Aalto University

Approximations to the solution of the Kushner-Stratonovich equation for the stochastic chemostat

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Outline

The stochastic chemostat

Prior knowledge: the Kolmogorov forward equation

Posterior knowledge: the Kushner-Stratonovich equation

Approximations to the solution of the Kushner-Stratonovich equation

$$\kappa s \Longrightarrow b + \gamma CH_4$$

Goal

$$\kappa s \Longrightarrow b + \gamma \mathrm{CH}_4$$

We want to estimate concentrations of substrate s and biomass b.

The chemostat

- $b(t)$: concentration of biomass at time t
- $s(t)$: concentration of substrate at time t
- D : dilution rate
- s_{in} : incoming concentration of substrate
- $\mu(\cdot)$: specific growth function (assumption: $s \mapsto \mu(s)$)

$$d\begin{bmatrix} b(t) \\ s(t) \end{bmatrix} = \begin{bmatrix} (\mu(\cdot) - D)b(t) \\ D(s_{in} - s(t)) - \kappa\mu(\cdot)b(t) \end{bmatrix} dt, \qquad \begin{bmatrix} b(0) \\ s(0) \end{bmatrix} = \begin{bmatrix} b_0 \\ s_0 \end{bmatrix}.$$

The chemostat

- $b(t)$: concentration of biomass at time t
- $s(t)$: concentration of substrate at time t
- D : dilution rate
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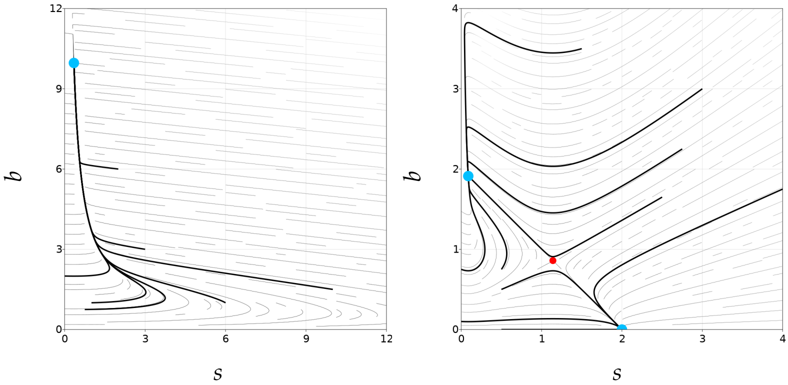
$$\underbrace{d\begin{bmatrix} b(t) \\ s(t) \end{bmatrix}}_{x(t)} = \underbrace{\begin{bmatrix} (\mu(\cdot) - D)b(t) \\ D(s_{in} - s(t)) - \kappa\mu(\cdot)b(t) \end{bmatrix}}_{f(t,x(t))} dt, \qquad \underbrace{\begin{bmatrix} b(0) \\ s(0) \end{bmatrix}}_{x(0)} = \underbrace{\begin{bmatrix} b_0 \\ s_0 \end{bmatrix}}_{x_0}.$$

Given x_0 at $t = 0$, we know $x(t)$ for all $t > 0$.

The chemostat



(a) Monod growth (b) Haldane growth

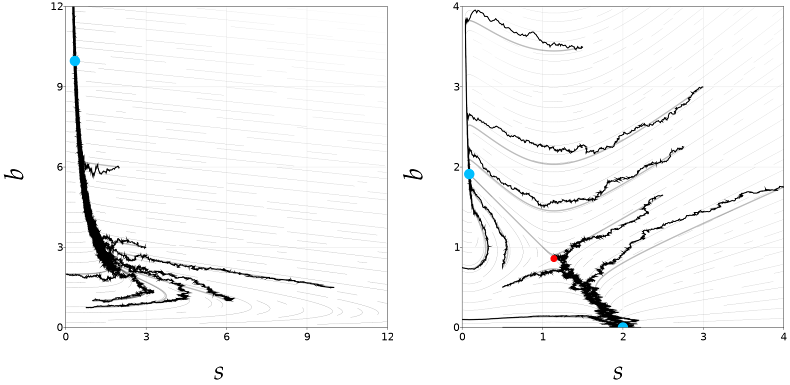
(●) stable steady states (●) unstable steady state.

The stochastic chemostat

The stochastic chemostat

$$\underbrace{d\begin{bmatrix} b_t \\ s_t \end{bmatrix}}_{X_t} = \underbrace{\begin{bmatrix} (\mu(s_t) - D)b_t \\ D(s_{in} - s_t) - \kappa\mu(s_t)b_t \end{bmatrix}}_{f(t,X_t)} dt + \underbrace{\begin{bmatrix} \omega_b b_t & 0 \\ 0 & \omega_s s_t \end{bmatrix}}_{g(t,X_t)} d\underbrace{\begin{bmatrix} B_t^b \\ B_t^s \end{bmatrix}}_{B_t^x},$$

with initial condition $x_0 = (b_0, s_0)^\top$, $x_0 \sim \pi_{X_0}$.



