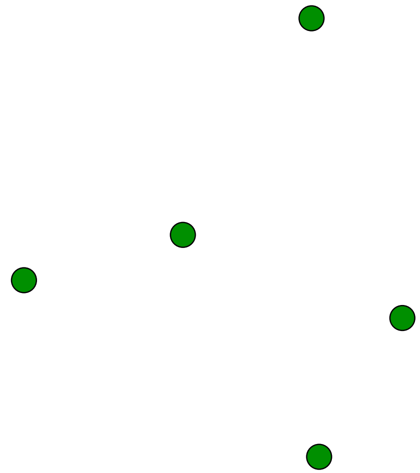
Fast Smallest-Enclosing-Ball Computation in High Dimensions

Martin Kutz
FU Berlin

joint work with Bernd Gärtner and Kaspar Fischer, ETH Zürich

The Smallest Enclosing Ball

given: finite point set $\color{green}{S}$ in $\mathbb{R}^d$



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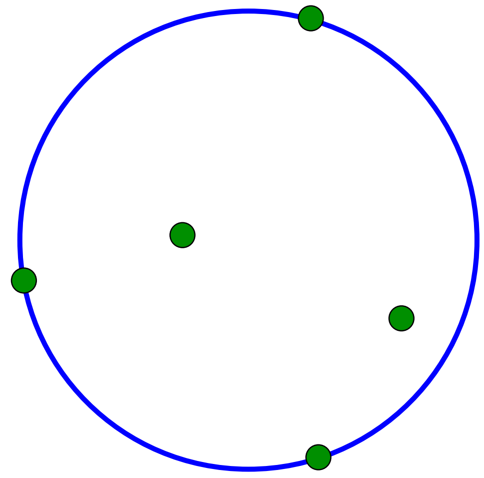
given: finite point set S in $\mathbb{R}^d$

wanted: smallest ball B
$= B(c, r) := \{x : \|x - c\| \leq r\}$
containing S



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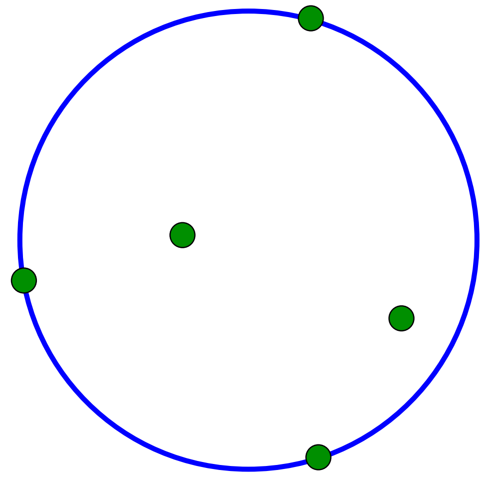

Call this unique minimal B the *smallest enclosing ball* of S, denoted $\mathrm{seb}(S)$.

Applications

- visibility culling and bounding sphere hierarchies in 3D computer graphics
- clustering (e.g. for support-vector machines) — many dimensions
- nearest neighbor search

Previous Work

- Welzl proposed randomized combinatorial algorithm, implemented by Gärtner, fast for $d \leq 30$, impractical above.

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- Quadratic-programming approach by Gärtner & Schönherr, uses exact arithmetic, up to $d = 300$.
- General-purpose QP-solver CPLEX, solves $d \leq 3{,}000$.
- Zhou, Toh, and Sun use interior-point method to find approximate solution, up to $d = 10{,}000$.
- Kumar, Mitchell, Yildrum compute approximation with core sets, results given up to $d = 1{,}400$.

Our Algorithm

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- similar to LP simplex-method
- equipped with pivot scheme to avoid cycling
- C++ floating-point implementation: solves several thousand points in a few thousand dimensions
- idea not completely new; Hopp & Reeve presented similar algorithm but without proofs, some details unclear, 3D only

The Basic Idea: Deflating a Ball

Iteratively shrink an enclosing Ball $B = B(c, T)$ represented by

- a current center c,
- an affinely independent subset $T \subseteq S$ of points at a common distance from c — the *support set*

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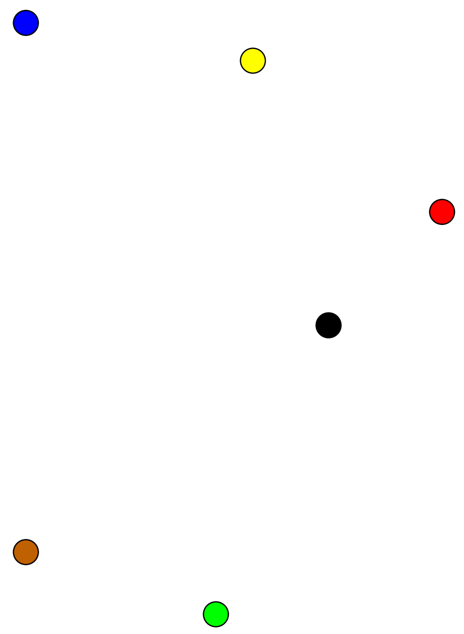
Invariants:

$$\begin{aligned} T &\subset \partial B(c, T) \\ S &\subset B(c, T) \end{aligned}$$

2D "Example"



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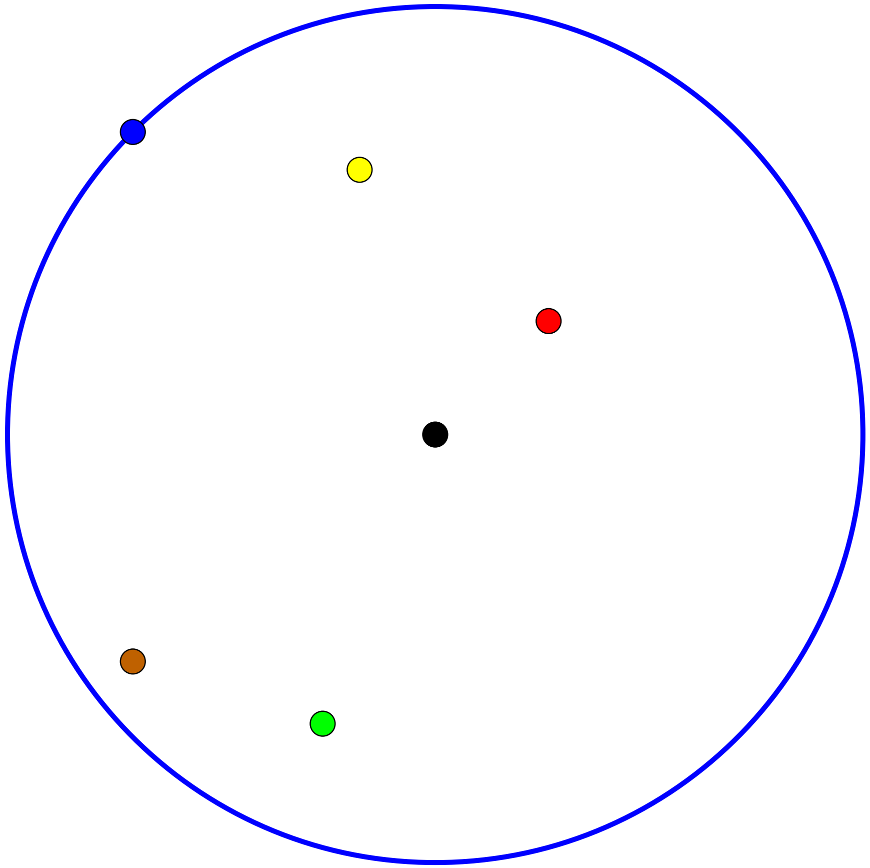

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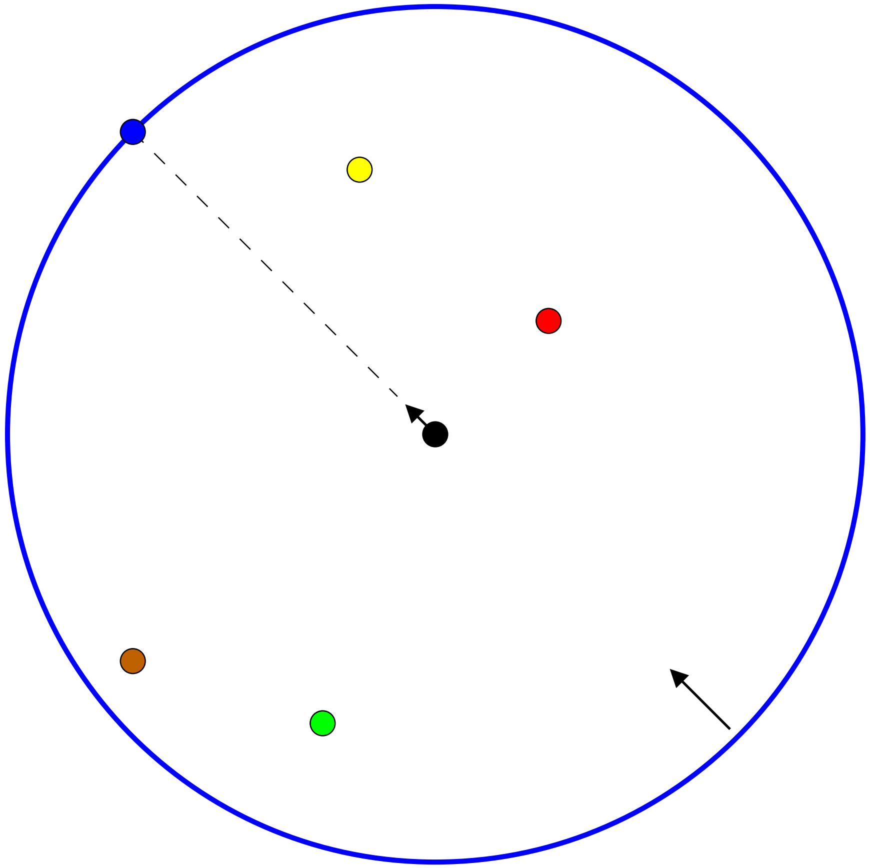

