

# Geometric Data analysis

## Random walks, Sampling, Volume

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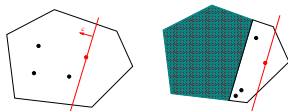
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May 20, 2022

- 1 Sampling
- 2 Random walks
- 3 Convex Volumes
  - Poly-time approximation
  - V-polytopes
  - Nonlinear bodies
  - Oracles by ANN
- 4 Financial modeling

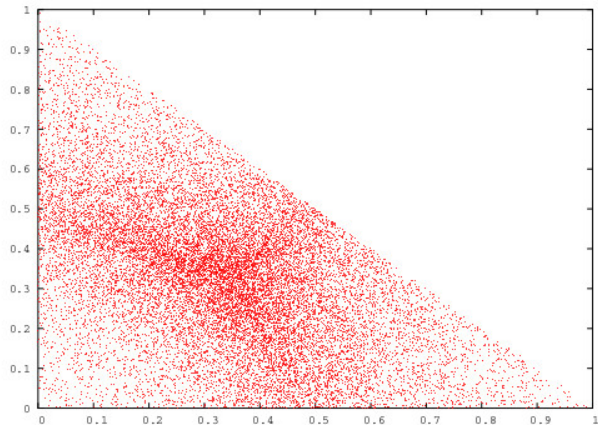
- Monte Carlo Integration (which generalizes volume)

- Optimization



- Sparse representation, check conjectures (# linear extensions)
- Contingency tables, underconstrained linear systems
- Systems biology [Chalkis et al.21], ...

# Simplex sampling



Sample each coordinate uniformly and normalize is too naive.

# Unit Simplex

## Distinct uniform variables

1. Pick 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  $d < 80$  using Bloom filter (rather than hashing).

## 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].

**Arbitrary** with vertices  $v_i$ :  $x \in$  unit simplex,  $\sum_{i=1}^{d+1} x_i v_i$  is uniform.

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# Geometric Random walks

- Rejection shall not work: exponentially many points in bounding cube / simplex but outside  $P$ . Curse of dimensionality.
- Continuous (geometric) version of random walks on discrete structures (graphs).
- 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

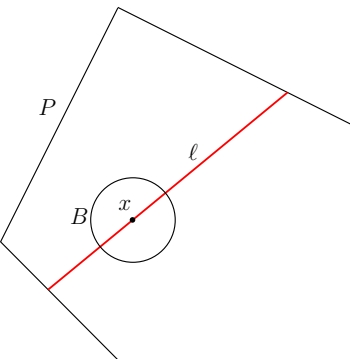
year	walk	mixing time	step cost
87	Coordinate HnR	?	$m$
06	Hit-and-Run	$d^3$	$md$
09	Dikin	$md$	$md^2$
14	Billiard	?	$Rmd$
16	Geodesic	$md^{3/4}$	$md^2$
17	Ball	$d^{2.5}$	$md$
17	Vaidya	$m^{1/2}d^{3/2}$	$md^2$
17	Riemmanian HMC	$md^{2/3}$	$md^2$
18	HMC w/reflections	?	$md$
19	sublinear Ball	$d^{2.5}$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



dimension  $d$ ,  $m$  facets,  $R$  bounds billiard reflections



# Random Directions Hit-and-Run (RDHR)



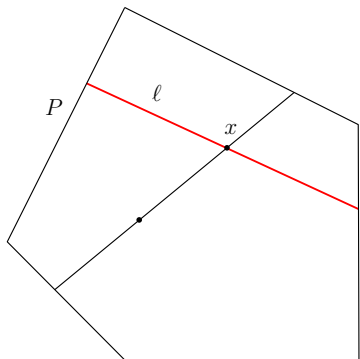
**Input:** point  $x \in P$  and polytope  $P \subset \mathbb{R}^d$

**Output:** a new point in  $P$

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

Perform  $W$  steps, return  $x$ .

# Random Directions Hit-and-Run (RDHR)



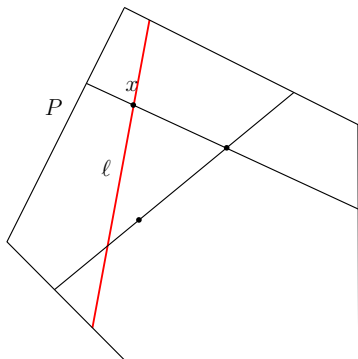
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Perform  $W$  steps, return  $x$ .

