Large Deviations
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Spectral theory of large deviations in birth-death systems

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Assaf and Meerson, PRL **97,** 200602 (2006)

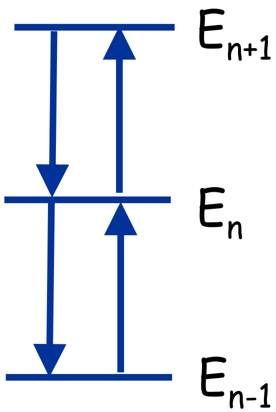
Assaf and Meerson, PRE **74,** 041115 (2006)

Assaf and Meerson, PRE **75,** 154703 (2007)

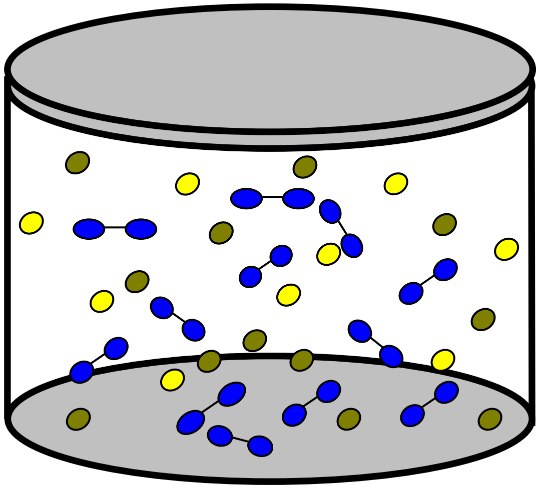
Introduction

Birth-death processes: Markov processes involving transitions, with known rules, within an ensemble of microscopic states

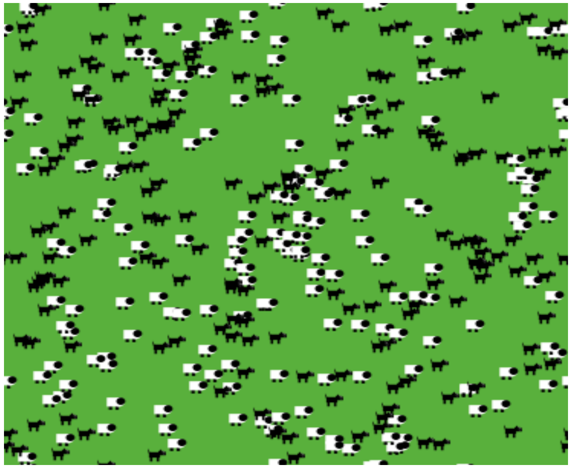
Numerous examples in physics, chemistry and astrochemistry, population biology, epidemiology, cell biochemistry etc…



Atomic processes and quantum optics



Chemical reactions
recombination, dissociation, desorption…



Population dynamics
birth, death, emigration/immigration, competition etc.

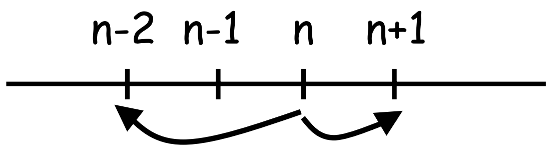
Extinction and meta-stability

Example: a **branching-annihilation** process

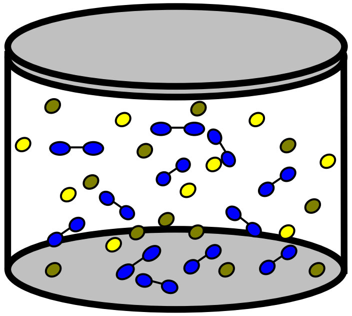
$$2A \xrightarrow{\mu} 0$$

$$A \xrightarrow{\lambda} 2A$$

(chemical reactions $2A \rightarrow B$, $A + C \rightarrow 2A + D$; population dynamics…)



a *two-step* birth-death process



What does the *rate equation* predict?

