Log-concave Sampling (Part 1)

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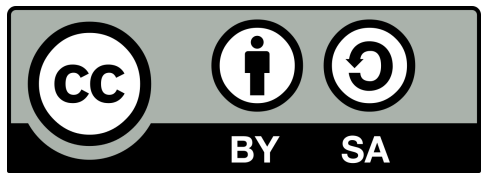

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Homepage: `https://github.com/GeomScale/volume_approximation`

About today's talk / tutorial

Today's talk will concentrate on
Sampling from high-dimensional log-concave densities

1. Introduction to log-concave sampling.
2. ODE Solvers.
3. Boundary Oracles.

Google Summer of Code 2020

The current GSoC project aims to provide implementations (and theoretical insights) to log-concave sampling problems for the GeomScale project.
Milestones

1. Milestone I (ODE Solvers)
   - Implement ODE solvers (Euler, Runge-Kutta, Collocation, etc.)
   - Efficiently address boundary oracles
2. Milestone II (Samplers)
   - Implement samplers (HMC, Langevin etc.).
   - Provide theoretical guarantees on truncated settings.
3. Milestone III (R bindings)
   - Port C++ functionality of

Today's talk will mostly concentrate on **Milestone I**.

Basics

Our project involves taking samples from distributions with probability density functions of the form

$$\pi(x) \propto \exp(-f(x)) \qquad x \in K$$

where K is either: (a) $\mathbb{R}^d$, or (b) a convex body, and f is a convex function that is L-smooth and m-strongly convex.

Convex Functions I

A domain K is convex iff (if and only if) for all $x, y \in K$ it holds that for all $t \in [0, 1]$

$$tx + (1 - t)y \in K$$

The domain K is a convex body iff it is convex, closed and bounded.
A function $f : K \to \mathbb{R}$ is convex iff for all $x, y \in K$ we have that for all $t \in [0, 1]$

$$f(tx + (1 - t)y) \leq tf(x) + (1 - t)f(y)$$

Convex functions have some very nice properties, and their use is widespread in optimization.

Convex Functions II

If the function is twice differentiable with gradient ∇f and Hessian matrix $\nabla^2 f$ then

- We say that f is L-smooth iff $\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$ or $\nabla^2 f(x) \preceq L \cdot I_d$.
- We say that f is m-strongly convex iff

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{m}{2}\|x - y\|^2$$

  or $\nabla^2 f(x) \succeq m \cdot I_d$.
- We define the **condition number** of f to be the ratio of max/min eigenvalues of the Hessian, that is $\kappa = L/m$.

Log-concave Sampling I

Our goal is sampling from $\pi(x) \propto \exp(-f(x))$.

Directly sampling from $\pi(x)$ is very difficult since one has to account for the normalization constant $\int_K \exp(-f(x))dx$ which is in general **intractable**.

Idea. The distribution $\pi(x)$ can be thought as the stationary measure of a Markov Chain that is $\pi(x) = \lim_{k\to\infty} \pi_k(x)$.

Log-concave Sampling II

One of the first algorithms to do it is the Metropolis-Hastings Algorithm. The general idea of Metropolis Hastings is

1. Assume that you are at a state x
2. Perform a transition to a new nearby state y and make a proposal
3. Accept the proposal to move to y with probability (Metropolis Filter)

$$\min\left\{1, \frac{a(x,y)\pi(y)}{a(y,x)\pi(x)}\right\}$$

where a is a transition probability function.

It can be shown analytically that the above process converges to a stationary distribution $\pi(x)$.
Intuition when $a(x,y) = a(y,x)$**:** The sampler has incentive to move towards higher-density areas (but lower density areas are also allowed)

Algorithmic Challenges

The main Algorithmic Challenges for (log-concave) sampling are in general

1. The **Mixing Time** of the Markov Chain, that is how fast (# iterations) a Markov Chain with transition operator $\mathcal{T}$ starting from an initial distribution π_0 reaches π within Total Variation Distance of at most $\delta > 0$ (more next time)

$$t_{mix}(\delta) = \inf \left\{ k \geq 0 | \| \mathcal{T}^k(\pi_0) - \pi \|_{TV} \leq \delta \right\}$$

where $\|P - Q\|_{TV} = \sup_{A \in \mathcal{F}} |P(A) - Q(A)|$ and $\mathcal{F}$ is a σ-algebra on the state space K.

