High-dimensional sampling and volume computation

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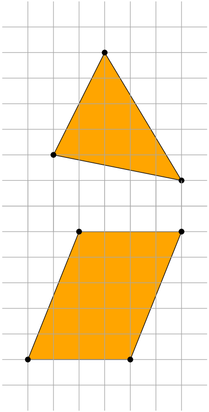
KULeuven, 30/01/2020

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.



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

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

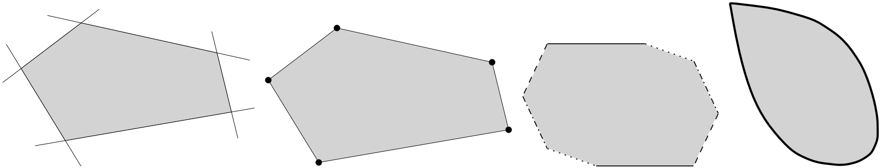
Convex bodies

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

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

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

LMI : $P = A_0 + x_1 A_1 + x_2 A_2 + \cdots + x_d A_d \succeq 0$, 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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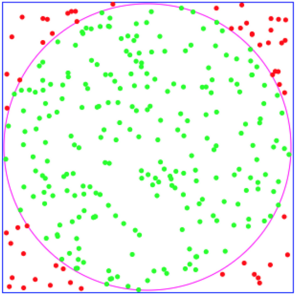
- Triangulation (or sign decomposition) methods – exponential size in d
- Sampling/rejections techniques (sample from bounding box) fail in high dimensions



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

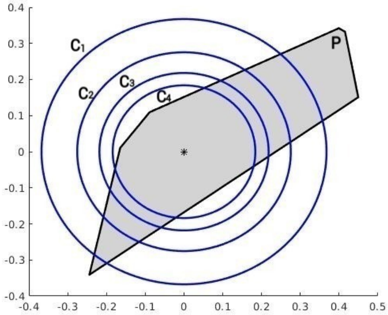
Volume algorithms parts

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 computes a ratio of integrals or volumes via sampling (2)
- geometric random walks are Markov chains where each "event" is a d-dimensional point
- Algorithmic complexity is polynomial in d [Dyer, Frieze, Kannan'91]

Multiphase Monte Carlo



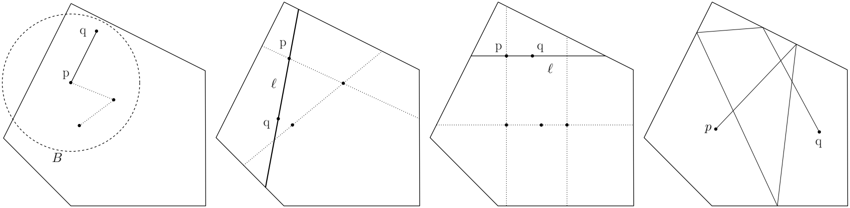
- Sequence of convex bodies $C_1 \supseteq \cdots \supseteq C_m$ intersecting P, then:

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

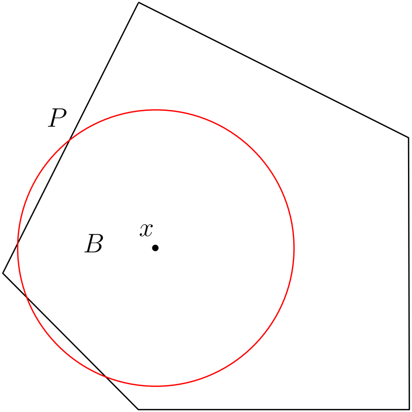
  where $P_i = C_i \cap P$ for $i = 1, \ldots, m$.
- Estimate ratios by sampling.

Four random walks

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



Ball walk



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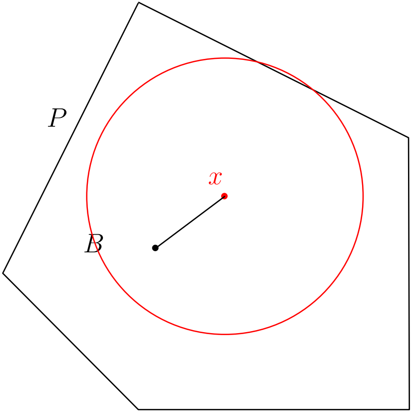

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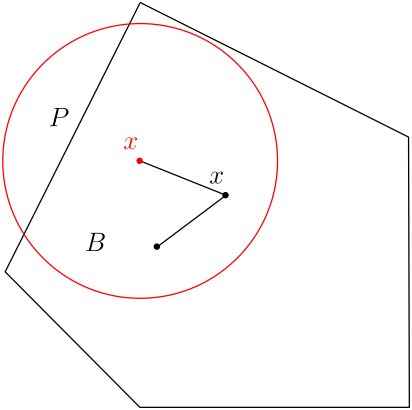