$$\dot{n} = -\mu n^2 + \lambda n$$

attracting fixed point $n_s = \dfrac{\lambda}{\mu} \equiv \Omega >> 1$

a natural large parameter

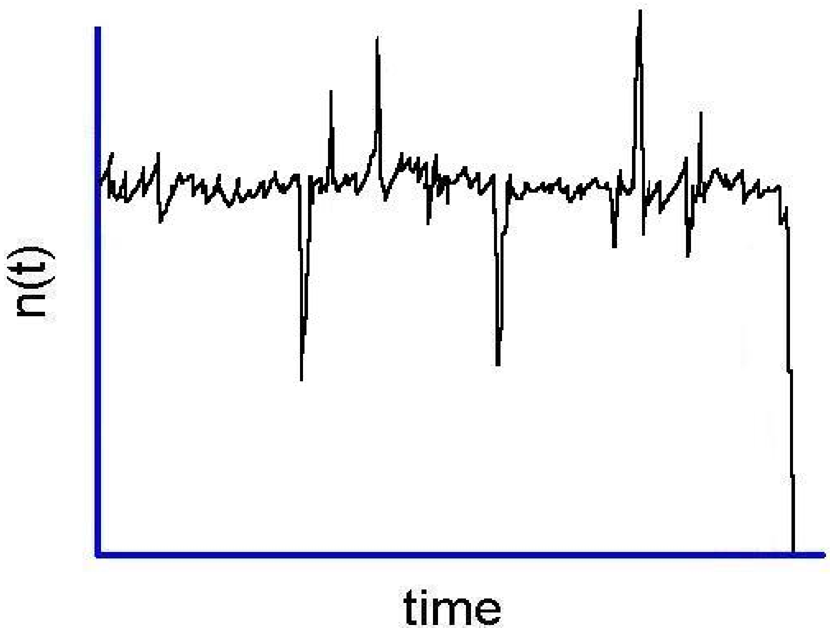
System stays at $n=\Omega$ forever

In the master equation formulation this result breaks down at long times

- existence of absorbing state at n=0
- Particle discreteness brings fluctuations, ultimately driving the system to absorbing state

Fluctuations work against deterministic effect ⇒ extinction time exponentially large

the stable (attracting) fixed point of the rate equation becomes ***meta-stable***



Interesting to calculate:

- quasi-stationary distribution
- extinction time statistics

Master equation

$$2A \xrightarrow{\mu} 0$$

$$A \xrightarrow{\lambda} 2A$$

$$\begin{cases} \dot{P}_n = \underbrace{\frac{\mu}{2}\left[(n+2)(n+1)P_{n+2} - n(n-1)P_n\right]}_{\text{annihilation}} + \underbrace{\lambda\left[(n-1)P_{n-1} - nP_n\right]}_{\text{branching}} \\ \dot{P}_0 = \mu P_2 \end{cases}$$

A particular case of a general gain-loss master equation

$$\frac{dP_n(t)}{dt} = \sum_{m \neq n} W_{mn} P_m(t) - W_{nm} P_n(t)$$

W_{nm} – transition matrix

Master equations are rarely soluble analytically

Existing methods of dealing with single- and multi-step birth-death systems

- Fokker-Planck (FP) approximation - good for “typical behavior”, fails for extreme statistics (Gaveau, Moreau, and Toth 1996, Doering, Sargsyan, and Sander 2005)

- Eikonal approximations: in the master equation (Dykman *et. al.* 1994), or in the PDE for the generating function (Elgart and Kamenev 2004) – significantly improve over FP, give new insight (optimal paths), but miss pre-exponents

Recent work by Kessler and Shnerb (2007) on branching-annihilation: WKB approximation etc. to *quasi-stationary* master equation

No general and self-contained analytical method to accurately calculate complete (incl. time-dependent) statistics, even for univariate problems

Can one go beyond the optimal path approximation?

Here comes the spectral method

Step 1: employing the generating function

Define $$G(x,t)=\sum_{m=0}^{\infty}x^m P_m(t)$$

The probabilities are recovered from $$P_n(t)=\frac{1}{n!}\frac{\partial^n G(x,t)}{\partial x^n}\bigg|_{x=0}=\frac{1}{2\pi i}\oint\frac{G(x,t)}{x^{n+1}}\,dx$$

Master equation collapses into a single PDE $$\frac{\partial G(x,t)}{\partial t}=\hat{L}(x)G(x,t)$$

$$\begin{array}{lllll}
0\rightarrow jA & & P_n(t) & & G(x,t) \\
A\rightarrow kA & \Longleftrightarrow & nP_n(t) & \Longleftrightarrow\ \sim & \partial_x G(x,t) \\
2A\rightarrow mA & & (1/2)n(n-1)P_n(t) & & \partial_x^2 G(x,t)
\end{array}$$

One boundary condition is universal $$G(x=1,t)=\sum_{m=0}^{\infty}x^m P_m(t)\bigg|_{x=1}=\sum_{m=0}^{\infty}P_m(t)=1$$

The mean extinction time $$<\tau_{ext}>=\frac{\int_0^\infty t\dot{P}_0(t)dt}{\int_0^\infty \dot{P}_0(t)dt}=\frac{\int_0^\infty t\frac{\partial G(0,t)}{\partial t}dt}{G(0,\infty)-G(0,0)}$$