2. The **Cost-Per Iteration** that is

$$\begin{pmatrix} \text{Cost-per} \\ \text{iteration} \end{pmatrix} = \begin{pmatrix} \text{Cost-per} \\ \text{ODE step} \end{pmatrix} + \begin{pmatrix} \text{Cost-per boundary} \\ \text{oracle (if truncated)} \end{pmatrix}$$

Sampling in a continuous setting

Hamiltonian Monte Carlo I

The state-space is continuous and the samples can be proposed via solving Hamilton's equations for a particle with position x and velocity v under a conservative potential $f(x)$ that applies a force $-\nabla f(x)$.
The Hamiltonian of the particle is defined as

$$H(x, v) = \frac{1}{2}\|v\|^2 + f(x)$$

and Hamilton's equations simulate the particle's behaviour

$$\dot{x} = \frac{\partial H}{\partial v} = v$$
$$\dot{v} = -\frac{\partial H}{\partial x} = -\nabla f(x)$$

Hamiltonian Monte Carlo II

We start by choosing a direction $v \sim \mathcal{N}(0, I_d)$ and simulate one/many steps of the ODE arriving at a proposal $(\tilde{x}, \tilde{v})$.

The Metropolis Filter in this case for a proposal $(\tilde{x}, \tilde{v})$ given a state (x, v) is $\min\{1, \exp(H(\tilde{x}, \tilde{v}) - H(x, v)\}$.

Ideally note that $\dot{H} = \langle \nabla_{x,v} H, (\dot{x}, \dot{v}) \rangle = \langle (v, \nabla f(x)), (-\nabla f(x), v) \rangle = 0$ and hence the Metropolis probability is always 1.

However, the ODE must be discretized and the **discretization error** makes the decision non-trivial.

Hamiltonian Monte Carlo III

Finally, the ODE admits a separable stationary measure proportional to

$$\pi(x, v) \propto \exp(-H(x, v))$$

The marginal density with respect to x is therefore

$$\pi(x) = \int_{\mathbb{R}^d} \pi(x, v) dv \propto \exp(-f(x))$$

Langevin Dynamics I

Another method for sampling is via solving the Langevin Stochastic Differential Equation which is the Newton's Second Law together with a Brownian Motion W.

$$\dot{x} = v$$
$$\dot{v} = -\gamma v - \nabla f(x) + \sqrt{2\epsilon\gamma}\dot{W}$$

where $\dot{W}$ is the derivative of the Brownian motion, that is $dW \sim \mathcal{N}(0, dt)$. Under mild conditions the SDE accepts a stationary measure proportional to $\exp\left(-\frac{1}{2}\|v\|^2 - f(x)\right)$. The parameters γ (damping factor), ϵ determine the nature of the dynamics

1. when $\gamma > 1$ the system is overdamped (OLD equation)
2. when $\gamma < 1$ the system is underdamped (ULD equation)
3. when $\gamma = 1$ the system is critically damped

Langevin Dynamics II

Of particular interest is the ULD equation

$$\begin{aligned}\dot{x} &= v \\ \dot{v} &= -2v - u\nabla f(x) + 2\sqrt{u}\dot{W} \\ u &= 1/L\end{aligned}$$

which is widely used in log-concave sampling. (for more information see [LST20, LSV18, GP14]).

Sampling Applications

1. Integral Calculation (Volume Calculation etc.)
2. Control systems
3. Generative Adversarial Networks
4. Logistic Regression
5. Financial Modeling
6. Probabilistic Graphical Models

ODE Solvers

General Setting I

Our goal is to solve an ODE of the form

$$\dot{x}(t) = F(x(t), t) \qquad x(0) = x_0$$

Theorem

If F is Lipschitz continuous in x and continuous in t then the above has a unique solution $x(t) = \phi(t)$

The HMC equations have $F(x(t), v(t), t) = \begin{pmatrix} v(t) \\ -\nabla f(x(t)) \end{pmatrix}$ which is Lipschitz (continuous) since f is L-smooth and $v(t)$ is 1-Lipschitz

General Setting II

In a discrete setting the equation is solved at discrete timesteps $t_n = t_{n-1} + \eta$ where $\eta > 0$ is the step-size.