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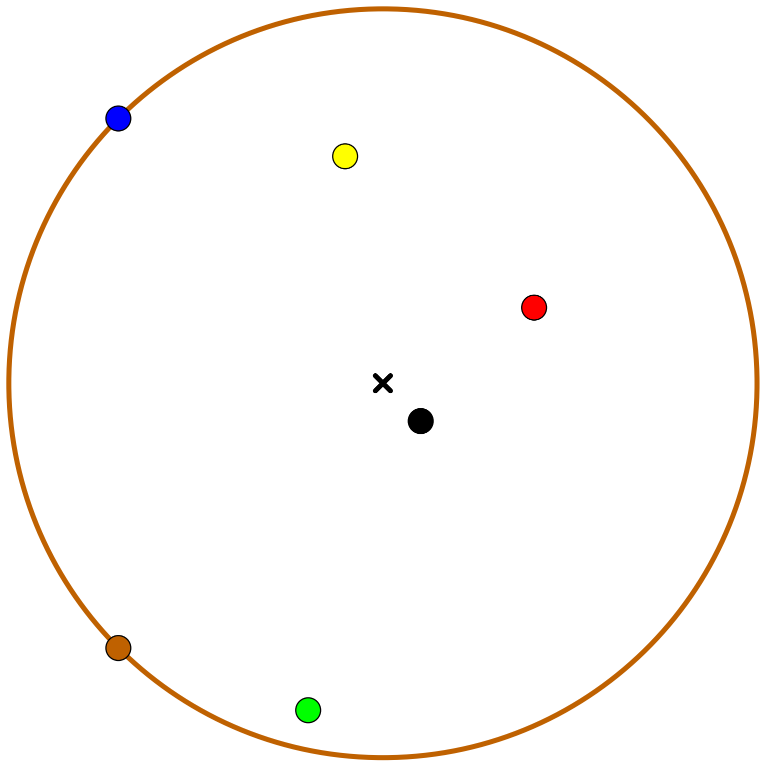

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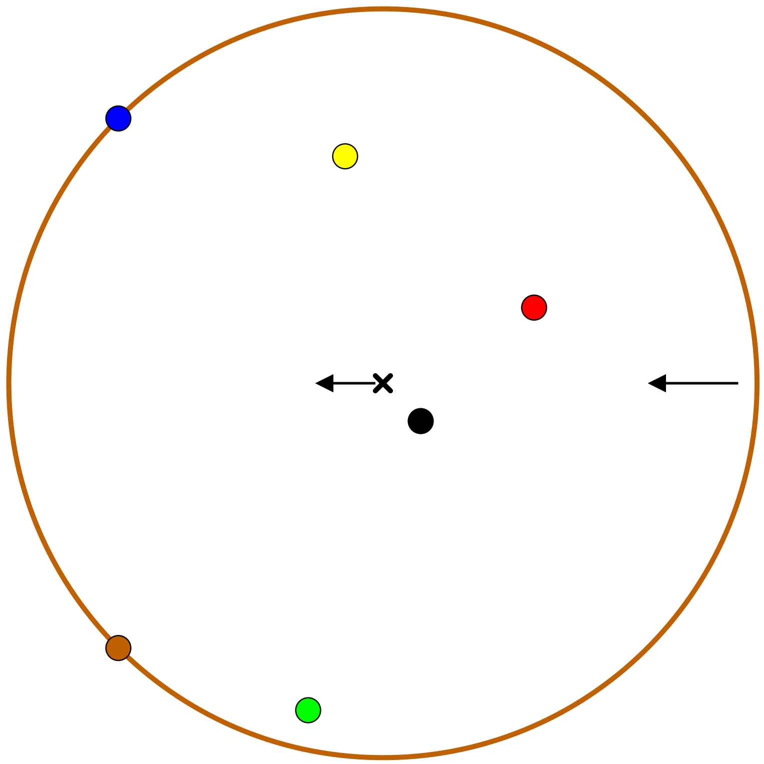

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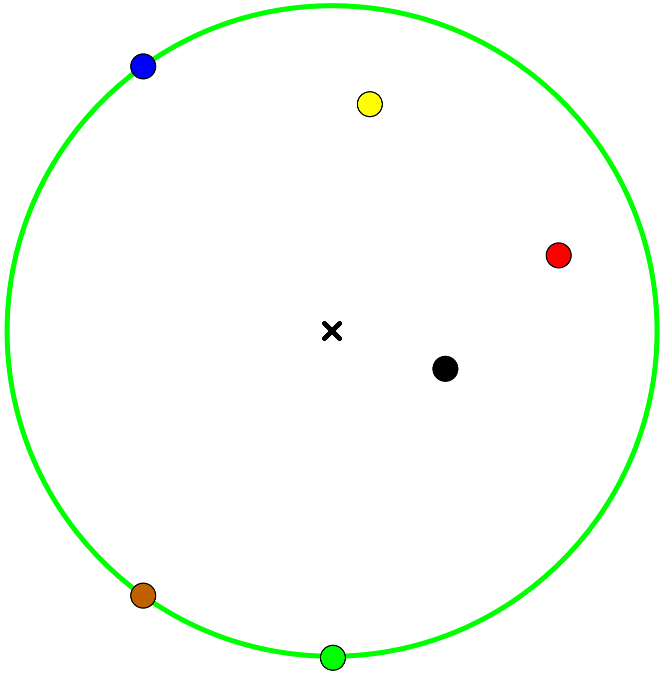

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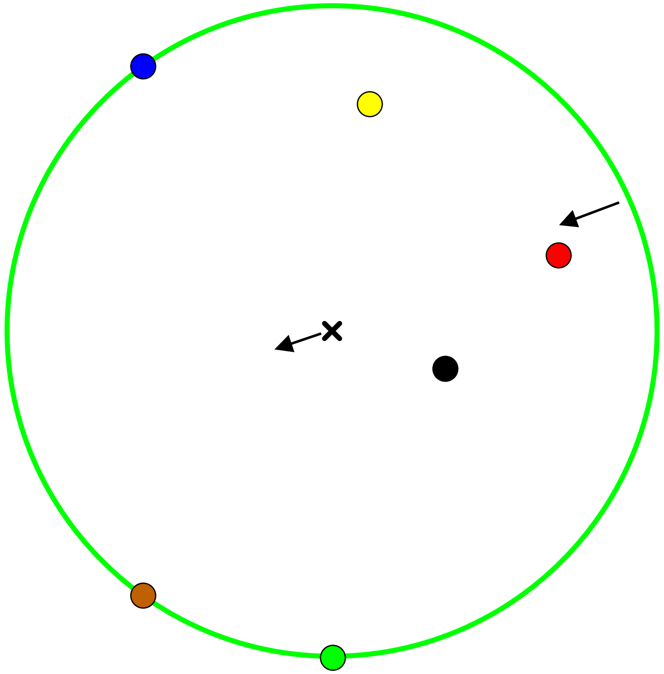

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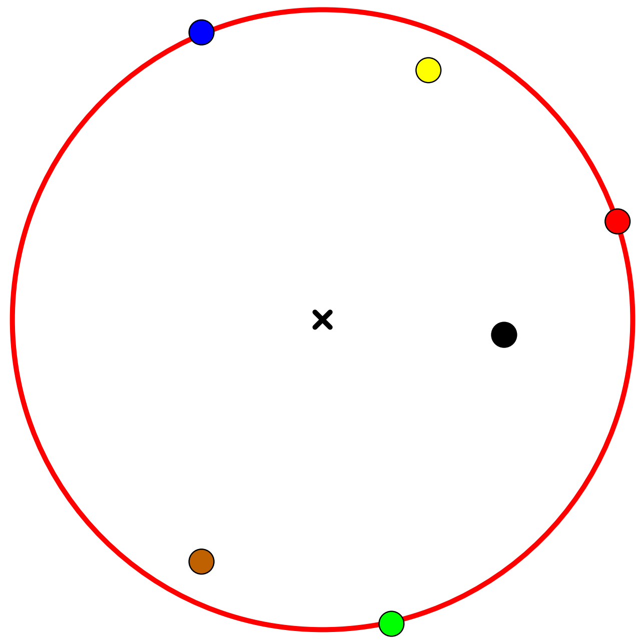
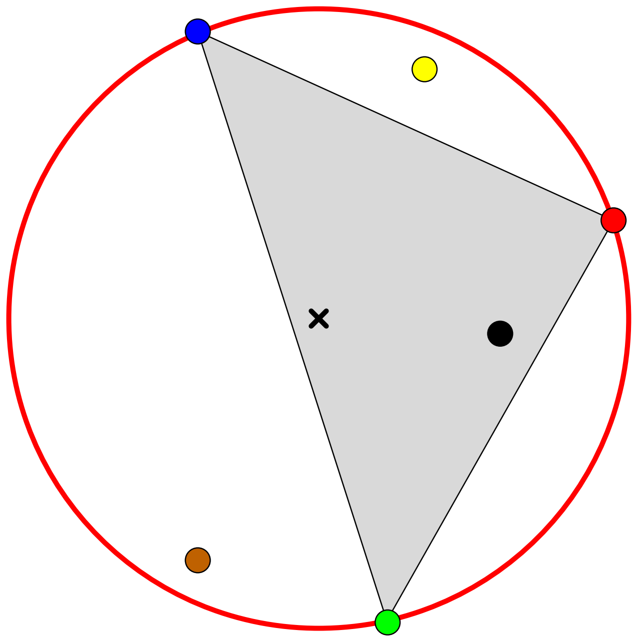


Termination Criterion



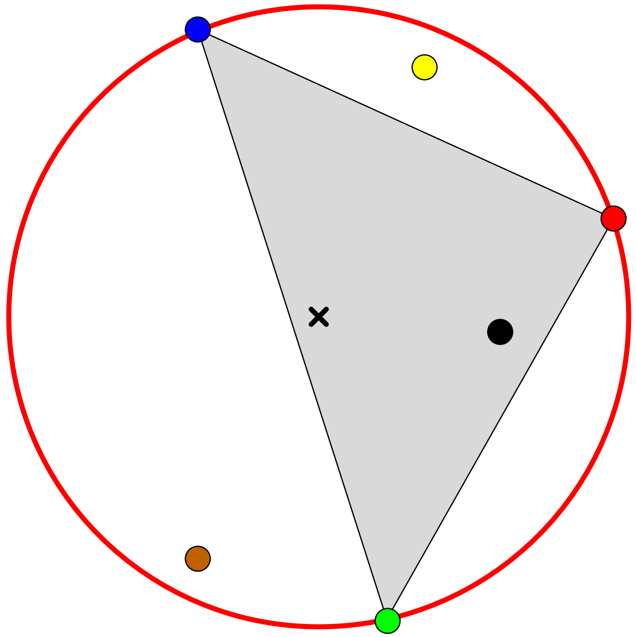
Termination Criterion

Lemma (Seidel).

Let T be set of points on boundary of some ball B with center c.