Back to branching-annihilation example

$$2A \xrightarrow{\mu} 0$$

$$A \xrightarrow{\lambda} 2A$$

$$\frac{\partial G(x,t)}{\partial t} = \frac{\mu}{2}(1-x^2)\frac{\partial^2 G(x,t)}{\partial x^2} + \lambda x(x-1)\frac{\partial G(x,t)}{\partial x}$$

n_0 particles at t=0: $G(x,0) = x^{n_0}$

First boundary condition $G(x=1,t)=1$

or we should rather say that the PDE is degenerate at x=1, so no BC is needed

Second boundary condition follows from demand that all probabilities be non-negative and normalizable to unity

In this example it emerges at the singular point x=-1 of the corresponding *ODE*, see later.

$$G(x=-1,t) = \sum_{m=0}^{\infty} P_{2m}(t) - \sum_{m=0}^{\infty} P_{2m+1}(t) < \infty$$

Step 2: steady state

Extinction, so we expect $\lim_{t\to\infty} P_0(t) = 1 \Rightarrow G_{st}(x) = 1$

Steady state equation $$0 = \frac{\mu}{2}(1 - x^2)G_{st}''(x) + \lambda x(x-1)G_{st}'(x)$$

G bounded at x=-1 $\Rightarrow \frac{d}{dx}G_{st}(x=-1) = 0 \Rightarrow G_{st}(x) = 1$

Step 3: expanding in eigenfunctions

$$g(x,t)=G(x,t)-G_{st}(x)=G(x,t)-1=\sum_{k=1}^{\infty}a_k e^{-\gamma_k t}\varphi_k(x)$$

$$(1-x^2)\varphi_k''(x)-2\Omega x(1-x)\varphi_k'(x)+2E_k\varphi_k(x)=0 \qquad E_k=\frac{2\gamma_k}{\mu}$$

boundedness of φ_k at x=-1 $\Longrightarrow$ $\begin{cases}\varphi_k(1)=0\\ 2\Omega\varphi_k'(-1)+E_k\varphi_k(-1)=0\end{cases}$

self-adjoint form $\begin{cases}\dfrac{d}{dx}\left[e^{-2\Omega x}(1+x)^{2\Omega}\dfrac{d\varphi_k(x)}{dx}\right]+E_k w(x)\varphi_k(x)=0\\ w(x)=2e^{-2\Omega x}(1+x)^{2\Omega}(1-x^2)^{-1}\end{cases}$

Solving the whole set of self-adjoint ODEs with the homogenous BCs yields a complete orthogonal set $\{\varphi_k(x),E_k\}_{k=0}^{\infty}$ by virtue of Sturm-Liouville theory

Step 4: projecting the initial condition and reconstructing G(x,t)

$$G(x,0)=\sum_{m=0}^{\infty}x^m P_m(t=0)=x^{n_0}$$

a_k determined by the initial condition

$$a_k=\frac{\int_{-1}^{1}(x^{n_0}-1)\varphi_k(x)w(x)dx}{\int_{-1}^{1}\varphi_k^2(x)w(x)dx},$$

where

$$\int_{-1}^{1}\varphi_k(x)\varphi_l(x)w(x)dx\propto\delta_{kl}$$

$$G(x,t)=1+\sum_{k=1}^{\infty}a_k\varphi_k(x)e^{-\mu E_k t}$$

G(x,t) encodes the complete statistics, including large deviations. For example,

$$<\tau_{ext}>=-\frac{1}{\mu}\sum_{k=1}^{\infty}\frac{a_k\varphi_k(0)}{E_k}$$

We obtained an exact mapping between solving the original, time-dependent master equation and finding the eigenvalues and eigenfunctions of a linear differential operator

Solving for the eigenvalues and eigenfunctions

$$(1-x^2)\varphi_k''(x) - 2\Omega x(1-x)\varphi_k'(x) + 2E_k\varphi_k(x) = 0$$

This eqn. can be transformed into a zero-energy Schrödinger eqn.

$$\left\{-\frac{1}{2}\frac{d^2}{dx^2} + V(x, E_k)\right\}\psi_k(x) = 0 \qquad \begin{cases} \psi_k(x) = (1+x)^{\Omega} e^{-\Omega x}\varphi_k(x) \\ V(x) = \dfrac{\Omega^2 x^2 - \Omega}{2(1+x)^2} - \dfrac{E_k}{1-x^2} \end{cases}$$

$$E_2, E_3, \ldots \sim O(\Omega)$$

E_1 exponentially small in Ω → Mean extinction time exponentially large in Ω

→ $G(x,t) \cong 1 + a_1\varphi_1(x)e^{-\mu E_1 t}$ for $\mu t >> \Omega^{-1}$

Highly lying states can be accurately calculated via WKB approx. (Assaf and Meerson 2006)

