Metastability and Complex Eigenvalues for Markov processes

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## Outline

I  Markov Process Assumptions  
II  Metastability  
III  Complex Spectra  
IV  Quasi-Periodic Orbits  
V  Conclusions
Markov Process Assumptions

- Aperiodic, hypoelliptic diffusion. The state space $\mathbb{X}$ is an open, connected subset of $\mathbb{R}^d$.

- Differential generator $\mathcal{D} = u \cdot \nabla + \frac{1}{2} \text{trace} ( \Sigma \nabla^2 )$.

For $C^2$ functions

$$\mathcal{D}h = \sum_i u_i(x) \frac{d}{dx_i} h(x) + \frac{1}{2} \sum_{ij} \Sigma_{ij}(x) \frac{d^2}{dx_i dx_j} h(x)$$
Markov Process Assumptions

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  For $C^2$ functions

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- Condition (V4): For constants $b < \infty$, $\Gamma > 0$, a compact set $K \subset X$, and a function $V : X \rightarrow [1, \infty)$

  $\mathcal{D}V \leq -\Gamma V + b 1_K$
Ornstein-Uhlenbeck Process

\[ dX(t) = AX(t)dt + BdN(t) \]

- Hypo-elliptic: \((A, B)\) controllable
- Differential generator:
  \[ Dh = \sum_i (Ax)_i \frac{d}{dx_i} h(x) + \frac{1}{2} \sum_{ij} (BB^T)_{ij} \frac{d^2}{dx_i dx_j} h(x) \]
- Condition (V4): \( \lambda(A) < -\bar{\Gamma} < 0 \)
  \[ V(x) = 1 + \frac{1}{2} x^T M x \quad M > 0 \quad A^T M + MA = -I \]
  \[ \mathcal{D}V \leq -\bar{\Gamma} V + b 1_K \]
Eigenfunction Assumptions

For an open set $M$ and a function $h: \mathbb{X} \rightarrow \mathbb{R}$, $\Gamma_0 < \bar{\Gamma}$,

$$\mathcal{D}h(x) = -\Gamma_0 h(x) \quad \text{for } x \in M.$$

- $h$ is $C^2$ in a neighborhood of the closure $\bar{M}$
- Positive on $M$
- Zero on the boundary of $M$
- $\nabla h \neq 0$ for $x \in \partial M$. 
Outline

I Markov Process Assumptions

II Metastability

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Twisted Process

\[ \mathcal{D} h(x) = -\Gamma_0 h(x) \quad \text{for } x \in \mathbb{M}. \]

Doob’s \( h \)-transform:

\[ \mathcal{D} = I_{h^{-1}} \mathcal{D} I_h + \Gamma_0 I \]

\( I_h \) is the multiplication operator: \( I_h g = h \cdot g \)
Twisted Process

Doob’s $h$-transform: \[
\tilde{\mathcal{D}} = I_{h^{-1}} \mathcal{D} I_h + \Gamma_0 I
\]

Defines a differential generator for a diffusion $\tilde{X}$ on $\mathbb{X}$,

\[
\tilde{\mathcal{D}} = \mathcal{D} + \langle \Sigma(\nabla H), \nabla \rangle,
\]

\[
H(x) = \log(h(x))
\]
Twisted Process

Doob’s $h$-transform: \[ \mathcal{D} h(x) = -\Gamma_0 h(x) \quad \text{for } x \in M. \]

Doob’s $h$-transform: 
\[
\mathcal{D} = I_{h^{-1}} \mathcal{D} I_h + \Gamma_0 I \\
= \mathcal{D} + \langle \Sigma(\nabla H), \nabla \rangle
\]

Representation w.r.t. $X$: For any bounded function $g$,
\[
\mathcal{E}_x[g(\tilde{X}(t))] := \mathbb{E}_x[m_h(t)g(X(t))\mathbf{1}(T_\bullet > t)]
\]

where $T_\bullet$ is the first exit time from $M$, and
\[
m_h(t) := h(x)^{-1}h(X(t))e^{\Gamma_0 t}, \quad t \in \mathbb{T}
\]
Ornstein-Uhlenbeck Process

In one dimension: \( dX(t) = -aX(t)\,dt + \sigma\,dN(t) \)

Differential generator: \( \mathcal{D} = -ax\frac{d}{dx} + \frac{1}{2}\sigma^2\frac{d^2}{dx^2} \)

Eigenvalues:
\[ \{ \Lambda_k = -(k - 1)a : k = 1, 2, \ldots \} \]

First four eigenfunctions:
\[ h_1 \equiv 1 \]
\[ h_3(x) = \frac{1}{2}x^2 - \frac{\sigma^2}{4a} \]
\[ h_2(x) = x \]
\[ h_4(x) = \frac{1}{3}x^3 - \frac{\sigma^2}{2a}x \]
Ornstein-Uhlenbeck Process

