Inference in Time Series

Cheng Soon Ong
Marc Peter Deisenroth

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Setting

- Time-series model

$$\boldsymbol{x}_{t+1} = f(\boldsymbol{x}_t) + \boldsymbol{\epsilon}, \qquad \boldsymbol{x}_0 \sim p(\boldsymbol{x}_0), \quad \boldsymbol{\epsilon} \sim \mathcal{N}\big(\mathbf{0}, \boldsymbol{Q}\big)$$

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- Compute an expected utility of a state trajectory $\boldsymbol{\tau} := (\boldsymbol{x}_0, \ldots, \boldsymbol{x}_T)$

$$\mathbb{E}_{\boldsymbol{\tau}}[U(\boldsymbol{\tau})]$$

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  - Reinforcement learning and optimal control
  - Demand forecasting (logistics)
  - Weather/climate forecasts

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  - Reinforcement learning and optimal control
  - Demand forecasting (logistics)
  - Weather/climate forecasts

- Challenge: Long-term predictions and uncertainty propagation

Approaches

- **Deterministic inference via iterative computation**
  - Iteratively determine marginal distributions $p(\boldsymbol{x}_1), \ldots, p(\boldsymbol{x}_T)$
  - Compute expectations $\mathbb{E}_{\boldsymbol{x}_t}[u(\boldsymbol{x}_t)]$ and compute utilities of the form

$$\mathbb{E}_{\boldsymbol{\tau}}[U(\boldsymbol{\tau})] = \sum_{t=0}^{T} \mathbb{E}_{\boldsymbol{x}_t}[u(\boldsymbol{x}_t)] = \sum_{t=0}^{T} \int u(\boldsymbol{x}_t) p(\boldsymbol{x}_t) d\boldsymbol{x}_t$$

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- **Stochastic inference via trajectory sampling**
  - Generate sample trajectories $\boldsymbol{\tau}^{(s)} = (\boldsymbol{x}_0^{(s)}, \ldots, \boldsymbol{x}_T^{(s)})$
  - Monte-Carlo integration

$$\mathbb{E}_{\boldsymbol{\tau}}[U(\boldsymbol{\tau})] \approx \frac{1}{S} \sum_{s=1}^{S} U(\boldsymbol{\tau}^{(s)})$$

Deterministic Approximate Inference

Deterministic approximate inference

- Iteratively compute marginals

$$p(\boldsymbol{x}_{t+1}) = \int p(\boldsymbol{x}_{t+1}|\boldsymbol{x}_t)p(\boldsymbol{x}_t)d\boldsymbol{x}_t$$

$$= \int \mathcal{N}\big(f(\boldsymbol{x}_t),\, \boldsymbol{Q}\big)p(\boldsymbol{x}_t)d\boldsymbol{x}_t$$

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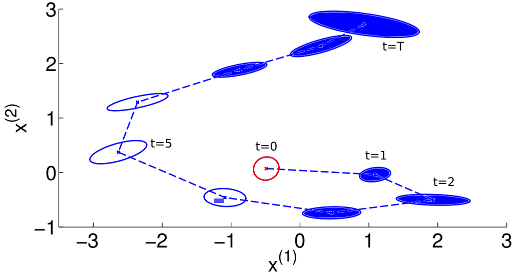
No closed-form solution for nonlinear f

Iterative Gaussian approximation

- Common approach: Iterative Gaussian approximation of marginals:

$$p(\boldsymbol{x}_t) \approx \mathcal{N}\big(\boldsymbol{\mu}_t,\, \Sigma_t\big)$$



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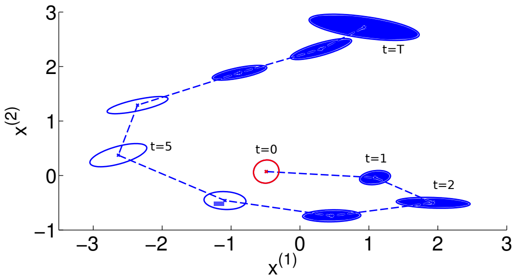

