High-dimensional sampling and volume computation

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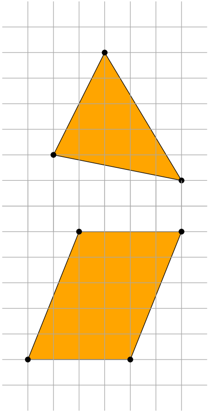
Our problem

Given P a convex body in $\mathbb{R}^d$ compute the volume of P.

Some elementary polytopes (simplex, cube) have simple determinantal formulas.



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

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

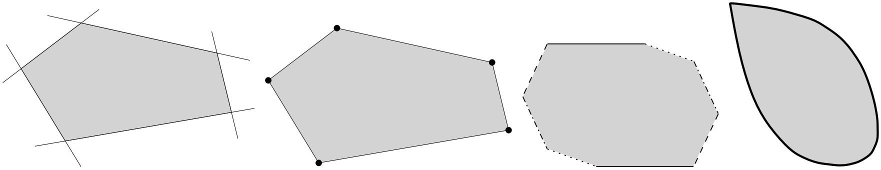
Convex bodies

H-polytope : $P = \{x \mid Ax \leq b,\ A \in \mathbb{R}^{q \times d},\ b \in \mathbb{R}^q\}$

V-polytope : P is the convex hull of a set of points in $\mathbb{R}^d$

Z-polytope : Minkowski sum of segments (projections of d-cubes)

LMI : $P = A_0 + y_1 A_1 + y_2 A_2 + \cdots + y_m A_m \succeq 0$, where A_i: symmetric matrices, $B \succeq 0$: B is positive semidefinite



First thoughts for volume computation

- Triangulation (or sign decomposition) methods – exponential size in d

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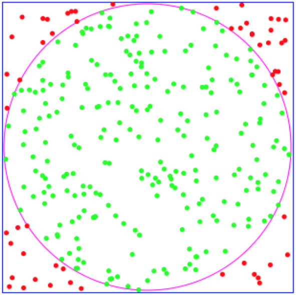
- Triangulation (or sign decomposition) methods – exponential size in d
- Sampling/rejections techniques (sample from bounding box) fail in high dimensions



volume(unit cube) $= 1$
volume(unit ball) $\sim (c/d)^{d/2}$
–*drops exponentially with* d

Volume computation is hard!

- #P-hard for V-, H-, Z-polytopes [DyerFrieze'88]
- no deterministic poly-time algorithm can compute the volume with less than exponential relative error (oracle model) [Elekes'86]
- open problem if V-polytope and H-polytope representations available

Randomized algorithms

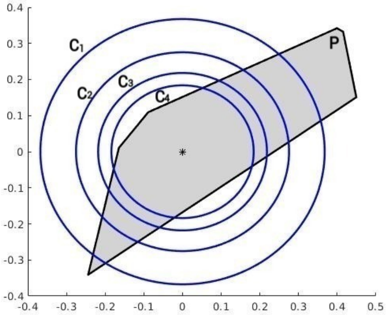
Volume algorithms parts

1. **M**ultiphase **M**onte **C**arlo (MMC)
   e.g. Sequence of balls, Annealing of functions
2. Sampling via geometric random walks
   e.g. grid-walk, ball-walk, hit-and-run, billiard walk

Notes:

- MMC (1) at each phase solves a sampling problem (2)
- geometric random walks are (most of the times) Marcov chains where each "event" is a d-dimensional point
- Algorithmic complexity is polynomial in d [Dyer, Frieze, Kannan'91]

