Deterministic Computational Methods for the Study of Stochastic Processes

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Rare Events and Large Deviation Theory

Deterministic dynamical system

$$\frac{dx}{dt} = b(x) \tag{1}$$

perturbed by small noise:

$$dx = b(x)dt + \sqrt{\epsilon}dw \tag{2}$$

$b(x)$: C^1-vector field, dw : Brownian motion, ϵ : small parameter

$\boxed{\text{Arbitrarily small } \epsilon \text{ changes the dynamics of (1)}}$

We'd like to calculate:

- Expected escape times from basins of attraction
- Maximum likelihood escape paths
- quasi-invariant probability measures in neighborhoods of attractors

Gradient v Nongradient SDEs

Gradient case

$$dx = -\nabla V(x)dt + \sqrt{\epsilon}dw$$

With potential V :

- Compute transition rates between attractors: $\rightarrow$ Arrhenius Formula
- Compute invariant probability measure: $\rightarrow$ Gibbs Measure

Nongradient case

$$dx = b(x)dt + \sqrt{\epsilon}dw$$

Task: Find analogue of potential

- Compute transition rates between attractors
- Compute quasi-invariant probability measure

Appears in biological and ecological models:

- Population Dynamics models (Touboul et al 2018)
- Genetic Switch models (Lv et al 2014)

Computing The Quasipotential on a Mesh

quasipotential

$$U(x) = \inf_{\psi, L}\{S(\psi)|\psi(0) \in A, \phi(L) = x\}$$

Geometric Action Functional(Heymann et al 2007)

$$S(\psi) = \int\limits_0^L (||b(\psi)||_2 \; ||\psi'||_2 - b(\psi) \cdot \psi')ds$$

Simpler problem:

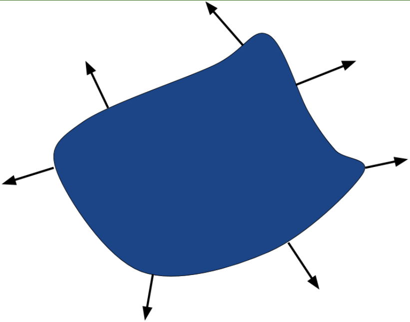
$$U(x) = \inf_{\psi, L} \left\{ \int_0^L \underbrace{\text{slowness}(\psi)}_{>0} ds | \psi(0) \in A, \phi(L) = x \right\}$$

$$\Updownarrow$$

$$||\nabla U(x)|| = \text{slowness}(x)$$

- Dijkstra-like Hamilton-Jacobi(HJ) Solvers
- $\boxed{\textbf{Simplest}}$: Sethians Fast Marching Method(1996)

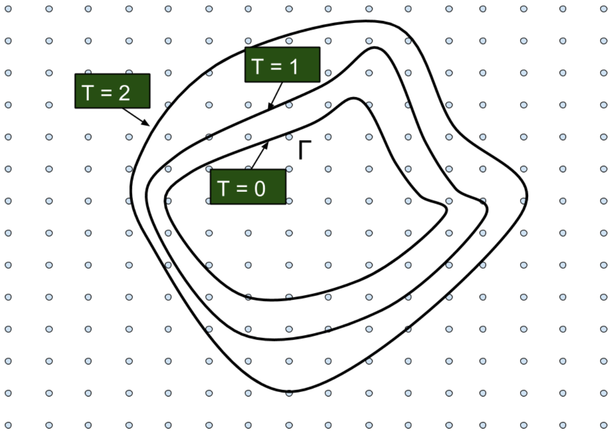
Task: Fast Marching Method



$$||\nabla U(\hat{x})|| = \frac{1}{F(\hat{x})} \quad U_\Gamma = 0 \quad \hat{x} \in \mathbb{R}^d,$$

- Γ : initial location of boundary
- F : given speed function of boundary
- $\boxed{U(\hat{x}) : \text{Arrival time of front at } x}$

