Large deviations of linear diffusions

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- Work with
  Johan du Buisson and Thamu Mnyulwa
  PRE **107** 2023; PRE **108** 2023

Dynamical large deviations

- Markov process: $X_t,\ t \in [0, T]$
- Observable: $A_T[x]$

Probability distribution

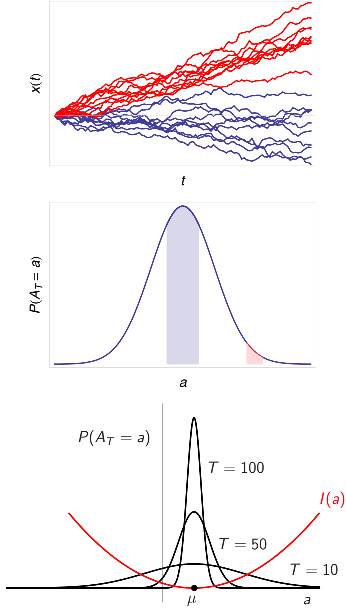
$$P(A_T = a) \approx e^{-T\,I(a)}$$

Generating function

$$E[e^{TkA_T}] \approx e^{T\lambda(k)}$$

Effective process

- How are fluctuations created?
- Conditioned process: $X_t | A_T = a$
- Markov when $T \to \infty$



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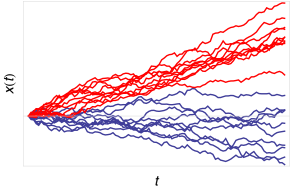

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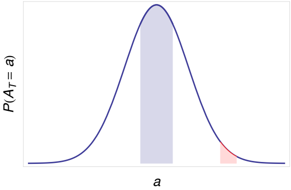

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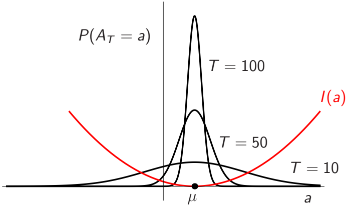

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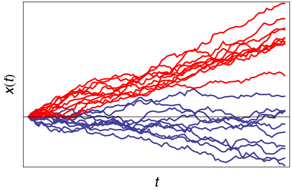
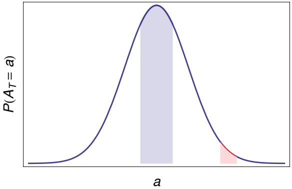
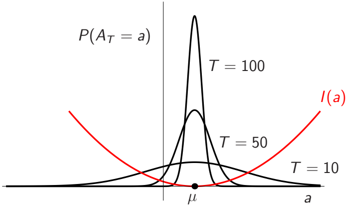
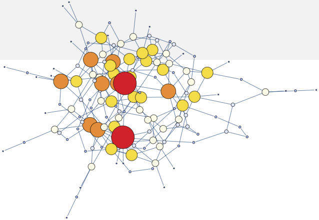




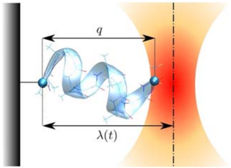


Applications



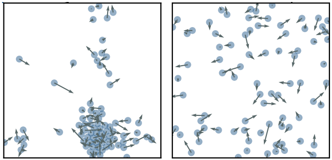
Markov chains

- Random walks
- Jump processes
- Occupation, displacement, currents



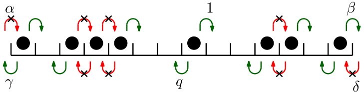
Diffusions

- Langevin equations, SDEs
- Work, heat, entropy production
- Active OUP



Many-particle dynamics

- Zero-range process
- Exclusion process
- Harmonic chains
- Density and current



[Reviews: HT 2009, 18; Derrida 07; Bertini et al 07]