Multiphase Monte Carlo



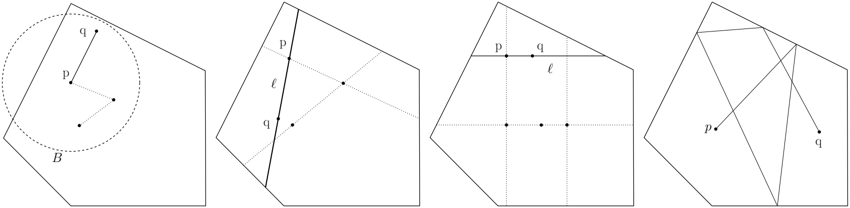
- Sequence of convex bodies $C_1 \supseteq \cdots \supseteq C_m$ intersecting P, then:

$$\mathrm{vol}(P) = \mathrm{vol}(P_m)\frac{\mathrm{vol}(P_{m-1})}{\mathrm{vol}(P_m)}\cdots\frac{\mathrm{vol}(P_1)}{\mathrm{vol}(P_2)}\frac{\mathrm{vol}(P)}{\mathrm{vol}(P_1)}$$

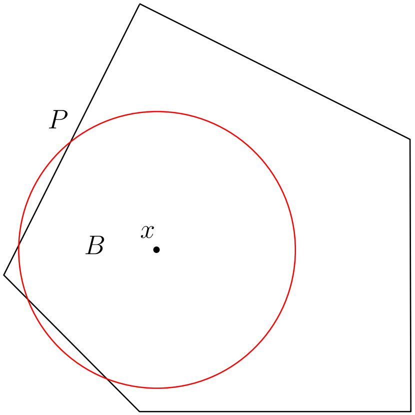
  where $P_i = C_i \cap P$ for $i = 1, \ldots, m$.
- Estimate ratios by sampling.

Four random walks

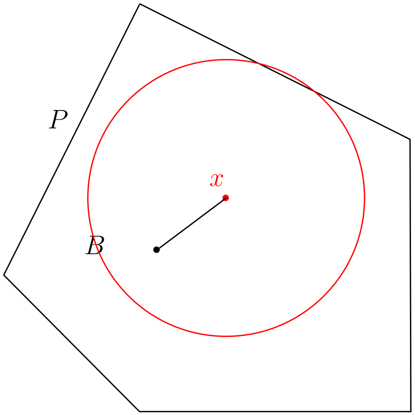
- Ball walk
- Random directions hit and run (rdhr)
- Cooridnate directions hit and run (cdhr)
- Billiard walk



Ball walk



Ball walk



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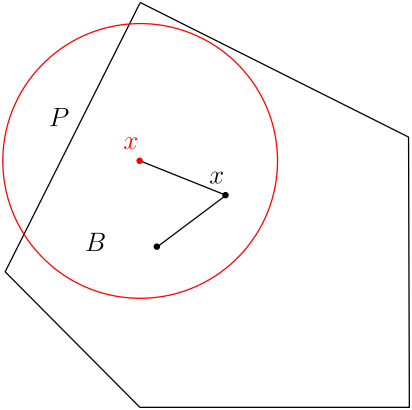

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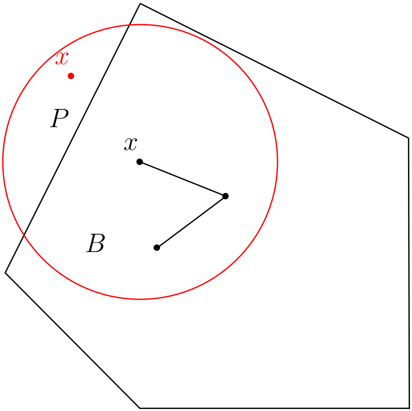

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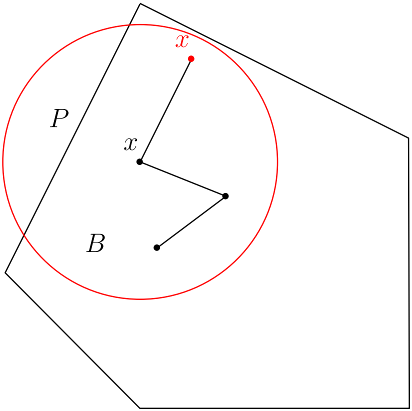
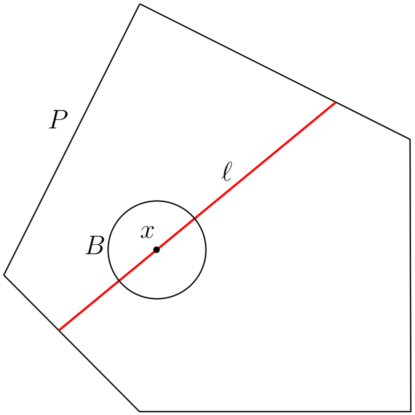