- **Linearization**

⏩ Extended Kalman filter

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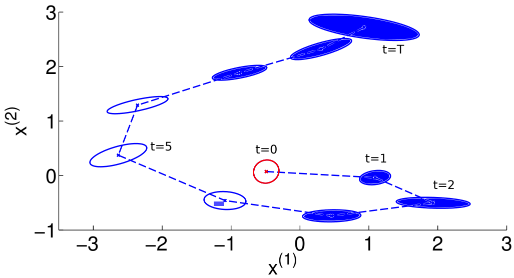

- **Linearization** ⏩ Extended Kalman filter
- **Unscented transformation** ⏩ Unscented Kalman filter

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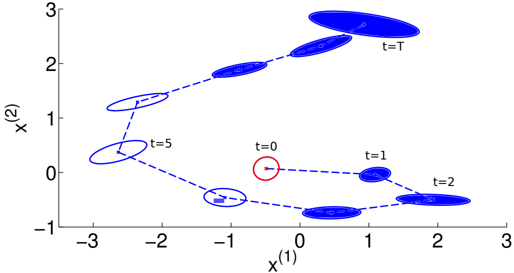

- **Linearization** ⏩ Extended Kalman filter
- **Unscented transformation** ⏩ Unscented Kalman filter
- **Moment matching** ⏩ Assumed density filter

Two approaches

$$p(\boldsymbol{x}_{t+1}) = \int \mathcal{N}\left(\boldsymbol{x}_{t+1} \middle| f(\boldsymbol{x}_t), \boldsymbol{Q}\right) p(\boldsymbol{x}_t) d\boldsymbol{x}_t \approx \mathcal{N}\left(\boldsymbol{x}_{t+1} \middle| \boldsymbol{\mu}_{t+1}, \boldsymbol{\Sigma}_{t+1}\right)$$

Two approaches

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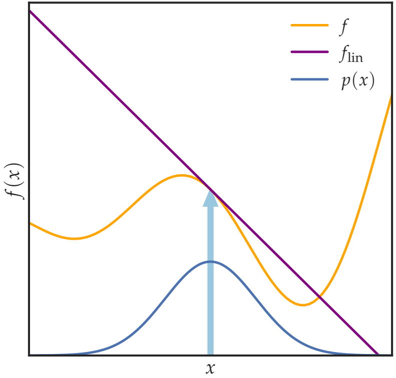
- Approximate f ⏩ Linearization (e.g., Smith et al., 1962)
- Approximate $p(\boldsymbol{x}_t)$ ⏩ Unscented transformation (Julier & Uhlmann, 1995)

Approach 1: Linearization

Key idea (e.g., Smith et al., 1962; Ohab & Stubberud, 1965)

1. Locally linearize f around mean $\boldsymbol{\mu}_t$
2. Compute predictive distribution (Gaussian) for linearized function in closed form



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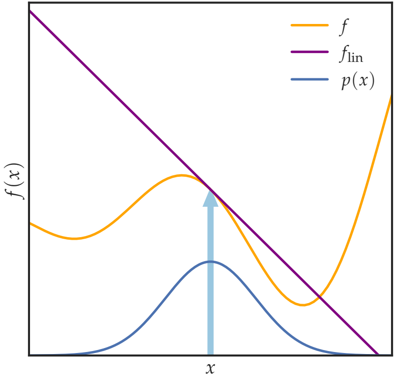
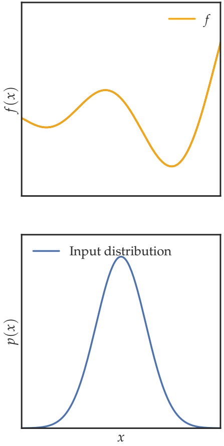


- Linearization: First-order Taylor-series expansion around $\boldsymbol{\mu}_t$
  - Gradient (Jacobian) $df/d\boldsymbol{x}_t$ of f evaluated at $\boldsymbol{\mu}_t$
- Key insight: Gaussians can be pushed through linear functions in closed form

How it works

- Compute gradient $\boldsymbol{J}_t := df/d\boldsymbol{x}_t|_{\boldsymbol{x}_t=\boldsymbol{\mu}_t}$



