A Quasi-Stationary Distribution Approach to Transient Dynamics

Zhongwei Shen

Department of Mathematical and Statistical Sciences
University of Alberta

Retreat for Young Researchers in Probability and areas of Application
BIRS

September 28, 2019

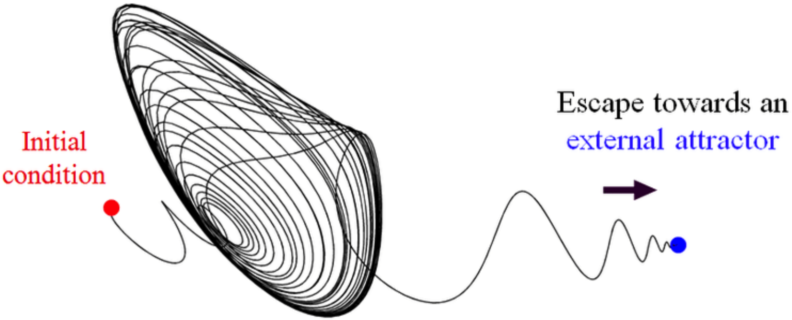
Collaborators

Shirou Wang
Yingfei Yi

Outline

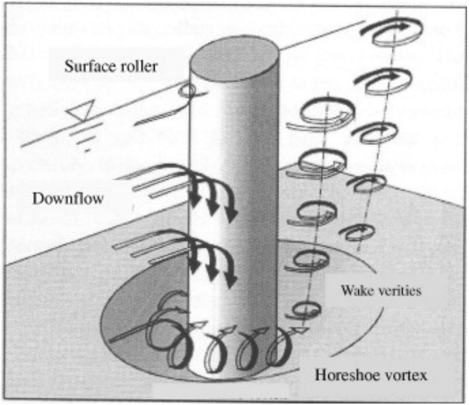
Transient dynamics

Illustration of transient dynamics (from R. Capeáns, J. Sabuco and M. A. F. Sanjuán, DCDS-B, 2018)



Transient dynamics

Illustration of the flow at a circular pier (from B.W. Melville and S.E. Coleman, Bridge Scour Water, 2000)



Transient dynamics

Three-species food chain model with cooperative hunting (from J. Duarte, C. Januário, N. Martins and J. Sardanyés, Chaos, 2009):

$$\begin{aligned}
&\text{(Resource)} \quad \dot{R} = R\left(1 - \frac{R}{K}\right) - \frac{x_c y_c C R}{R + R_0}, \\
&\text{(Consumer)} \quad \dot{C} = -x_c C + \frac{x_c y_c C R}{R + R_0} - \phi(P)\frac{x_p y_p C}{C + C_0}, \\
&\text{(Predator)} \quad \dot{P} = -x_p P + \phi(P)\frac{x_p y_p C}{C + C_0},
\end{aligned}$$

where

$$\phi(P) = (1 - \sigma)P + \sigma P^2.$$

Transient dynamics

Three-species food chain model with cooperative hunting (from J. Duarte, C. Januário, N. Martins and J. Sardanyés, Chaos, 2009):

$$
\begin{aligned}
\text{(Resource)} \quad & \dot{R} = R\left(1 - \frac{R}{K}\right) - \frac{x_c y_c C R}{R + R_0}, \\
\text{(Consumer)} \quad & \dot{C} = -x_c C + \frac{x_c y_c C R}{R + R_0} - \phi(P)\frac{x_p y_p C}{C + C_0}, \\
\text{(Predator)} \quad & \dot{P} = -x_p P + \phi(P)\frac{x_p y_p C}{C + C_0},
\end{aligned}
$$

where

$$\phi(P) = (1 - \sigma)P + \sigma P^2.$$

- $\sigma \in [0, 1]$ is a measure of the degree of cooperation inside the population of predators.

