



Spectral Theory and Model Reduction for Markov Models

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Questions

- When is there a spectral gap? A discrete spectrum?
- What can we learn from eigenfunctions and eigenvalues?
- Can we approximate by a finite state space Markov chain?

So what?

Applications to model reduction.

Also, LDP theory, simulation, ...

Spectral theory in practice ...

- *Fiedler* Fiedler cuts in graph theory
- *Hendrickson and Leland*. Computation
- *Bovier* Neural nets, and theoretical foundations for diffusions
- *Garcia* (and Dellnitz, Schuette) Protein folding
- *Vanden-Eijnden* Various applications, computation for diffusions
- *Kleinberg's* HITS algorithm for web page ranking
- *Mehta, Hagen* Jet engines
- *Mezic, Banaszuk* Fuel cells, ...
- *Roberts et. al.* CDMA

Outline

I Generators & Spectrum

II Lyapunov Functions and Spectra

III Metastability

IV Example: Three-Well Potential

V Example: Jet Engine Dynamics

VI Conclusions

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Generator for an ODE

$$\frac{d}{dt}x(t) = \phi(x(t))$$

The generator is defined for C^1 functions,

$$\mathcal{D}h(x) := \left. \frac{d}{dt}h(x(t)) \right|_{\substack{t=0 \\ x=x(0)}} = \langle \phi(x), \nabla h(x) \rangle$$

Fundamental Theorem of Calculus,

$$h(x(T)) = h(x(0)) + \int_0^T \mathcal{D}h(x(t)) dt$$

Generator for an SDE

$$dX(t) = \phi(X(t)) dt + B(X(t))dN(t)$$

The generator is defined for C^2 (extra nice) functions ,

$$\begin{aligned} \mathcal{D}h(x) &:= \frac{d}{dt} \mathbb{E}[h(X(t)) \mid X(0) = x] \Big|_{t=0} \\ &= \langle \phi(x), \nabla h(x) \rangle + \frac{1}{2} \text{trace}(\Sigma(x) \nabla^2 h(x)) \end{aligned}$$

$$\Sigma(x) = B(x)B(x)^T$$

Martingale Representation

$$\mathbb{E} \left[h(X(T)) - \int_0^T \mathcal{D}h(X(t)) dt \right] = h(X(0))$$

Eigenfunction for an ODE $\mathcal{D}h = \lambda h$

$z(t) = h(x(t))$ solution to linear ODE,

$$\frac{d}{dt}z(t) = \lambda z(t)$$

Applications

Decomposition:

If λ is nearly zero, level sets of h are *almost invariant*

The set $\{h(x) > 0\}$ is *invariant*

Eigenfunction for an ODE $\mathcal{D}h = \lambda h$

$z(t) = h(x(t))$ solution to linear ODE,

$$\frac{d}{dt}z(t) = \lambda z(t)$$

Applications

Model reduction: $z(t) = (z_1(t), \dots, z_n(t)) = (h_1(x(t)), \dots, h_n(x(t)))$

Simple linear description,

$$\frac{d}{dt}z(t) = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & \\ \vdots & & \ddots & \\ 0 & & & \lambda_n \end{pmatrix} z(t)$$

Eigenfunction for an SDE $\mathcal{D}h = \lambda h$

$Z(t) = h(X(t))$ solution to *almost* linear SDE,

$$dZ(t) = \lambda Z(t) + dN_Z(t)$$

white noise

$$dN_Z(t) := \nabla h(X(t)) \cdot B(X(t)) dN_X(t)$$

Applications ...

Decompositions ? model reduction ??

This is the subject of this talk!

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Markov Process Assumptions

- Aperiodic, hypoelliptic diffusion. The state space X is an open, connected subset of \mathbb{R}^d
- Differential generator $\mathcal{D} = \phi \cdot \nabla + \frac{1}{2} \text{trace}(\Sigma \nabla^2)$.
For C^2 functions

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

Exponential Ergodicity

Condition (V4): For some $V: X \rightarrow [1, \infty)$, $b < \infty$, $\delta > 0$
 K compact

$$\mathcal{D}V \leq -\delta V + b\mathbb{I}_K$$

Under a density assumption, the diffusion is exponentially ergodic,

There is a spectral gap

Ornstein-Uhlenbeck Process

$$dX(t) = AX(t)dt + BdN(t)$$

- Hypo-elliptic: (A, B) controllable
- Differential generator:

$$\mathcal{D}h = \sum_i (Ax)_i \frac{d}{dx_i} h(x) + \frac{1}{2} \sum_{ij} (BB^T)_{ij} \frac{d^2}{dx_i dx_j} h(x)$$

- Condition (V4):

$$\mathcal{D}V \leq -\bar{\Gamma}V + b\mathbf{1}_K$$

$$V(x) = 1 + \frac{1}{2} x^T M x \quad M > 0 \quad A^T M + M A = -I$$

Exponential Ergodicity

Condition (V4): For some $V: X \rightarrow [1, \infty)$, $b < \infty$, $\delta > 0$
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$$\mathcal{D}V \leq -\delta V + b\mathbb{I}_K$$

Exponential ergodicity?

Choose weighted norm, $L_\infty^V = \left\{ f : \|f\|_V \triangleq \sup_{x \in X} \frac{|f(x)|}{V(x)} < \infty \right\}$

$$\|P^t - \pi\|_V \triangleq \sup_{\|f\|_V=1} \left(\|P^t f - \pi(f)\|_V \right) \rightarrow 0 \quad \text{Exponentially fast}$$

Exponential Ergodicity

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Spectral gap?

Choose weighted norm, $L_\infty^V = \left\{ f : \|f\|_V \triangleq \sup_{x \in X} \frac{|f(x)|}{V(x)} < \infty \right\}$

$$[Iz - \mathcal{D}]^{-1} \text{ Isolated pole at } z = 0 \quad \mathcal{D}\mathbf{1} = 0 \quad \pi\mathcal{D} = 0$$

$$[Iz - (\mathcal{D} - \mathbf{1} \otimes \pi)]^{-1} \text{ exists for } z \sim 0$$

Drift condition of Donsker & Varadhan

The nonlinear generator is defined by, $\mathcal{H}(F) = e^{-F} \mathcal{D}e^F$

Condition (DV3): For some $V, W : X \rightarrow [1, \infty)$, $b < \infty$,
 K compact

$$\mathcal{H}(V) \leq -W + b\mathbb{I}_K$$

W has compact sublevel sets

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Example: $dX(t) = AX(t) dt + B dN(t)$

(A, B) controllable
 $\lambda(A) < 0$

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Example: $dX(t) = AX(t) dt + B dN(t)$

$$V(x) = 1 + \frac{\varepsilon}{2} x^T M x$$

$$W(x) = 1 + \delta \|x\|$$

(A, B) controllable
 $\lambda(A) < 0$

$$M > 0$$

$$A^T M + M A = -I$$

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Under a density assumption a global LDP is established,
the rate function is identified as relative entropy,
and

the spectrum is discrete

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Proof: (for those of you following this week's short course)

$$R \approx \sum s_i \otimes \nu_i \quad \text{on } S_n = \{x : W(x) \leq n\}$$

under density assumption on R

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$$\|R - I_{S_n^c} R I_{S_n^c}\|_v = \varepsilon(n) \quad \text{if and only if (DV3) holds}$$

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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 $x \in \partial M$.

Twisted Process

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

$$\text{Doob's } h\text{-transform: } \check{\mathcal{D}} = I_{h^{-1}} \mathcal{D} I_h + \Gamma_0 I$$

I_h is the multiplication operator: $I_h g = h \cdot g$

Twisted Process

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$$\text{Doob's } h\text{-transform: } \check{\mathcal{D}} = I_{h^{-1}} \mathcal{D} I_h + \Gamma_0 I$$

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

$$\check{\mathcal{D}} = \mathcal{D} + \langle \Sigma(\nabla H), \nabla \rangle,$$

$$H(x) = \log(h(x))$$

Twisted Process

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

$$\begin{aligned} \text{Doob's } h\text{-transform: } \check{\mathcal{D}} &= I_{h^{-1}} \mathcal{D} I_h + \Gamma_0 I \\ &= \mathcal{D} + \langle \Sigma(\nabla H), \nabla \rangle \end{aligned}$$

Representation w.r.t. \check{X} : For any bounded function g ,

$$\check{\mathbb{E}}_x[g(\check{X}(t))] := \mathbb{E}_x[m_h(t)g(X(t))\mathbf{1}(T_\bullet > t)]$$