Ground state calculation: a matched asymptotic expansion

Ground state problem $$(1-x^2)\varphi_1''(x) - 2\Omega x(1-x)\varphi_1'(x) + 2E_1\varphi_1(x) = 0$$

with homogenous BCs $$\begin{cases} \varphi_1(1) = 0 \\ \varphi_1'(-1) \cong 0 \end{cases}$$

We solve the ODE separately in two different regions

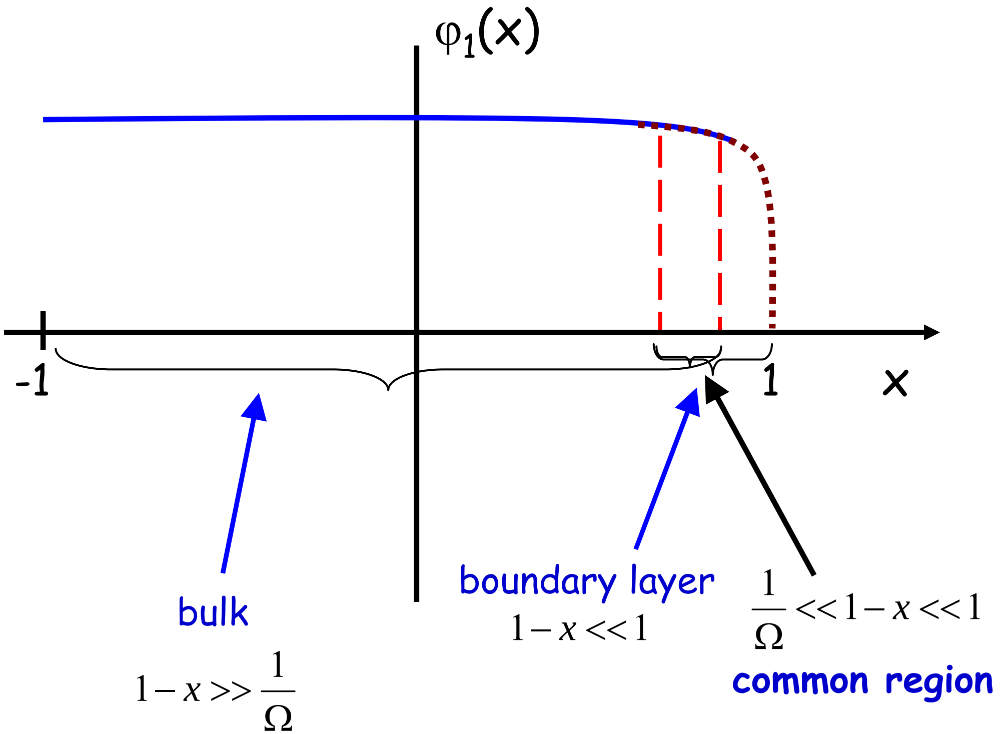
$$\varphi_{bulk}(x) = 1 + \delta\varphi(x) \qquad \delta\varphi << 1$$

$$\delta\varphi''(x) - \frac{2\Omega x}{1+x}\delta\varphi'(x) \cong -\frac{2E_1}{1-x^2}$$

$$\boxed{\varphi_{bulk}(x) = 1 - E_1 \delta\tilde{\varphi}(x)}$$

$$\varphi_{bl}''(x) - \frac{2\Omega x}{1+x}\varphi_{bl}'(x) \cong 0$$

$$\boxed{\varphi_{bl}(x) = C\left[1 - \frac{2^{2\Omega}}{e^{2\Omega}}\frac{e^{2\Omega x}}{(1+x)^{2\Omega}}\right]}$$