Transient dynamics

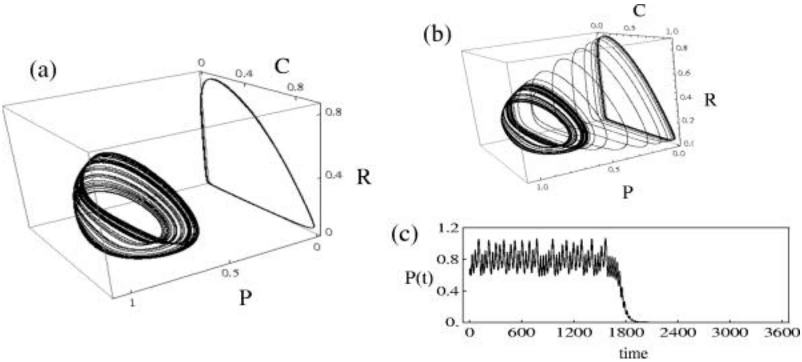


Figure: (a) $\sigma = 0$, McCann-Yodzis model; (b) (c) $0 < \sigma \ll 1$

Transient dynamics

More examples:

- Dispersion of volcanic ash;

Transient dynamics

More examples:

- Dispersion of volcanic ash;
- Pollutant spreading in the atmosphere;

Transient dynamics

More examples:

- Dispersion of volcanic ash;
- Pollutant spreading in the atmosphere;
- Process of decision making.

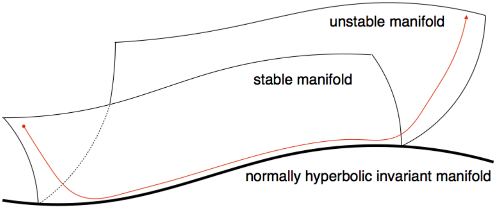
Transient dynamics

More examples:

- Dispersion of volcanic ash;
- Pollutant spreading in the atmosphere;
- Process of decision making.

Traditional approaches:

- normally hyperbolic invariant manifold;



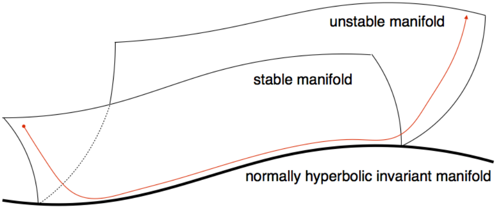
Transient dynamics

More examples:

- Dispersion of volcanic ash;
- Pollutant spreading in the atmosphere;
- Process of decision making.

Traditional approaches:

- normally hyperbolic invariant manifold;



- identifying the time scales;

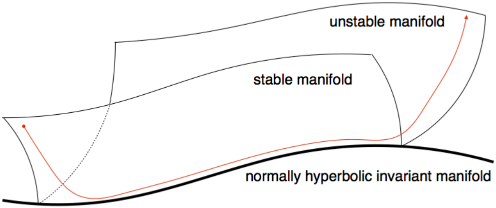
Transient dynamics

More examples:

- Dispersion of volcanic ash;
- Pollutant spreading in the atmosphere;
- Process of decision making.

Traditional approaches:

- normally hyperbolic invariant manifold;



- identifying the time scales;
- perturbing chaotic systems + measure of complexity (Lyapunov exponent, entropy, dimension, etc.).

Stochastic chemical reaction models

Chemical reactions:

$$A + X \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2X, \quad X \xrightarrow{k_2} C,$$

- reaction rates: k_1, k_{-1}, k_2,
- open system, the number of A molecules held fixed n_A,
- scaling parameter $V =$ volume $\times$ Avogadro number.

Stochastic chemical reaction models

Chemical reactions:

$$A + X \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2X, \quad X \xrightarrow{k_2} C,$$

- reaction rates: k_1, k_{-1}, k_2,
- open system, the number of A molecules held fixed n_A,
- scaling parameter V = volume $\times$ Avogadro number.

Continuous-time Markov jump process:

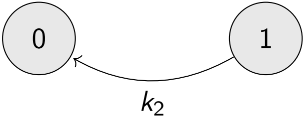
- X_t^V: the process counting the number of X molecules,
- $\frac{X_t^V}{V}$: the process for the concentration.

