

Geometric Data analysis

Random walks, Sampling, Volume

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Fall 2020

Outline

1 Random walks for sampling

2 Convex Volumes

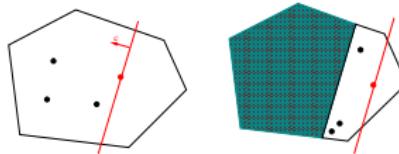
- Poly-time approximation
- Structured inputs
- V-polytopes

Sampling

Sampling is important for:

- Monte Carlo Integration (which generalizes volume)

- Optimization



- Sparse Representation of domains, check conjectures
- Contingency tables, underconstrained linear systems
- Systems biology, ...

Geometric Random walks

- In arbitrary polytopes: Markov (memoryless) chains of points which “mix” to the desired distribution (typically uniform); complexity depends on (warm) start, roundedness of body.
- Each point generated with desired probability distribution after a number of steps: this number is the mixing time.
- Continuous uniform distribution: point in $A \subset P$ with probability $\text{vol}(A)/\text{vol}(P)$. Then, probability density function is $1/\text{vol}(P)$, and

$$\int_P \frac{dv}{\text{vol}(P)} = 1.$$

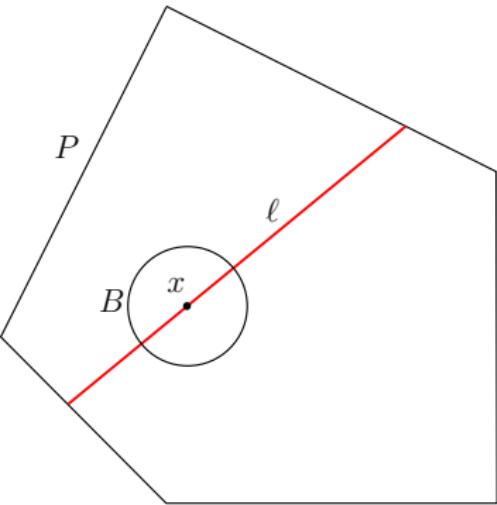
Main existing walks

year	walk	mixing time	step cost
87	Coordinate HnR	?	m
06	Hit-and-Run	d^3	md
09	Dikin	md	md^2
14	Billiard	?	Rmd
16	Geodesic	$md^{3/4}$	md^2
17	Ball	$d^{2.5}$	md
17	Vaidya	$m^{1/2}d^{3/2}$	md^2
17	Riemmanian HMC	$md^{2/3}$	md^2
18	HMC w/reflections	?	md
19	sublinear Ball	$d^{2.5}$	m

dimension d , m facets, R bounds billiard reflections



Random Directions Hit-and-Run (RDHR)



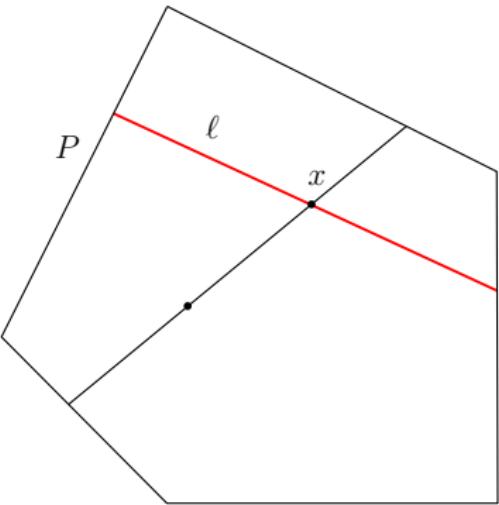
Input: point $x \in P$ and polytope $P \subset \mathbb{R}^d$

Output: a new point in P

1. line ℓ through x , uniform on $B(x, 1)$
2. new x uniform on $P \cap \ell$

Perform W steps, return x .

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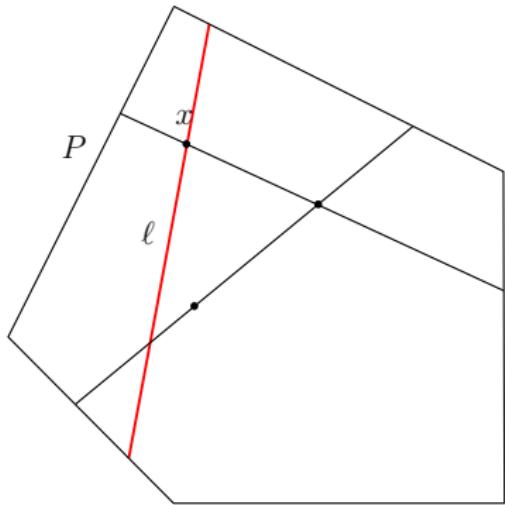


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- x is uniformly distributed in P after $W \sim 10^{11}d^3$ steps [LV'06].

Sample distribution

p_u : distribution on taking **one step** from $u: A \subset P$ reached w/prob. $p_u(A)$

Theorem

For $u \in P$, the pdf of point $v \in P$ **at next step** is

$$f_u(v) = \frac{2}{\text{vol}_{d-1}(S_d)} \frac{1}{\ell(u, v)|v - u|^{d-1}}$$

where $\ell(u, v) = \text{length of chord through } u, v$, sphere $S_d \subset \mathbb{R}^d$.

Proof. It suffices to prove $p_u(A) = \frac{2}{\text{vol}_{d-1}(S_d)} \int_A \frac{dv}{\ell(u, v)|v - u|^{d-1}}$ for infinitesimally small A : $\ell(u, v) \approx \ell$, $\forall v \in A$; $|v - u| \approx t$. Given chord L through u , $\text{Prob}[v \in A] = \text{vol}_1(A \cap L)/\ell$. Now $p_u(A) = \text{average over all } L$:

$$\mathbb{E}_L \left(\frac{\text{vol}_1(A \cap L)}{\ell} \right) = \frac{2}{\text{vol}(S_d)t^{d-1}} \frac{\text{vol}(A)}{\ell} = \frac{2}{\text{vol}(S_d)} \int_A \frac{1}{\ell t^{d-1}} dv$$

because $\text{vol}(S_d)t^{d-1} = \text{vol}(t\text{-sphere})$ counts directions of L .