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:

$$\{\Lambda_k = -(k-1)a : k = 1, 2, \dots\}$$

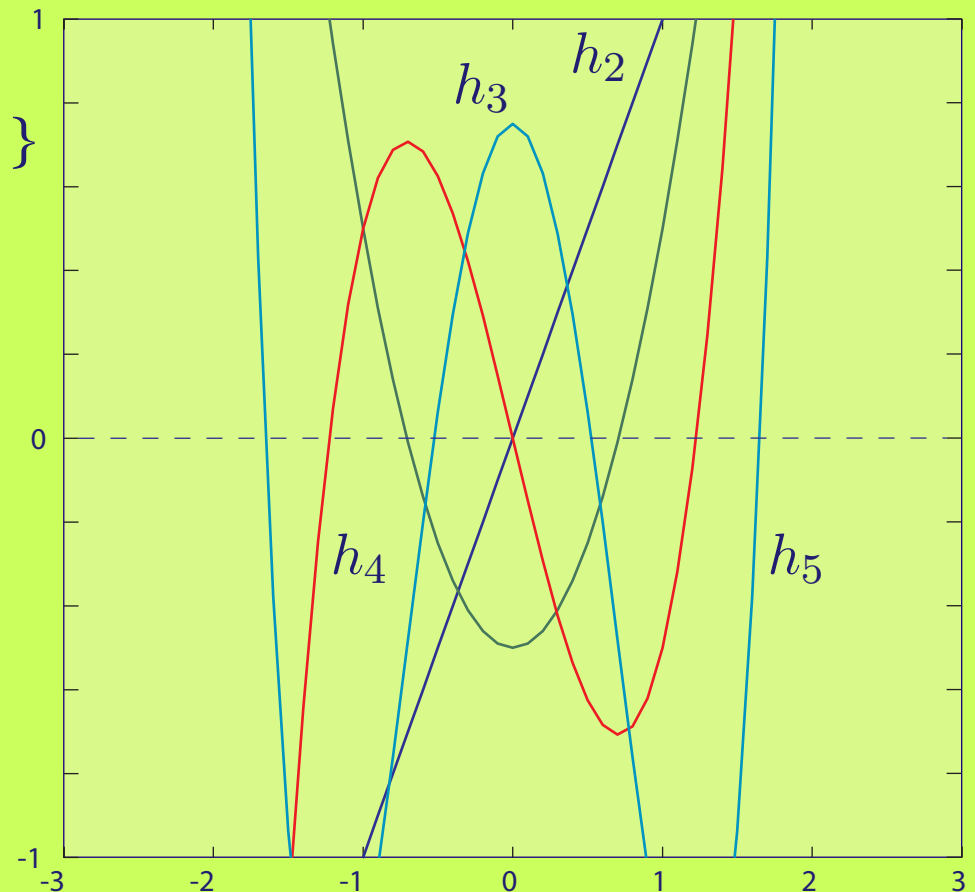
First four eigenfunctions:

$$h_1 \equiv 1$$

$$h_3(x) = \frac{1}{2}x^2 - \frac{\sigma^2}{4a}$$

$$h_2(x) = x$$

$$h_4(x) = \frac{1}{3}x^3 - \frac{\sigma^2}{2a}x$$

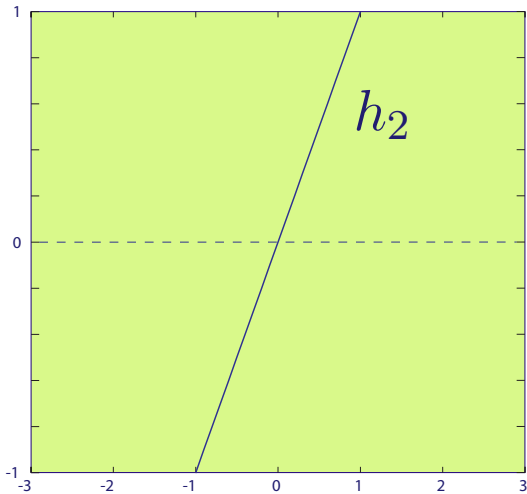


Ornstein-Uhlenbeck Process

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 :

$$\check{\mathcal{D}} = \mathcal{D} + \sigma^2 H_2' dx = (-ax + \sigma^2/x)dx + \frac{1}{2}\sigma^2 dx^2$$

Twisted process is ergodic on the positive real line \mathbb{R}_+

Ergodicity of the Twisted Process

Twisted process is \check{V} -uniformly ergodic

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

$$\alpha < 1$$

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Twisted process is \check{V} -uniformly ergodic

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$$\alpha < 1$$

$$\begin{aligned} \check{D}\check{V} &\leq -\frac{1}{2}(\bar{\Gamma} - \Gamma_0)h^{-1}V + h^{-1}b\mathbf{1}_K \\ &\quad + h^{\alpha-1}\left[(1-\alpha)\Gamma_0 + \frac{1}{2}(\bar{\Gamma} - \Gamma_0) + bh^{-\alpha}\mathbf{1}_K \right. \\ &\quad \quad \left. - \frac{1}{2}(\bar{\Gamma} - \Gamma_0)Vh^{-\alpha} \right. \\ &\quad \quad \left. - \frac{1}{2}h^{-2}\alpha(1-\alpha)\nabla h^T\Sigma\nabla h\right] \\ &\leq -\frac{1}{2}(\bar{\Gamma} - \Gamma_0)\check{V} + b_0\mathbf{1}_{K_{n_0}} \end{aligned}$$

K_{n_0} compact subset of M
(sublevel set of H)

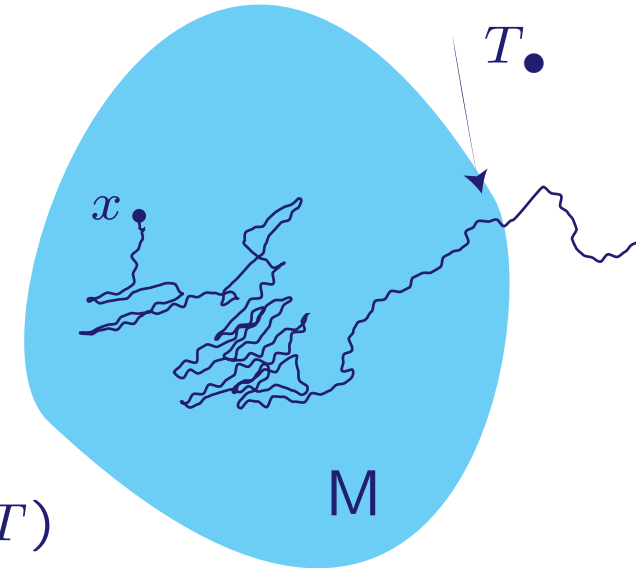
Ergodicity of the Twisted Process: Consequences

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

The exit time from M is approximately exponentially distributed:

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

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



MGF for exponential rv

Quasi steady-state on M

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

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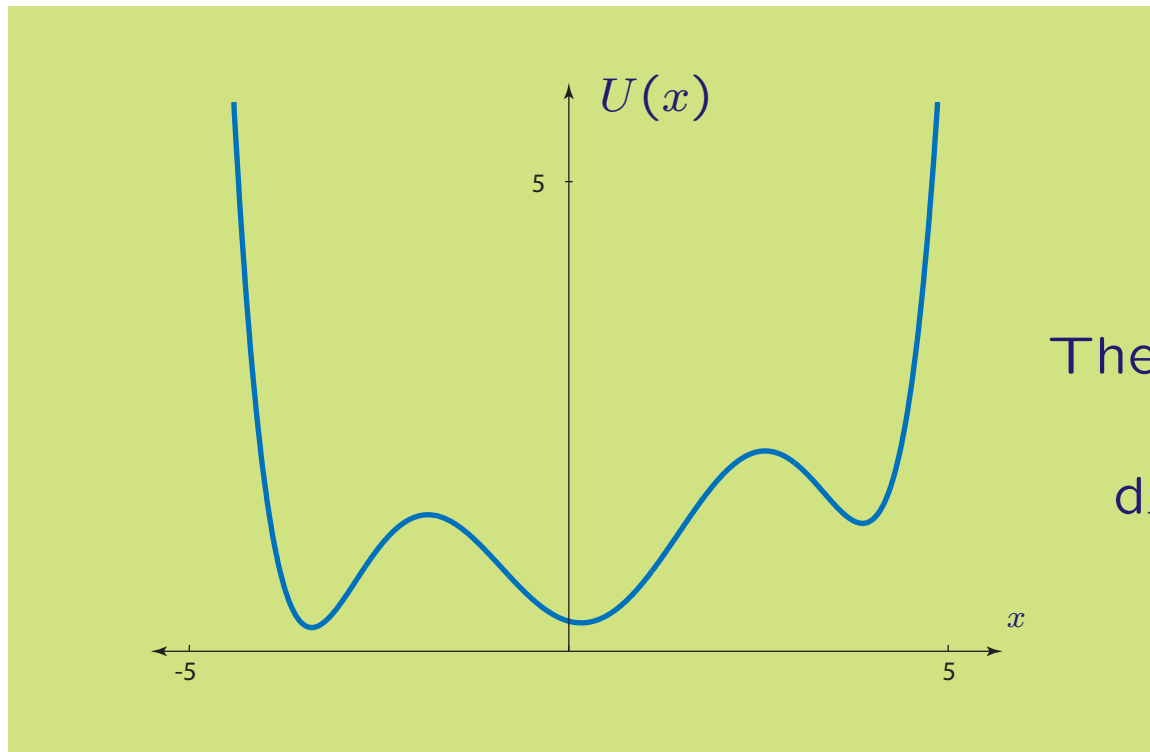
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The three-well potential