In one dimension: \[ dX(t) = -aX(t)dt + \sigma dN(t) \]

Differential generator:
\[ \mathcal{D} = -ax \frac{d}{dx} + \frac{1}{2} \sigma^2 \frac{d^2}{dx^2} \]

Second eigenvalue: \[ \Lambda_2 = -a \]
Second eigenfunction: \[ h_2(x) = x \]

Generator for twisted process using \( h_2 \):
\[ \tilde{\mathcal{D}} = \mathcal{D} + \sigma^2 H'_2 dx = (-ax + \sigma^2/x)dx + \frac{1}{2} \sigma^2 dx^2 \]

Twisted process is ergodic on the positive real line \( \mathbb{R}_+ \)
Ergodicity of the Twisted Process

Twisted process is $\tilde{V}$-uniformly ergodic

$$\tilde{V} := h^{-1}(V + e^{\alpha H}) = h^{-1}(V + h^\alpha)$$

$\alpha < 1$
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$$\tilde{\mathcal{D}} \tilde{V} \leq -\frac{1}{2}(\Gamma - \Gamma_0) h^{-1} V + h^{-1} b \mathbf{1}_K$$

$$+ h^{\alpha-1} \left[ (1 - \alpha) \Gamma_0 + \frac{1}{2}(\Gamma - \Gamma_0) + bh^{-\alpha} \mathbf{1}_K 
- \frac{1}{2}(\Gamma - \Gamma_0)V h^{-\alpha} 
- \frac{1}{2}h^{-2}\alpha(1 - \alpha) \nabla h^T \Sigma \nabla h \right]$$

$$\leq -\frac{1}{2}(\Gamma - \Gamma_0) \tilde{V} + b_0 \mathbf{1}_{K_{n_0}}$$

$K_{n_0}$ compact subset of $M$ (sublevel set of $H$)
Ergodicity of the Twisted Process: Consequences

Based on $\tilde{V}$-ergodicity of the twisted process and the representation of $X$ and $\tilde{X}$ statistics we obtain:

The exit time from $M$ is approximately exponentially distributed:

$$P_x\left\{ \exp \left( \beta (T_\bullet - T) \right) \mid T_\bullet > T \right\} = \frac{\Gamma_0}{\Gamma_0 - \beta} + \mathcal{E}(x, T)$$

$$E_x[f(X(T)) \mid T_\bullet > T] = \tilde{\pi}(f) + \mathcal{E}(x, T)$$

MGF for exponential rv

Quasi steady-state on $M$

$$\mathcal{E} = O\left( v(x)h(x)^{-1}e^{-cT} \right)$$

Huisinga M. Schuette '03
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Complex Eigenvalues

Suppose that $\Lambda$ is a complex eigenvalue, written as

$$\Lambda = -\Gamma + i\vartheta$$

with $\Gamma > 0$, and $\vartheta \neq 0$. 
Periodicity

Consider sampled process, or skeleton chain,

\[ X(\beta + \tau k) \quad k = 0, 1, 2, \ldots \]

\( \tau \): Sampling time

Eigenvalues in unit circle:

\[ \lambda = e^{\tau \Lambda} \]

\[ \Lambda = -\Gamma + iv\theta \]

If \( \Gamma = 0 \) then periodicity ...
Periodicity

Eigenvalue on unit circle $\lambda = e^{i\tau\vartheta}$

Periodicity

Sampling time $\tau = 2\pi\vartheta^{-1}$
Periodicity

Eigenvalue on unit circle \( \Rightarrow \) Periodicity

Sampling time

\[ \tau = 2\pi \theta^{-1} \]

\[ \lambda = e^{i\tau \theta} \]

\[ \Rightarrow \text{Skeleton chain} \]

\[ X(\beta + \tau k) \]

is ergodic on subset \( X_\beta \)
Periodicity

Eigenvalue on unit circle $\rightarrow$ Periodicity $\rightarrow$ Sampling time

$\lambda = e^{i\tau \theta}$

Skeleton chain is ergodic on subset $X_{\beta}$

Distinct skeleton chains are mutually singular:

$X_{\beta_1} \cap X_{\beta_2} = \emptyset \quad \beta_1 \neq \beta_2$

$\tau = 2 \pi \theta^{-1}$
Procedure:  1. Compute POD modes from given data.