Linear diffusions

- Quadratic observables: Bercu et al 1997
- Entropy production: Visco 2006; Chernyak et al 2006; Jaksic et al 2016
- Nonequilibrium work: Kwon, Noh & Park 2011, Noh 2014
- Coupled oscillators: Kundu et al 2011, Sabhapandit, 2012; Pal & Sabhapandit 2013
- More general setting: Mazzolo & Monthus 2023

This work

- General linear SDEs in $\mathbb{R}^n$
- More general class of observables
- Not based on path integrals
- Derive effective process (remains linear)
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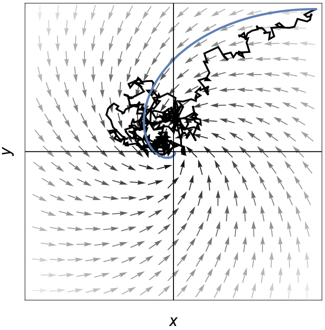
Linear diffusions

- Dynamics:

$$dX(t) = -MX(t)dt + \sigma dW(t)$$

  - $X(t) \in \mathbb{R}^n$, $W(t) \in \mathbb{R}^m$
  - M positive definite, $\sigma > 0$

- Applications:
  - Laser tweezers (thermal noise)
  - Electric circuits (Nyquist noise)
  - Noisy controlled systems



Stationary density

$$p^*(x) \propto e^{-\frac{1}{2}x\cdot C^{-1}x}$$

$$D = MC + CM^{\mathsf{T}}$$

Stationary current

$$J^*(x) = Hxp^*(x)$$

$$H = \frac{D}{2}C^{-1} - M$$

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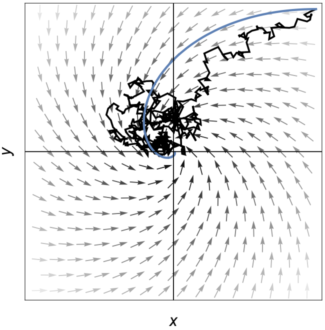

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Example 1: Gradient diffusions

- Conservative drift:

$$\boldsymbol{F}(\boldsymbol{x}) = -\nabla U(\boldsymbol{x})$$

- Noise matrix: $\sigma = \epsilon \boldsymbol{I}$

- 2D example:

$$M = \begin{pmatrix} \gamma & 0 \\ 0 & \gamma \end{pmatrix}$$

- Density:

$$p^*(\boldsymbol{x}) = \frac{\gamma}{\pi\epsilon^2} \exp\left(-\frac{\gamma}{\epsilon^2}\|\boldsymbol{x}\|^2\right)$$

- Current: $\boldsymbol{J}^* = 0$

Equilibrium or reversible system

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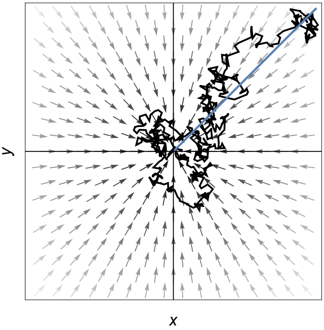

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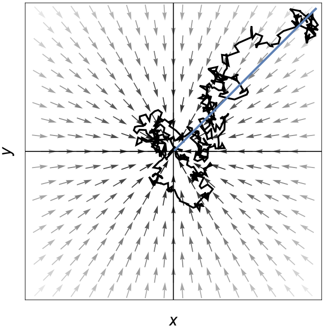

Equilibrium or reversible system

Example 2: Transverse diffusions

- Drift:

$$\boldsymbol{F} = -\nabla U + \boldsymbol{A}, \quad \boldsymbol{A} \cdot \nabla U = 0$$

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$$M = \begin{pmatrix} \gamma & \xi \\ -\xi & \gamma \end{pmatrix}$$

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$$\boldsymbol{J}^*(\boldsymbol{x}) = \xi \begin{pmatrix} -y \\ x \end{pmatrix} p^*(\boldsymbol{x})$$

