Spectral theory and model reduction for complex Markov processes

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Outline

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Generator for an ODE

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

The generator is defined for C^1 functions ,

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

Fundamental Theorem of Calculus,

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

Generator for an SDE $dX(t) = \delta(X(t))\,dt + B(X(t))dN(t)$

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

$$\mathcal{D}h\,(x) := \frac{d}{dt}\mathsf{E}[h(X(t))\ |X(0)=x]\Big|_{t=0}$$

$$= \langle \delta(x), \nabla h(x)\rangle + \tfrac{1}{2}\mathrm{trace}\,(\Sigma(x)\nabla^2 h(x))$$

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

Martingale Representation

$$\mathsf{E}\Big[h(X(T)) - \int_0^T \mathcal{D}h\,(X(t))\,dt\Big] = h(X(0))$$

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,

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Applications

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

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!

Outline

Exponential Ergodicity

Condition (V4): For some $V : \mathsf{X} \to [1, \infty)$, $b < \infty$, $\delta > 0$

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

Exponential Ergodicity

Condition (V4): For some $V\colon \mathsf{X} \to [1,\infty)$, $b < \infty$, $\delta > 0$
K compact

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

Example:

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

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

$$V(x) = 1 + \tfrac{1}{2}\varepsilon x^T M x \qquad M > 0 \qquad A^T M + MA = -I$$

Exponential Ergodicity

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Exponential ergodicity?

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

$$|||P^t - \pi|||_V \triangleq \sup_{\|f\|_V=1} \Big(\|P^t f - \pi(f)\|_V \Big) \to 0$$ *Exponentially fast*

Down, M., Tweedie '95
Kontoyiannis & M. '03

Exponential Ergodicity

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Spectral gap?

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

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

Down, M., Tweedie '95
Kontoyiannis & M. '03

Drift condition of Donsker & Varadhan

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

Condition (DV3): For some $V, W : \mathsf{X} \to [1,\infty),\ b < \infty,$

W has compact sublevel sets

$$\mathcal{H}(V) \le -W + b$$

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Example: $dX(t) = AX(t)dt + BdN(t)$ (A, B) controllable $\lambda(A) < 0$

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

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This is a relaxation of D&V's conditions for Large Deviations

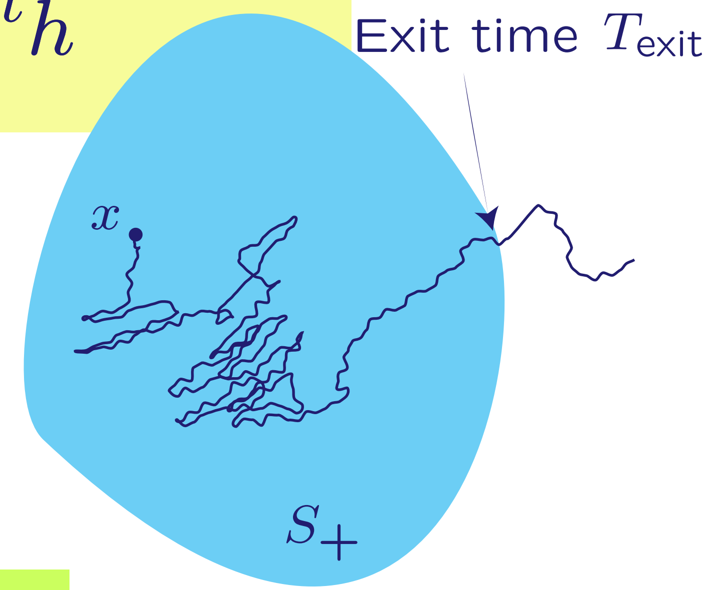
Under a density assumption a global LDP is established,
the rate function is identified as relative entropy,
and

the spectrum is discrete

Kontoyiannis & M. '05

Outline

Metastability & $P^t h = e^{-\Gamma t} h$



In continuous time,

$\Gamma > 0$, h is the second eigenfunction

$S_+ =$ connected component of $\{h > 0\}$

The exit time from a positive set S_+ is approximately exponentially distributed:

$$\mathsf{P}_x\Big\{\exp\Big(\beta(T_{\text{exit}} - T)\Big) \mid T_{\text{exit}} > T\Big\} = \frac{\Gamma}{\Gamma - \beta} \quad + \quad \mathcal{E}(x,T)$$