Stationary distribution

- Recall p_u is distribution obtained on taking one step from $u \in P$:
 $A \subset P$ is reached with probability $p_u(A)$, and $p_u(P) = 1$.
- Distribution Q on P is **stationary** if one step gives same distribution:

$$\int_P p_u(A) dQ(u) = Q(A), \quad \text{for any } A \subset P.$$

- Symmetry/reversibility: $f_u(v) = f_v(u)$.

If Q is uniform on P then, $Q(A) = \text{vol}(A)/\text{vol}(P)$, and:

$$\begin{aligned} \int_P p_u(A) dQ(u) &= \int_P \int_A f_u(v) dQ(v) dQ(u) = \int_A \int_P f_v(u) dQ(u) dQ(v) = \\ &= \int_A p_v(P) dQ(v) = \int_A \frac{dv}{\text{vol}(P)} = \frac{\text{vol}(A)}{\text{vol}(P)} = Q(A). \end{aligned}$$

- Hence the uniform distribution is stationary. Is it unique?

Uniform distribution

Theorem (Smith'86)

Any symmetric (has the **reversibility** property) random walk with positive transition pdf converges to the uniform distribution, and it is the unique such distribution.

Examples: RDHR, Billiard walk.

Similarly for non-negative transition pdf, e.g. CDHR.

Mixing time

- Q_T : distribution after T steps.
- **Mixing time:** T steps s.t. $\|Q_T - Q\| \leq \epsilon$, for $\epsilon \rightarrow 0^+$.

Theorem

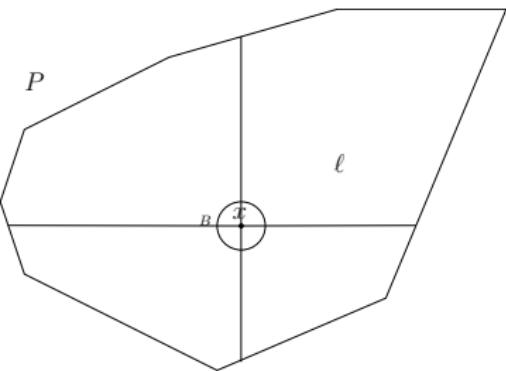
$T \approx 10^{11}d^3$ for RDHR and uniform distribution Q .

Proof

$T = O(1/\phi^2)$, where ϕ is the **conductance** of a (geometric) random walk, defined as:

$$\phi = \min_{0 \leq Q(A) \leq 1/2} \frac{\int_A p_u(P \setminus A) dQ(u)}{Q(A)}, \quad \text{out of some } A \subset P.$$

Coordinate Directions Hit-and-Run (CDHR)

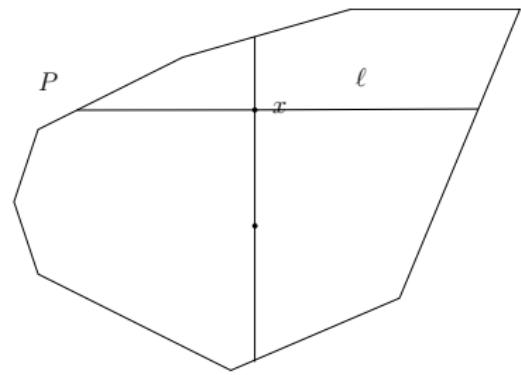


Input: point $x \in P$.

Output: a new point in P .

1. line ℓ through x , uniform on $\{e_1, \dots, e_d\}$, $e_i = (\dots, 0, 1, 0, \dots)$
2. x uniformly $\in P \cap \ell$.

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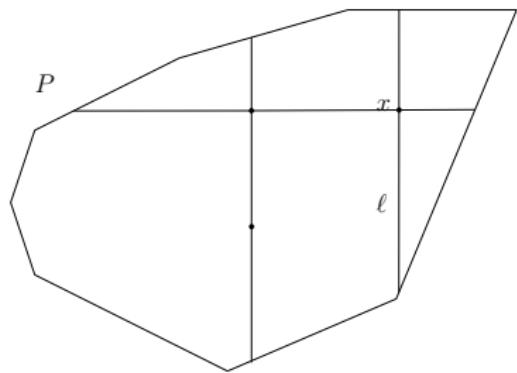


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Perform W steps, return x .

“Continuous” grid walk: Converges to uniform, unknown mixing.

Boundary oracle

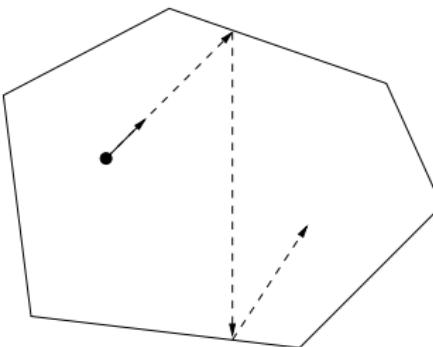
Compute intersection of line ℓ with boundary ∂P , given m hyperplanes:

- RDHR step in $O(md)$.
- CDHR = $O(m)$ per step: solve 1d (linear) problem per facet.
- Duality reduces oracle to farthest point search (max inner product) among m points: same asymptotics, practical if large m (16-dim cross-polytope: $m = 2^{16}$, 40x speedup).

