Estimation of pattern formation in stochastic reaction-diffusion systems with the Block Particle Filter

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Non-linear Filtering

◇ Assume X to be a Markov chain with underlying probability space $(\Omega, \mathcal{F}, \mathbb{P})$, where

$$X : \mathbb{N} \times \Omega \ni (k, \omega) \mapsto X_k(\omega) \in \mathbb{R}^{N_x}.$$

◇ Consider a sequence of observations $(y_k)_{k\in\mathbb{N}}$.

PROBLEM: Estimate the stochastic process $\pi = (\pi_k)_{k\in\mathbb{N}}$, where $\pi_k(\mathcal{A}) = \mathbb{P}(X_k \in \mathcal{A} | Y_{1:k} = y_{1:k})$ for all $\mathcal{A} \in \mathcal{B}(\mathbb{R}^{N_x})$.

The filters π_k can be computed recursively via

$$\pi_{k-1} \xrightarrow{\text{prediction}} \widetilde{\pi}_k = \mathrm{P}_k \pi_{k-1} \xrightarrow{\text{correction}} \pi_k = \mathrm{C}_k \widetilde{\pi}_k, \tag{1}$$

with operators P_k and C_k satisfying

$$(\mathrm{P}_k \pi_{k-1})(\mathcal{A}) \triangleq \int \mathrm{P}_k(x, \mathcal{A}) \pi_{k-1}(dx), \quad (\mathrm{C}_k \widetilde{\pi}_k)(\mathcal{A}) \triangleq \frac{\int_{\mathcal{A}} \mathrm{C}_k(x) \widetilde{\pi}_k(dx)}{\widetilde{\pi}_k(\mathrm{C}_k)}.$$

Classical particle filters:

Let particles $\{X_k^{(n)}\}_{n=1}^{N_p}$ be N_p mutually independent stochastic processes, with common distribution π_k with density p_k. Let π^{N_p} be the sequence of empirical distributions

$$\pi_k^{N_p} \triangleq \frac{1}{N_p} \sum_{n=1}^{N_p} \delta_{X_k^{(n)}}, \quad X_k^{(n)} \sim p_k.$$

Since p_k is unavailable, we sample $\{X_k^{(n)}\}_{n=1}^{N_p}$ from importance distributions with density q_k instead (normalised Importance Sampling), resulting in

$$\frac{1}{N_p} \sum_{n=1}^{N_p} w_k(X_k^{(n)}) \delta_{X_k^{(n)}}, \qquad w_k(x) = \frac{p_k(x)}{q_k(x)}, \qquad X_k^{(n)} \sim q_k,$$

with the support of q_k containing the support of p_k.

Once q_k is chosen, procedure **(1)** is approximated via

$$\pi_{k-1}^{N_p} \xrightarrow{\text{prediction/sampling}} \widetilde{\pi}_k^{N_p} = \mathrm{P}_k \pi_{k-1}^{N_p} \xrightarrow{\text{correction}} \pi_k^{N_p} = \mathrm{C}_k \widetilde{\pi}_k^{N_p}.$$

Block particle filtering [1]:

To address the curse of dimensionality, we assume that the dynamics and observations at a spatial location depend only on state-variables associated with its neighbourhood.

Once q_k is chosen, procedure **(1)** is instead approximated via

$$\pi_{k-1}^{N_p} \xrightarrow{\text{prediction/sampling}} \widetilde{\pi}_k = \mathrm{P}_k \pi_{k-1}^{N_p} \xrightarrow{\text{blocking/correction}} \pi_k^{N_p} = \mathrm{C}_k \mathrm{B} \widetilde{\pi}_k^{N_p},$$

where the operator B is built in the following way:

◇ (X_k, Y_k) is a random field $(X_k, Y_k)_{v\in V}$ indexed by a (finite) undirected graph $\mathcal{G} = (V, W)$;

◇ Graph $\mathcal{G}$ has vertex set $V = \{v \in \mathbb{N}^2 : 1 \le v_i \le \overline{V}, i \in \{1,2\}, \overline{V} \in \mathbb{N}\}$;

