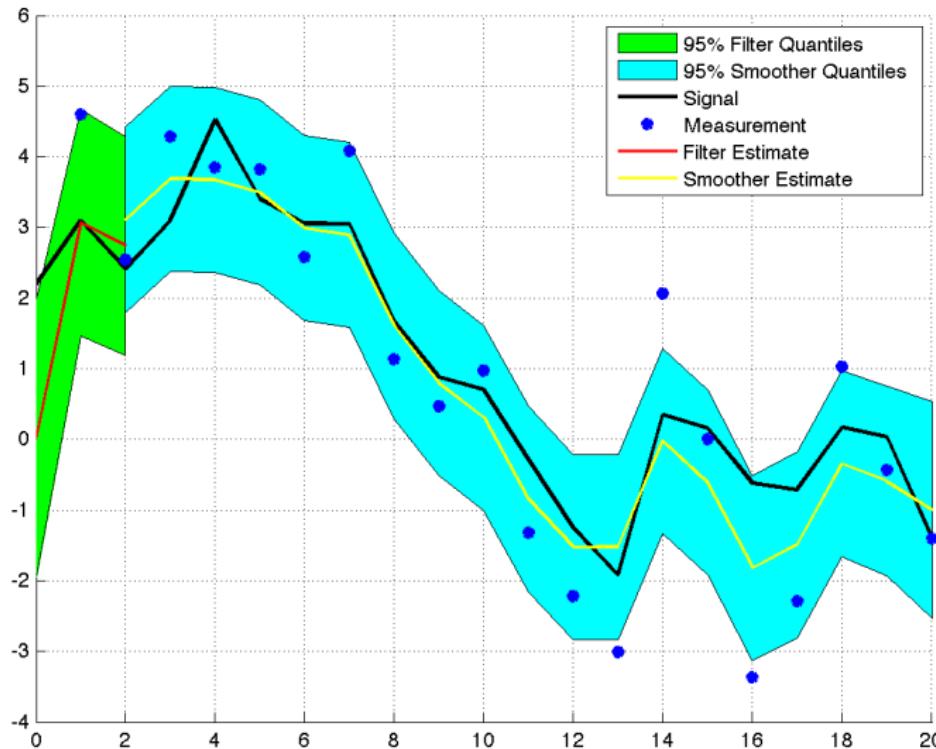
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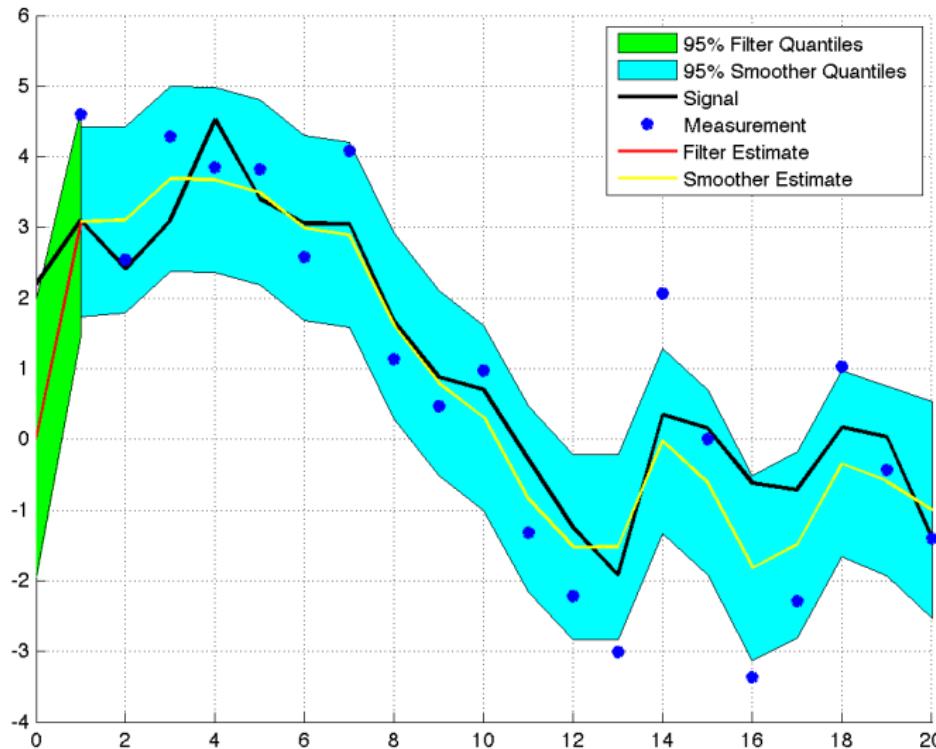
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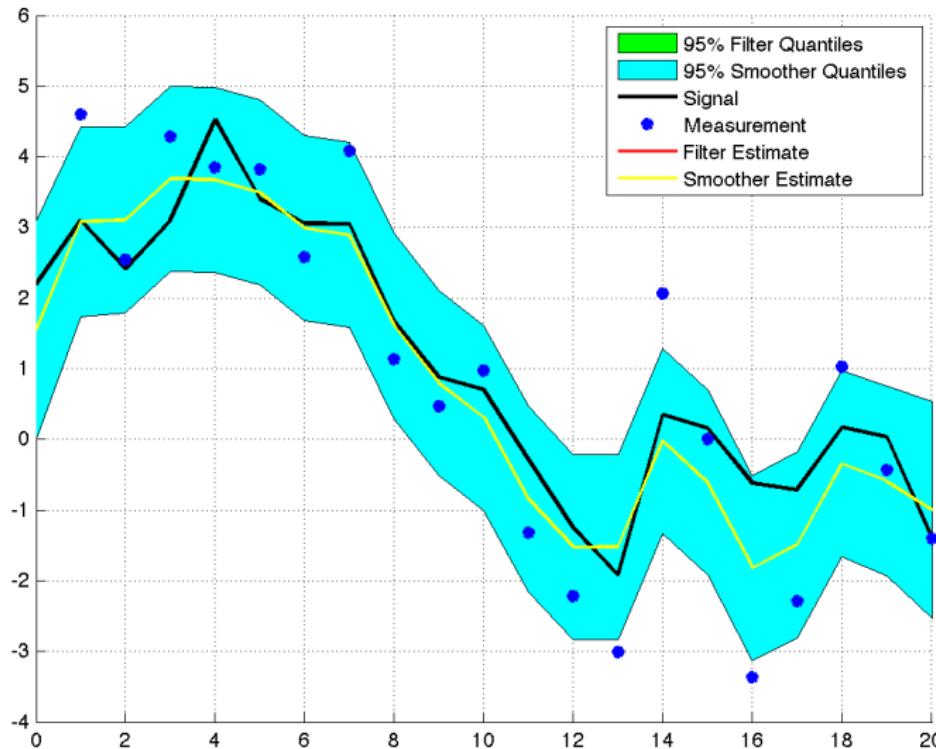
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Continuous-time Limit of the Random Walk Model [1/3]

- Our discrete-time random walk model had the form

$$x_k = x_{k-1} + w_{k-1}, \quad w_{k-1} \sim N(0, q)$$

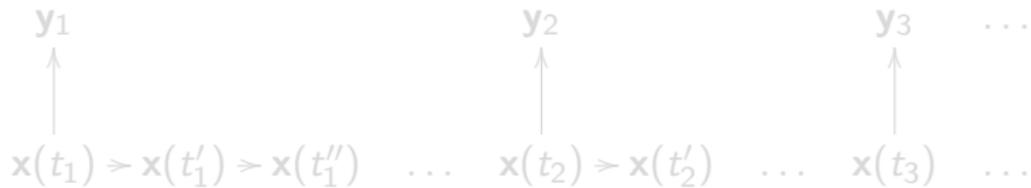
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- Assume that, in fact, it was a *discretely-observed* random walk model

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- Between the measurements we actually have n intermediate steps:



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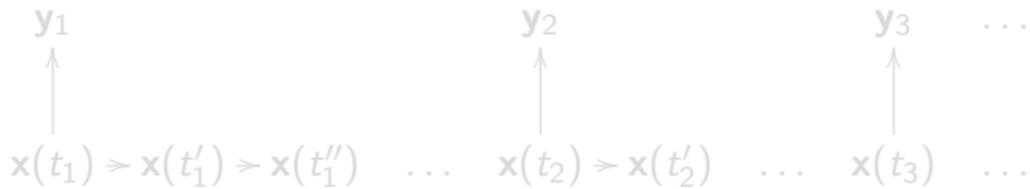
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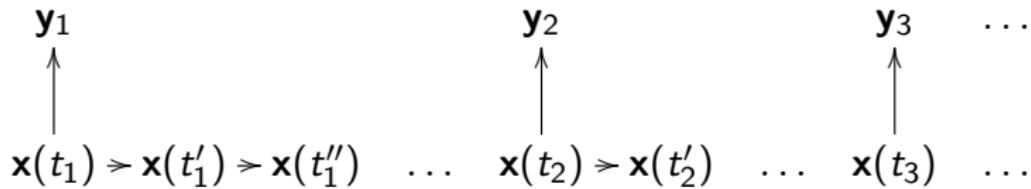
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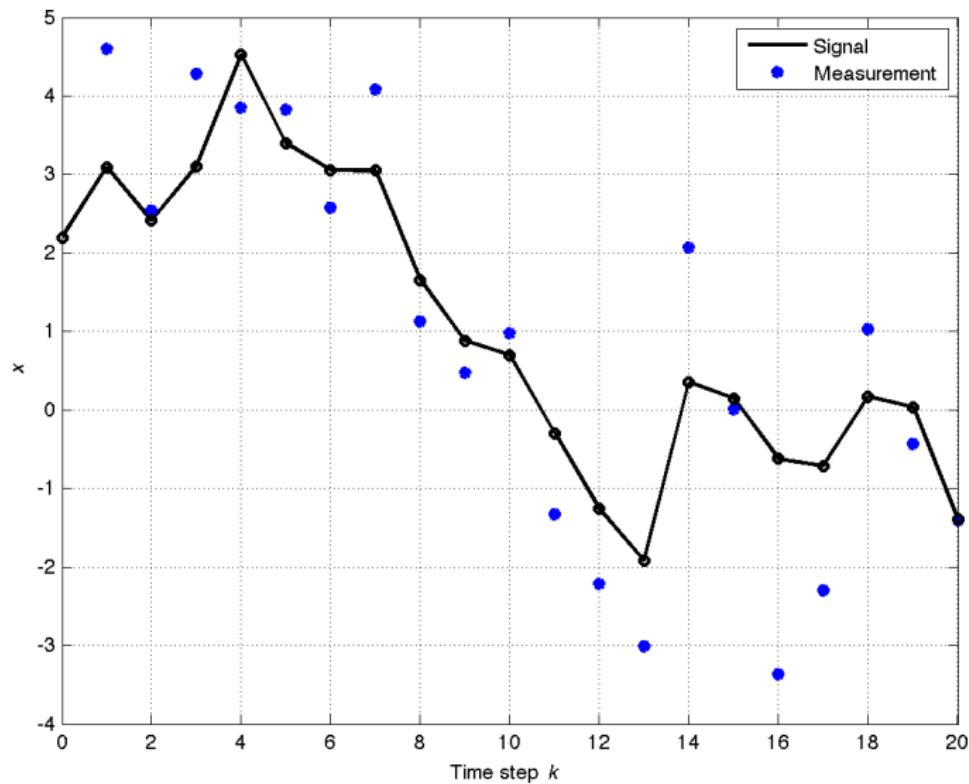
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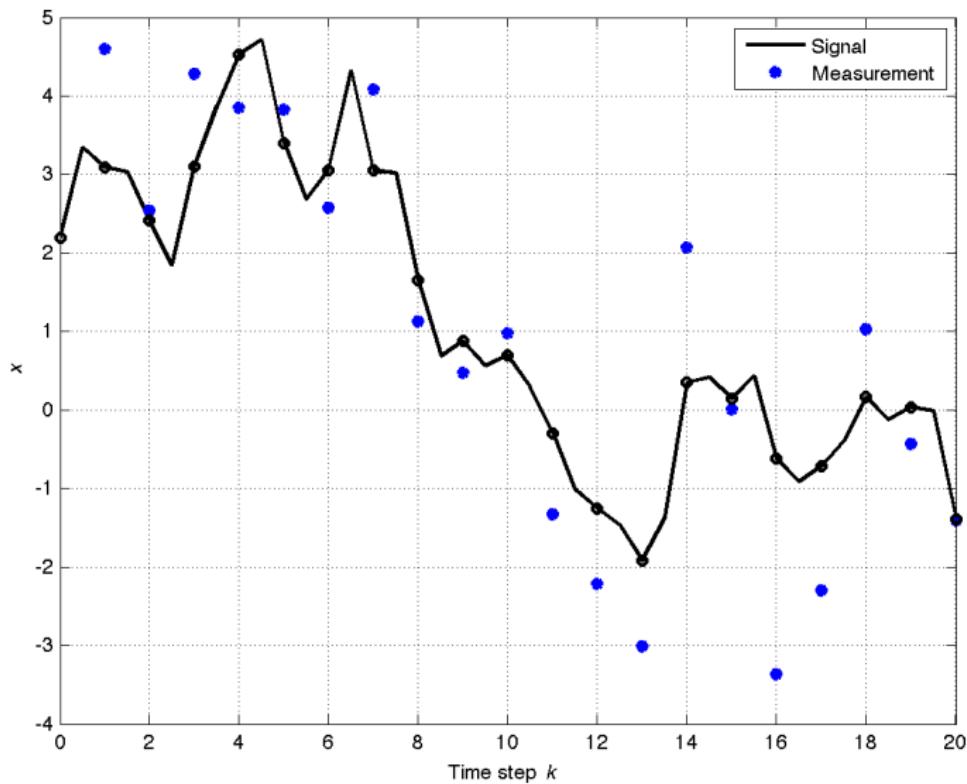
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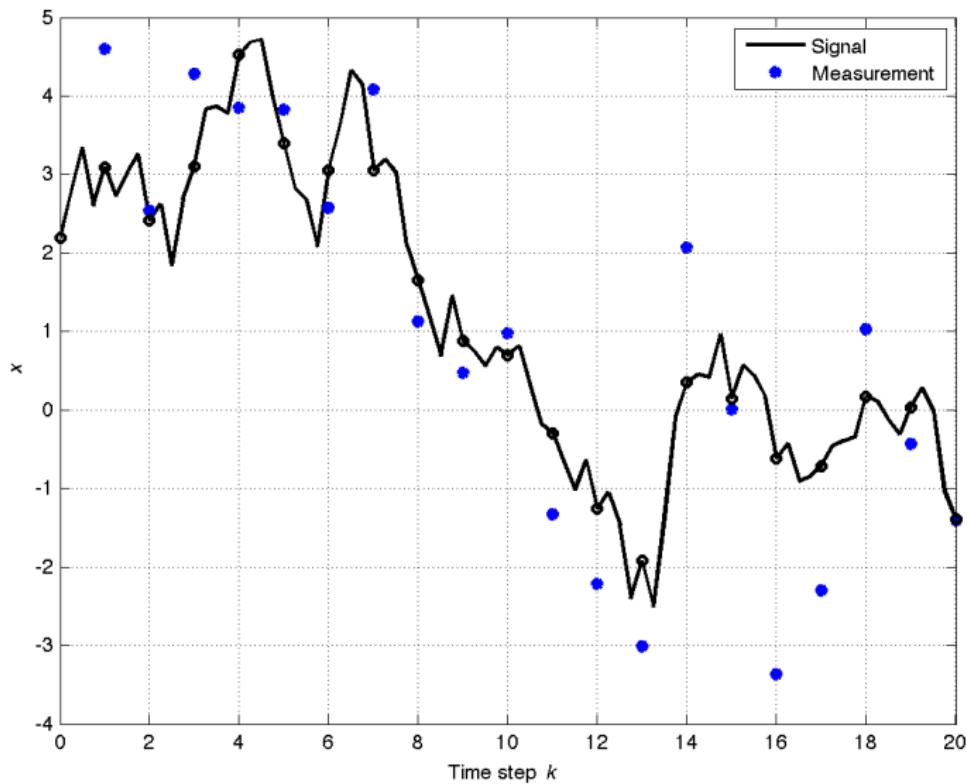
Continuous-time Limit of the Random Walk Model [2/3]



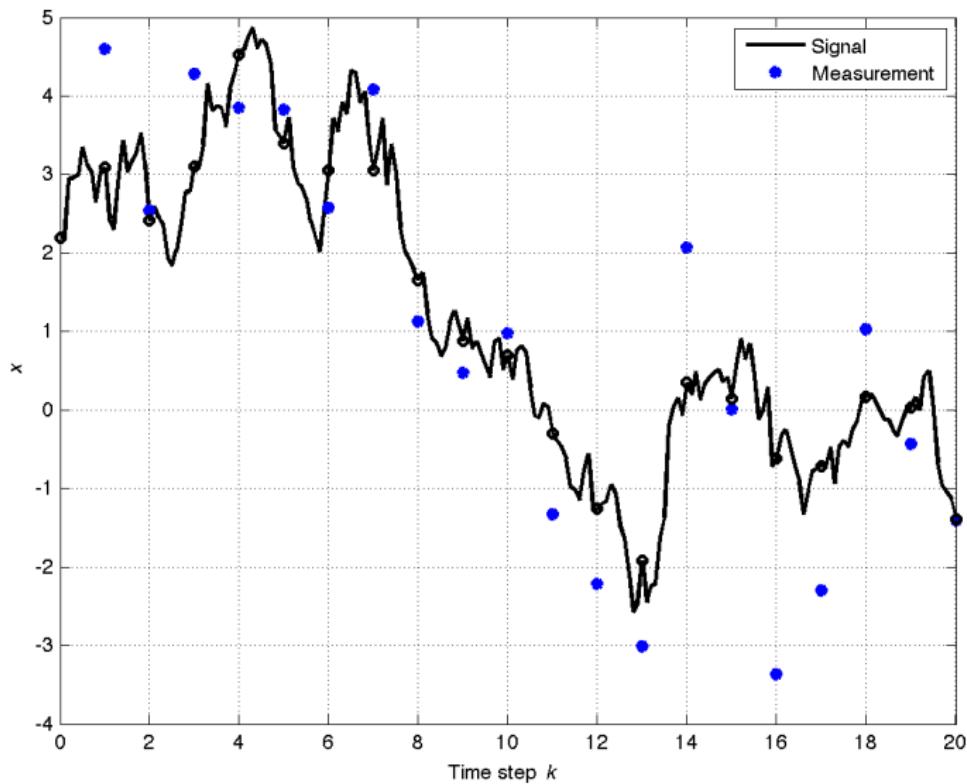
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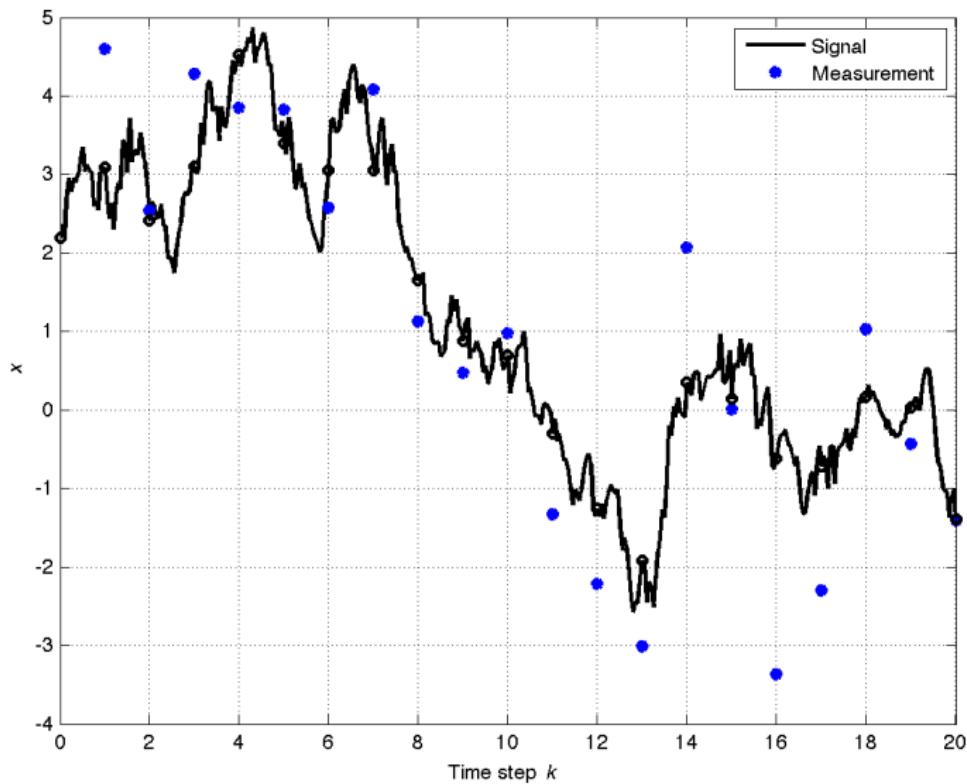
Continuous-time Limit of the Random Walk Model [2/3]



Continuous-time Limit of the Random Walk Model [2/3]



Continuous-time Limit of the Random Walk Model [2/3]



Continuous-time Limit of the Random Walk Model [3/3]

- With $n = \infty$ intermediate steps we get a discretely observed stochastic differential equation (SDE) model:

$$\frac{dx(t)}{dt} = w(t),$$

$$y_k = x(t_k) + e_k, \quad e_k \sim N(0, r).$$

- Now $w(t)$ is a continuous-time white noise with spectral density q .
- The process defined as $dx(t)/dt = w(t)$ is called Brownian motion.
- Hence, we actually have a Gaussian process regression model

$$x(t) \sim GP(0, q \min(t, t')),$$

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- Kalman filter and RTS smoother can still be used to compute the posterior of $x(t)$ given the observations y_1, \dots, y_T
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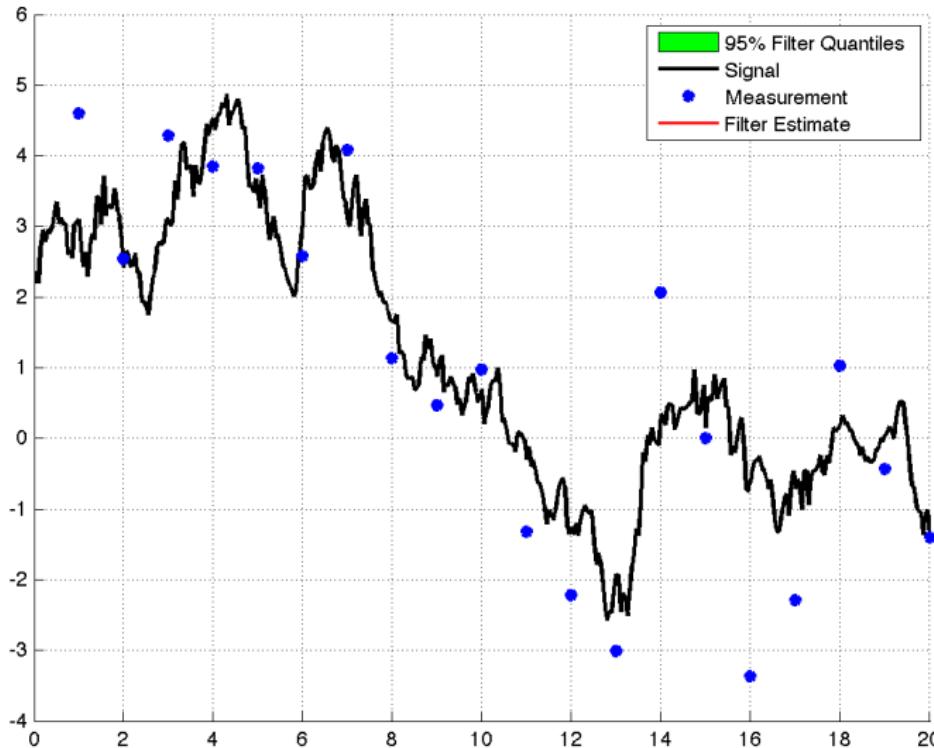
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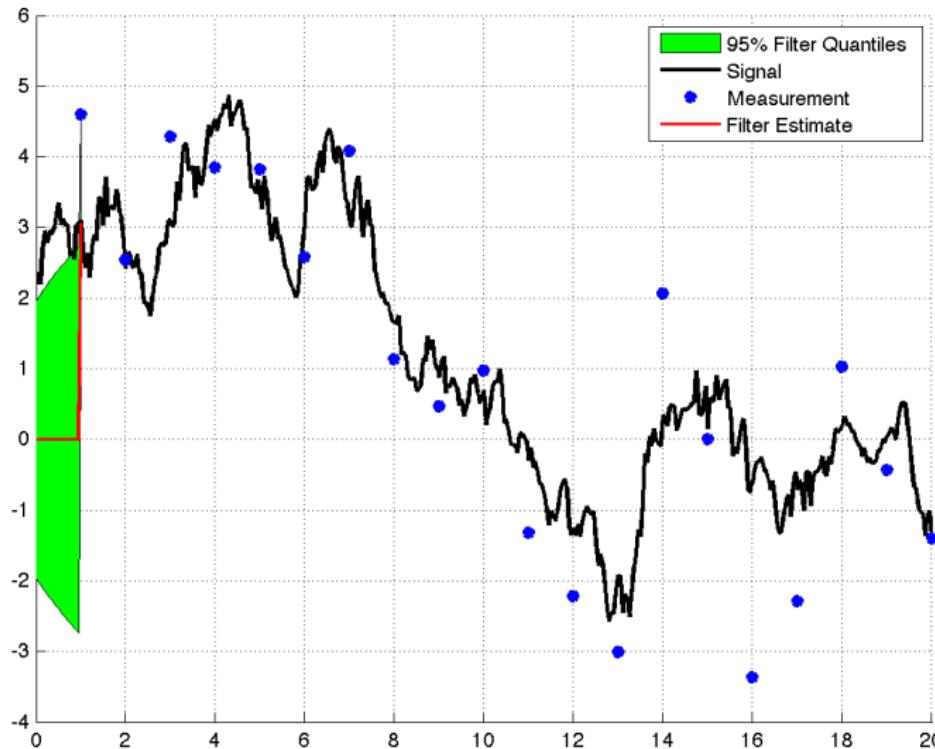
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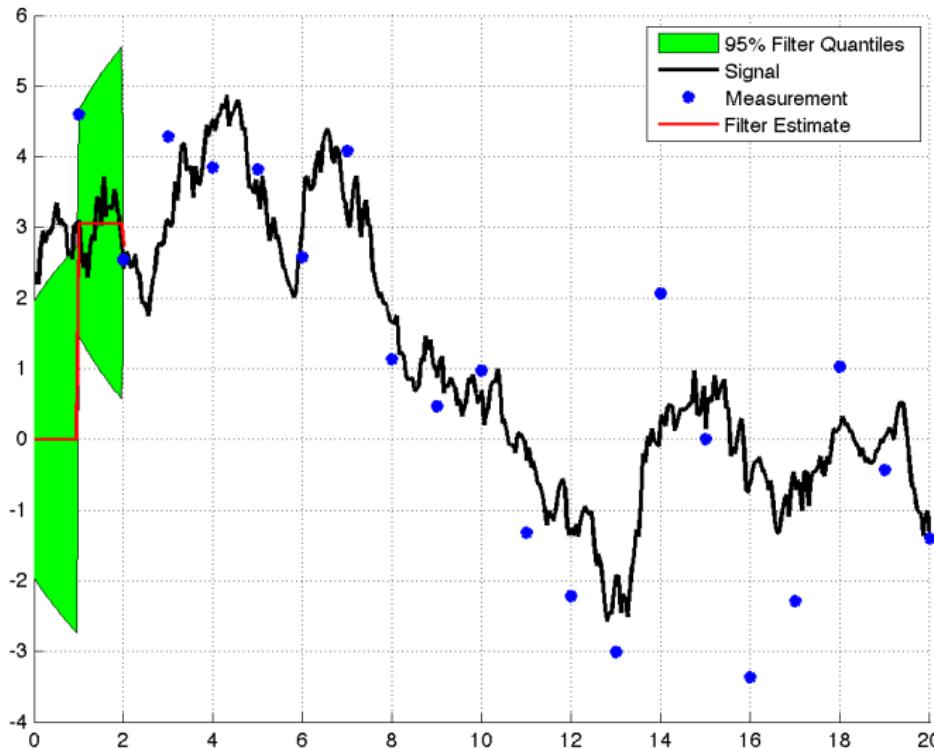
Continuous-discrete (-time) Filter and Smoother Example