Let x_n denote the solution provided by the discrete solver at step n and $\phi_n = \phi(t_n)$ be the "ideal point" at step n

We define the **error** ϵ_n to be

$$\epsilon_n = x_n - \phi_n$$

The dynamical behaviour of $\{\epsilon_n\}_{n \geq 0}$ provides inshights regarding the methods' accuracy.

Euler Solver

The Euler Solver is the simplest one

$$t_n = t_{n-1} + \eta$$
$$x_n = x_{n-1} + \eta F(x_{n-1})$$

It can be proven that

$$\|\epsilon_n\| \leq \frac{\eta m}{2L} \left(\exp(t_n - t_0) - 1\right) = K(t_n) \cdot \eta$$

Hence the error of the Euler Solver is $O(\eta)$.

Runge-Kutta Methods I

The idea is to "break" every step of size η to smaller sub-steps and interpolate to find the next position. Each Runge-Kutta (RK) method is given by the following table (Butcher Tableau)

0				
c_2	a_{21}			
c_3	a_{31}	a_{32}		
$\vdots$				
c_m	a_{m1}	$\dots$	$a_{m,m-1}$	
	b_1	$\dots$	b_{m-1}	b_m

Table: Butcher's Tableau

where $\sum_{j=1}^{m} b_j = 1$ and $c_j = \sum_{r=1}^{j-1} a_{jr}$

Runge-Kutta Methods II

The RK iteration proceeds in sub-steps where

$$t_n^j = t_{n-1} + c_j \eta \qquad j \in [m]$$

$$k_j = F\left(\sum_{r=1}^{j-1} a_{j,r} k_r, t_n^j\right)$$

$$x_{n+1} = \sum_{j=1}^{m} b_j k_j$$

$$t_{n+1} = t_n + \eta$$

The global truncation error $\|\epsilon_n\|$ is $O(\eta^m)$.

Collocation Methods I

The collocation method assumes that the solution is locally approximated as

$$p(t) = \sum_{j=0}^{m} a_j \phi_j(t) \tag{1}$$

where $\{\phi_j\}_{0 \le j \le m}$ are basis functions (e.g. polynomials). The constants $\{a_j\}_{0 \le j \le m}$ are found by interpolation on the derivative of x at points given by $t_{n+1}^j = t_n + c_j \eta$ as in the RK methods.
As choices for bases one has many choices, some of which being

1. Polynomials $\phi_n^j(t) = (t - t_n)^j$
2. Lagrange polynomials $\phi_n^j(t) = \prod_{r \neq j} \frac{t - t_r}{t_j - t_r}$
3. Rational functions $\phi_n^j(t) = \frac{p_n^j(t)}{q_n^j(t)}$ with $q_n^j(t) \neq 0$ in the ROIs.

Collocation Methods II

The system of equations for the interpolation is given by

$$\begin{aligned} t_{n+1}^j &= t_n + c_j \eta \\ p_{n+1}(t_{n+1}^0) &= x_n \\ \dot{p}_{n+1}(t_{n+1}^j) &= F(p_{n+1}(t_{n+1}^j)) \qquad j \in [m]^* \end{aligned}$$

Alternatively if F is a linear mapping one solves an $m \times m$ system of the form $\dot{\Phi}_{n+1} a_{n+1} = \dot{X}_{n+1}$. If the matrix of the basis derivatives is not full-rank then a solution to $\min_{a_{n+1}} \frac{1}{2} \|\dot{\Phi}_{n+1} a_{n+1} - \dot{X}_{n+1}\|_2^2$ is seeked (e.g. using SVD).