(a) Monod growth (b) Haldane growth

(●) stable steady states. (●) unstable steady state.

Prior knowledge: the Kolmogorov forward equation

The Kolmogorov forward equation

Sample infinitely many paths X_t from

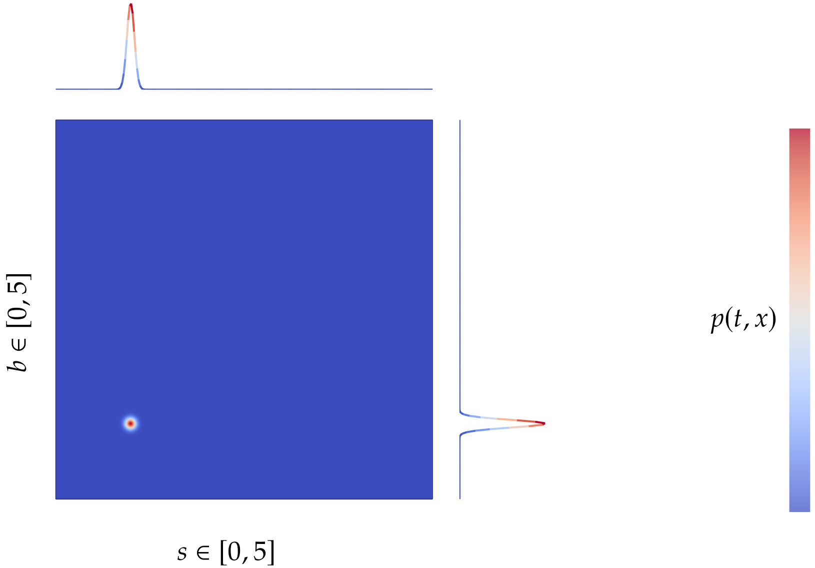
$$dX_t \quad = \quad f(t, X_t)dt + g(t, X_t)dB_t^x, \quad \text{with initial condition } X_0.$$

$$\sim$$

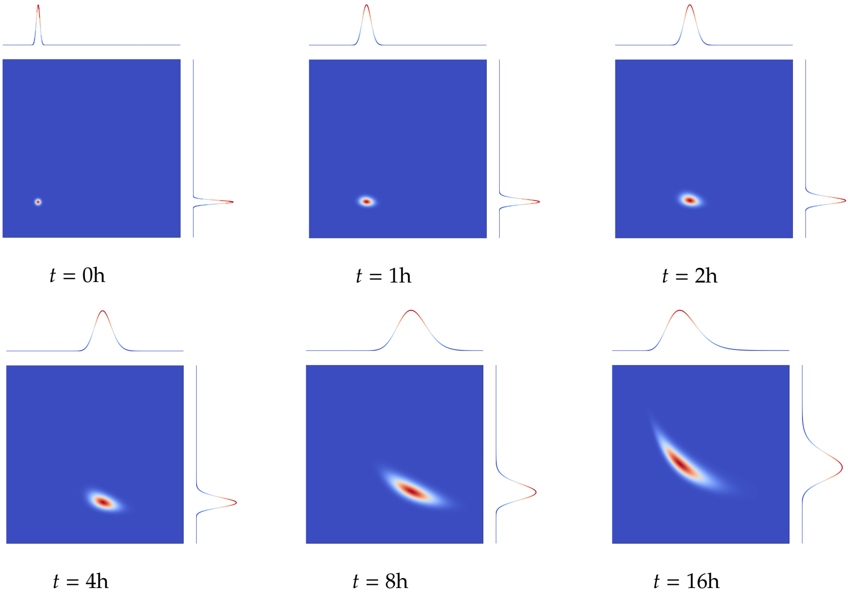
Solve the following partial differential equation:

$$\frac{\partial}{\partial t}p(t,x) = -\sum_{d_x=1}^{2} \frac{\partial}{\partial x_{d_x}}[f_{d_x}(t,x)p(t,x)] + \sum_{d_x=1}^{2}\sum_{d'_x=1}^{2} \frac{\partial^2}{\partial x_{d_x}\partial x_{d'_x}}[G_{d_x d'_x}(t,x)p(t,x)],$$