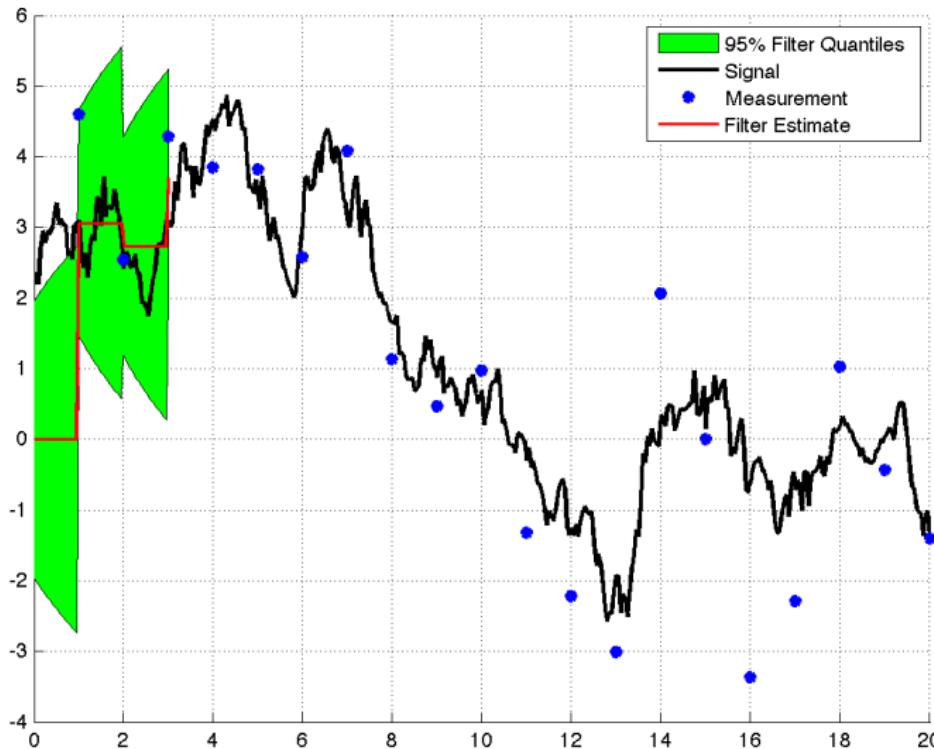
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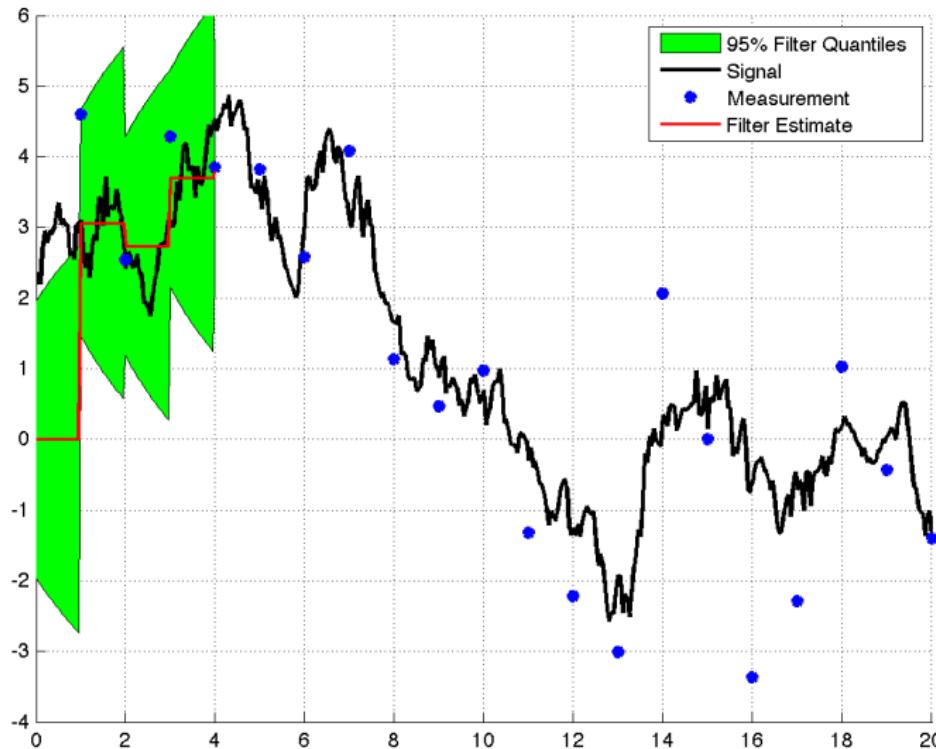
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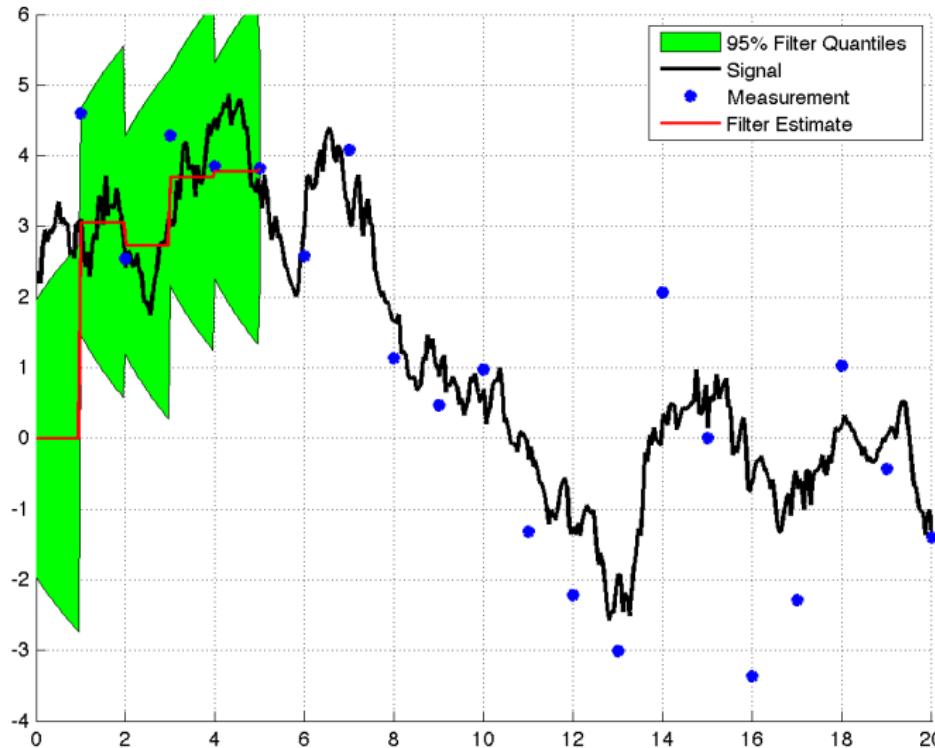
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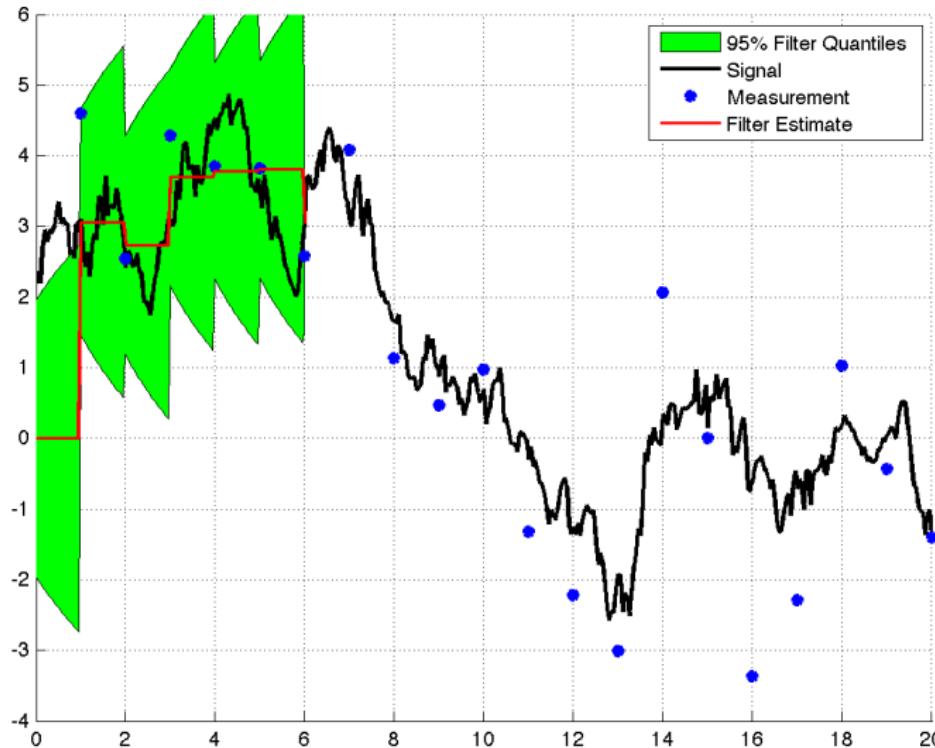
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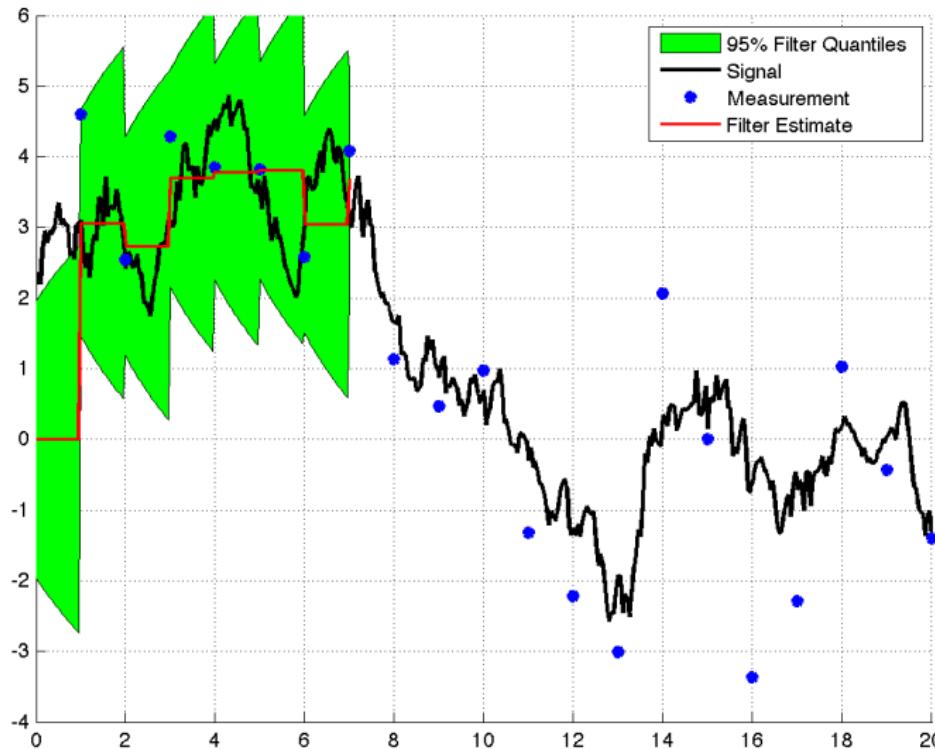
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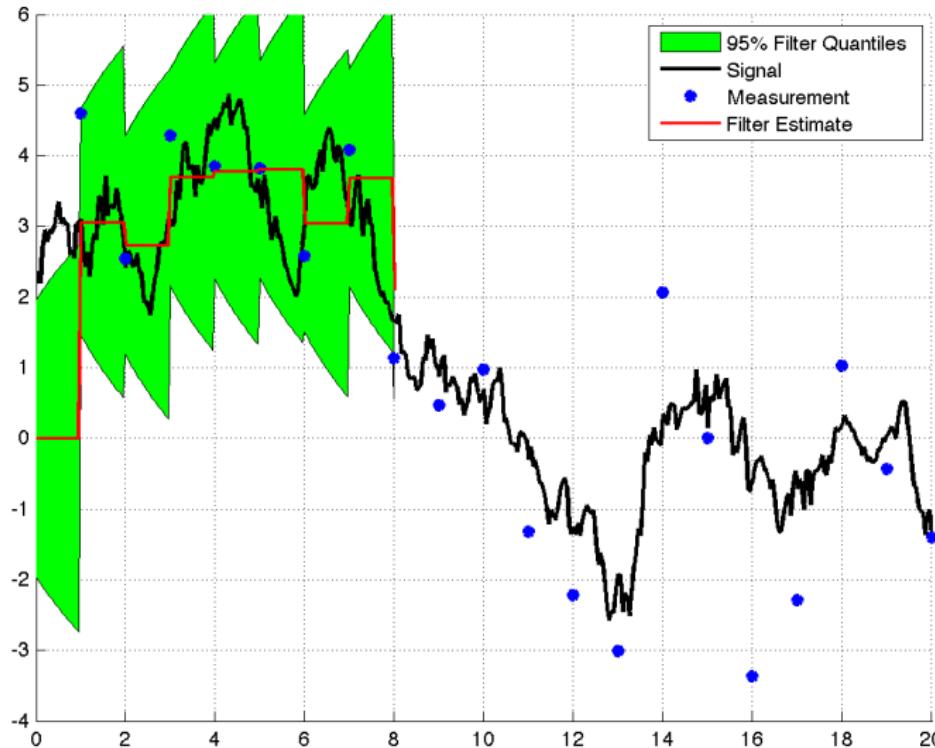
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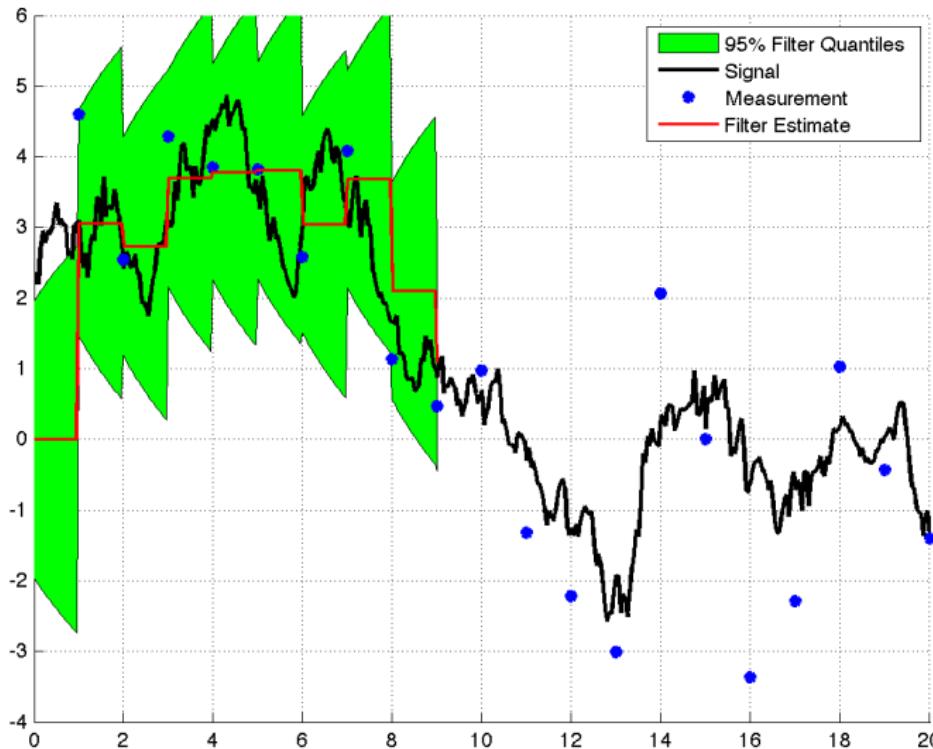
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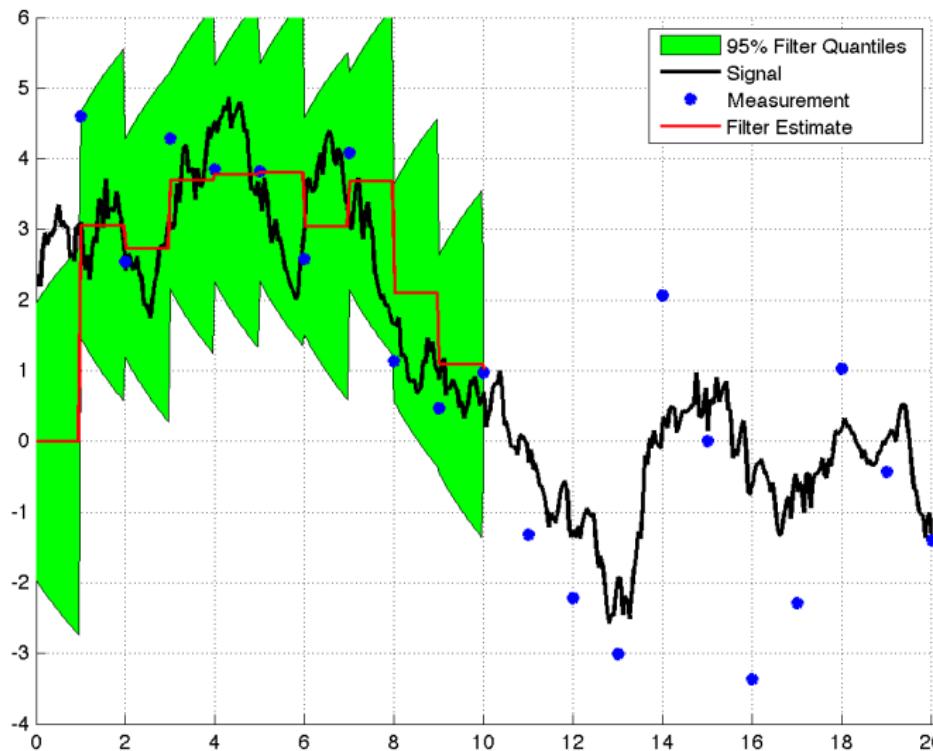
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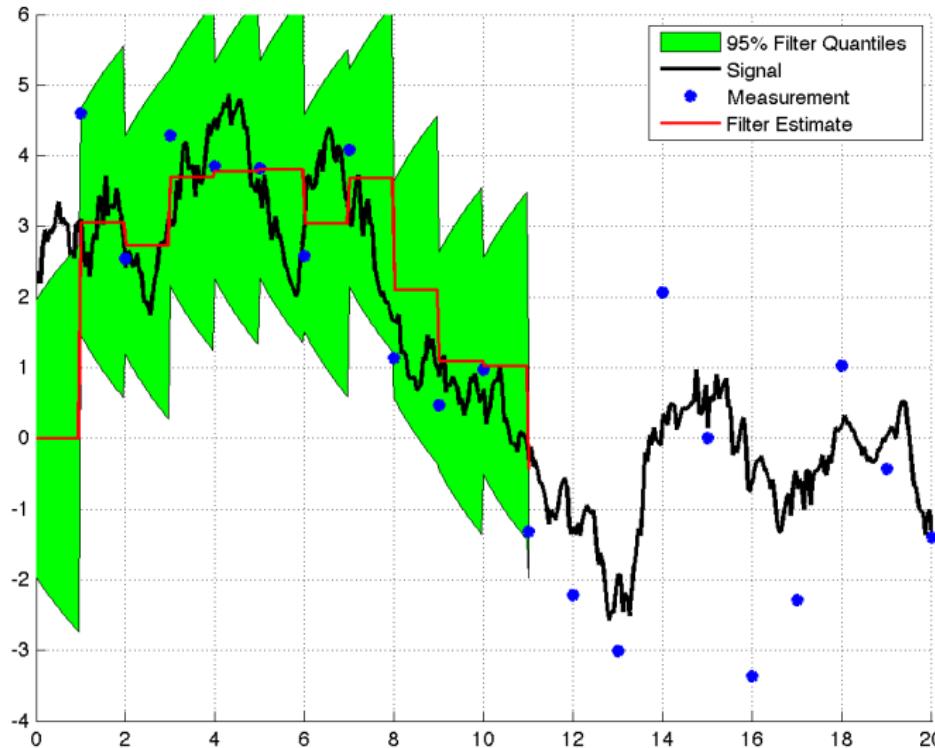
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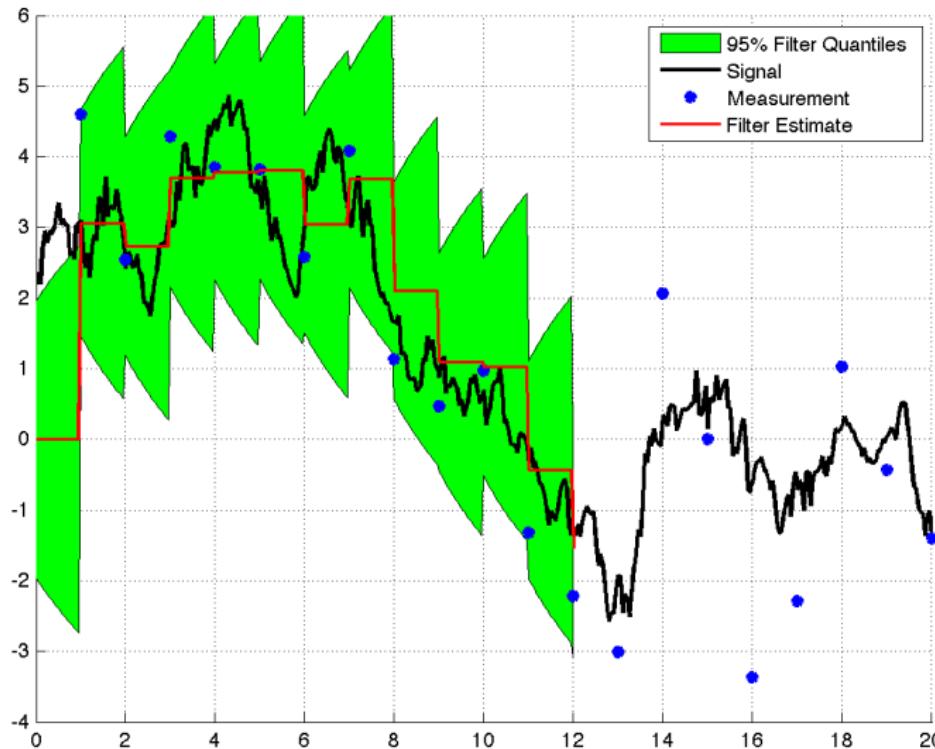
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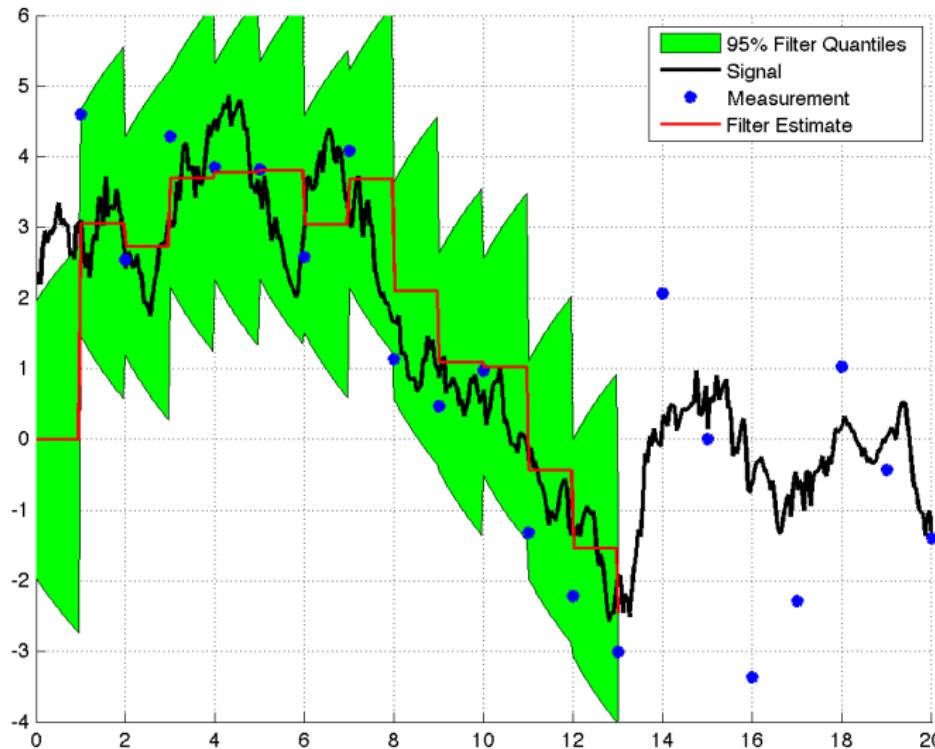
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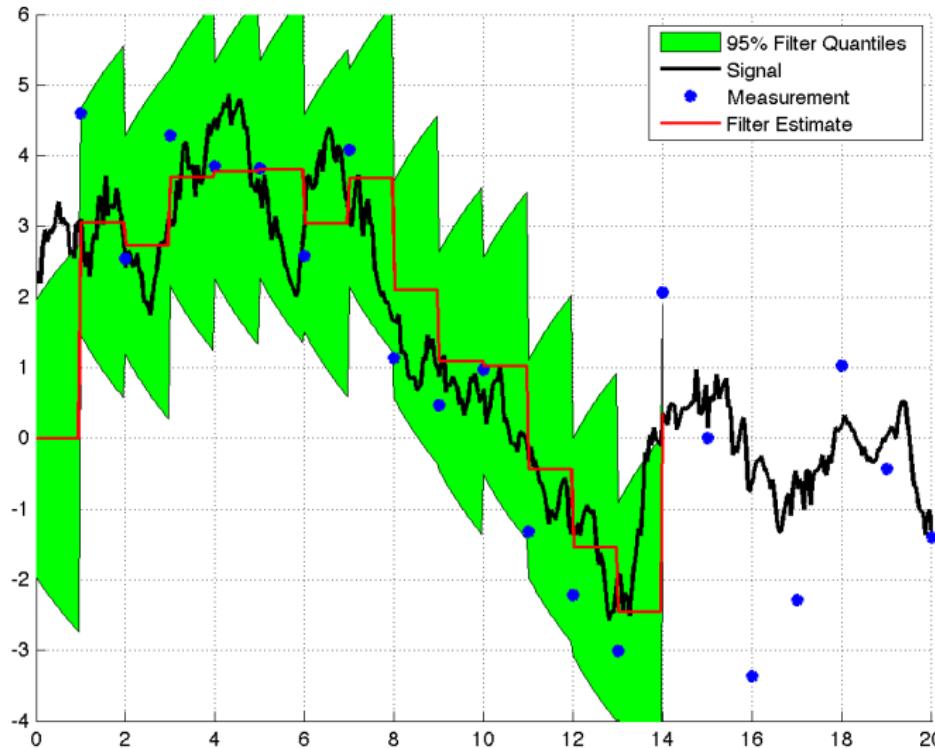
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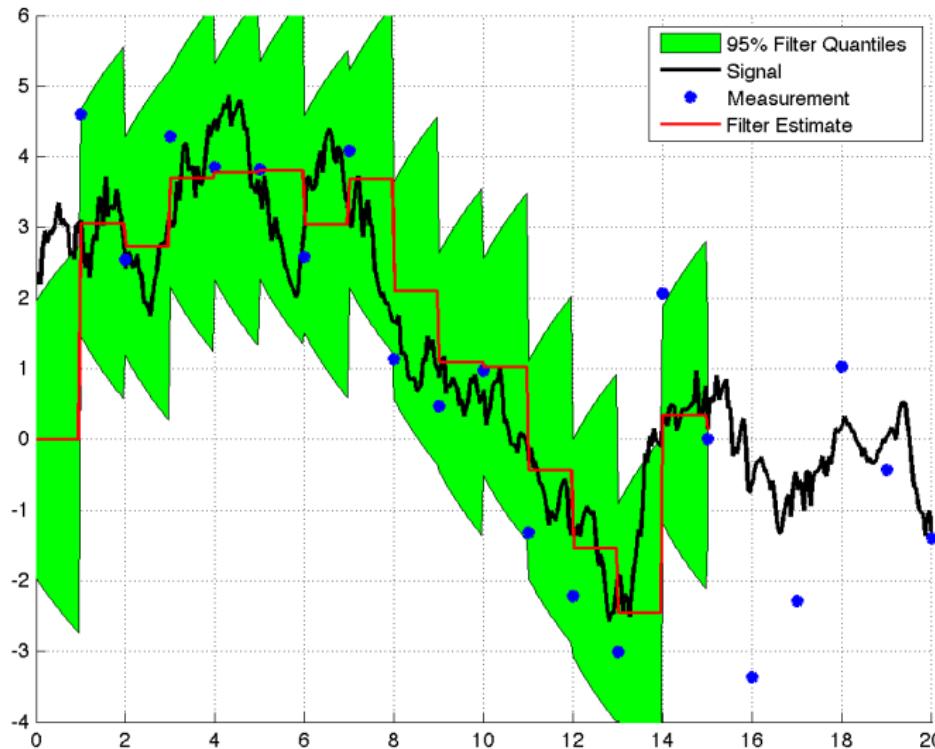