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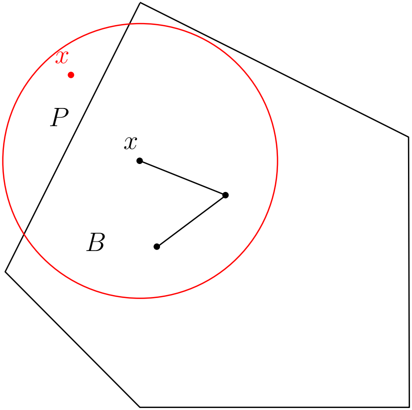

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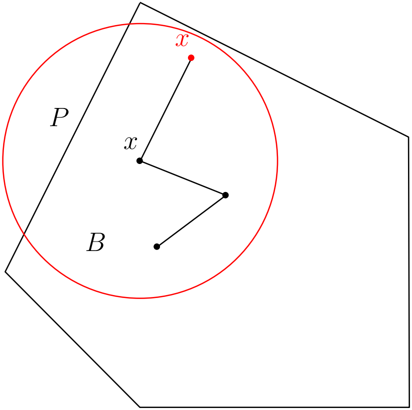
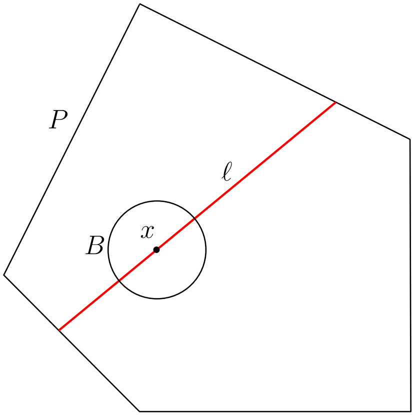


Random directions hit and run



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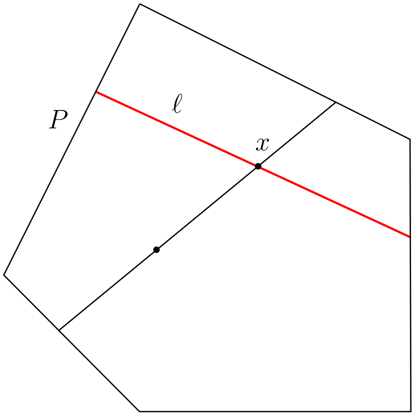

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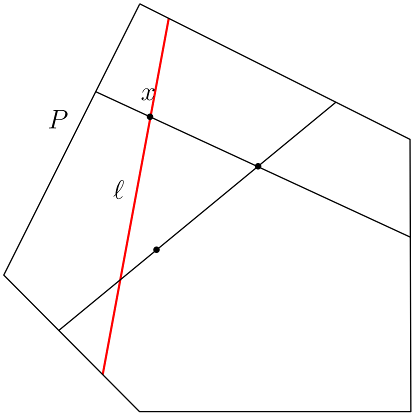
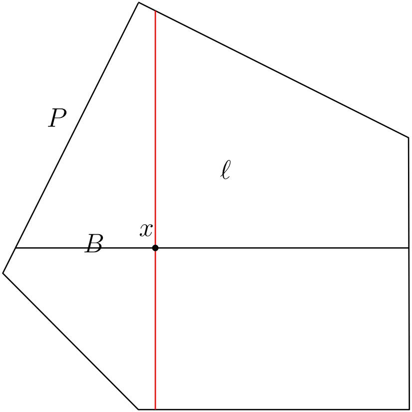


Coordinate directions hit and run



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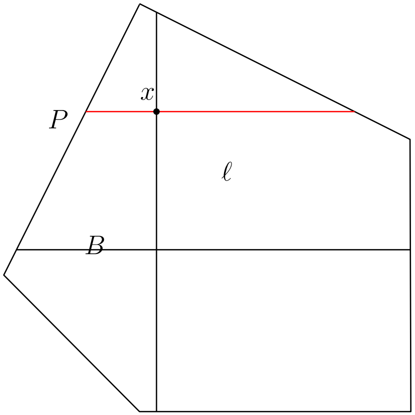

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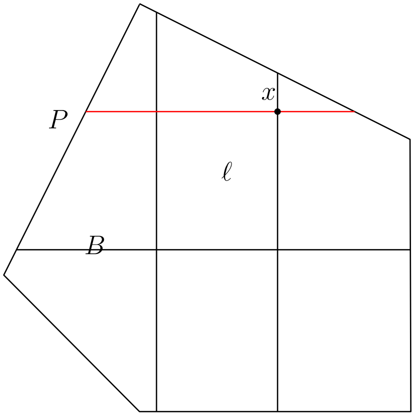