MGF for exponential rv

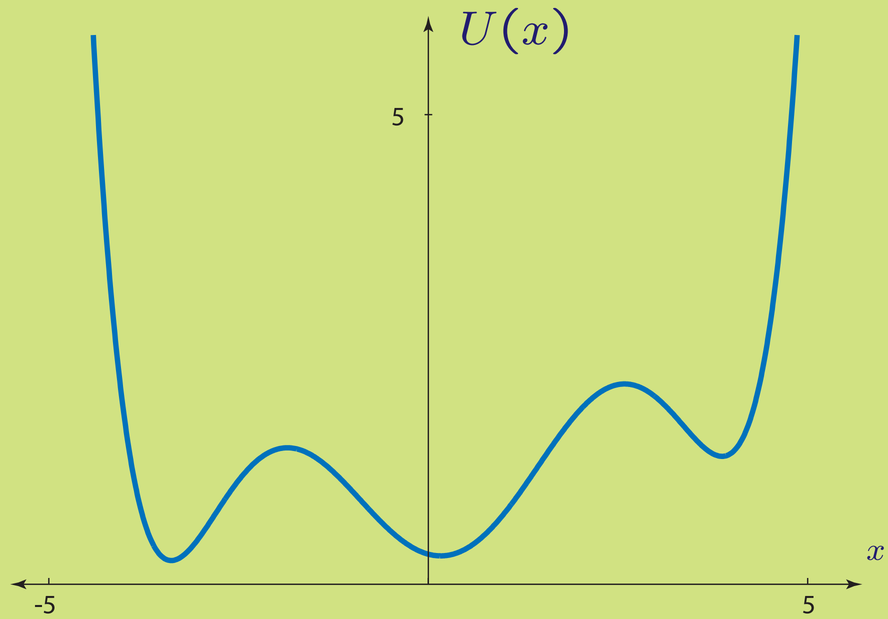
$$\mathsf{E}_x[f(\Phi(T)) \mid T_{\text{exit}} > T] = \check{\pi}(f) \quad + \quad \mathcal{E}(x,T)$$

Quasi steady-state on S_+

$$\mathcal{E}(x,T) = O\Big(v(x)h(x)^{-1}e^{-cT}\Big)$$

Huisinga M. Schuette '03

The three-well potential



The Smoluchowski equation

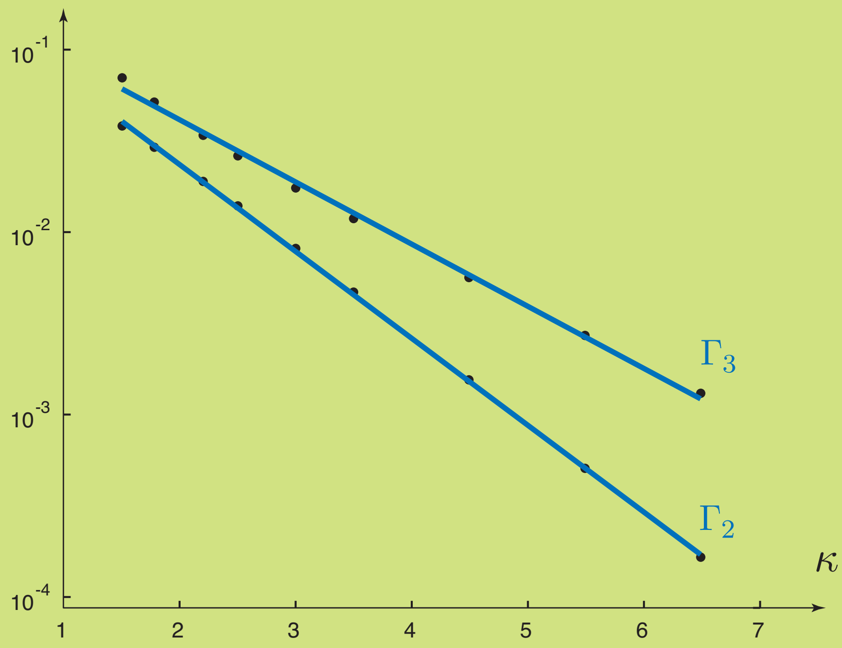
$$\mathrm{d}X = -\frac{1}{\gamma}\nabla U(X)\,\mathrm{d}t + \frac{\sigma}{\gamma}\,\mathrm{d}W$$