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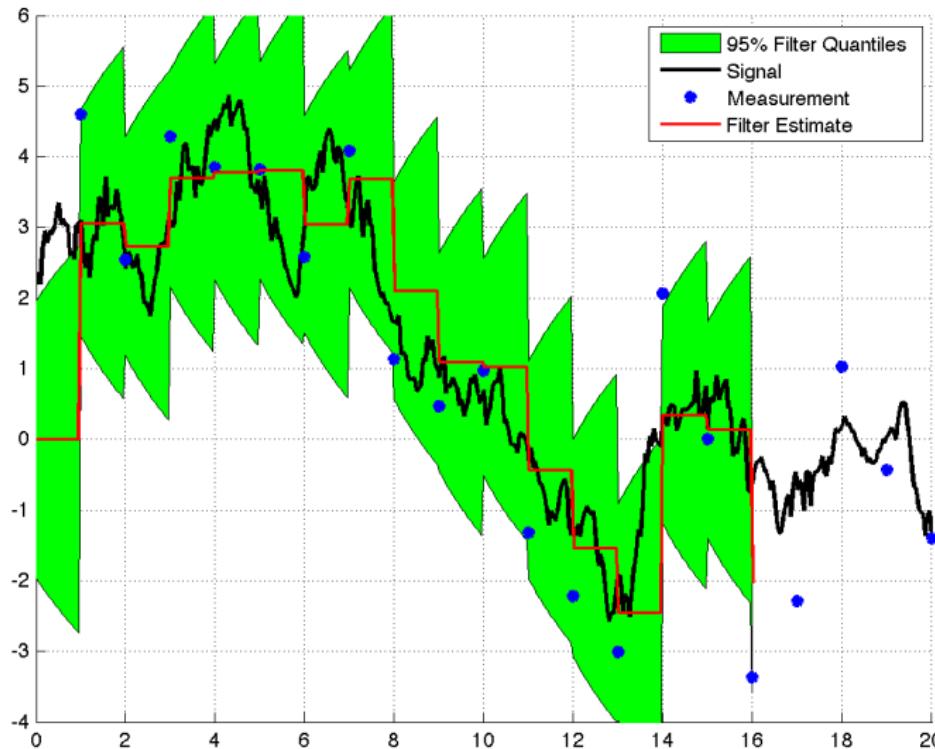
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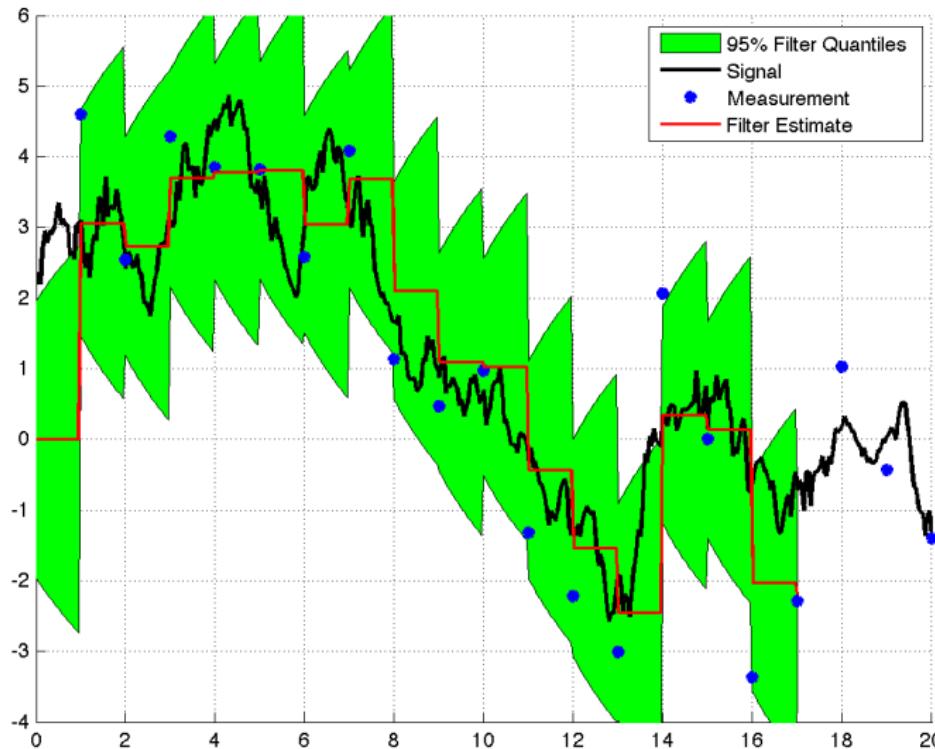
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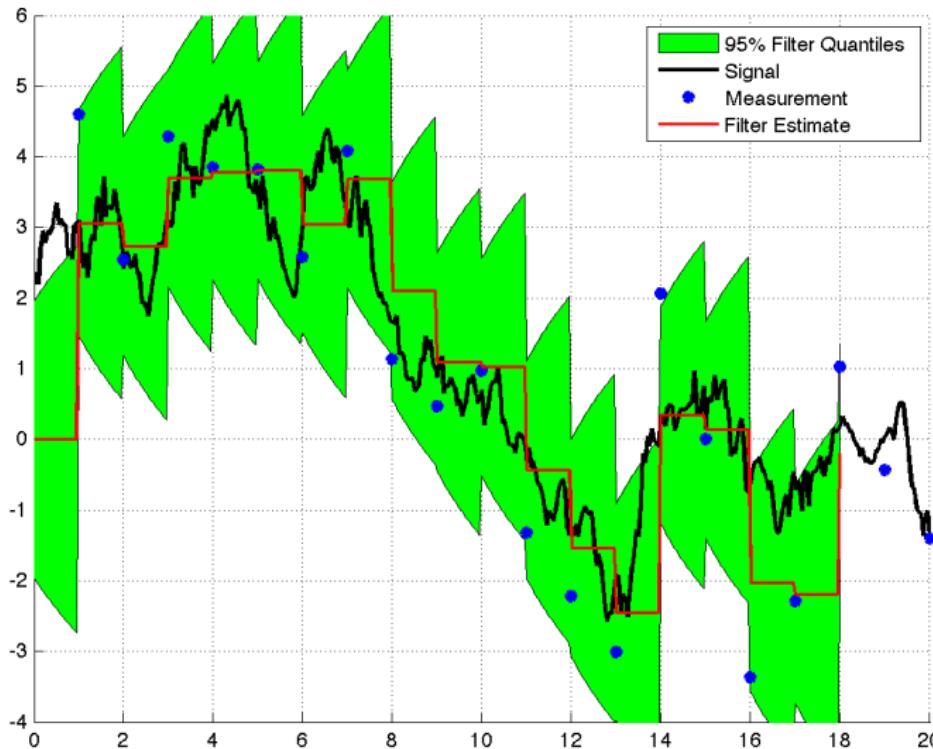
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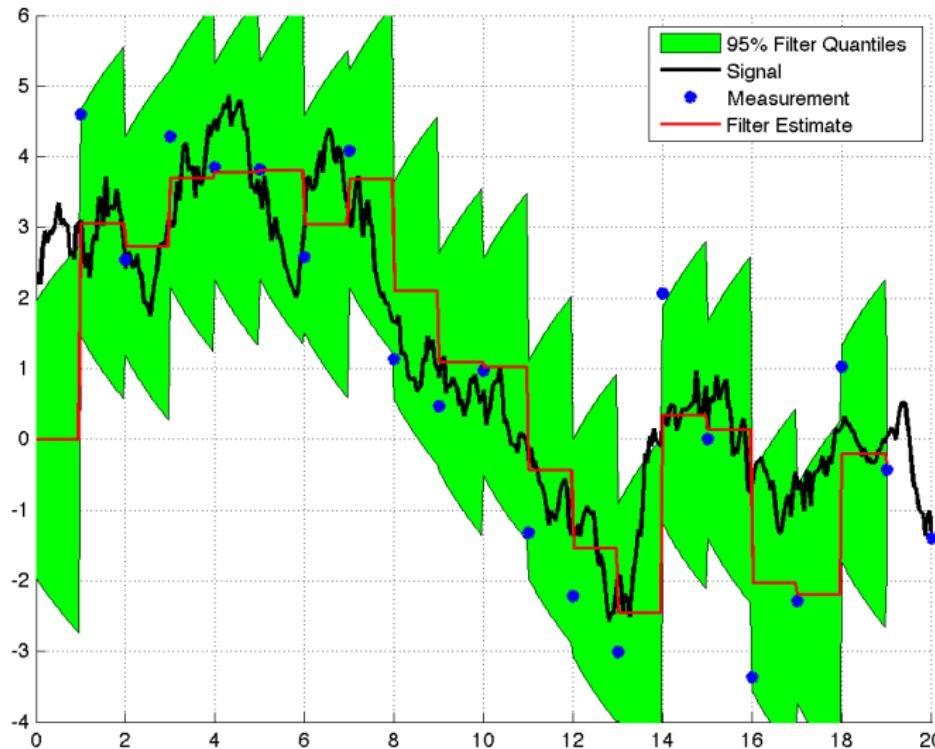
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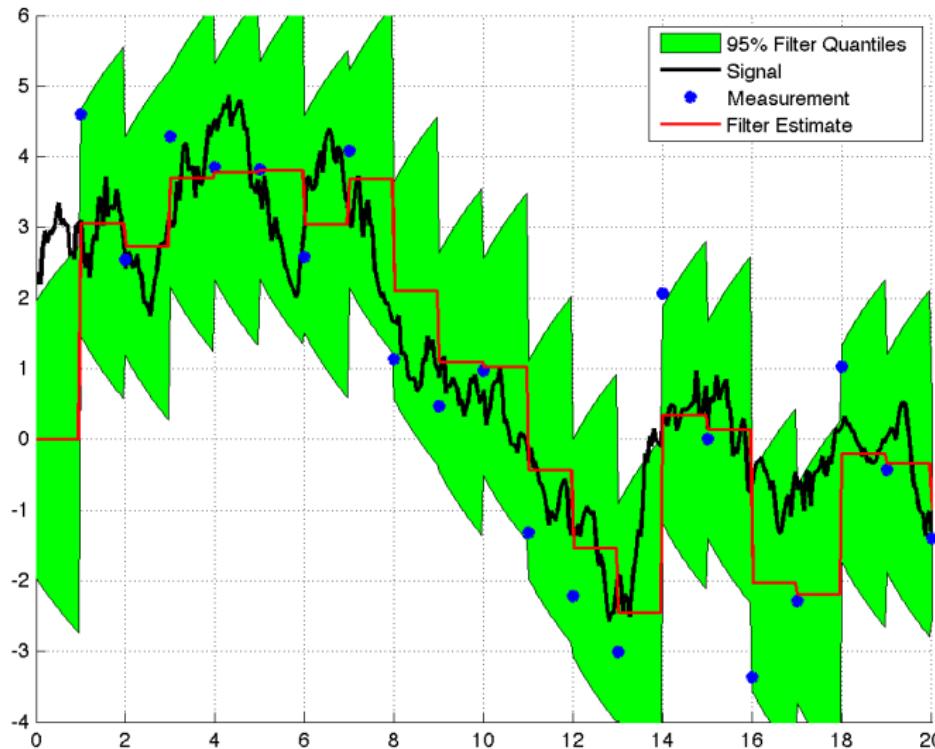
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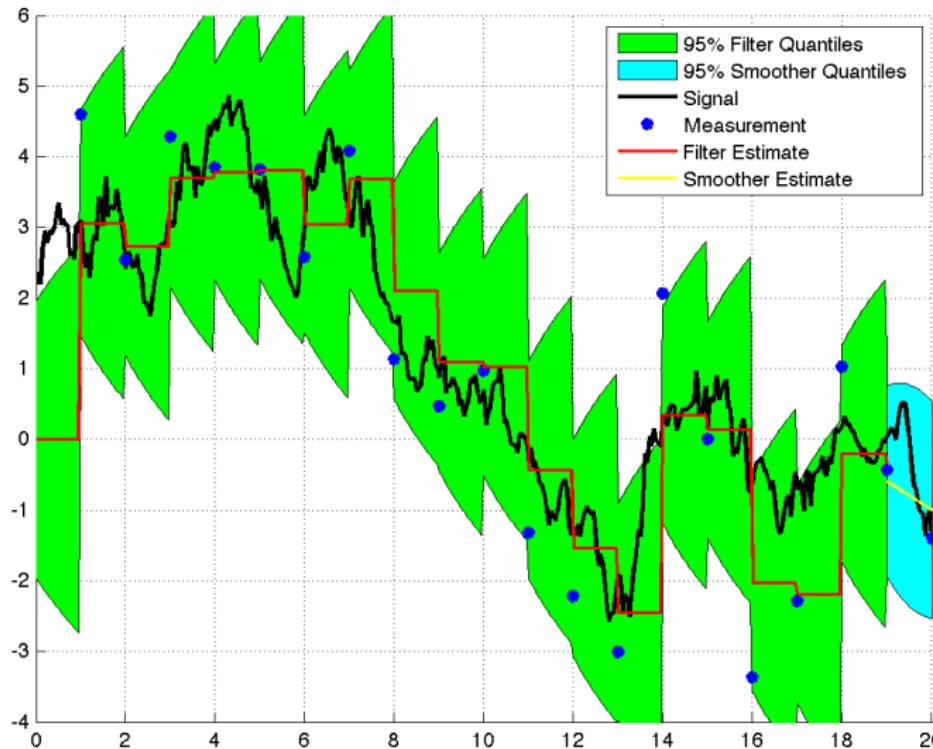
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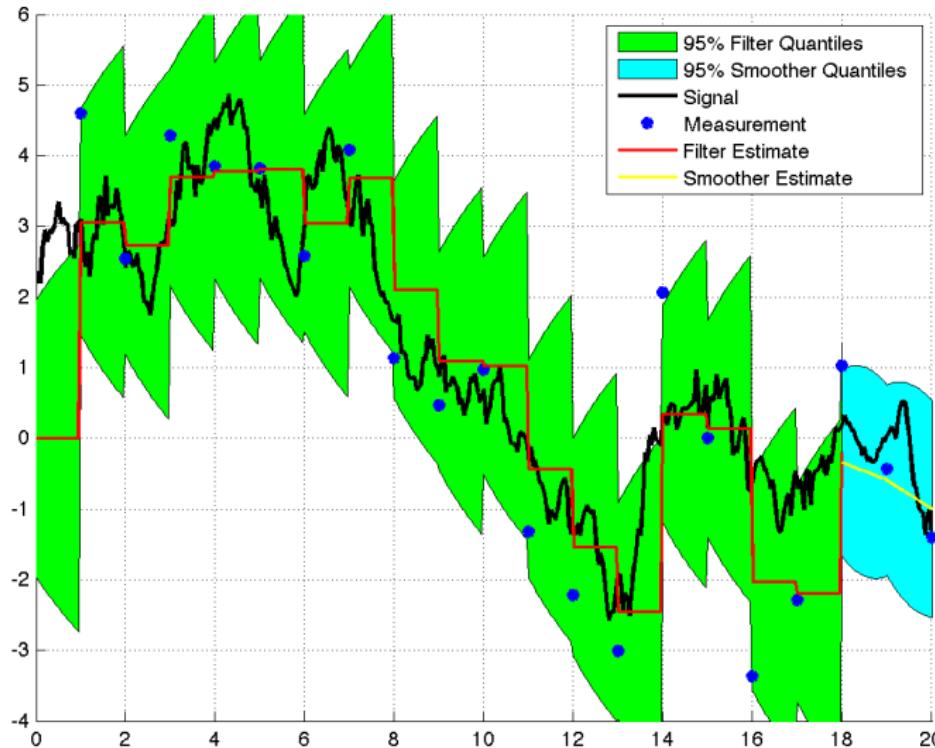
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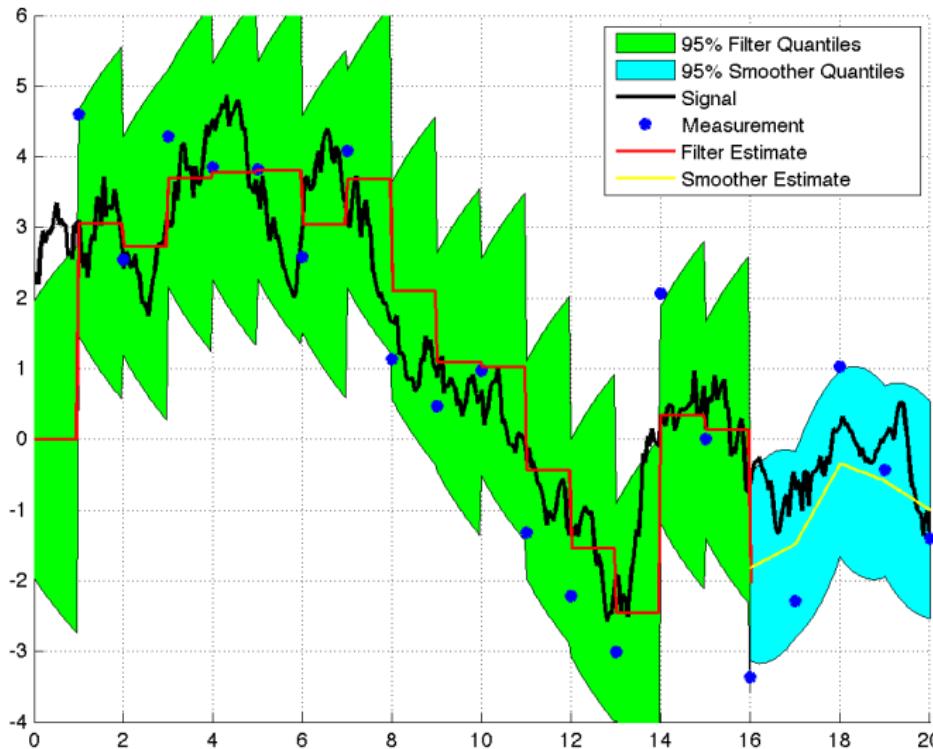
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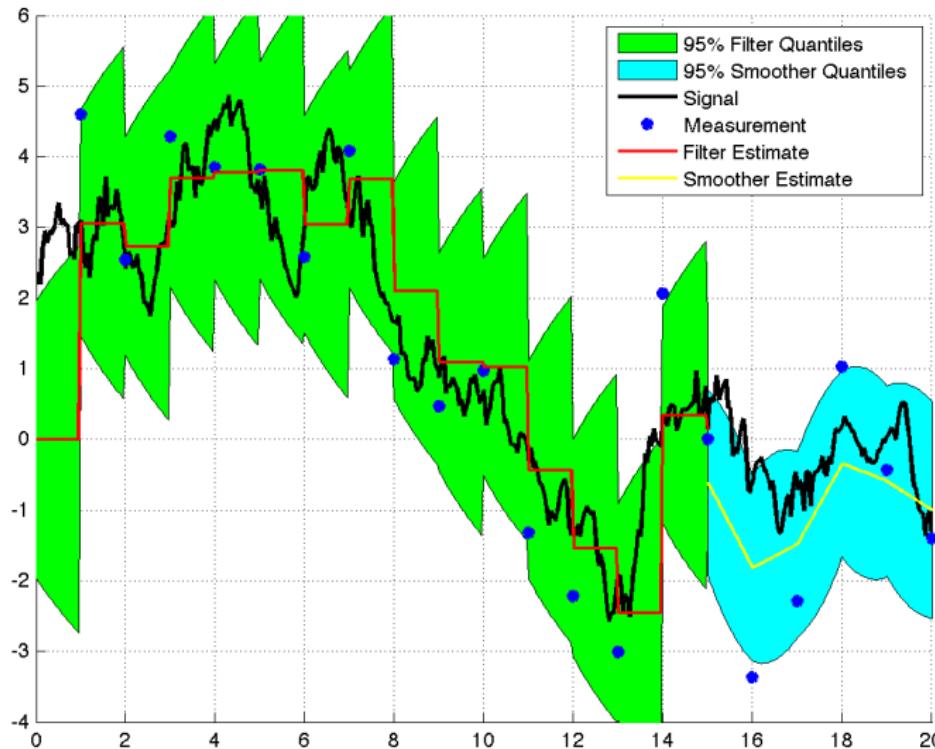
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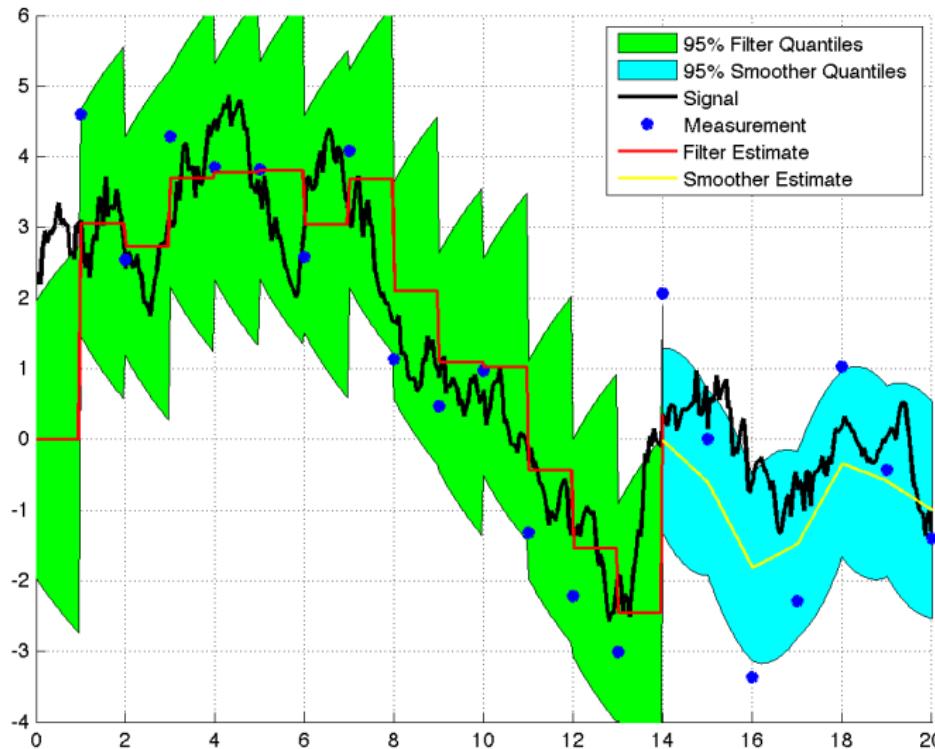
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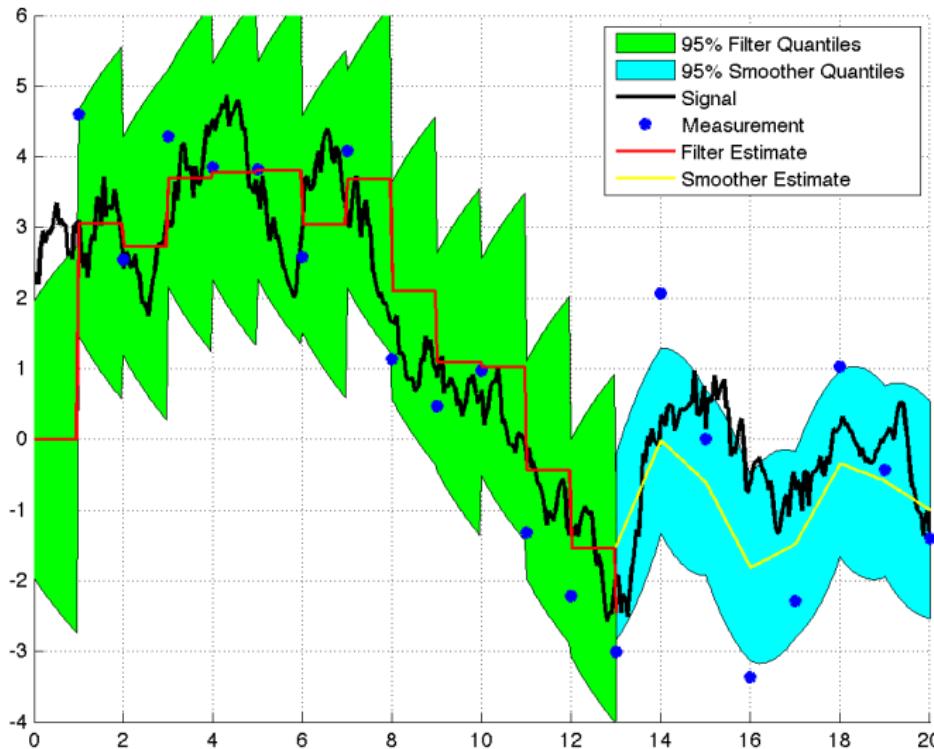
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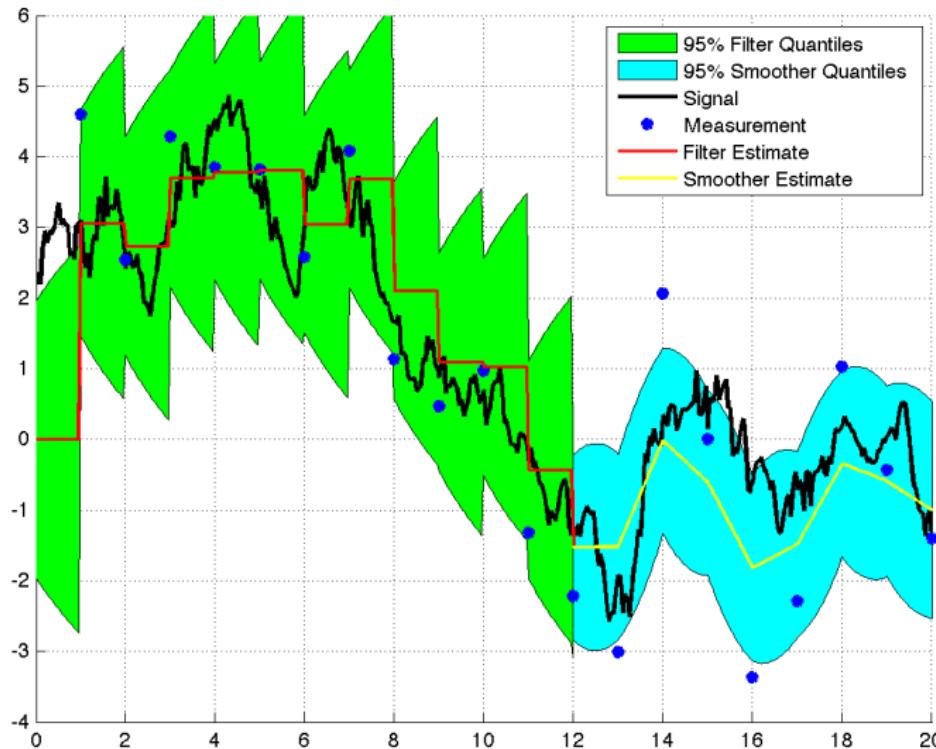
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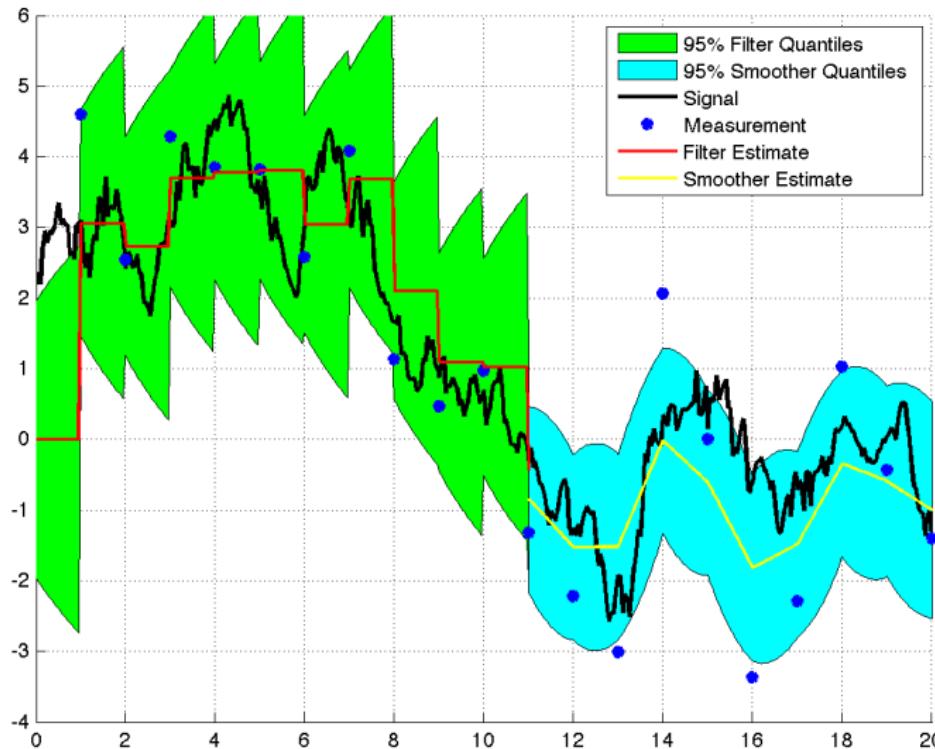