◇ Vertices of $\mathcal{G}$ can be partitioned in $V = \bigcup_{V_b \in \mathcal{K}} V_b, V_b \cap V_{b'} = \emptyset$ for $V_b \neq V_{b'}, V_b, V_{b'} \in \mathcal{K}$;

◇ $\mathcal{K}$ is a collection of non-overlapping blocks $\{(v_0 + \{1, \dots, \overline{V}_b\}^2) \cap V : v_0 \in \overline{V}_b \mathbb{N}^2\}$.

$$\mathrm{B}\pi_k := \bigotimes_{V_b \in \mathcal{K}} \mathrm{B}^{V_b} \pi_k, \text{ where } \mathrm{B}^{V_b}\pi_k \text{ is the marginal distribution of } \pi_k \text{ on } \prod_{v\in V_b} \mathbb{R}^{N_x(v)}.$$

This work

◇ We examine two choices for the importance density q_k in the context of the Block particle filter (together with a resampling procedure):

standard choice (stand. SIR)

$$q_k(x) = p(x | x_{k-1}^{(n)})$$

optimal choice (optimal. SIR, minimal MSE)

$$q_k(x) = \frac{p(y_k | y_{1:k-1}, x_{0:k-1}, x) p(x | x_{k-1})}{p(y_k | y_{1:k-1}, x_{0:k-1})};$$

◇ We reconstruct the concentrations of chemical substances in a reactive-diffusion system using noisy spectral observations.

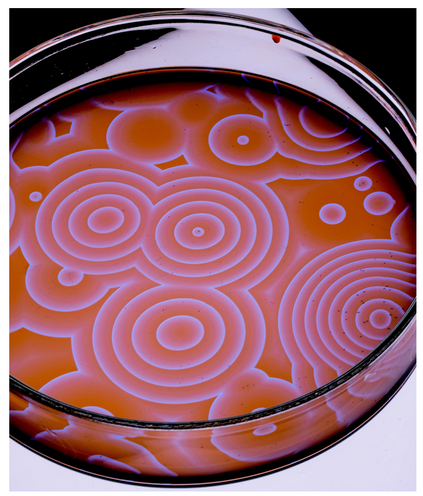

Figure 1: An oscillatory chemical reaction propagating across a petri dish.

Case-study: The Oregonator System [2]

A reaction-diffusion system with

◇ a quasi-two-dimensional space $U = \{u \in \mathbb{R}^2 : 0 \le u_i < \overline{U}, i \in \{1,2\}\}$ (e.g. a petri dish);

◇ sets of chemical species $\mathcal{S} = \{\mathcal{S}_1, \dots, \mathcal{S}_6\}$ distributed over U

$$2\mathcal{S}_1 \xrightarrow{\kappa_1} \mathcal{S}_4 + \mathcal{S}_5 \qquad \mathcal{S}_1 + \mathcal{S}_3 \xrightarrow{\kappa_2} 2\mathcal{S}_5 \qquad \mathcal{S}_2 + \mathcal{S}_6 \xrightarrow{\kappa_5} 0.5\sigma\mathcal{S}_3;$$
$$\mathcal{S}_1 + \mathcal{S}_4 \xrightarrow{\kappa_3} 2\mathcal{S}_1 + 2\mathcal{S}_2 \qquad \mathcal{S}_3 + \mathcal{S}_4 \xrightarrow{\kappa_4} \mathcal{S}_1 + \mathcal{S}_5$$

◇ a discretisation $V = \{v \in \mathbb{N}^2 : 1 \le v_i \le \overline{V}, i \in \{1,2\}, \overline{V} = (\overline{U}/\Delta u)\}$ of evenly-spaced grid points;