Then

$$B = \mathrm{seb}(T) \quad \Longleftrightarrow \quad c \in \mathrm{conv}(T).$$



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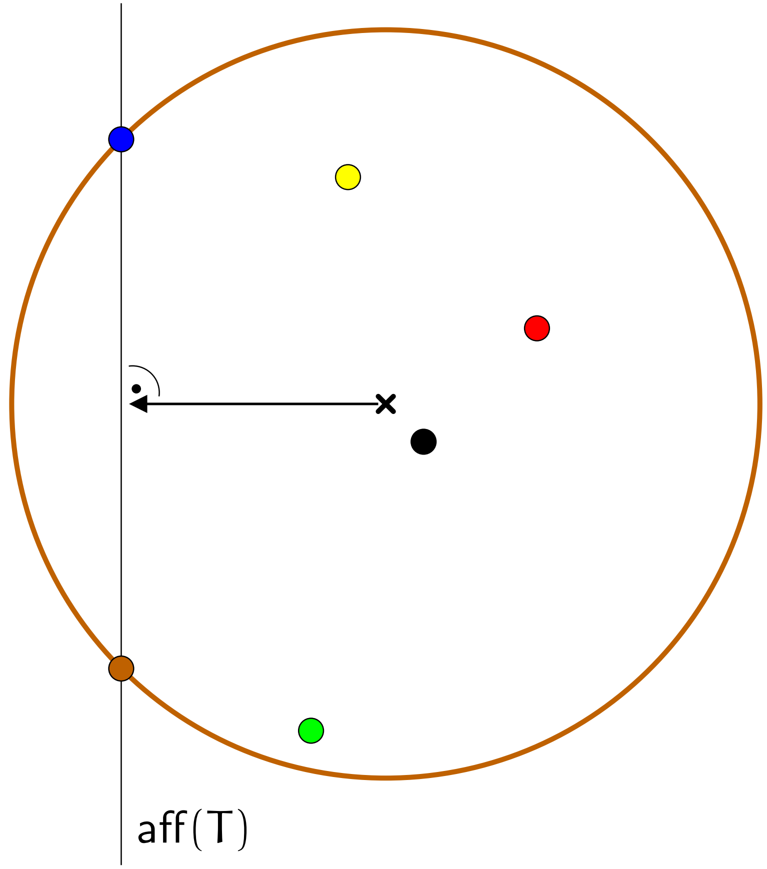
Moving Step [Precondition $c \notin \mathrm{aff}(T)$]

Move c orthogonally towards $\mathrm{aff}(T)$,
i.e., heading for closest point in $\mathrm{aff}(T)$.



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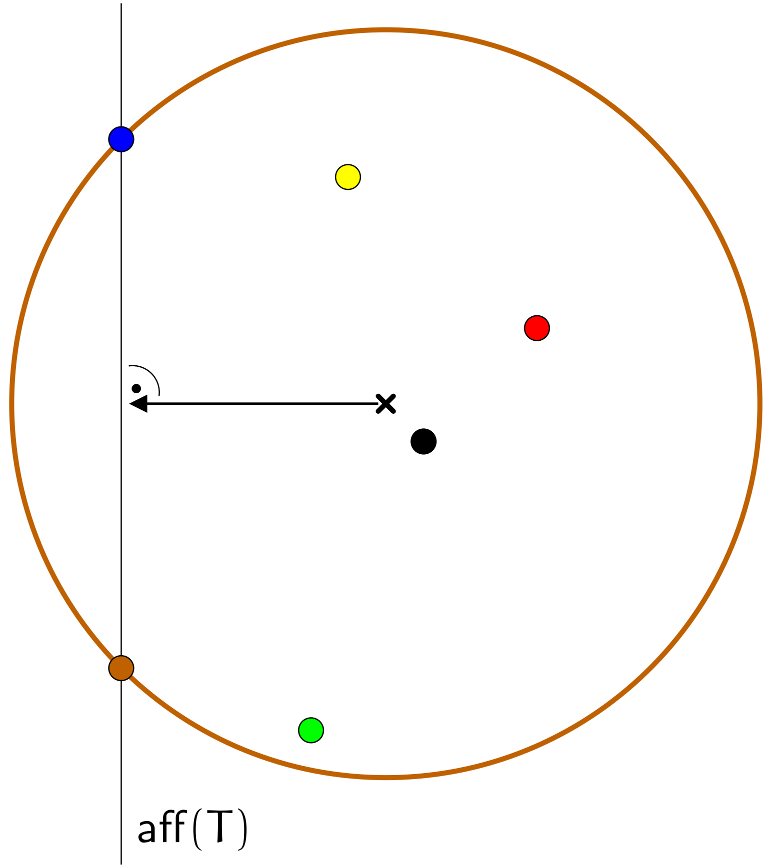
Especially, our target point is the center of the unique sphere through T in $\text{aff}(T)$, called circumcenter of T.



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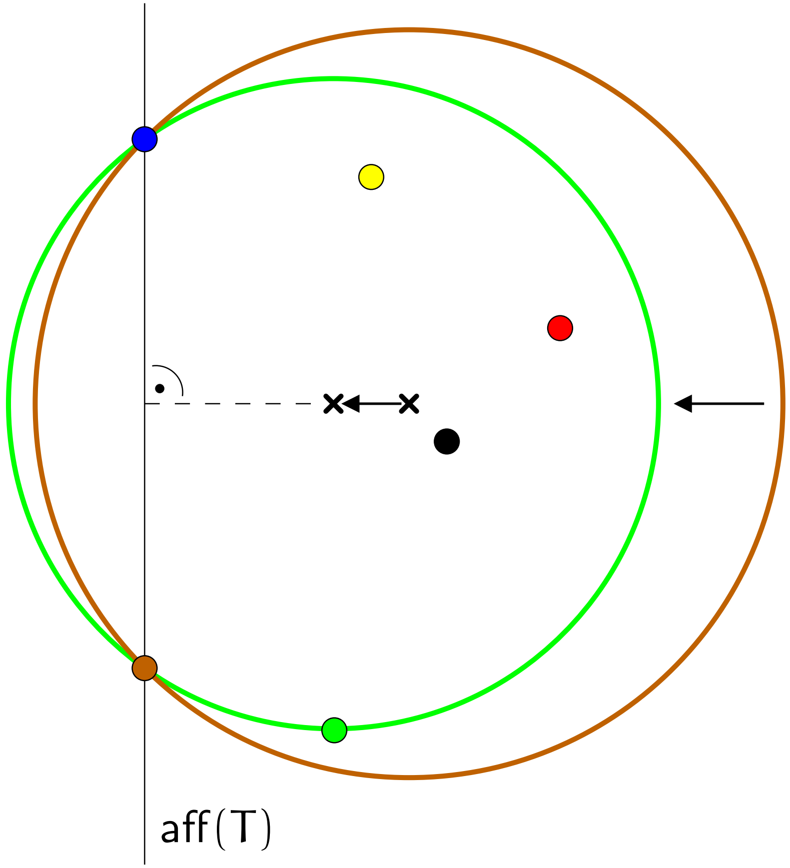
Stop movement when shrinking boundary
hits new point of S, insert it into T;
otherwise just stop with c in $\mathrm{aff}(T)$.



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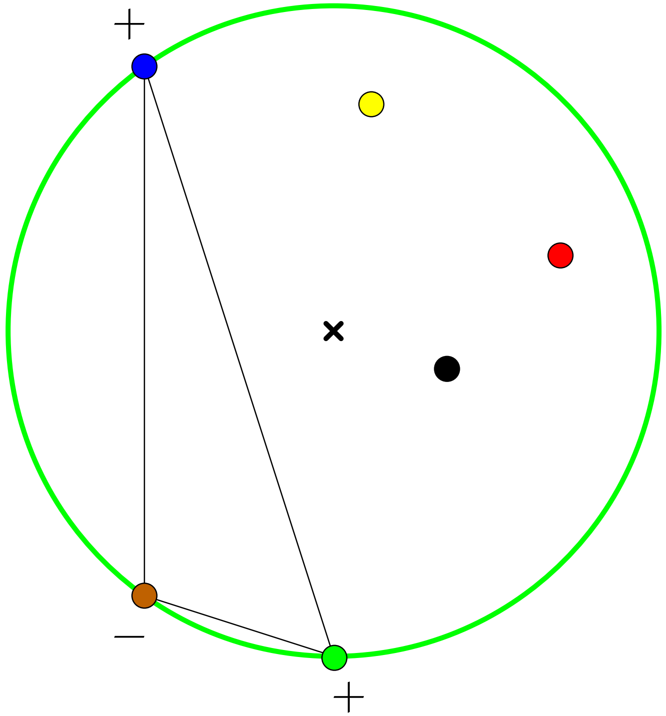

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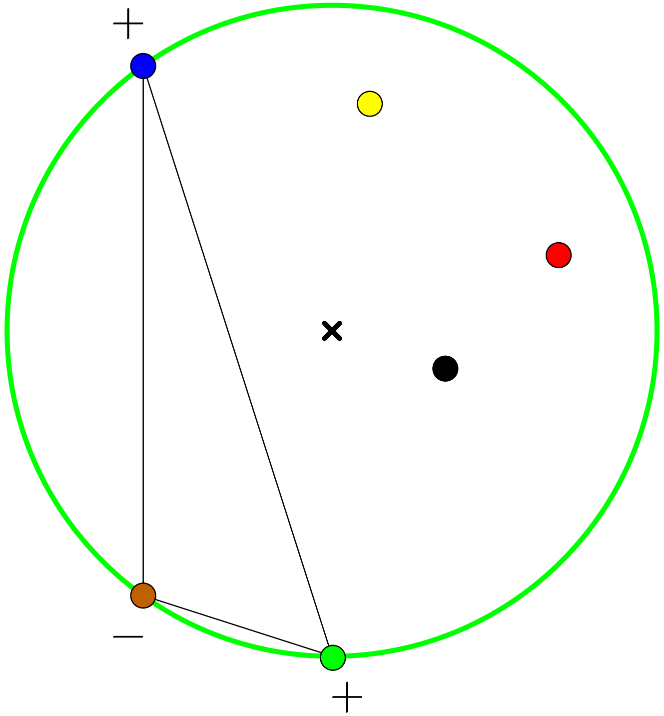

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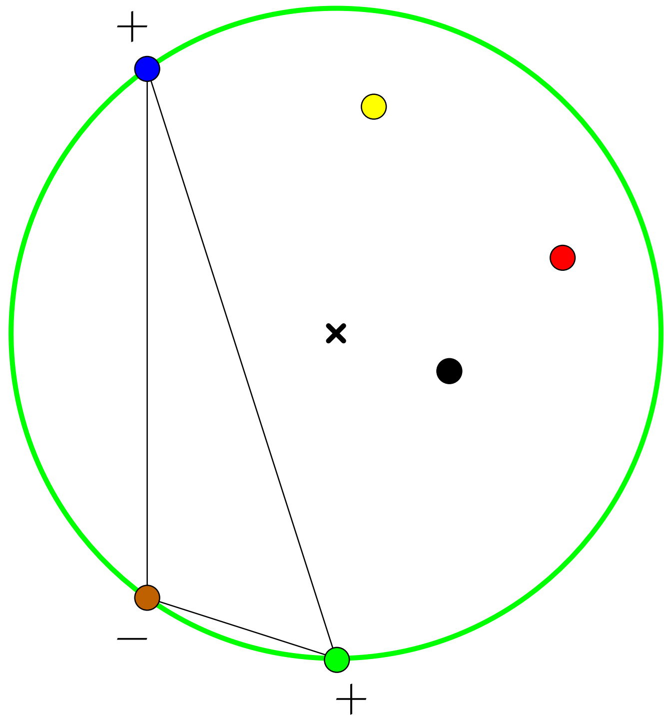
Afterwards, c lies outside the new $\mathrm{aff}(T)$, so it we can move again.
The next move will *not* recollect the dropped point.