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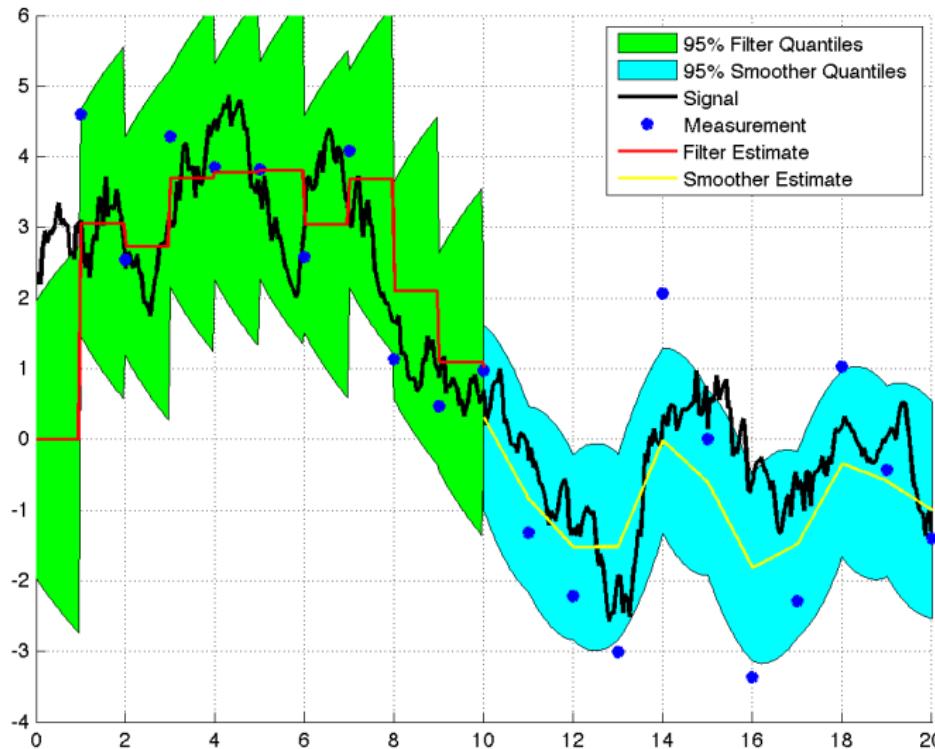
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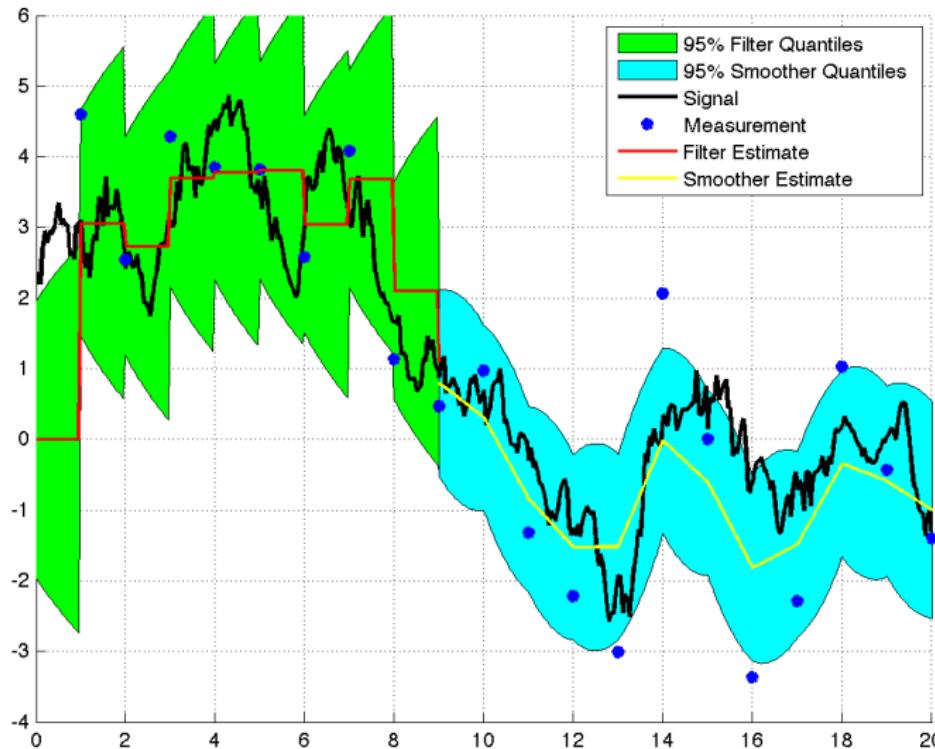
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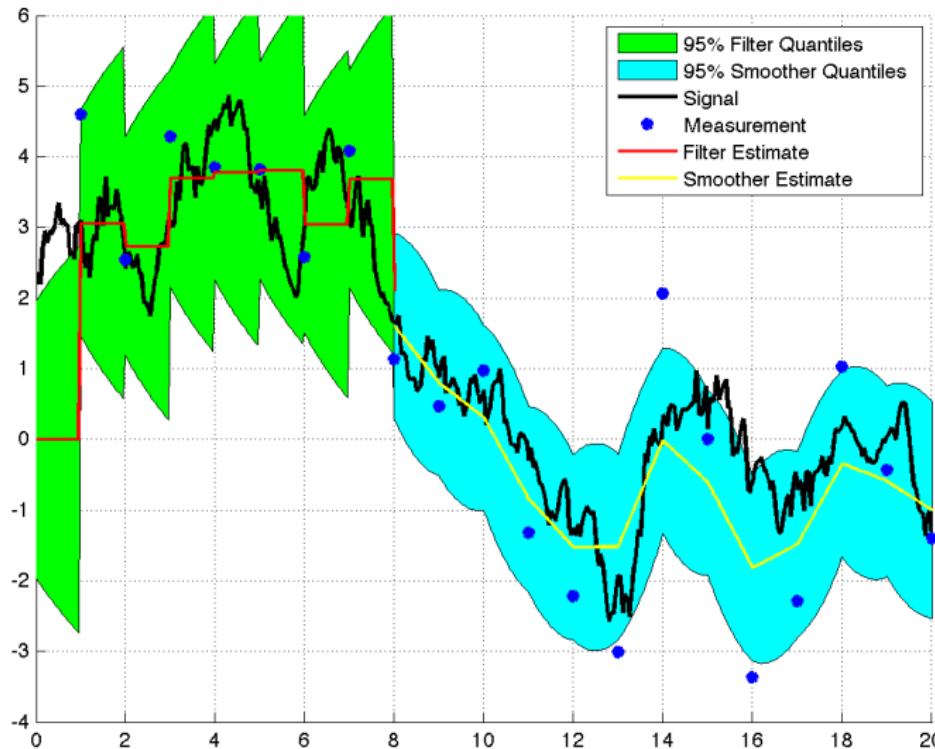
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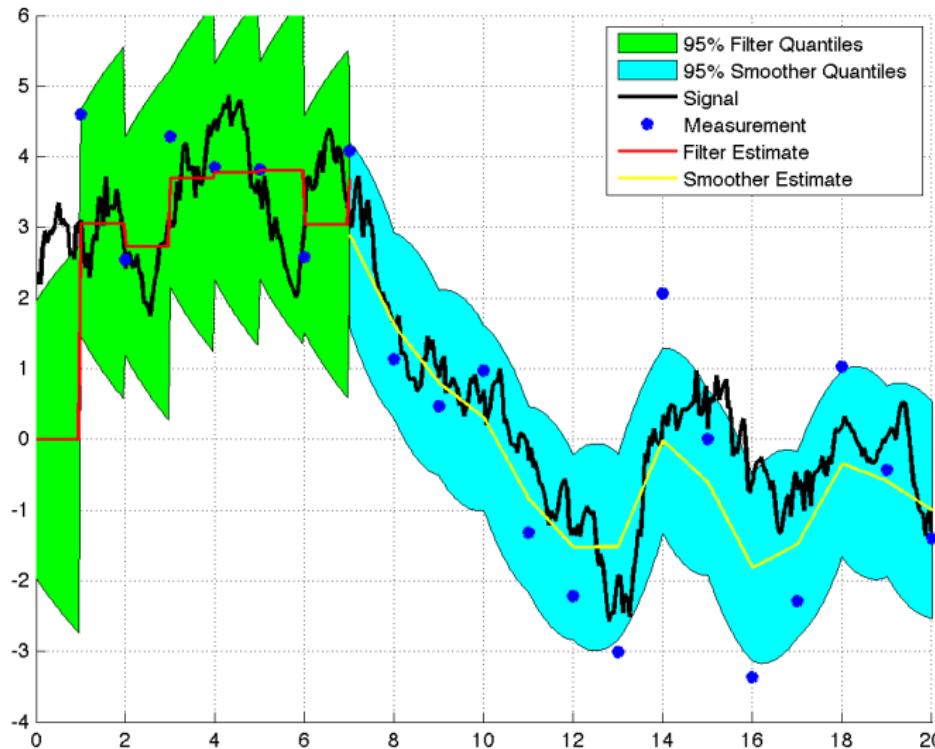
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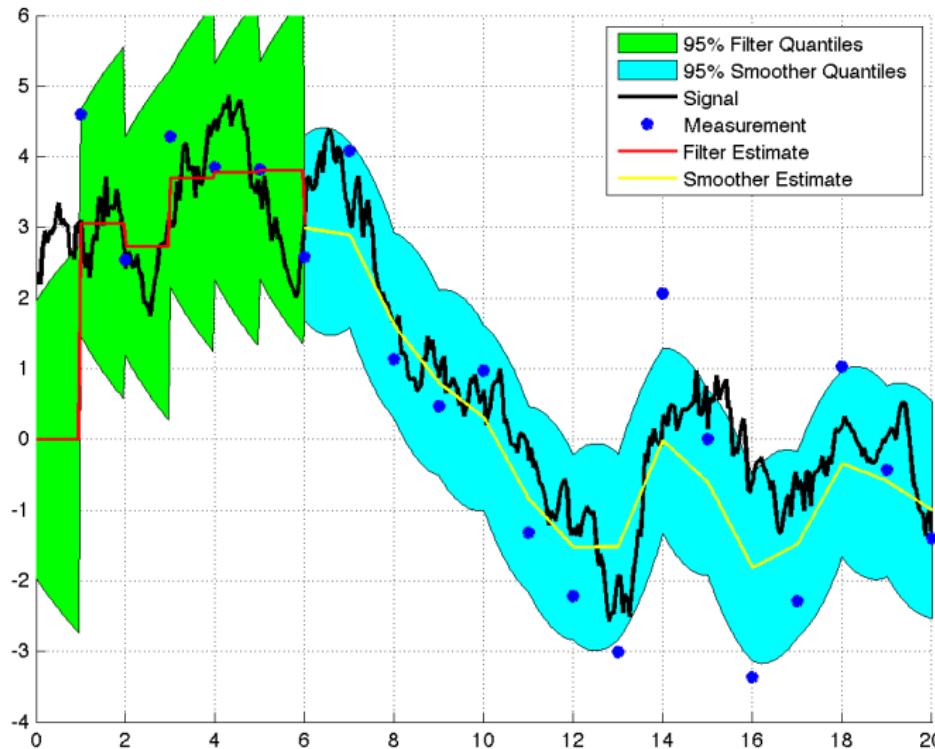
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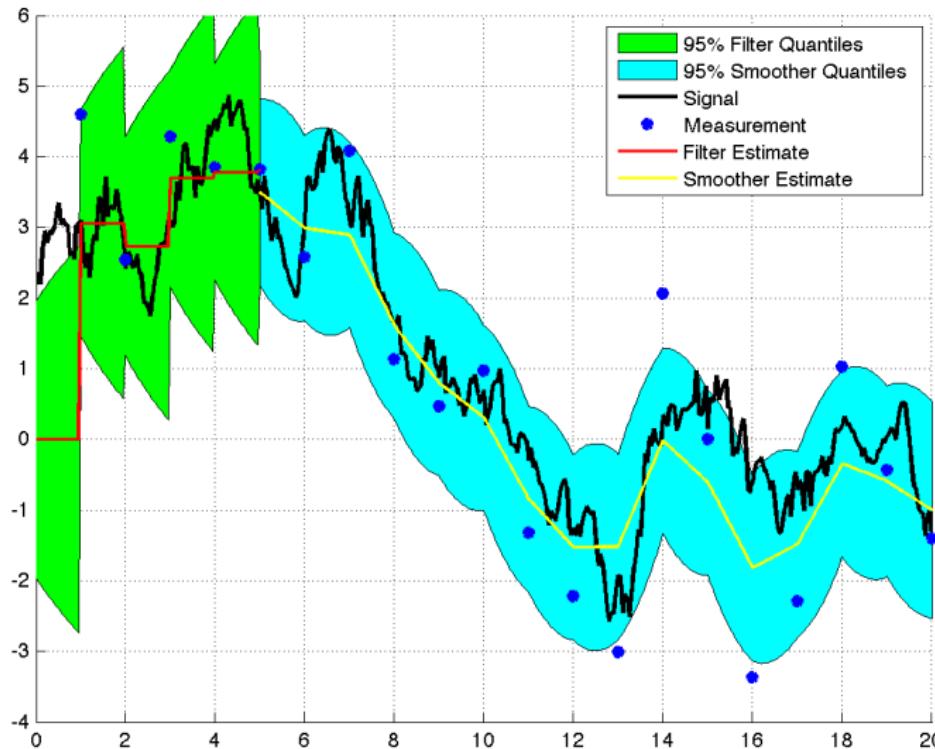
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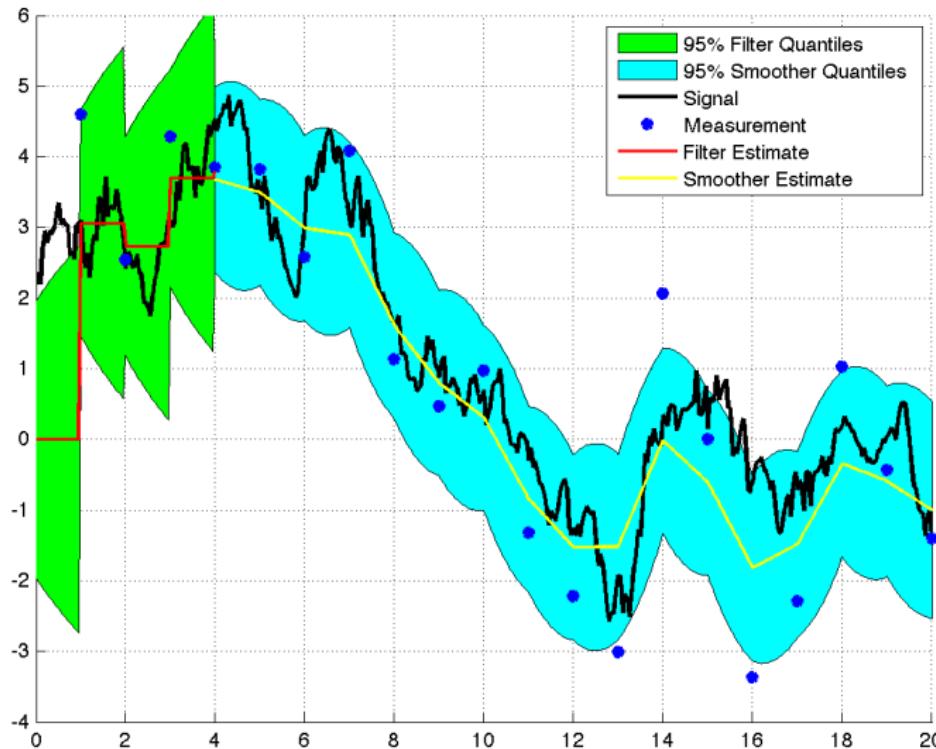
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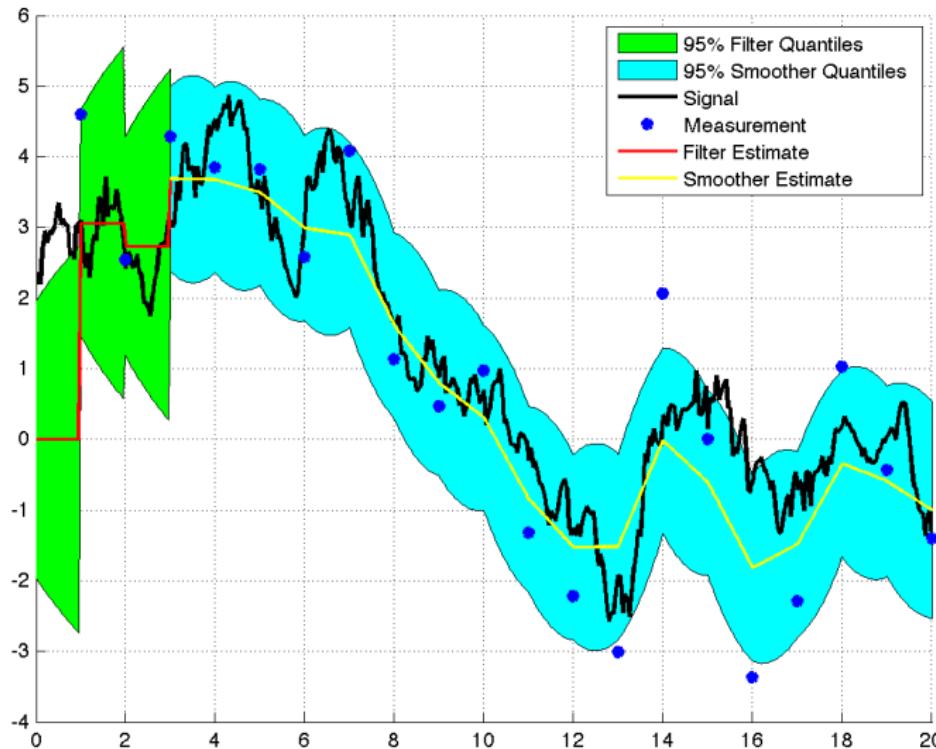
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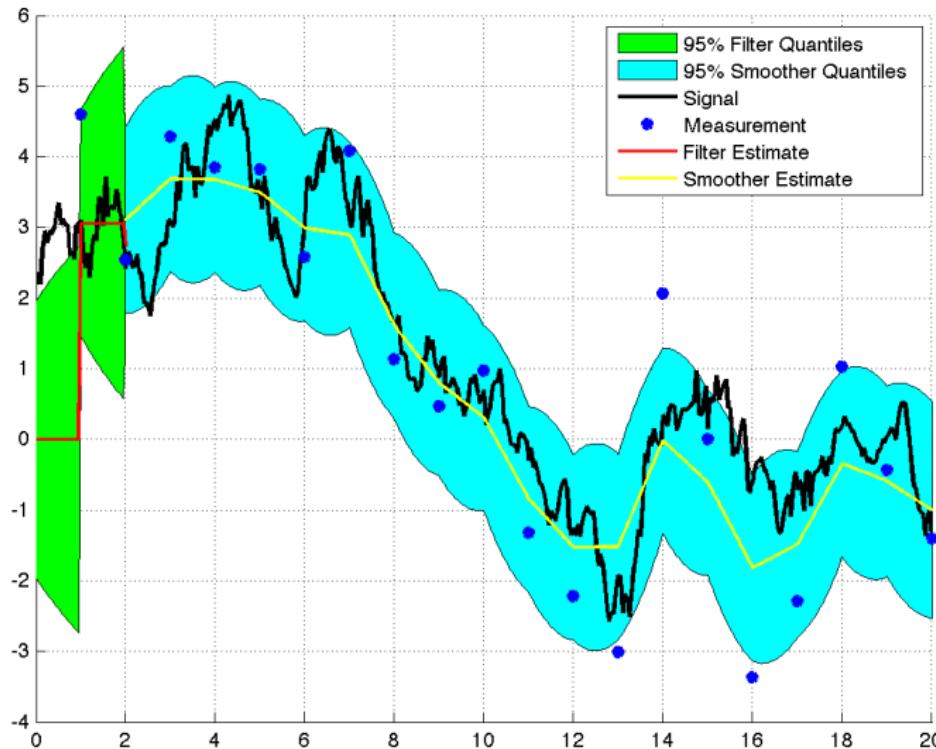
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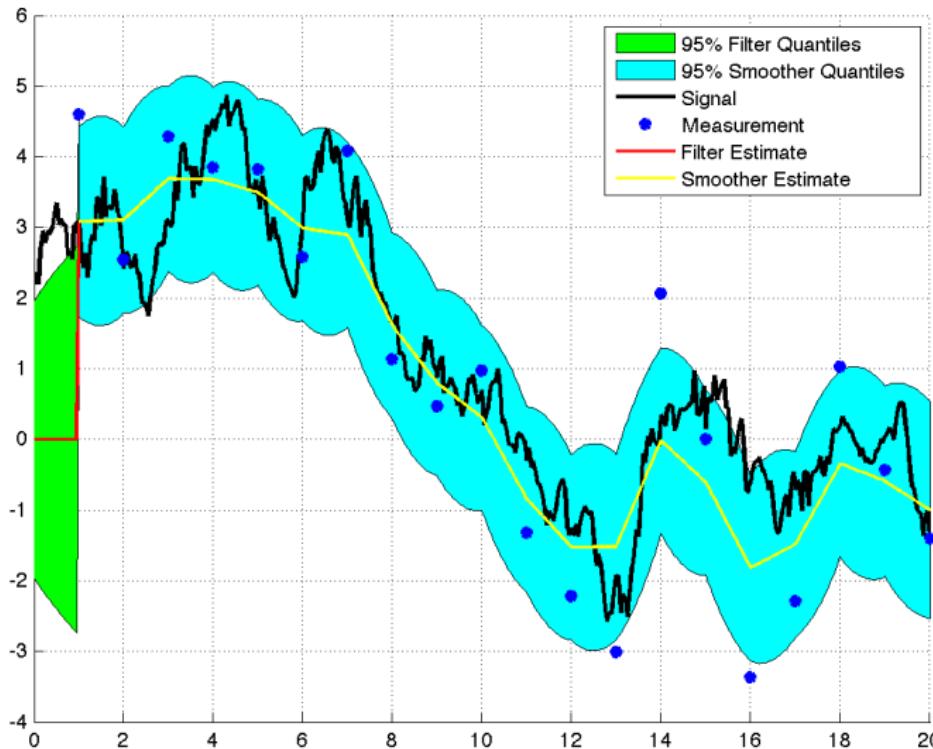
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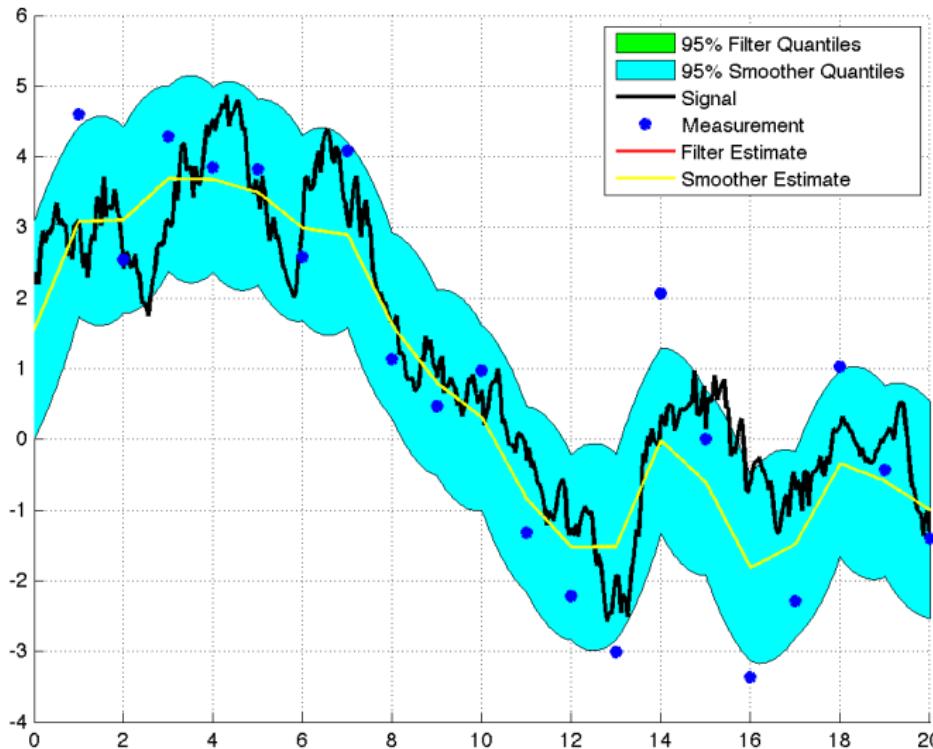
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Continuous-Discrete Bayesian Filtering