- $x$  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  $\ell(u,v)$  = 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  $p_u(A) =$  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?

## 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

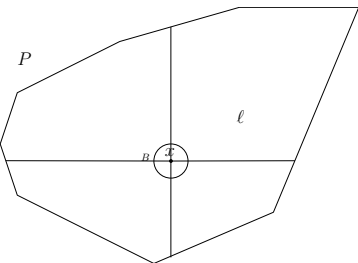
$T \approx 10^{11} d^3$  for RDHR and uniform distribution  $Q$ .

## Proof

$T = O(1/\phi^2)$ , where  $\phi$  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)



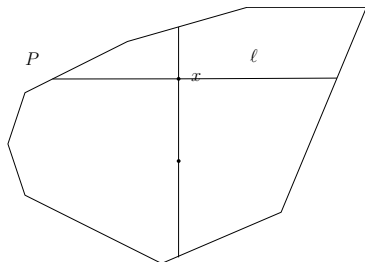
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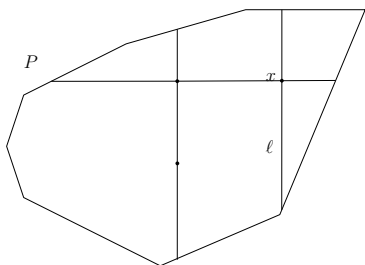


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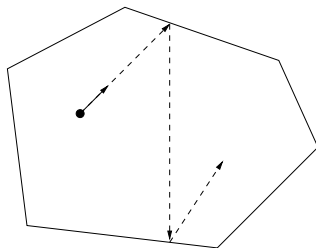
“Continuous” grid walk: Converges to uniform, mixing =  $O(d^{11}R^2)$  [2020].

Compute intersection of line  $\ell$  with boundary  $\partial P$ , given  $m$  hyperplanes:

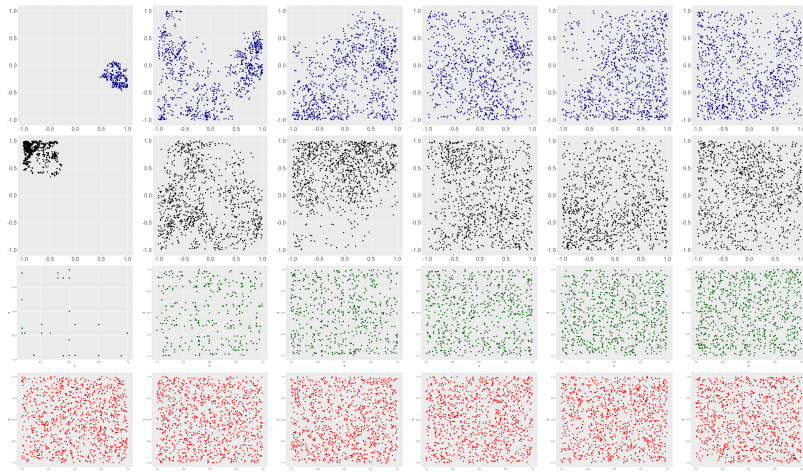
- RDHR step in  $O(md)$ .
- CDHR =  $O(m)$  per step: solve 1d (linear) problem per facet.
- Duality reduces oracle to farthest point search (max inner product) among  $m$  points: same asymptotics, practical if large  $m$  (16-dim cross-polytope:  $m = 2^{16}$ , 40x speedup).

**BW-step** (polytope  $P$ , point  $p_i$ , real  $\tau$ , 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  $\partial P$  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**  $p_{i+1} = p_i$ .



