Finding the Quasipotential for Nongradient SDE's

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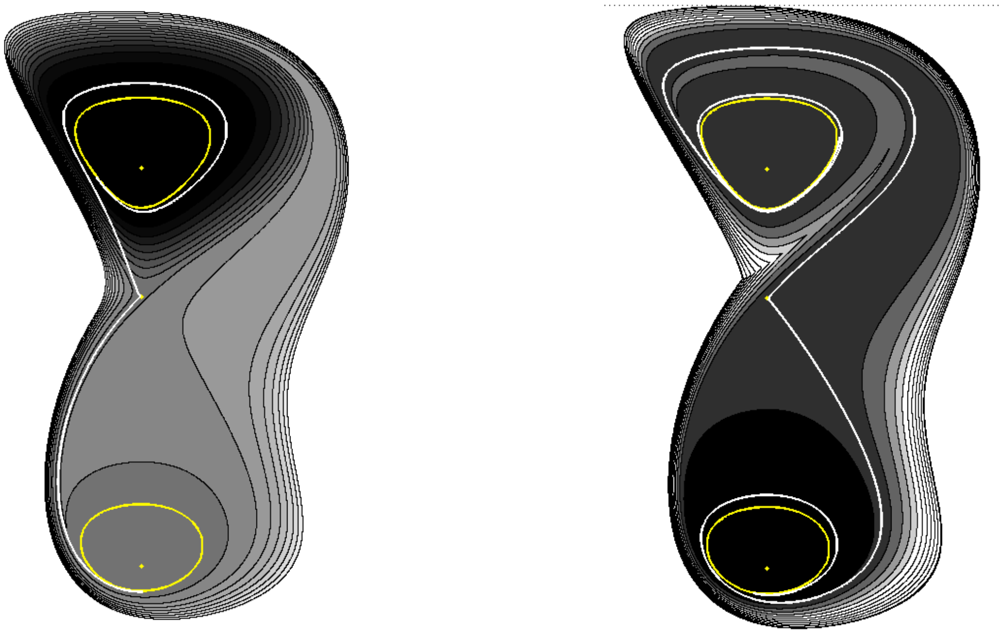
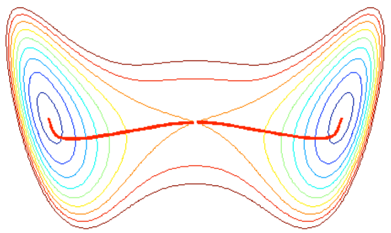


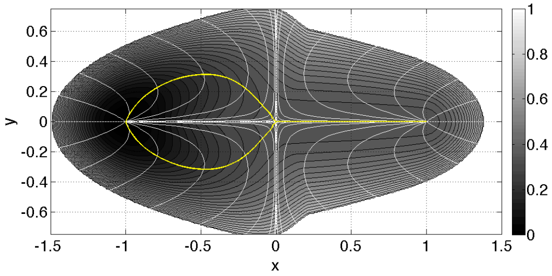
Stochastic dynamics:
Gradient vs Nongradient

$$dx = -\nabla V(x)dt + \sqrt{2\beta^{-1}}dw$$



Freidlin and Wentzell,
1979, 1998

$$dx = b(x)dt + \sqrt{2\beta^{-1}}dw$$



The most likely transition paths:

$$\phi_s \parallel \nabla V(x)$$

$b(x) = -(1/2)\nabla U(x) + l(x)$,
$\nabla U(x) \perp l(x)$,

$-(1/2)\nabla U(x)$ = potential component of $b(x)$
$l(x)$ = rotational component of $b(x)$

$$\phi_s \parallel (1/2)\nabla U + l$$

Equilibrium probability density:

$$m(x) = Z^{-1} \exp(\ \beta V(x)\ )$$

In some neighborhood of an asymptotically stable equilibrium

$$m(x) \sim \exp(\ (1/2)\beta U(x)\ )$$

$U(x)$ = the quasipotential

Attractors of nongradient systems

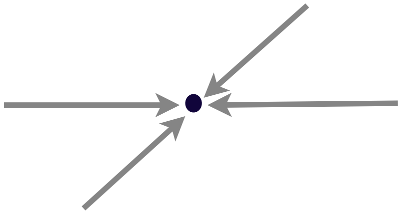
$$dx = b(x)dt + \sqrt{2\beta^{-1}}dw$$

$$x \in R^n$$

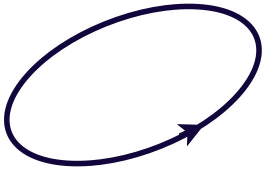
dw - standard Brownian Motion in R^n

$\sqrt{2\beta^{-1}}$ - small parameter

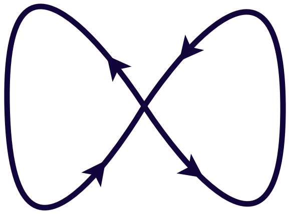
Unperturbed equation $x'=b(x)$ can have various types of attractors, i.e.



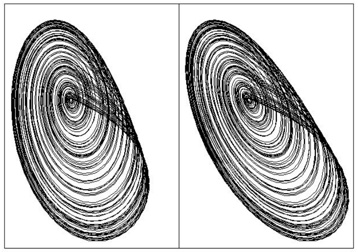
Stable equilibrium



Stable limit cycle



Saddles and connecting them homoclinic or heteroclinic trajectories



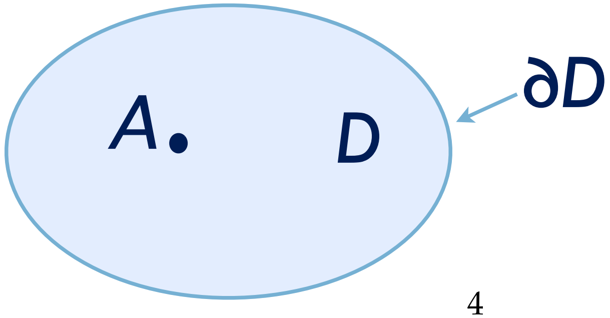
Strange attractor (Roessler attractor)

Transitions between different attractors of the system happen under the influence of small noise

The Large Deviation Theory

Freidlin, Wentzell, 1979, 1998

- SDE $$dx = b(x)dt + \sqrt{2\beta^{-1}}dw$$
- Freidlin-Wentzell Action $$S_T(\varphi) = \frac{1}{2}\int_0^T \left|\varphi_t - b(\varphi(t))\right|^2 dt$$
- Quasipotential $$U_A(x) = \inf_{\varphi,T}\left\{S_T(\varphi)\middle|\varphi(0) = A, \varphi(T) = x\right\}$$
- The first passage time $$\tau_A(D) \sim \min_{x\in\partial D} e^{\frac{\beta}{2}U_A(x)}$$



Goals

- To understand the theoretical behavior of the quasipotential w.r.t. various types of attractors of the system
- To develop a numerical algorithm for computing the quasipotential on a mesh

