Log-concave Sampling (Part 1)

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About today's talk / tutorial

Today's talk will concentrate on

Sampling from high-dimensional log-concave densities

- Introduction to log-concave sampling.
- ODE Solvers.
- 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

- Milestone I (ODE Solvers)
 - Implement ODE solvers (Euler, Runge-Kutta, Collocation, etc.)
 - Efficiently address boundary oracles
- Milestone II (Samplers)
 - Implement samplers (HMC, Langevin etc.).
 - Provide theoretical guarantees on truncated settings.
- 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

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

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 $f: \mathcal{K} \to \mathbb{R}$ is convex iff for all $x,y \in \mathcal{K}$ 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

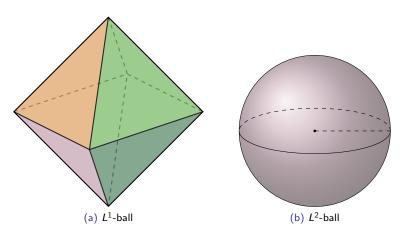


Figure: Examples of convex bodies.

Convex Functions III

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

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

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

or
$$\nabla^2 f(x) \succeq m \cdot I_d$$
.

- The above generalize in a looser setting as well.
- We define the **condition number** of f to be the ratio of max/min eigenvalues of the Hessian, that is $\kappa = L/m$.



Random Walks and 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 $\pi(x) = \lim_{k \to \infty} \pi_k(x)$.

The dependence on the dimension d and the condition number κ of f are interesting.

Random Walks and Sampling II

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

- Assume that you are at a state x
- Perform a transition to a new nearby state y and make a proposal for transitioning to y
- 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 I

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

• 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)

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

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.

The Cost-Per Iteration that is

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



Algorithmic Challenges II

Method	Support	Mixing Time	Distance
MALA/HMC [DCWY19]	\mathbb{R}^d	$ ilde{ ilde{O}}(\max\{\kappa d,\kappa^{1.5}\sqrt{d}\})$	TVD
MALA/HMC [LST20]	\mathbb{R}^d	$ ilde{O}(\kappa d)$	TVD
ULD [SL19]	\mathbb{R}^d	$\tilde{O}(\kappa^{7/6}/\epsilon^{1/3} + \kappa/\epsilon^{2/3})$	\mathcal{W}_2
Our conjecture (log-	K	$ ilde{O}(\kappa d)$	TVD
concave)			
Coord. Hit-and-Run	K	$O(d^2)$	TVD
[HCT ⁺ 17]			
Our conjecture (Billiard)	K	$ ilde{O}(d)$	TVD

Table: Known results for the mixing time of random-walk methods. Above: First-order Methods. Below: Zero-order Methods. K is a convex body. The notation $\tilde{O}(\cdot)$ ignores logarithmic factors. The logarithmic factors (in the case of convex-body support) depend on the condition number and the "shape" of the polytope.

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 $-\nabla f(x)$. [DKPR87] The Hamiltonian of the particle is defined as

$$H(x, v) = \underbrace{\frac{1}{2} \|v\|^2}_{\text{kinetic energy}} + \underbrace{f(x)}_{\text{potential energy}}$$

Hamiltonian Monte Carlo II

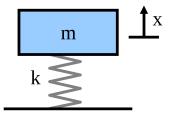


Figure: 1D Mass-Spring System with mass m=1 and spring constant k=1 has a Hamiltonian $H(x,v)=\frac{1}{2}v^2+\frac{1}{2}x^2$

Hamiltonian Monte Carlo III

Hamilton's equations simulate the particle's behaviour in the conservative field

$$\dot{x} = \frac{\partial H}{\partial v} = v$$

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

In our previous example $\dot{x}=v$ and $\dot{v}=-x$ that is $\ddot{x}+x=0$ which gives rise to the well-known simple harmonic oscilator $x(t)=A\cos(\omega t+\phi)$

Hamiltonian Monte Carlo IV

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 (i.e. with infinite precision) 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 V

Correctness. 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

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

Hence the sequence of samples x_1, \ldots, x_i, \ldots that the algorithm produces are ϵ -close (in total variation distance) from the distribution $\pi(x)$. We need to make sure that the chain has "mixed" before "trusting" the samples.

Hamiltonian Monte Carlo VI

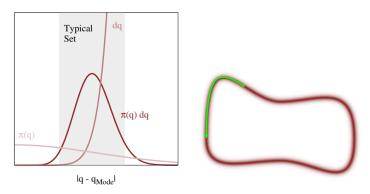


Figure: The typical set of a Markov Chain. Formally, the typical path is defined the set of points x where the product $\pi(x)dx$ is concentrated

Hamiltonian Monte Carlo VII

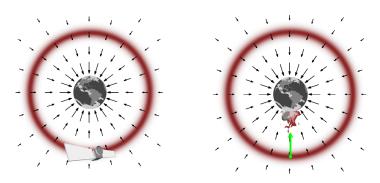


Figure: Intuition behind HMC Sampling from [Bet17]. Left: The vector field of f is pointing towards the minimizer of f, that is x^* . The goal of the sampler (satelite) is to move on the red trajectory where the running sample mean approaches the expected value of x, that is $\mathbb{E}_{\pi}[x]$. Right: A gradient-inspired method (steepest descent $\dot{x} = -\nabla f(x)$) fails to maintain orbit around Earth (minimizer) and crushes into it.