Random directions hit and run



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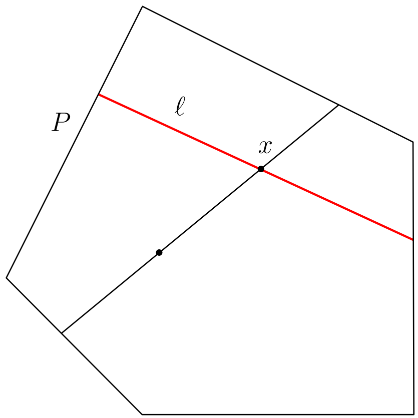

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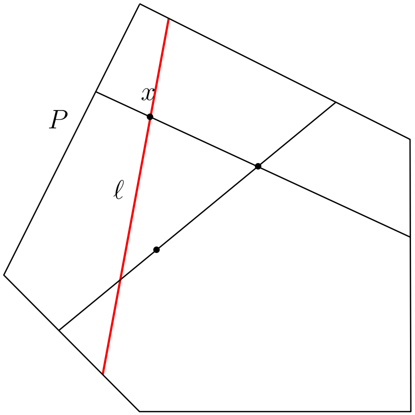
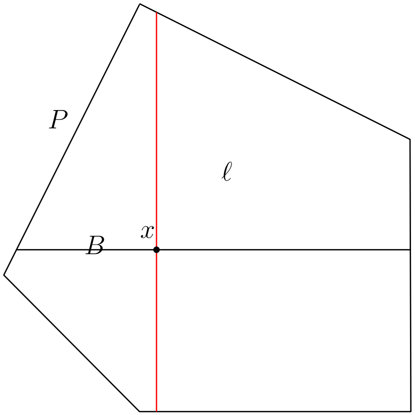


Coordinate directions hit and run



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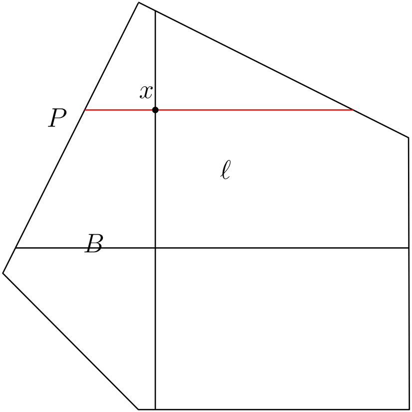

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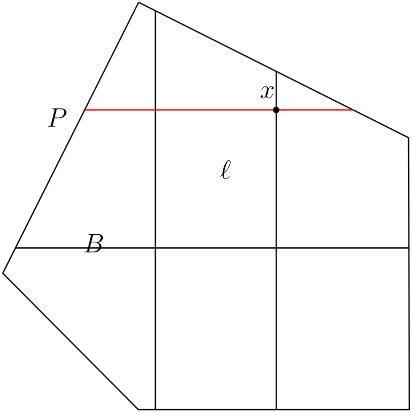