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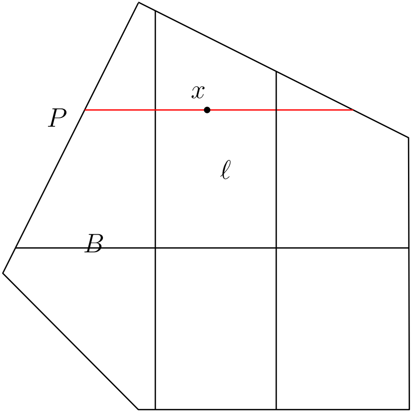
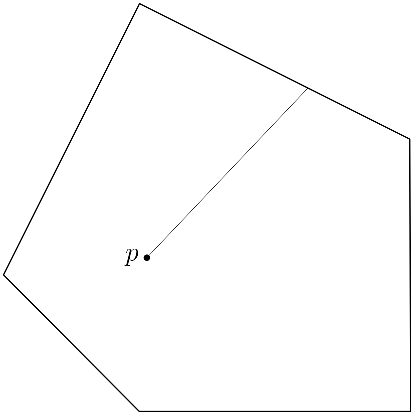


Billiard walk



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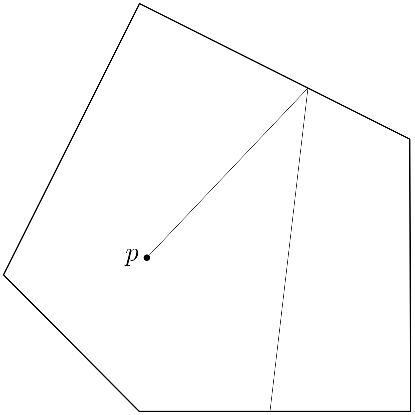

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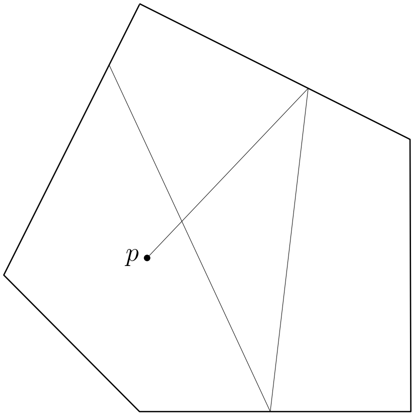

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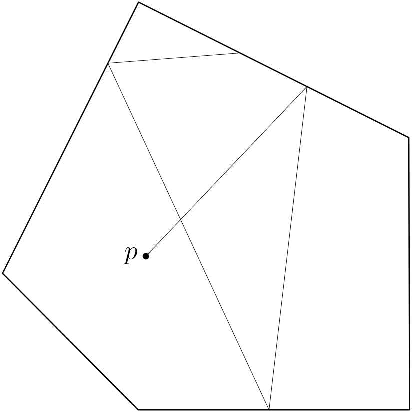

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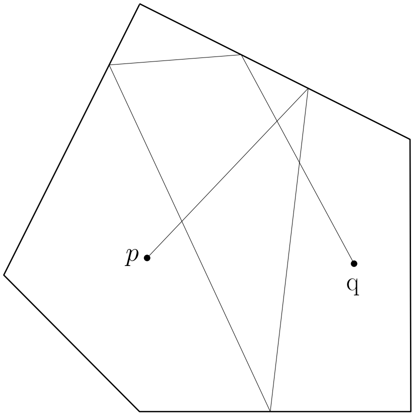

Complexity of random walks

Year & Authors	Random walk	Mixing time	cost per step
[Berbee et al.'87]	Coordinate Hit-and-Run	??	$O(m)$
[Lovasz et al.'06]	Hit-and-Run	$O^*(d^3)$	$O(md)$
[Kannan et al.'09]	Dikin walk	$O(md)$	$O(md^2)$
[Polyak et al.'14]	Billiard walk	??	$O(mR + md)$
[Lee et al.'16]	Geodesic walk	$O(md^{3/4})$	$O(md^2)$
[Lee et al.'17]	Ball walk	$O^*(d^{2.5})$	$O(md)$
[Chen et al.'17]	Vaidya walk	$O(m^{1/2}d^{3/2})$	$O(md^2)$
[Lee et al.'17]	Riemmanian HMC	$O(md^{2/3})$	$O(md^2)$
[Chevallier et al.'18]	HMC with reflections	??	$O(md)$
[Mangoubi et al.'19]	sublinear Ball walk	$O(d^{4.5})$	$\sim O(m)$