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- Compute gradient $\boldsymbol{J}_t := df/d\boldsymbol{x}_t|_{\boldsymbol{x}_t=\boldsymbol{\mu}_t}$
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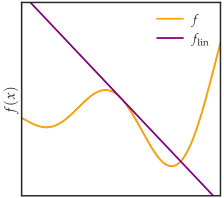
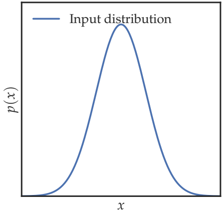
$$f(\boldsymbol{x}) \approx f(\boldsymbol{\mu}_t) + \boldsymbol{J}_t(\boldsymbol{x} - \boldsymbol{\mu}_t)$$





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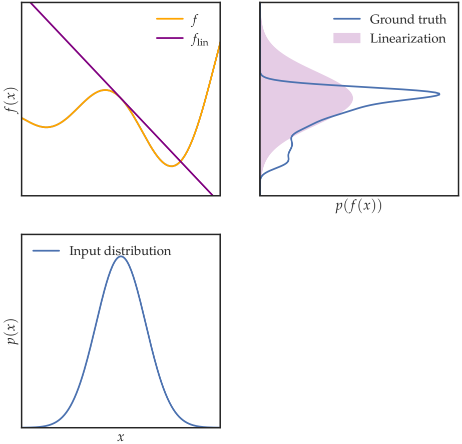
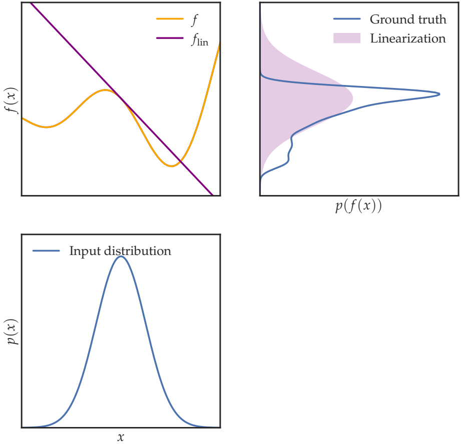
- Approximate predictive distribution is Gaussian:

$$p(f(\boldsymbol{x}_t)) \approx \mathcal{N}\left(f(\boldsymbol{\mu}_t),\ \boldsymbol{J}_t\boldsymbol{\Sigma}_t\boldsymbol{J}_t^\top\right)$$
$$p(\boldsymbol{x}_{t+1}) \approx \mathcal{N}\left(f(\boldsymbol{\mu}_t),\ \boldsymbol{J}_t\boldsymbol{\Sigma}_t\boldsymbol{J}_t^\top + \boldsymbol{Q}\right)$$



Linearization: Properties

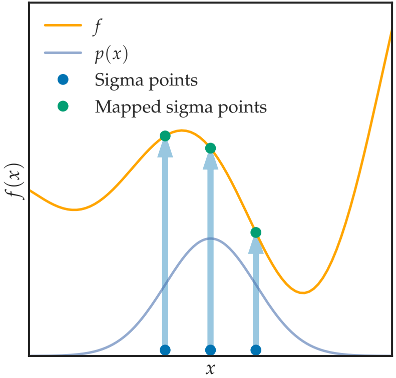
- Conceptually straightforward
- Requires differentiable f
- Tends to underestimate true covariance matrix ⏩ Overconfidence
- Scales cubically in the dimension of $\boldsymbol{x}$
- Widely used in engineering
  (e.g., navigation systems, GPS, Apollo missions)



Approach 2: Unscented transformation

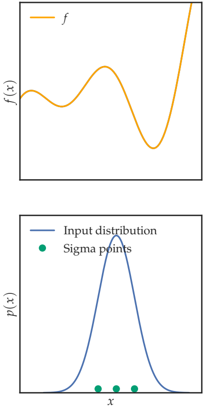
Key idea (Julier & Uhlmann, 1995)

1. Approximate $p(\boldsymbol{x}_t)$ using a small set of deterministically chosen sigma points
2. Map sigma points through f
3. Compute a weighted average of the mean and covariance of the predictive distribution.