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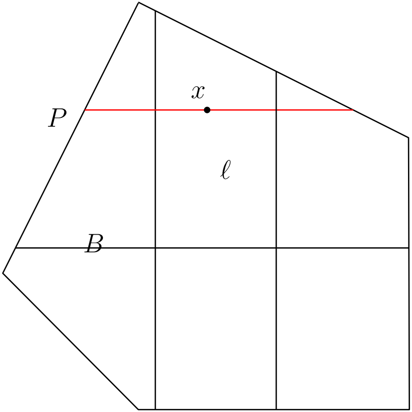
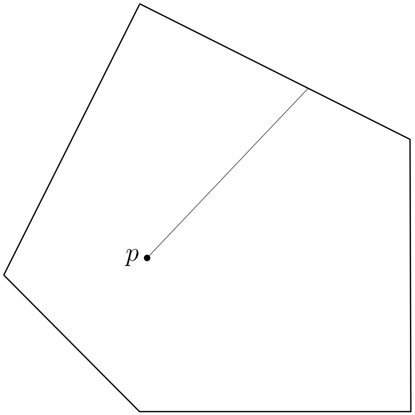


Billiard walk



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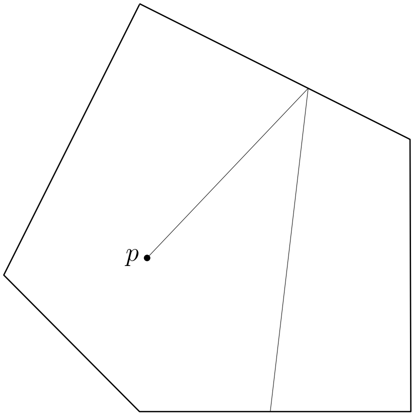

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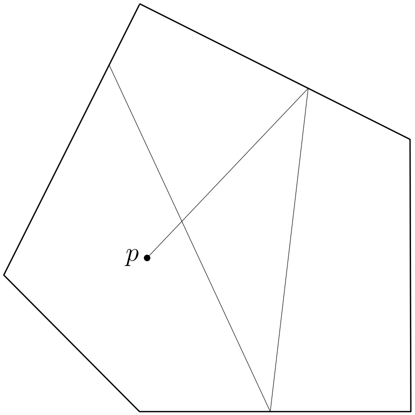

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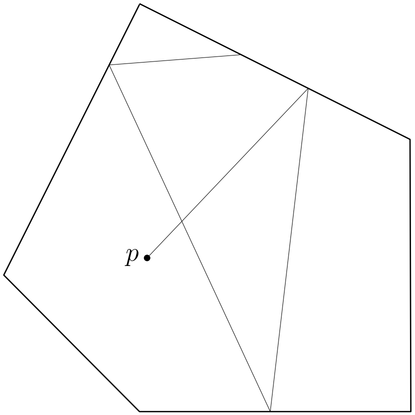

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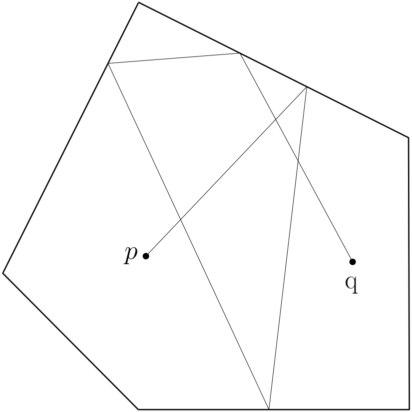

State-of-the-art

Theory:

Authors-Year	Complexity (oracle steps)	Algorithm
[Dyer, Frieze, Kannan'91]	$O^*(d^{23})$	Seq. of balls + grid walk
[Kannan, Lovasz, Simonovits'97]	$O^*(d^5)$	Seq. of balls + ball walk + isotropy
[Lovasz, Vempala'03]	$O^*(d^4)$	Annealing + hit-and-run
[Cousins, Vempala'15]	$O^*(d^3)$	Gaussian cooling (* well-rounded)
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Software:

1. [Emiris, F'14] Sequence of balls + coordinate hit-and-run
2. [Cousins, Vempala'16] Gaussian cooling + hit-and-run
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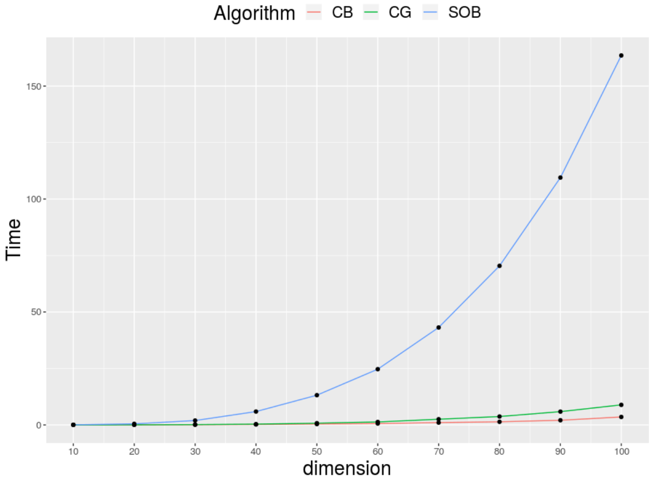
Notes:

- (2) is (theory + practice) faster than (1)
- (1),(2) efficient only for H-polytopes
- (3) efficient also for V-,Z-polytope, non-linear convex bodies
- C++ implementation of (2) $\times$10 faster than original (MATLAB)

Performance

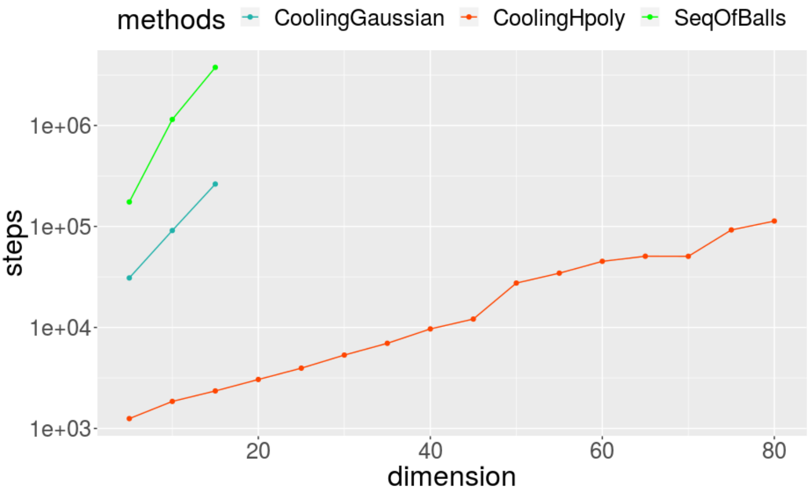
H-polytopes



Sequence Of Balls (SOB), Cooling Gaussians (CG), Cooling Balls (CB)

Performance

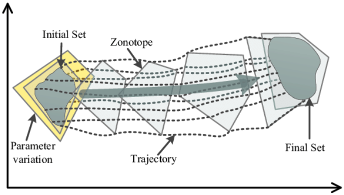
Z-polytopes

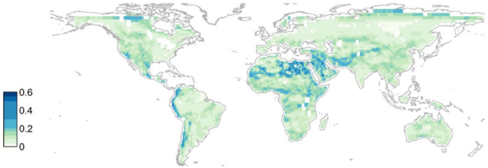


Applications

Biogeography & engineering

- Volume of zonotopes is used to test methods for order reduction which is important in several areas: autonomous driving, human-robot collaboration and smart grids [Althoff et al.]
- Volumes of intersections of polytopes are used in bio-geography to compute biodiversity and related measures e.g. [Barnagaud, Kissling, Tsirogiannis, F, Villeger, Sekercioglu'17]





Applications

Combinatorics & Machine Learning

- Volume can be used for counting linear extensions of a partially ordered set. This arises in sorting [Peczarski 2004], sequence analysis [Mannila et al.2000], convex rank tests [Morton et al.2009], preference reasoning [Lukasiewicz et al.2014], partial order plans [Muise et al.2016], learning graphical models [Niinimäki et al. 2016] See also [Talvitie et al.AAAI'2018]
- *e.g.* elements a, b, c
  partial order $a < c$
  3 linear extensions: abc, acb, bac