- General continuous-discrete filtering model:

$$\frac{d\mathbf{x}}{dt} = \mathbf{a}(\mathbf{x}) + \mathbf{L}(\mathbf{x}) \mathbf{w}(t)$$
$$\mathbf{y}_k \sim p(\mathbf{y}_k | \mathbf{x}(t_k)).$$

Continuous-Discrete Bayesian Optimal filter

- Prediction step: Solve the Fokker-Planck-Kolmogorov PDE

$$\frac{\partial p}{\partial t} = - \sum_i \frac{\partial}{\partial x_i} (a_i(\mathbf{x}) p) + \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} \left([\mathbf{L}(\mathbf{x}) \mathbf{Q} \mathbf{L}^\top(\mathbf{x})]_{ij} p \right)$$

- Update step: Apply the Bayes' rule.

$$p(\mathbf{x}(t_k) | \mathbf{y}_{1:k}) = \frac{p(\mathbf{y}_k | \mathbf{x}(t_k)) p(\mathbf{x}(t_k) | \mathbf{y}_{1:k-1})}{\int p(\mathbf{y}_k | \mathbf{x}(t_k)) p(\mathbf{x}(t_k) | \mathbf{y}_{1:k-1}) d\mathbf{x}(t_k)}$$

Continuous-Discrete Bayesian Filtering

- General continuous-discrete filtering model:

$$\frac{d\mathbf{x}}{dt} = \mathbf{a}(\mathbf{x}) + \mathbf{L}(\mathbf{x}) \mathbf{w}(t)$$
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Continuous-Discrete Bayesian Optimal filter

- Prediction step: Solve the Fokker-Planck-Kolmogorov PDE

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- Continuous-discrete **non-linear Kalman filters** are considered with models of the form:

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

- Kalman filters form a **Gaussian (process) approximation** to the posterior of the process $\mathbf{x}(t)$.
- The resulting approximation is of the form

$$p(\mathbf{x}(t) | \mathbf{y}_{1:k}) \approx N(\mathbf{x}(t) | \mathbf{m}(t), \mathbf{P}(t)), \quad t \in [t_k, t_{k+1}),$$

where $\mathbf{m}(t)$ and $\mathbf{P}(t)$ are computed by the **non-linear Kalman filter**.

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Continuous-Discrete Bayesian Smoothing

- Continuous-discrete (-time) smoothing refers to recursive computation of the distributions

$$p(\mathbf{x}(t) | \mathbf{y}_{1:T}), \quad t \in [t_0, t_T].$$

- Discrete-time smoothing: compute $p(\mathbf{x}(t_k) | \mathbf{y}_{1:T})$ for $k = 1, \dots, T$.
- The (discrete-time) Bayesian smoothing equation is

$$\begin{aligned} p(\mathbf{x}(t_k) | \mathbf{y}_{1:T}) &= p(\mathbf{x}(t_k) | \mathbf{y}_{1:k}) \\ &\times \int \frac{p(\mathbf{x}(t_{k+1}) | \mathbf{y}_{1:T}) p(\mathbf{x}(t_{k+1}) | \mathbf{x}(t_k))}{p(\mathbf{x}(t_{k+1}) | \mathbf{y}_{1:k})} d\mathbf{x}(t_{k+1}). \end{aligned}$$

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Contents

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- 2 Bayesian Filtering and Smoothing
- 3 State Space Representation of Gaussian Process Regression
- 4 Spatio-Temporal Systems, Latent Force Models and Other Extensions
- 5 Application examples
- 6 Summary

Definition and Notation of Gaussian Processes in Regression

- **Spatial Gaussian process** (GP) or Gaussian **field** is a random function $\mathbf{f}(\mathbf{x})$, such that all finite-dimensional distributions $p(\mathbf{f}(\mathbf{x}_1), \dots, \mathbf{f}(\mathbf{x}_n))$ are Gaussian.
- Note that \mathbf{x} is the **input** – not the **state!** – BEWARE of the notation!
- Can be defined in terms of **mean** and **covariance functions**:

$$\mathbf{m}(\mathbf{x}) = E[\mathbf{f}(\mathbf{x})]$$

$$\mathbf{K}(\mathbf{x}, \mathbf{x}') = E[(\mathbf{f}(\mathbf{x}) - \mathbf{m}(\mathbf{x})) (\mathbf{f}(\mathbf{x}') - \mathbf{m}(\mathbf{x}'))^\top].$$

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

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

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Gaussian Process Regression as State Estimation

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$$y_k = f(t_k) + e_k, \quad e_k \sim N(0, \sigma^2).$$

- The **covariance function** of $f(t)$ can be, e.g.,

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

- We now assert that it is possible to form a **state space model**

$$\frac{d\mathbf{f}(t)}{dt} = \mathbf{A}\mathbf{f}(t) + \mathbf{L}w(t)$$

$$y_k = \mathbf{H}\mathbf{f}(t_k) + e_k.$$

such that a linear **Kalman filter/smooth**er computes the **GP-regression solution**.

- The solution has complexity $O(T)$ when GP-regression has $O(T^3)$.

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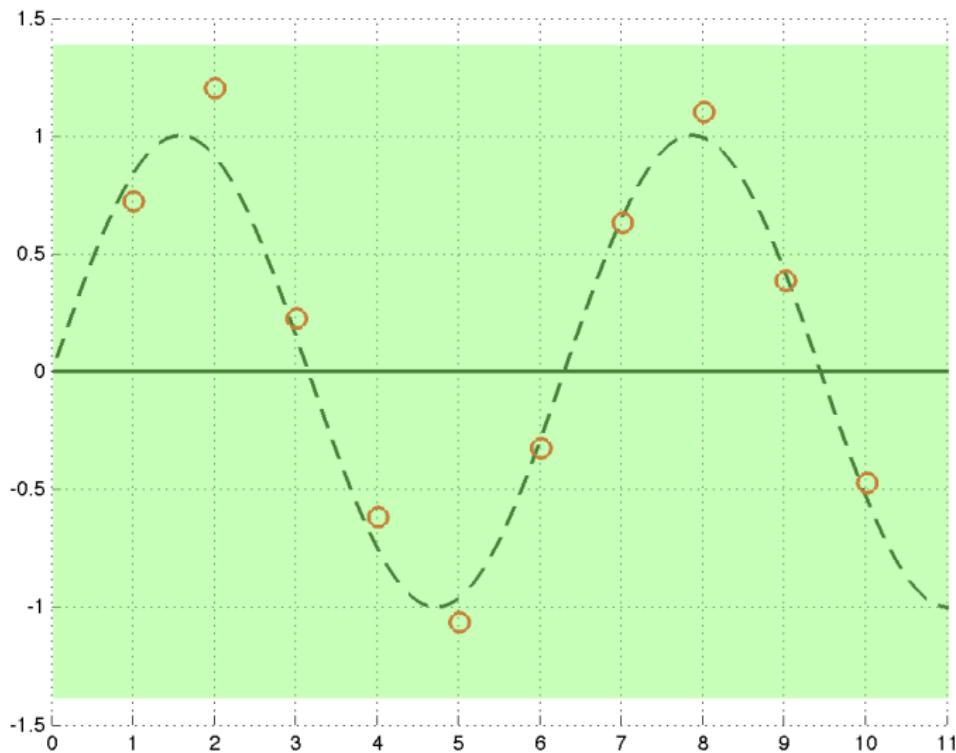
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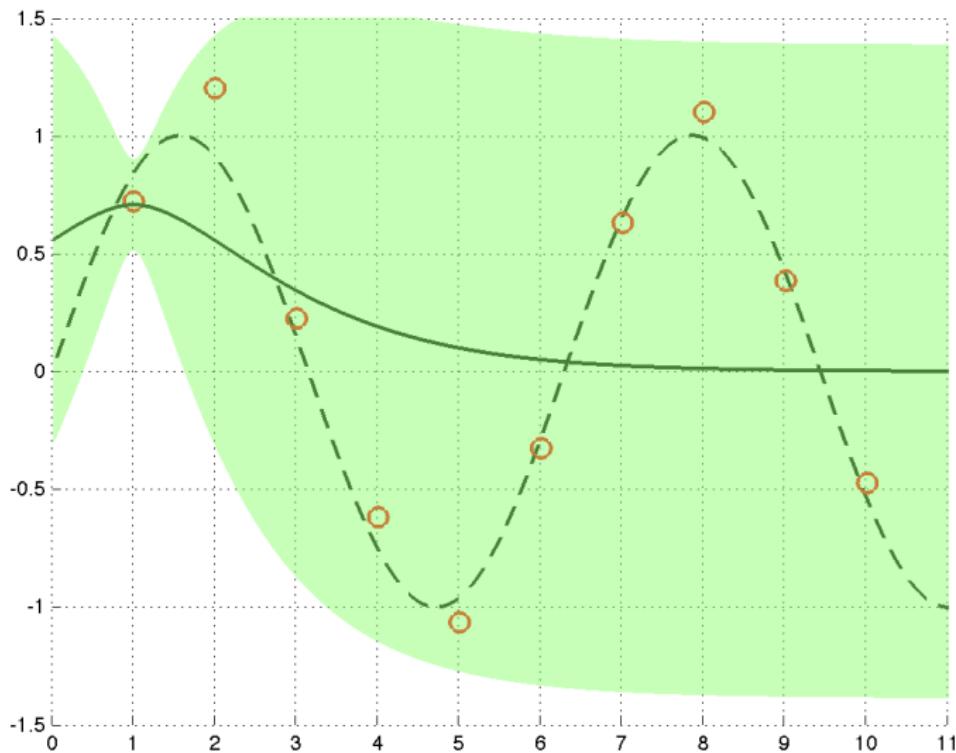
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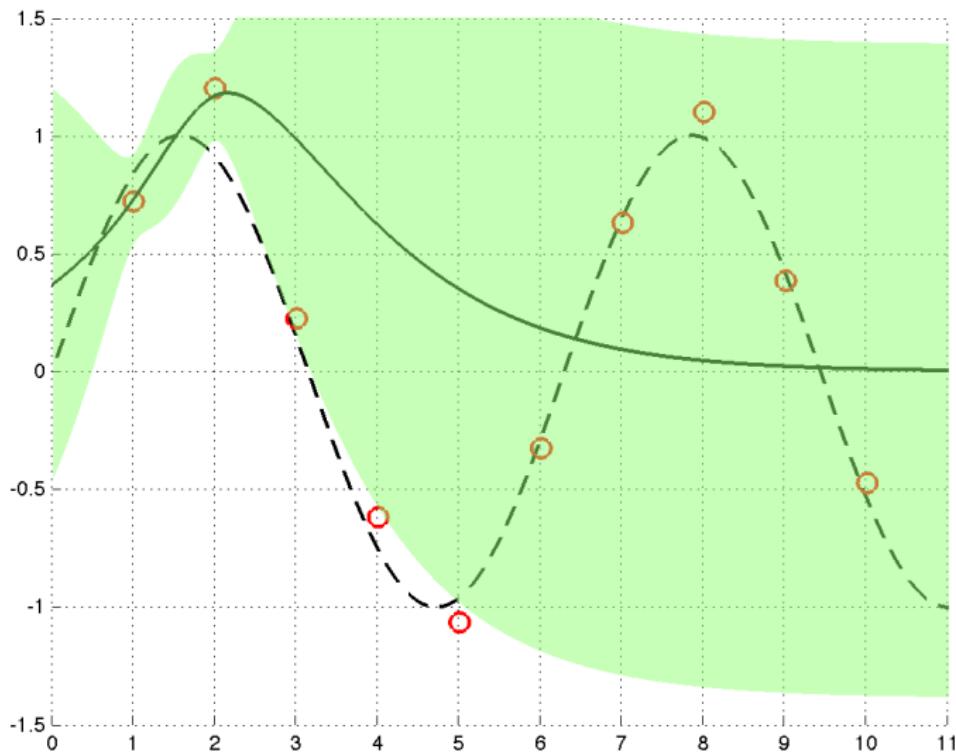
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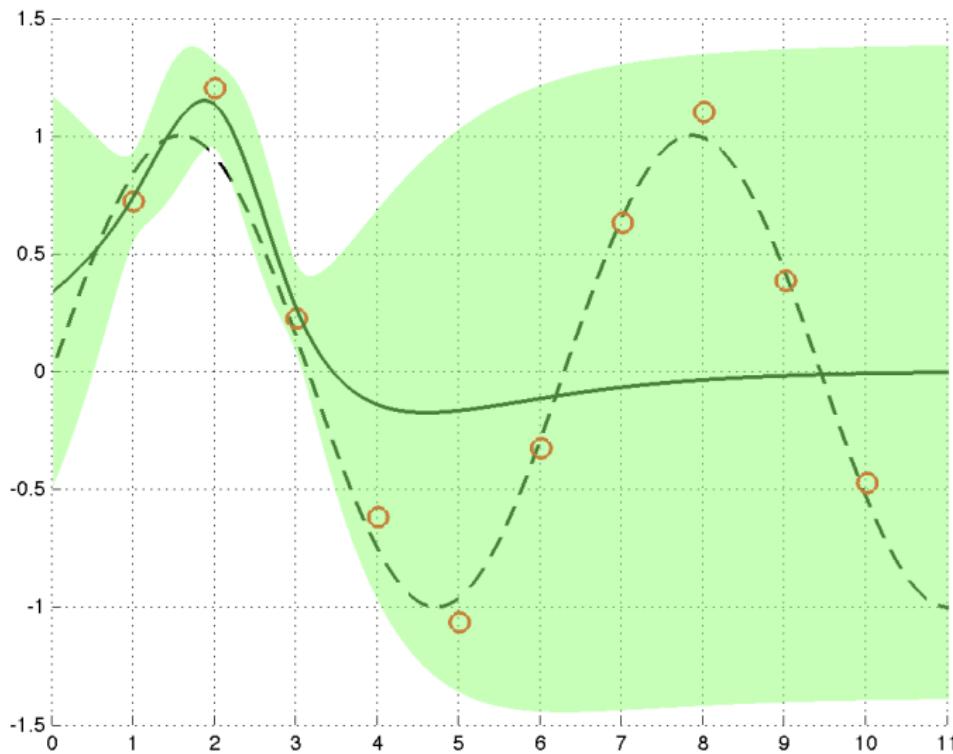
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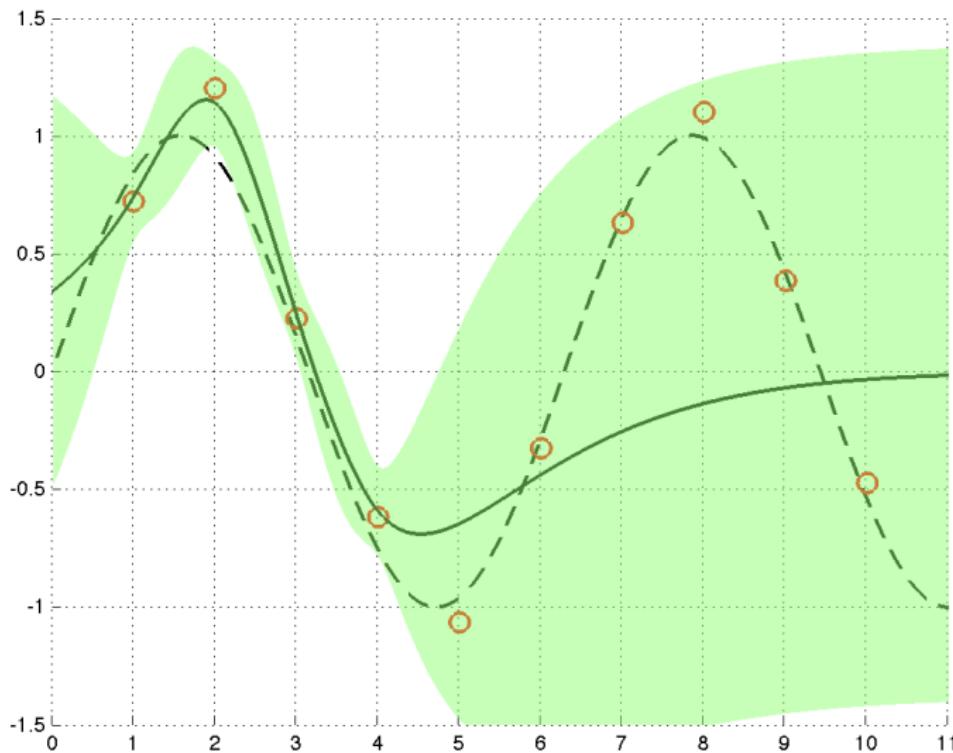
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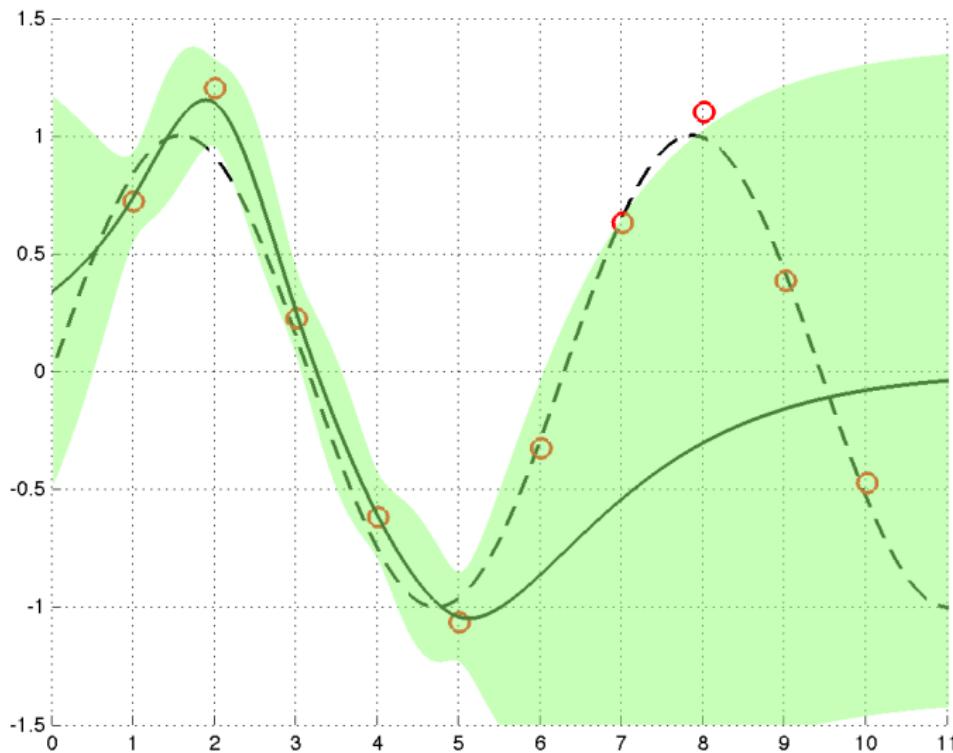
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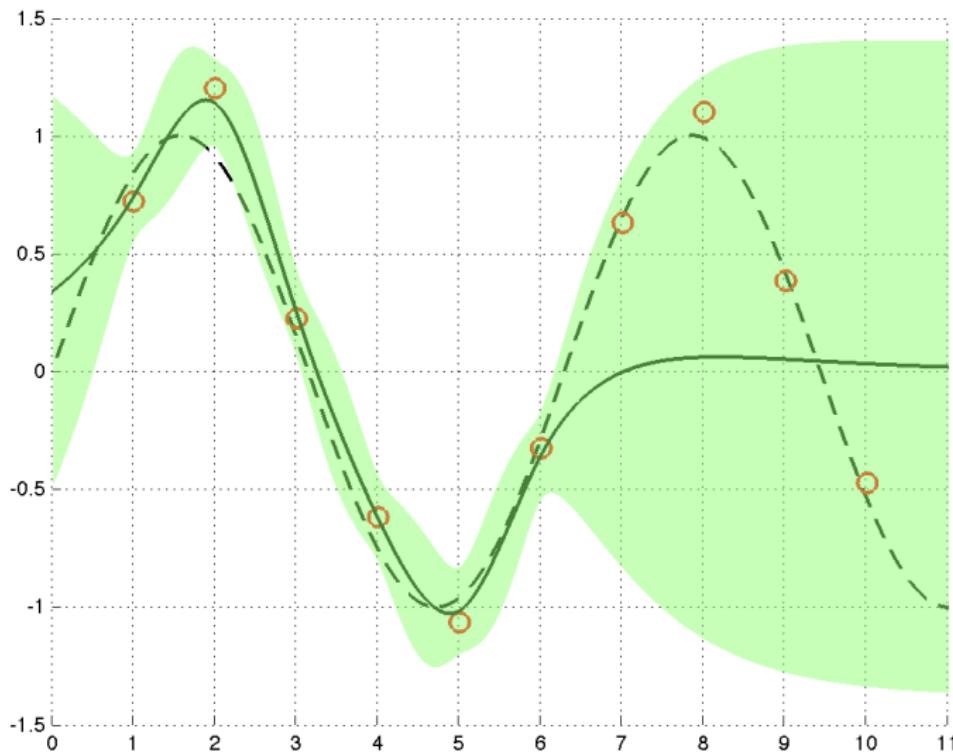
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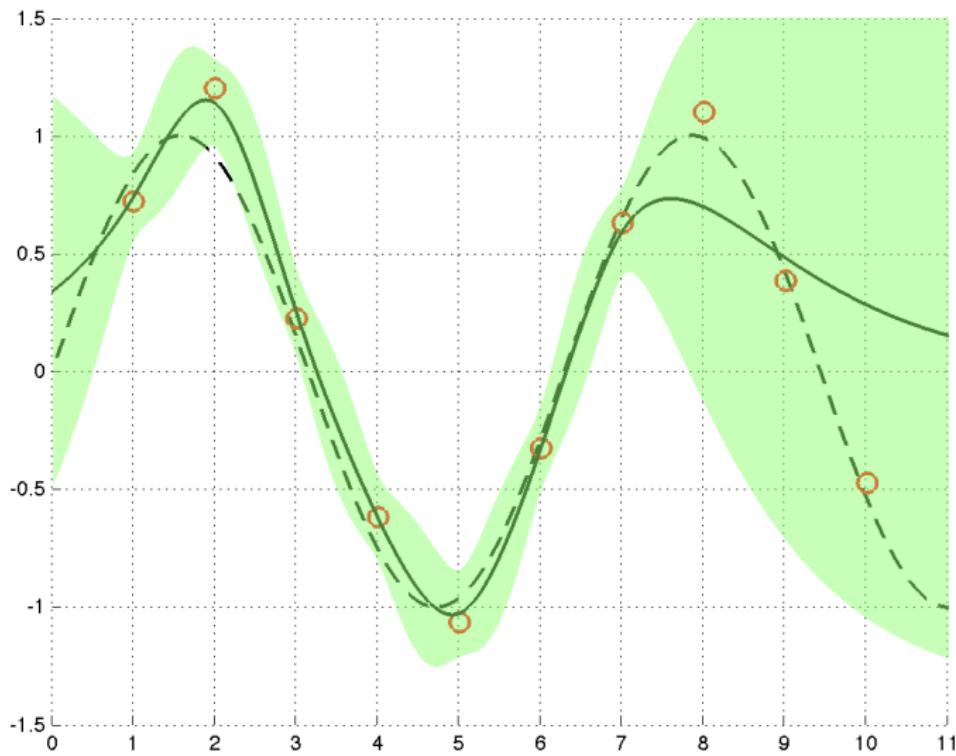
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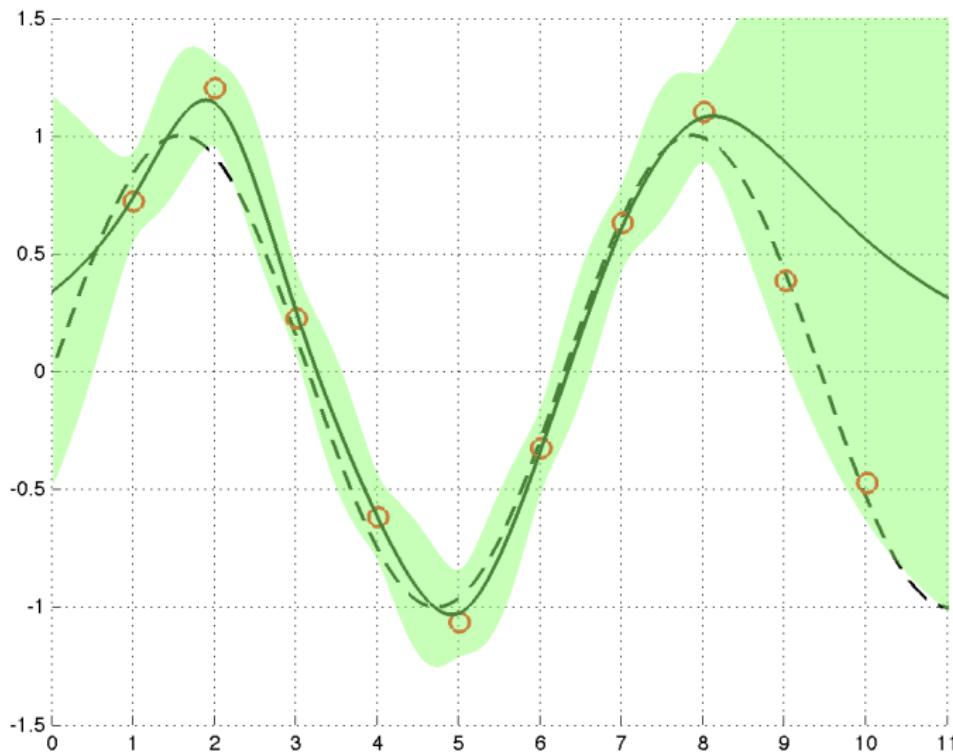
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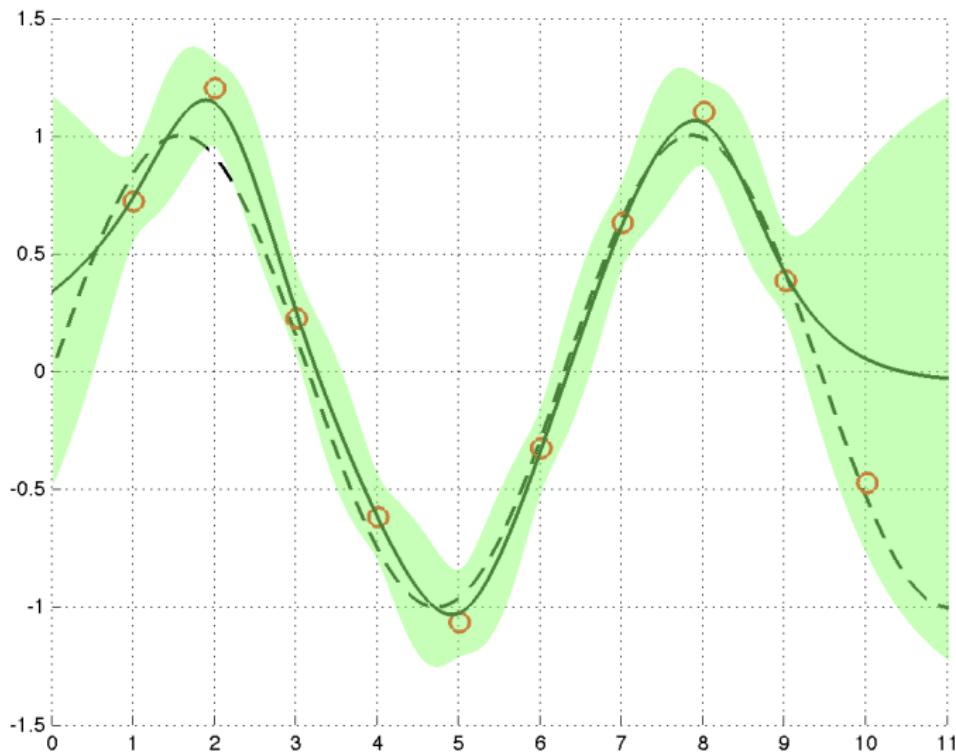
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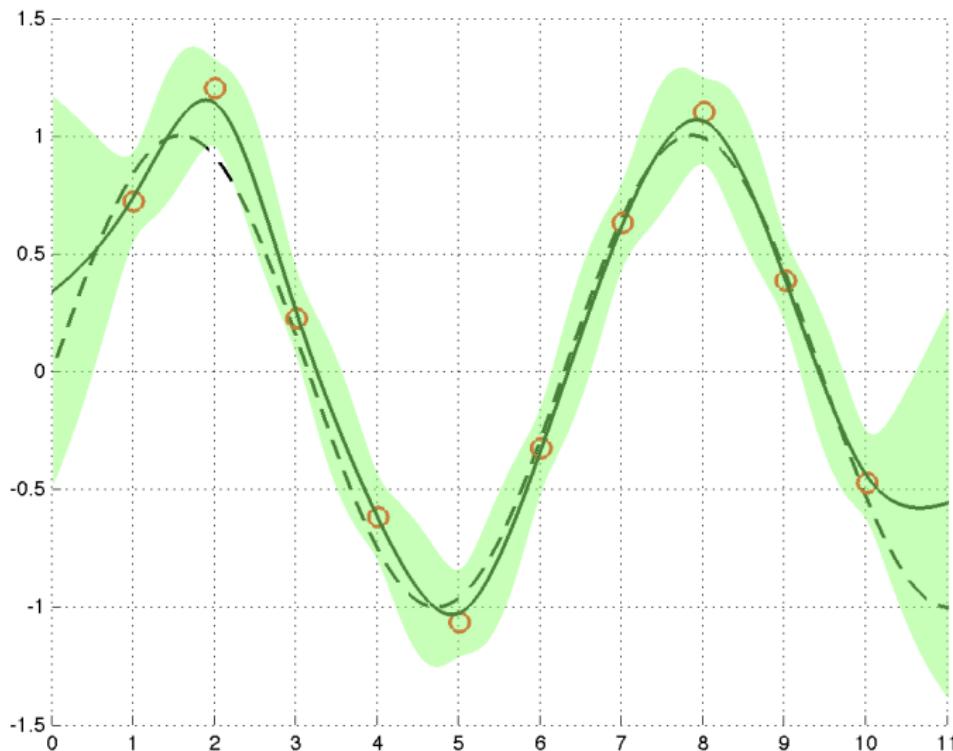
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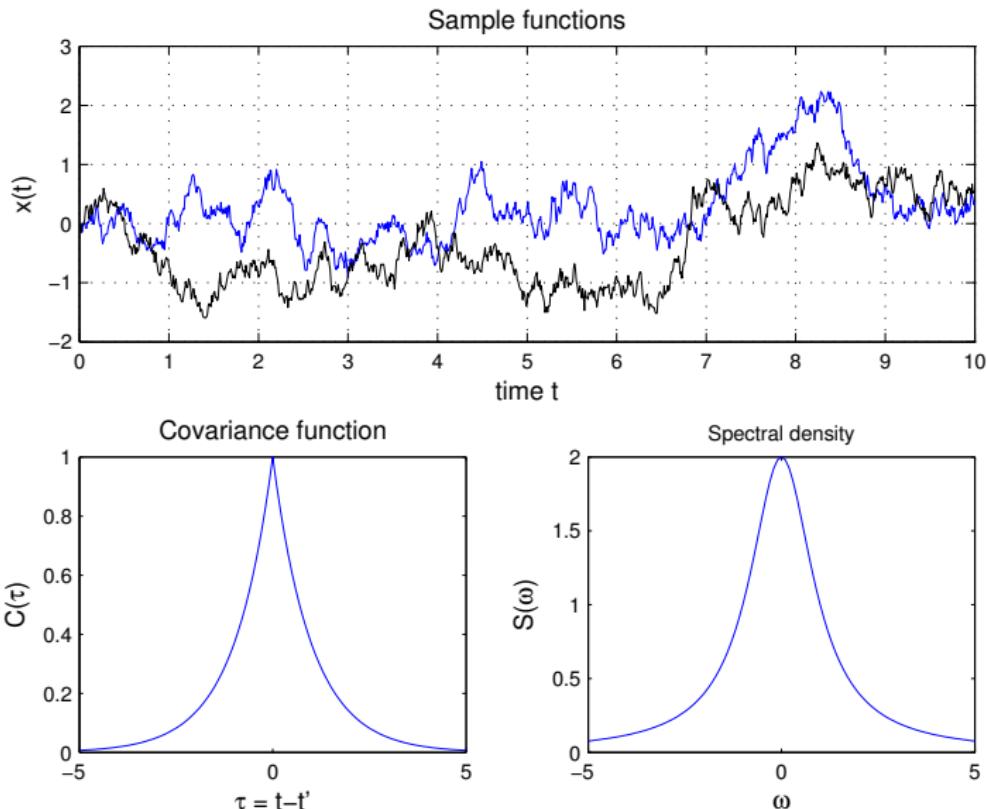
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Representations of Temporal Gaussian Processes