2. Observe time-evolution of first two POD coefficients (projection of data onto first two POD modes)

3. Construct Perfect-Prediction Markov model
Markov Model from Jet Engine Data

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1. Compute POD modes from given data.
2. Observe time-evolution of first two POD coefficients (projection of data onto first two POD modes)
3. Construct Perfect-Prediction Markov model

Phase portrait of first two POD coefficients
Invariant measure for Markov model
Spectrum from Jet Engine Model

\[ \lambda = e^{\tau \Lambda} \]

\( \tau \): Sampling time
\( \Lambda = -\Gamma + iv^\theta \)
Phase of second eigenfunction:
Degenerate model: Spectrum of skeleton is entirely real

Spectrum from Jet Engine Model

Spectrum of $P$

Spectrum of $P^{67}$
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Suppose that $\Lambda$ is a complex eigenvalue, written as

$$\Lambda = -\Gamma + iv$$

with $\Gamma > 0$, and $v \neq 0$.

Introduce the clock process:

$$\Phi(t) = \Phi(0)e^{ivt}, \quad t \geq 0$$
Complex Eigenvalues

Suppose that $\Lambda$ is a complex eigenvalue, written as

$$\Lambda = -\Gamma + iv\vartheta$$

with $\Gamma > 0$, and $\vartheta \neq 0$.

Introduce the clock process:

$$\Phi(t) = \Phi(0)e^{i\vartheta t}, \quad t \geq 0$$

Bivariate process is another diffusion:

$$Y(t) = \begin{pmatrix} X(t) \\ \Phi(t) \end{pmatrix}, \quad t \geq 0$$

Its spectrum is continuous, since this is true for $\Phi$. 
Suppose that \( h \) is an eigenfunction for \( X \)

Define for real-valued \( \beta \in \mathbb{R} \)

\[
g_\beta(y) = \text{Re} \left( \left( e^{i\beta}/\phi \right) h(x) \right), \quad y = (x, \phi) \in Y
\]
Suppose that \( h \) is an eigenfunction for \( X \)

Define for real-valued \( \beta \in \mathbb{R} \)

\[
g_\beta(y) = \text{Re} \left( \frac{e^{i\beta}}{\phi} h(x) \right), \quad y = (x, \phi) \in Y
\]

**Proposition:** The function \( g_\beta \) is an eigenfunction for \( Y \), with real eigenvalue

\[
\Lambda_Y = -\Gamma
\]
Suppose that $h$ is an eigenfunction for $X$.

Define for real-valued $\beta \in \mathbb{R}$

$$g_\beta(y) = \Re \left( \left( e^{i\beta} / \phi \right) h(x) \right), \quad y = (x, \phi) \in Y$$

**Proposition:** The function $g_\beta$ is an eigenfunction for $Y$, with real eigenvalue

$$\Lambda_Y = -\Gamma$$

Conclusion: We can define a twisted process, provided we can verify previous assumptions.
EigenfunctionTranslation

\[ Y(t) = \begin{pmatrix} X(t) \\ \Phi(t) \end{pmatrix} \]

\[ M \subset Y \text{ is an open connected component of } \{ y \in Y : g_0(y) > 0 \} \]

\[ g_\beta(y) = \text{Re} \left( (e^{i\beta} / \phi) h(x) \right) \]
Eigenfunction Translation

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\( M \subset Y \) is an open connected component of

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Assume as before:

- \( h \) and hence \( g_\beta \) is \( C^2 \)
- \( g_0 \) positive on \( M \)
- \( g_0 \) zero on the boundary of \( M \)
\[ Y(t) = \begin{pmatrix} X(t) \\ \Phi(t) \end{pmatrix} \]

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Assume as before:

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- \( g_0 \) positive on \( M \)
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Strengthen remaining assumptions:

- Ellipticity: \( \Sigma(x) > 0 \) for all \( x \)
- \( \nabla_x g_0(y) = \text{Re} \left( \phi^{-1}\nabla h(x) \right) \neq 0 \) for all \( y = (x, \phi) \in \partial M \)
Metastability

\[ Y(t) = \begin{pmatrix} X(t) \\ \Phi(t) \end{pmatrix} \]

\( Y(t) \) remains in the set \( M \) for a time period approximately exponentially distributed, with parameter \( \Gamma \)
Metastability

\[ Y(t) = \begin{pmatrix} X(t) \\ \Phi(t) \end{pmatrix} \]

\( Y(t) \) remains in the set \( M \) for a time period approximately exponentially distributed, with parameter \( \Gamma \).

\( X(t) \) remains in a set-valued periodic orbit for the same time period.
Phase of second eigenfunction:

\[ e^{-i\vartheta t} h(X(t)) \]

remains positive-real for exp. distributed period
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Conclusions

**Main result:**

Complex spectra carry wealth of information!

When there is a spectral gap then trajectory evolves as a quasi-periodic orbit, lasting approximately \( \exp(\Gamma) \) seconds.

**Questions:**

*Examples, Applications:*

- Dynamical insight, optimization, inference

*Learning:*

- Insight for non-Markov models & perfect prediction
- Error bounds for learning coarse Markov model