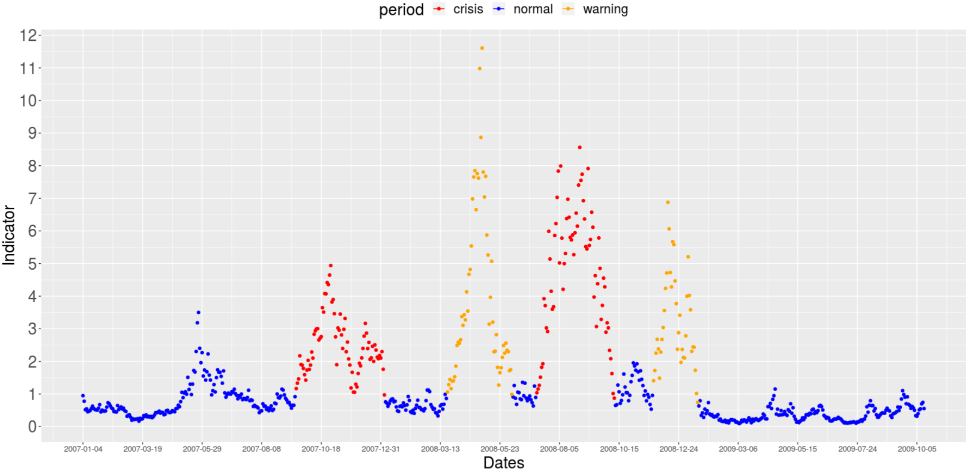
- In Weighted Model Integration (WMI), given is a SMT formula and a weight function, then we want to compute the weight of the SMT formula.
- e.g. SMT formula:

$$(A \;\&\; (X > 20) \mid (X > 30)) \;\&\; (X < 40)$$

  Boolean formula + comparison operations. Let X has a weight function of $w(X) = X^2$ and $w(A) = 0.3$.
- WMI answers the question of the weight of this formula i.e. integration of a weight function over convex sets.
- [P.Z.D. Martires et al.2019]

Applications in finance

When is the next financial crisis?



Cales, Chalkis, Emiris, Fisikopoulos - Practical volume computation of structured convex bodies, and an application to modeling portfolio dependencies and financial crises, SoCG 2018

VolEsti package: sampling and volume estimation

https://github.com/GeomScale/volume_approximation

- C++, R-interface, python bindings (limited)
- open source, LGPL3
- since 2014, CGAL (not any more), Eigen, LPSolve, Boost
- 3 volume algorithms, 4 sampling algorithms
- design: mix of obj oriented + templates
- C++11 dependence (mostly C++03)
- main developers: Vissarion Fisikopoulos, Tolis Chalkis

VolEsti package

- R package on CRAN
  https://cran.r-project.org/package=volesti
- Documentation
  https://github.com/GeomScale/volume_approximation/blob/develop/README.md

How to contribute (github account is needed):

- first star and fork the repo :D
- then follow the contribution tutorial

VolEsti on Google Summer of Code 2020

- Applying this year as an organization for GSoC 2020.
- See this wiki for more details.
- Tentative plan:
  - MCMC integration
  - sampling for structural biology
  - randomized algorithms for convex optimization
  - sampling in higher dimensions (reach the thousands)
- Communication channels: gitter, `geomscale-gsoc@googlegroups.com`

VolEsti tutorial

https://vissarion.github.io/tutorials/volesti_tutorial_pydata.html

CRAN mode (recommended!)

- in Rtudio install CRAN package "volesti"
- follow this https://github.com/GeomScale/volume_approximation/blob/tutorial/tutorials/volesti_tutorial.Rmd

develop mode

- `git clone git@github.com:GeomScale/volume_approximation.git`
- `git checkout tutorial`
- in Rtudio open `R-proj/volesti.Rproj` and then click `build source Package` and then `Install and Restart` in `Build` tab at the menu bar.
- follow this https://github.com/GeomScale/volume_approximation/blob/tutorial/tutorials/volesti_tutorial_1_1_0.Rmd