If F is non-linear one can in general use iterative methods (NR) to compute the coefficients $\{a_{n+1}^j\}_{n \geq 0, j \in [m]}$

Leapfrog Integrator (2nd order)

The Leapfrog integrator is used to solve the equation $\ddot{x} = F(x, t)$

The method proceeds as follows

$$v_{i+1/2} = v_i + \frac{\eta}{2} F(x_i)$$
$$x_{i+1} = x_i + \eta v_{i+1/2}$$
$$v_{i+1} = v_{i+1/2} + \frac{\eta}{2} F(x_{i+1})$$

Examples of interest. Particle dynamics (HMC, Langevin)

Boundary Oracles

Boundary Conditions I

In HMC the domain of (x, v) is $K \times \mathbb{R}^d \subseteq \mathbb{R}^d \times \mathbb{R}^d$. Where $K \neq \mathbb{R}^d$ one has to account for **boundary conditions** for the position x.

There are three main types of boundary conditions

1. Neumann Conditions (Boundary Reflections) where $\frac{\partial x}{\partial n} = 0$
2. Dirichlet Conditions $x = g$
3. Robin (mixed) Conditions $a\frac{\partial x}{\partial n} + g = 0$

where the domain of a, g is the boundary ∂K.
It has been proven [PP14] that HMC admits boundary conditions equivalent to the **Neumann Conditions**.

Boundary Conditions II

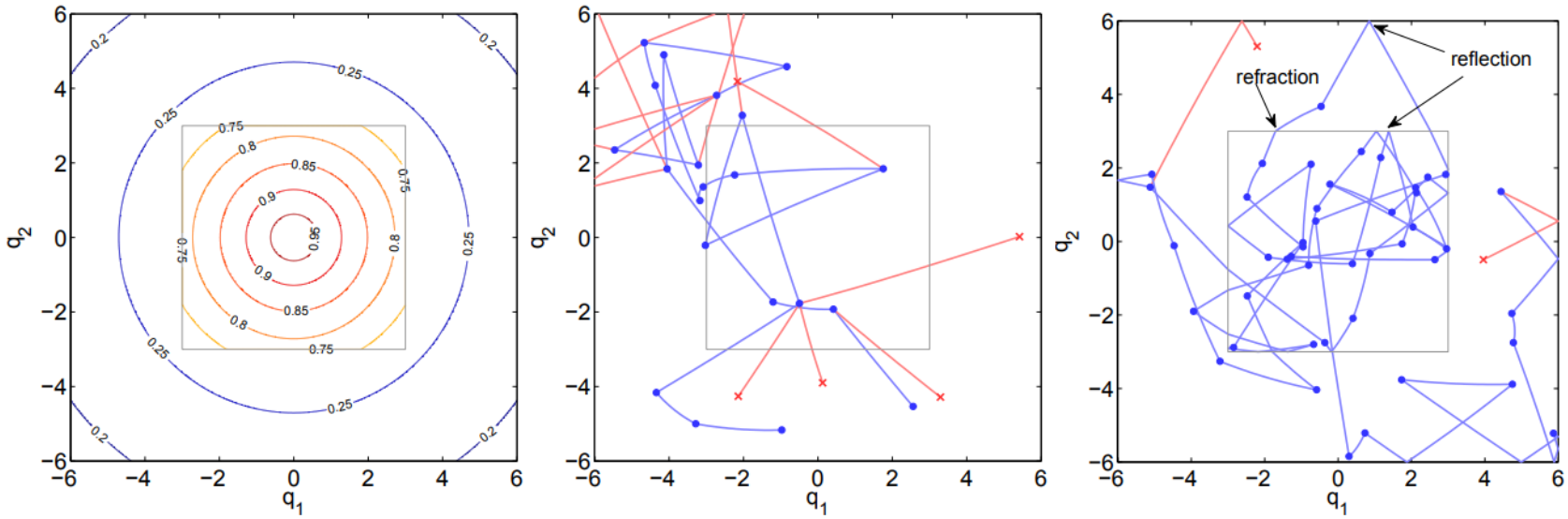

Figure: Baseline and Reflective HMC. Taken from [AD15].

The Reflection Operator I

A point x reflects at the boundary point $\tilde{x}$ with normal n.