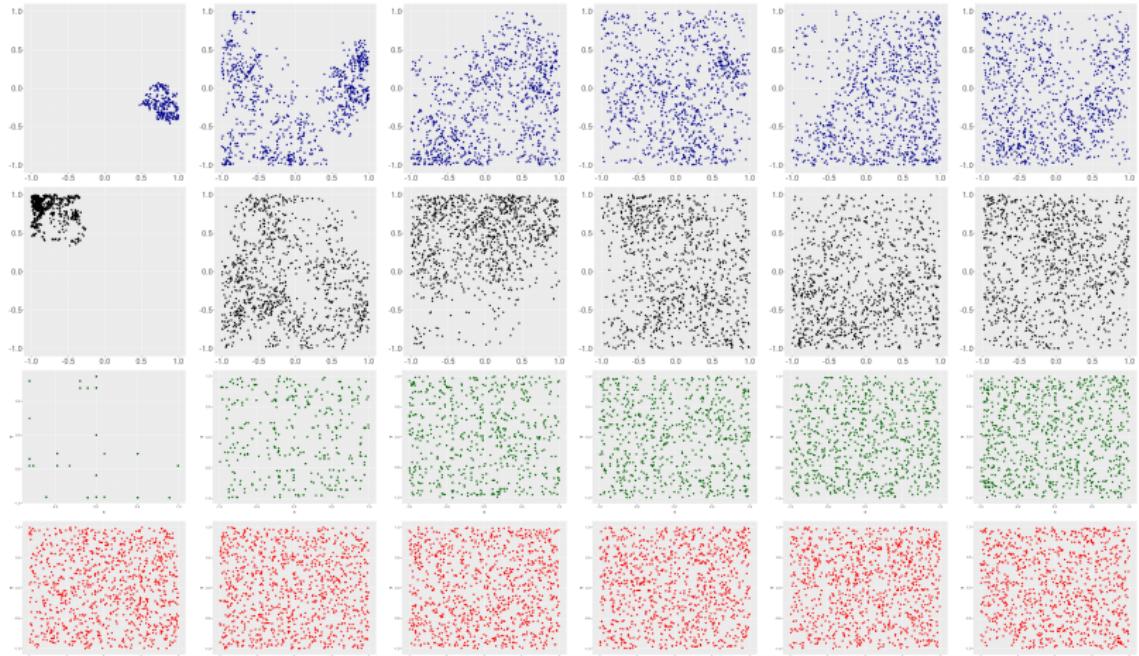
Billiard walk

BW-step (polytope P , point p_i , real τ , integer R) [Polyak'14]

1. Set length of trajectory $L = -\tau \ln \eta$, for random $\eta \sim U(0, 1)$.
2. Pick uniform direction v to start the trajectory at p_i .
3. When trajectory meets ∂P with inner normal s , $\|s\| = 1$,
the direction changes to $v - 2\langle v, s \rangle s$.
4. **return** the end of trajectory as p_{i+1} .
If number of reflections exceeds R then **return** $p_{i+1} = p_i$.



Experimental comparison



Sampling the 100d cube with **Ball Walk**, **RDHR**, **CDHR**, **Billiard walk**.
Walk length = 1,20,40,60,80,100.

Outline

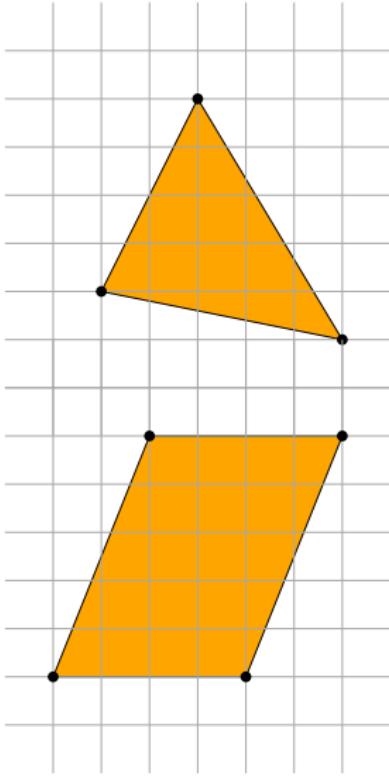
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Easy cases

Some elementary polytopes have determinantal formulas.



$$\begin{vmatrix} 1 & 2 & 1 \\ 3 & 6 & 1 \\ 6 & 1 & 1 \end{vmatrix} / 2! = 11$$

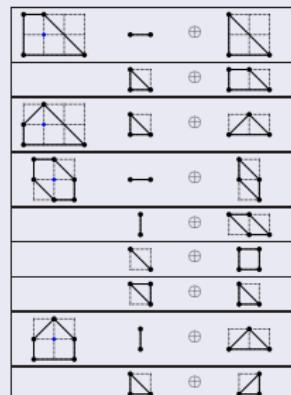
$$\begin{vmatrix} 2 & 5 \\ 4 & 0 \end{vmatrix} = 20$$

Convex polytope

- Convex polytopes are defined by
 - the set of all convex combinations of a finite set of points (V-rep):
easy point generation, membership requires LP;
 - the intersection of a finite number of halfspaces (H-rep):
easy membership, ray-shooting reduces to F linear systems.
- Further representations include Minkowski (vector) sums:

- of a finite number of polytopes,
- of segments v_i : zonotope (Z-rep)
"generated" as follows:

$$\sum_{i=1}^t \lambda_i v_i, \quad 0 \leq \lambda_i \leq 1.$$



Hardness

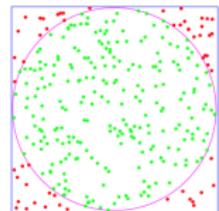
IN: H-polytope $P := \{x \in \mathbb{R}^d \mid Ax \leq b, A \in \mathbb{R}^{m \times d}, b \in \mathbb{R}^m\}$,
which has m linear inequalities (maybe some redundant).

V-polytope defined by points (vertices) $v_i \in \mathbb{R}^d$:
 $P := \{\lambda_1 v_1 + \dots + \lambda_n v_n \in \mathbb{R}^d \mid \sum_i \lambda_i = 1, \lambda_i \geq 0\}$

OUT: Euclidean volume of P .