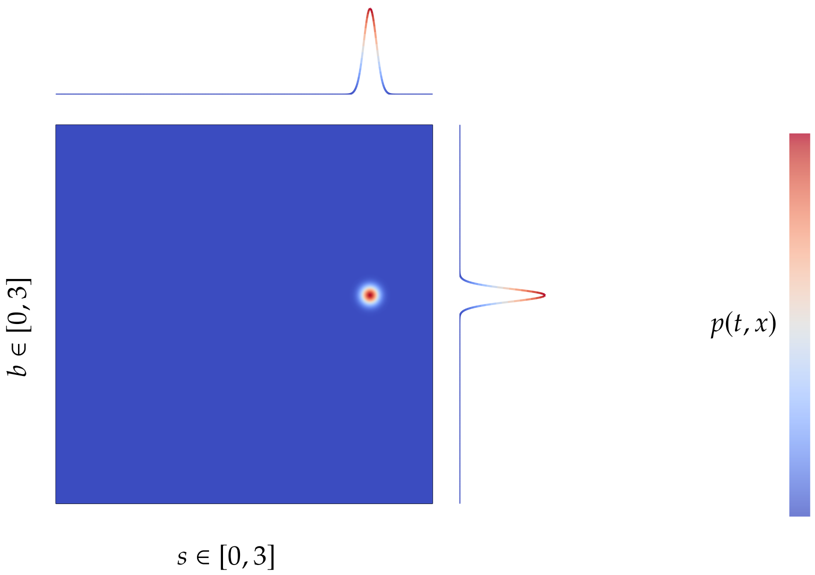
with diffusion terms $G_{d_x d'_x}(t,x) = \frac{1}{2}\sum_{m=1}^{2} g_{d_x m}(t,x) g_{d'_x m}(t,x)$ and initial condition $p(0,x)$.



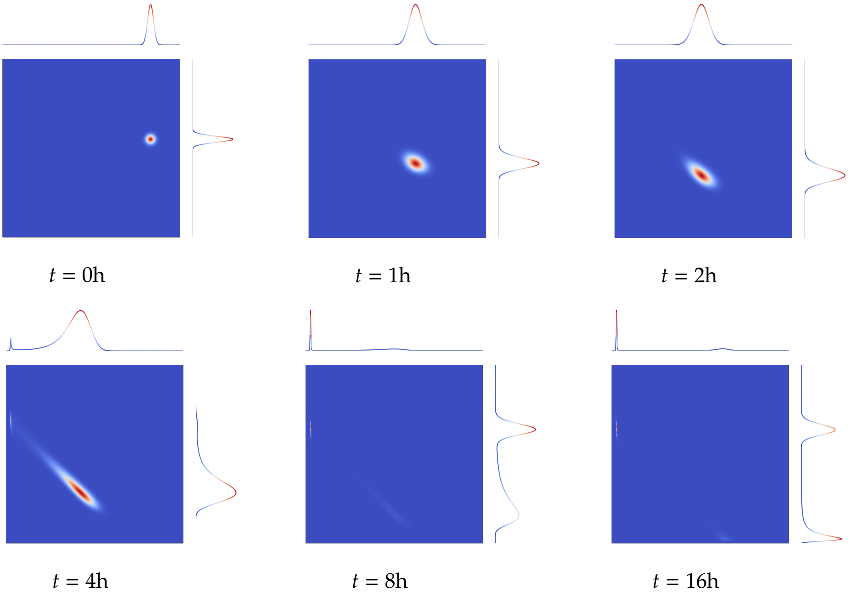
Initial condition for the Kolmogorov forward equation with Monod growth kinetics.



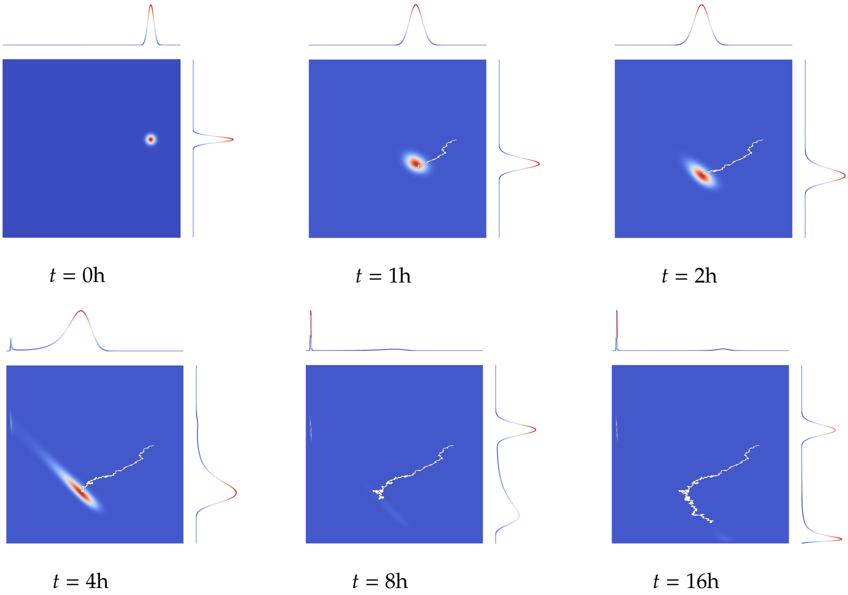
Solution to the Kolmogorov forward equation with Monod growth kinetics.