We define the reflection operator refl such that

$$\mathrm{refl}(x) = -2(a^T n)n + a + \tilde{x}$$

where $a = \tilde{x} - x$ is the ray between the initial and the boundary points. Note that in general $\mathrm{refl}(x)$ may not lie in K. We compose the reflection operator k times such that $\mathrm{refl}^k(x) = \mathrm{refl} \circ \cdots \circ \mathrm{refl}(x) \in K$. In our setting we assume that at each step the proposal point cannot reflect more than $\ell \in \mathbb{N}^*$ times.

The Reflection Operator II

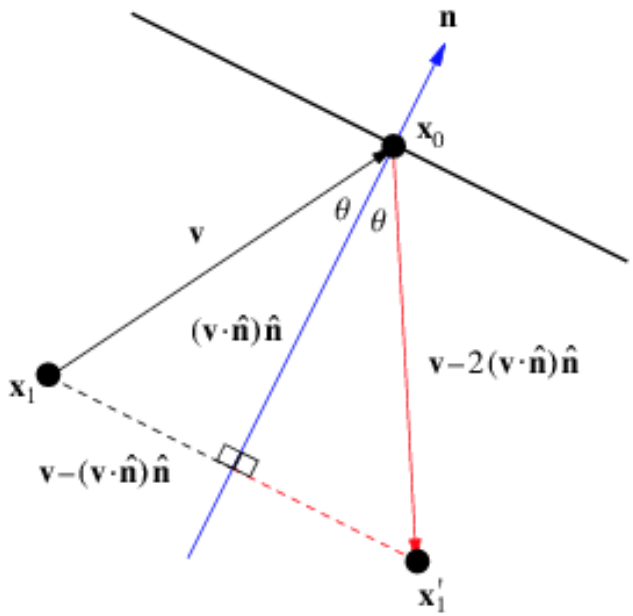

Figure: Reflection Illustration. x_1' is the reflection of x_1 about x_0 with normal n. Source: `https://mathworld.wolfram.com/Reflection.html`

Computing Intersections with ∂K I

Of particular interest is the computation of the intersection of an (implicit) curve between a point x inside the convex body K and a proposal $\tilde{x} \notin K$.

Case 1. The curve is a *line segment* and K is a convex polytope.
We parametrize the line segment between x and $\tilde{x}$ with $\gamma(t) = tx + (1-t)\tilde{x}$ where $t \in [0,1]$. We seek $t_u = \sup\{t \in [0,1] | \gamma(t) \in \partial K\}$ and $u = \gamma(t_u)$ as the solution to the boundary intersection problem.

We use the Cyrus-Beck [CB78] algorithm

Computing Intersections with ∂K II

Let $z \in \partial K$ be known and let n represent the normal vector at z. We compute the quantity

$$n^T(\gamma(t) - z) \begin{cases} = 0 & \gamma(t) \in \partial K \\ < 0 & \gamma(t) \notin K \\ > 0 & \gamma(t) \in K \setminus \partial K \end{cases}$$

Solving the equation $n^T(\gamma(t) - z)$ for t we get

$$t = \frac{n^T(z - x)}{n^T(\tilde{x} - x)}$$

We compute the above for all the N normals of the polytope and keep the maximum value that lies in $[0, 1]$. The min value can also be kept in case we want the other intersetion point as well. Complexity is $O(Nd)$

Computing Intersections with ∂K III

H-polytope. The polytope is given by the form $Ax \leq b$ where A consists of N row vectors $a_1, \ldots, a_N \in \mathbb{R}^d$ and $b = (b_1, \ldots, b_N)^T$. On each facet we use a_i as normal vector and if $b_i = 0$ then we use $\vec{0}$ as a point on the facet. If $b_i \neq 0$, there exists at least one index r such that $a_r \neq 0$ (otherwise the problem is trivial) we use the point $u = (0, 0, \ldots, b_i/a_r, \ldots, 0)^T$ which lies on the hyperplane, that is $a_i^T u = b_i$. Worst-case complexity is $O(Nd)$.