The Smoluchowski equation

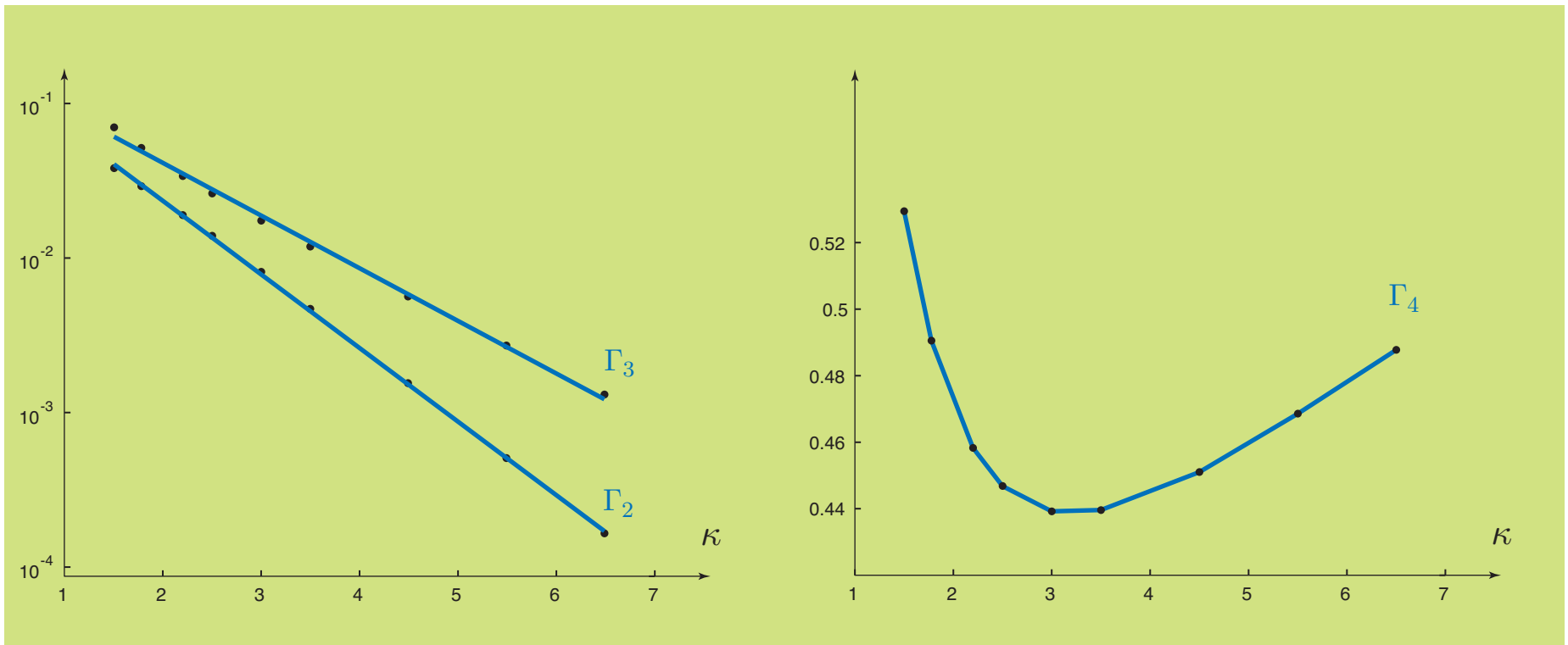
$$dX = -\frac{1}{\gamma} \nabla U(X) dt + \frac{\sigma}{\gamma} dW$$

$V(x) = e^{\eta U(x)}$ solves (DV3)