The unknowns E_1 and C are found by asymptote matching in the common region

$$\varphi_1(x) = \begin{cases} 1 - 2E_1 \int_0^x \frac{e^{2\Omega s}}{(1+s)^{2\Omega}} ds \int_{-1}^s \frac{e^{-2\Omega r}(1+r)^{2\Omega}}{1-r^2} dr, & 1 - x \gg \frac{1}{\Omega} \\ 1 - e^{2\Omega(1-\ln 2)} \frac{e^{2\Omega x}}{(1+x)^{2\Omega}}, & 1 - x \ll 1 \end{cases}$$

$$E_1 = \frac{\Omega^{3/2} e^{-2\Omega(1-\ln 2)}}{2\sqrt{\pi}}$$

$$\longrightarrow \quad G(x,t) \cong 1 - \varphi_1(x) e^{-\mu E_1 t}$$

Indeed, for $n_0 \gg 1$

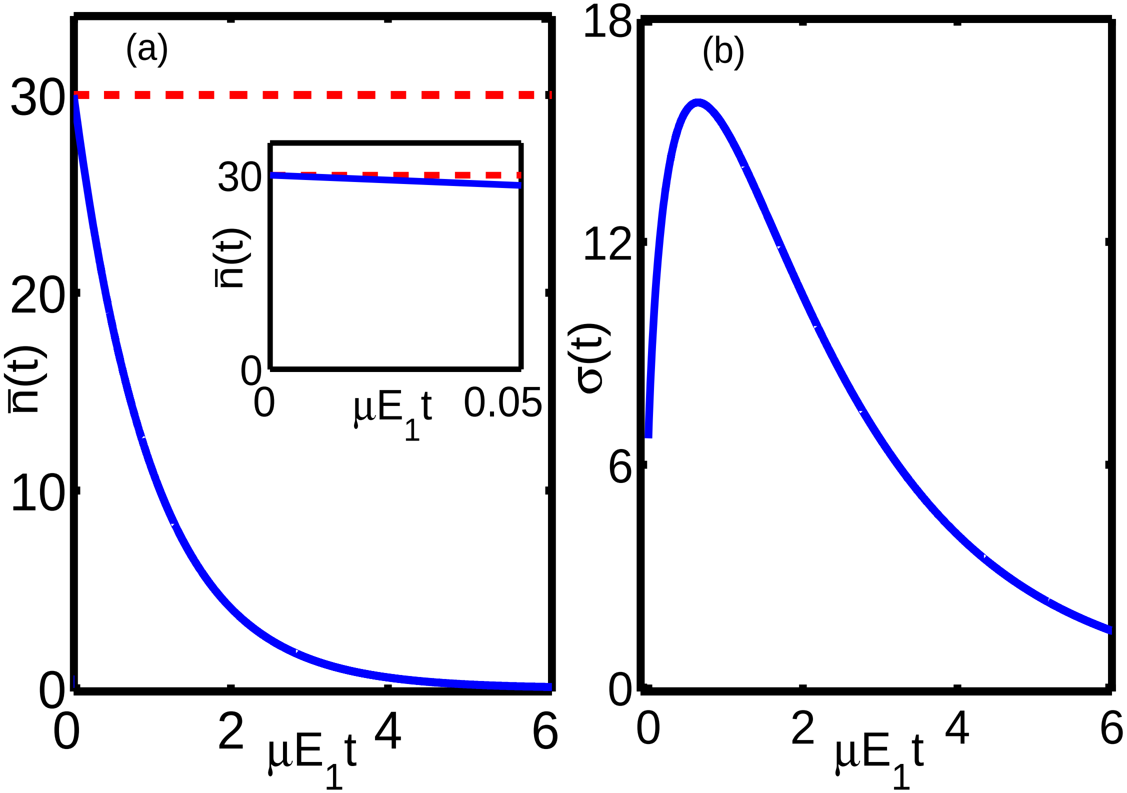
$$a_1 = \frac{\int_{-1}^{1} \varphi_1(x)(x^{n_0} - 1) 2e^{-2\Omega x}(1+x)^{2\Omega}(1-x^2)^{-1} dx}{\int_{-1}^{1} \varphi_1^2(x) 2e^{-2\Omega x}(1+x)^{2\Omega}(1-x^2)^{-1} dx} \cong -1$$

Average and variance of distribution

$$\begin{cases} \bar{n}(t) = \sum_{n=0}^{\infty} nP_n(t) = \partial_x G(x=1,t) \\ \sigma^2 = \sum_{n=0}^{\infty} n^2 P_n(t) - \left(\sum_{n=0}^{\infty} nP_n(t)\right)^2 = \partial_x^2 G(x=1,t) + \partial_x G(x=1,t) - \left[\partial_x G(x=1,t)\right]^2 \end{cases}$$

$$\bar{n}(t) = \Omega e^{-\mu E_1 t}$$

$$\sigma^2 = \left[\frac{3}{2}\Omega + \Omega^2\left(1 - e^{-\mu E_1 t}\right)\right] e^{-\mu E_1 t}$$