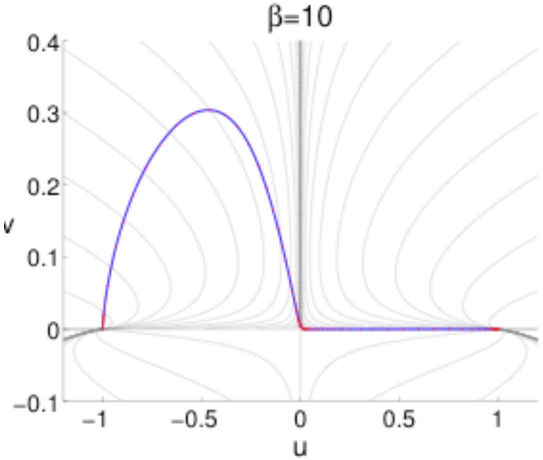
Numerical Methods
for nongradient systems with noise

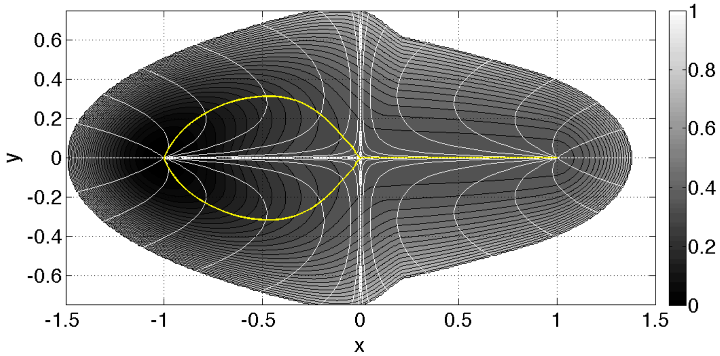
Previous works

- Geometric Minimum Action Method, Heymann and Vanden-Eijnden, 2008
- Adaptive Minimum Action Method, Zhou, Ren, and E, 2008

This work

Dijkstra-like solver for finding the quasipotential on a regular mesh, based on the Ordered Upwind Method. Adjustment for unbounded speed function and numerical analysis





Important advantage: always finds the global minimizer and no initial guess is required.

Outline for the rest of the talk

- Theoretical part
  - Quasipotential as a function defined on compact sets. General properties
  - Quasipotential and the Hamilton-Jacobi-Bellman equation
  - Behavior near stable orbits in 2D
    - Linear systems
    - Nonlinear systems with stable equilibria
    - Systems with limit cycles
- Numerical part
  - Background: Hamilton-Jacobi solvers and path-based methods
  - Adjusted Ordered Upwind Method. Error analysis
  - Examples

Theoretical part

Geometric action

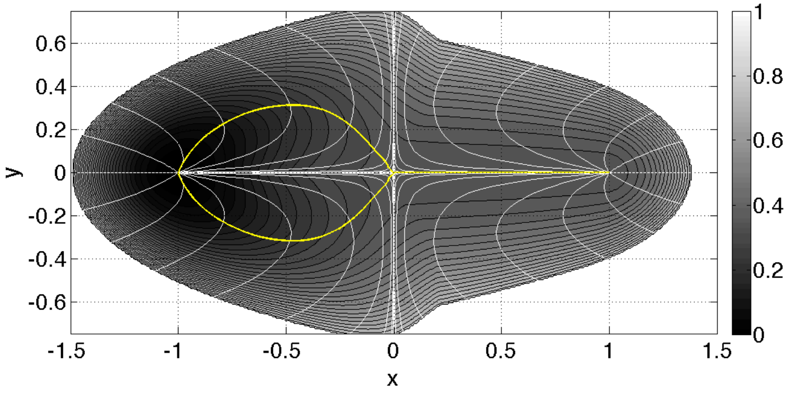
Freidlin, Wentzell, 1979; Heymann, Vanden-Eijnden, 2008

$$S_T(\varphi) = \frac{1}{2}\int_0^T |\varphi_t - b(\varphi)|^2\,dt = \frac{1}{2}\int_0^T \left\{|\varphi_t|^2 + |b(\varphi)|^2 - 2\varphi_t \bullet b(\varphi)\right\}dt \ge$$

$$\int_0^T \left\{|\varphi_t||b(\varphi)| - \varphi_t \bullet b(\varphi)\right\}dt = \int_0^L \left\{|\varphi_s||b(\varphi)| - \varphi_s \bullet b(\varphi)\right\}ds$$

$$"=" \Leftrightarrow |\varphi_t| = |b(\varphi)|$$

$$\boxed{S(\varphi) = \int_0^L \left\{|\varphi_s||b(\varphi)| - \varphi_s \bullet b(\varphi)\right\}ds = \int_0^1 \left\{|\varphi_\alpha||b(\varphi)| - \varphi_\alpha \bullet b(\varphi)\right\}d\alpha}$$

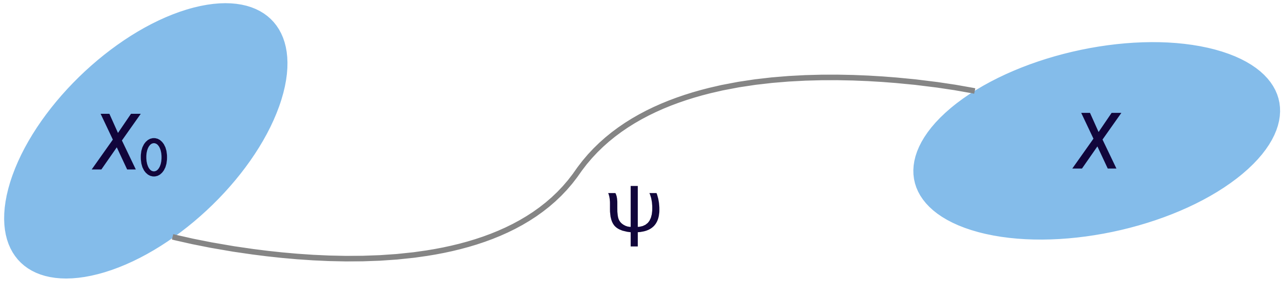


Quasipotential as a function on compact sets

Definition: For any pair of compact sets $X_0, X \subset R^n$ we define the quasipotential as

$$U(X_0,X)=\inf_{\psi}\left\{S(\psi)\middle|\psi(0)\in X_0,\psi(L)\in X\right\},$$

$$S(\psi)=\int_0^L\left\{|\psi_s||b(\psi)|-\psi_s\bullet b(\psi)\right\}ds.$$



General Properties

Assumption: $b(x)$ is continuously differentiable

Lemma 1. $D \subset R^n$ is convex and compact. Then $U(X_0,X)$ is Lipschitz-continuous w.r.t. Hausdorff metric in D.

(Hausdorff metric: $d_H(X, Y) = \max\{ \sup_{x\in X} \inf_{y\in Y} | x-y | , \sup_{y\in Y} \inf_{x\in X} | x-y | \}$.)

Theorem 1. Let X_0 be a compact set. Let $C = \{ x(t) \mid t \geq 0 \}$ be a trajectory of $x_t = b(x)$, and F be its ω-limit set. Then

1. $U(X_0, y) = U(X_0, F)$ for all $y \in F$.

2. $U(y, X_0) = U(F, X_0)$ for all $y \in F$.