How it works

- Determine $2D+1$ sigma points
  $\mathcal{X}_t = \{\boldsymbol{\mu}_t \pm \alpha\left(\sqrt{\boldsymbol{\Sigma}_t}\right)_i, \; i = 1, \ldots, D\}$



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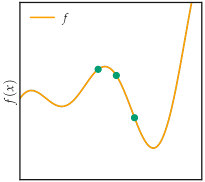

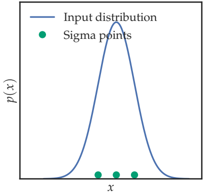

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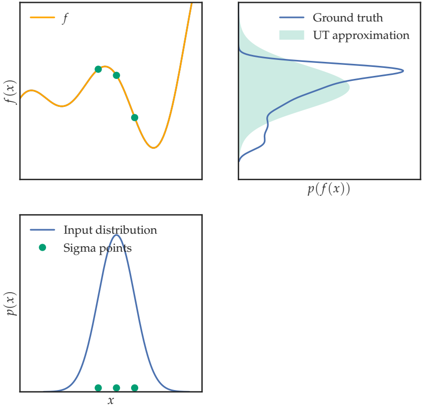
- Map sigma points through f to get $f(\mathcal{X}_t)$
- Compute mean/covariance of predictive distribution $p(f(\boldsymbol{x}_t))$ as a weighted average

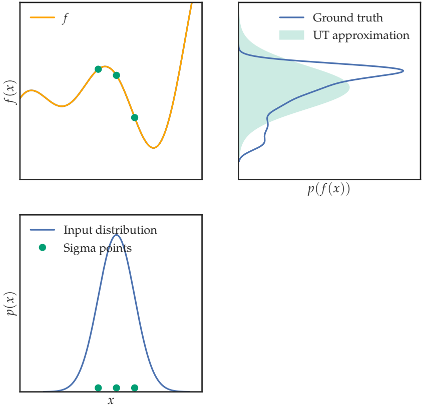
$$\boldsymbol{\mu}_{t+1} \approx \sum_{d=1}^{2D+1} w_d^{\mu} f(\mathcal{X}_t^{(d)})$$

$$\boldsymbol{\Sigma}_{t+1} \approx \sum_{d=1}^{2D+1} w_d^{\Sigma} \big(f(\mathcal{X}_t^{(d)}) - \boldsymbol{\mu}_{t+1}\big)\big(f(\mathcal{X}_t^{(d)}) - \boldsymbol{\mu}_{t+1}\big)^\top$$



Unscented transformation: Properties

- Not a Monte-Carlo method: Sigma points are deterministic, not random
- No explicit calculation of Jacobians
  ⏩ f can be non-differentiable
- Input distribution does not need to be Gaussian
- Higher accuracy (covariance) than linearization (Julier & Uhlmann, 2004)



Stochastic Approximate Inference

Stochastic approximate inference

- Sample trajectories $\boldsymbol{\tau}^{(i)} = \left(\boldsymbol{x}_0^{(i)}, \dots, \boldsymbol{x}_T^{(i)}\right)$:
  1. Sample initial state: $\boldsymbol{x}_0^{(i)} \sim p(\boldsymbol{x}_0)$
  2. For $t = 1, \dots, T$:

$$\boldsymbol{x}_t^{(i)} \sim p(\boldsymbol{x}_t | \boldsymbol{x}_{t-1}^{(i)}) = \mathcal{N}\left(\boldsymbol{x}_t \middle| f(\boldsymbol{x}_{t-1}^{(i)}), \boldsymbol{Q}\right)$$

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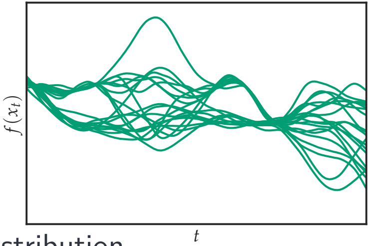
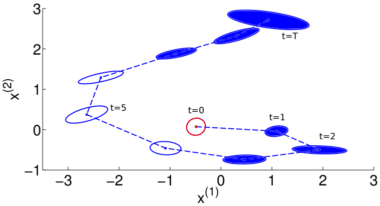
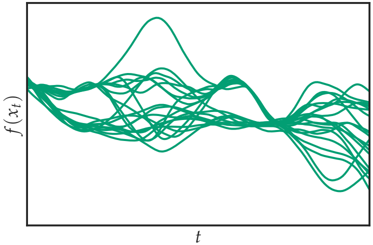