The Whole Algorithm

$\mathsf{c} :=$ any point of S;
$\mathsf{T} := \{p\}$, with some $p \in S$ at maximal distance from c;

while $\mathsf{c} \notin \mathsf{conv}(\mathsf{T})$ **do**
  [Invariant: $B(\mathsf{c}, \mathsf{T}) \supset \mathsf{S}$, $\partial B(\mathsf{c}, \mathsf{T}) \supset \mathsf{T}$, and T affinely independent]

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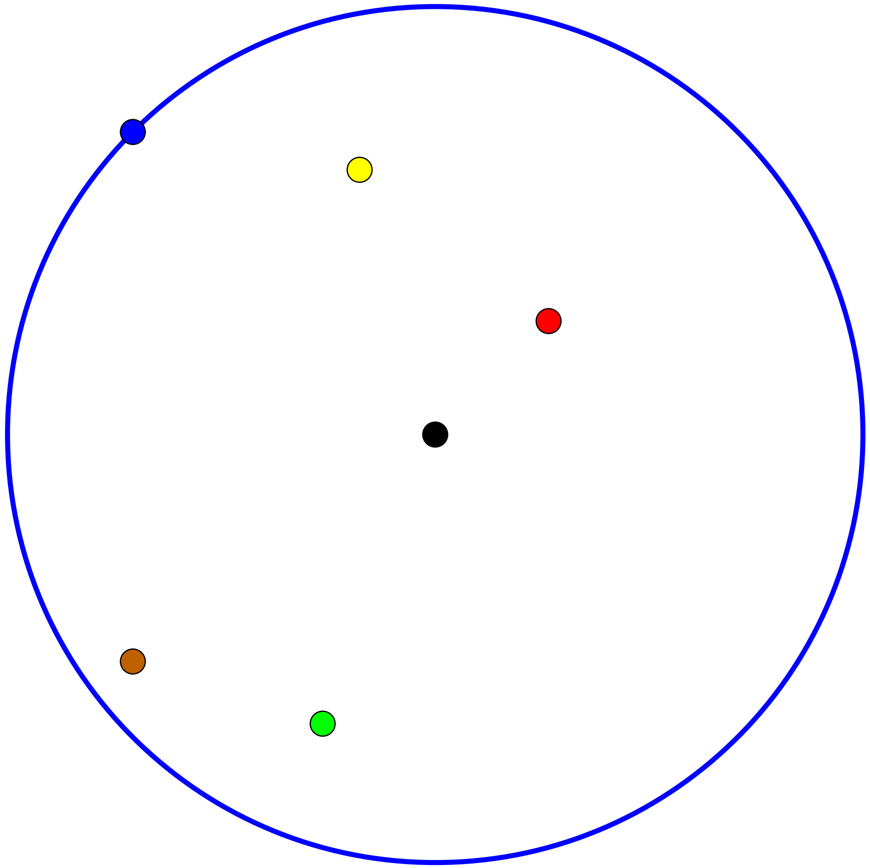

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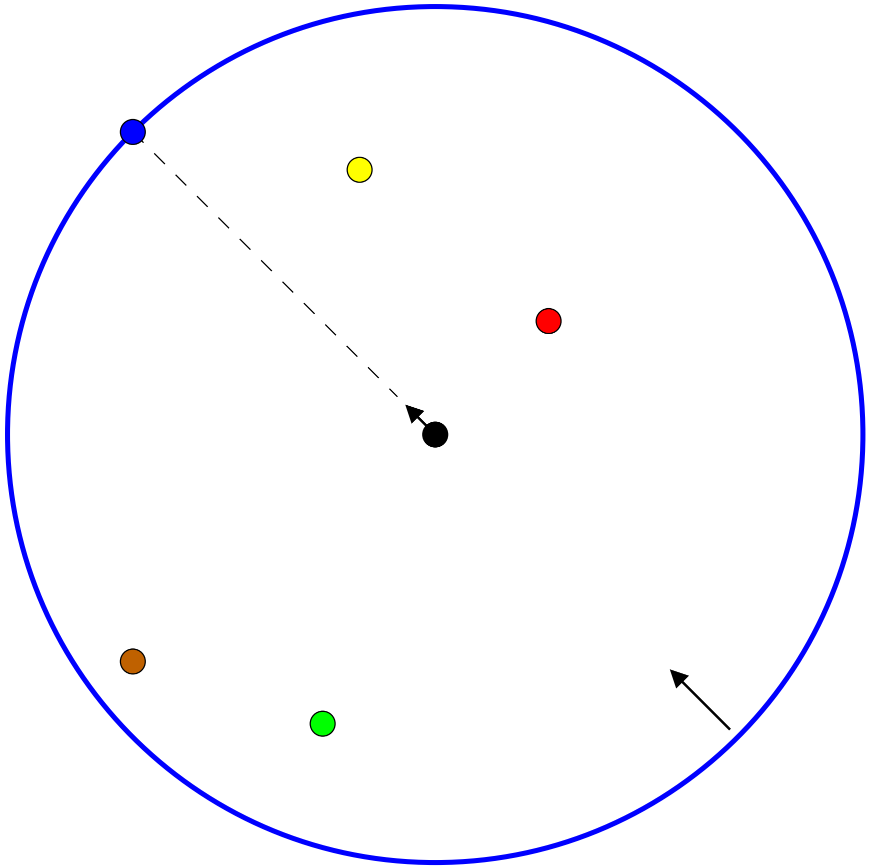

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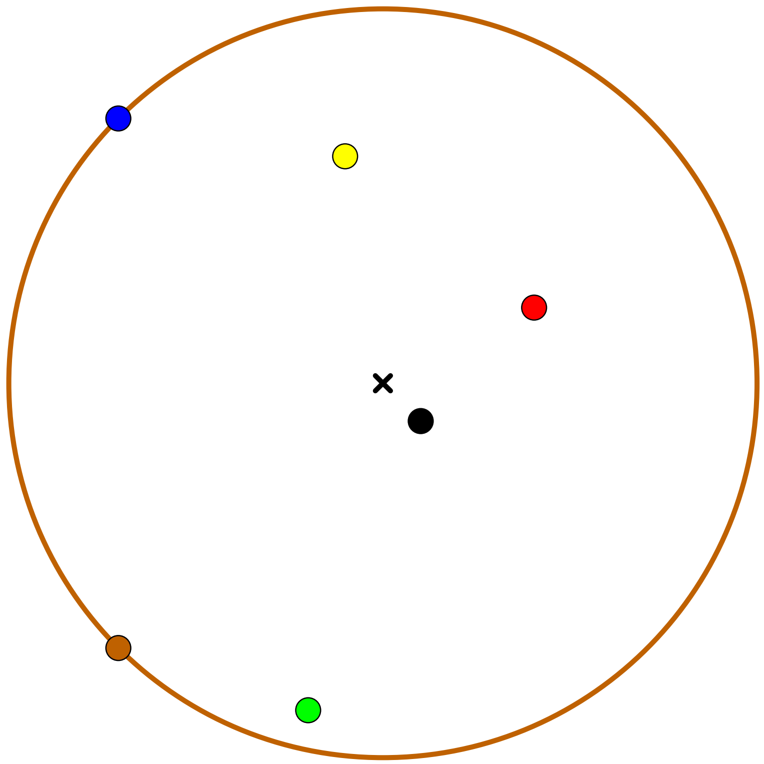

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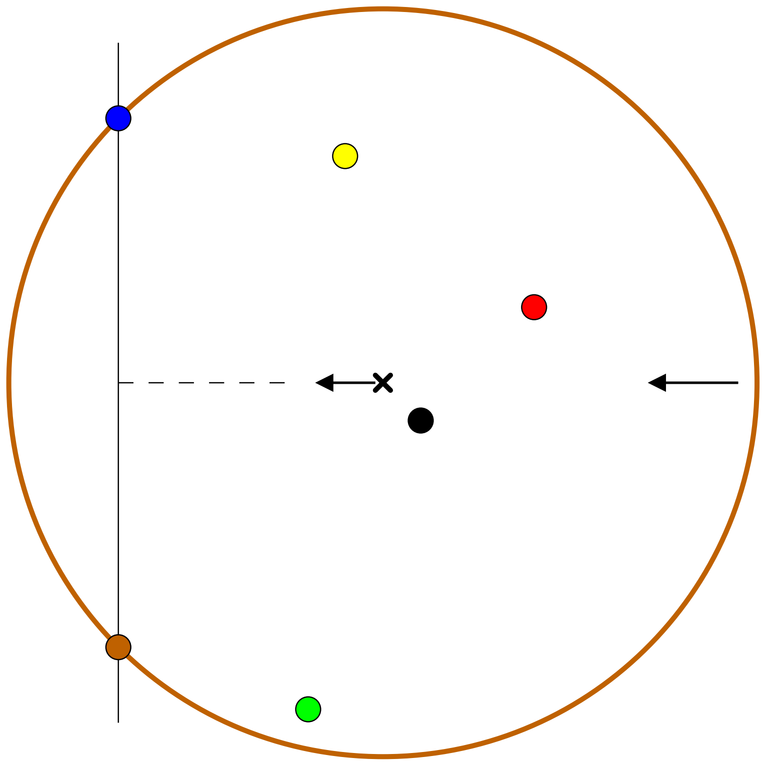