Stochastic chemical reaction models

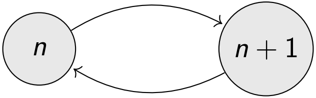
Master equation for $\frac{X_t^V}{V}$:

$$\frac{d}{dt}p(t,\tfrac{n}{V})=\lambda_{n-1,V}\,p(t,\tfrac{n-1}{V})-(\lambda_{n,V}+\mu_{n,V})p(t,\tfrac{n}{V})+\mu_{n+1,V}\,p(t,\tfrac{n+1}{V}),$$

where $p(t,\frac{n}{V}) = \mathbb{P}\left[\frac{X_t^V}{V} = \frac{n}{V}\right]$, and $\lambda_{n,V}, \mu_{n,V}$ are determined by law of mass action.



$$\lambda_{n,V} := \frac{k_1 n_A n}{V}$$



$$\mu_{n+1,V} := \frac{k_{-1}n(n+1)}{V} + k_2(n+1)$$

$$\frac{k_{-1}n(n+1)}{V} = \frac{k_{-1}}{V^{2-1}}2!\binom{n+1}{2},$$

$$A + X \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2X, \quad X \xrightarrow{k_2} C.$$

Stochastic chemical reaction models

Mean-field approximation of $\frac{X_t^V}{V}$:

$$\dot{x} = b(x), \quad x \in [0, \infty)$$

where

$$b(x) = k_1 x_A x - k_{-1} x^2 - k_2 x = k_{-1} x \left(\frac{k_1 x_A - k_2}{k_{-1}} - x \right).$$

Stochastic chemical reaction models

Mean-field approximation of $\frac{X_t^V}{V}$:

$$\dot{x} = b(x), \quad x \in [0, \infty)$$

where

$$b(x) = k_1 x_A x - k_{-1} x^2 - k_2 x = k_{-1} x \left(\frac{k_1 x_A - k_2}{k_{-1}} - x \right).$$

- x_A is concentration of A molecules ($\frac{n_A}{V} \to x_A$ as $V \to \infty$).

Stochastic chemical reaction models

Mean-field approximation of $\frac{X_t^V}{V}$:

$$\dot{x} = b(x), \quad x \in [0, \infty)$$

where

$$b(x) = k_1 x_A x - k_{-1} x^2 - k_2 x = k_{-1} x \left(\frac{k_1 x_A - k_2}{k_{-1}} - x \right).$$

- x_A is concentration of A molecules ($\frac{n_A}{V} \to x_A$ as $V \to \infty$).
- Assume $k_1 x_A > k_2$. Positive equilibrium $x_e := \frac{k_1 x_A - k_2}{k_{-1}}$.

Stochastic chemical reaction models

Mean-field approximation of $\frac{X_t^V}{V}$:

$$\dot{x} = b(x), \quad x \in [0, \infty)$$

where

$$b(x) = k_1 x_A x - k_{-1} x^2 - k_2 x = k_{-1} x \left(\frac{k_1 x_A - k_2}{k_{-1}} - x \right).$$

- x_A is concentration of A molecules ($\frac{n_A}{V} \to x_A$ as $V \to \infty$).
- Assume $k_1 x_A > k_2$. Positive equilibrium $x_e := \frac{k_1 x_A - k_2}{k_{-1}}$.
- Dynamics:

$$x(t) \to x_e \quad \text{exponentially as} \quad t \to \infty.$$

Stochastic chemical reaction models

Diffusion approximation of $\frac{X_t^V}{V}$:

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t, \quad x \in [0, \infty),$$

where $\epsilon = \frac{1}{\sqrt{V}}$ and

$$a(x) = k_1 x_A x + k_{-1} x^2 + k_2 x.$$

Stochastic chemical reaction models

Diffusion approximation of $\frac{X_t^V}{V}$:

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t, \quad x \in [0, \infty),$$

where $\epsilon = \frac{1}{\sqrt{V}}$ and

$$a(x) = k_1 x_A x + k_{-1} x^2 + k_2 x.$$

- Extinction state 0 is an absorbing state.
- δ_0 is the unique stationary distribution.