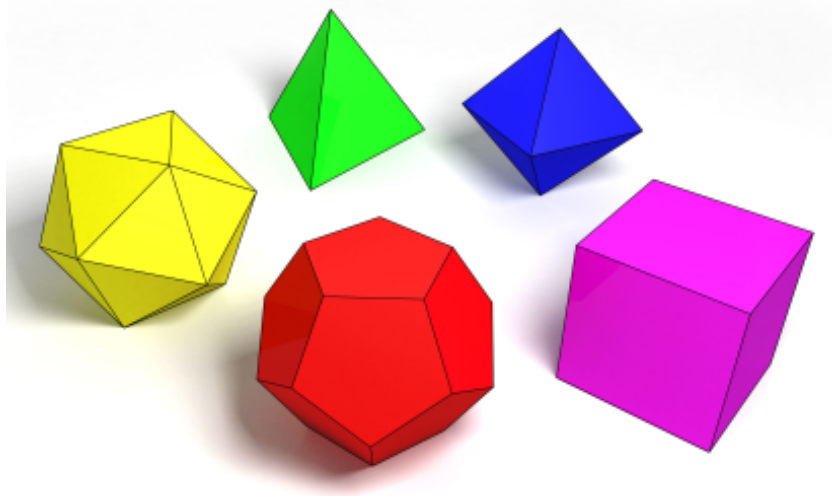
# Experimental comparison



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

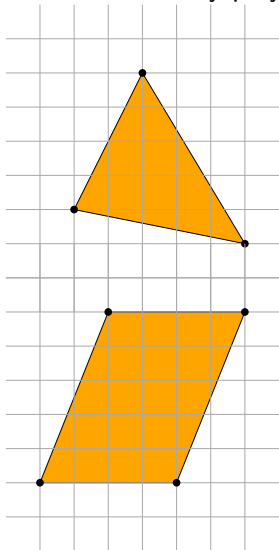
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# Famous polytopes



# Easy cases

Some elementary polytopes have determinantal formulas.



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

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

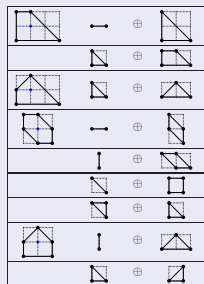


# Convex polytope

- 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:

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



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].

**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  $\leq 10$  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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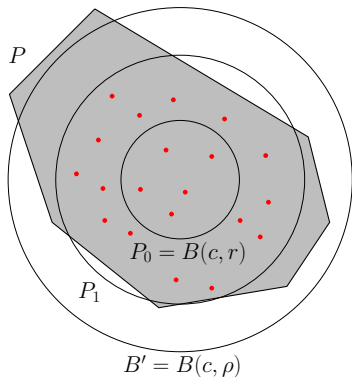
# Algorithmic ingredients

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



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

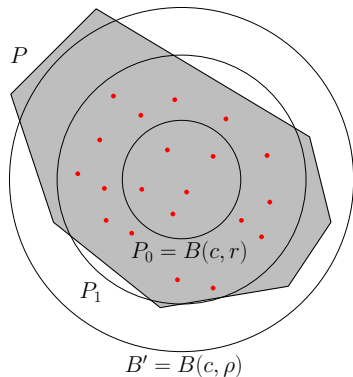
# Ball sequence



- Cocentric ball  $B(c, 2^{i/d})$  sequence: centered at point  $c \in P$ , sequence of radii  $r, 2r, \dots, \rho$ , for  $i = \lfloor d \log r \rfloor, \dots, \lceil d \log \rho \rceil$  s.t.  $B(c, r) \subset P \subseteq B(c, \rho)$ .
- Define convex  $P_i := P \cap B(c, 2^{i/d})$ .

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

# Multiphase Monte Carlo



The  $P_i$ 's are sampled uniformly.

Partial inverse point generation:

1. Let  $N$  uniform points in  $P_i$ .
2. Count (+ keep)  $\nu$  in  $P_{i-1}$ .
3. Sample  $N - \nu$  in  $P_{i-1}$ .

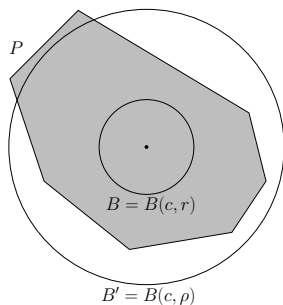
$$\text{vol}(P) = \text{vol}(P_{d \log r}) \prod_{i=\lfloor d \log r \rfloor + 1}^{\lceil d \log \rho \rceil} \frac{\text{vol}(P_i)}{\text{vol}(P_{i-1})}.$$

where each **ratio** is approximated by rejection sampling (step 2).