Hamilton-Jacobi-Bellman equation

$$S(\psi) = \int_0^L \left\{ |\psi_s||b(\psi)| - \psi_s \bullet b(\psi) \right\} ds,$$

Geometric action

$$U(x) = \left\{ \inf_{\psi} \int_0^L \left\{ |\psi_s||b(\psi)| - \psi_s \bullet b(\psi) \right\} ds : \psi(0) \in X_0, \psi(L) = x \right\}$$

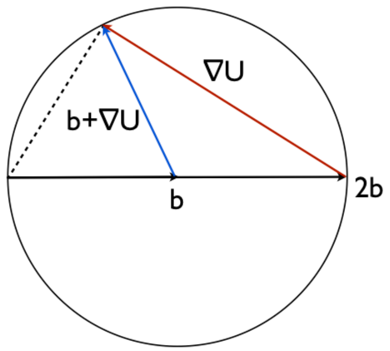
Quasipotential = Value Function

$$H(x, \nabla U) \triangleq \inf_{\psi_s \in S^{n-1}} \left\{ |b(x)| - \left(b(x) + \nabla U \right) \bullet \psi_s \right\} = 0$$

Hamiltonian

The infimum is achieved if $\psi_s = \dfrac{b + \nabla U}{|b + \nabla U|}$

The infimum is zero if $\psi_s = \dfrac{b + \nabla U}{|b|}, \quad \nabla U = |b|\psi_s - b$



Hamilton-Jacobi-Bellman equation

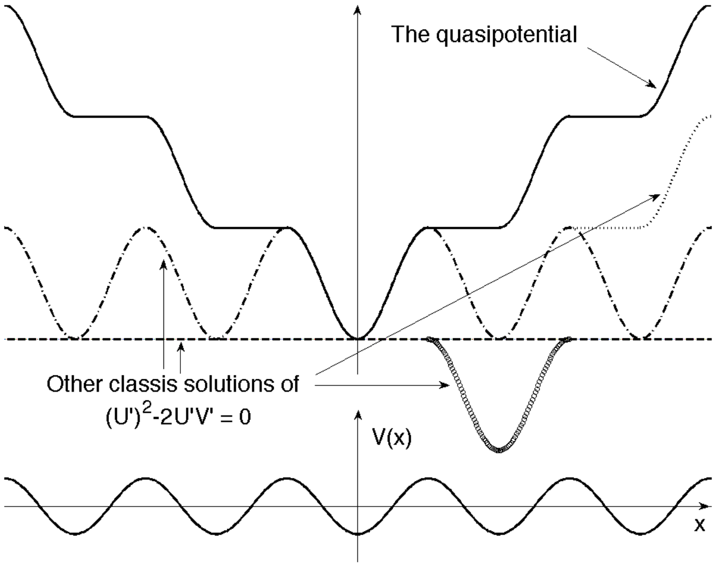
U(*x*) = quasipotential at the point *x* w.r.t. the set X_0

$$\boxed{|\nabla U(x)|^2 + 2\nabla U(x) \bullet b(x) = 0, \quad U\big|_{X_0} = 0.}$$

Problem: the viscosity solution is NOT UNIQUE in general

Viscosity solutions for $|\nabla U|^2 + 2b(x)\bullet\nabla U = 0$

The 1D case:
$(U')^2 - 2U'V' = 0$
Hence $U' = 0$ or $U' = 2V'$
Multiple classic solutions
each of which is a viscosity solution



Theorem (H. Ishii (1987):)

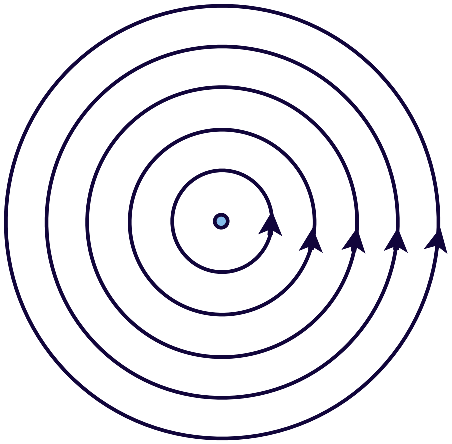
$$\begin{aligned} |\nabla U|^2 + 2b(x)\bullet\nabla U &= 0, & x &\in \Omega, \\ U &= 0, & x &\in \partial\Omega \end{aligned}$$

If for there is a function $\varphi(x) \in C^1(\Omega)$ such that

$b(x) \cdot \nabla\varphi \geq 1,$

then there is at most one viscosity solution of class $C(\Omega)$

2D. Periodic trajectories

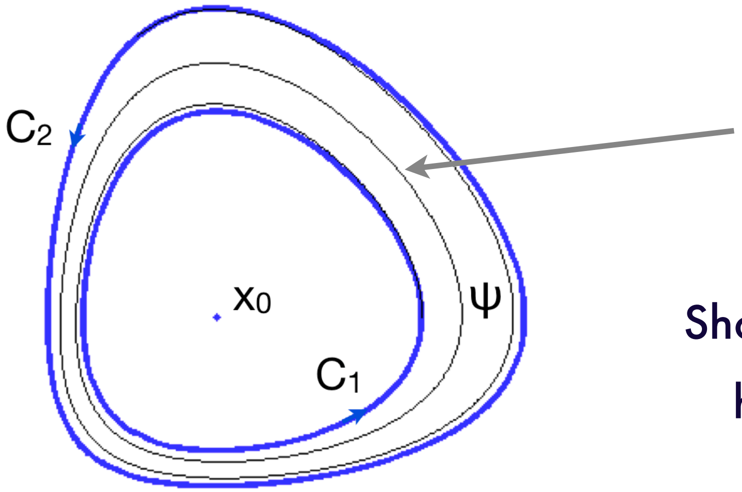


Theorem 2. Let x_0 be an equilibrium of $x_t = b(x)$, $x \in R^2$, and all trajectories in some neighborhood

D of x_0 containing no other critical points are periodic. Then

$$U(x, y) = 0 \text{ for all } x, y \in D.$$

Sketch of proof



$$\psi_s = \frac{b(\psi)+\varepsilon b^{\perp}(\psi)}{\left|b(\psi)+\varepsilon b^{\perp}(\psi)\right|}.$$

Show that the geometric action $S(\psi) \propto \epsilon$,

hence can be made arbitrarily small.

2D linear systems

Theorem 3. Let the origin x_0 be an asymptotically stable equilibrium of

$$x_t = Ax, \quad x \in R^2, \text{ where } \quad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \qquad \text{Let} \qquad (Ax)^{\perp} = \begin{pmatrix} -c & -d \\ a & b \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$

Then the vector field Ax can be decomposed as $Ax = - 1/2\, \nabla U(x) + l(x)$, where

$$-\frac{\nabla U(x)}{2} = Ax\sin^2\theta - (Ax)^{\perp}\sin\theta\cos\theta, \qquad \cot\theta = \frac{c-b}{a+d}$$

$$l(x) = Ax\cos^2 + (Ax)^{\perp}\sin\theta\cos\theta,$$

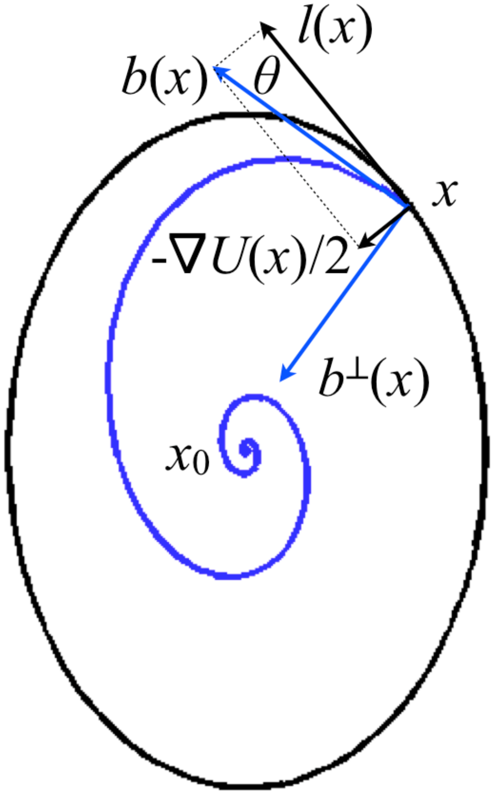
$U(x)$ is the quasipotential for the linear SDE

$$dx = Axdt + \sqrt{2\beta^{-1}}\,dw,$$

w.r.t the origin. It is given by

$$U(x) = -x_1^2(a\sin^2\theta + c\sin\theta\cos\theta) - x_2^2(d\sin^2\theta - b\sin\theta\cos\theta) - 2x_1x_2\left(b\sin^2\theta + d\sin\theta\cos\theta\right).$$