Stochastic chemical reaction models

Diffusion approximation of $\frac{X_t^V}{V}$:

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t, \quad x \in [0, \infty),$$

where $\epsilon = \frac{1}{\sqrt{V}}$ and

$$a(x) = k_1 x_A x + k_{-1} x^2 + k_2 x.$$

- Extinction state 0 is an absorbing state.
- δ_0 is the unique stationary distribution.
- Long time dynamics:
  - $x_\epsilon(t) \to \delta_0$ in distribution as $t \to \infty$,

Stochastic chemical reaction models

Diffusion approximation of $\frac{X_t^V}{V}$:

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t, \quad x \in [0, \infty),$$

where $\epsilon = \frac{1}{\sqrt{V}}$ and

$$a(x) = k_1 x_A x + k_{-1}x^2 + k_2 x.$$

- Extinction state 0 is an absorbing state.
- δ_0 is the unique stationary distribution.
- Long time dynamics:
  - $x_\epsilon(t) \to \delta_0$ in distribution as $t \to \infty$,
  - Extinction time T_ϵ satisfies $\mathbb{E}[T_\epsilon] < \infty$.

Stochastic chemical reaction models

Diffusion approximation of $\frac{X_t^V}{V}$:

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t, \quad x \in [0, \infty),$$

where $\epsilon = \frac{1}{\sqrt{V}}$ and

$$a(x) = k_1 x_A x + k_{-1} x^2 + k_2 x.$$

- Extinction state 0 is an absorbing state.
- δ_0 is the unique stationary distribution.
- Long time dynamics:
  - $x_\epsilon(t) \to \delta_0$ in distribution as $t \to \infty$,
  - Extinction time T_ϵ satisfies $\mathbb{E}[T_\epsilon] < \infty$.
- Stochastic stability: small noise stabilizes/de-stabilizes the unstable/stable equilibrium.

Stochastic chemical reaction models

Two-scale dynamics of the diffusion approximation

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t,$$

- Eventual extinction dynamics.

Stochastic chemical reaction models

Two-scale dynamics of the diffusion approximation

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t,$$

- Eventual extinction dynamics.
- Transient dynamics: stay near x_e for a (long) finite time period.

Stochastic chemical reaction models

Two-scale dynamics of the diffusion approximation

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t,$$

- Eventual extinction dynamics.
- Transient dynamics: stay near x_e for a (long) finite time period.
  - Large deviation. For each $T > 0$,

$$\text{SDE}_\epsilon \approx \text{ODE on } [0, T]$$

for all $0 < \epsilon \ll 1$.

Stochastic chemical reaction models

Two-scale dynamics of the diffusion approximation

$$dx = b(x)dt + \epsilon\sqrt{a(x)}dW_t,$$

- Eventual extinction dynamics.
- Transient dynamics: stay near x_e for a (long) finite time period.
  - Large deviation. For each $T > 0$,

    $$\text{SDE}_\epsilon \approx \text{ODE on } [0, T]$$

    for all $0 < \epsilon \ll 1$.
  - Beyond large deviation. For each $0 < \epsilon \ll 1$, there is T_ϵ such that

    $$\text{SDE}_\epsilon \approx \text{ODE on } [0, T_\epsilon],$$
    $$\text{SDE}_\epsilon \not\approx \text{ODE on } (T_\epsilon, \infty).$$

Stochastic chemical reaction models

Questions:

- How to rigorously characterize the transient dynamics?
  Is it a corresponding state, called transient state?
  What properties does the transient state have?

Stochastic chemical reaction models

Questions:

- How to rigorously characterize the transient dynamics?
  Is it a corresponding state, called transient state?
  What properties does the transient state have?

- How long do solutions stay with the transient state?