- No parametric restriction to a specific kind of distribution
- Have to store all samples (particles) ⏩ Potential memory issue
- Sequential Monte Carlo (particle filter)
  (e.g., Doucet et al., 2000; Thrun et al., 2005;)

Discussion: Long-term predictions

	Deterministic	Stochastic
Density representation	Parametric	Particles
Bias	Yes	No
Time correlation	No	Yes
Speed	Fast	(Slow)
Parallelization		Easy
Memory consumption	Low	(High)
Gradients	Deterministic	Stochastic





Inference in Gaussian Process Time Series Models

Setting

- Time-series model

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Setting

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$$x_{t+1} = f(x_t) + \epsilon, \qquad x_0 \sim p(x_0), \quad \epsilon \sim \mathcal{N}(\mathbf{0}, \boldsymbol{Q}), \quad f \sim GP(\mu, k)$$

- Two approaches for long-term predictions:
  - Deterministic approximate inference of the marginals $p(\boldsymbol{x}_1), \ldots, p(\boldsymbol{x}_T)$
  - Stochastic approximate inference by sampling trajectories $\boldsymbol{\tau}^{(i)} = (\boldsymbol{x}_0^{(i)}, \ldots, \boldsymbol{x}_T^{(i)})$

Deterministic approximate inference

$$p(\boldsymbol{x}_{t+1}) = \int p(\boldsymbol{x}_{t+1}|\boldsymbol{x}_t)p(\boldsymbol{x}_t)d\boldsymbol{x}_t$$

Deterministic approximate inference

$$\begin{aligned} p(\boldsymbol{x}_{t+1}) &= \int p(\boldsymbol{x}_{t+1}|\boldsymbol{x}_t)p(\boldsymbol{x}_t)d\boldsymbol{x}_t \\ &= \int \int p(f(\boldsymbol{x}_t)|f, \boldsymbol{x}_t)p(f)df\, p(\boldsymbol{x}_t)d\boldsymbol{x}_t \end{aligned}$$

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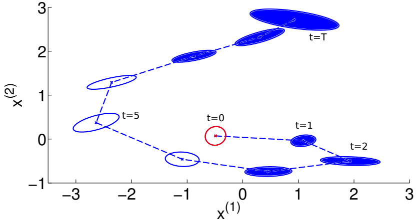
Approaches:

- Linearization (e.g., Ko & Fox, 2009)
- Unscented transformation (e.g., Ko & Fox, 2009)
- Moment matching (e.g., Deisenroth et al., 2009)

Long-term predictions

- Iteratively compute $p(\boldsymbol{x}_1), \dots, p(\boldsymbol{x}_T)$



Long-term predictions

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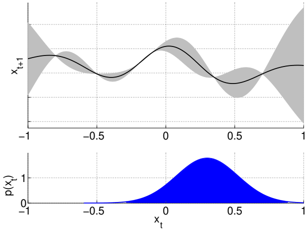
$$\underbrace{p(\boldsymbol{x}_{t+1}|\boldsymbol{x}_t)}_{\text{GP prediction}} \underbrace{p(\boldsymbol{x}_t)}_{\mathcal{N}(\boldsymbol{\mu}_t, \boldsymbol{\Sigma}_t)}$$



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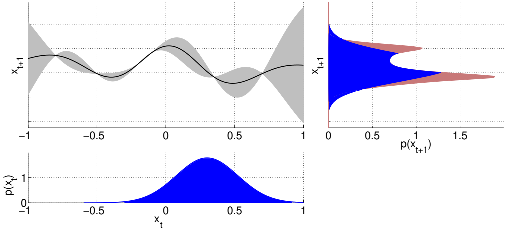