Sketch of proof:



Modify the vector field $b(x)$ by rotating it by a constant angle θ to be defined:
$x_t = Ax \cos\theta + (Ax)^{\perp} \sin\theta$

so that the trajectories of the new equation are periodic.

Denote $l_0(x) = Ax \cos\theta + (Ax)^{\perp} \sin\theta$

and set and orthogonal to it field

$u(x) = - Ax \sin\theta + (Ax)^{\perp} \cos\theta.$

Show that the desired decomposition
$Ax = -1/2 \, \nabla U(x) + l(x)$
can be obtained by scaling the vector fields $l_0(x)$ and $u(x)$.

Remarks

- Chen and Freidlin (2005), general formula for linear equations

$$U(x) = \frac{1}{2}\left(\left(\int_0^{\infty} e^{At} e^{A^* t}\, dt\right)^{-1} x, x\right).$$

This formula can be simplified if $AA^T = A^T A$. In 2D this means $A = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$ *or* $A = \begin{pmatrix} a & -c \\ c & a \end{pmatrix}$.

- This construction is not applicable for 2D nonlinear systems as the angle between $b(x)$ and $\nabla U(x)$ is not constant in this case.

- The equilibrium probability density (the invariant probability measure) **equals exactly** to

$m(x) = Z^{-1}\exp(-\beta U(x)/2)$ **iff** div $l(x) = 0$.

This is so in the case of 2D linear systems.

2D nonlinear equations with asymptotically stable equilibrium

Theorem 4. Let the x_0 be an asymptotically stable equilibrium of

$$x_t = b(x), \quad x \in R^2, \quad b \in C^1(R^2).$$

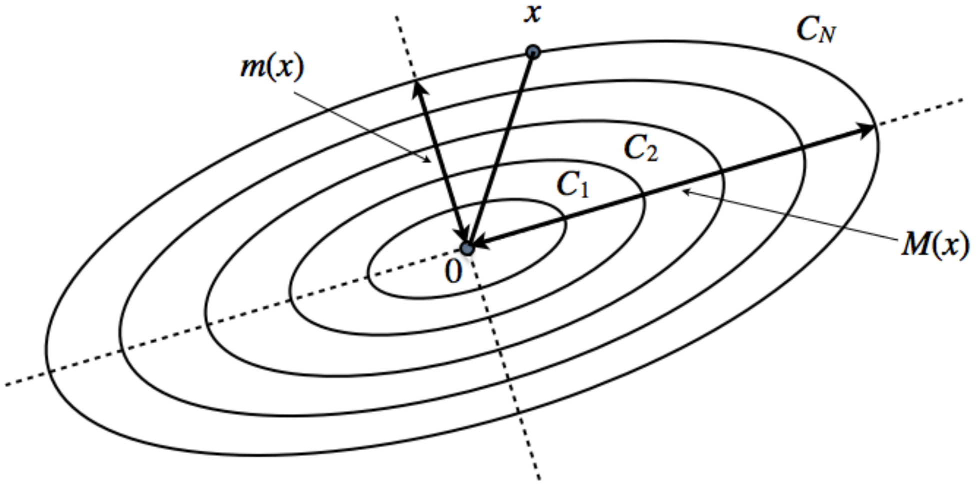
Let the eigenvalues of $A \equiv \nabla b(x_0)$ have negative real parts.

Then there is a neighborhood of x_0 where the quasipotential $U(x_0, x)$ grows quadratically, i.e.,

$$a_1 |x - x_0|^2 < U(x) < a_2 |x - x_0|^2$$

for some positive constants a_1, a_2.

Sketch of proof:



Consider *N* evenly spaced level sets of the quasipotential for the linearized system, bound the infimum of geometric action between every pair of them.

Let *N* go to infinity.

2D. Stable limit cycles

Theorem 5. Let C be a closed curve representing a stable limit cycle of
$x_t = b(x)$, $x \in R^2$.

Let Ω be a neighborhood of C lying in its basin of attraction where one can introduce
local coordinates (s,y), s = arclength of C, y = signed distance to C.

Suppose $b(x) = b_{||}(x) + b_\perp(x)$ in Ω,

where $q(x)$ is parallel to C, and $p(x)$ is orthogonal to C. Suppose

$$f_1(|y|) \le |b_\perp(x)| \le f_2(|y|)$$

for some continuous functions f_1 and f_2 , positive in Ω\C. Then in Ω we have

$$2\int_0^L f_1(z)dz \quad \le \quad U(C,x) \quad \le \quad 2\int_0^L f_2(z)dz$$

where L = distance between the point x and the curve C.

Numerical part

Methods for finding Minimum Action Paths

1. "Geometric Minimum Action Method", Heymann and Vanden-Eijnden, 2008

   Idea: Solve the Euler-Lagrange equation for the geometric action by steepest descent combined with reparametrization.

2. "Adaptive Minimum Action Method", Zhou, Ren, and E, 2008

   Idea: Minimize discretized Freidlin-Wentzell action equipped with a monitor function that controls the distribution of the points along the path.