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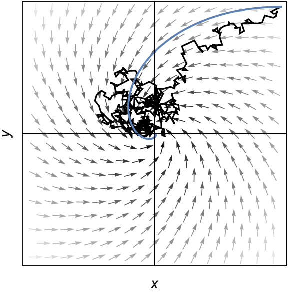
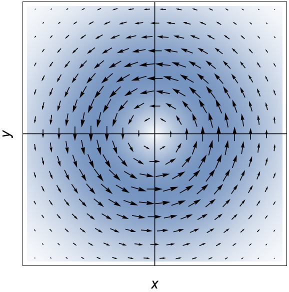
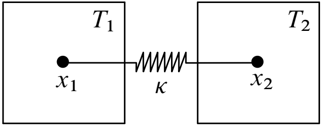




Example 3: Brownian gyrator

[Exartier & Peliti 1999; Filiger & Reimann 2007]



- Drift:

$$M = \begin{pmatrix} \gamma + \kappa & -\kappa \\ -\kappa & \gamma + \kappa \end{pmatrix}$$

- Noise matrix:

$$\sigma = \begin{pmatrix} \sqrt{2T_1} & 0 \\ 0 & \sqrt{2T_2} \end{pmatrix}$$

- $J^* \neq 0$ iff $\kappa > 0$ and $T_1 \neq T_2$

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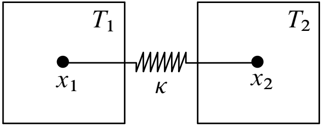

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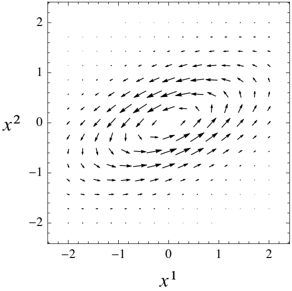

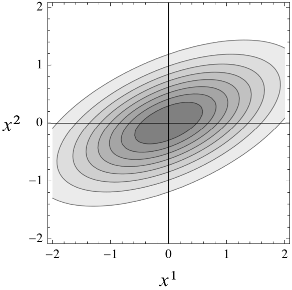

Observables

- Linear forms:

$$A_T = \frac{1}{T}\int_0^T \eta \cdot \boldsymbol{X}(t)dt$$

- Quadratic forms:

$$A_T = \frac{1}{T}\int_0^T \boldsymbol{X}(t) \cdot Q\boldsymbol{X}(t)dt$$

- Current-type forms:

$$A_T = \frac{1}{T}\int_0^T \Gamma\boldsymbol{X}(t) \circ d\boldsymbol{X}(t)$$

Examples

- Mechanical work W_T
- Heat exchanged Q_T
- Entropy prod Σ_T
- Integrated currents J_T
- Residence times
- Control costs, reward
- Statistical estimators

Large deviation approximation

$$P(A_T = a) \approx e^{-TI(a)}$$

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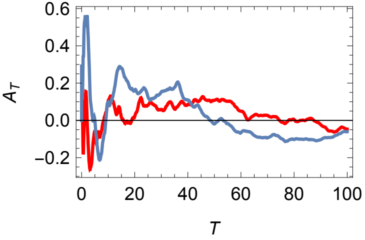

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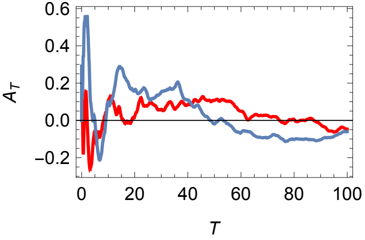

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Large deviation theory

[Donsker & Varadhan 1970s; Gärtner 1977]