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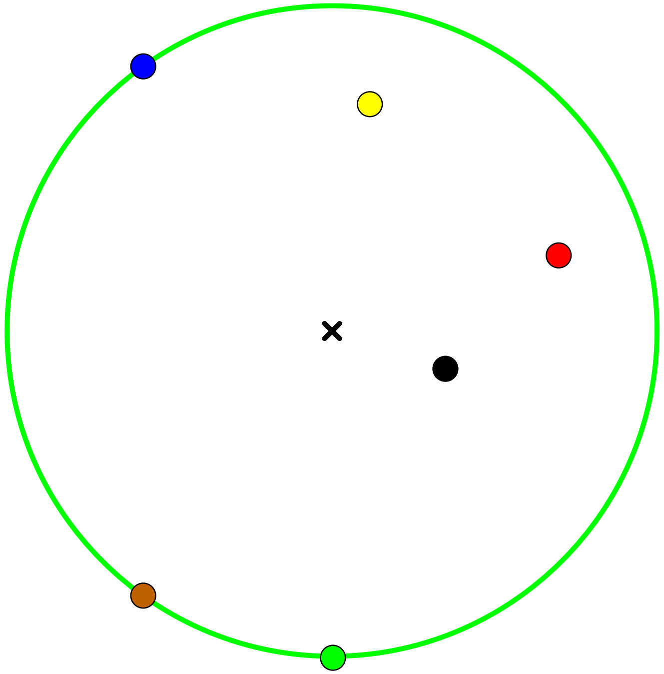

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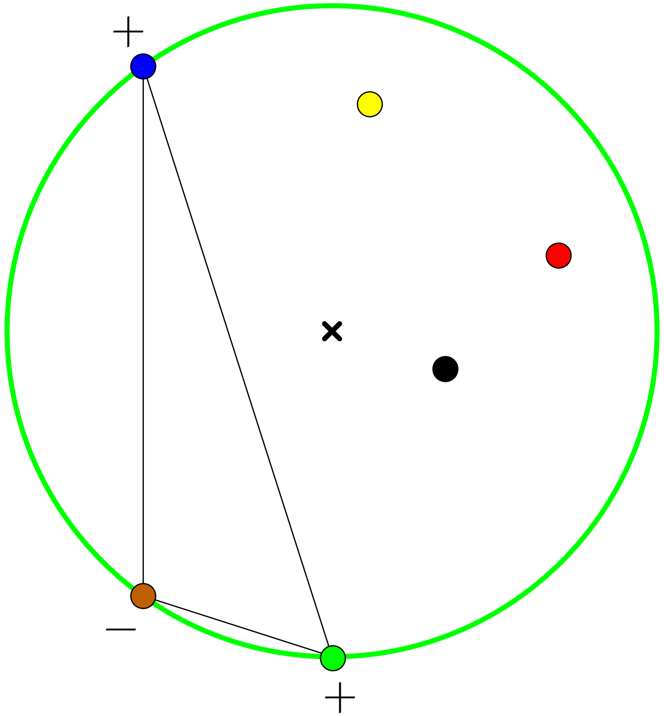

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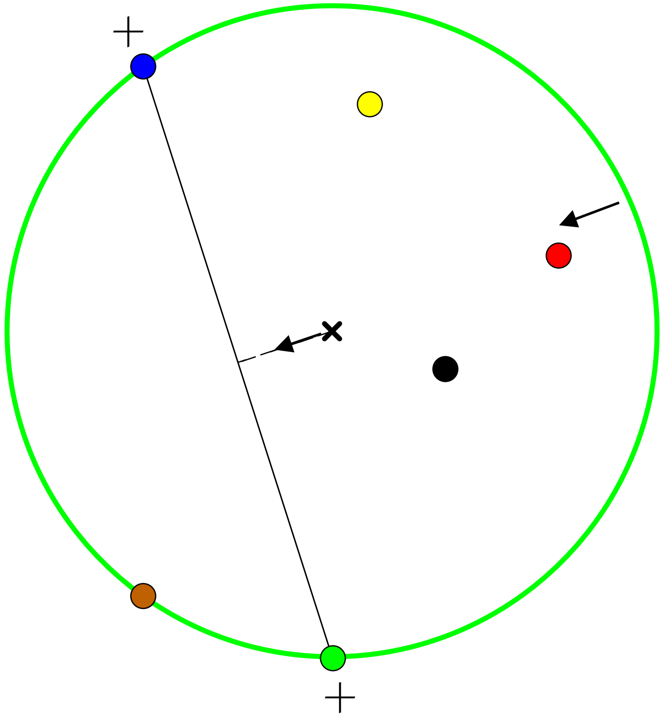

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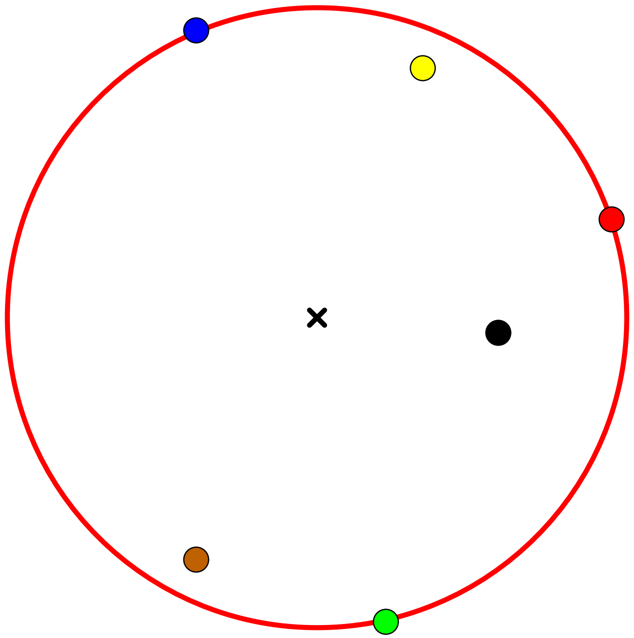

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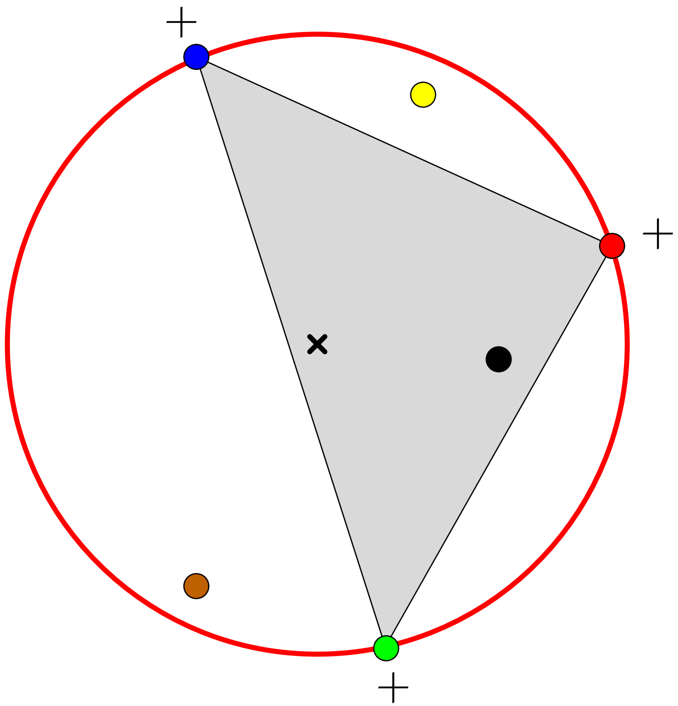

