Qualitative parameter inference:
Automated Detection of Chaotic and Oscillatory Regimes

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Motivation – Elusive behaviours

- Traditional quantitative driven parameter inference methods can fail for certain types of data.
Motivation – System design

- System design – finding parameter combinations that give rise to desired types of behaviour.
Outline

1 Motivation

2 Background and Methods
   - Encoding Dynamical Behaviour via Lyapunov Exponents
   - Kalman Filtering
   - The Unscented Kalman Filter
   - Adapting the Unscented Kalman Filter

3 Results
   - Detecting Chaos
   - Detecting Oscillations
   - Detecting Hyperchaos

4 Summary

5 Ongoing work
Lyapunov spectra, \( \{ \lambda_i \} \), measure the long term average rate of contraction/expansion of nearby trajectories.

- Computationally expensive inference procedure.
Probabilistic inference

Allows the estimation of hidden system parameters from a sequence of incomplete and noisy observations.

- Posterior distribution $p(\theta_t | y_{1:t})$

\[ x_{t+1} = f(x_t, n_t^p; \theta) \]

\[ y_t = g(x_t, n_t^m; \theta) \]
Probabilistic inference

- Allows the estimation of hidden system parameters from a sequence of incomplete and noisy observations.
  - Posterior distribution $p(\theta_t|y_{1:t})$
- Also applicable to state and dual estimation problems.
The optimal solution

\[ p(\theta_k | y_{1:k}) = \frac{p(\theta_k | y_k)p(\theta_k | y_{1:k-1})}{p(y_k | y_{1:k-1})} \]

- Terms in the Bayesian estimation update correspond to multi-dimensional integrals.
- In general, closed form solutions are only available for linear systems.
  - Known as Kalman filtering.
Filtering for non-linear systems

- Models of biological systems are often non-linear.
- Our method requires the use of highly non-linear functions.

- The extended Kalman filter
- Particle filtering
- Sigma-point Kalman filters

Figure adapted from *The Unscented Kalman Filter for Nonlinear Estimation* - E. A. Wan and R. van der Merwe
The Unscented Kalman Filter (Van der Merwe 2004)

Intuition: *Probability density functions may be easier to approximate than highly non-linear systems.*

- Propagated means and covariances are accurate to third order in the Taylor expansion.
- Computationally very efficient.

Figure adapted from *The Unscented Kalman Filter for Nonlinear Estimation* - E. A. Wan and R. van der Merwe
UKF $t^{th}$ iteration

$P(\theta | y_i < t)$
Summarize parameter distribution with sigma-points
Propagate sigma-points through the observation model $g$
Update parameter distribution using observation $y_t$

$$P(\theta | y_i < t)$$

$$P(\theta | y_i < t + 1)$$
Adapting the UKF for qualitative inference

The idea

- Exploit the flexibility of the observation function, $g$, and observations, $y_t$.
- Choose $g$ to output the Lyapunov exponents of the model for parameter vector $\hat{\theta}^i$.
- Fix $y_t = \Lambda_t = \Lambda$ as the constant desired Lyapunov spectrum.

\[
\begin{align*}
\theta_{t+1} &= \theta_t + v_t \\
y_t &= g(x_t, \theta_t) + u_t,
\end{align*}
\]
Adapting the UKF for qualitative inference

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Results – Chaos in the Lorenz system

\[
\begin{align*}
\dot{x} &= \sigma(y - x) \\
\dot{y} &= x(\rho - z) - y \\
\dot{z} &= xy - \beta z,
\end{align*}
\]
\[ \dot{M} = -k_{\text{deg}} M + 1/(1 + (P_2/P_0)^h) \]
\[ \dot{P}_1 = -k_{\text{deg}} P_1 + \nu M - k_1 P_1 \]
\[ \dot{P}_2 = -k_{\text{deg}} P_2 + k_1 P_1 \]
Results – Chaotification

\[ \dot{x} = y \]
\[ \dot{y} = ay - x - z \]
\[ \epsilon \dot{z} = b + y - c(e^z - 1), \]

Very large Lyapunov exponents give trajectories similar properties to white noise.
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Lyapunov spectrum = (31.8, 16.8, −19.1, −71.4), over twice as large as previously found.
The Unscented Kalman filter may be adapted for qualitative parameter inference.
Parameters may be inferred such that a model exhibits a chosen Lyapunov spectrum.
Example applications successfully identify chaotic, oscillatory and hyperchaotic regimes.
Ongoing work

- Can we infer model structure as well?
Ongoing work

- Can we infer model structure as well?
- Scan the space of 3 and 4 node networks for chaos/oscillations. Hope to identify common and necessary motifs for different types of behaviour.
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