QSDs and transient states

Quasi-stationary distribution: a QSD μ_ϵ is a probability measure on $(0,\infty)$ s.t.

$$\mathbb{P}_{\mu_\epsilon}\left[x_\epsilon(t) \in \bullet \middle| T_\epsilon > t\right] = \mu_\epsilon, \quad \forall t > 0.$$

Stationary distribution for the conditioned process; expect to capture the dynamics before the extinction.

QSDs and transient states

Quasi-stationary distribution: a QSD μ_ϵ is a probability measure on $(0, \infty)$ s.t.

$$\mathbb{P}_{\mu_\epsilon}\left[x_\epsilon(t) \in \bullet | T_\epsilon > t\right] = \mu_\epsilon, \quad \forall t > 0.$$

Stationary distribution for the conditioned process; expect to capture the dynamics before the extinction.

- existence, uniqueness and regularity of QSD

$$d\mu_\epsilon = u_\epsilon dx;$$

QSDs and transient states

Quasi-stationary distribution: a QSD μ_ϵ is a probability measure on $(0, \infty)$ s.t.

$$\mathbb{P}_{\mu_\epsilon}[x_\epsilon(t) \in \bullet | T_\epsilon > t] = \mu_\epsilon, \quad \forall t > 0.$$

Stationary distribution for the conditioned process; expect to capture the dynamics before the extinction.

- existence, uniqueness and regularity of QSD

$$d\mu_\epsilon = u_\epsilon dx;$$

- principal eigen-pair:

$$\mathcal{L}^\epsilon u_\epsilon = -\lambda_\epsilon u_\epsilon,$$

where $\lambda_\epsilon > 0$ and $\mathcal{L}^\epsilon u = \frac{\epsilon^2}{2}(au)_{xx} - (bu)_x$;

QSDs and transient states

- extinction time:

$$\mathbb{P}_{\mu_\epsilon}[T_\epsilon > t] = e^{-\lambda_\epsilon t}, \quad \forall t > 0;$$

QSDs and transient states

- extinction time:

$$\mathbb{P}_{\mu_\epsilon}[T_\epsilon > t] = e^{-\lambda_\epsilon t}, \quad \forall t > 0;$$

- conditioned dynamics:

$$\mathbb{P}[x_\epsilon(t) \in \bullet | T_\epsilon > t] \xrightarrow{t \to \infty} \mu_\epsilon \quad \text{exponentially with rate } \eta_\epsilon,$$

where η_ϵ is the gap between $-\lambda_\epsilon$ and the second eigenvalue.

QSDs and transient states

- extinction time:

$$\mathbb{P}_{\mu_\epsilon}\left[T_\epsilon > t\right] = e^{-\lambda_\epsilon t}, \quad \forall t > 0;$$

- conditioned dynamics:

$$\mathbb{P}\left[x_\epsilon(t) \in \bullet | \, T_\epsilon > t\right] \xrightarrow{t\to\infty} \mu_\epsilon \quad \text{exponentially with rate } \eta_\epsilon,$$

  where η_ϵ is the gap between $-\lambda_\epsilon$ and the second eigenvalue.
- due to P. Cattiaux, P. Collet, A. Lambert, S. Martinez, S. Meleard and J. San Martin, Ann. Probab., 2009.

QSDs and transient states

- extinction time:

$$\mathbb{P}_{\mu_\epsilon}[T_\epsilon > t] = e^{-\lambda_\epsilon t}, \quad \forall t > 0;$$

- conditioned dynamics:

$$\mathbb{P}[x_\epsilon(t) \in \bullet | T_\epsilon > t] \xrightarrow{t\to\infty} \mu_\epsilon \quad \text{exponentially with rate } \eta_\epsilon,$$

  where η_ϵ is the gap between $-\lambda_\epsilon$ and the second eigenvalue.
- due to P. Cattiaux, P. Collet, A. Lambert, S. Martinez, S. Meleard and J. San Martin, Ann. Probab., 2009.

Problem: λ_ϵ Vs η_ϵ.