Initial condition for the Kolmogorov forward equation with Haldane growth kinetics.



Solution to the Kolmogorov forward equation with Haldane growth kinetics.



However, we are interested in estimating one possible realization of the system!

Posterior knowledge: the Kushner-Stratonovich equation

Observations

$$y_{t_i} \quad = \quad h(t_i, X_{t_i}) + \text{noise}, \qquad i = 1, 2, \ldots$$

We work with the integrated process Y_t instead of y_{t_i}. For example:

- Measurements corrupted by Gaussian noise:

$$dY_t \quad = \quad h(t, X_t)dt + k(t)dB_t^y, \qquad Y_0 = 0$$

- Measurements coming in the form of a series of events:

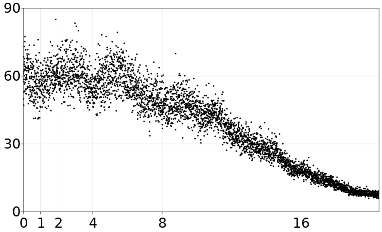
$$dY_t \quad \sim \quad \text{Poisson}(\, h(t, X_t)dt \,), \qquad Y_0 = 0$$

Observation function $h(t, X_t)$

$$\kappa s \Longrightarrow b + \gamma \mathrm{CH}_4$$

- Let Q denote the flow rate of biogas production;
- The flow rate is proportional to the microbial activity,

$$Q(s(t), b(t)) = \gamma \mu(s(t)) b(t).$$



Time (h)

We choose the following model:

$$dY_t = \underbrace{\left[\log Q(s(t), b(t))\right]}_{h(t, X_t)} dt + \underbrace{\left[\omega_y\right]}_{k(t)} d\left[B_t^y\right].$$

Objective | Dynamics + Measurements

We started with the density of the distribution of X_t given an initial condition X_0,

$$p(t, x \,|\, X_0).$$

We now want the density of the distribution of X_t given an initial condition X_0 and some information F^y_τ from measurements up to time t,

$$p(t, x \,|\, X_0, F^y_{\tau \leq t}).$$

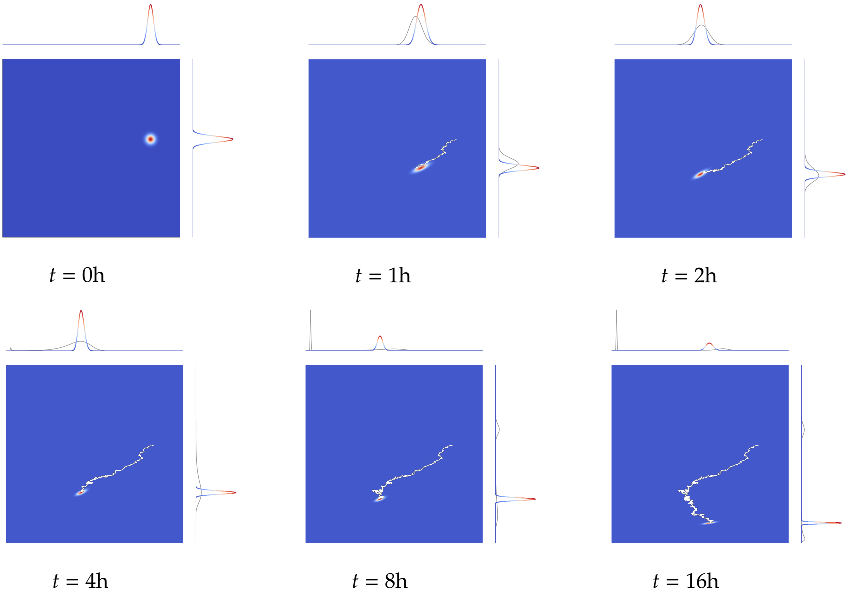
We use the measurements of biogas flow rate to refine our knowledge about the state variables $(b(t), s(t))$.