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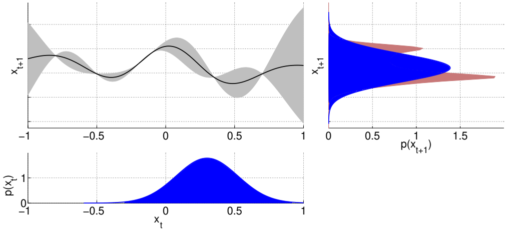
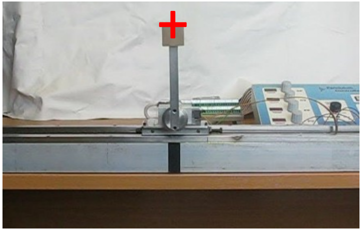


  - GP moment matching (Girard et al., 2003; Quiñonero-Candela et al., 2003)
  - Key ingredient: Computing kernel expectations

Example: Model-based reinforcement learning

- Learn dynamics of a physical system from data ⏩ Gaussian process

$$\boldsymbol{x}_{t+1} = f(\boldsymbol{x}_t, \boldsymbol{u}_t) + \boldsymbol{\epsilon}, \quad f \sim GP$$
$$\boldsymbol{u}_t = \pi(\boldsymbol{x}_t; \boldsymbol{\theta})$$



From Deisenroth & Rasmussen (2011)
https://www.youtube.com/PilcoLearner

Example: Model-based reinforcement learning

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- Given the learned system, find policy parameters $\boldsymbol{\theta}^*$ that minimize an expected long-term cost

$$\mathbb{E}_{\boldsymbol{\tau}}[U(\boldsymbol{\tau})] = \sum_{t=1}^{T} \mathbb{E}_{\boldsymbol{x}_t}[c(\boldsymbol{x}_t)]$$

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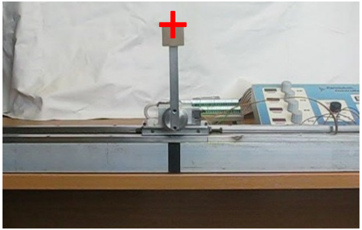

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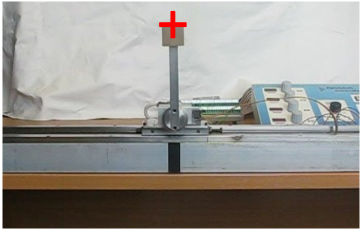

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- GP moment matching for long-term predictions
- Gradient descent to find $\boldsymbol{\theta}^*$

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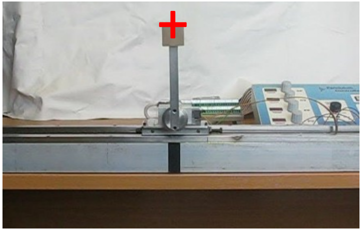

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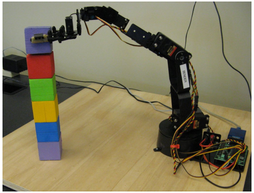
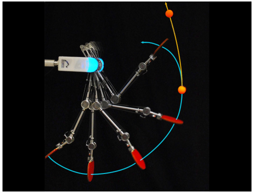
https://www.youtube.com/PilcoLearner

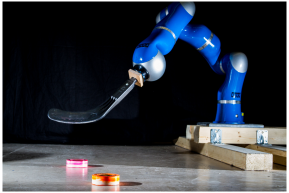
Wide Applicability



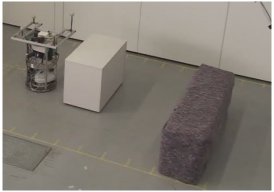
Deisenroth et al. (2011)



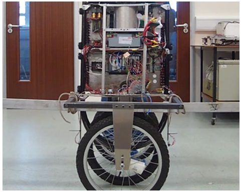
Englert et al. (2013)



Kupcsik et al. (2017)



Bischoff et al. (2013b)



McHutchon (2014)

Bischoff et al. (2013a)

▶▶▶ Application to a wide range of robotic systems

Stochastic approximate inference

- Generating a function draw: Sampling from a T-dimensional multivariate Gaussian
  T: Number of query points