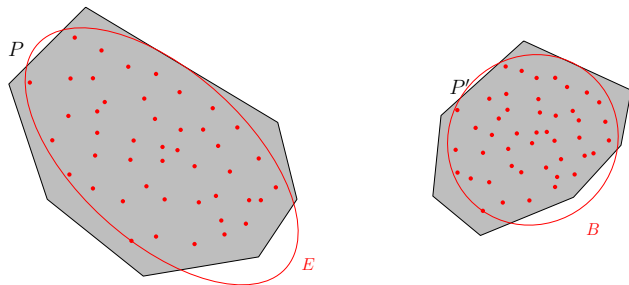
# Sandwiching (Schedule)

- 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:  $P \subseteq B(c, \rho)$



# 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.

## 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.

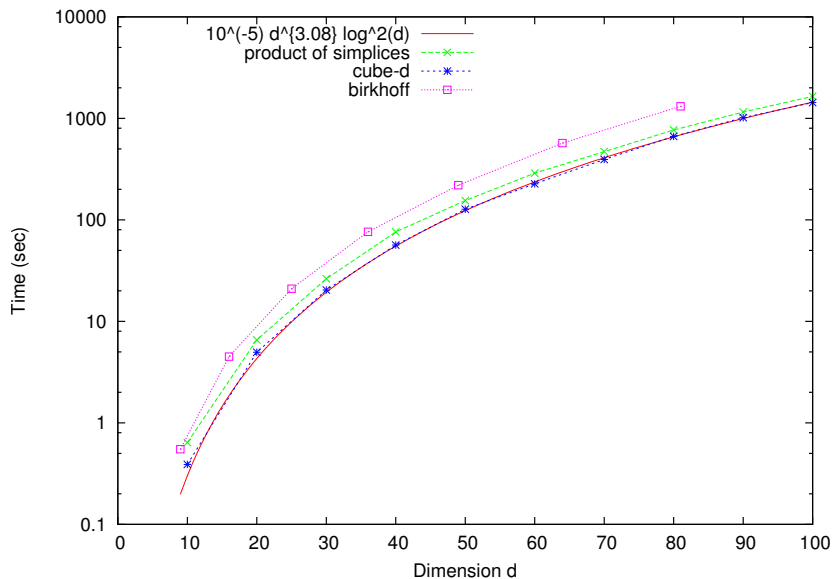
## Runtime

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

- CDHR: **boundary oracle** =  $O(m)$ .
- **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](https://github.com/GeomScale)
- CGAL for LP, min-ellipsoid; Eigen for linear algebra
- Google summer of code 2018: R interface [Chalkis]

- approximate the volume of **polytopes** (cubes, random, cross, Birkhoff) up to dimension 100 in  $< 2$ hrs 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  $\sim 1$  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 <small>[CanfieldMcKay09]</small>	<u>estimate</u> asympt.	exact	<u>exact</u> 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	?	?

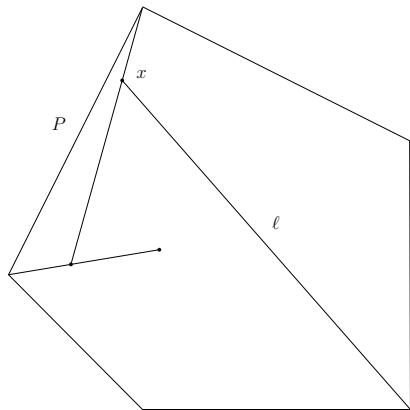
All volumes in few hrs; exact  $V(B_{10})$  in  $\sim 1$  year [\[BeckPixton03\]](#).

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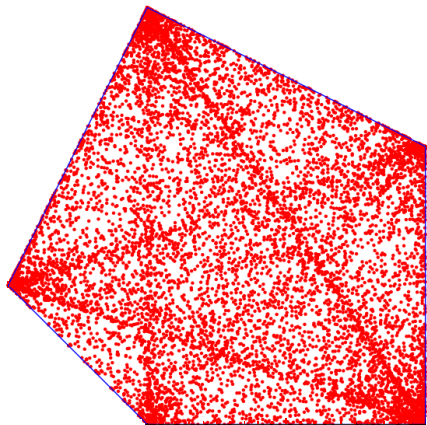
# Open: V-polytopes

Given by **optimization oracle**



# Open: V-polytopes

Given by **optimization oracle**

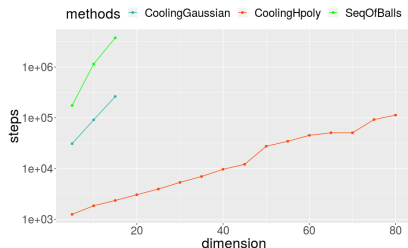
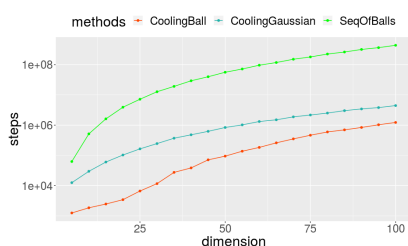