- #P hard for vertex, halfspace representations [Dyer,Frieze'88]
- Open if both vertex & halfspace representations are available.
- APX-hard in oracle model: deterministic poly-time approximations have exponential error [Elekes'86]

Volume Approximation (H-rep)



- Curse of dimensionality:
 - Triangulation is exponential in d .
 - $V(\text{unit ball}) = \pi^{d/2} / \Gamma(1 + d/2) = \Theta((2\pi e/d)^{d/2} / \sqrt{d}) = O((1/d)^d)$
Hence rejection sampling does not scale.
- det. poly-time approximation with error $\leq d!$ [Betke, Henk'93]
- Fully Poly-time Randomized Approx. Scheme: arbitrarily small error with high probability; grid random walk, **telescoping sphere sequence** [D,F,Kannan'91] in $O^*(d^{23})$.
- Ball walk [K,Lovász,Simonovits'97] $O^*(d^5)$.
 $O^*(d^4 m)$ [LVempala'04] by simulated annealing, **Hit-and-Run**.
If rounded $O^*(d^3 F)$ [CousinsV'14] by Gaussian cooling.
Hamiltonian walk $O^*(d^{2/3} F)$ [LeeV'18].

Implementations

Exact: VINCI [Bueler et al'00], Latte [deLoera et al], Qhull [Barber et al]

- too slow in high dimensions (e.g. > 20)

Randomized for H-polytopes:

- [Lovász,Deák'12] only in ≤ 10 dimensions.
- Zonotopes via LP oracles, shake-and-bake [Fukuda et al.]
- Ours: based on Sampling [DFK'91], [Kannan,Lovász,Simonovits'97]; few hrs for few hundred dimensions.
- Matlab code by Cousins & Vempala based on [LV04], needs #facets.
- Hit-and-run in non-convex regions [Abbasi-Yadkori et al.'17]

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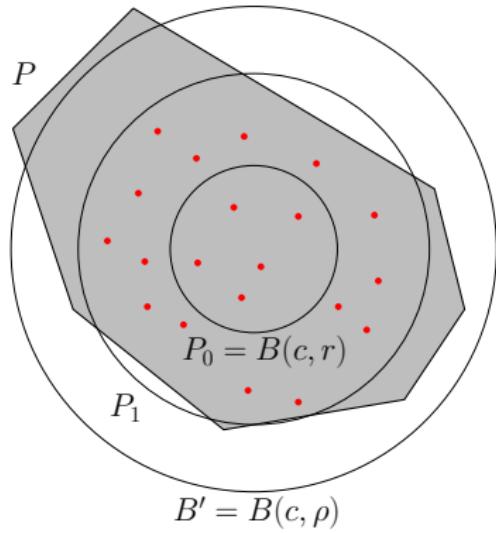
Algorithmic ingredients

- ✓ Sampling by Hit-and-Run
- Telescoping (multiphase) sequence of balls;



- Sandwiching input P between balls;
- Rounding input P .

Multiphase Monte Carlo (ball sequence)



- Cocentric balls $B(c, 2^{i/d})$,
 $i = \lfloor d \log r \rfloor, \dots, \lceil d \log \rho \rceil$,
 $B(c, r) \subset P \subseteq B(c, \rho)$.
- $P_i := P \cap B(c, 2^{i/d})$.

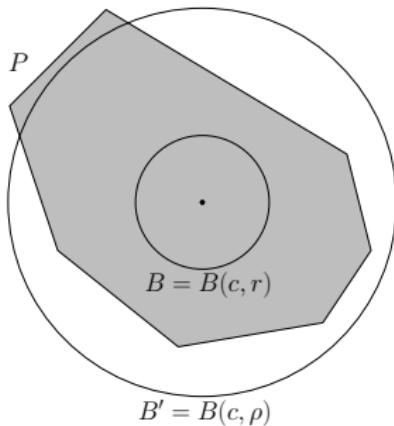
Partial inverse generation:

1. Let N uniform points in P_i
2. Count ν in P_{i-1}
3. Keep ν , sample $N - \nu$ in P_{i-2}

$$\text{vol}(P) = \text{vol}(P_{d \log r}) \prod_{i=\lfloor d \log r \rfloor + 1}^{\lceil d \log \rho \rceil} \frac{\text{vol}(P_i)}{\text{vol}(P_{i-1})} \quad [\text{DFK91}]$$

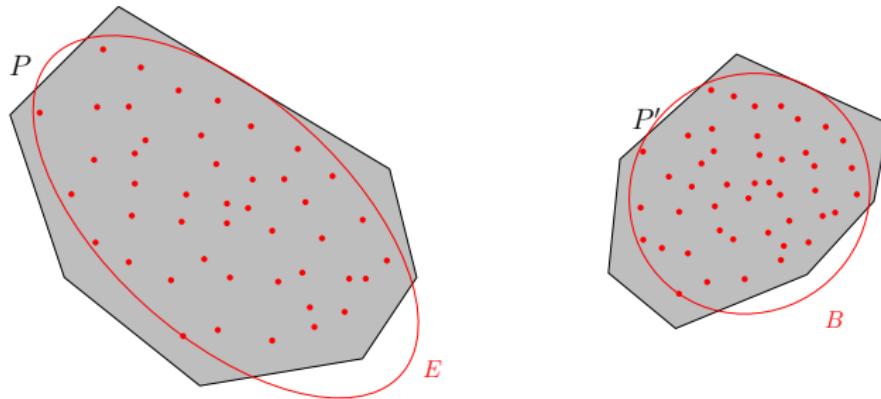
Sandwiching (Schedule)

- compute max inscribed ball $B(c, r)$ of P , by LP:
$$\max r : A_i c + r \|A_i\|_2 \leq b_i, i = 1, \dots, m.$$
- get uniformly distributed $p \in B(c, r)$; sample N uniform points $\in P$
- $\rho = \max$ distance between c and N points: $P \subset B(c, \rho)$



Well-Rounding

1. given set S of s uniformly distributed points $\in P$
2. compute (approximate) min-volume ellipsoid E covering S :
$$S \subset E = \{x : (x - c)^T L^T L(x - c) \leq 1\}$$
3. compute L mapping E to unit ball B : apply L to P



Iterate till ratio of max over min ellipsoid axes reaches threshold.
Note: Isotropic position (identity covariance) implies well-rounded.