- Mixing times are unrealistically high for practical purposes
- Billiard walk, CDHR and HMC with reflections seems the most efficient in practice but there is not guarantee on the mixing time

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
3. [Chalikis, Emiris, F'20] Convex body annealing + billiard walk

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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)

Convex body annealing

New features

- MMC using convex bodies (balls or H-polytopes that "fit well" and are "easy" to sample from)
- New annealing method. Bound each ratio $\mathrm{vol}(P_{i+1})/\mathrm{vol}(P_i)$ to a given interval with high probability thus reduces the sequence of bodies
- Billiard walk (constant number of steps in practice)

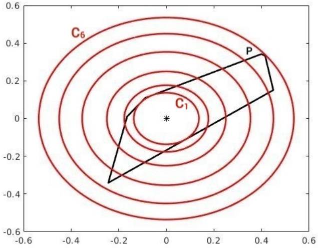
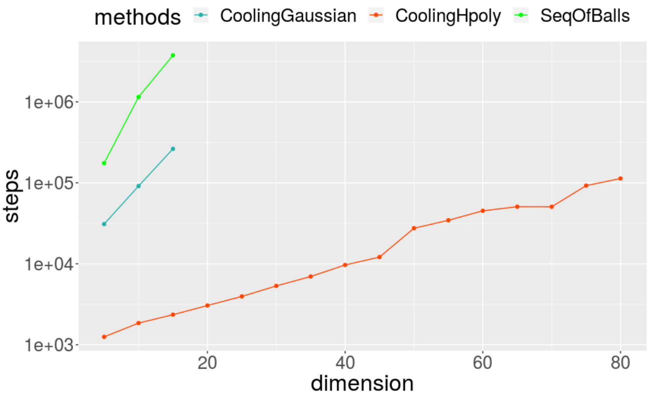


Figure. Sequence of balls vs. ball annealing

Comparison with state-of-the-art

Zonotopes

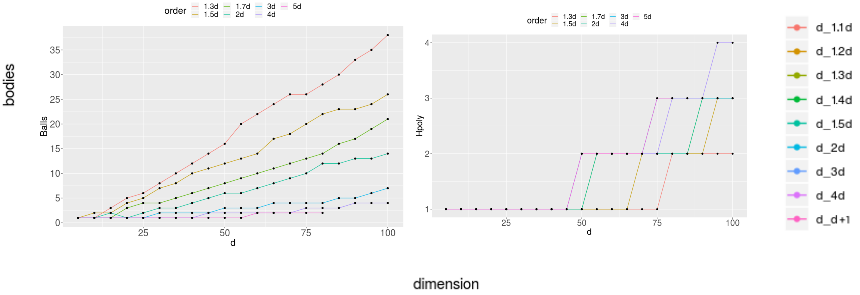


The number of steps for random zonotopes of order 2

- Our method is asymptotically better
- `CoolingGaussian` and `SeqOfBalls` takes $> 2hr$ for $d > 15$.
- for higher orders the difference is larger

Zonotopes

Number of phases



Two types of bodies: balls (left) symmetric H-polytopes (right)

- For low order (i.e. $\#generators/d$) zonotopes, ≤ 4, the number of bodies is smaller than the case of using balls
- For balls the number of phases reduces as the order increases for a fixed dimension

Zonotopes

Performance

Experimental results for zonotopes.						
z-d-k	*Body*	*order*	*Vol*	*m*	*steps*	*time*(sec)
z-5-500	Ball	100	4.63e+13	1	0.1250e+04	22
z-20-2000	Ball	100	2.79e+62	1	0.2000e+04	1428
z-50-65	Hpoly	1.3	1.42e+62	1	1.487e+04	173
z-50-75	Hpoly	1.5	2.96e+66	2	1.615e+04	253
z-100-150	Hpoly	1.5	2.32+149	3	15.43e+04	2992
z-60-180	Hpoly	3	8.71e+111	2	5.059e+04	417
z-100-200	Hpoly	3	5.27e+167	3	15.25e+04	2515

- *z-d-k*: random zonotope in dimension d with k generators; *Body*: the type of body used in MMC; m: number of bodies in MMC
- Used to evaluate zonotope approximation methods in engineering [Kopetzki'17]