## H-polytopes [E-Fisikopoulos14]

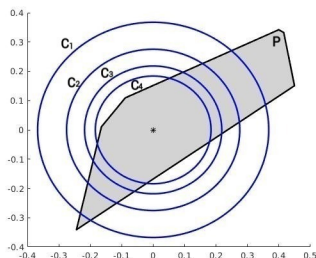
- CDHR amortized  $O(1)$ ,  $\lfloor 10 + d/10 \rfloor$  vs.  $\simeq 10^{11}d^3$  random walks.
- $d \leq 100$ :  $< 2$ hrs,  $< 1\%$  error.

## 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  $P = P_0$ ,  $P_i = C_i \cap P$ ,  $i = 1, \dots, m$ :

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

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.

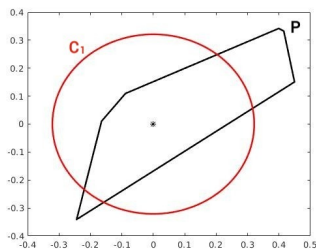
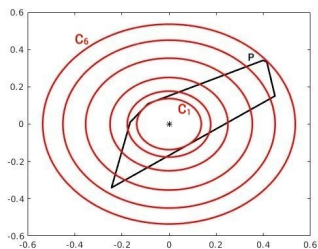
**Input:** Polytope  $P$ , error  $\epsilon$ , cooling parameters  $r, \delta > 0$  s.t.  $0 < r + \delta \ll 1$ .

**Output:** A sequence of convex bodies  $C_1 \supseteq \cdots \supseteq C_m$  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]:  $\frac{\text{vol}(C_2 \cap P)}{\text{vol}(C_1 \cap P)} \cdots \frac{\text{vol}(C_6 \cap P)}{\text{vol}(C_5 \cap P)} \text{vol}(C_1)$ .
- 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  $\nu$  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  $\hat{\mu} = \text{mean of } \nu \text{ ratios}$ .

**testL**( $P_i, P_{i+1}, r, \delta$ ):

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

**Successful** if we **reject**  $H_0$

**testR**( $P_i, P_{i+1}, r, \delta$ ):

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

**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**( $P_i, P_{i+1}, r, \delta$ ):

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

**Successful** if we **reject**  $H_0$

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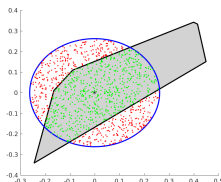


Figure: **testL**: **successful**, **testR**: **fails**

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

# Statistical tests

**testL**( $P_i, P_{i+1}, r, \delta$ ):

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

**Successful** if we **reject**  $H_0$

**testR**( $P_i, P_{i+1}, r, \delta$ ):

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

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

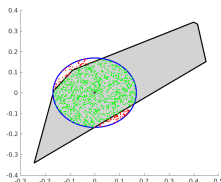


Figure: **testL**: fails, **testR**: succeeds

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

# Statistical tests

**testL**( $P_i, P_{i+1}, r, \delta$ ):

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

**Successful** if we **reject**  $H_0$

**testR**( $P_i, P_{i+1}, r, \delta$ ):

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

**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.

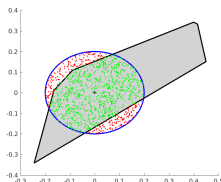


Figure: **testL**: succeeds, **testR**: succeeds

- 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**( $P_i, P_{i+1}, r, \delta$ ):

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

**Successful** if we **reject**  $H_0$

**testR**( $P_i, P_{i+1}, r, \delta$ ):

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

**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.

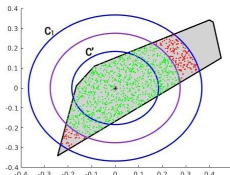


Figure: **testL**: succeeds, **testR**: succeeds

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

- The annealing schedule terminates with constant probability.
- #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.