Complexity

Theorem (Kannan,Lovász,Simonovits'97; Lovász'99)

Let a polytope P be well-rounded: $B(c, r = 1) \subseteq P \subseteq B(c, \rho)$, for $c \in P$. The algorithm computes, with probability $\geq 3/4$, an estimate of $\text{vol}(P)$ in $[(1 - \epsilon)\text{vol}(P), (1 + \epsilon)\text{vol}(P)]$, by

$$O^*(d^4\rho^2) = O^*(d^5)$$

oracle calls, with probability $\geq 9/10$, where $\rho = O^*(\sqrt{d})$ by isotropic sandwiching, and $\epsilon > 0$ is fixed.

Runtime

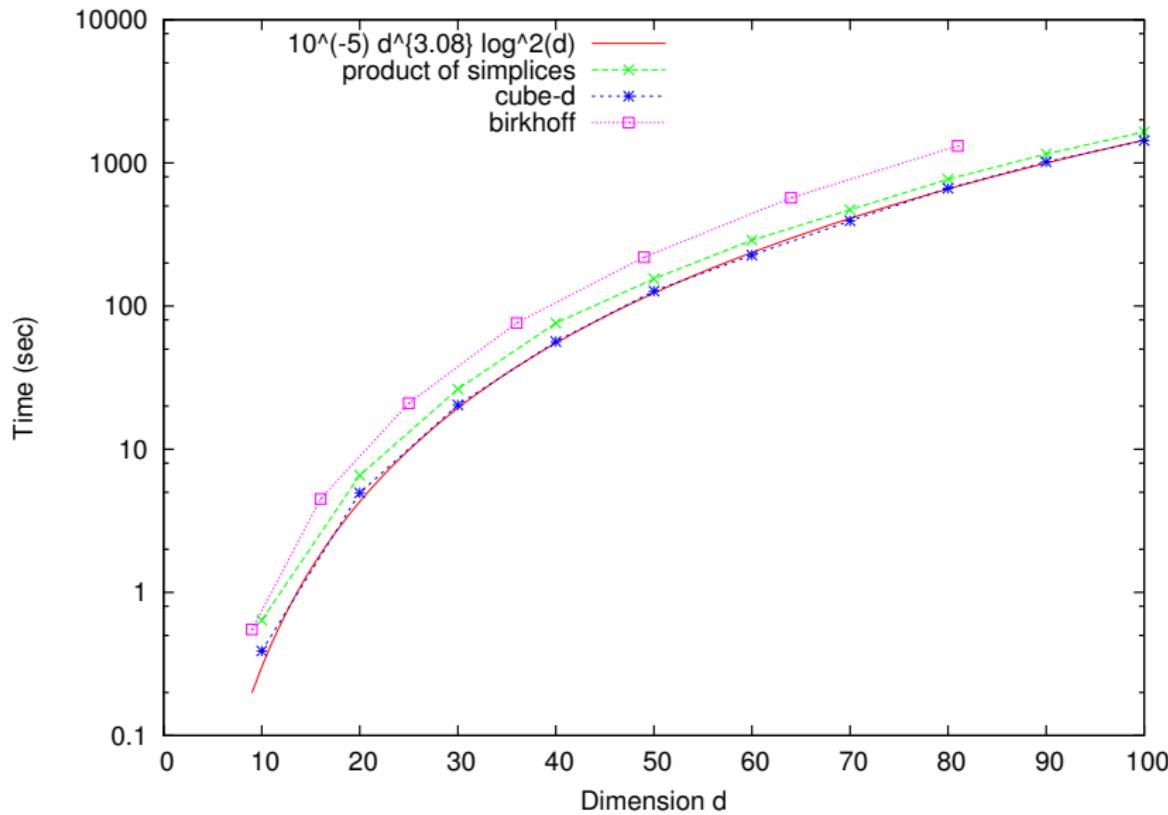
- $N = 400d \log d / \epsilon^2 = O^*(d)$ random points per P_i ,
- each point computed after $W \sim 10^{11}d^3$ walk steps.

- CDHR: boundary oracle = $O(m)$ per step.
- Set $W = \lfloor 10 + d/10 \rfloor$ walk steps, also [LovDeák]: achieves $< 1\%$ error in $d \leq 100$. Hence our algorithm takes $O^*(md^3)$ ops.
- sample partial generations of $\leq N$ points per ball $\cap P$, starting from largest; saves constant fraction per ball.
- rounding = $O^*(sd^2) = O^*(d^3)$ [Khachiyan'96]; k iterations in $O^*(k(md + d^3))$, typically $k = 1$.
- 2.5K lines C++, github.com/GeomScale
- CGAL for LP, min-ellipsoid; Eigen for linear algebra
- Google summer of code 2018: R interface [Chalkis]

Experimental results

- approximate the volume of **polytopes** (cubes, random, cross, Birkhoff) up to dimension 100 in < 2hrs with mean error < 1%
- estimate **always** in $[(1 - \epsilon)\text{vol}(P), (1 + \epsilon)\text{vol}(P)]$, with $W = \Theta(d)$
- **CDHR** faster (and more accurate) than RDHR
- volume of Birkhoff polytopes B_{11}, \dots, B_{15} in few hrs; exact specialized software **computed B_{10}** in ~ 1 year [BeckPixton03]