Task: Fast Marching Method



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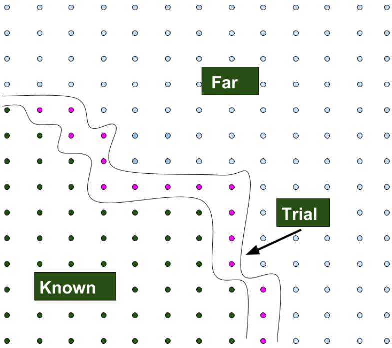
FMM Algorithm



- Initialize points
- While *Far* points still exist:
  1. $\boxed{\text{Find } \textit{Trial} \text{ point } x^* \text{ with lowest } T \text{ value}}$
  2. Tag x^* as *Known*, remove x^* from *Trial*
  3. Tag all neighbors of x^* not *Known* as *Trial* and remove *Far* label if necessary
  4. Compute **upwind update** for all *Trial* neighbors of x^*

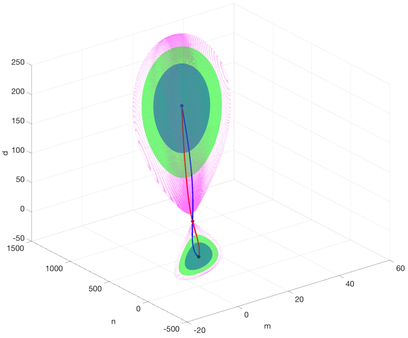
Task: Ordered Line Integral Methods

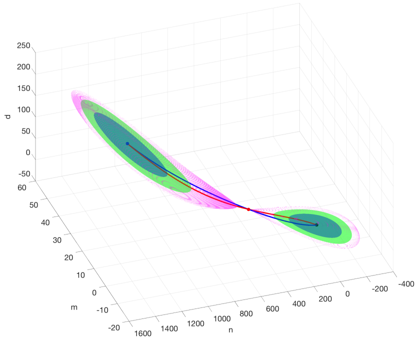
- FMM is fast: heap-sort
- FMM fails for the quasipotential

Ordered Line Integral Methods(OLIMs)
(Cameron,Dahiya,Potter,Yang, 2017,2018)
Idea: Solve minimization directly

- Geometric action $S(\psi)$ solved with quadrature rules, e.g. midpoint
- Dijkstra-like Solver
- State-of-the-art for quasipotential solvers on mesh

2D Solvers in 3D





(Yang,Potter,Cameron,2018) Quasipotential level sets computed for 3D genetic switch model(Lv,Li,Li,Li, 2014)

Goal for this project: Promote OLIM solvers to higher dimensions!

Project Goals / Research Plan

1. (October - November): Implement QP solvers
   - Implement FMM from scratch
   - Implement and optimize 2D OLIM
2. (December - Mid-February): Apply solvers with example-specific dim. reduction
   - Compute 2D quasipotential for 3D genetic switch(Lv et al, 2014) following example of Lorenz quasipotential in(Yang, Cameron 2018)
   - Explore 3D and 4D Savannah plant systems from (Touboul, 2018) find intrinsic dimensionality
3. (Spring Semester): Implement Manifold Learning algorithms, combine with solvers
   - Manifold Learning, Combination with quasipotential solvers

Current Status

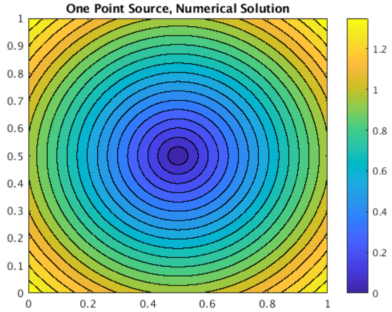
Accomplishments so far:

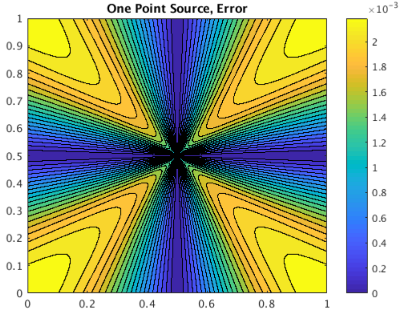
- Implemented binary heap in C from scratch
- Implemented FMM in C for point sources on the mesh
- Basic validation for FMM, agrees with the literature so far
- Extras: my first makefile! my first git branch and merge!