1 Sampling

2 Random walks

3 **Convex Volumes**

- Poly-time approximation
- V-polytopes
- **Nonlinear bodies**
- Oracles by ANN

4 Financial modeling

For ellipsoids we generalized:

- Boundary oracle: univariate quadratic equation.
- Compute internal point, inscribed ball, enclosing ball.
- Sequence of concentric balls: Stop when all rays first hit inscribed ball

- Transform ellipsoid to sphere  $H_0$ , transform simplex similarly.
- Find  $B(p, r)$  of max radius  $r$ , satisfying constraints:

$$\text{dist}(p, H_i) \geq r \Leftrightarrow a_i^T p + b_i \geq r \|a_i\|,$$

$$\text{dist}(p, H_0) \geq r \Leftrightarrow \|p - c_0\| \leq r_0 - r.$$

This is a Second Order Cone Program. In general, polytope intersection with  $O(1)$  balls.

- Solved by SDP / interior-point method in poly-time.
- Inverse transform yields inscribed ellipsoid, maybe not max. Center is good internal point.
- Get max inscribed ball by taking distance of  $p$  to  $H_i$ 's.



- 1 Sampling
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- 3 Convex Volumes**
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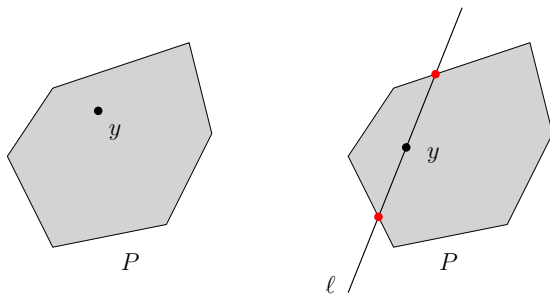
# Polytope Oracles

## Membership oracle

Given point  $y \in \mathbb{R}^d$ , return yes if  $y \in P$  otherwise return no.

## Boundary oracle

Given  $y \in P$ , ray  $\ell$  through  $y$ , return points  $\ell \cap \partial P$ .



# Approximation

Given is polytope  $P \subset \mathbb{R}^d$  and approximation parameter  $\epsilon \in (0, 1)$ :

## Definition (Approximate Polytope Membership)

Preprocess  $P$  into data-structure so that, given query point  $q$ , decide whether  $q \in P$  or not. If  $d(q, \partial P) \leq \epsilon \cdot \text{diam}(P)$  the data structure can answer either way.

## Definition (Approximate Polytope Boundary)

Preprocess  $P$  into data-structure so that given query ray  $r$  emanating from  $y \in P$ , compute point  $r^*$ , s.t.

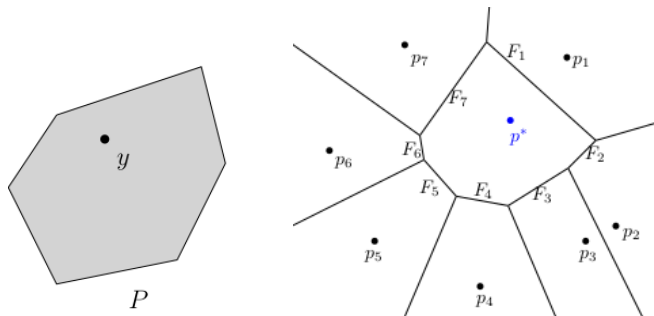
$$r^* \in r \text{ and } d(r^*, \partial P) \leq \epsilon \cdot \text{diam}(P).$$

Previous approaches have complexity exponential in  $d$ .

# Reduction

## Exact setting [Aurenhammer'87]

Let  $P \subset \mathbb{R}^d$  have  $n$  facets.  $\forall p^* \in P \setminus \partial P$ , compute set  $S$  of  $n$  points: membership of  $q$  reduces to finding its Nearest Neighbor in  $S \cup \{p^*\}$



# Approximate membership

Let  $P^{-\epsilon} = \{x \in P \mid d(x, \partial P) > \epsilon \cdot \text{diam}(P)\} \neq \emptyset$ .

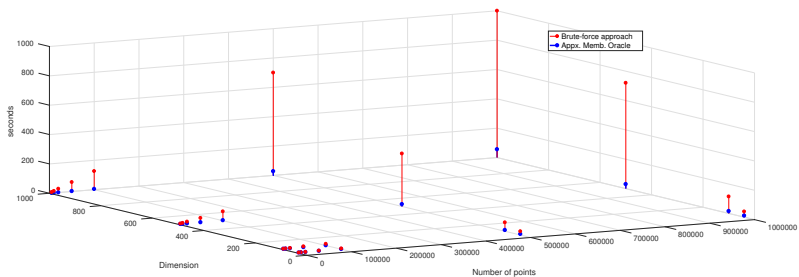
Approximate Membership reduces to  $\epsilon$ ANN on  $S \cup \{p^*\}$ ,  $p^* \in P^{-\epsilon}$ .