Invariant distribution with density $p(x) = \gamma e^{-\kappa U(x)}$

where $\kappa = 2\gamma/\sigma^2$ is the *inverse temperature*

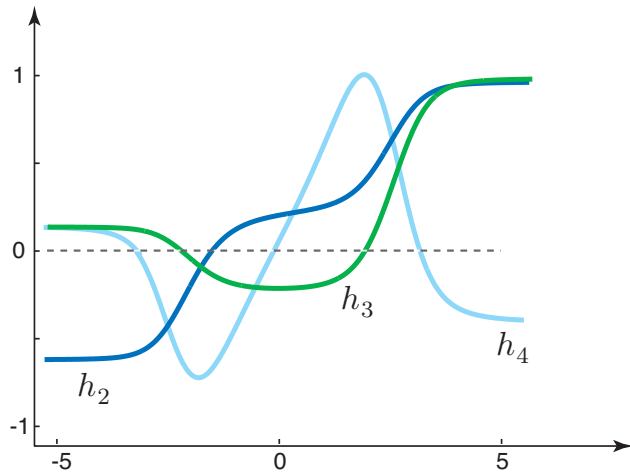
Eigenvalues as a function of κ



The second and third eigenvalues converge to zero

The fourth eigenvalue is bounded away from zero

Eigenfunctions and decompositions



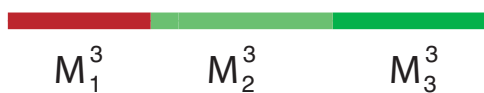
Three eigenfunctions



Decomposition based on zeros of h_2h_3

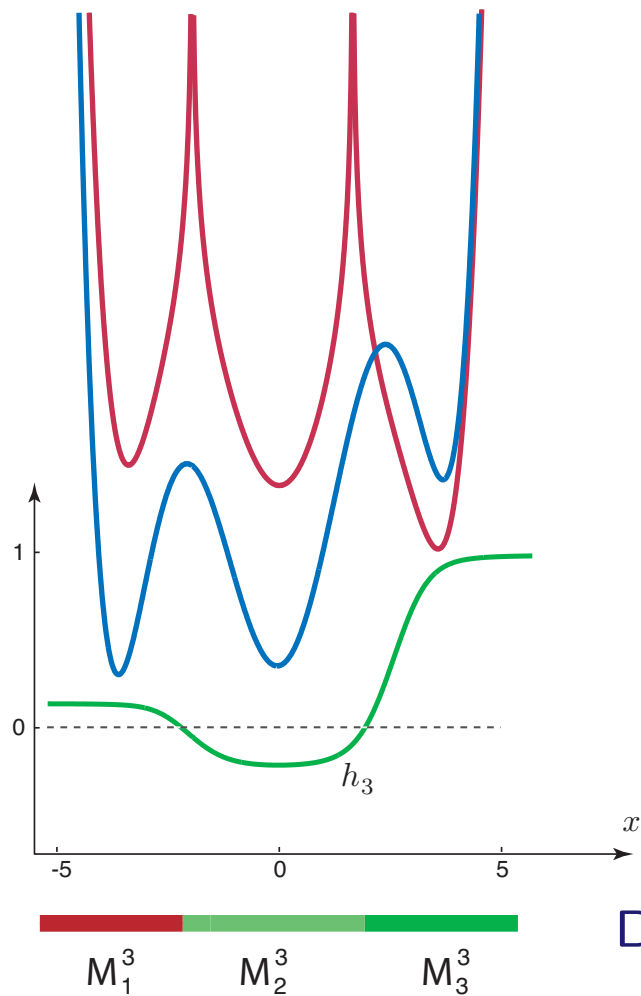


Decomposition based on zeros of h_2



Decomposition based on zeros of h_3

The twisted potential



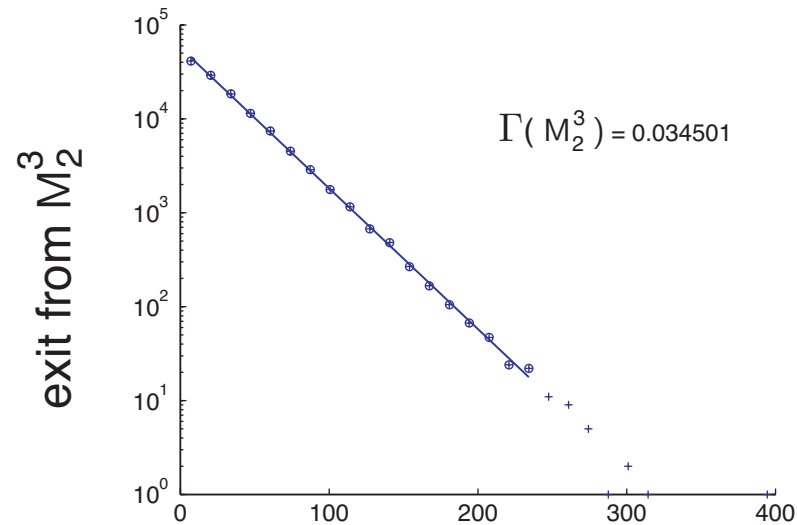
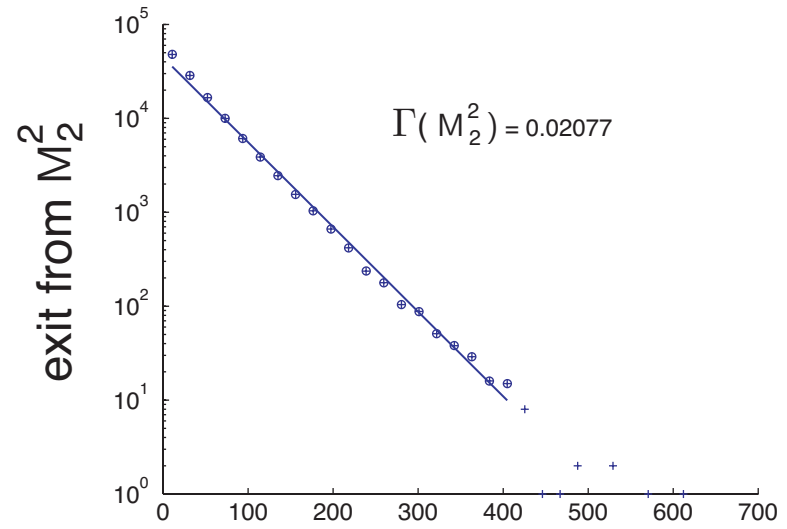
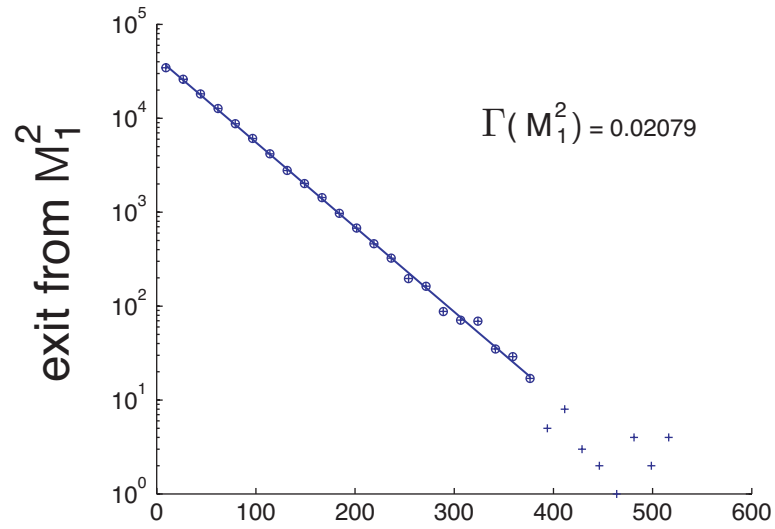
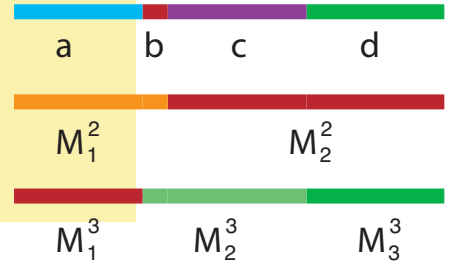
— The potential function $U(x)$

— The twisted potential function:

$$U_3(x) = U(x) - \sigma^2 \log(|h_3(x)|)$$

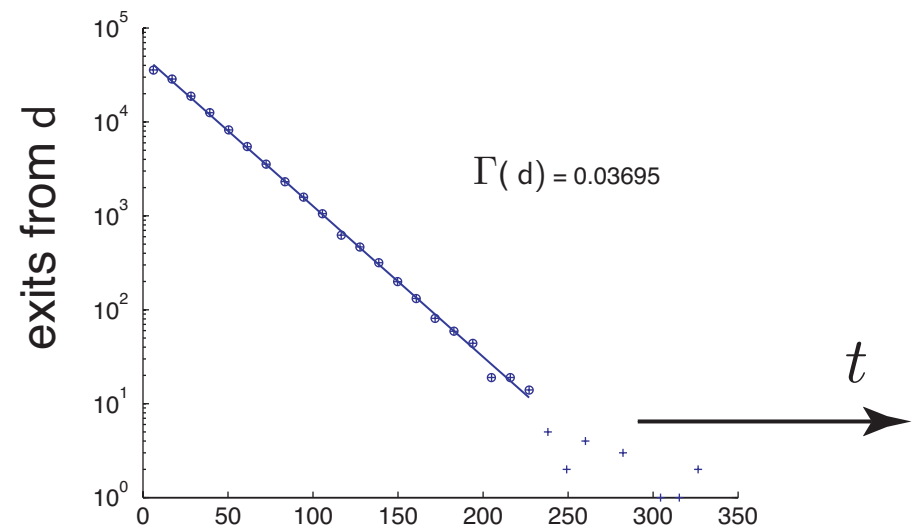
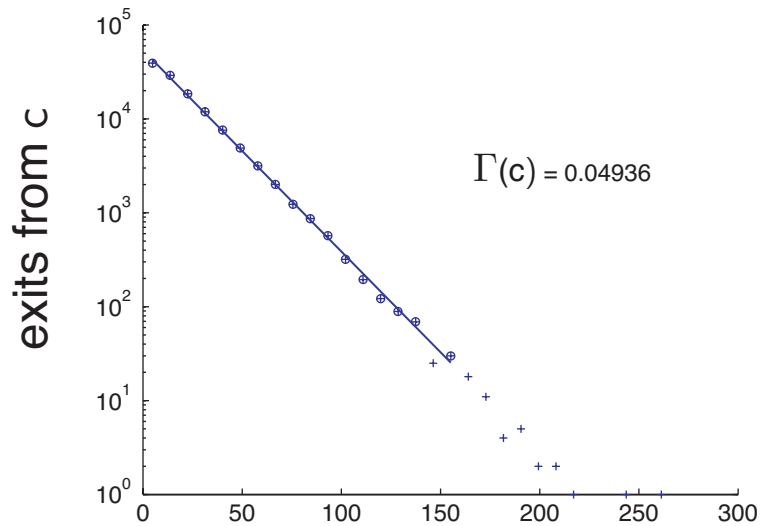
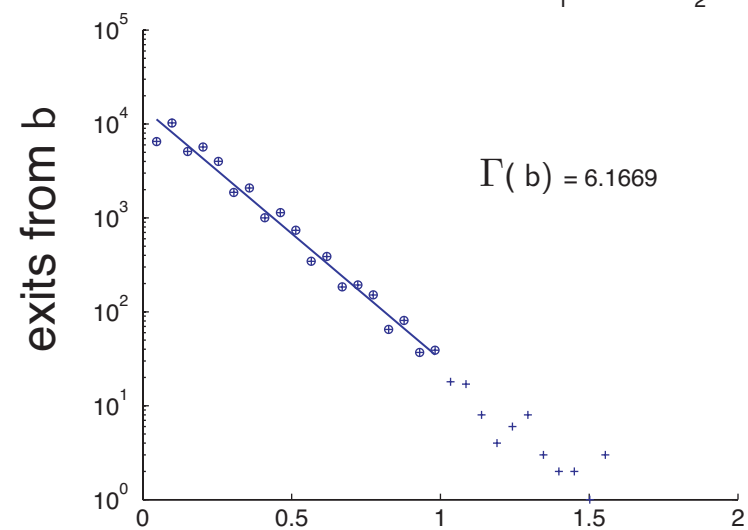
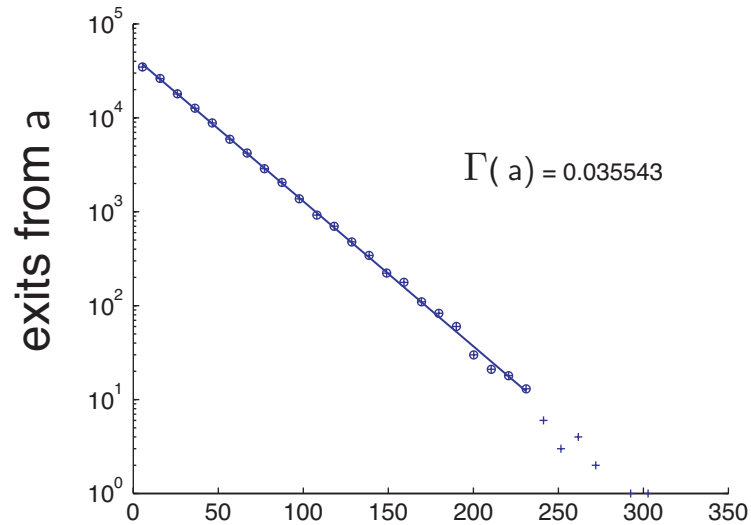
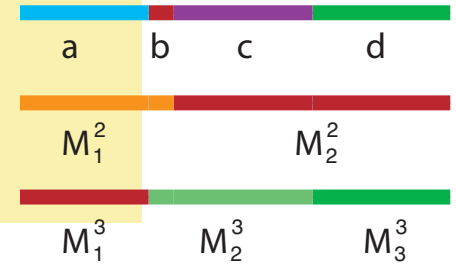
Decomposition based on zeros of h_3

Exit time distributions



\longrightarrow
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Exit time distributions



