The String Method as a Dynamical System

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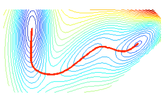
Minimum energy paths (MEP's)

We are considering an SDE $dx = -\nabla V(x) + \varepsilon dw$ where ε is small. Such a system spends most of the time at the minima of the potential V and performs rare transitions from one minimum to another. The transition probability along the path φ in time T is proportional to $\exp(-S_T / 2\varepsilon)$, where S_T is the Wentzel-Freidlin action. The smaller the action is, the larger is the probability. If the two minima are separated by a single mountain pass then the minimum of the W-F action in both φ and T is achieved along the MEP as $T \to \infty$.



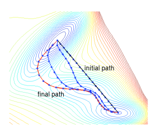
Definition 1. An MEP in a potential field ∇V is any path φ satisfying $\nabla V^{\perp}(\varphi) = 0$, i.e., it is a path which consists only of critical points and heteroclinic trajectories.

The string method

(W. E, W. Ren, E. Vanden-Einden, 2002, 2007)

A path $\varphi(\alpha, t),\ \alpha \in [0,1],\ t \ge 0,$ evolves in time according to

$$\varphi_t = -\nabla V(\varphi) + \lambda \hat{\tau},\ \ \varphi(\alpha, 0) = \varphi_0(\alpha),$$



where $\hat{\tau}$ is the unit tangent vector to the path. The factor λ is such that the path is uniformly parameterized at all times.

Goal and results

Goal: mathematical analysis of the string method in continuous-time, continuous-space setting.

Results:

- Curve evolution according to the string method does not necessarily converge to any MEP (if MEP's are not isolated).
- Complex dynamics is linked to the presence of critical points of Morse index ≥ 2.
- The string method always succeeds to find an MEP in practice, but the result should be interpreted with care.

Limit set

Definition 2. x_0 is a limit point of the path $\varphi(\alpha, t)$, if there are sequences $\{\alpha_n\}$ and $\{t_n\} \to \infty$ s. t. $\lim_{n\to\infty} \varphi(\alpha_n, t_n) = x_0$.

The limit set is the collection of the limit points.

Key fact. The limit set of a path evolving according to $\varphi_t = -\nabla V(\varphi) + \lambda \hat{\tau}$ and $\varphi_t = -\nabla V(\varphi)$ coincide!

Definition 3. The path converges to its limit set if the Hausdorff distance between the path and its limit set tends to 0 as $t \to \infty$.

We consider only potentials V satisfying the following conditions.

(i) V is twice continuously differentiable,

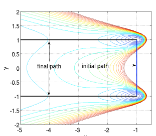
(ii) the critical points are isolated and nondegenerate,

(iii) the initial path is of finite length and contained in a compact connected component of a sublevel set of V.

Theorem 1. The limit set is compact, connected and consists only of critical points and heteroclinic trajectories.

However,

- the limit set of a path is not necessarily a curve: it might be multidimensional,
- the path does not necessarily converge to its limit set.



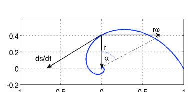
An example where Condition (iii) is violated. The initial path is not lying in any compact connected component of sublevel set of the potential and its limit set is not compact.

Affirmative results

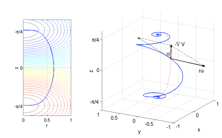
Theorem 2. If the potential has only a finite number of critical points, and all of them are of the Morse index ≤ 1 then the limit set of a path is a curve.

Theorem 3. If the limit set of a path is a curve then the path converges to it.

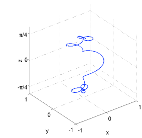
Examples



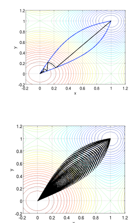
Motivation. A logarithmic spiral $r(\theta) = e^{-\theta \tan\alpha}$ revolves with a constant angular velocity $\omega = \tan\alpha$ in the quadratic potential .



1. Revolving path. We take a cylindrically symmetric potential with one maximum and one minimum lying on the axis of symmetry. We pick a trajectory (r(s),z(s)) going from the maximum to the minimum and construct a path $(r(s), \theta(s), z(s))$ on its surface of revolution. Given a constant angular velocity ω we can compute $\theta(s)$. The limit set of this path is the surface of revolution, and the path does not converge to it.

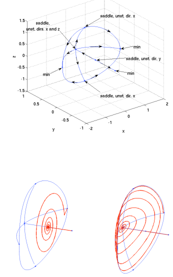


2. A path whose limit set is 3D. We upgrade the path from the previous example by replacing r(s) with $\frac{1}{2} r(s)(1 + \cos b\theta(s))$, where b is irrational. The time evolution of the resulting path is a complicated aperiodic motion, and its limit set is the entire 3D body of revolution of (r(s),z(s)).



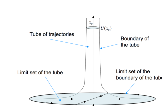
3. Filling a region. We take a four-well potential and pick two symmetric trajectories connecting its maximum and one of its minima. Then we construct an initial path from the circle arcs of radii n^{-2}, n=2,3,..., and segments of straight lines connecting them. The initial path has finite length. Its limit set is the entire region between the two trajectories, and the path converges to it, i.e., fills the region.

In all of these examples the initial path passes through a critical point of Morse index ≥ 2. The next example shows that it does not have to do so in order to have a multidimensional limit set.



4. Sliding to a Morse index 2 saddle. We take a potential whose heteroclinic structure is shown in the figure and is reminiscent to an umbrella . Any path from the minimum at the end of the "handle" to a minimum at the edge of the "canopy" evolves to a path passing through the index 2 saddle at the top of the "canopy". Moreover, a path passing nowhere close to the index 2 saddle might have a 2D limit set as shown in the figure.

Theorems



Definition 4. Consider a collection of trajectories passing through a small disc normal to some given trajectory. We call it a tube. Tubes corresponding to a nested family of discs form a nested family of tubes.

Theorem 4. The limit set of a path is not a curve iff there is a nested family of tubes such that the initial path leaves and enters each tube of the family infinitely many times.

Theorem 5. If the potential is piecewise analytic and the path is piecewise linear, then the limit set of a path is a curve and the path converges to it.