Bayesian Spatio-Dynamic Modelling in Cell Motility Studies: Learning Nonlinear Taxic Fields Guiding Immune Response: 3-dimensional synthetic example

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We develop a 3-dimensional synthetic example to illustrate our methods described in the main text, using the same notation.

1 Illustration and evaluation using 3-dimensional synthetic data

A p = 3-dimensional data set of C = 100 cells was generated from the model with the following specifications, which have been calibrated to match the posterior estimates (in 'standardized' units) of all the parameters in the real data analysis described in the main text. We assume trajectories are observed with noise with $\Sigma = 0.001 I$, and each cell has a trajectory of length $T_c \sim 2 + Po(25)$ time steps every $\Delta t = 18/60$, with $a_\zeta = 20, b_\zeta = 4$, such that $\zeta^2_c \sim IG(20, 20 \times / 4)$, and $a_\gamma = 20, b_\gamma = 2$ such that $\gamma_c \sim G(20, 20/2)$. The taxic field is generated through a potential surface with $K = 4$ and parameters $\alpha_{1:4} = [-20, 10, -15, 5], \mu_1 = (0, -2, 0)', \mu_2 = (1, 3, 1)', \mu_3 = (-3, 0, 2)', \mu_4 = (-4, -4, 3)', and \Sigma_1 = [(1, -0.1, 0); (-0.110); (001)], \Sigma_2 = [(211); (121); (112)], \Sigma_3 = [(0.5 - 0.20); (-0.20.50); (000.5)] and $\Sigma_4 = [(0.5, -0.4, 0); (-0.4, 0.5, 0); (0, 0, 0.5)]$. The potential function can be realized through isosurfaces of an intensity function in Figure 1(b) with resulting observed cell trajectories in Figure 1(a).

We implement our MCMC sampler, setting $b_\gamma \sim IG(2, 0.001), b_\zeta \sim IG(2, 200)$, for the cell motion hyperparameters and $\Sigma \sim IW(p + 1, 0.001)$ for the noise variance. On the gradient field potential model parameters we set $M = 10I, r = 1$ and $R = 10I, a_\alpha = 1$ and $b_\alpha = 10^{-4}$ for the kernel weight priors, and $K = 10$. The resulting estimated posterior mean of the potential surface is shown in Figure 2(a); posterior distributions, summarized as box-plots, for the hyper-parameters
Figure 1: (a) The noisy 3-dimensional trajectories used in the synthetic example, and (b) The taxic field shown through isosurfaces of the potential function.

$b_\zeta$ and $b_\gamma$, as well as the error variance $\Sigma$, are in Figure 3. As indicated by the box-plots, the model successfully separates the error variance $\Sigma$ and stochastic variance $\zeta$. The posterior mean of the potential function identifies the two regions of attraction, shown in blue in Figure 2(a). The nature of the model, however, implies that there will be fewer observations around regions of repulsion, especially in high dimensions; more data (either more cells or longer trajectories) are required for the regions of repulsion to be accurately estimated. In order to visualize the posterior mean surface in combination with the corresponding posterior variance, we plot a signal-to-noise ratio surface in Figure 2(b); at each point $x$, this is the reciprocal of the estimated posterior coefficient of variation of $U(x)$. 


Figure 2: Panel (a) shows isosurfaces of the posterior mean inferred potential function, and panel (b) shows the corresponding isosurfaces of the signal-to-noise ratio surface computed as the reciprocal of the estimated posterior coefficient of variation at each location.

Figure 3: Box plots summarizing the posterior for each of the following hyper-parameters: (a) $b_\gamma$ and (b) $b_\zeta$, representing locations of the cellular population distributions of $\gamma$ and $\zeta^2$ and respectively, and (c) marginal posterior error variance $\Sigma_{11}$, $\Sigma_{22}$ and $\Sigma_{33}$. 