Exit time distribution for the sets $S = \{a, b, c, d\}$ and their combinations

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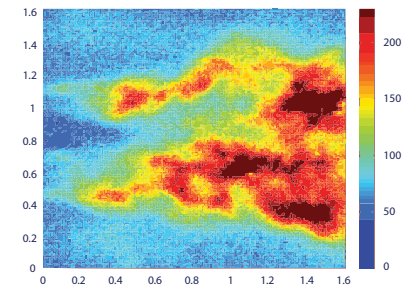
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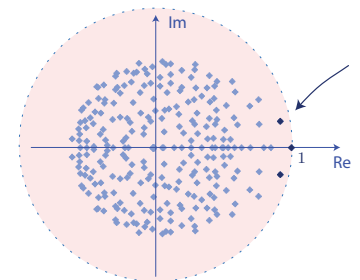
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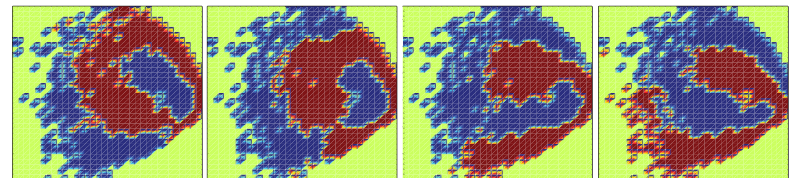
VI Conclusions



Flame Dynamics



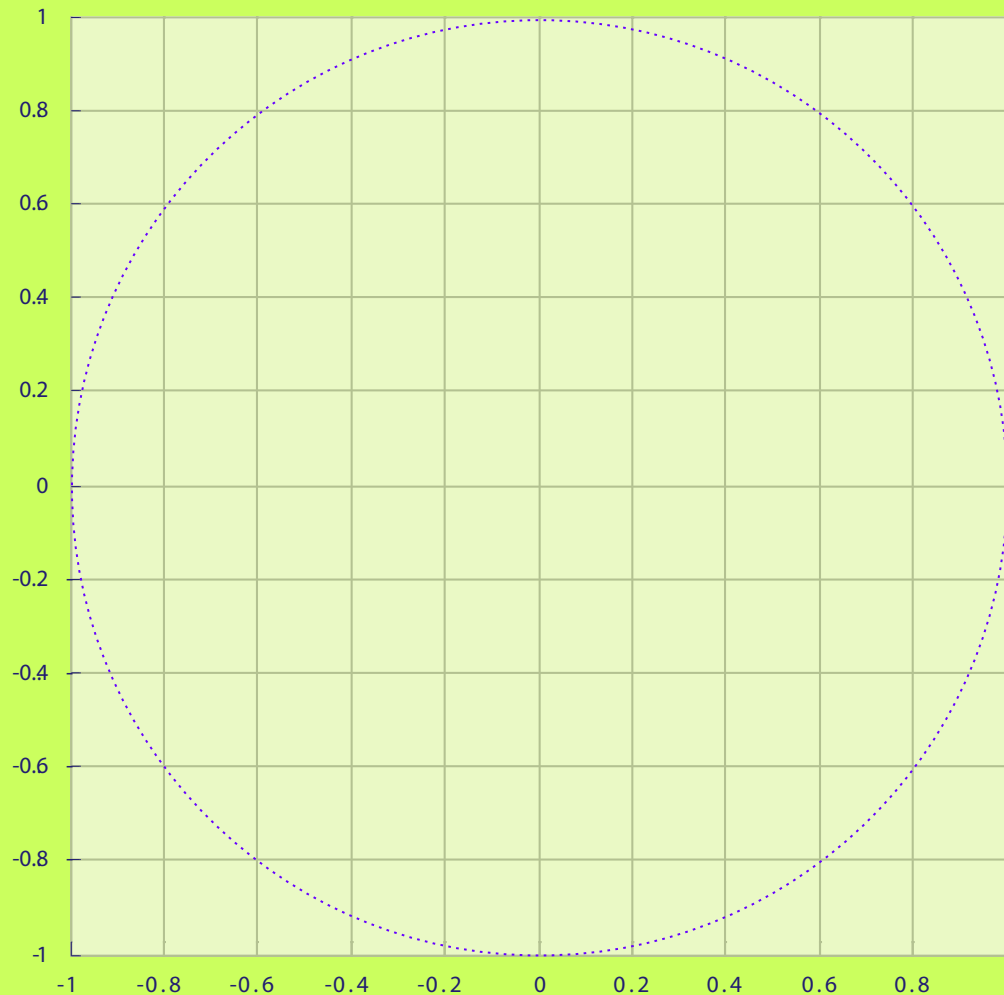
Spectrum



Quasi-Periodicity

Periodicity

Consider sampled process, or *skeleton chain*,



$$X(\beta + \tau k) \quad k = 0, 1, 2, \dots$$

τ : Sampling time

Eigenvalues in unit circle:

$$\lambda = e^{\tau\Lambda}$$

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

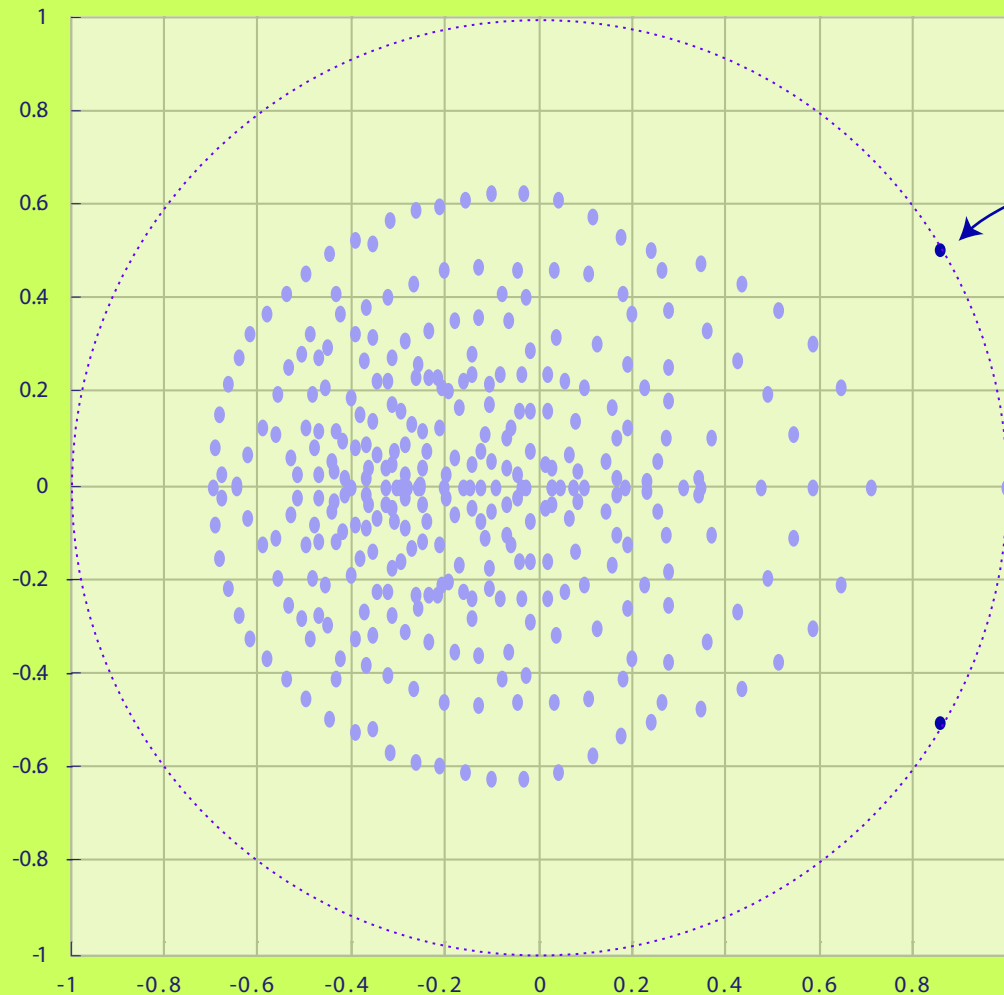
If $\Gamma = 0$ then periodicity ...