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- 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 $\{f(s'), s' > t\}$.

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State Space Form of Linear Time-Invariant SDEs

- Consider a **Nth 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 $\mathbf{f} = (f, \dots, d^{N-1}f/dt^{N-1})$, we get a **state space model**:

$$\begin{aligned}\frac{d\mathbf{f}}{dt} &= \underbrace{\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ -a_0 & -a_1 & \cdots & -a_{N-1} \end{pmatrix}}_A \mathbf{f} + \underbrace{\begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}}_L w(t) \\ f(t) &= \underbrace{\begin{pmatrix} 1 & 0 & \cdots & 0 \end{pmatrix}}_H \mathbf{f}.\end{aligned}$$

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

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

- 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.:

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

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- Spectral factorization finds rational stable transfer function

$$G(i\omega) = \frac{b_m(i\omega)^m + \cdots + b_1(i\omega) + b_0}{a_n(i\omega)^n + \cdots + a_1(i\omega) + a_0}$$

such that

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- The procedure practice:
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Example: Matérn Covariance Function

Example (1D Matérn covariance function)

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- **Conventional GP regression:**

- ➊ Evaluate the covariance function at the training and test set points.
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- ➊ Form the state space model.
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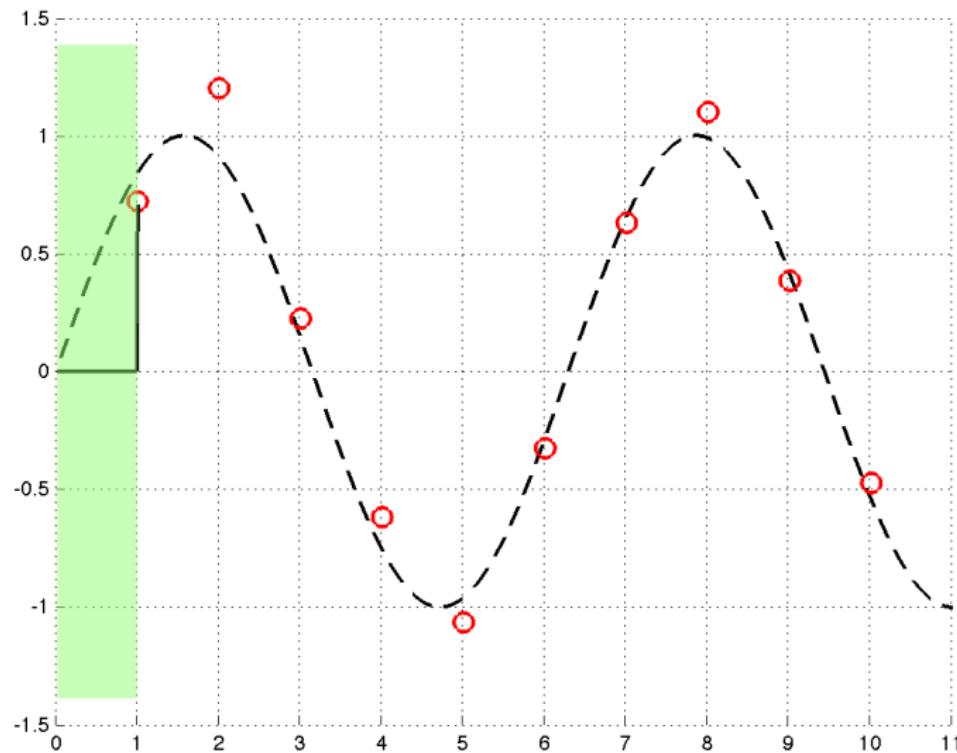
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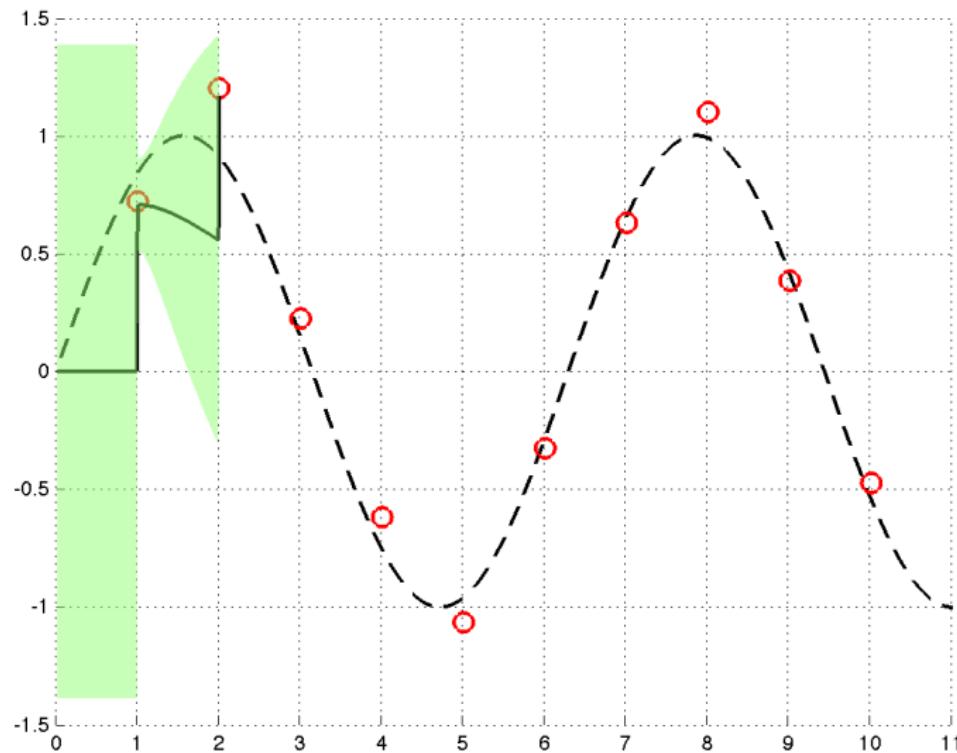
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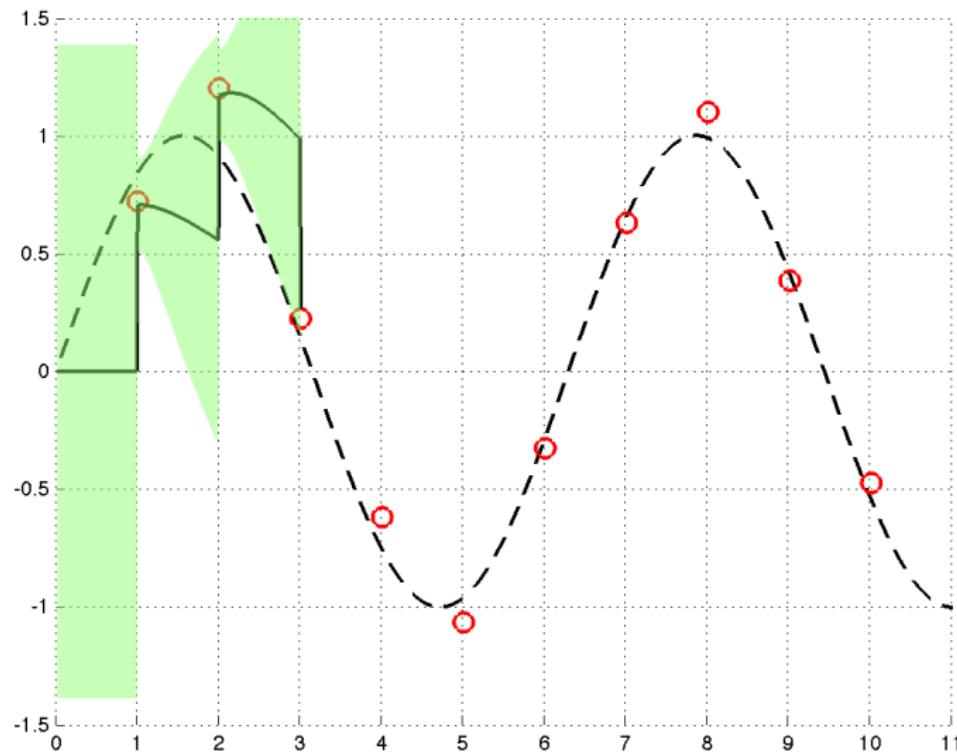
State-Space GP Regression Demo