Hamilton-Jacobi Solvers

Solvers for Eikonal Equation

$$F(x)|\nabla U(x)| = 1$$

1. Fast Marching Method,
   Sethian 1996

2. Fast Sweeping Method,
   proposed by Dupuis and Boue, 1999,
   analysed and promoted by H. Zhao

3. Fast Marching Characteristics
   Based Schemes,
   Cacace, Cristiani

Solvers for Hamilton-Jacobi Equation

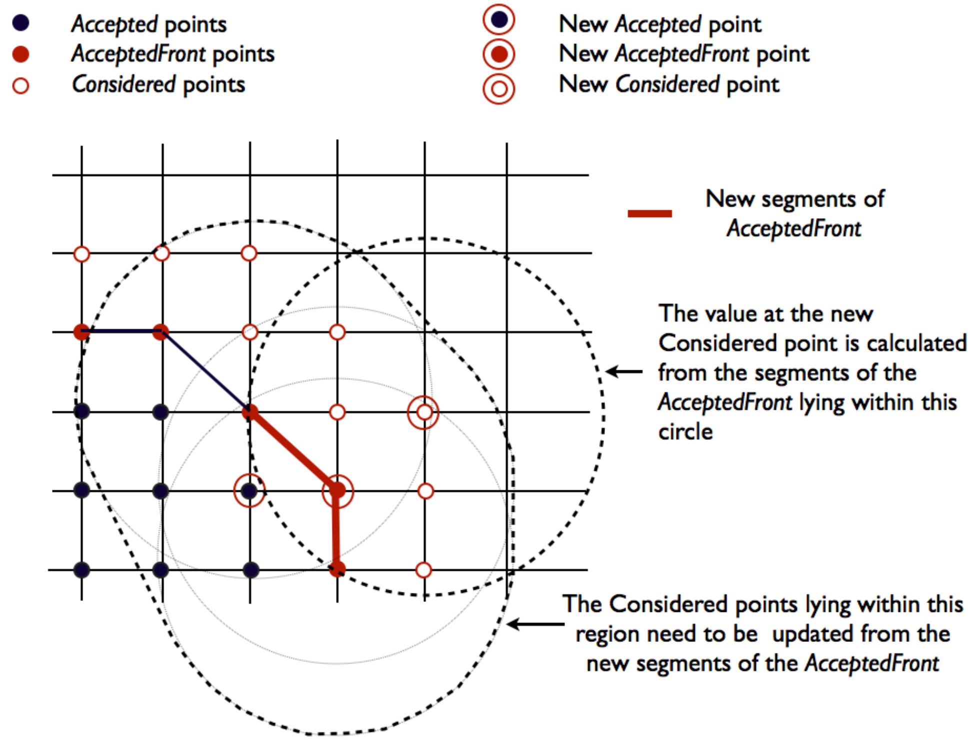
$$F\left(x, \frac{\nabla U}{|\nabla U|}\right)|\nabla U(x)| = 1$$

1. Ordered Upwind Method,
   Sethian, Vladimirsky, 2001, 2003

2. Fast Marching Characteristics
   Based Schemes,
   Cacace, Cristiani

Ordered Upwind Method

Sethian, Vladimirsky, 2001, 2003



The value at the new Considered point is calculated from the segments of the *AcceptedFront* lying within this circle

The Considered points lying within this region need to be updated from the new segments of the *AcceptedFront*

$$F\left(x, \frac{\nabla U}{|\nabla U|}\right)|\nabla U(x)| = 1,$$

$$0 < F_1 \le F(x,a) \le F_2 < \infty$$

Four kinds of mesh points:
Accepted
AcceptedFront
Considered
Unknown

At each step, a Considered point with smallest tentative value of U becomes AcceptedFront or Accepted depending on whether it has Considered neighbors or not.

Key concept: update radius

$$\rho = h\frac{F_2}{F_1} < \infty$$

Minimization problem for finding the quasipotential

The minimization problem for the qualipotential

$$U(x) = \left\{ \inf_{\psi} \int_0^L \left\{ |\psi_s||b(\psi)| - \psi_s \bullet b(\psi) \right\} ds : \psi(0) \in X_0, \psi(L) = x \right\}$$

The Hamilton-Jacobi-Bellman equation

$$|\nabla U(x)|^2 + 2\nabla U(x) \bullet b(x) = 0, \quad U\big|_{X_0} = 0.$$

$$\frac{1}{-2b(x)\bullet a}|\nabla U(x)| = 1, \quad a \equiv \frac{\nabla U(x)}{|\nabla U(x)|}$$

$$F(x,a) = \frac{1}{-2b(x)\bullet a},$$

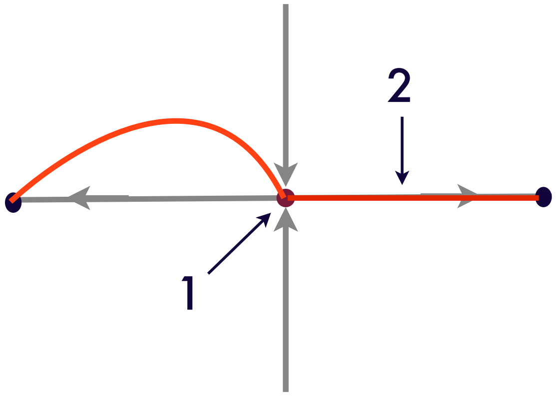
$$0 < \frac{1}{2|b(x)|} \le F(x,a) \le \infty$$

By design, the numerical procedure automatically avoids parasite solutions of the H-J-B equation

Difficulty: the speed function is unbounded from above.

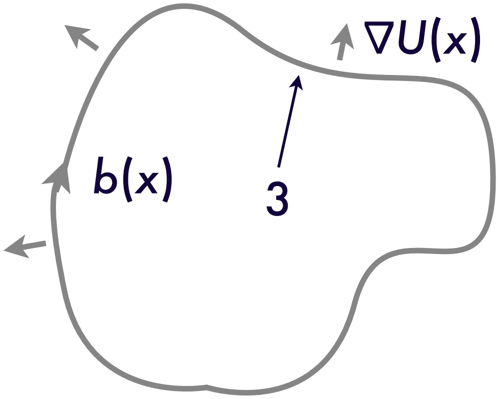
Where $F(x,a) \to \infty$?

1. Where $b(x) \to 0$, e.g. near saddle points.



2. Where $\nabla U(x) \neq 0$ and $b(x) \neq 0$, but $\nabla U(x) \perp b(x)$,

   e.g. along trajectories $\varphi_t = b(\varphi)$ going downhill where $U(\varphi) = \text{constant}$.



3. Where $\nabla U(x) = 0$ but $b(x) \neq 0$,

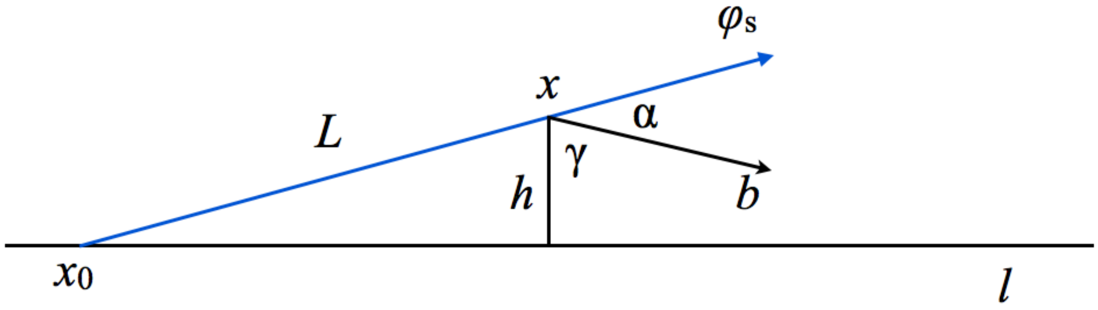
   e.g. near limit cycles.

Fighting the difficuly: Setting a finite update radius

We set a finite update radius

ρ = *Kh*,

where h is the mesh step, and *K* is a positive integer, e.g., *K*=10, 20, or 40.