Periodicity

Eigenvalue on unit circle \Rightarrow Periodicity

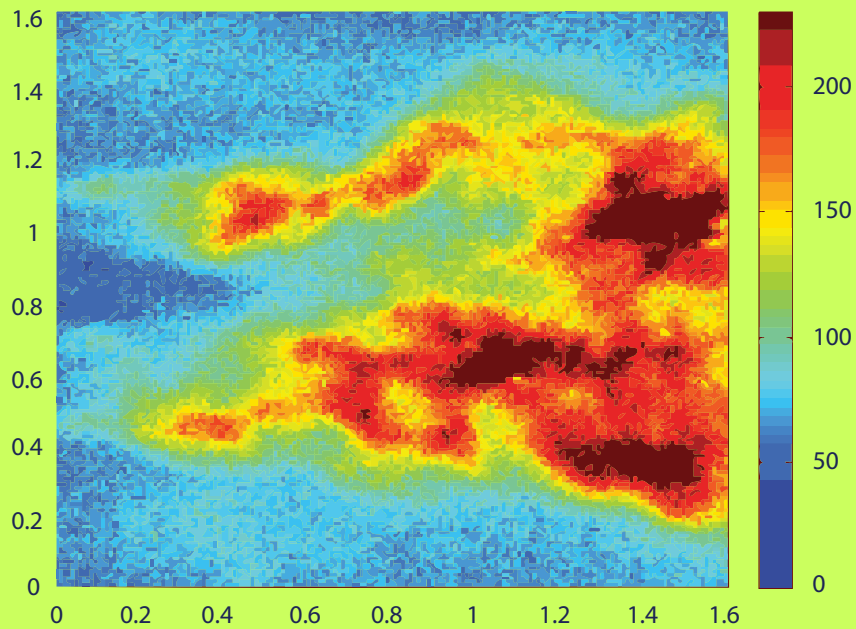
Sampling time

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



$$\lambda = e^{i\pi\vartheta}$$

Markov Model from Jet Engine Data



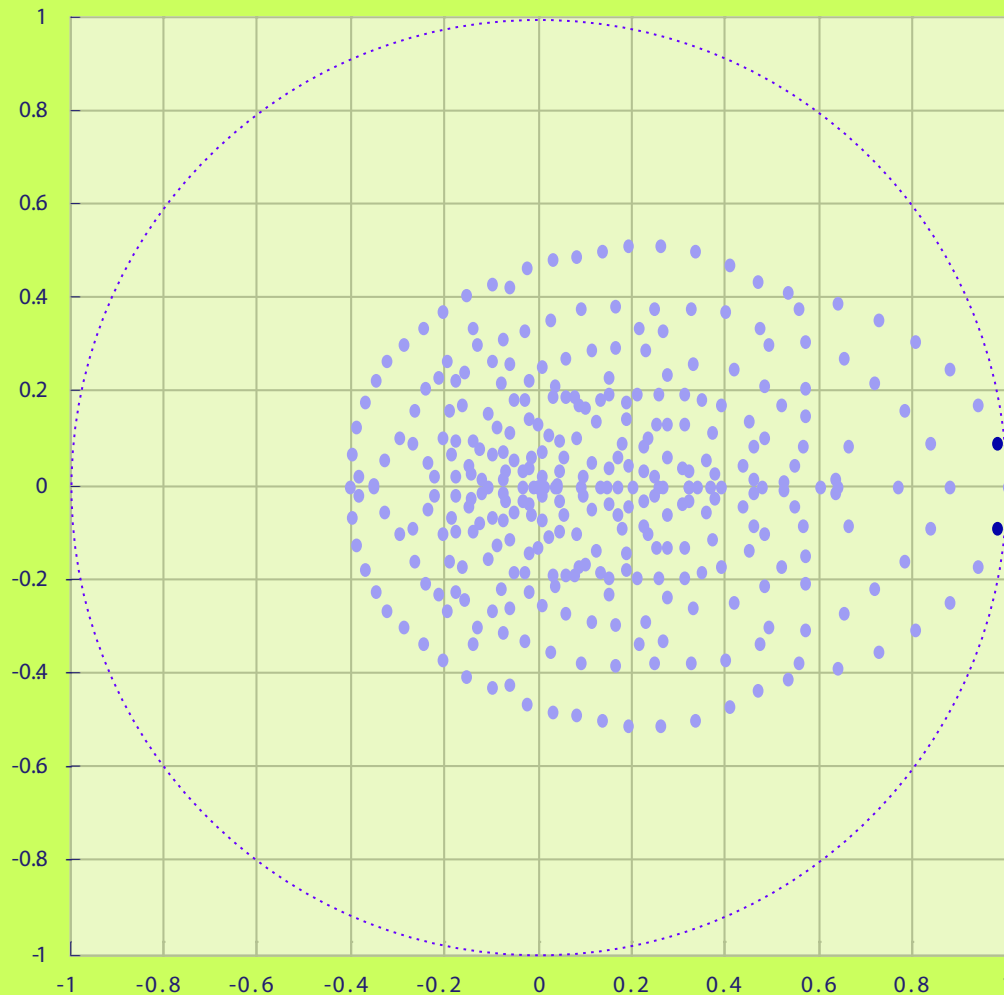
Flame Dynamics

Markov model obtained using Bayes' Rule

- [16] K. A. Teerlinck, G. Hagen, A. Banaszuk, J. A. Lovett, J. M. Cohen, A. Ateshkadi, and B. V. Kiel. Demonstration of thermoacoustic instability control in a three-flameholder combustor. *53rd JANNAF (Joint Army-Navy-NASA-Air Force) Propulsion Meeting, Monterey, CA, Dec 5-8, 2005*.
- [17] U. Vaidya and G. Hagen. Empirical model extraction from time resolved image data. *Proceedings of the American Control Conference, 2008*.

Spectrum from Jet Engine Model

Spectrum:



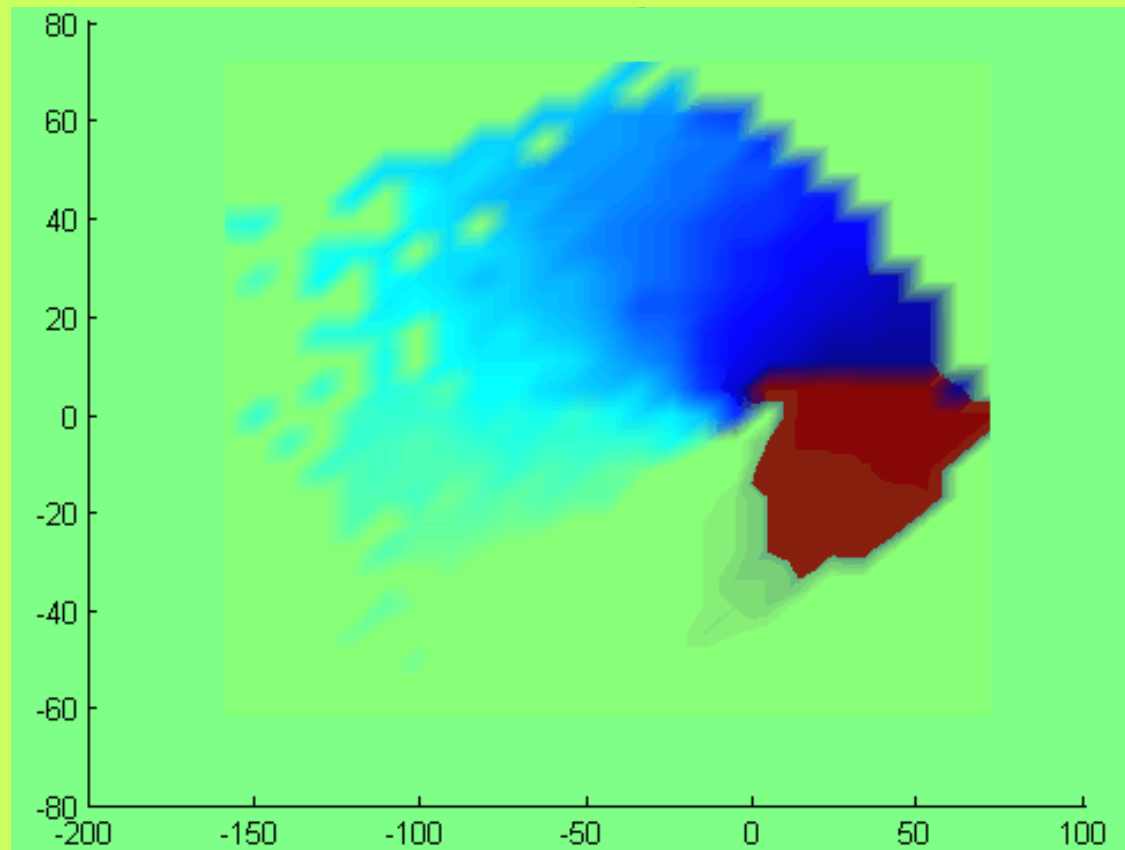
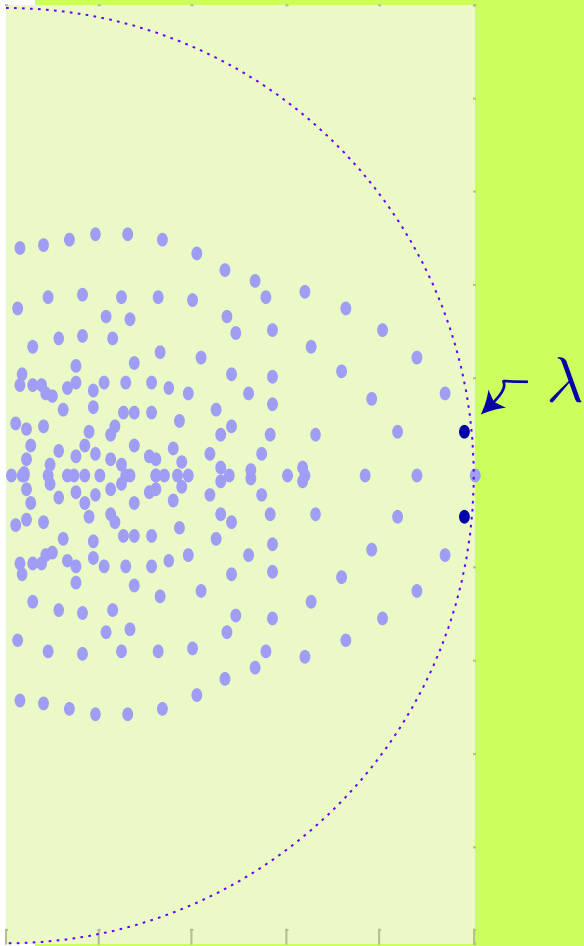
$$\lambda = e^{\tau\Lambda}$$

