Modelling of Biochemical Reactions in Cells

UPPSALA UNIVERSITET

Jonathan Andersson
Jonathan.Andersson.
8055@student.uu.se

Agnes Johansson
Agnes.Johanssson.
9036@student.uu.se

Aim

Compare different methods for time stepping in the hybrid method by investigating the accuracy they have in different systems.

Hybrid method

Split the set of chemical species into two parts $\mathbf{Z} \rightarrow (\mathbf{X}, \mathbf{Y})$.

The species $\mathbf{Y}$ have low statistic variation and can be approximated deterministically using ODE:s. The species $\mathbf{X}$ have low copy number or large variation, and need to be treated stochastically and is therefore simulated with the Stochastic Simulation Algorithm (SSA).

A time step (Δt) is used to determine how often the deterministic and the stochastic parts are synchronized.

Algorithm

The hybrid method was implemented with Euler, Lie-Trotter (LT-sd and LT-ds), and Strang splitting, and applied on different systems.

A reference solution of each system was computed with the Piecewise-Deterministic Markov Process (PDMP)[1].

Conclusion

For a simple example with two species X and Y, the coupling factor between the species have a great impact on how well the different method works.

For a Circadian Rhythm a too big Δt increases the randomness in both the amplitude and period of the species.
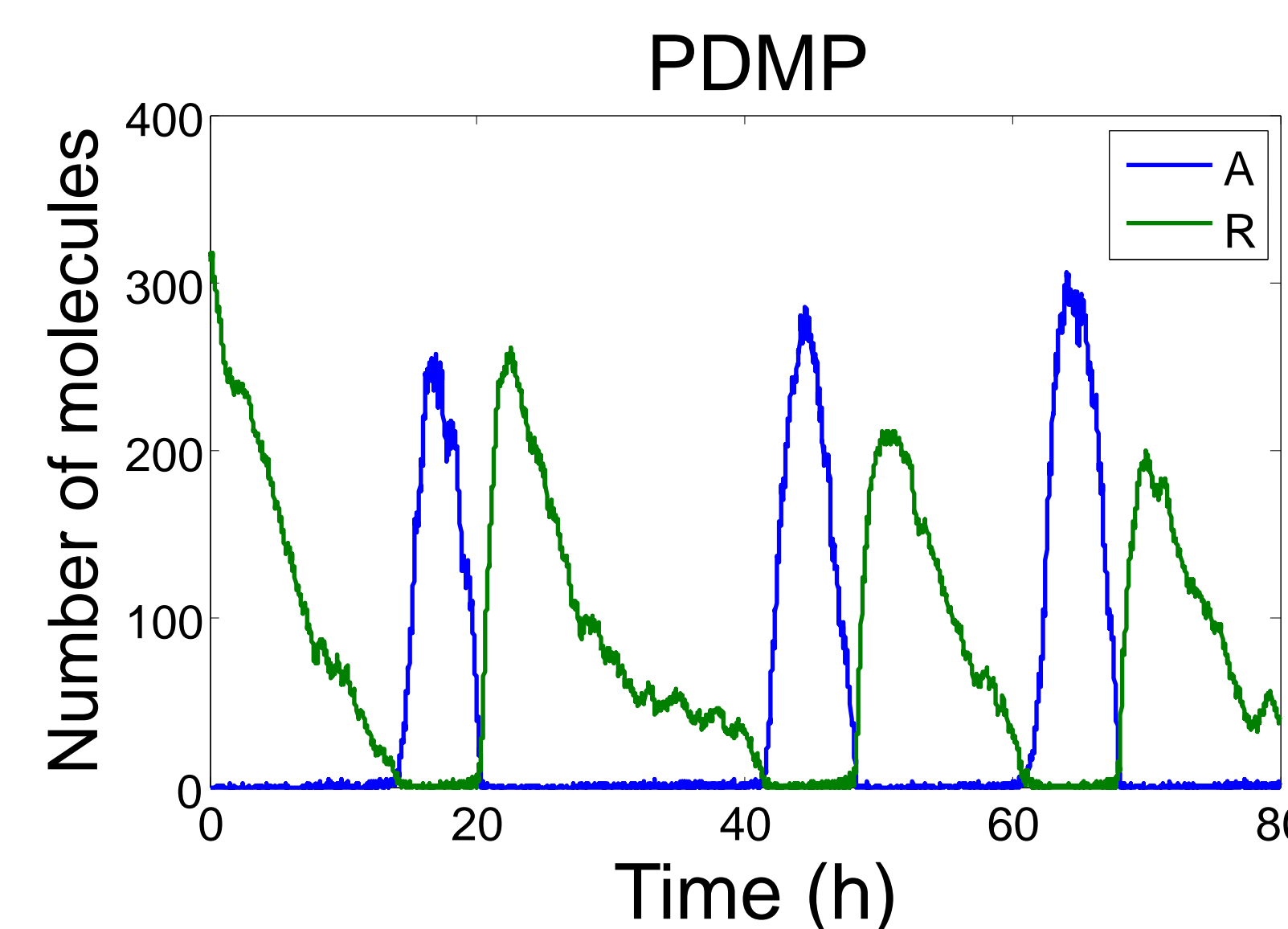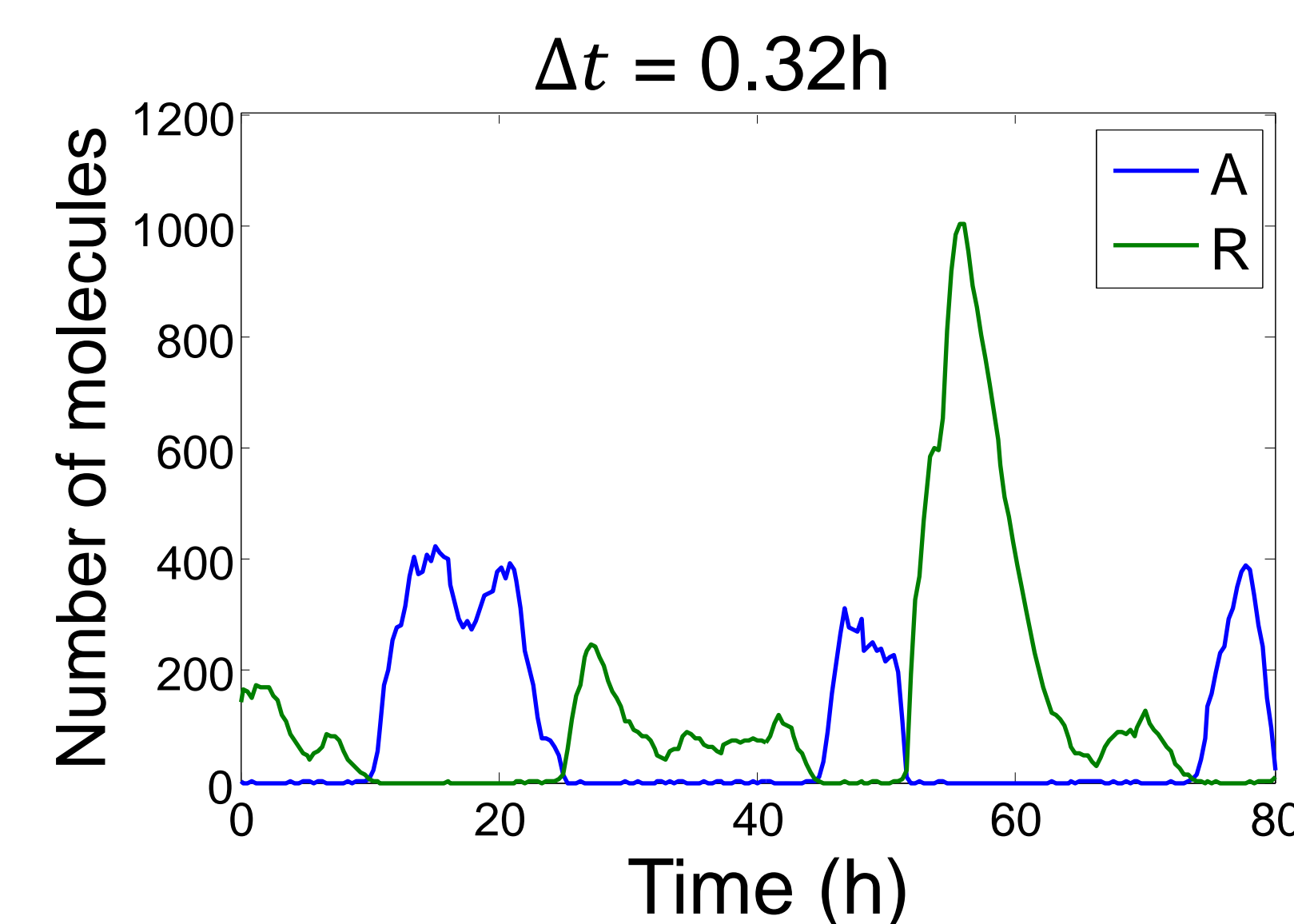
Result