The Kushner-Stratonovich equation (KSE)

$$\frac{\partial}{\partial t} p_t = -\sum_{d_x=1}^{2} \frac{\partial}{\partial x_{d_x}} [f_{d_x}(t,x) p_t] + \sum_{d_x=1}^{2} \sum_{d'_x=1}^{2} \frac{\partial^2}{\partial x_{d_x} \partial x_{d'_x}} [G_{d_x d'_x}(t,x) p_t]$$
$$+ p_t \times \{h(t,x) - \mathbb{E}_t[h(t,x)]\}^\top \times \left\{((k^2(t))^{-1}(dY_t - \mathbb{E}_t[h(t,x)]\, dt)\right\}.$$

- Posterior density: $p_t \overset{def.}{=} p(t, x \mid X_0, F^y_\tau)$;
- Measurement process: dY_t;
- Nonlinear terms $p_t \times \mathbb{E}_t[h(t,x)]$, where $\mathbb{E}_t[h(t,x)] = \int h(t,x) p_t \, dx$.

$$dX_t = f(t, X_t)dt + g(t, X_t)dB^x_t$$
$$dY_t = h(t, X_t)dt + k(t)dB^y_t$$

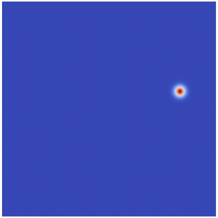


Solution to the Kushner-Stratonovich equation with Haldane growth kinetics.

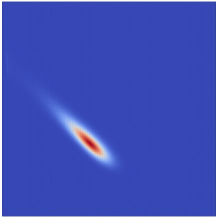
Approximations to the solution of the Kushner-Stratonovich equation

Methods for Partial Differential Equations

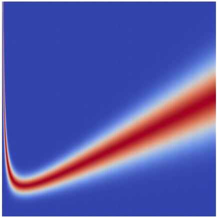
- Idea
  (step 1) solve the Kolmogorov forward equation (KFE)
  (step 2) update the result with the likelihood
- Examples
  1. Upwind-scheme for the KFE + Kallianpur-Striebel formula for the likelihood
  2. Spectral methods
- How it looks like:



Initial condition



KFE

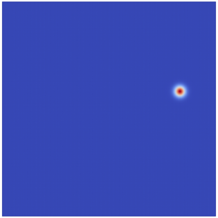


Likelihood

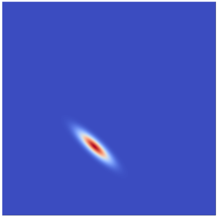
PDE

Linearisation methods

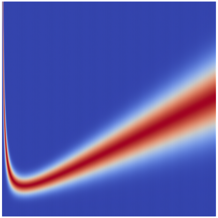
- Idea
  (step 0) linearise the dynamics for X_t
  (step 1) solve the Kolmogorov forward equation (KFE) (closed-form solution!)
  (step 2) update the result with the likelihood
- Example: Extended Kalman Filter (EKF)
- How it looks like:



Initial condition



KFE for a Gaussian

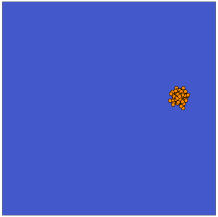


Likelihood

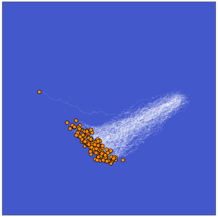
EKF

Sequential Monte Carlo methods

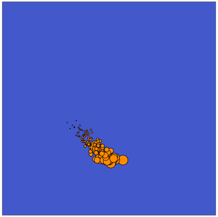
- Idea
  (step 0) sample collection of particles $\{x_0^i\}, i = 1 \dots, N$, all copies of X_0
  (step 1) evolve particles according to a proposal distribution
  (step 2) weigh particles according to the likelihood
  (step 3) resample particles with replacement
  (final step) approximate $\int \phi(x) p(t, x \mid X_0, F_\tau^y) dx$ with $\frac{1}{N} \sum_{i=1}^N \phi(x_i) \delta(x - x_i) dx$
- Examples: Bootstrap Particle Filter (BPF)
- How it looks like:



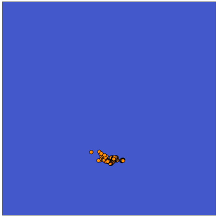
Initial condition



Proposed evolution



Weighing



BPF

Overview

Stochastic Model

$\Downarrow$

Prior knowledge:
Kolmogorov forward equation

$\Downarrow$

Stochastic model for the measurements

$\Downarrow$

Refined knowledge:
Kushner-Stratonovich equation

Outlook

How about other Sequential Monte Carlo methods?

- their theoretical properties
- their computational cost