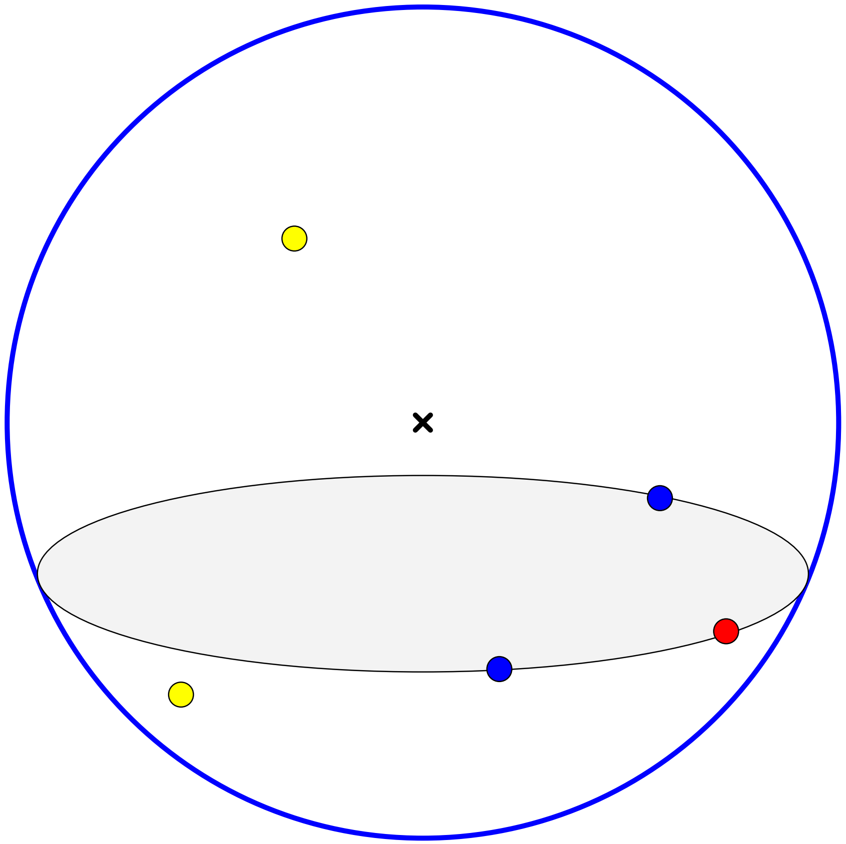

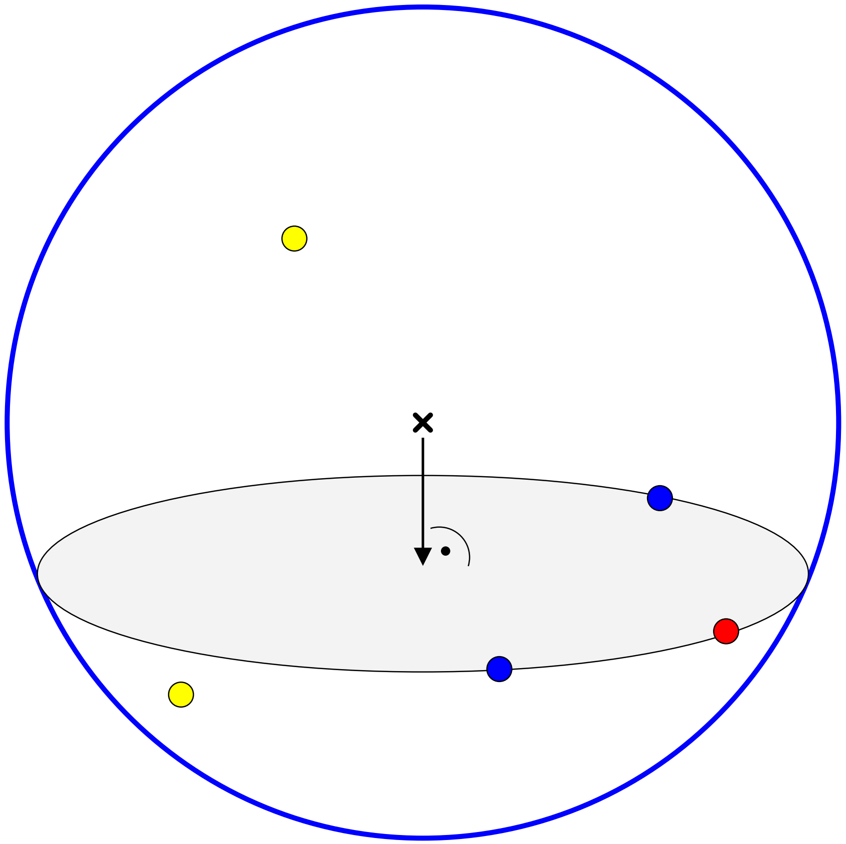

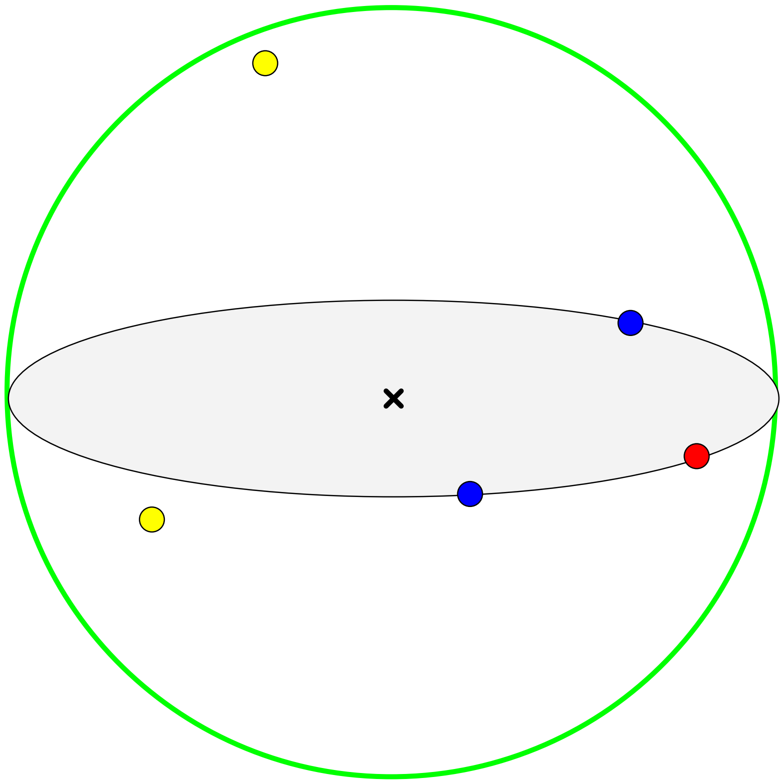

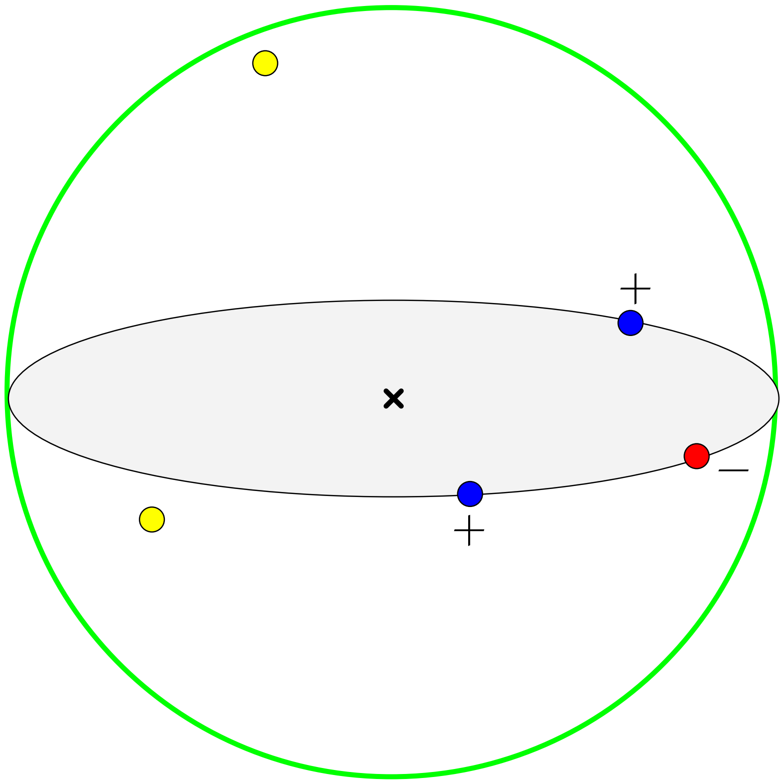

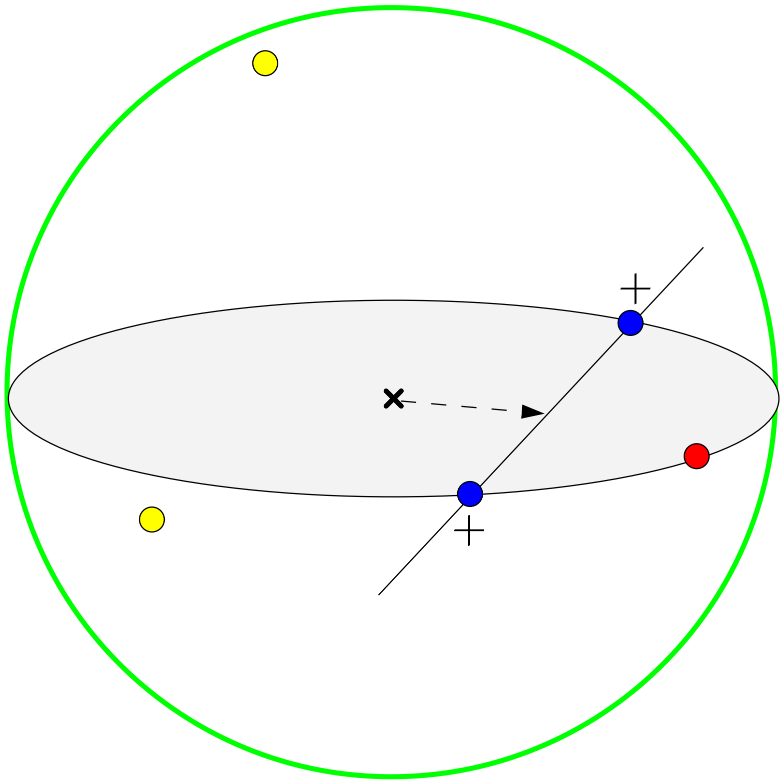

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Proof:

- Negative-coefficient rule prevents immediate re-insertion after drop.
- Radius decreases after dropping step.
- At least 1 out of d consecutive iterations performs a drop.
- Set of all possible balls $B(c, T)$ preceding drops is finite.

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Theorem. *Using "Bland's rule" our algorithm terminates.*

Technical Details

Data structure for support set T needed that allows requests

- compute orthogonal projection onto $\mathrm{aff}(T)$ (for walking),
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and updates

- insert point into T and
- delete point from T.

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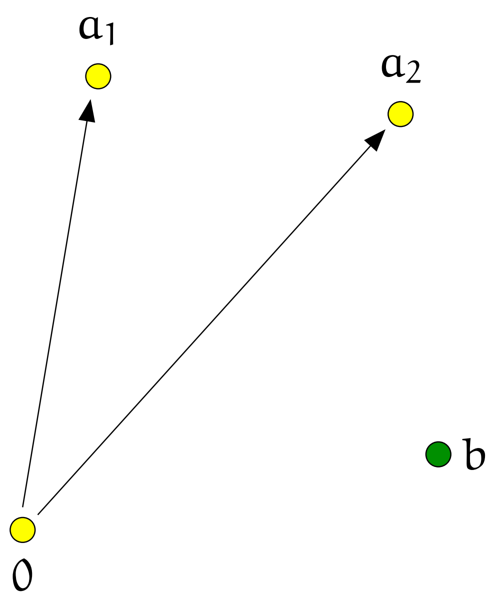

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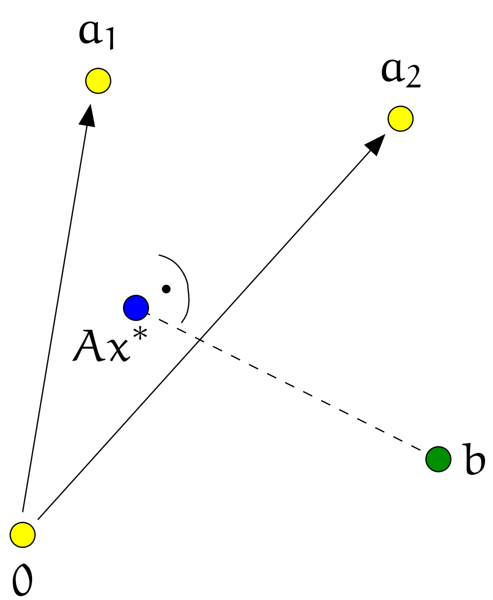

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then Ax^* is the orthogonal projection of b onto $\langle a_1, a_2, \ldots, a_k \rangle$.