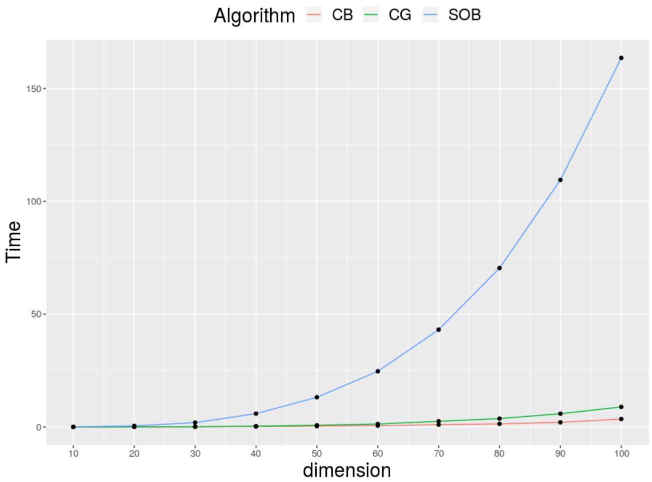
V-polytopes

P	Vol	m	steps	error	time(sec)	exact Vol	exact time
cross-60	1.27e-64	1	20.6e+03	0.08	60	−−	−−
cross-100	1.51e-128	2	94.2e+03	0.11	406	−−	−−
Δ-60	1.08e-82	10	77.4e+04	0.1	899	1.203-82	0.02
Δ-80	1.30e-119	13	187e+04	0.07	4140	1.39e-119	0.07
cube-10	1052.4	1	1851	0.03	54	−−	−−
cube-13	7538.2	1	2127	0.08	2937	−−	−−
rv-10-80	3.74e-03	1	0.185e+04	0.08	3	3.46e-03	7
rv-10-160	1.59e-02	1	0.140e+04	0.06	6	1.50e-03	59
rv-15-30	2.73e-10	1	0.235e+04	0.02	3	2.79e-10	2
rv-15-60	4.41e-08	1	0.235e+04	−−	6	−−	−−
rv-20-2000	2.89e-07	1	0.305e+04	−−	457	−−	−−
rv-80-160	5.84e-106	3	11.3e+04	−−	891	−−	−−
rv-100-200	1.08e-141	4	24.5e+04	−−	2312	−−	−−

time: the average time in seconds; ex. Vol: the exact volume; ex. time: the time in seconds for the exact volume computation i.e. `qhull` in `R` (package `geometry`); m is the number of phases. $--$ implies that the execution failed due to memory issues or exceeded 1 hr.

Performance

H-polytopes

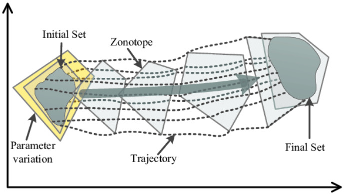


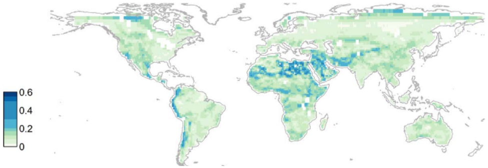
Sequence Of Balls (SOB), Cooling Gaussians (CG), Cooling Balls (CB)

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

Applications
Computing integrals for AI

- 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:

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

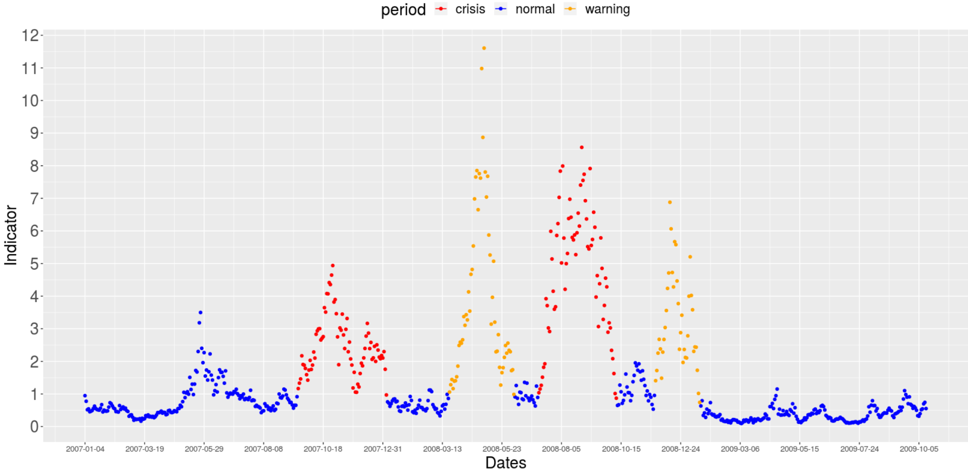
Boolean formula + comparison operations. Let X has a weight function of $w(X) = X^2$ and $w(A) = 0.3$.

- 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, Apostolos 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

Thank you!