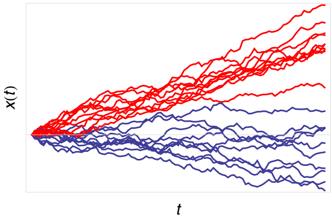
LD functions

- Rate function:

$$I(a) = \max_{k\in\mathbb{R}}\{ka - \lambda(k)\}$$

- SCGF:

$$\lambda(k) = \text{dom eigval}(\mathcal{L}_k)$$



Fluctuation process

$$d\tilde{\boldsymbol{X}}_t = \tilde{\boldsymbol{F}}_k(\tilde{\boldsymbol{X}}_t)dt + \sigma d\boldsymbol{W}_t$$

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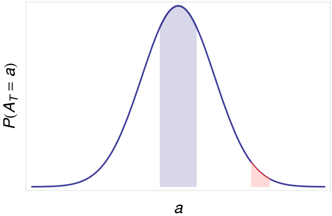

- Effective process creating fluctuation [Chetrite & HT 2013, 2015]
- Effective density and current: p_k^*, $\boldsymbol{J}_k^*$

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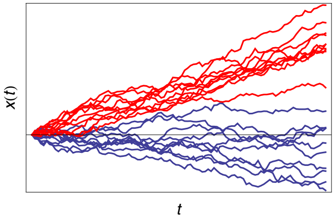

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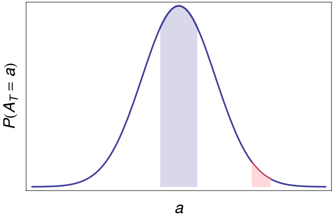

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Main result

[du Buisson PhD 2023; du Buisson & HT 2023]

- Generating function:

$$G_k(\boldsymbol{x}, t) = E[e^{ktA_t} | \boldsymbol{X}(0) = \boldsymbol{x}]$$

- Feynman-Kac equation:

$$\partial_t G_k(\boldsymbol{x}, t) = \mathcal{L}_k G_k(\boldsymbol{x}, t), \quad G(\boldsymbol{x}, 0) = 1$$

- Solution:

$$G_k(\boldsymbol{x}, t) = e^{\boldsymbol{x} \cdot B_k(t) \boldsymbol{x}} e^{\int_0^t \mathrm{Tr}[D B_k(s)] ds} \overset{t \to \infty}{\sim} e^{\boldsymbol{x} \cdot B_k^* \boldsymbol{x}} e^{t \, \mathrm{Tr}(D B_k^*)}$$

LD solution

- SCGF: $\lambda(k) = \mathrm{Tr}(D B_k^*)$
- Riccati matrix: B_k^*
- Eigenfunction: $r_k(\boldsymbol{x}) = e^{\boldsymbol{x} \cdot B_k^* \boldsymbol{x}}$
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Current observables

$$A_T = \frac{1}{T}\int_0^T \Gamma \boldsymbol{X}(t) \circ d\boldsymbol{X}(t)$$

- Tilted generator:

$$\mathcal{L}_k = -kM\boldsymbol{x}\cdot\Gamma\boldsymbol{x} + (-M + kD\Gamma)\boldsymbol{x}\cdot\nabla + \frac{1}{2}\nabla\cdot D\nabla + \frac{k^2}{2}\Gamma\boldsymbol{x}\cdot D\Gamma\boldsymbol{x}$$

- Algebraic Riccati equation:

$$\frac{k^2}{2}\Gamma^{\mathsf{T}}D\Gamma - \frac{k}{2}(M^{\mathsf{T}}\Gamma - \Gamma M) - (M - kD\Gamma)^{\mathsf{T}}B_k^* - B_k^*(M - kD\Gamma) + 2B_k^*DB_k^* = 0$$

$$C + AB + BA + BQB = 0$$

Effective process

$$M_k = M - 2DB_k^* - kD\Gamma$$

$$p_k^*(\boldsymbol{x}) \propto e^{-\frac{1}{2}\boldsymbol{x}\cdot C_k{}^{-1}\boldsymbol{x}}, \qquad D = M_kC_k + C_kM_k^{\mathsf{T}}$$