Complete probability distribution

$$P_n(t) = \frac{1}{n!}\frac{\partial^n G(x,t)}{\partial x^n}\bigg|_{x=0} = \delta_{0n} - \frac{1}{n!}\frac{d^n \varphi(x=0)}{dx^n} e^{-\mu E_1 t}$$

slowly decaying (quasi-stationary) distribution

$$\begin{cases} P_0(t) \approx 1 - e^{-\mu E_1 t} \\ P_{n>0}(t) = \dfrac{2E_1 (2\Omega)^{n-1} e^{2\Omega}\Gamma(2\Omega)}{n\Gamma(2\Omega+n)} {}_1F_1(2\Omega, n+2\Omega, -2\Omega) e^{-\mu E_1 t} \end{cases}$$

$$\mu t >> \Omega^{-1}$$

Kummer confluent hypergeometric function.
(Actually, one must use the $\Omega >> 1$ asymptote
of this result, see Assaf and Meerson 2007)

For $\left|n-\Omega\right| << \Omega$ $\qquad P_n^C(t) \cong \dfrac{1}{\sqrt{3\pi\Omega}} e^{-\frac{(n-\Omega)^2}{3\Omega} - \mu E_1 t}$

A Gaussian with mean Ω
and variance $3\Omega/2$

$$< \tau_{ext} > = \int_0^\infty t \frac{dP_0(t)}{dt} dt \approx (\mu E_1)^{-1} = \frac{2\sqrt{\pi}}{\mu \Omega^{3/2}} e^{2\Omega(1-\ln 2)}$$

agrees with Turner and Malek-Mansour (1978);
exponent agrees with Elgart and Kamenev (2004)

Comparison with Fokker-Planck approximation

Assume n>>1 and expand in Taylor series up to the second order in 1/Ω

$$\dot{P}_n = \frac{\mu}{2}\left[(n+2)(n+1)P_{n+2} - n(n-1)P_n\right] + \lambda\left[(n-1)P_{n-1} - nP_n\right]$$

$$P(n-1,t) \cong P(n,t) - \frac{\partial P(n,t)}{\partial n} + \frac{1}{2}\frac{\partial^2 P(n,t)}{\partial n^2}$$

$$P(n+2,t) \cong P(n,t) + 2\frac{\partial P(n,t)}{\partial n} + 2\frac{\partial^2 P(n,t)}{\partial n^2}$$

Kramers - Moyal expansion $\quad n \to \Omega x \qquad \frac{\partial}{\partial n} \to \frac{1}{\Omega}\frac{\partial}{\partial x}$

$$\Rightarrow \quad \frac{\partial P(n,t)}{\partial t} = \frac{\mu}{2}\frac{\partial}{\partial n}\left\{-2n(\Omega - n)P(n,t) + \frac{1}{2}\frac{\partial}{\partial n}\left[2n(2n+\Omega)P(n,t)\right]\right\}$$

(Zero flux) steady state probability distribution

$$P^{FP}(n,t) \cong \frac{1}{\sqrt{3\pi\Omega}} e^{\Omega - n + \frac{3}{2}\Omega \ln\frac{2n+\Omega}{3\Omega}}$$