Mean value of X
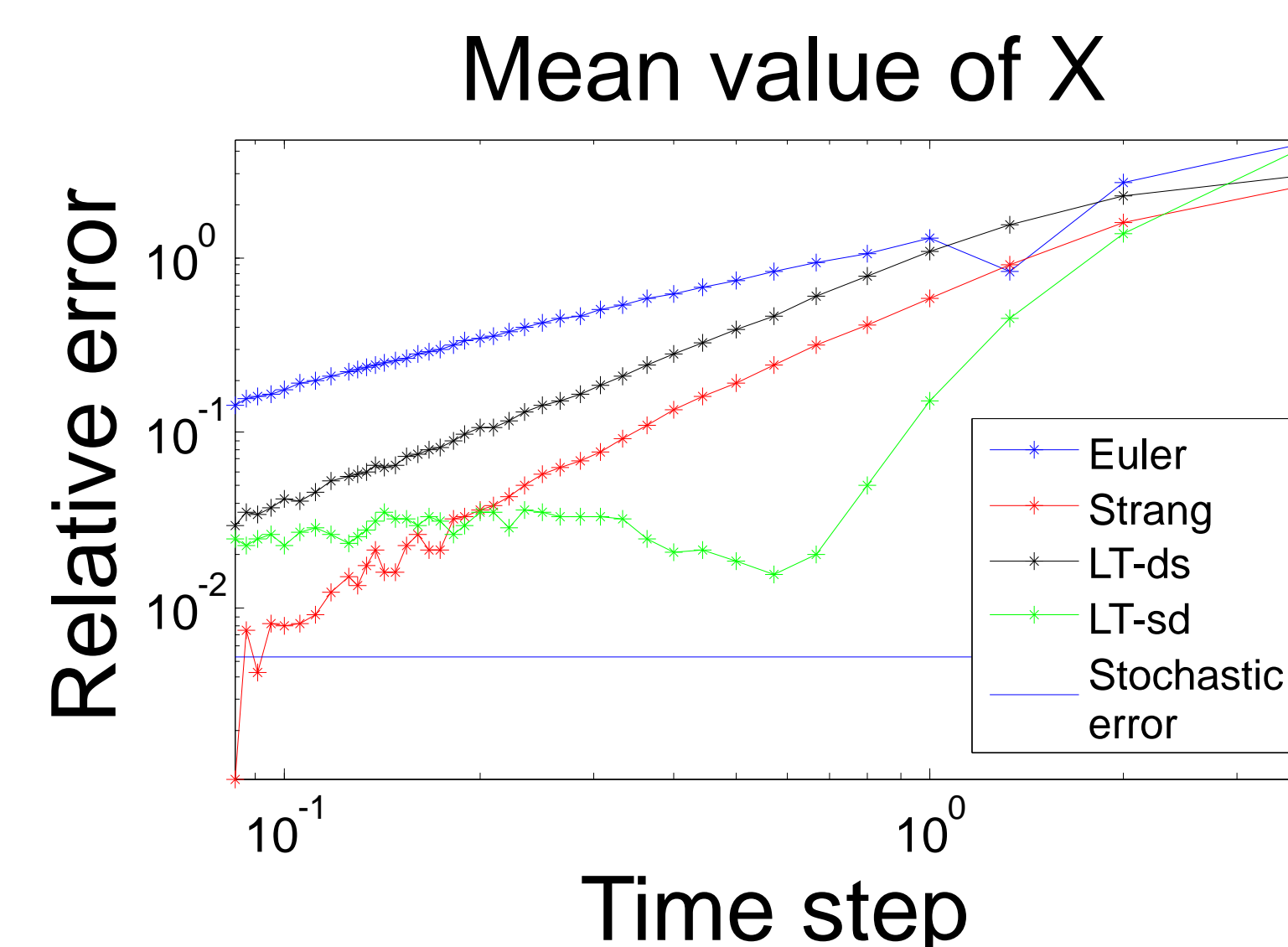
Simulation of a simple example with two species X and Y, showing convergence rates of the different methods.