Level set $U = U_0$

$$S(\alpha) = U_0 + L(\alpha)|b|(1-\cos\alpha),$$
$$U(x) = \inf_{\alpha}\{S(\alpha)\},$$
$$U(x) = \begin{cases} S(\alpha = \pi - 2\gamma) = U_0 + 2|b|h\cos\gamma, & \gamma < \dfrac{\pi}{2}, \\ S(\alpha = 0) = U_0, & \gamma \geq \dfrac{\pi}{2} \end{cases}$$

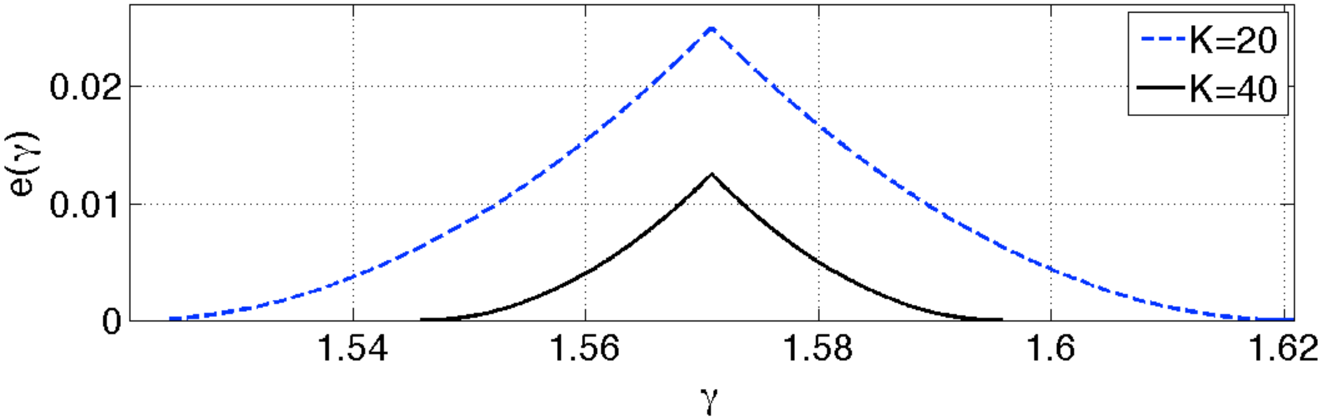
Additional consistency error

Theorem 6. Let $U_h(x) = \inf_\alpha \{ S(\alpha) \mid L(\alpha) \le Kh \}$.

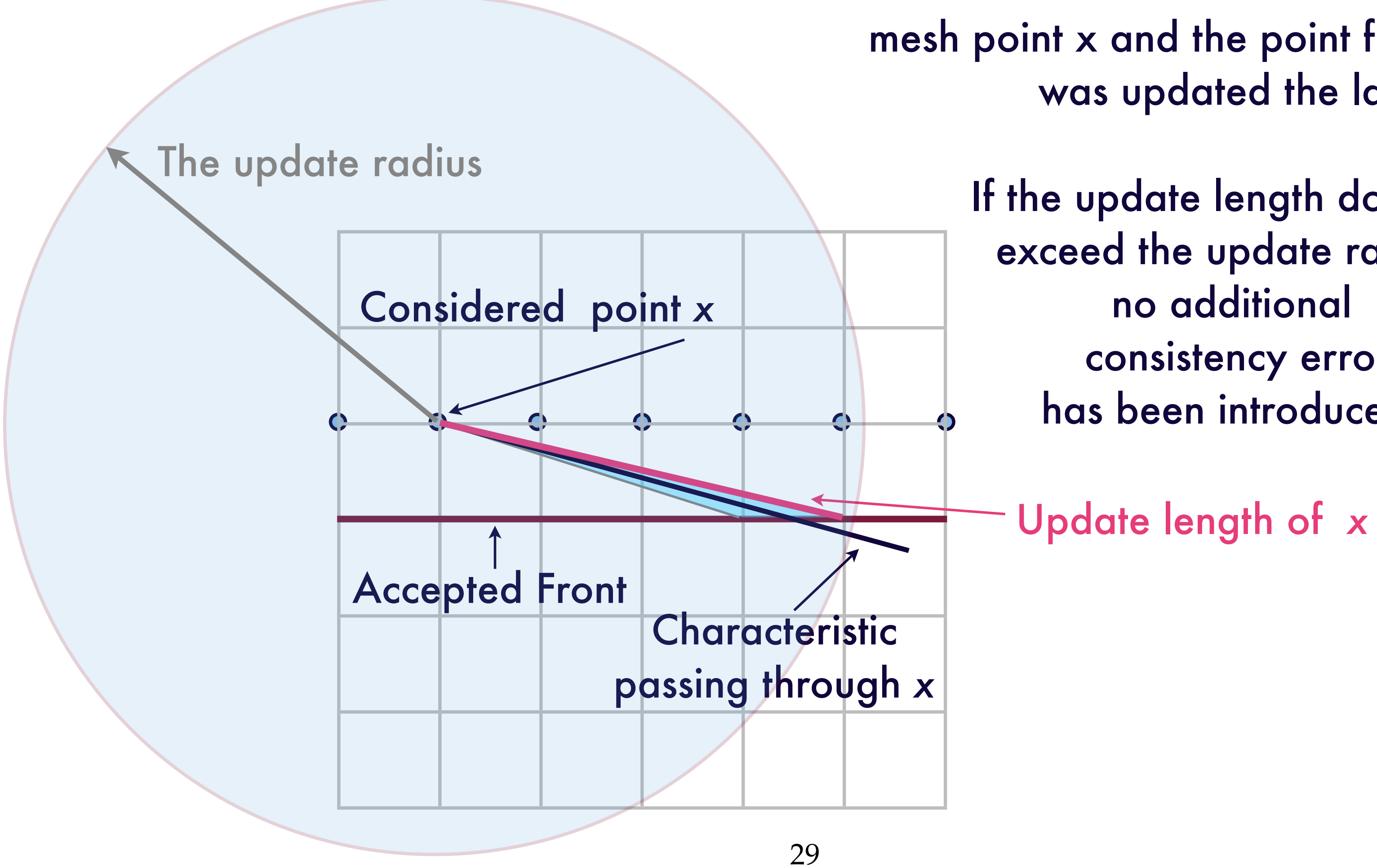
Then $U_h(x) = U(x)$ if $\gamma < \arccos(1/K)$ or $\gamma > \pi - \arccos(1/K)$, and

$$U_h(x) - U(x) = \begin{cases} h|b|\left(K\left[1+\cos\left(\gamma + \arccos\frac{1}{K}\right)\right] - 2\cos\gamma\right), & \arccos\frac{1}{K} < \gamma < \frac{\pi}{2} \\ h|b|\left(K\left[1+\cos\left(\gamma + \arccos\frac{1}{K}\right)\right]\right), & \frac{\pi}{2} \le \gamma < \pi - \arccos\frac{1}{K}, \end{cases}$$

and the maximal difference is achieved at $\gamma = \pi/2$ and equals $|b|h \{ 1/(2K) + O(1/K^3) \}$.



Error monitoring

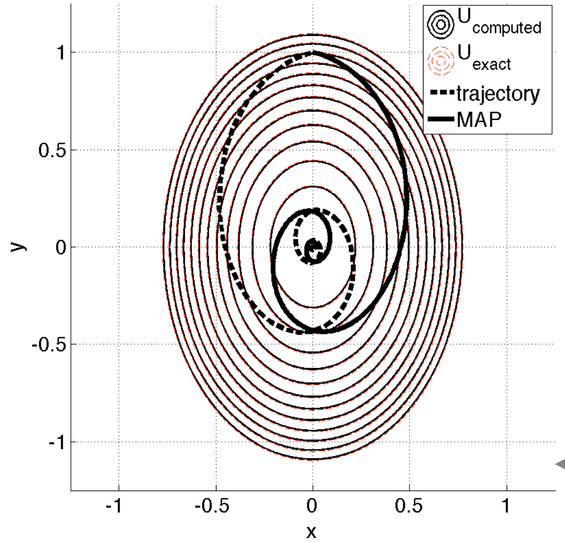


One can monitor the update length, i.e. the distance between the current mesh point x and the point from which it was updated the last.