For $|n - \Omega| << \Omega$

$$P^{FP}(n,t) = \frac{1}{\sqrt{3\pi\Omega}} e^{-\frac{(n-\Omega)^2}{3\Omega}}$$

ok

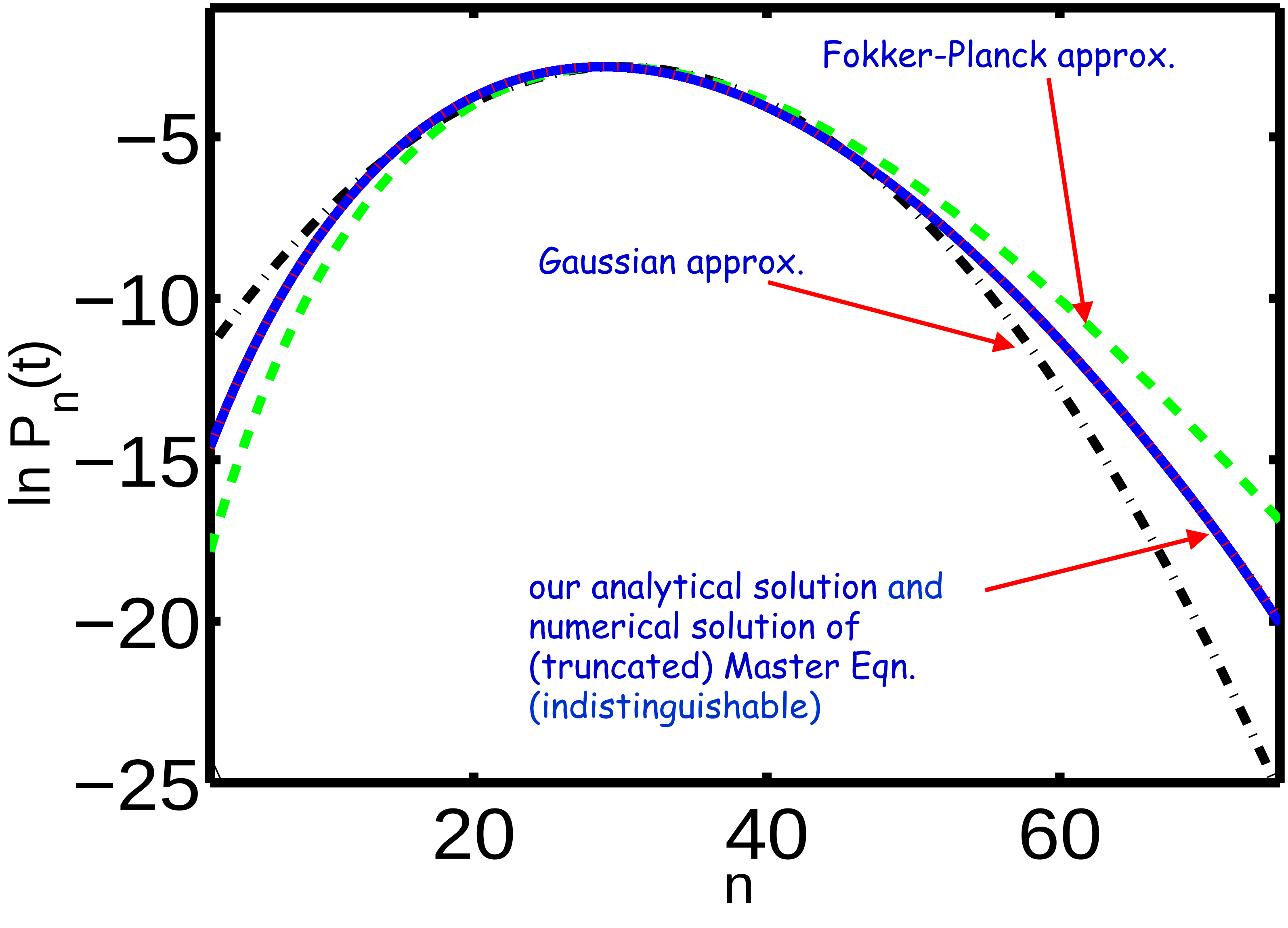
$$\left|1 - \frac{P^{FP}(n+1,t)}{P^{FP}(n,t)}\right| \cong 1 - e^{-\frac{1}{3\Omega}} << 1$$