Hamiltonian Monte Carlo VIII



Figure: HMC Idea. (Left) The position x of the sampler (orbiter) is corrected with a momentum term v that counteracts the effects of "gravity" and keeps the sampler into orbit. The HMC equations $\dot{x}=v$ and $\dot{v}=-\nabla f(x)$ assist the satelite to maintain orbit. Middle: Adding too little momentum and the satelite crushes to the center again. Right: Adding to much momentum acts like a slingshot.

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)
- when $\gamma = 1$ the system is critically damped



Langevin Dynamics II

Of particular interest is the ULD equation

$$\dot{x} = v$$

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

$$u = 1/L$$

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

Sampling Applications I

- Integral Calculation (Monte-Carlo Integration)
- Control systems
- Generative Adversarial Networks
- Logistic Regression
- Financial Modeling
- Probabilistic Graphical Models

Example: Monte-Carlo Integration. We are interested in computing $\int_K \pi(x)g(x)dx$. Given samples x_1,\ldots,x_N from π (truncated in K) the integral is a.a.s. approximated as

$$\int_{K} \pi(x)g(x)dx \approx \frac{1}{N} \sum_{i=1}^{N} g(x_{i})$$



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

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

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)

Table: Butcher's Tableau

where
$$\sum_{i=1}^{m} b_i = 1$$
 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

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

where $\{\phi_j\}_{0\leq j\leq m}$ are basis functions (e.g. polynomials). The constants $\{a_j\}_{0\leq j\leq m}$ 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

- 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

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

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

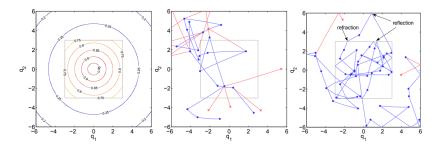


Figure: Baseline and Reflective HMC. Taken from [AD15].

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

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

where $a=\tilde{x}-x$ is the ray between the initial and the boundary points. Note that in general $\operatorname{refl}(x)$ may not lie in K. We compose the reflection operator k times such that $\operatorname{refl}^k(x)=\operatorname{refl}\circ\cdots\circ\operatorname{refl}(x)\in K$. 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

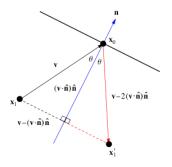


Figure: Reflection Illustration. x_1' is the reflection of x_1 about x_0 with normal n. Source: https://mathworld.wolfram.com/Reflection.html

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 $\partial K \coprod$

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 $A_{ir} \neq 0$ (otherwise the problem is trivial) we use the point $u = (0, 0, \ldots, b_i/A_{ir}, \ldots, 0)^T$ 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 $\gamma(t_0)=\sum_{i=1}^M\lambda_iv_i$, which translates to the following LP problem which has O(Md) constraints

maximize
$$t$$
 subject to $0 \le t \le 1$
$$\lambda_i \ge 0 \qquad \qquad i \in [M]$$

$$\sum_{i=1}^M \lambda_i = 1$$

$$tx + (1-t)\tilde{x} - \sum_{i=1}^M \lambda_i v_i = 0$$

Solvable via lp_solve (functionality already exists)



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Computing Intersections with $\partial K V$

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.

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

Complexity is O(NdRm) where R is the maximum number of iterations the NR solver must be called to find a root.

Alternatively. Solve optimization problem $\max_{t\geq 0} t$ subject to $A\gamma(t)\leq b$. The constraint translates to $\tilde{A}\Phi\leq b$ where Φ is a column vector that contains $\phi_j(t)$ and \tilde{A} is the product of the matrix A and the coefficient matrix.

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

maximize
$$t$$
 subject to $t\geq 0$
$$\lambda_i\geq 0 \qquad \qquad i\in [M]$$

$$\sum_{i=1}^M \lambda_i=1$$

$$\sum_{i=1}^M a_i\phi_j(t)-\sum_{i=1}^M \lambda_i v_i=0$$

Can be solved via interior-point-methods such as line-search filters (e.g. using the COIN-OR IPOPT toolbox)



Computing Intersections with ∂K VII

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

Examples. L₂ 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.

- 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 $g(x_{i+1}) = \max_{1 \le j \le M} g_j(x_{i+1})$. If $|g(x_{i+1})| \le \epsilon$, output x_{i+1}, t_{i+1} , else repeat.

Progress Report for GSoC

The working repository can be found here

https://github.com/papachristoumarios/volume_approximation

What has been implemented (including testing and source code docs)

- ODE Solvers (include/ode_solvers)
 - Euler Sovler
 - RK Solvers (RK4, Midpoint, etc.)
 - Leapfrog Solver
 - Bulirsch-Stoer-Richardson Solver
 - 6 Collocation Method (ongoing)
- Research Paper (ongoing)
- **3** Boundary Oracles curves of the form $\gamma(t) = \sum_i a_i \phi_i(t)$ (ongoing)
- Samplers: HMC with reflections

Next Steps. SDEs (Langevin), R bindings, more Documentation, more Testing

Next Talk(s)

Next talk(s) will be occupied with

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

Thank you!

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