Runtime vs. dimension



Birkhoff polytopes

$B_n = \{x \in \mathbb{R}^{n \times n} \mid x_{ij} \geq 0, \sum_i x_{ij} = 1, \sum_j x_{ij} = 1, 1 \leq i, j \leq n\}$:
perfect matchings of $K_{n,n}$, or Newton polytope of determinant.

n	d	estimate	asymptotic [CanfieldMcKay09]	estimate asympt.	exact	exact asympt.
4	9	6.79E-002	7.61E-002	0.89194	6.21E-002	0.81593
5	16	1.41E-004	1.69E-004	0.83444	1.41E-004	0.83419
6	25	7.41E-009	8.62E-009	0.85987	7.35E-009	0.85279
7	36	5.67E-015	6.51E-015	0.87139	5.64E-015	0.86651
8	49	4.39E-023	5.03E-023	0.87295	4.42E-023	0.87786
9	64	2.62E-033	2.93E-033	0.89608	2.60E-033	0.88741
10	81	8.14E-046	9.81E-046	0.83052	8.78E-046	0.89555
11	100	1.40E-060	1.49E-060	0.93426	?	?
12	121	7.85E-078	8.38E-078	0.93705	?	?
13	144	1.33E-097	1.43E-097	0.93315	?	?
14	169	5.96E-120	6.24E-120	0.95501	?	?
15	196	5.70E-145	5.94E-145	0.95938	?	?

All volumes in few hrs; exact $V(B_{10})$ in ~ 1 year [BeckPixton03].

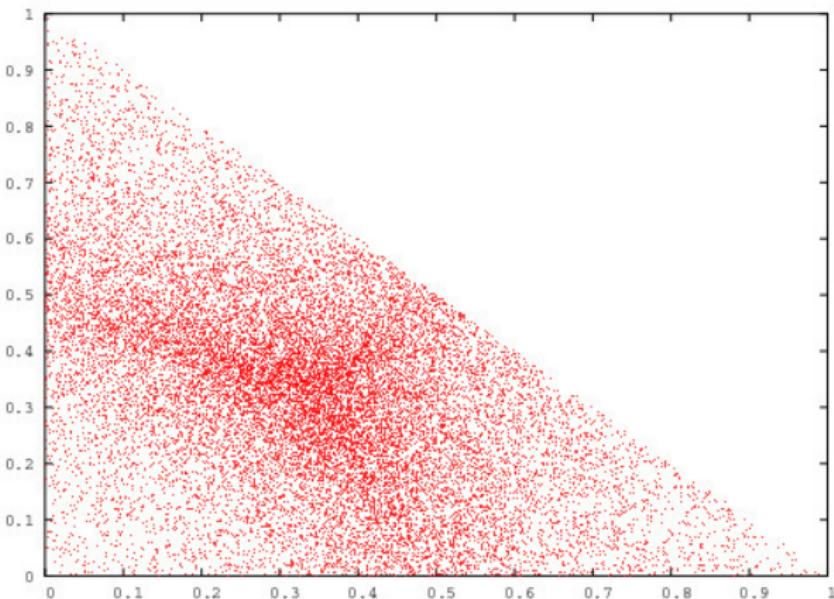
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Uniform simplex coordinates



Sample d coordinates and normalize is too naive.

Unit Simplex

Distinct uniform variables

1. Pick d uniform **distinct** integers; then sort:

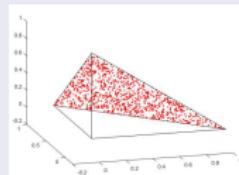
$$x_0 = 0 \leq x_1 < \dots < x_d \leq x_{d+1} = M.$$

2. Point $[y_i = (x_i - x_{i-1})/M : i = 1, \dots, d]$ is uniform.

Complexity = $O(d \log d)$ [Smith, Tromble'04].

Fastest for $d < 80$ with Bloom filter (rather than hashing)

Check: $\sum_i y_i \leq 1$.



Exponential random variables

1. Pick uniform $x_i \in (0, 1)$; set $y_i = -\ln x_i$, $i = 1, \dots, d + 1$.
2. Let $T = \sum_{i=1}^{d+1} y_i$, then $[y_1/T, \dots, y_d/T]$ is uniform.

Complexity = $O(d)$ [Rubinstein, Melamed'98].

Halfspace intersecting simplex

$H = \{x : a^T x \leq a_0, a = (a_1, \dots, a_d)\}$, S is the unit simplex.

1. Let $y_i = a_i - a_0$ if ≥ 0 , $i = 1, \dots, K \geq 0$,
 $z_i = a_i - a_0$ if < 0 , $i = 1, \dots, J$, s.t. $J + K = d$.
2. Initialize $A_0 = 1, A_1 = \dots = A_K = 0$.
3. For $j = 1, \dots, J$ do:

$$A_k \leftarrow \frac{y_k A_k - z_j A_{k-1}}{y_k - z_j}, \quad k = 1, \dots, K.$$

For $j = J$,

$$A_K = \text{vol}(S \cap H) / \text{vol}(S) : \quad \text{frustum.}$$

Complexity = $O(d^2)$ [Varsi'73, Ali'73, Gerber'81].

Example of frustum

$H = \{x : x_1 - x_2 \leq 0\}$, $S \subset \mathbb{R}^2$ is the unit triangle.

1. Let $y_1 = 1 - 0 \geq 0$, $K = 1$, $z_1 = -1 - a_0 < 0$, $J = 1$.

Initialize $A_0 = 1$, $A_1 = 0$.