◇ dynamics of $z^{(v)}(t) = z\big((v_1, v_2)\Delta u, t\big)$ approximated as

$$dz^{(v)} = \left[(\overline{S} - \underline{S})^{\mathsf{T}} \nu\big(z^{(v)}\big) + D_z \nabla^2 z^{(v)}\right] dt, \quad \forall v \in V,$$

with stoichiometric matrix $\underline{S} \in \mathbb{N}^{5\times 5}$ for the reactants and $\overline{S} \in \mathbb{N}^{5\times 5}$ for the products;

◇ environmental perturbations added in the form of Brownian Motion B^z

$$dz(u,t) = f_z(z(u,t), \nabla^2 z(u,t))\, dt + g_z(z(u,t)) dB_t^z;$$

◇ an output equation of the form $y^{(v)}(t) = H_z z^{(v)}(t) + e_z(t)$, with $y^{(v)}(t) = y((v_1, v_2)\Delta u, t)$.

For this reaction network,

$$\big([\mathcal{S}_4], [\mathcal{S}_5], [\mathcal{S}_6] = \text{ constant }\big) \wedge \big([\mathcal{S}_3] \text{ slowly varying}\big) \xrightarrow{[3]} z^{(v)}(t) \in \mathbb{R}^2, H_z \in \mathbb{R}^{10\times 2}.$$

We let $X_k = (z^{(v_1,v_2)}(t_k))_{v_1,v_2=1}^{\overline{V}}$ and $Y_k = (y^{(v_1,v_2)}(t_k))_{v_1,v_2=1}^{\overline{V}}$.

$$\Big((\overline{V}/\overline{V}_b)^2 = 400\Big) \wedge \Big(\text{block size } \overline{V}_b = 5\Big) \longrightarrow X_k \in \mathbb{R}^{2\cdot(100)^2}, Y_k \in \mathbb{R}^{10\cdot(100)^2}.$$

References

[1] Patrick Rebeschini and Ramon van Handel. Can local particle filters beat the curse of dimensionality? The Annals of Applied Probability, 25(5):2809 – 2866, 2015.

[2] Richard J. Field and Richard M. Noyes. Oscillations in chemical systems. iv. limit cycle behavior in a model of a real chemical reaction. Journal of Chemical Physics, 60:1877–1884, 1974.

[3] James P. Keener and John J. Tyson. Spiral waves in the belousov-zhabotinskii reaction. Physica D: Nonlinear Phenomena, 21(2):307–324, 1986.

Figure 2: Snapshots of $(X_k)_1$ (4 first columns) and $(X_k)_2$ (4 last columns) for the Oregonator model at different times t_k. First row shows a draw for X_k used to generate observation y_k. We estimated $\hat{X}_k$ with the Block Particle Filter (for each block $N_p = 128$ particles) with a standard (2nd row) and with an optimal (3rd row) choice of importance densities q_k. $[f_z]_1 = a^{-1}(z_1(1 - z_1) - \frac{bz_2(z_1 - c)}{z_1 + c}) + D_{z_1}\nabla^2 z_1$, $\quad [f_z]_2 = (z_1 - z_2) + D_{z_2}\nabla^2 z_2$, with constants $(a, b, c) = (0.08, 0.95, 0.0075)$, $(D_{z_1}, D_{z_2}) = (5 \times 10^{-4}, 5 \times 10^{-6})$. The process noise has coefficient $g(X_{k-1}) = 10^{-2}\mathtt{diag}(X_{k-1})$. The measurement process is defined by $H = [I_{\overline{V}^2} \otimes \mathcal{M}_{\mathcal{S}_1}\ I_{\overline{V}^2} \otimes \mathcal{M}_{\mathcal{S}_2}]$ with spectra $(\mathcal{M}_{\mathcal{S}_1}, \mathcal{M}_{\mathcal{S}_2})$ collected at 10 equally-spaced wavelengths $r \in [0, 50)$ through response functions $m_{\mathcal{S}_1}(r) = \exp\left(-\frac{(r-10)^2}{30}\right)$ and $m_{\mathcal{S}_2}(r) = \exp\left(-\frac{(r-40)^2}{30}\right)$.