Currently:

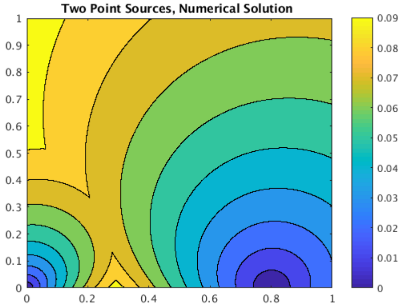
- More Validation for FMM: more complicated speed functions
- Implementing point sources off mesh
- Implementing initial curves

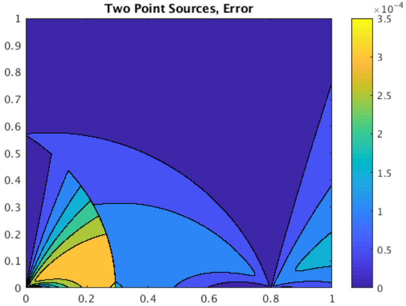
FMM: One Point Source





FMM: Two Point Sources





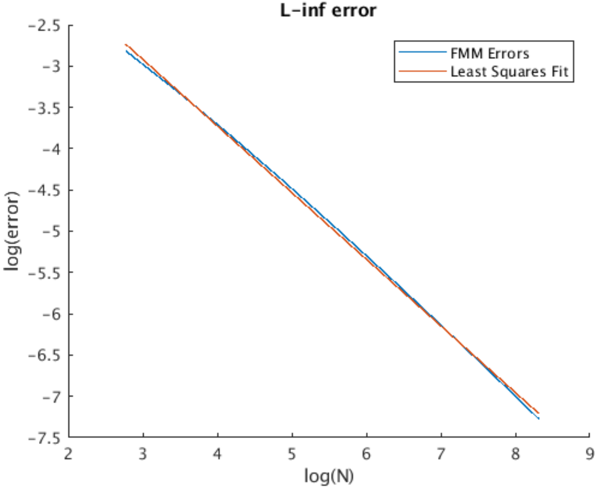
FMM: First Order?

$$||\nabla U(\hat{x})|| = 1$$

on domain $[0, 1] \times [0, 1]$, point source at $(0, 0)$
Mesh sizes: $N = 16, 32, 64, 128, 256, 512, 1024, 2049, 4088$

Error SHOULD be $\mathcal{O}(h)$

FMM: $\mathcal{O}(h \log(1/h))$?



Indicates not quite first-order, but DOES match relevant literature on this.

References I

M. Cameron and S. Yang.
Visualization and analysis of stochastic lorenz'63 by means of computing the quasipotential.
arXiv preprint arXiv:1809.09987, 2018.

M. Crosskey and M. Maggioni.
Atlas: a geometric approach to learning high-dimensional stochastic systems near manifolds.
Multiscale Modeling & Simulation, 15(1):110–156, 2017.

M. Freidlin and A. D. Wentzell.
Random perturbations of dynamical systems.
Springer-Verlag, 3rd edition, 2012.

References II

M. Heymann and E. Vanden-Eijnden.
The geometric minimum action method.
polymer, 3:2, 2009.

C. Lv, X. Li, F. Li, and T. Li.
Constructing the energy landscape for genetic switching system driven by intrinsic noise.
PLoS one, 9(2):e88167, 2014.

J. A. Sethian.
Level set methods and fast marching methods: evolving interfaces in computational geometry, fluid mechanics, computer vision, and materials science, volume 3.
Cambridge university press, 1999.

References III

J. D. Touboul, A. C. Staver, and S. A. Levin.
On the complex dynamics of savanna landscapes.
Proceedings of the National Academy of Sciences, 2018.

S. Yang, S. F. Potter, and M. K. Cameron.
Computing the quasipotential for nongradient SDEs in 3D.
ArXiv e-prints, Aug. 2018.