Figure: Generated with GPflow (Matthews et al., 2017)

Stochastic approximate inference

- Generating a function draw: Sampling from a T-dimensional multivariate Gaussian
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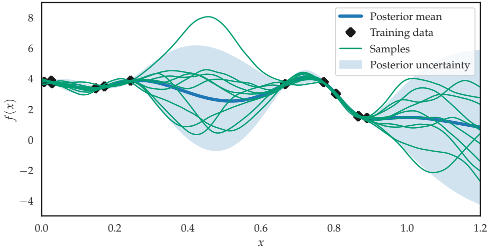
- Drawing a sample from a GP **scales cubically in T**



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Stochastic approximate inference

- Generating a function draw: Sampling from a T-dimensional multivariate Gaussian
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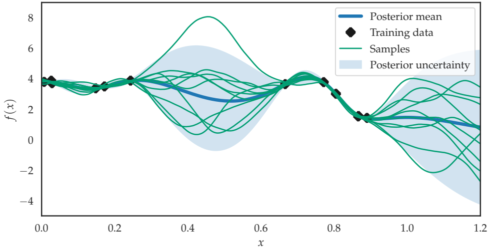

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Stochastic approximate inference

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  - Let's try something else

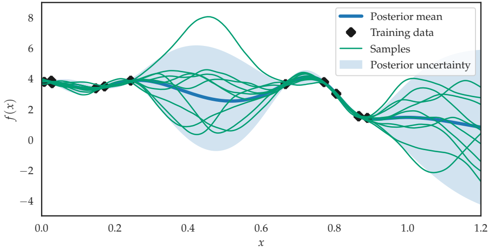

Figure: Generated with GPflow (Matthews et al., 2017)

Decoupled sampling (Wilson et *a*l., 2020*a*)

Key idea

Sample functions from a Gaussian process by exploiting **Matheron's rule** (for Gaussian random variables):

$$\text{posterior} = \text{prior} + \text{data-dependent update}$$

Decoupled sampling (Wilson et al., 2020*a*)

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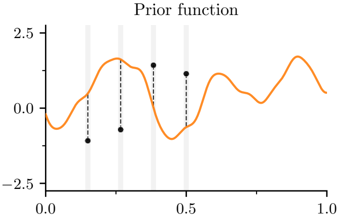
Key idea

Sample functions from a Gaussian process by exploiting **Matheron's rule** (for Gaussian random variables):

$$\text{posterior} = \text{prior} + \text{data-dependent update}$$

- Think about the posterior in terms of samples, not in terms of (conditional) distributions
- Samples from the posterior can be obtained through a two-step procedure:
  1. Sample from prior ⏩ Source of randomness
  2. "Correct" sample using a data-dependent update term
     ⏩ Deterministic transformation

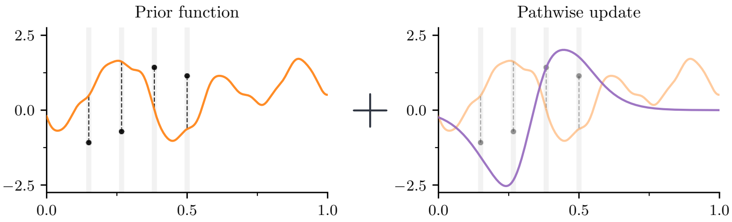
Illustration: Decoupled sampling (Wilson et al., 2020*a*)



$$\underbrace{f^{(s)}(\cdot)}_{\text{sample from prior}}$$

1. Sample from the prior

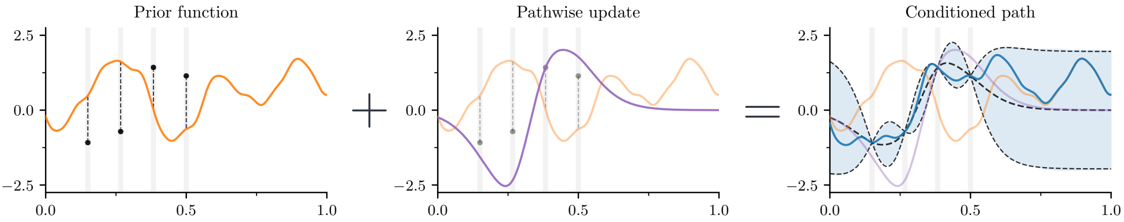
Illustration: Decoupled sampling (Wilson et al., 2020*a*)



$$\underbrace{f^{(s)}(\cdot)}_{\text{sample from prior}} + \underbrace{k(\cdot, \boldsymbol{X})\boldsymbol{K}^{-1}(\boldsymbol{y} - f^{(s)}(\boldsymbol{X}))}_{\text{data-dependent update}}$$