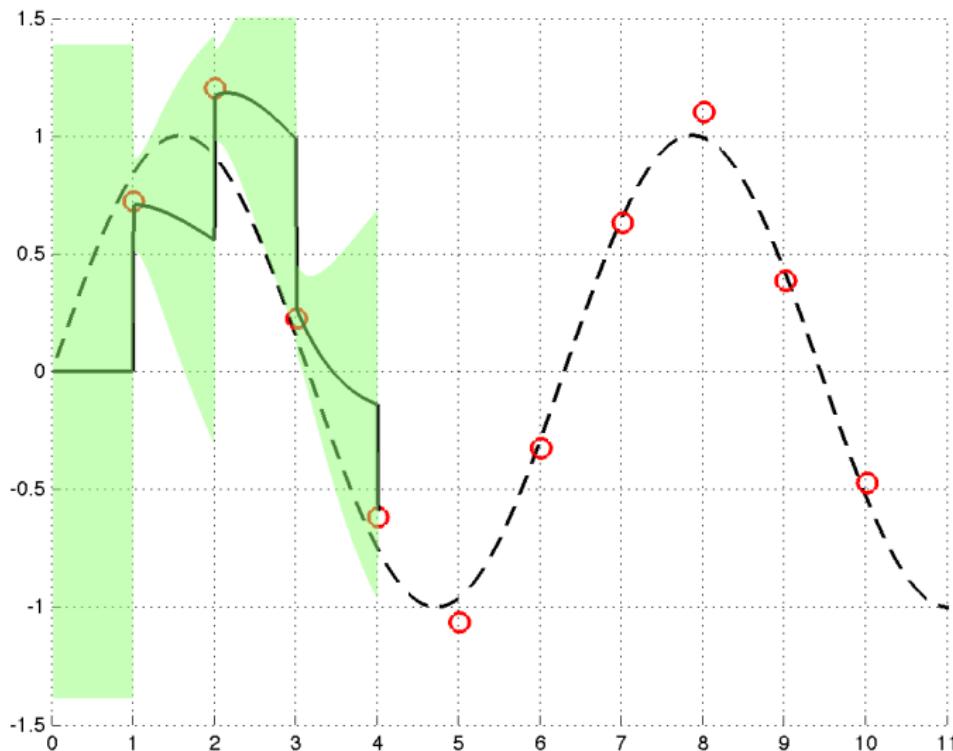
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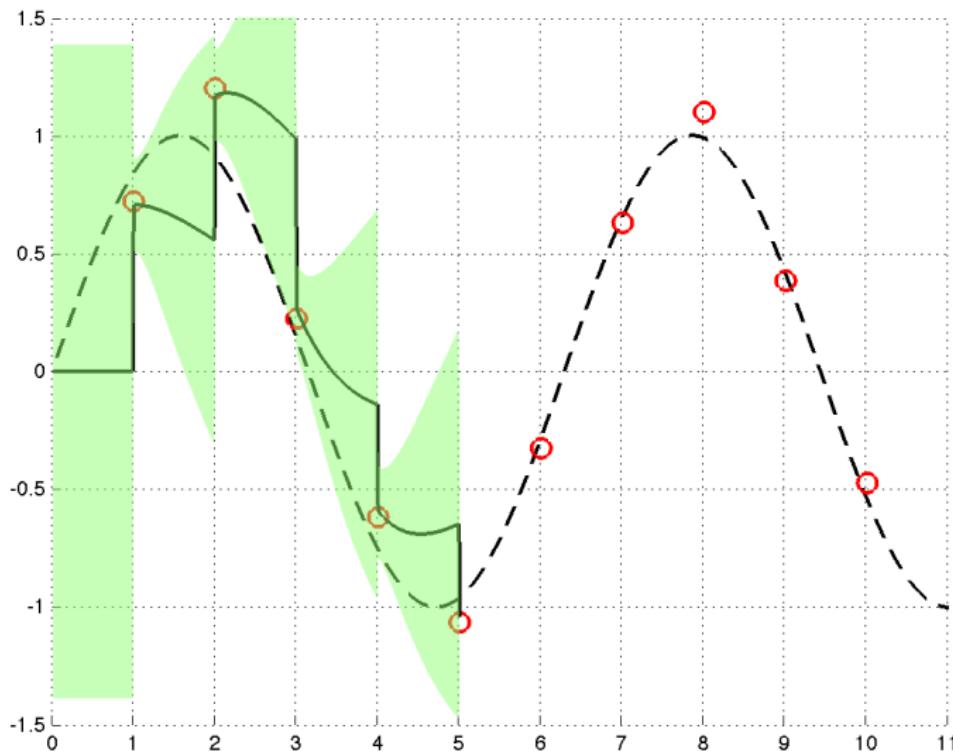
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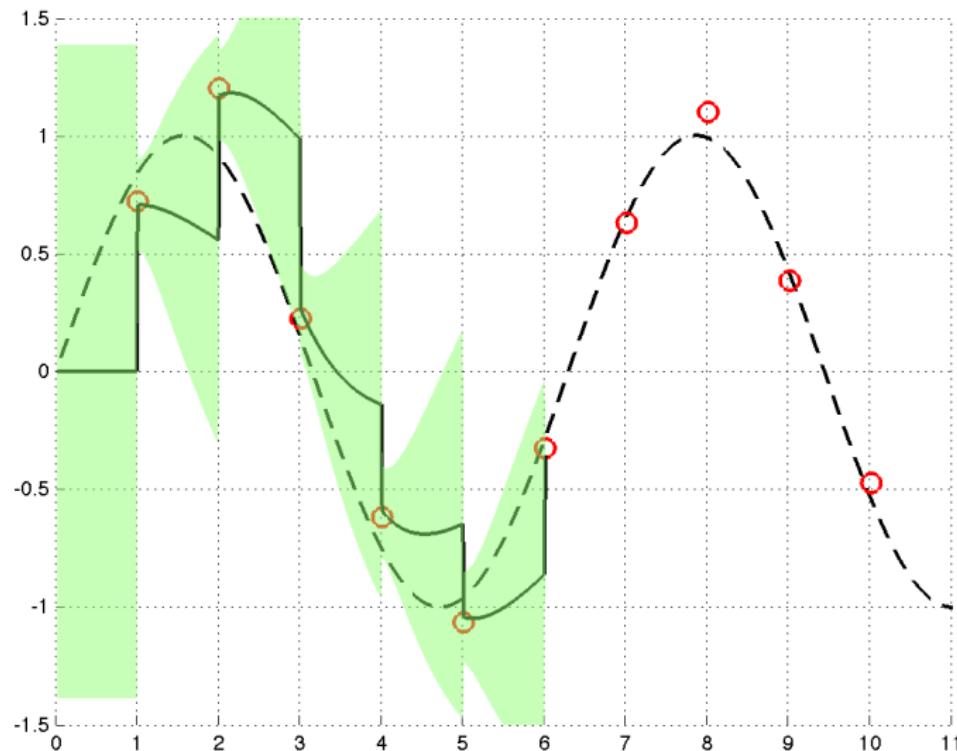
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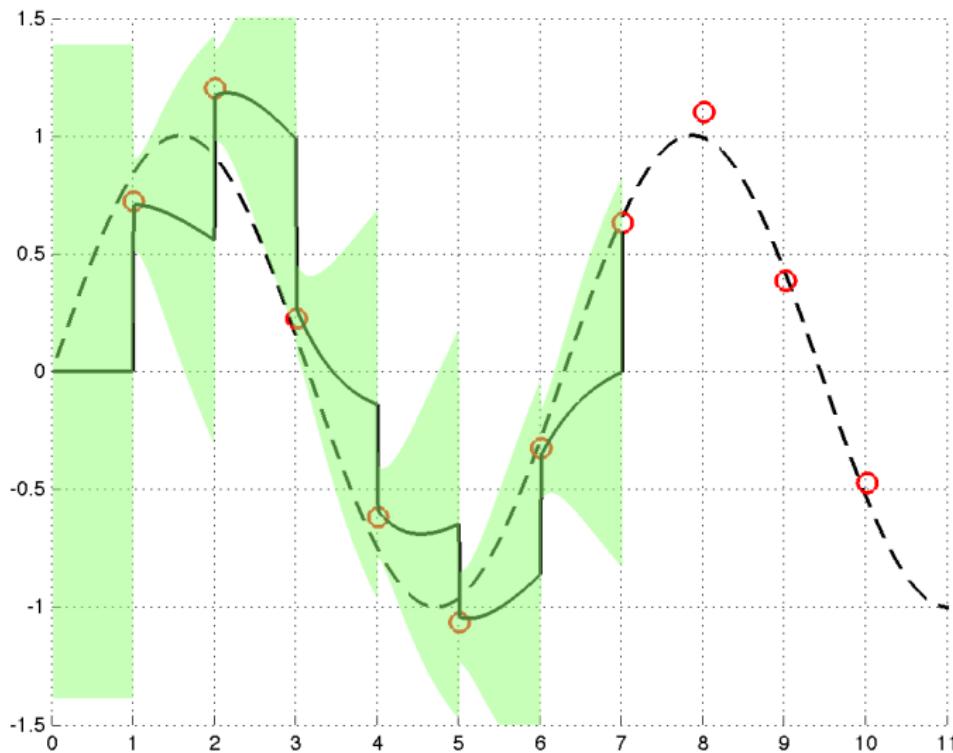
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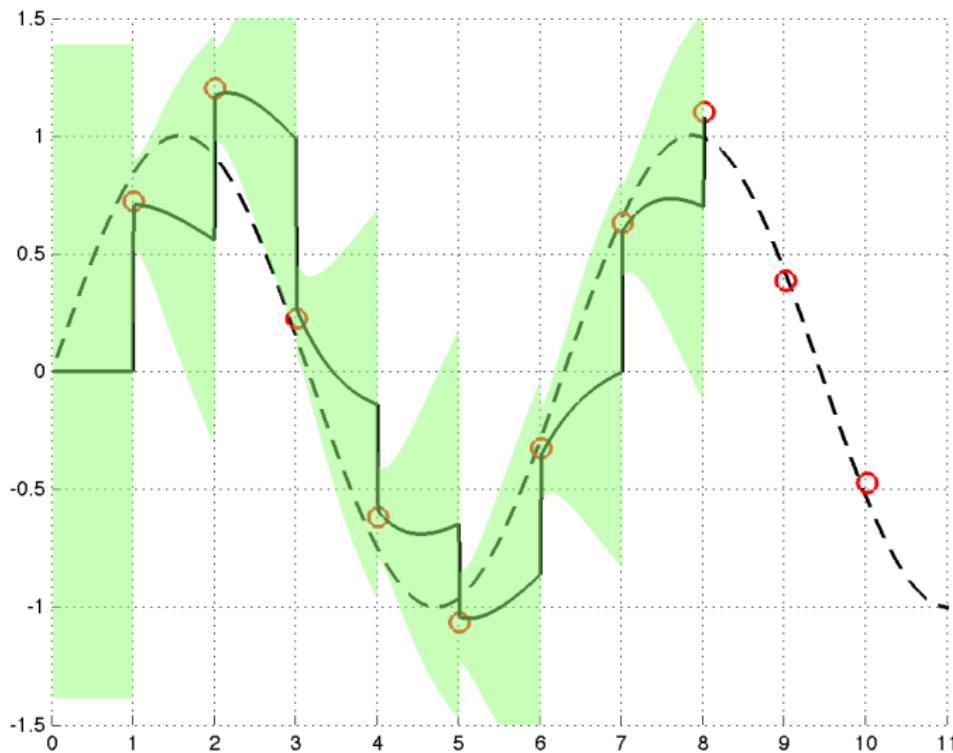
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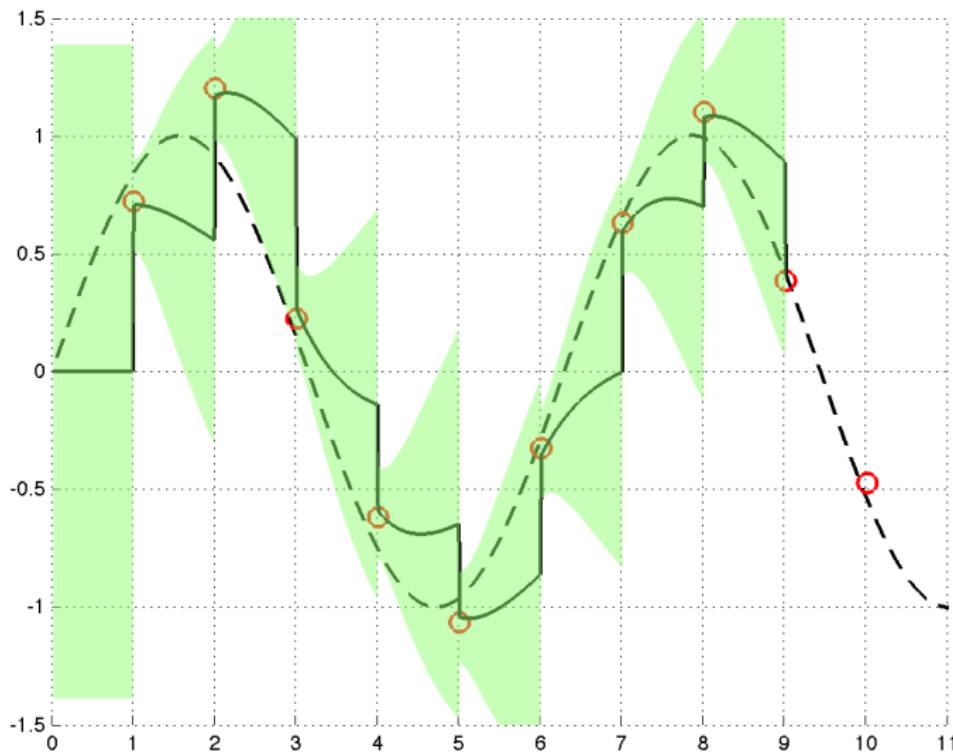
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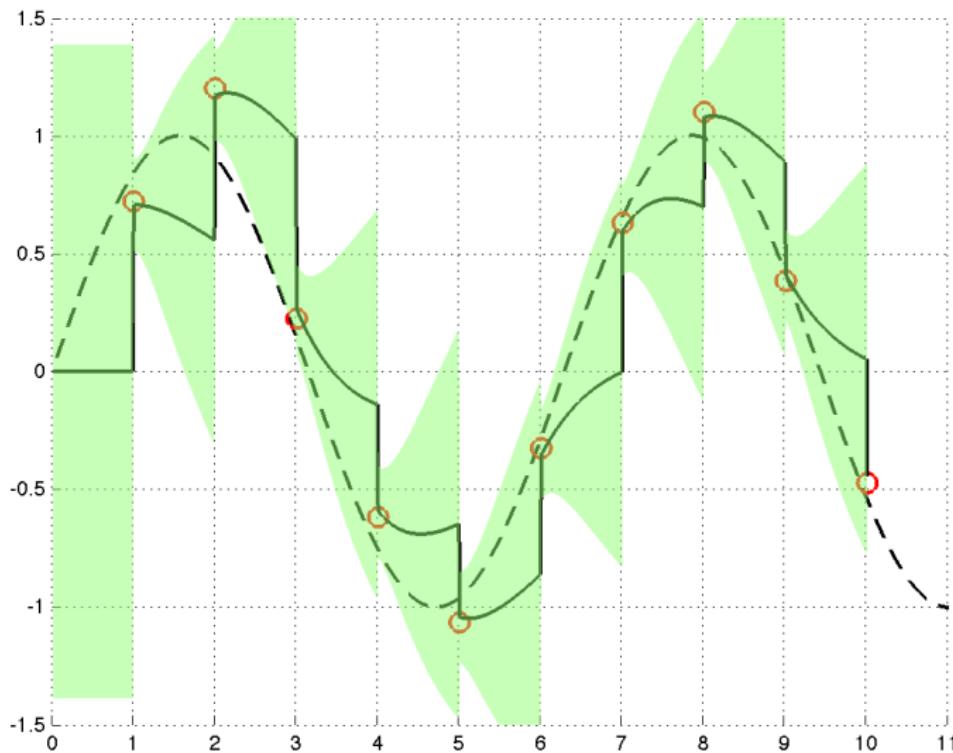
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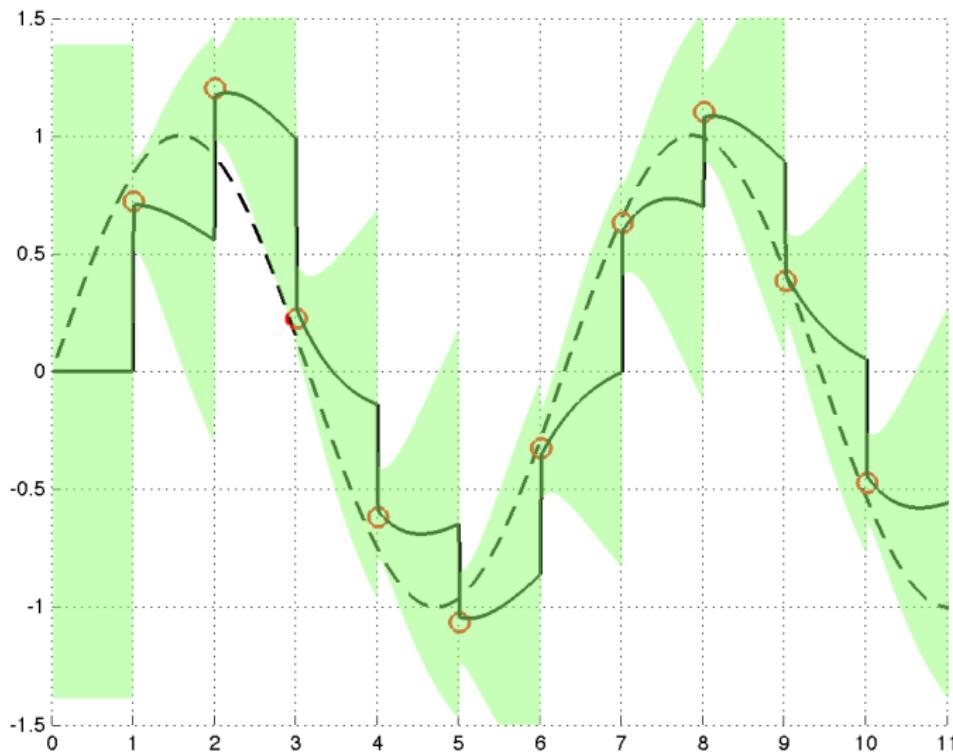
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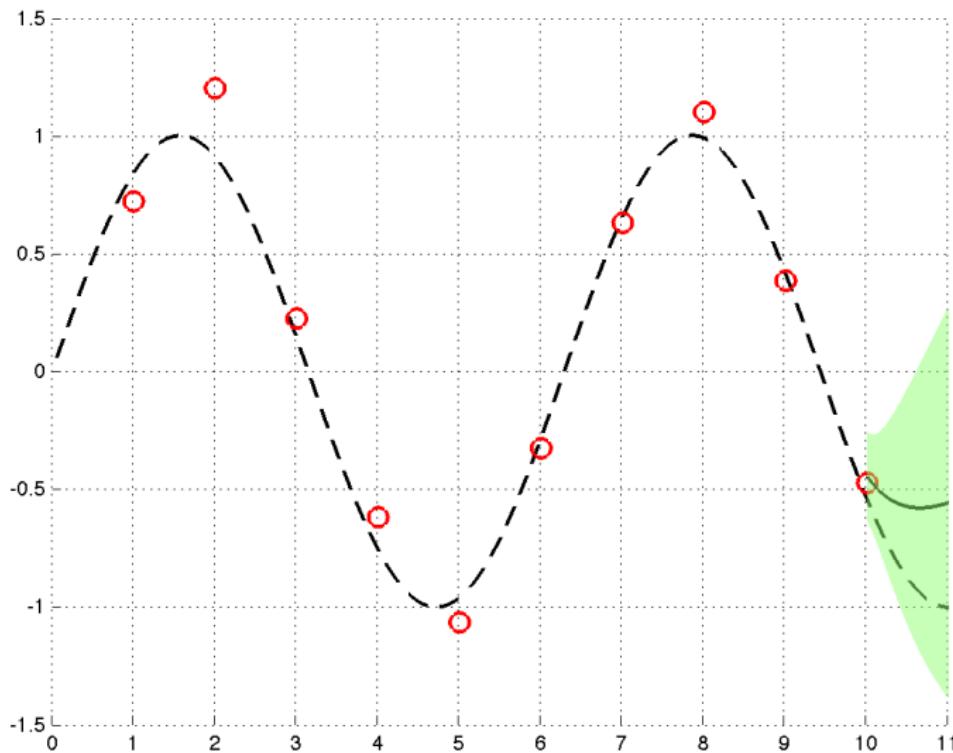
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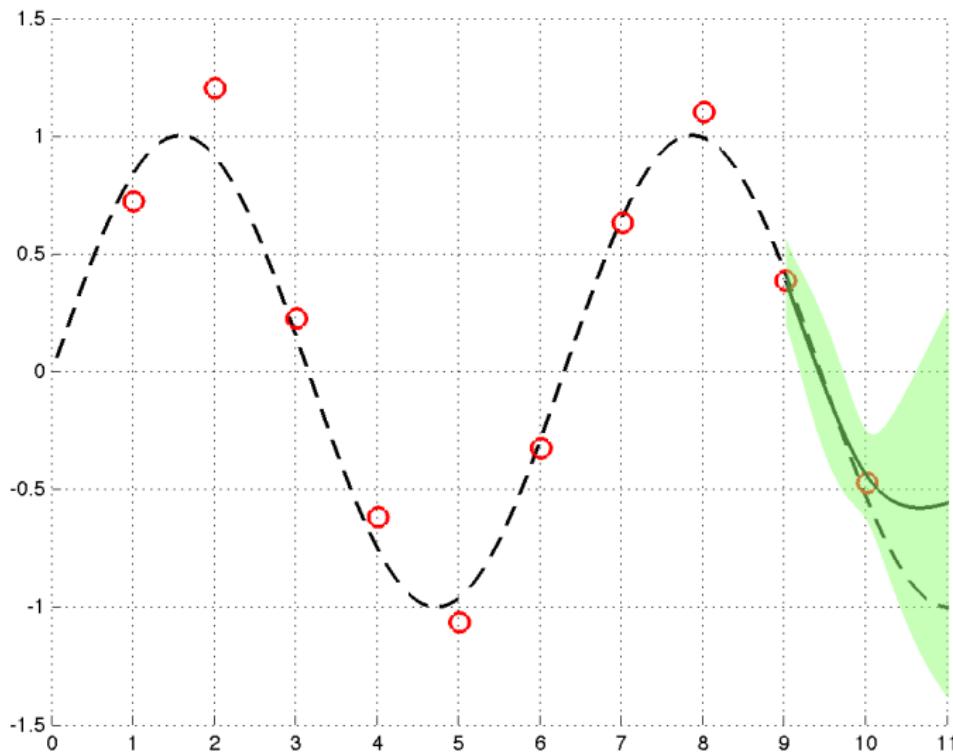
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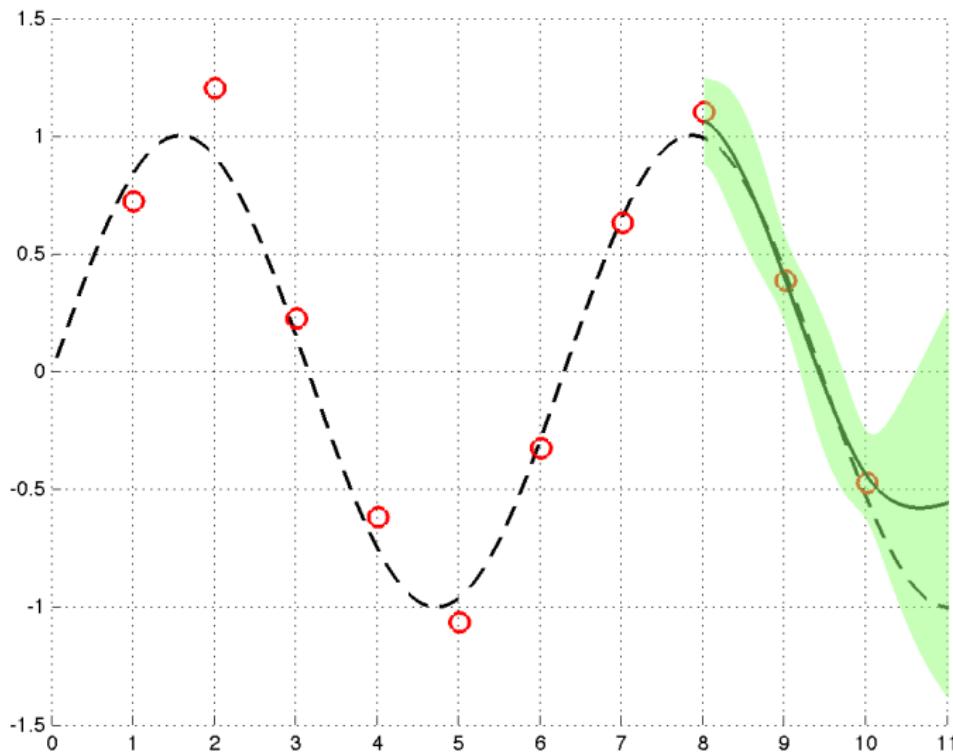
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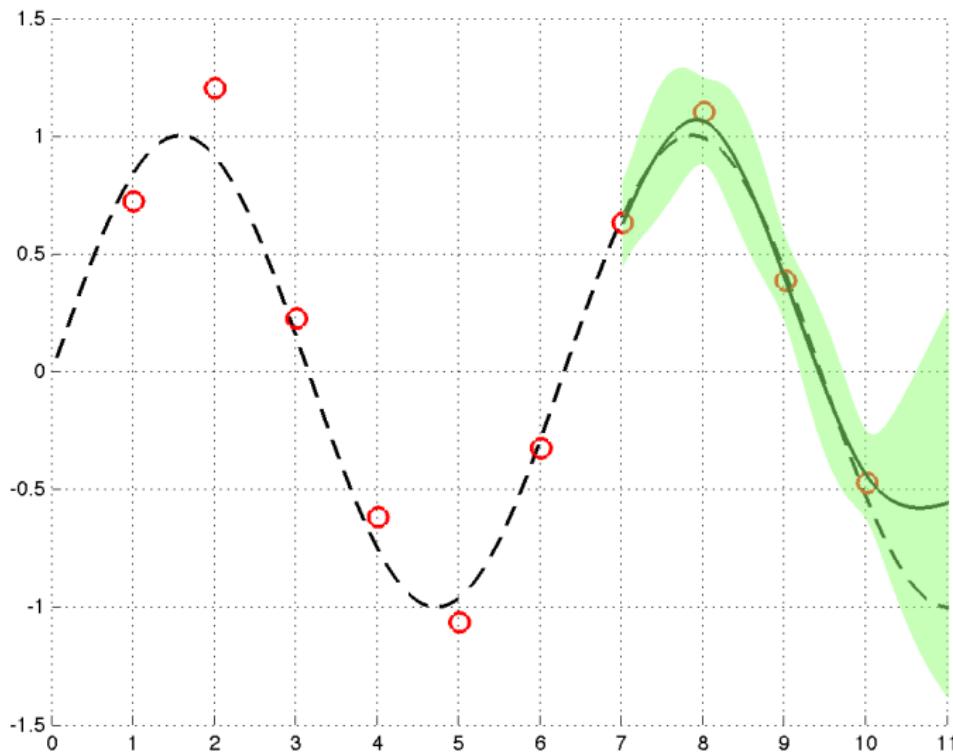
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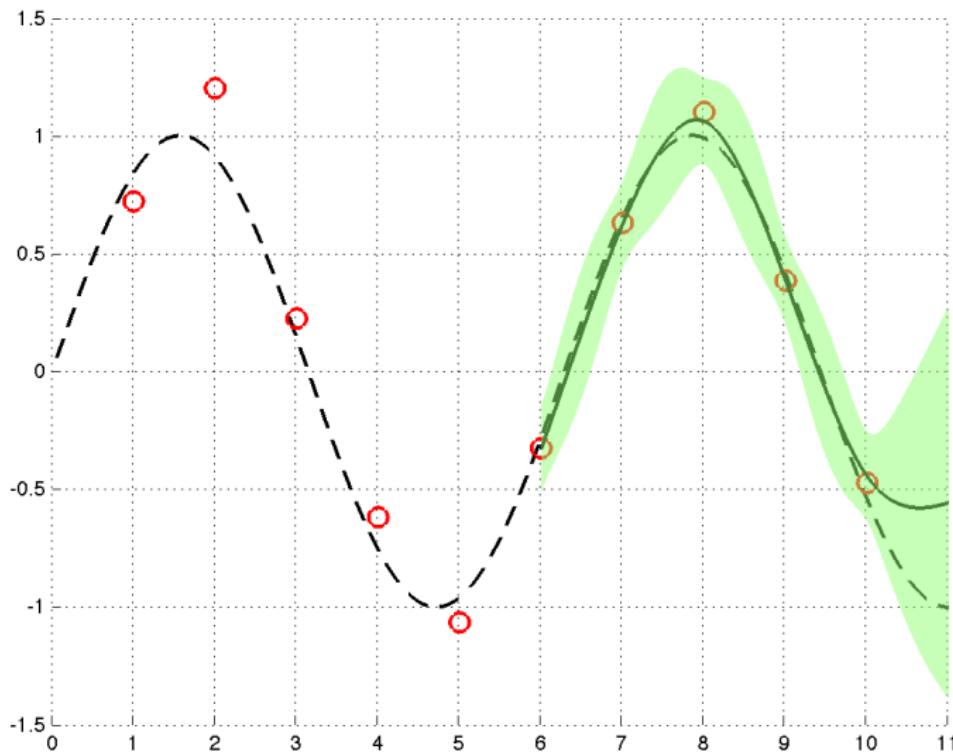
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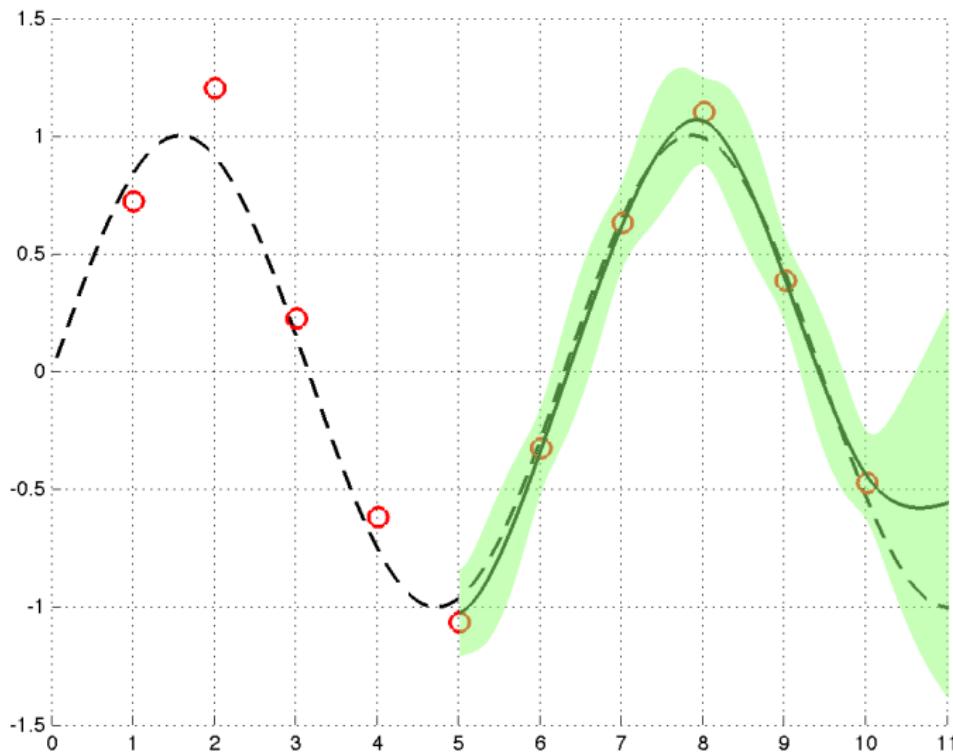
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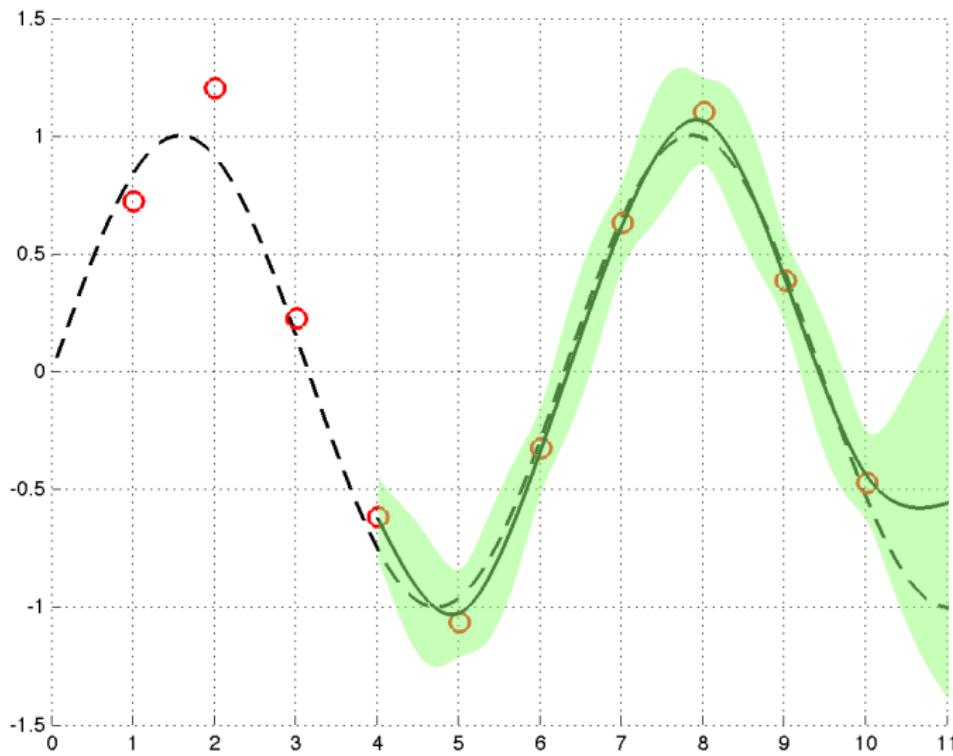
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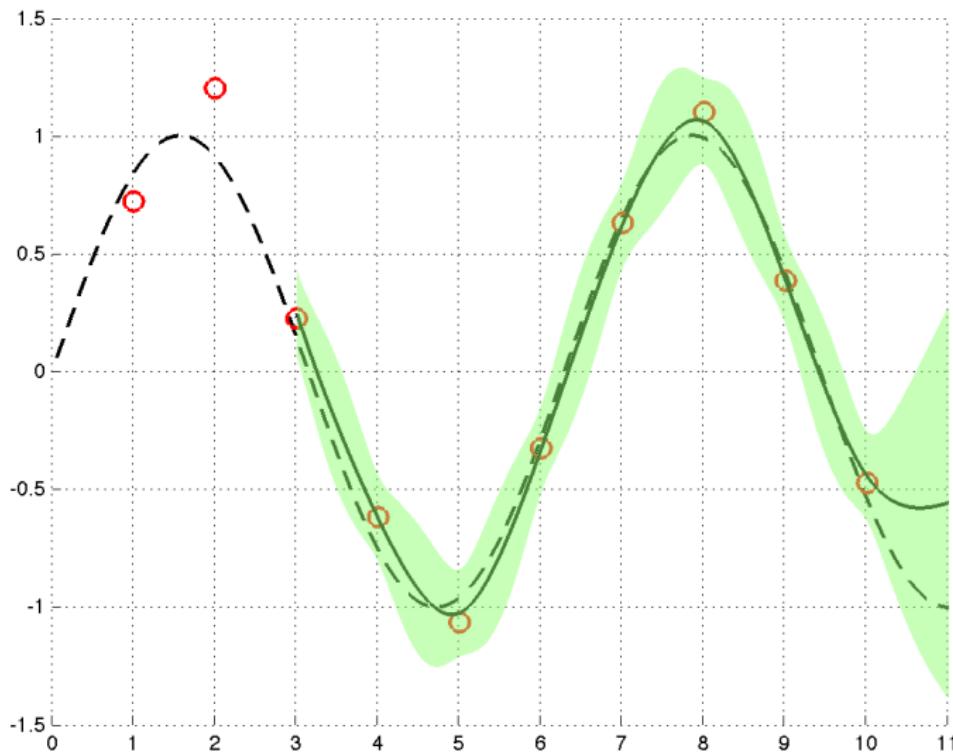
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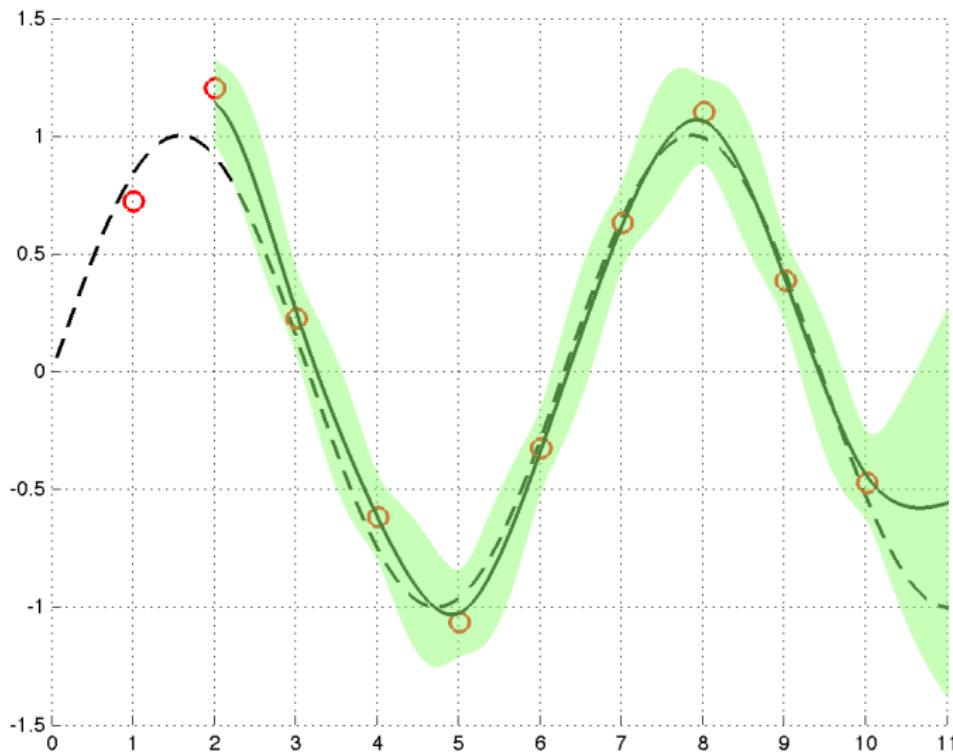
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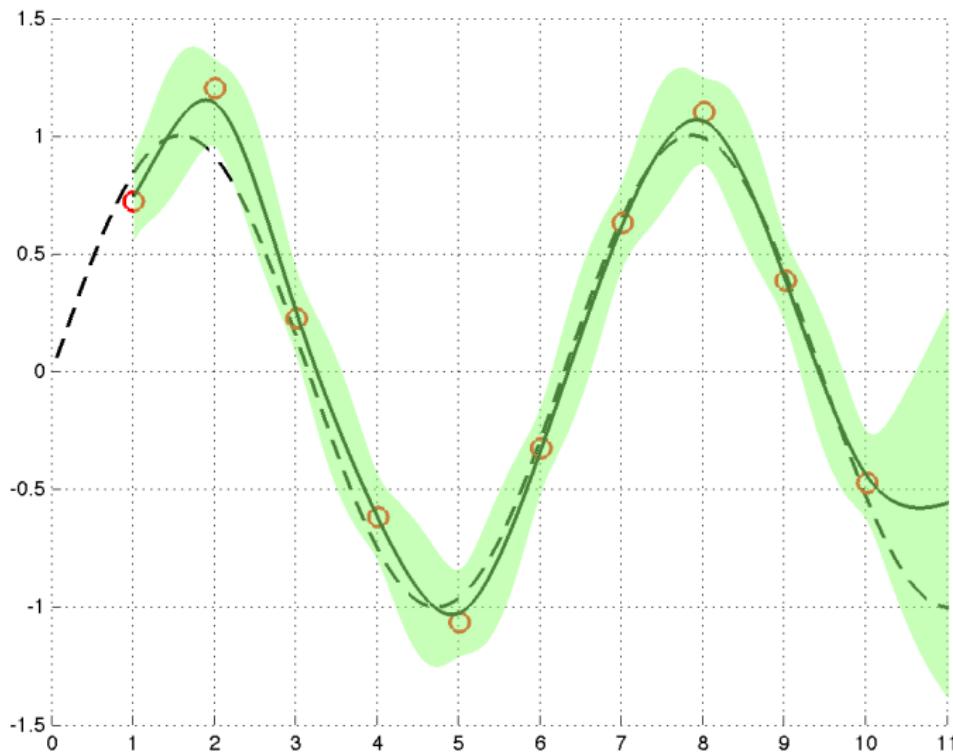
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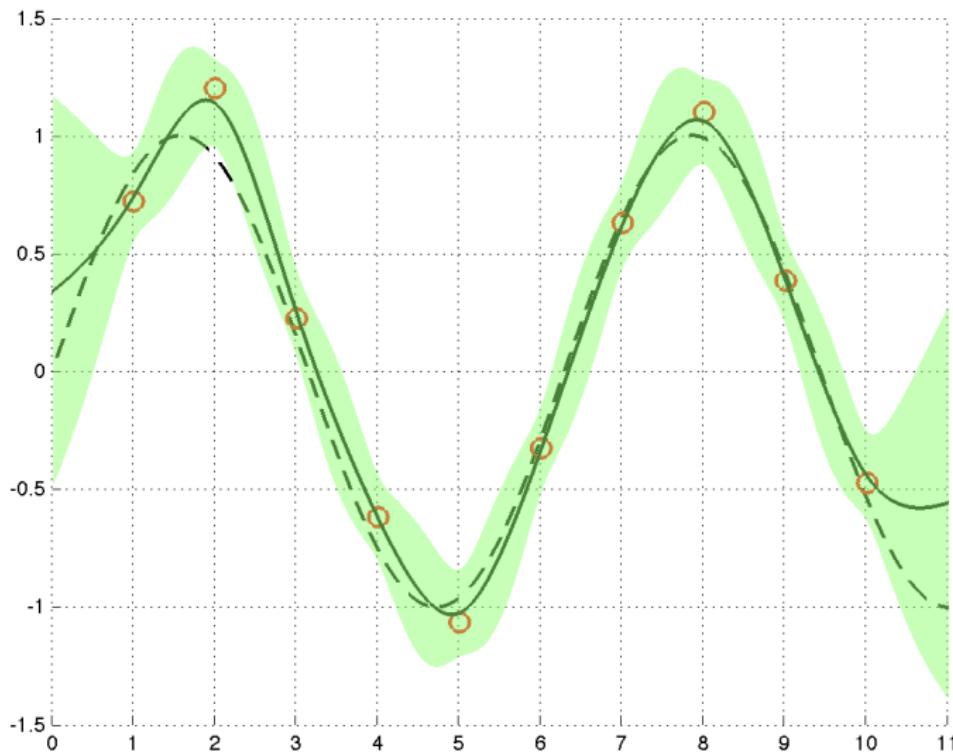
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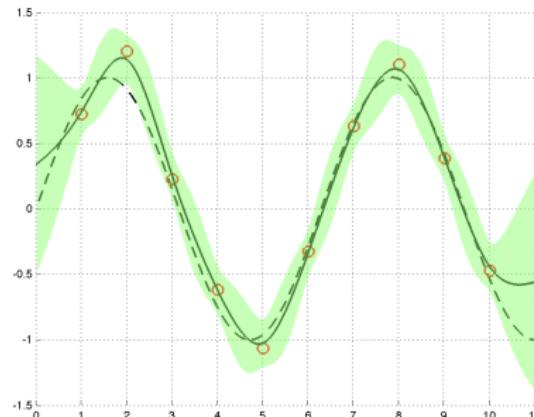
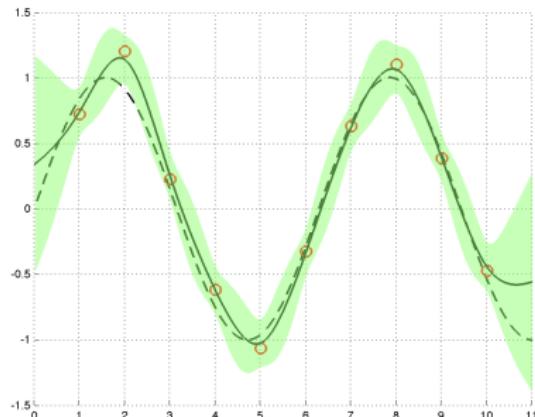