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

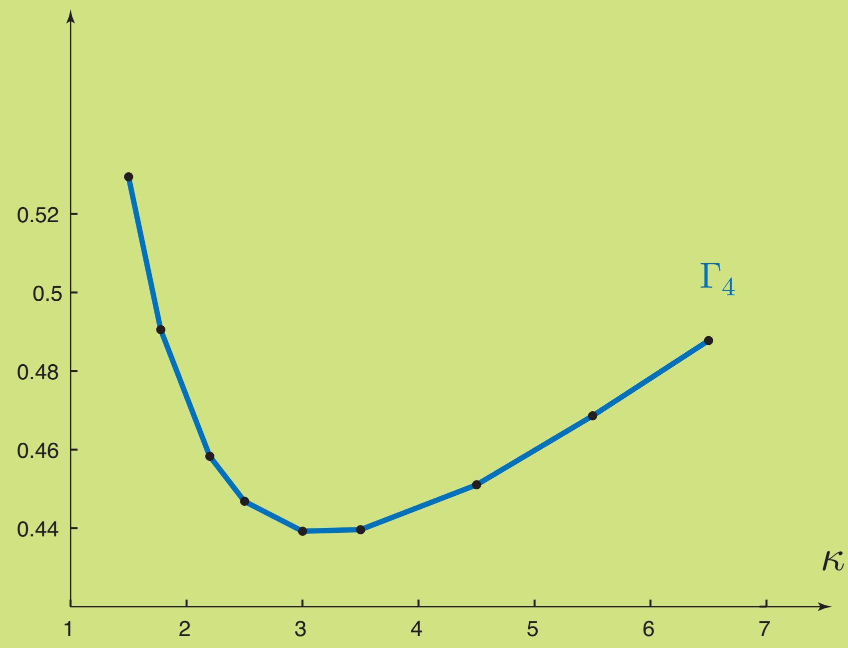
Invariant distribution with density $p(x) = \gamma e^{-\kappa U(x)}$