For n>>Ω

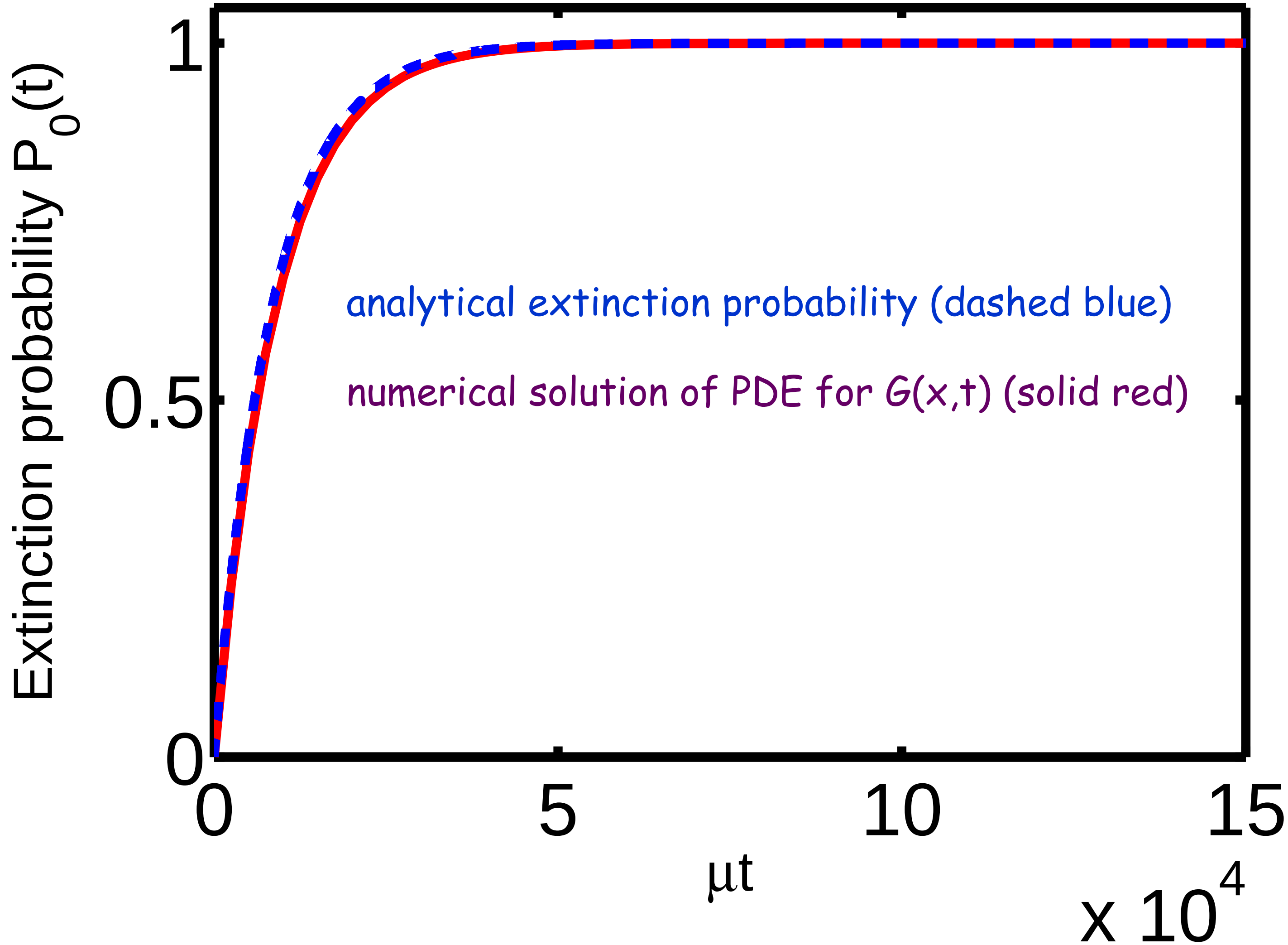
$$\left|1 - \frac{P^{FP}(n+1,t)}{P^{FP}(n,t)}\right| \cong 1 - e^{-1} \not\ll 1$$

$\Rightarrow$ FP fails in tails

For n~1 FP is inapplicable too.



Fokker-Planck approx.
Gaussian approx.
our analytical solution and
numerical solution of
(truncated) Master Eqn.
(indistinguishable)
−5
−10
−15
−20
−25
ln P_n(t)
20
40
60
n



Extinction time (spectral method) ~ $\mathrm{Exp}[\Omega(2-2\ln 2)]$

Extinction time (Fokker-Planck) ~ $\mathrm{Exp}\{\Omega\,[(3/2)\ln 3-1]\}$

includes an exponentially large error

Different definitions related to quasi-stationarity/metastability

1. Quasi-stationary distribution = amplitude $P_n^{(0)}$ of long-time asymptote of the time-dependent pdf

$$P_{n>0}(t) = P_n^{(0)} e^{-\mu E_1 t} = -\frac{1}{n!}\frac{d^n\varphi(x=0)}{dx^n} e^{-\mu E_1 t}$$

2. *Stationary* distribution obtained by assuming zero flux to n=0

Definitions 1 and 2 are different

In the branching-annihilation example def. 2 gives the same result as def. 1 *in the leading order in* $1/\Omega$. Sub-leading terms might be different. In the SIS problem def. 2 gives a different result already in the leading order, Nåsell 2001. It might be meaningless to pursue to a high accuracy while using def. 2.

Is spectral method generalizable to two and more species?

Generating function for two species $$G(x_1, x_2, t) = \sum_{m,n=0}^{\infty} x_1^{\ m} x_2^{\ n} P_{mn}(t)$$

The master equation transforms to $$\frac{\partial G(\mathbf{x}, t)}{\partial t} = \hat{L}(\mathbf{x}) G(\mathbf{x}, t), \quad \mathbf{x} = (x_1, x_2)$$

This parabolic PDE demands, in addition to the initial condition, a boundary condition on a closed curve (finite or infinite) in the plane (x_1,x_2). This BC must follow from the boundedness and non-negativeness of the probabilities, and is yet unknown.

The eikonal approaches circumvent the need for the explicit BC.

Conclusions

- We developed a simple spectral approach for univariate birth-death processes that employs the generating function technique in conjunction with Sturm-Liouville theory

- The spectral approach yields accurate rare-event statistics for single-step and multiple-step processes, where other methods in general fail