If the update length does not exceed the update radius, no additional consistency error has been introduced.

Examples

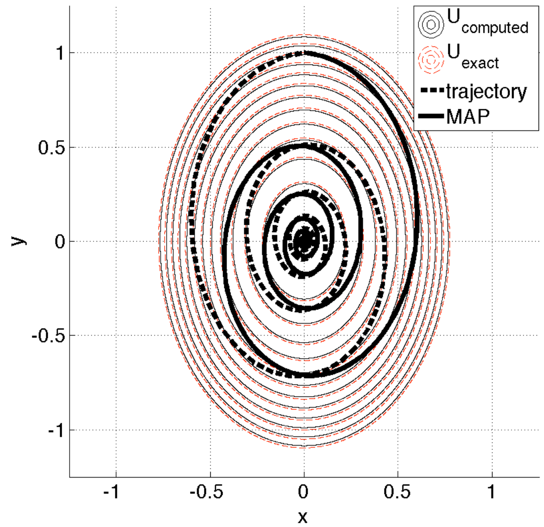
Example 1. Test on a linear equation



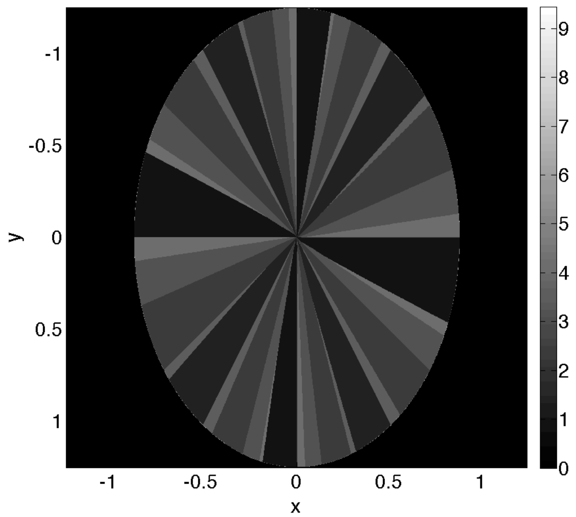
$$dx = (-2x - ay)dt + \sqrt{2\beta^{-1}}dw_1$$