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

Eigenvalues as a function of κ

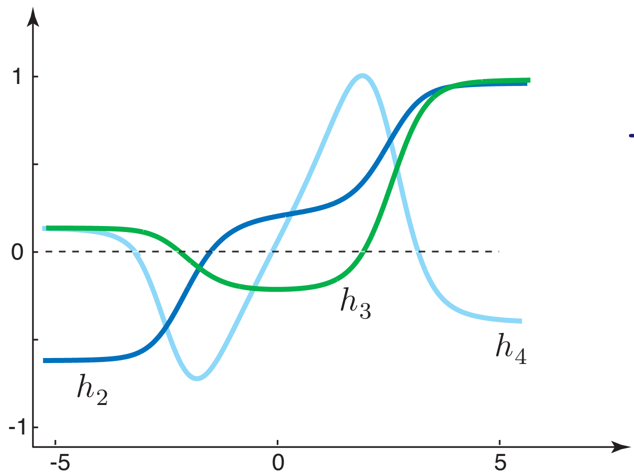


The second and third eigenvalues converge to zero

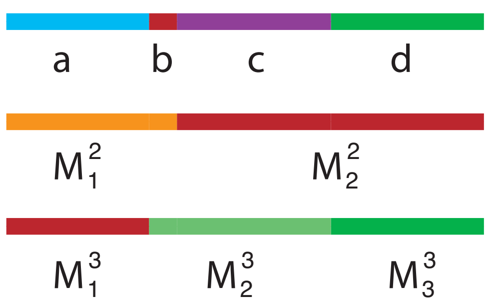


The fourth eigenvalue is bounded away from zero

Eigenfunctions and decompositions



Three eigenfunctions