2. For $j = 1$ do:

$$A_1 \leftarrow \frac{1 \cdot 0 - (-1)1}{1 - (-1)} = \frac{1}{2} = \text{vol}(S \cap H) / \text{vol}(S).$$

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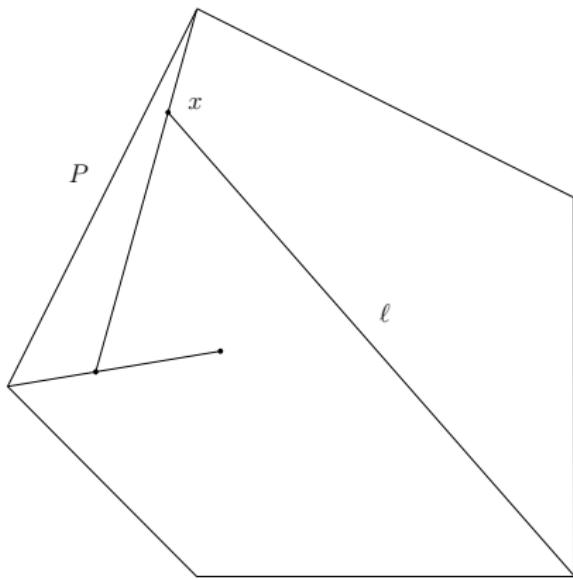
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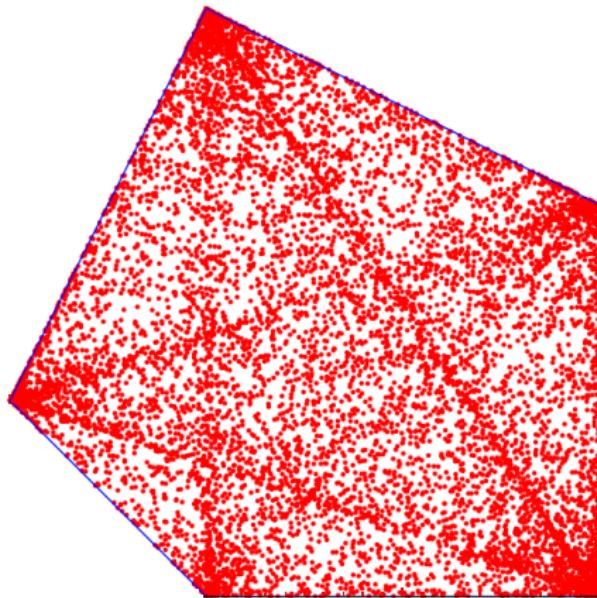
Open: V-polytopes

Given by optimization oracle



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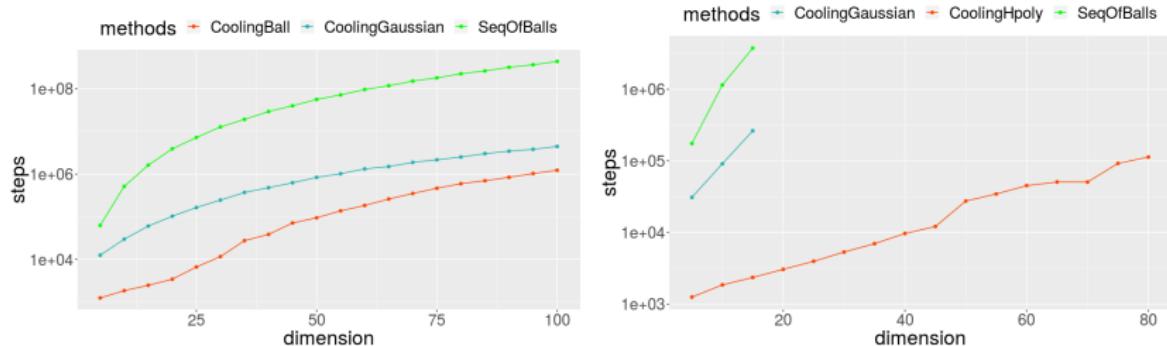


H-polytopes [E-Fisikopoulos14]

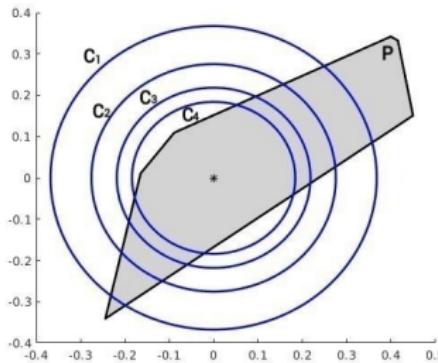
- CDHR amortized $O(1)$, $\lfloor 10 + d/10 \rfloor$ vs. $\simeq 10^{11}d^3$ random walks.
- $d \leq 100$: < 2hrs, < 1% error.

H/V-polytopes, zonotopes [Chalkis-E-Fisikopoulos'19]

- Sequence of convex bodies: good fit, easy sampling (rejection)
- Simulated annealing to construct sequence
- Statistical criterion of convergence



New Multiphase Monte Carlo



Convex $C_1 \supseteq \dots \supseteq C_m$ intersect $P = P_0$, $P_i = C_i \cap P$, $i = 1, \dots, m$:

$$\text{vol}(P) = \frac{\text{vol}(P_0)}{\text{vol}(P_1)} \cdots \frac{\text{vol}(P_{m-1})}{\text{vol}(P_m)} \cdot \frac{\text{vol}(P_m)}{\text{vol}(C_m)} \cdot \text{vol}(C_m),$$

is good sequence provided ratios computed fast, m small;
inner ratio may be approximated by rejection sampling.

Annealing schedule: body sequence

Employ (ideas of) simulated annealing to reduce length of sequence by adapting to the problem: non-deterministic, varying steps.