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$$A_T = \frac{1}{T}\int_0^T \Gamma \boldsymbol{X}(t) \circ d\boldsymbol{X}(t)$$

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$$\mathcal{L}_k = -kM\boldsymbol{x}\cdot\Gamma\boldsymbol{x} + (-M + kD\Gamma)\boldsymbol{x}\cdot\boldsymbol{\nabla} + \frac{1}{2}\boldsymbol{\nabla}\cdot D\boldsymbol{\nabla} + \frac{k^2}{2}\Gamma\boldsymbol{x}\cdot D\Gamma\boldsymbol{x}$$

- Algebraic Riccati equation:

$$\frac{k^2}{2}\Gamma^{\mathsf{T}}D\Gamma - \frac{k}{2}(M^{\mathsf{T}}\Gamma - \Gamma M) - (M - kD\Gamma)^{\mathsf{T}}B_k^* - B_k^*(M - kD\Gamma) + 2B_k^*DB_k^* = 0$$

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Example: Stochastic area

[Lévy 1940, 1950, 1951; Teitsworth et al 2017, 2019]

- Process in $\mathbb{R}^2$: $((X_t, Y_t))_{t=0}^{T}$
- Green's theorem:

$$\mathcal{A}_T = \frac{1}{2}\int_0^T X_t dY_t - Y_t dX_t$$

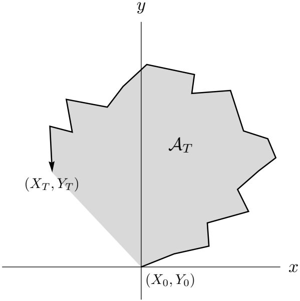
- Brownian motion:

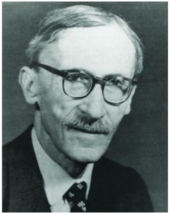
$$p(A_T = a) = \frac{1}{T}\operatorname{sech}\left(\frac{\pi a}{T}\right), \quad \operatorname{var}(\mathcal{A}_T) = \frac{T^2}{4}$$

- Linear diffusions:

$$a^* = \lim_{T\to\infty}\left\langle \frac{\mathcal{A}_T}{T}\right\rangle = \left(MC - \frac{D}{2}\right)_{1,2}$$

$\neq 0$ nonreversible systems





Paul Lévy (1886-1971)

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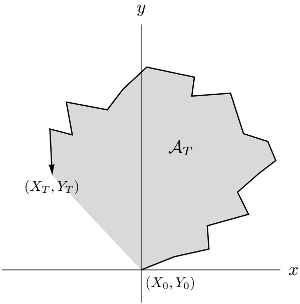

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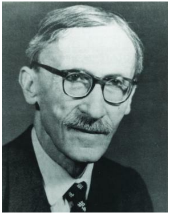

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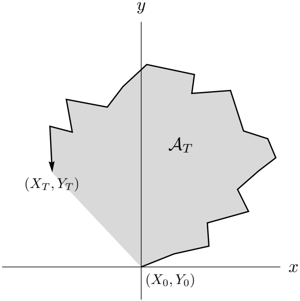

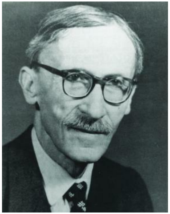

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Example: Transverse diffusions [du Buisson, Mnyulwa & HT 2023]

$$M = \begin{pmatrix} \gamma & \xi \\ -\xi & \gamma \end{pmatrix} \qquad A_T = \frac{1}{T}\int_0^T \Gamma \boldsymbol{X}(t) \circ d\boldsymbol{X}(t) \qquad \Gamma = \frac{1}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

- Typical area: $a^* = \frac{\epsilon^2 \xi}{2\gamma}$
- Riccati matrix: $B_k^* = b_k^* I$
- SCGF:

$$\lambda(k) = \gamma - \sqrt{\gamma^2 - \frac{k\epsilon^2(k\epsilon^2 + 4\xi)}{4}}$$