State-Space GP Regression Demo



State-Space GP Regression Demo (cont.)

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

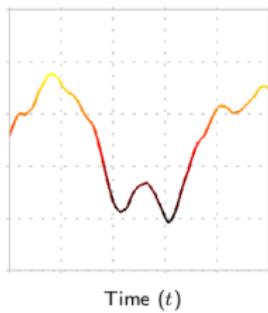


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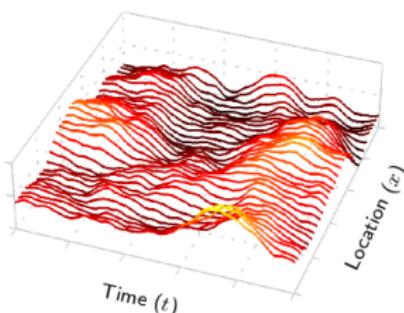
- 1 From Linear Regression to Kalman Filter and Beyond
- 2 Bayesian Filtering and Smoothing
- 3 State Space Representation of Gaussian Process Regression
- 4 Spatio-Temporal Systems, Latent Force Models and Other Extensions
- 5 Application examples
- 6 Summary

From Temporal to Spatio-Temporal Processes

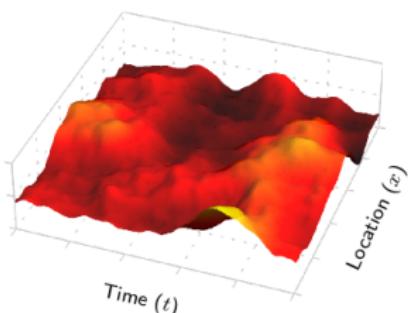
One Time Series ($n = 1$)



Multiple Time Series ($n = 34$)



Random Field ($n \rightarrow \infty$)



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

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

State Space Inference in Spatio-Temporal Processes

- Spatio-temporal GP-regression problem:

$$\mathbf{f}(\mathbf{x}, t) \sim \mathcal{GP}(0, \mathbf{K}(\mathbf{x}, \mathbf{x}'; t, t'))$$

$$\mathbf{y}_k = \mathbf{f}(\mathbf{x}_k, t_k) + \mathbf{e}_k$$

- We can convert this into infinite-dimensional state-space model with operators \mathcal{A} and \mathcal{H}_k :

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- We can use the infinite-dimensional Kalman filter and RTS smoother
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- We can approximate with PDE methods such as basis function expansions, FEM, finite-differences, spectral methods, etc.
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Example: 2D Matérn Covariance Function

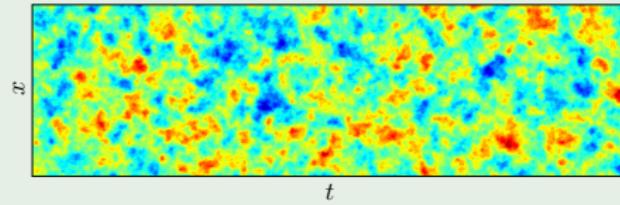
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- For example, if $\nu = 1$ and $d = 2$, we get the following:

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



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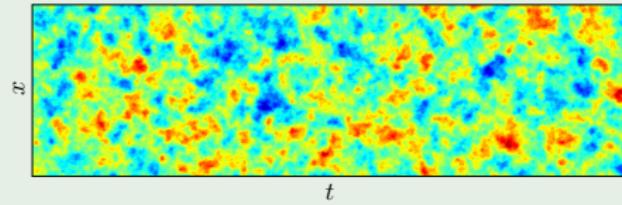
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State Space Inference in Latent Force Models

- A **latent force model** 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:

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

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

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Other Extensions

- **Change-detection** via combining state-space GPs with **switching models** and methods such as IMM or EC.
- **Distributed latent force models**, i.e., combined partial differential equation (PDE) and GP models.
- Outlier-robust GPs via **Student-t** measurement model or via classical **clutter rejection** methods.
- **Online parameter estimation** via sequential Monte Carlo, state-augmentation, online-EM, variational Bayes, and other methods.
- **Classification** corresponds to replacing the linear-Gaussian **measurement model** with a non-Gaussian one.
- **Non-linear spatio-temporal (PDE) models** via using non-linear infinite-dimensional Kalman filter and smoothers.

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GPS Satellite Orbit Prediction

- Accurate orbit prediction improves **Time To First Fix (TTFF)** when network is not available for A-GPS.
- The equation of motion for the satellite can be written as

$$\frac{d}{dt} \begin{bmatrix} \mathbf{r} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{v} \\ \mathbf{a}(\mathbf{r}, t) + \mathbf{u}(\mathbf{r}, \mathbf{v}, t) \end{bmatrix}.$$

- The **deterministic model** for acceleration is

$$\mathbf{a}(\mathbf{r}, t) = \mathbf{a}_g + \mathbf{a}_{\text{moon}} + \mathbf{a}_{\text{sun}} + \mathbf{a}_{\text{srp}}.$$

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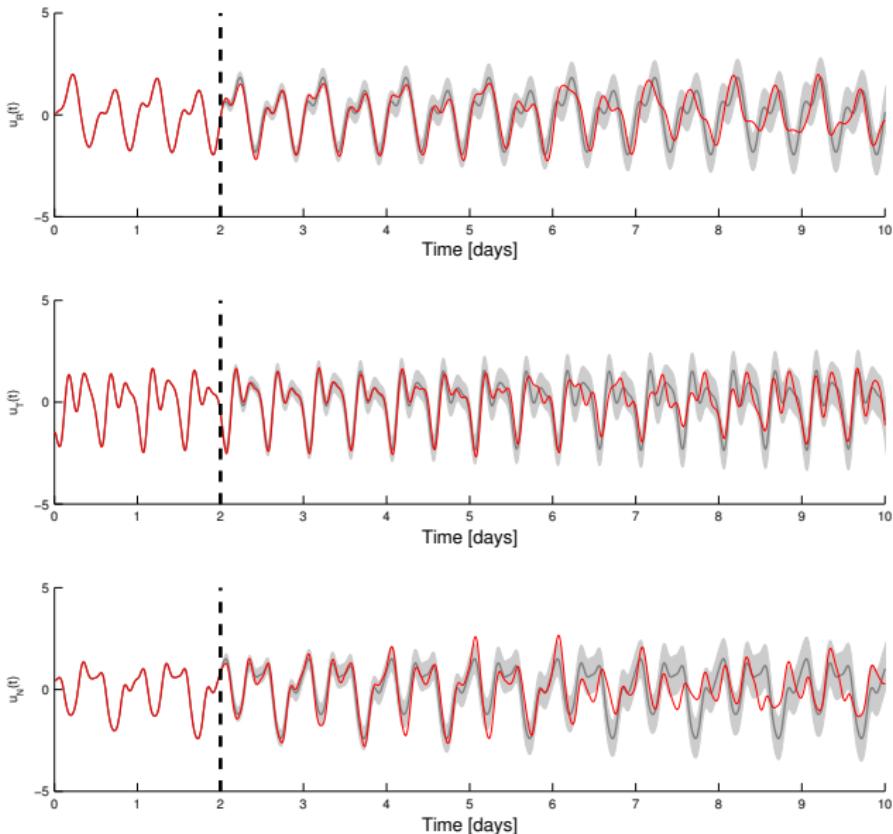
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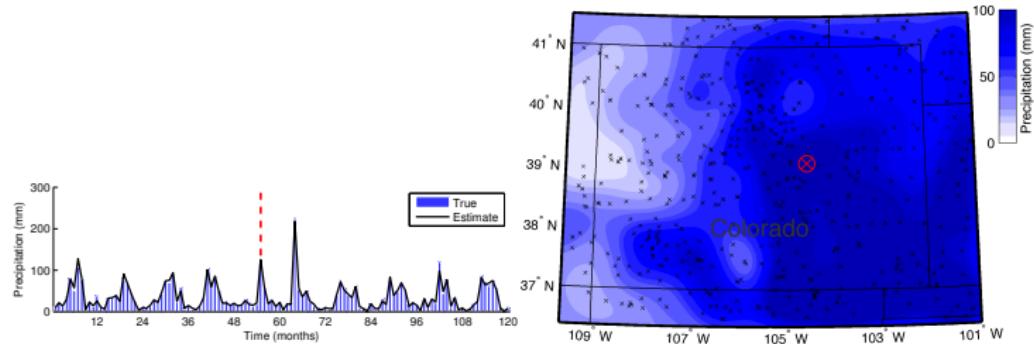
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GPS Satellite Orbit Prediction: Prediction Results

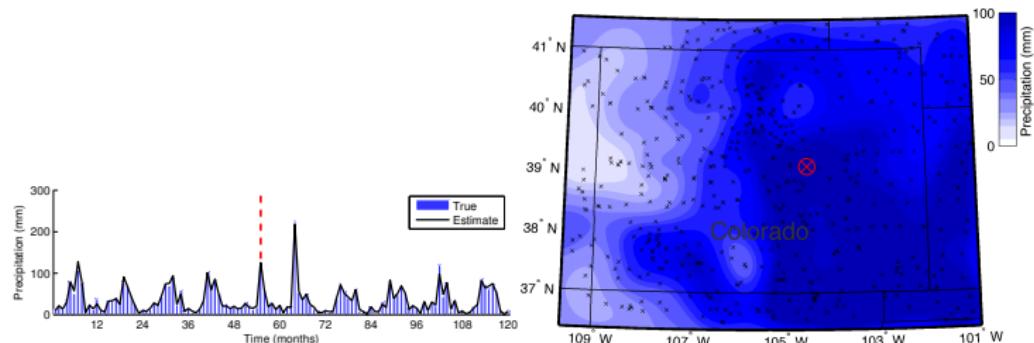


Spatio-Temporal Modeling of Precipitation



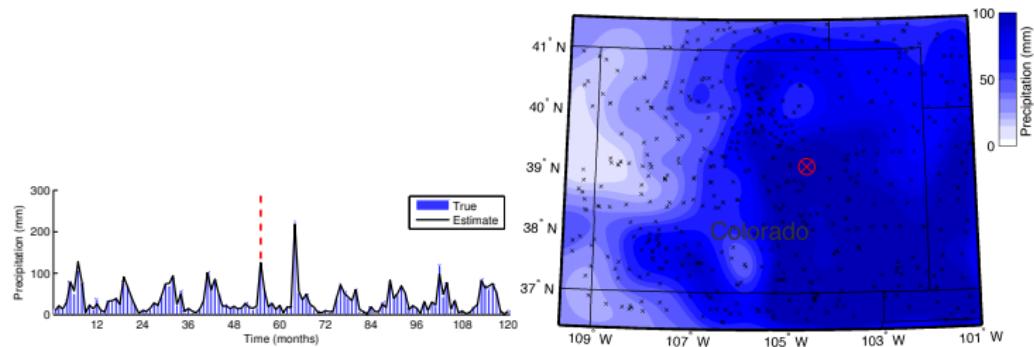
- Spatio-temporal interpolation of precipitation levels based on monthly data, years 1895–1997, Colorado, US.
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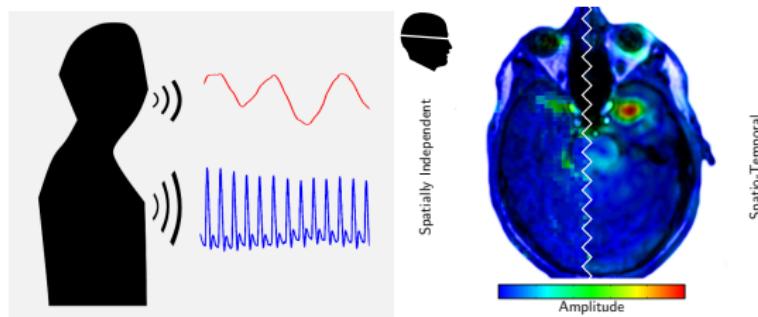
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Oscillatory Structures in fMRI Brain Data

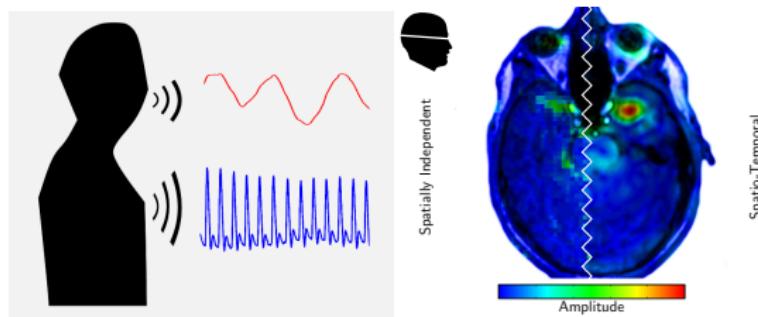


- Spatio-temporal estimation of heart beat induced oscillations in fMRI brain data (measured at AMI centre, Finland).
- Superposition of spatio-temporal oscillators (GPs as well):

$$\frac{\partial^2 f_j(\mathbf{x}, t)}{\partial t^2} + \mathcal{A}_j \frac{\partial f_j(\mathbf{x}, t)}{\partial t} + \mathcal{B}_j f_j(\mathbf{x}, t) = \xi_j(\mathbf{x}, t).$$

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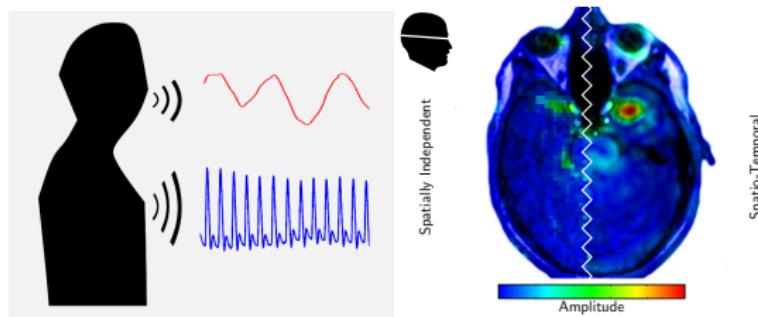


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