$$dy = (2ax - y)dt + \sqrt{2\beta^{-1}}dw_2$$

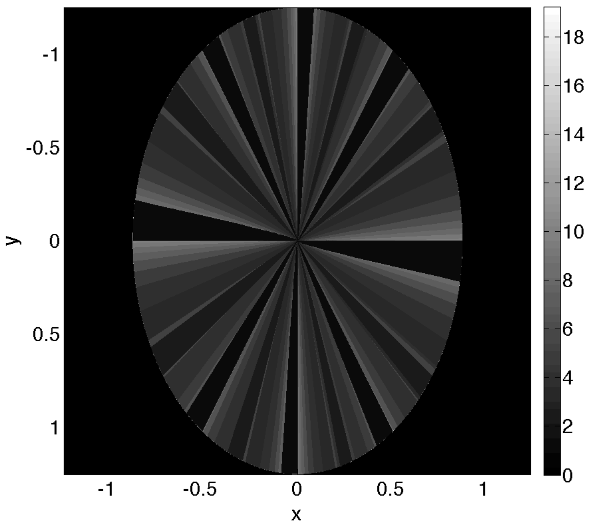
$$a = \frac{|l(x)|}{|0.5\nabla U(x)|}$$



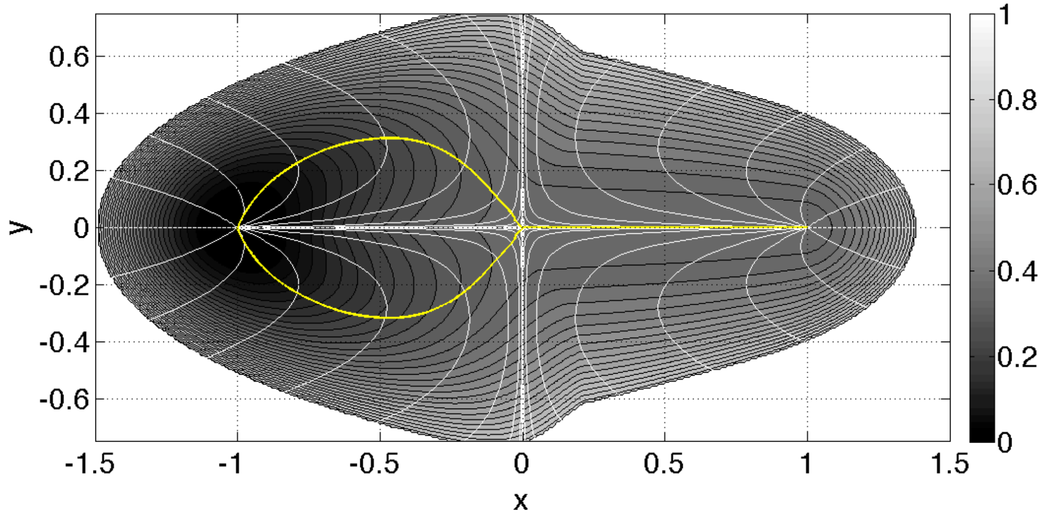
← $a = 4$ $a = 10$ →

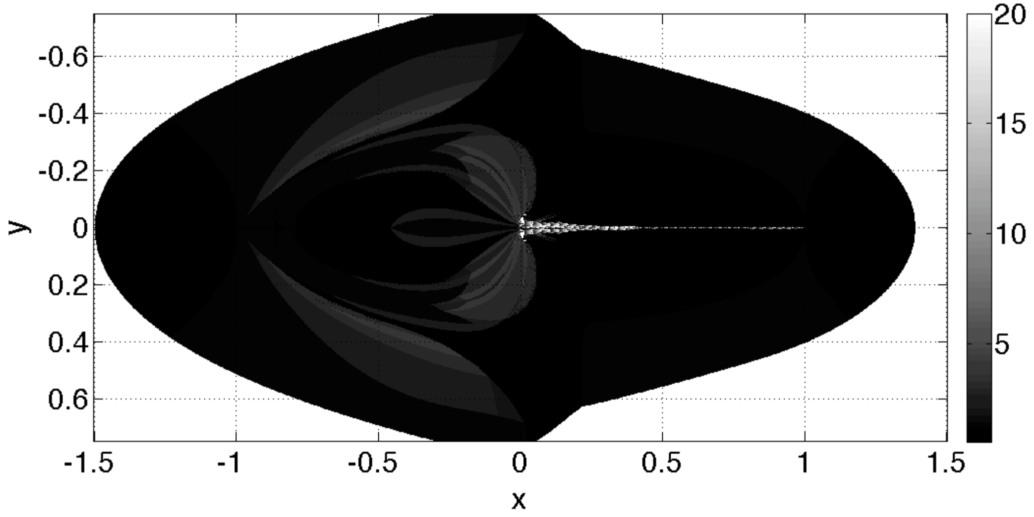


$U(x,y) = 2x^2 + y^2$



Example 2. Maier-Stein model



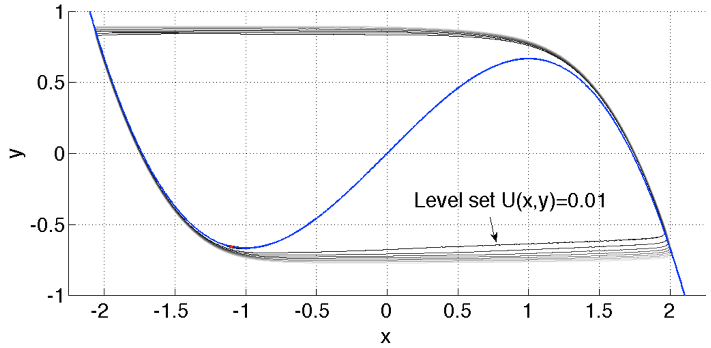


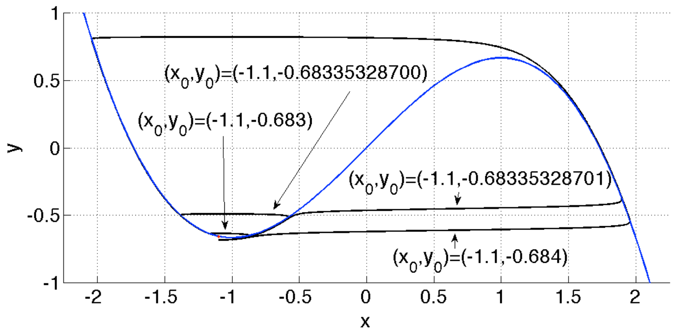
$$dx = (x - x^3 - 10xy^2)dt + \sqrt{2\beta^{-1}}dw_1$$
$$dy = -(1 + x^2)ydt + \sqrt{2\beta^{-1}}dw_2$$

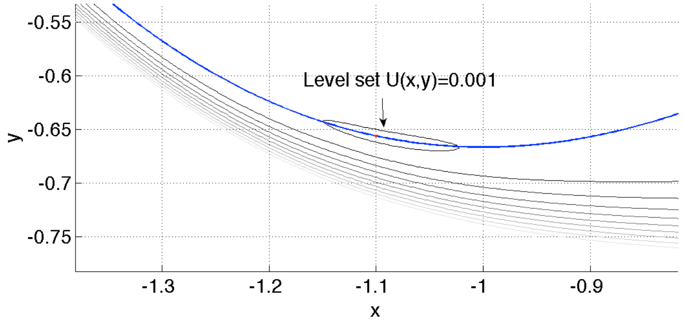
Example 3. A system with stochastic resonance

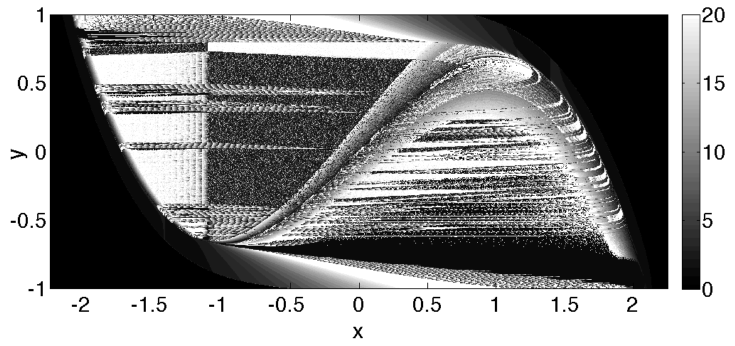
$$dx = \frac{1}{\varepsilon}\left(x - \frac{x^3}{3} - y\right)dt + \sqrt{2\beta^{-1}}\,dw_1$$

$$dy = (x + 1.1)dt + \sqrt{2\beta^{-1}}\,dw_2$$





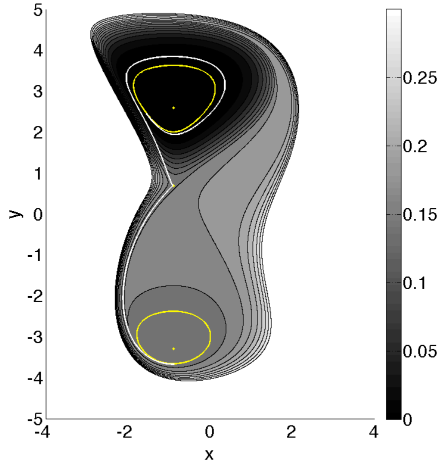


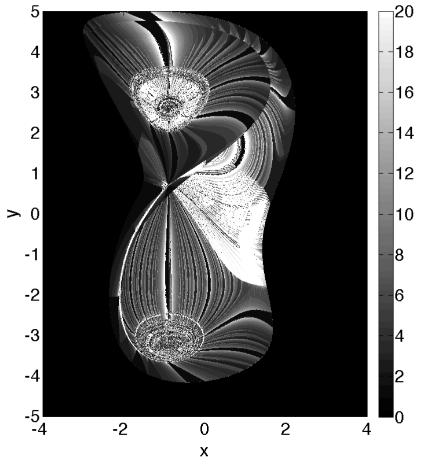


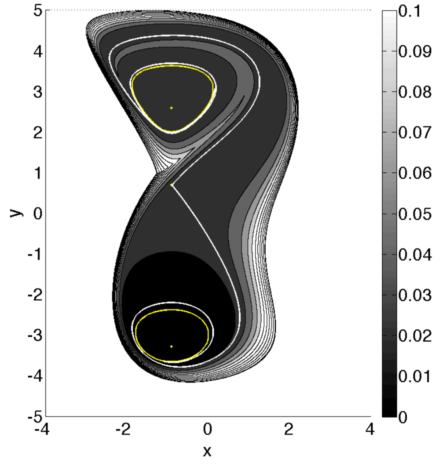
Example 4. A system with two stable limit cycles

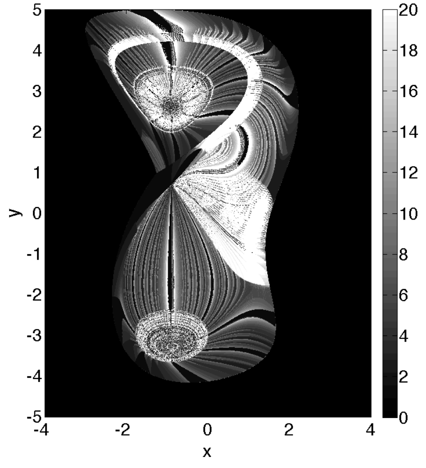
$$dx = \frac{1}{\varepsilon}\left(x - \frac{x^3}{3} + y - \frac{y^3}{9} \right) dt + \sqrt{2\beta^{-1}}\, dw_1$$

$$dy = (x + 0.9)dt + \sqrt{2\beta^{-1}}\, dw_2$$









Future research

- Theoretical behavior of the quasipotential near other kinds of attractors.
- Allowance of non-isotropic diffusion. How does it influence the quasipotential and the Hamilton-Jacobi solver.
- Development of a 3D Hamilton-Jacobi solver.
- Application for building a hierarchy of cycles.
- Investigation whether one can define an analog of the MaxFlux functional in the nongradient case.