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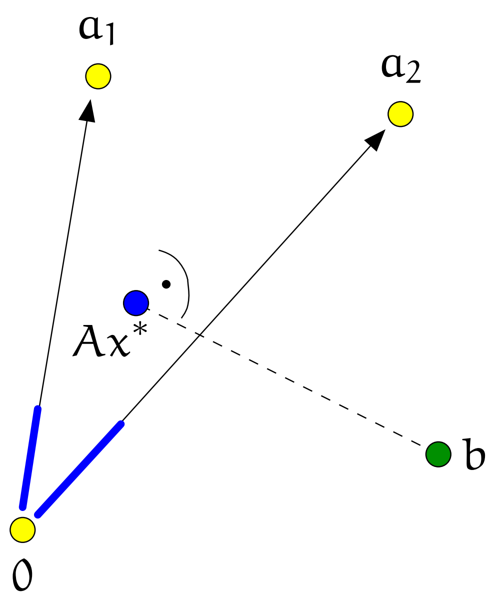

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$$||Ax - b||_2,$$

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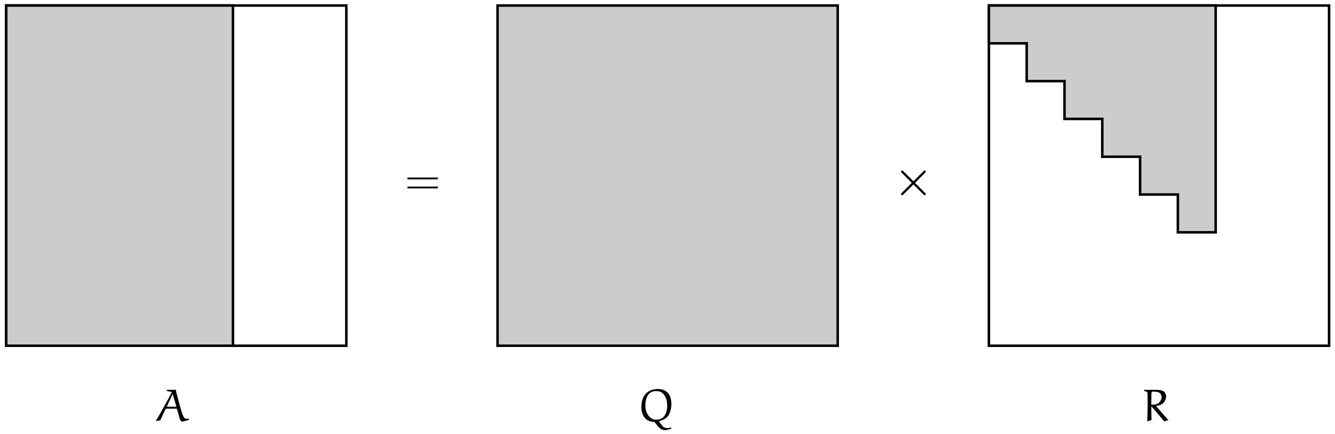
If $b \in \langle a_1, a_2, \ldots, a_k \rangle$ then the coefficients of x^* simply are the coefficients of b.

Technical Details

We compute the x^* that minimizes $\|Ax - b\|$ with QR-decomposition



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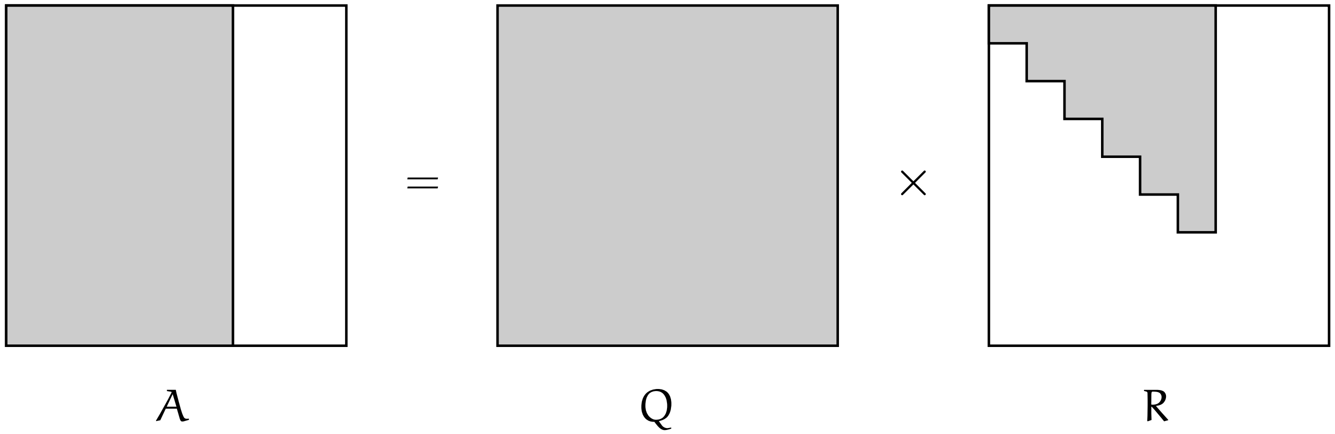

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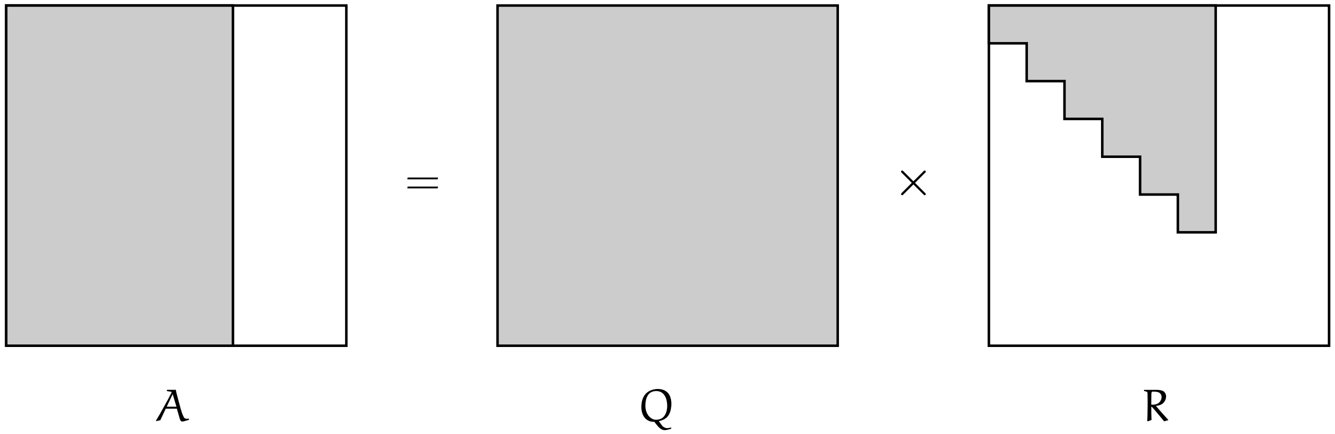

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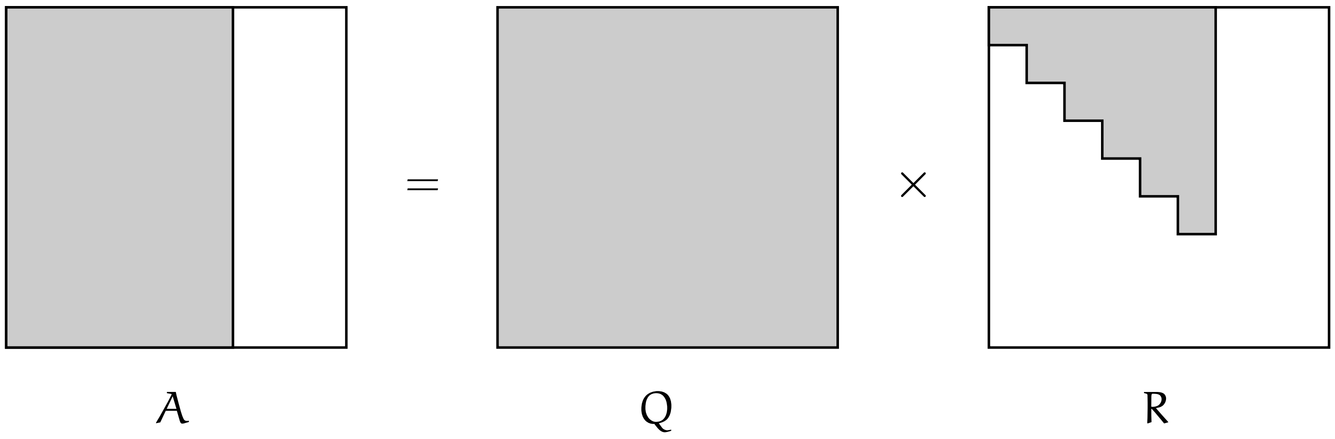
Let $y :\approx Q^T b$ with last entries zeroed
and then solve $Rx = y$ via back substitution.

Technical Details

Update QR-decomposition via Givens rotations.



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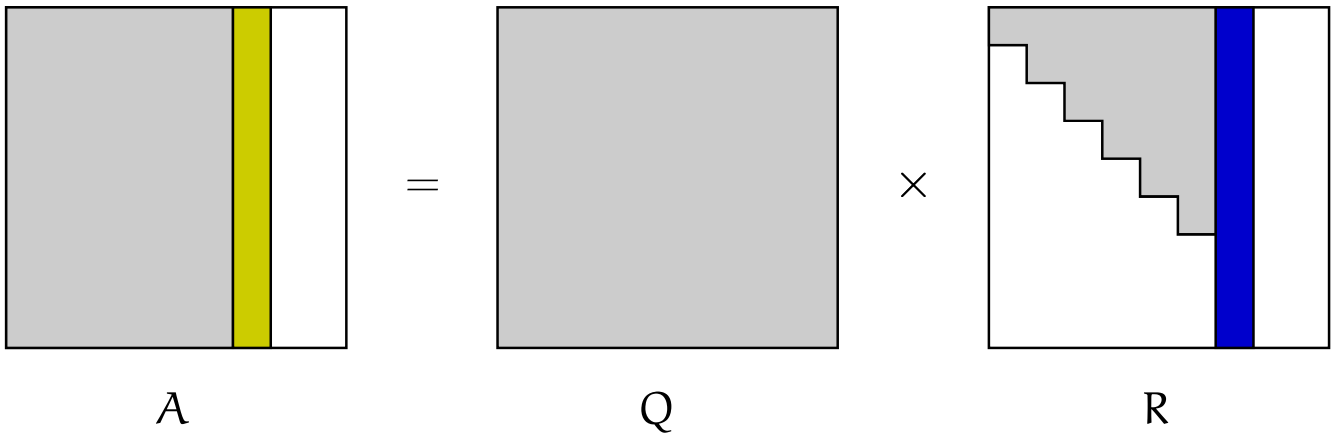

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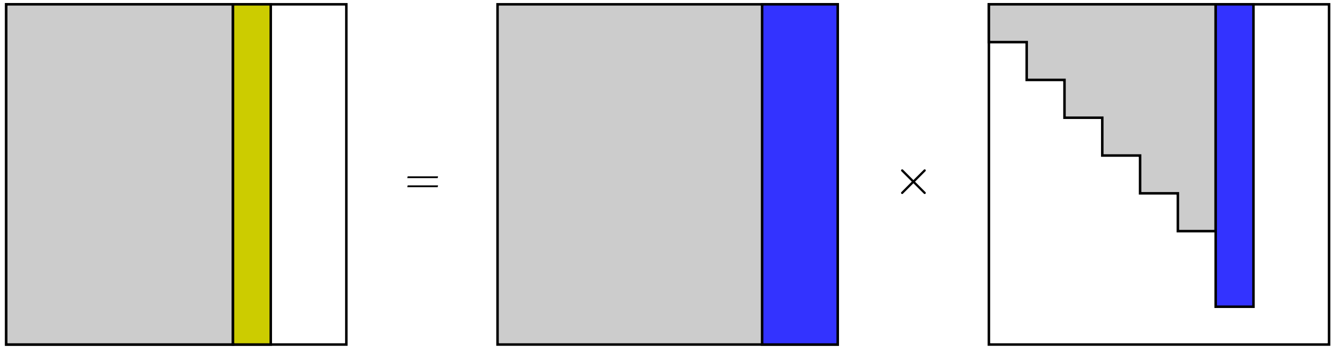