τ : Sampling time

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

Spectrum from Jet Engine Model

Phase of second eigenfunction:



Complex Eigenvalues

Suppose that Λ is a complex eigenvalue, written as

$$\Lambda = -\Gamma + i\vartheta \quad \text{with } \Gamma > 0, \text{ and } \vartheta \neq 0.$$

Introduce the clock process:

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

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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 Φ

Eigenfunction Translation

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

Suppose that h is an eigenfunction for X

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

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

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

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

Proposition: The function g_β is an eigenfunction for Y , with real eigenvalue

$$\Lambda_Y = -\Gamma$$

Eigenfunction Translation

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

Suppose that h is an eigenfunction for X

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

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

Proposition: The function g_β is an eigenfunction for Y , with real eigenvalue

$$\Lambda_Y = -\Gamma$$

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

Eigenfunction Translation

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

$M \subset Y$ is an open connected component of

$$\{y \in Y : g_0(y) > 0\}$$

$$g_\beta(y) = \operatorname{Re}((e^{i\beta}/\phi)h(x))$$

Eigenfunction Translation

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

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Assume as before:

- h and hence g_β is C^2
- g_0 positive on M
- g_0 zero on the boundary of M

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Assume as before:

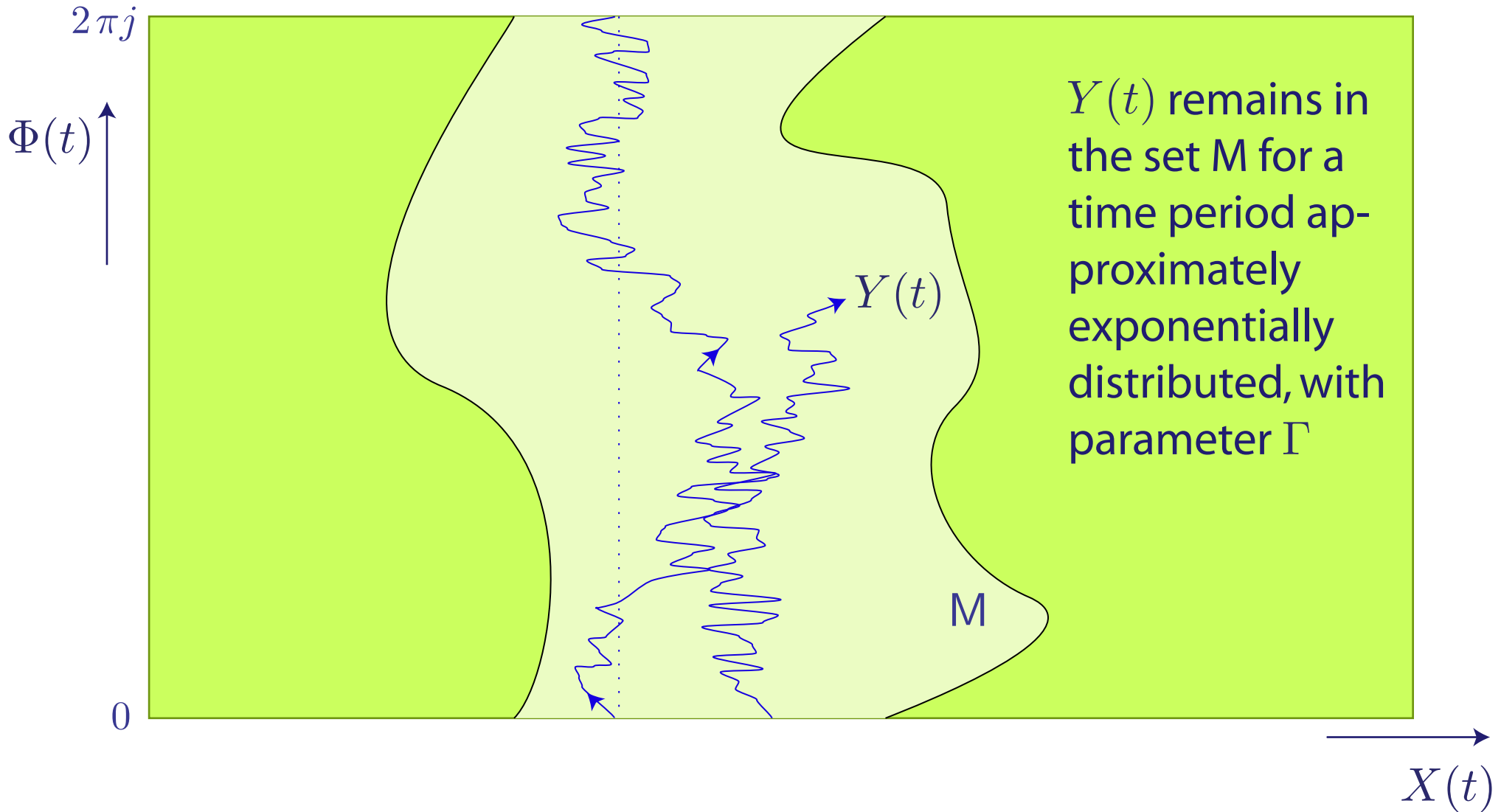
- h and hence g_β is C^2
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Strengthen remaining assumptions:

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

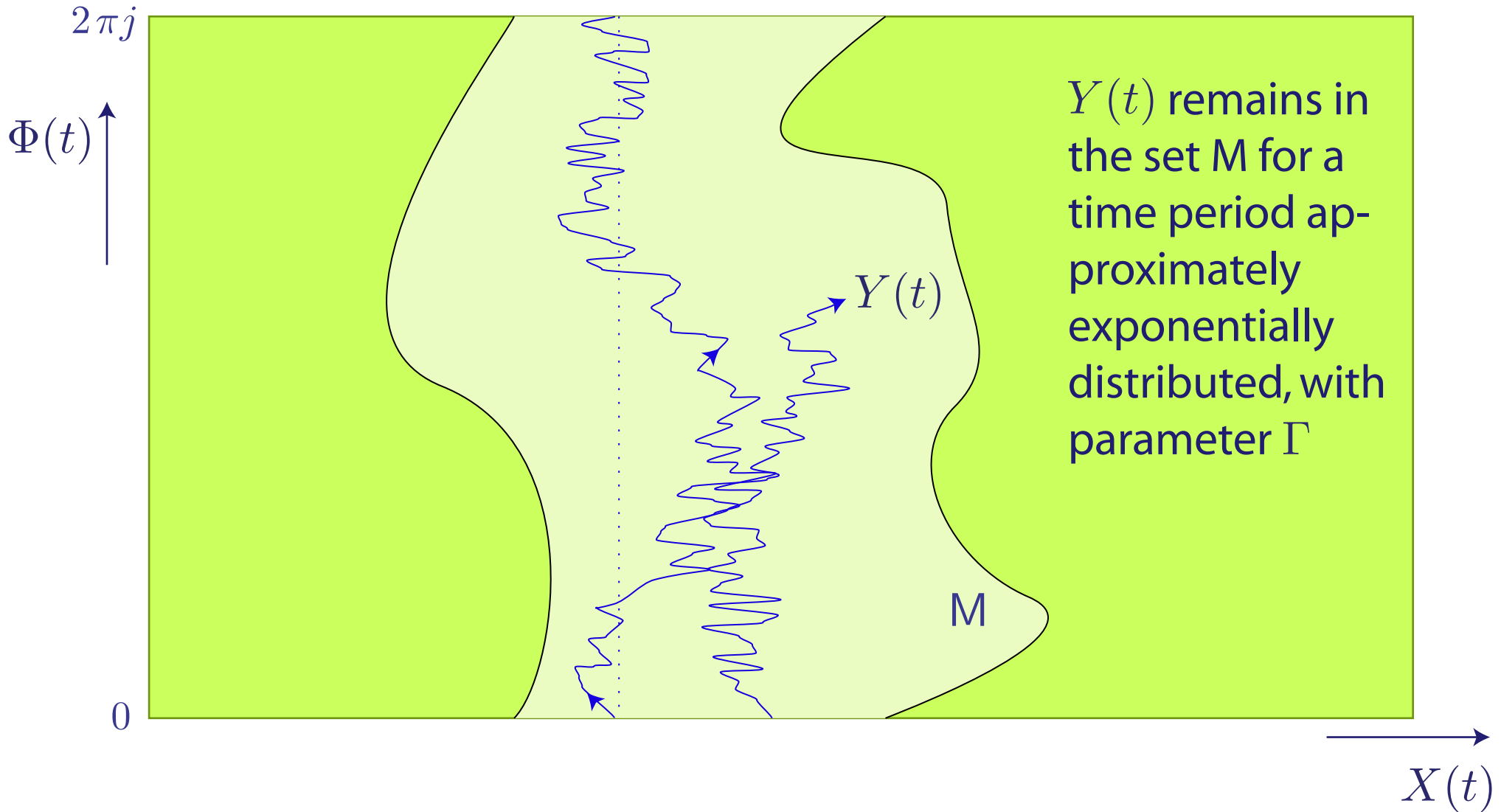
Metastability

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



Metastability

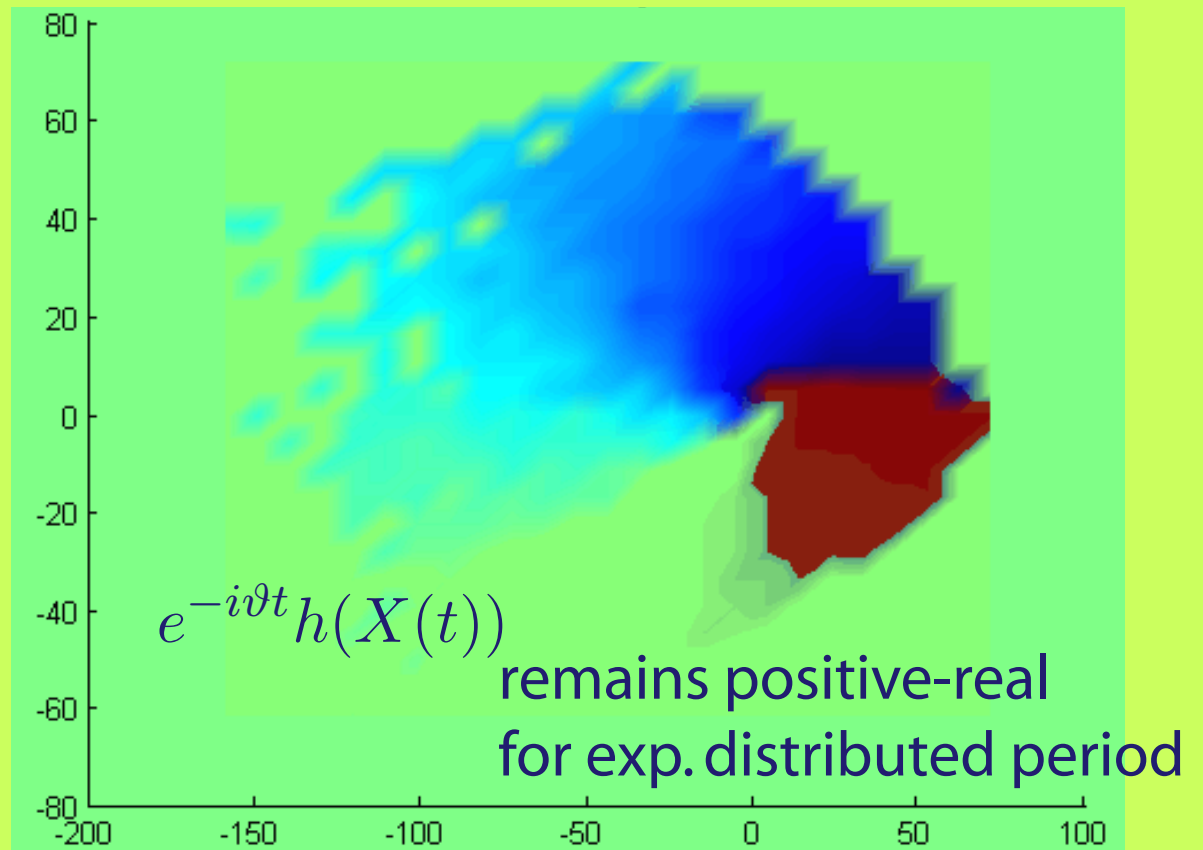
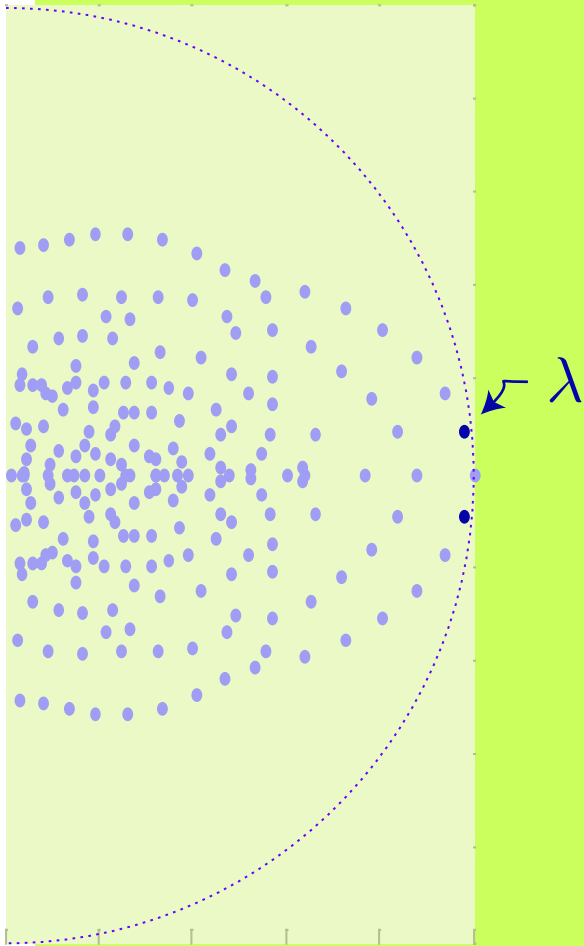
$$Y(t) = \begin{pmatrix} X(t) \\ \Phi(t) \end{pmatrix}$$



$X(t)$ remains in a set-valued periodic orbit for the same time period

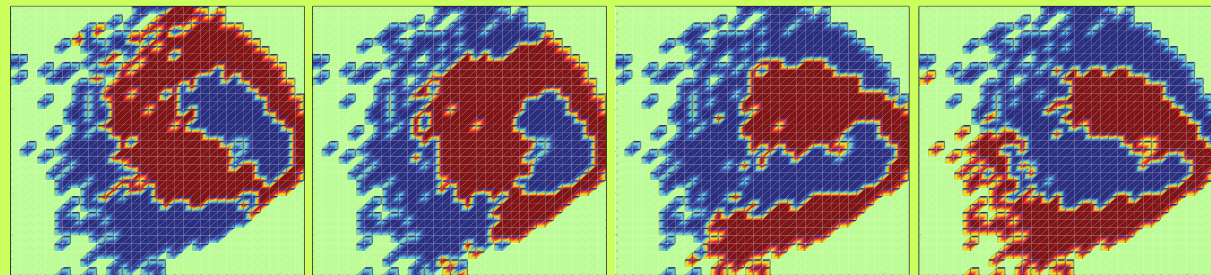
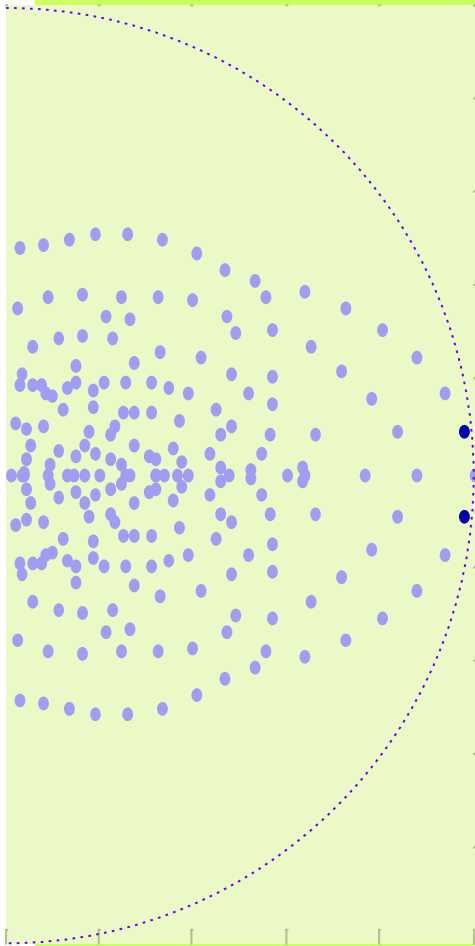
Spectrum from Jet Engine Model

Phase of second eigenfunction:



Spectrum from Jet Engine Model

Phase of second eigenfunction:



Quasi-Periodicity

Outline

I Generators & Spectrum

II Lyapunov Functions and Spectra

III Metastability

IV Example: Three-Well Potential

V Example: Jet Engine Dynamics

VI Conclusions

Conclusions

Contributions

- Markov spectra for insight and for model reduction
- Complex spectra carry wealth of information!
 - When there is a spectral gap then trajectory evolves as a quasi-periodic orbit, lasting approximately $1/\Gamma$ seconds

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Current Research

- Computation of optimal state partition
- Generalization: Finite-rank Markov models.
 - Interpretations and Computation
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$$R \approx \sum s_i \otimes \nu_i$$

\equiv Hidden Markov Model
on finite state space

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