1. Sample from the prior
2. Add data-dependent update term

Illustration: Decoupled sampling (Wilson et al., 2020a)



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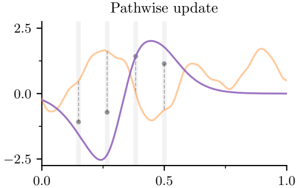
Sample from the posterior

Properties

$$\underbrace{f^{(s)}(\cdot)}_{\text{sample from prior}} + \underbrace{k(\cdot, \boldsymbol{X})\boldsymbol{K}^{-1}(\boldsymbol{y} - f^{(s)}(\boldsymbol{X}))}_{\text{data-dependent update}} = \underbrace{f^{(s)}(\cdot)|\boldsymbol{X}, \boldsymbol{y}}_{\text{sample from posterior}}$$



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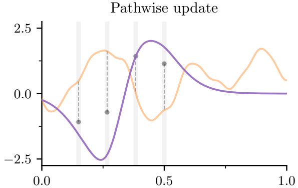

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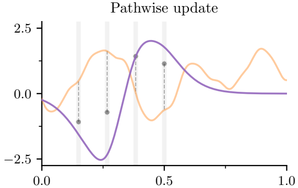

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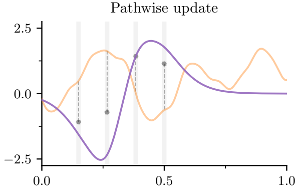

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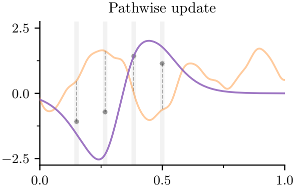

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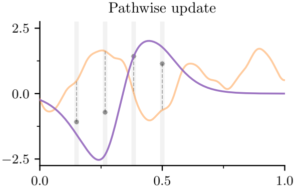

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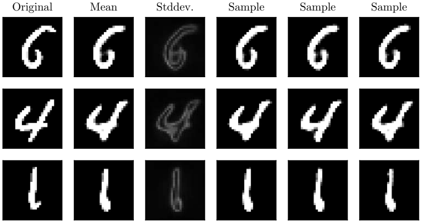
  - Update term can be computed linearly in the number T of test inputs
- **Functions can be sampled efficiently** (linearly in the number of test inputs)

Applications

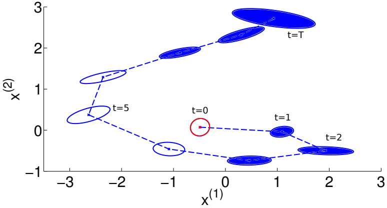


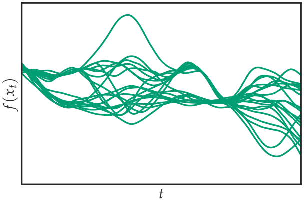
From Wilson et al. (2020b)

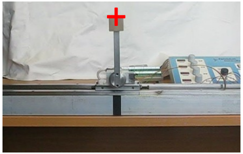
From Borovitskiy et al. (2020)

- Deep convolutional GP auto-encoders (Wilson et al., 2020b)
- Bayesian optimization with Thompson sampling (Wilson et al., 2020a)
- Sampling from GPs on manifolds (Borovitskiy et al., 2020)
- Model-based reinforcement learning

Summary







- Propagate uncertainty through a nonlinear dynamical system
- Deterministic approximate inference (linearization, unscented transformation)
- Stochastic approximate inference (sampling)
- Examples in the context of GP dynamical systems

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