Computing Intersections with ∂K IV

V-polytope. The polytope is given by its convex hull V which contains M points $v_1, \ldots, v_M \in \mathbb{R}^d$. The point $\gamma(t) = tx + (1-t)\tilde{x}$ is on the boundary for some $t_0 \in [0,1]$ (given that $x \in K$) if t_0 is the maximum value of $t \in [0,1]$ such that there exist $\lambda_1, \ldots, \lambda_M \geq 0$ with $\sum_{i=1}^{M} \lambda_i = 1$ and $\gamma(t_0) = \sum_{i=1}^{M} \lambda_i v_i$, which translates to the following LP problem which has $O(Md)$ constraints

$$
\begin{aligned}
\text{maximize} \quad & t \\
\text{subject to} \quad & 0 \leq t \leq 1 \\
& \lambda_i \geq 0 \qquad\qquad i \in [M] \\
& \sum_{i=1}^{M} \lambda_i = 1 \\
& tx + (1-t)\tilde{x} - \sum_{i=1}^{M} \lambda_i v_i = 0
\end{aligned}
$$

Solvable via `lp_solve` (functionality already exists)

Computing Intersections with ∂K V

Case 2. The curve has the form $\gamma(t) = \sum_{i=1}^{m} a_i \phi_i(t)$, $\{\phi_j\}_{j\in[m]}$ are basis functions, and K is a convex polytope.

H-polytope. We use the same procedure as above, however now we cannot solve directly for t. We, for example, can use the Newton-Raphson root finder to solve the transcendental equation.

$$t^{(r+1)} = t^{(r)} - \frac{\sum_{j\in[m]}(n^T a_j)\phi_j(t^{(r)}) - n^T z}{\sum_{j\in[m]}(n^T a_j)\dot{\phi}_j(t^{(r)})} \qquad r \in [R]$$

Complexity is $O(NdR)$ where R is the maximum number of iterations the NR solver must be called to find a root.
Problems. Convergence, Well-posedness (denominator getting too small)

Computing Intersections with ∂K VI

V-polytope. The problem of Case I is a general optimization problem

$$\begin{aligned} \text{maximize} \quad & t \\ \text{subject to} \quad & t \geq 0 \\ & \lambda_i \geq 0 \qquad\qquad i \in [M] \\ & \sum_{i=1}^{M} \lambda_i = 1 \\ & \sum_{i=1}^{M} a_j \phi_j(t) - \sum_{i=1}^{M} \lambda_i v_i = 0 \end{aligned}$$

Can be addressed using the KKT conditions.

Computing Intersections with ∂K VII

Case 3. The convex body K has the form $K = \{x \in \mathbb{R}^d | g(x) \leq 0\}$ where $g(x) = \max_{1 \leq i \leq M} g_i(x)$ where $g_1, \ldots, g_M$ are twice-differentiable convex functions that are μ-strongly-convex.

Examples. L_2 Balls, Spectrahedra etc.

Idea. Linearize the convex body around $x + h$

$$0 \geq g_i(x + h) \geq g_i(x) + \langle \nabla g_i(x), h \rangle + \frac{\mu \|h\|^2}{2}$$

The linearized convex polytope $P(x)$ around x is

$$J(x)h \leq b$$

where $J(x)$ is the Jacobian matrix around x with entries $J_{ij}(x) = \frac{\partial g_i(x)}{\partial x_j}$ and b has entries $b_i = -g_i(x)$.

Computing Intersections with ∂K VIII

The linear approximation error is at most $\frac{\mu}{2}\|h\|^2$. A high-level algorithm (Local-search-based) proceeds as follows.

We are given a curve $\gamma(t)$ and a starting point $x_0 = \gamma(0)$, an accuracy $\epsilon > 0$, and a step counter i initialized at 0.

1. Find $P(x_i)$ around x_i and the intersection point of $\gamma(t)$ with $P(x_i)$ (see Case 1, Case 2). Let that point be $x_{i+1} = \gamma(t_{i+1})$
2. Calculate $g(x_{i+1}) = \max_{1 \leq j \leq M} g_j(x_{i+1})$. If $|g(x_{i+1})| \leq \epsilon$, output x_{i+1}, t_{i+1}, else repeat.

Next Talk(s)

Next talk(s) will be occupied with

1. Algorithmic Issues for the sampling problem (mixing time, bounds etc.).
2. Theoretical contributions to the problem.
3. Implementation details.

Thank you!

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