- Rate function:

$$I(a) = \sqrt{\frac{\epsilon^4(\gamma^2+\xi^2)}{4a^2+\epsilon^4}} - \frac{2a\xi}{\epsilon^2} - \gamma + \frac{4|a|^3\left(\gamma^2+\xi^2\right)}{\sqrt{a^2\epsilon^4(4a^2+\epsilon^4)(\gamma^2+\xi^2)}}$$

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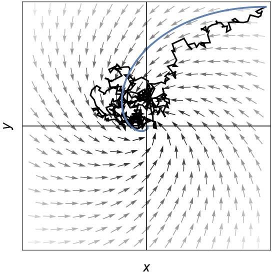

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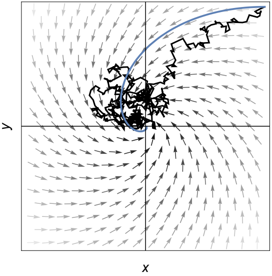

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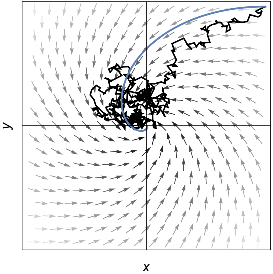

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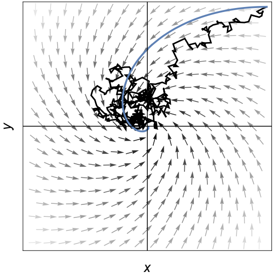

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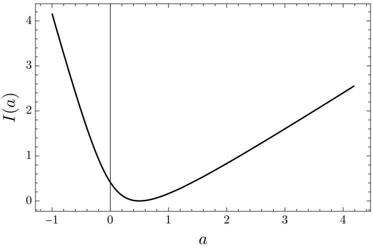

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Deconfinement

$0 < a < a^*$
Confinement

$a < 0$
Current reversal

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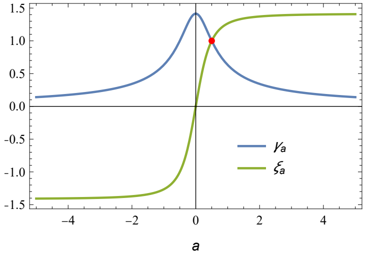

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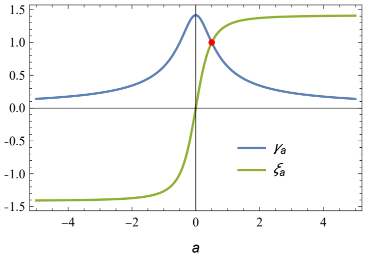

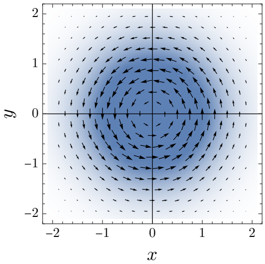

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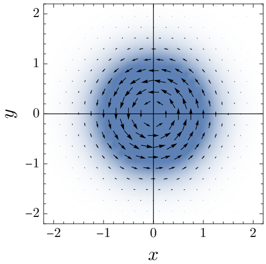

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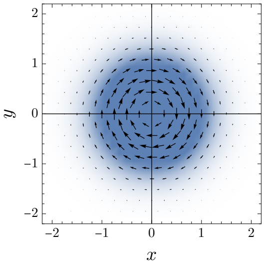

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Conclusions

- Similar results for other observables/processes
- Fluctuations created by effective (modified) linear process
- Underlying Gaussian density and current fluctuations
- Effective process = LQG optimal control

Current work

- Linear approximations for nonlinear SDEs/observables
- Numerical methods (Riccati or control)

[1] Johan du Buisson
Dynamical Large Deviations of Diffusions
PhD thesis, Stellenbosch University, 2022

[2] Johan du Buisson, HT
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