- $\lambda_\epsilon > \eta_\epsilon \implies$ extinction ahead of QSD;
- $\lambda_\epsilon < \eta_\epsilon \implies$ QSD ahead of extinction.

QSDs and transient states

Theorem (Z. Shen, S. Wang and Y. Yi, 2019)

- *For each* $\mathcal{O} \subset\subset (0,\infty) \setminus \{x_e\}$, *there are* $\gamma_{\mathcal{O}}$ *and* $\epsilon_{\mathcal{O}}$ *s.t.*

$$\mu_\epsilon(\mathcal{O}) \leq e^{-\frac{\gamma_{\mathcal{O}}}{\epsilon^2}}, \quad \forall \epsilon \in (0, \epsilon_{\mathcal{O}}).$$

QSDs and transient states

Theorem (Z. Shen, S. Wang and Y. Yi, 2019)

- *For each* $\mathcal{O} \subset\subset (0, \infty) \setminus \{x_e\}$, *there are* $\gamma_{\mathcal{O}}$ *and* $\epsilon_{\mathcal{O}}$ *s.t.*

$$\mu_\epsilon(\mathcal{O}) \le e^{-\frac{\gamma_{\mathcal{O}}}{\epsilon^2}}, \quad \forall \epsilon \in (0, \epsilon_{\mathcal{O}}).$$

- *The family* $\{\mu_\epsilon\}_\epsilon$ *is tight. Hence,* $\mu_\epsilon \to \delta_{x_e}$ *as* $\epsilon \to 0$.

QSDs and transient states

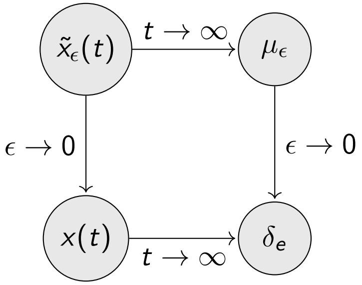
Theorem (Z. Shen, S. Wang and Y. Yi, 2019)

- *For each* $\mathcal{O} \subset\subset (0, \infty) \setminus \{x_e\}$, *there are* $\gamma_{\mathcal{O}}$ *and* $\epsilon_{\mathcal{O}}$ *s.t.*

$$\mu_\epsilon(\mathcal{O}) \leq e^{-\frac{\gamma_{\mathcal{O}}}{\epsilon^2}}, \quad \forall \epsilon \in (0, \epsilon_{\mathcal{O}}).$$

- *The family* $\{\mu_\epsilon\}_\epsilon$ *is tight. Hence,* $\mu_\epsilon \to \delta_{x_e}$ *as* $\epsilon \to 0$.

Commutative diagram:



Conclusion and vision

Conclusion:

- use QSDs to capture the transient states;
- study the concentration of QSDs;
- obtain results that are compatible with the intuition.

Conclusion and vision

Conclusion:

- use QSDs to capture the transient states;
- study the concentration of QSDs;
- obtain results that are compatible with the intuition.

Vision: stochastic model + QSD.

Conclusion and vision

Conclusion:

- use QSDs to capture the transient states;
- study the concentration of QSDs;
- obtain results that are compatible with the intuition.

Vision: stochastic model + QSD.

Advantages of stochastic theory of complicated transient dynamics:

- modeling: closer to reality;

Conclusion and vision

Conclusion:

- use QSDs to capture the transient states;
- study the concentration of QSDs;
- obtain results that are compatible with the intuition.

Vision: stochastic model + QSD.

Advantages of stochastic theory of complicated transient dynamics:

- modeling: closer to reality;
- math theory: could be simpler and more informative;

Conclusion and vision

Conclusion:

- use QSDs to capture the transient states;
- study the concentration of QSDs;
- obtain results that are compatible with the intuition.

Vision: stochastic model + QSD.

Advantages of stochastic theory of complicated transient dynamics:

- modeling: closer to reality;
- math theory: could be simpler and more informative;
- computation: could be more stable and accurate.

Thank you for your attention!