Mean value of X
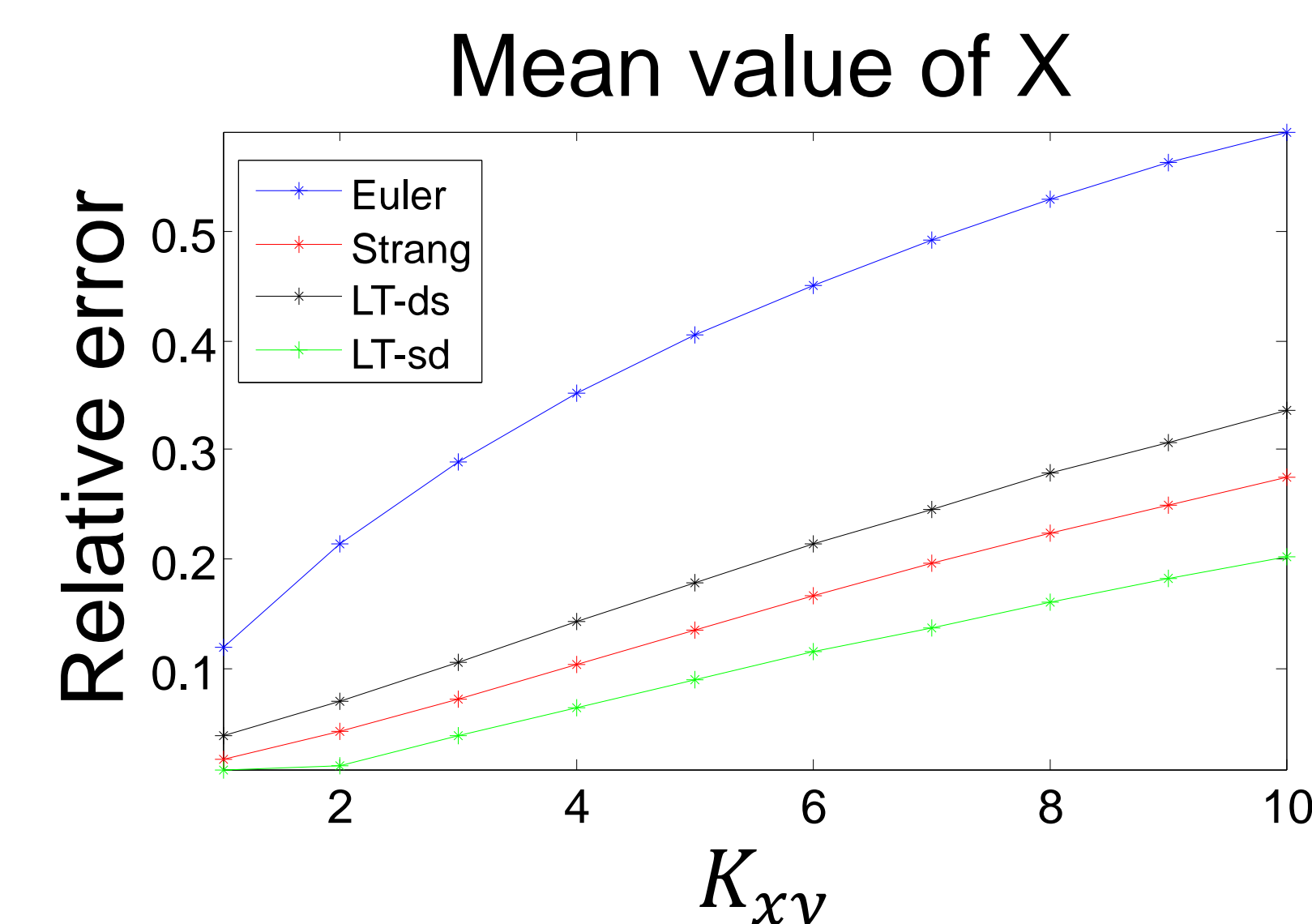
Simulation of a simple example with two species X and Y. Error for different values of the coupling factor K_{xy} between X and Y.

PDMP

Simulation of Circadian Rhythm. Typical behaviour when using PDMP.

$\Delta t = 0.32h$

Simulation of Circadian Rhythm. Typical behaviour when using Strang with too large time step.

[1] Davis, M.H.A.,1984, Piecewise-Deterministic Markov Processes: A General Class of Non-diffusion Stochastic Models, *Journal of the Royal Statistical Society, Series B*, 46 (3) pp. 353-388.