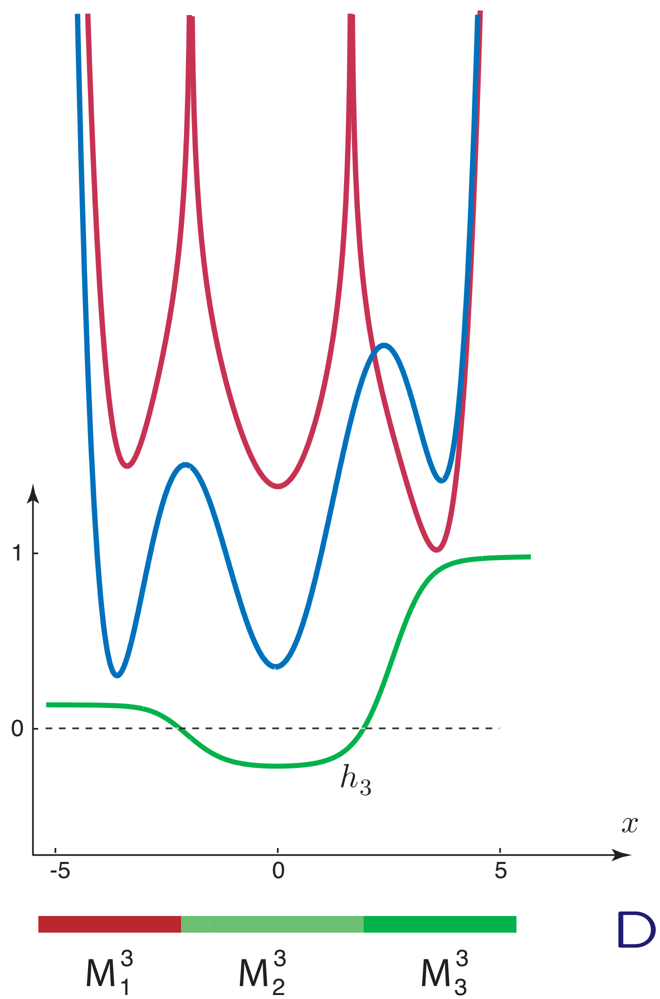


Decomposition based on zeros of $h_2 h_3$

Decomposition based on zeros of h_2

Decomposition based on zeros of h_3

The twisted potential



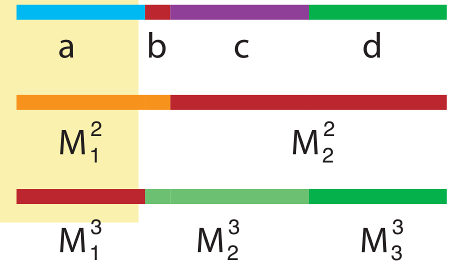
— The potential function $U(x)$

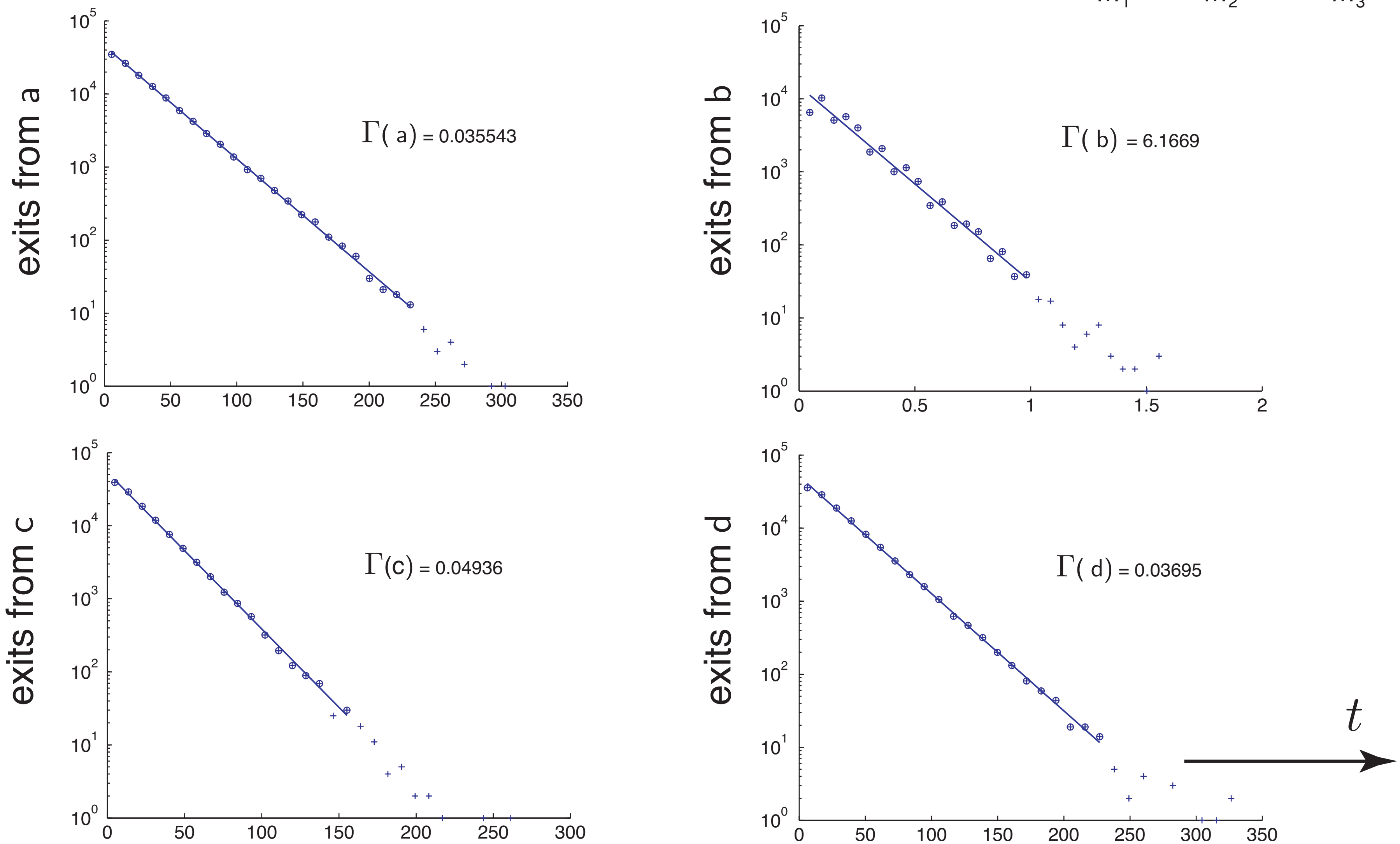
— The twisted potential function:

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

Decomposition based on zeros of h_3

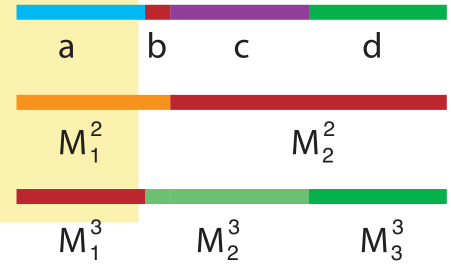
Exit time distributions

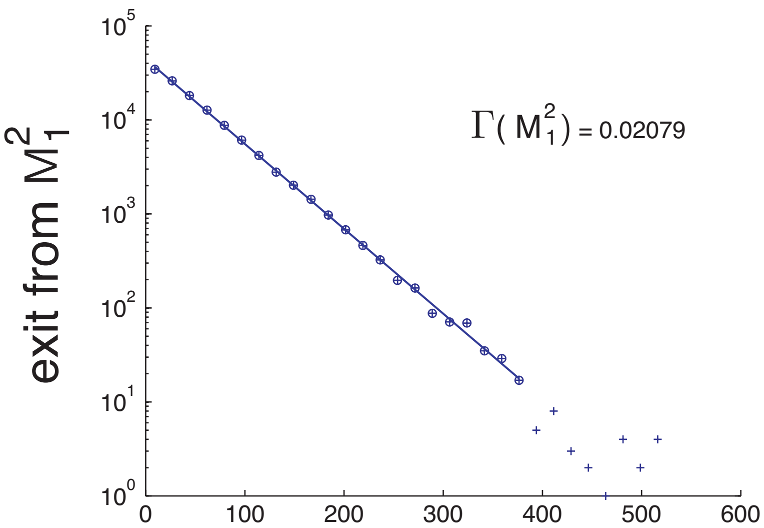


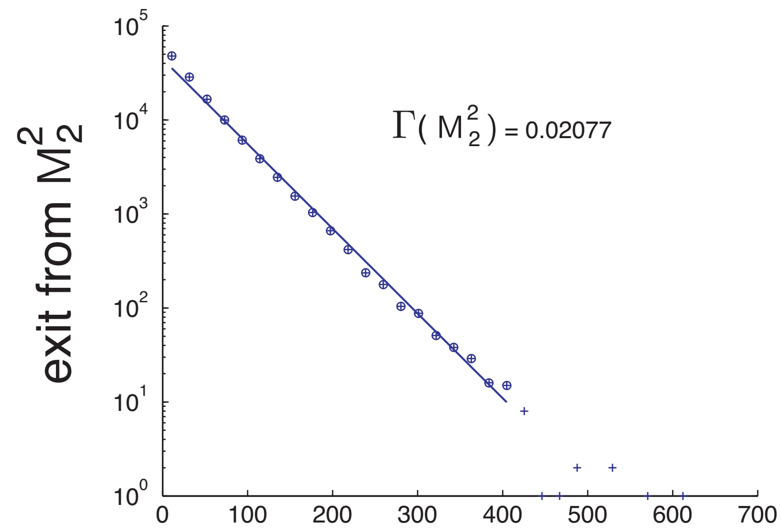


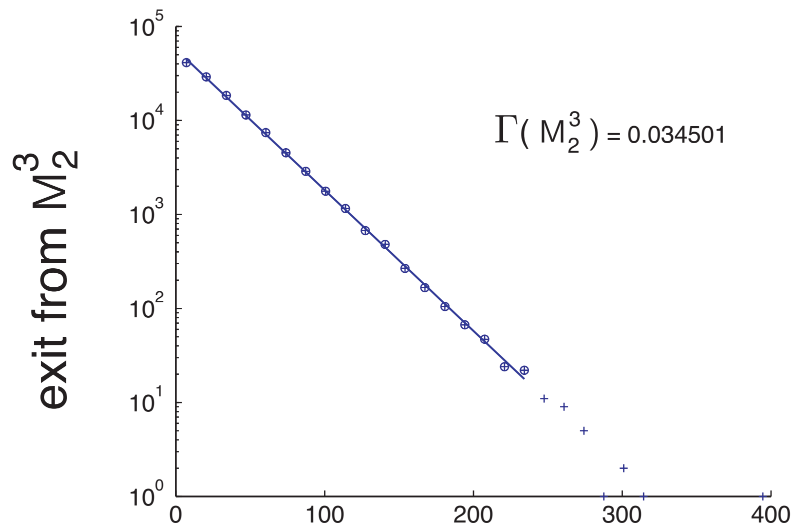
Exit time distribution for the sets $S = \{a, b, c, d\}$ and their combinations

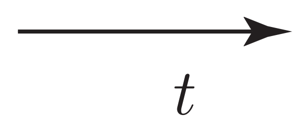
Exit time distributions











Outline

Finite approximations for P

(discrete time, densities, for simplicity)