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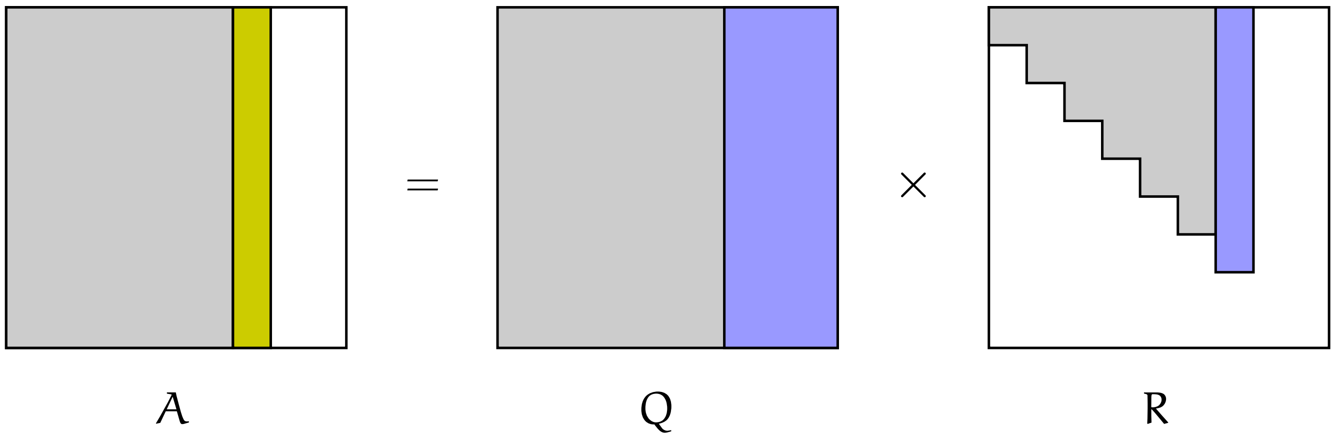

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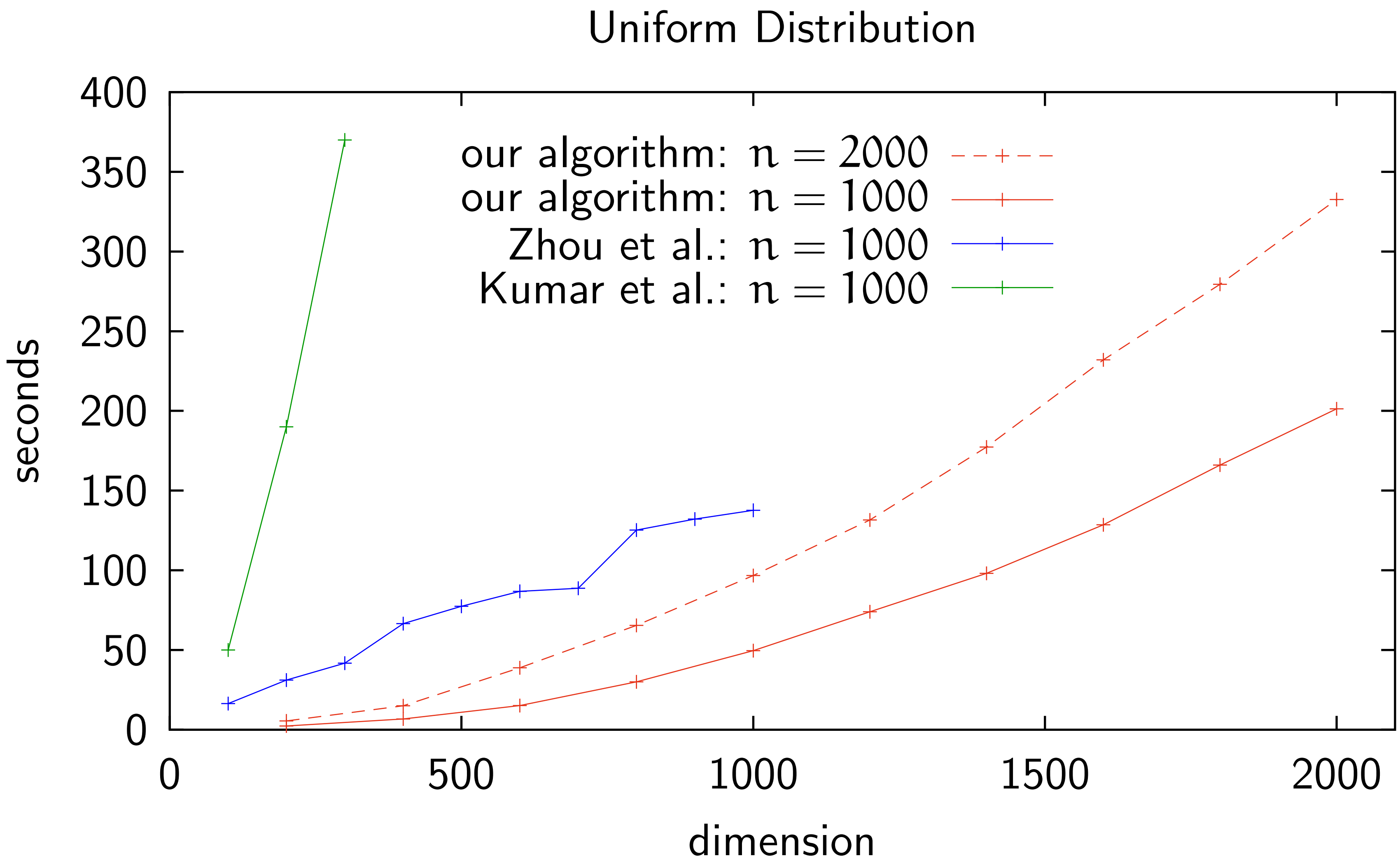
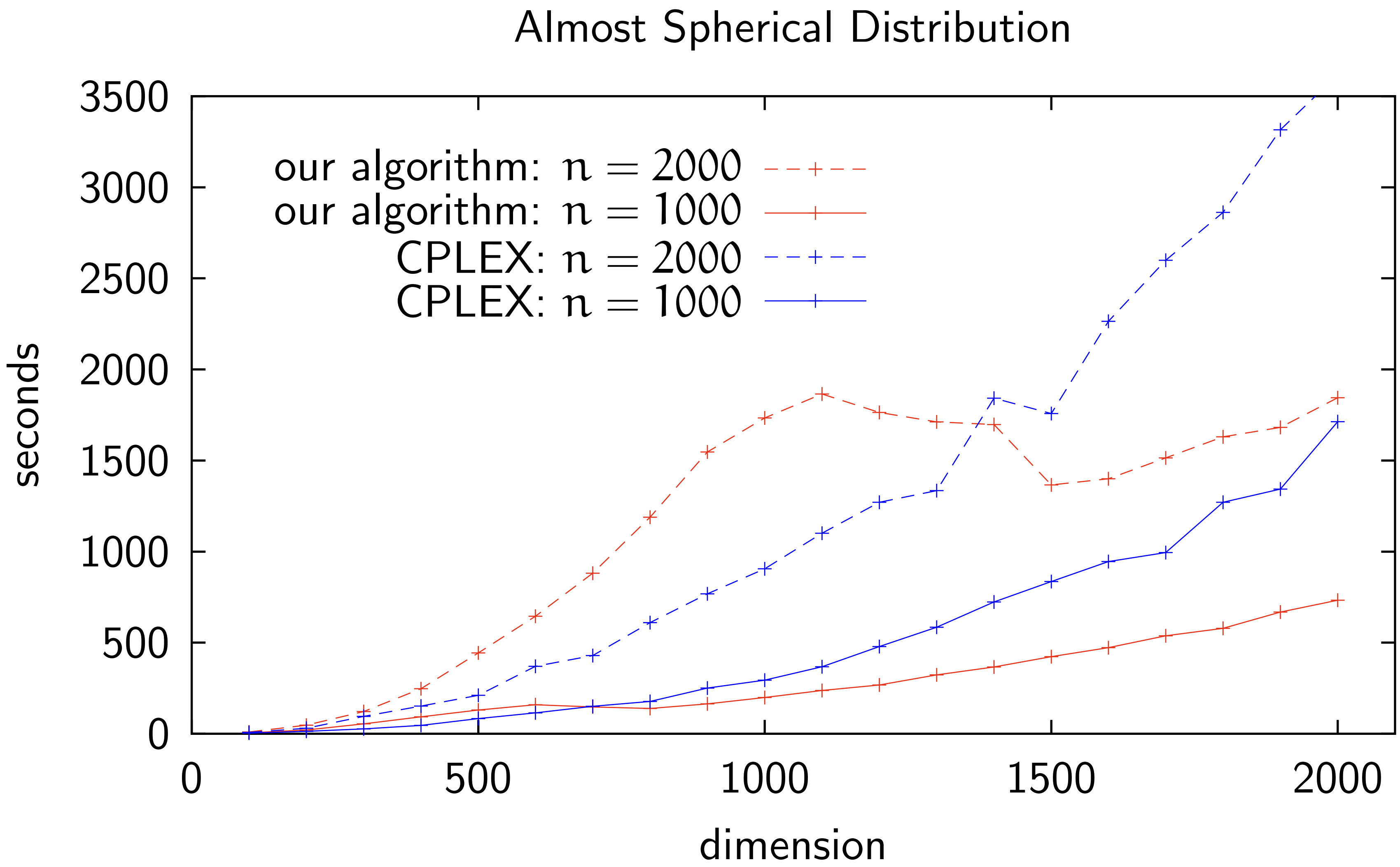
- QR decomposition numerically very stable
- very accurate results, about $1{,}000$ times machine precision


Uniform Distribution
our algorithm: $n = 2000$
our algorithm: $n = 1000$
Zhou et al.: $n = 1000$
Kumar et al.: $n = 1000$
seconds
dimension
0
50
100
150
200
250
300
350
400
0
500
1000
1500
2000



Almost Spherical Distribution
seconds
dimension
our algorithm: n = 2000
our algorithm: n = 1000
CPLEX: n = 2000
CPLEX: n = 1000
0
500
1000
1500
2000
2500
3000
3500
0
500
1000
1500
2000