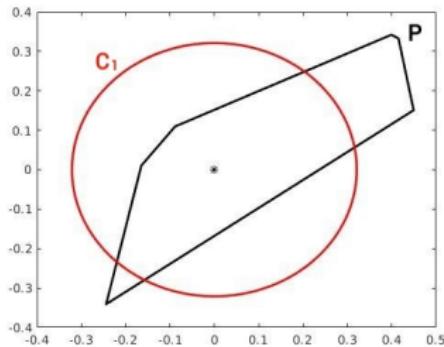
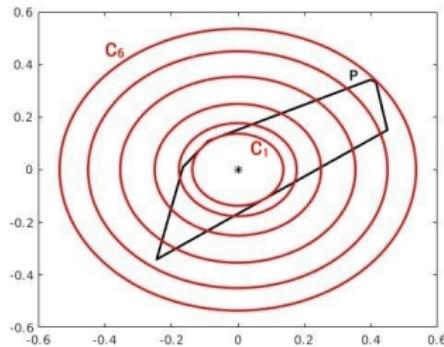
Input: Polytope P , error ϵ , cooling parameters $r, \delta > 0$ s.t. $0 < r + \delta \ll 1$.

Output: A sequence of convex bodies $C_1 \supseteq \dots \supseteq C_m$ s.t.

$$\text{vol}(P_{i+1})/\text{vol}(P_i) \in [r, r + \delta] \text{ with high probability}$$

where $P_i = C_i \cap P$, $i = 1, \dots, m$ and $P_0 = P$.

Annealing schedule: reduce number of phases



Six balls C_i (left), one by annealing $r=0.25$, $\delta=0.05$ (right)

- Classic MMC [LKS97]: $\frac{\text{vol}(C_2 \cap P)}{\text{vol}(C_1 \cap P)} \dots \frac{\text{vol}(C_6 \cap P)}{\text{vol}(C_5 \cap P)} \text{vol}(C_1)$.
- Annealing schedule: $\frac{\text{vol}(C_1 \cap P)}{\text{vol}(C_1)} \cdot \frac{\text{vol}(P)}{\text{vol}(C_1 \cap P)} \cdot \text{vol}(C_1)$.

Statistical tests to estimate volume ratio

Given $P_i \supseteq P_{i+1}$, $r, \delta > 0$, $0 < r + \delta \ll 1$, define null hypotheses H_0 :

testLeft: $H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \leq r + \delta$
testRight: $H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \leq r$

1. Sample set of N points from P_i , repeat ν times.
2. \forall set, binomial r.v. X counts points in P_{i+1} , success probability is unknown ratio $r_i = \text{vol}(P_{i+1})/\text{vol}(P_i)$.
3. Use $\hat{\mu} = \text{mean of } \nu \text{ ratios}$.

Statistical tests

testL(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \geq r + \delta$$

Successful if we **reject** H_0

testR(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \leq r$$

Successful if we **reject** H_0

- If both successful then $r_i = \text{vol}(P_{i+1})/\text{vol}(P_i) \in [r, r + \delta]$ whp.

Statistical tests

testL(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \geq r + \delta$$

Successful if we **reject** H_0

testR(P_i, P_{i+1}, r, δ):

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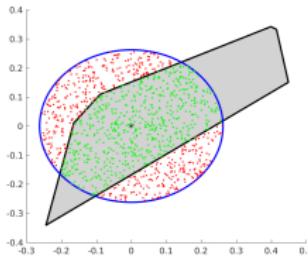


Figure: **testL**: succeeds, **testR**: fails

- Binary search a radius in $[r_{\max}, r_{\min}]$ until both tests are successful.

Statistical tests

testL(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \geq r + \delta$$

Successful if we **reject** H_0

testR(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \leq r$$

Successful if we **reject** H_0

- If both successful then $r_i = \text{vol}(P_{i+1})/\text{vol}(P_i) \in [r, r + \delta]$ whp.

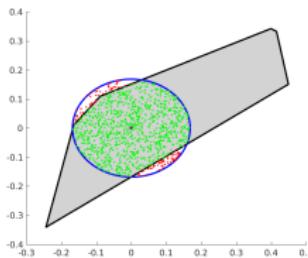


Figure: **testL**: fails, **testR**: succeeds

- Binary search a radius in $[r_{\max}, r_{\min}]$ until both tests are successful.

Statistical tests

testL(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \geq r + \delta$$

Successful if we **reject** H_0

testR(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \leq r$$

Successful if we **reject** H_0

- If both successful then $r_i = \text{vol}(P_{i+1})/\text{vol}(P_i) \in [r, r + \delta]$ whp.

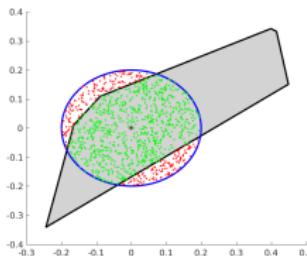


Figure: **testL**: succeeds, **testR**: succeeds

- Binary search a radius in $[r_{\max}, r_{\min}]$ until both tests are successful.

Statistical tests

Given convex bodies $P_i \supseteq P_{i+1}$, we define two statistical tests:

testL(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \geq r + \delta$$

Successful if we **reject** H_0

testR(P_i, P_{i+1}, r, δ):

$$H_0 : \text{vol}(P_{i+1})/\text{vol}(P_i) \leq r$$

Successful if we **reject** H_0

- If both successful then $r_i = \text{vol}(P_{i+1})/\text{vol}(P_i) \in [r, r + \delta]$ whp.

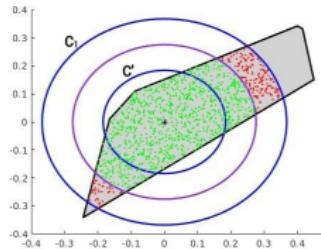


Figure: **testL**: succeeds, **testR**: succeeds

- Binary search a radius in $[r_{\max}, r_{\min}]$ until both tests are successful.

Bound #phases

- The annealing schedule terminates with constant probability.
- $\# \text{phases } m = O\left(\log(\text{vol}(P)/\text{vol}(C' \cap P))\right)$.
- If the body we use in MMC is a "good fit" to P , then $\text{vol}(C' \cap P)$ increases and m decreases.