Suppose that P has a continuous density,

$$P(x, dy) = p(x, y)\psi(dy)\,, \qquad x, y \in \mathsf{X}$$

On compact sets we can approximate,

$$p(x, y) \approx \sum_{i=1}^{n} s_i(x) p_i(y)\,,$$

$$Q(x, dy) = \sum_{i=1}^{n} s_i(x) \nu_i(dy)\,, \qquad x, y \in K.$$

Do we have $|||P - Q|||_v < \epsilon$ *?*

Can we assume that Q *is a transition kernel?*

Finite approximations for P

(discrete time, densities, for simplicity)

Suppose that $V, W : \mathsf{X} \to [1, \infty)$ are continuous with compact sublevel sets.

Suppose there exists $b < \infty$, satisfying (DV3):

$$\mathcal{H}(V) \triangleq \log(Pe^V) - V \leq -W + b$$

Then, for any $\epsilon > 0$, there exists $r \geq 1$ and a finite approximation on

$$K = \{x : W(x) \leq r\}.$$

Yes! We CAN assume that Q is a transition kernel

we have

$$|||P - Q|||_v < \epsilon$$

$$\sup_{t \geq 1} |||P^t - Q^t|||_v = O(\epsilon)$$

Dynamics for Q

$$Q(x, dy) = \sum_{i=1}^{n} s_i(x)\nu_i(dy)$$

A realization of the Markov chain Ψ under Q :

Process is a randomized function of a chain I on $\{1, \dots, n\}$

$$\Psi(0) = x$$

$$s(x) = [s_1(x), \dots, s_n(x)]^T$$

$$\mathsf{P}\{I(0) = i\} = s_i(x)$$

$$\mathsf{P}\{\Psi(1) \in A \mid I(0) = i\} = \nu_i\{A\}, \qquad A \in \mathcal{B}, \quad i = 1, \dots, n$$

$$\mathsf{P}\{I(1) = j \mid \Psi(0),\ \Psi(1)\} = s_j(\Psi(1))$$

Dynamics for Q

$$Q(x,dy) = \sum_{i=1}^{n} s_i(x)\nu_i(dy)$$

The process $I(k)$ is a Markov chain on $\{1,\dots,n\}$

Its transition law:

$$\mathsf{P}\{I(k) = j \mid I(k-1) = i\} = \nu_i(s_j)\,, \qquad i,j \in \{1,\dots,n\}$$

The finite chain serves as a sufficient statistic

$$\mathsf{P}\{\Psi(k) \in A \mid I(k-1) = i, \Psi(0),\dots,\Psi(k-1)\} = \nu_i(A)$$

Conclusion:

Anything that is true for I is also true for Ψ

and, with a bit more effort, true for Φ

Spectral theory for Q

Q has $\leq n$ eigenfunctions $\{h_1, \ldots, h_n\} \subset$ *span* $\{s_1, \ldots, s_n\}$

$\leq n$ eigenmeasures $\{\mu_1, \ldots, \mu_n\} \subset$ *span* $\{\nu_1, \ldots, \nu_n\}$

P has a finite spectrum within the region

$$B_\epsilon = \{z \in \mathbb{C} : |z| \geq \epsilon\},$$

and eigenvectors are approximated by those of Q

In particular,

$$P^t \rightarrow \mathbf{1} \otimes \pi$$
$$Q^t \rightarrow \mathbf{1} \otimes \varpi$$

with $\|\pi - \varpi\|_v = O(\epsilon)$.

Outline

Conclusions

- ▷ The DV drift condition allows a finite approximation of P *provided one considers the weighted* L_∞*-norm*
- ▷ Strong conclusions are possible without reversibility. Complex eigenvalues to be explored.
- ▷ Far weaker assumptions are possible, such as a relaxation of the one-step density conditions
- ▷ Recent applications to products of random matrices, and spectral decompositions for diffusions
- ▷ It seems likely that the finite approximations will find application in other areas **!**

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