## Theorem (Complexity)

*We answer Approximate Membership queries in  $O^*(dn^{\rho+o(1)})$ , using  $O^*(n^{1+\rho+o(1)} + dn)$  space, whp, where  $\rho \leq 1/(1 + 4\epsilon^2) < 1$ .*

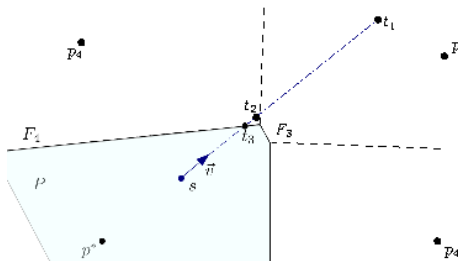
[Anagnostopoulos-E-Fisikopoulos'17]

# Membership experiments



# Approximate Boundary Oracle

1. Compute  $t_1 \notin P$ ,  $t_1 \in r$ , where  $r$  is ray shooting query.
2. For  $t_i \notin P$ , compute  $t_{i+1}$  closer to apex:  $p_i := \text{NN}(t_i)$ .
  - hyperplane  $H_i$  supports facet  $F_i$  defining  $p_i$ ;  $t_{i+1} := H_i \cap r$ .
3. Terminate by checking (approximate) membership oracle.



May get in local “optimum”: If  $t_i$  does not decrease distance to apex, set  $t_i := (t_{i-1} - r.apex) - r.unitdir \cdot \epsilon$ .

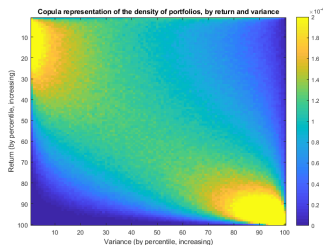
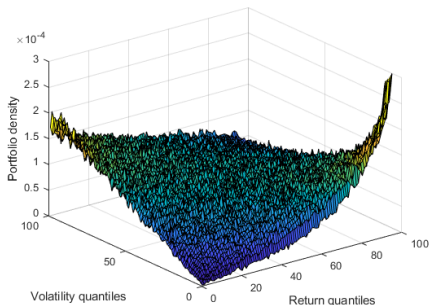
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# Financial markets

Stock markets exhibit 3 types of behavior:

- Normal: slightly positive returns, moderate volatility.
- Up-market (bubbles): high returns, low volatility.
- Crises: strongly negative returns, high volatility.



The **copula** is a volatility-return probability distribution.  
Figure: up-market and crisis: bubble burst in Sep. 2000.

- Portfolios of  $d + 1$  assets represented by simplex  $\Delta^d \subset \mathbb{R}^{d+1}$ .
- For portfolio  $\omega \in \Delta^d$ , returns  $R \in \mathbb{R}^{d+1}$ , total return  $f(\omega, R) = R^T \omega$  is linear combination of returns.
- Cross-sectional score of portfolio  $\omega^*$  is  $vol(\Delta^*)/vol(\Delta^d)$  s.t.

$$\Delta^* = \{\omega \in \Delta^d : f(\omega, R) \leq f(\omega^*, R)\}.$$

Score corresponds to cumulative distribution of  $f(\omega, C)$ .

- Volatility is quadratic form of returns.

- Let  $R_{ij}$  be the return at day  $i$  of asset  $j$ . Consider compound returns over  $k$  days starting at day  $i$ : define  $(d + 1)$ -vector  $v$  whose  $j$ -th coordinate,  $j = 1, \dots, d + 1$ , equals

$$v_j = (1 + R_{i,j})(1 + R_{i+1,j}) \cdots (1 + R_{i+k-1,j}) - 1.$$

Normal vector  $v$  defines family of hyperplanes.

- Volatility requires estimation of the returns' variance – covariance matrix, yielding concentric ellipsoids.
- Copula populated by intersecting  $\Delta^d$  along asset characteristics: Hyperplane families normal to two compound vectors, or to one vector and concentric ellipsoids.

# Formula for single halfspace

Let  $H: a^T x \leq a_0$ ,  $a = (a_1, \dots, a_d)$ , let  $S$  be the unit simplex.

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

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

For  $j = J$ ,

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

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

**Thank you!**