Solving Low-Dimensional Optimization Problems via Zonotope Vertex Enumeration

Nate Veldt

PUNLAG Seminar

February 22, 2017

Binary Quadratic Maximization (01QP)

Given: Matrix A symmetric, rational, n x n

$$\boxed{\begin{aligned} &\max\ \mathbf{x}^T\mathbf{A}\mathbf{x} \\ &\text{s.t. } \mathbf{x} \in \{0,1\}^n \end{aligned}}$$

NP-hard in general

Binary Quadratic Maximization (01QP)

Given: Matrix A symmetric, rational, n x n

$$\begin{aligned} &\max \ \mathbf{x}^T \mathbf{A} \mathbf{x} \\ &\text{s.t. } \ \mathbf{x} \in \{0,1\}^n \end{aligned}$$

Polynomial-time for rank-d, PSD matrices via zonotope vertex enumeration

Binary Quadratic Maximization (01QP)

Given: Matrix A symmetric, rational, n x n

$$\boxed{\begin{aligned} &\max \ \mathbf{x}^T \mathbf{A} \mathbf{x} \\ &\text{s.t. } \mathbf{x} \in \{0,1\}^n \end{aligned}}$$

Ferrez, Fukuda, Libeling. Solving the fixed rank convex quadratic maximization in binary variable by a parallel zonotope construction algorithm. *European Journal of Operational Research* 2005

Zonotope: the linear projection of a hypercube into a lower dimensional space

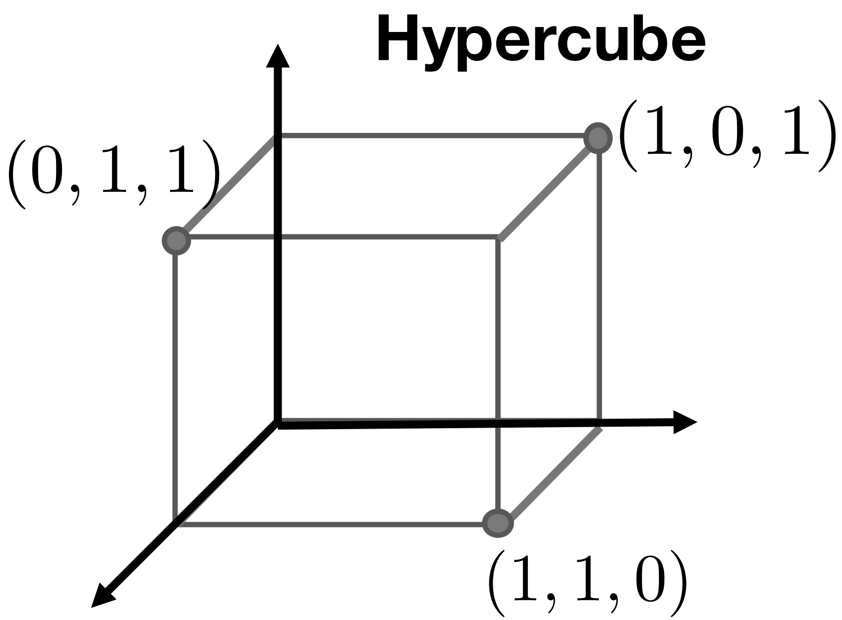
$$\mathbf{G} \in \mathbb{R}^{d \times n}$$

$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]^n\}$$

Zonotope: the linear projection of a hypercube into a lower dimensional space

$$\mathbf{G} \in \mathbb{R}^{d \times n}$$

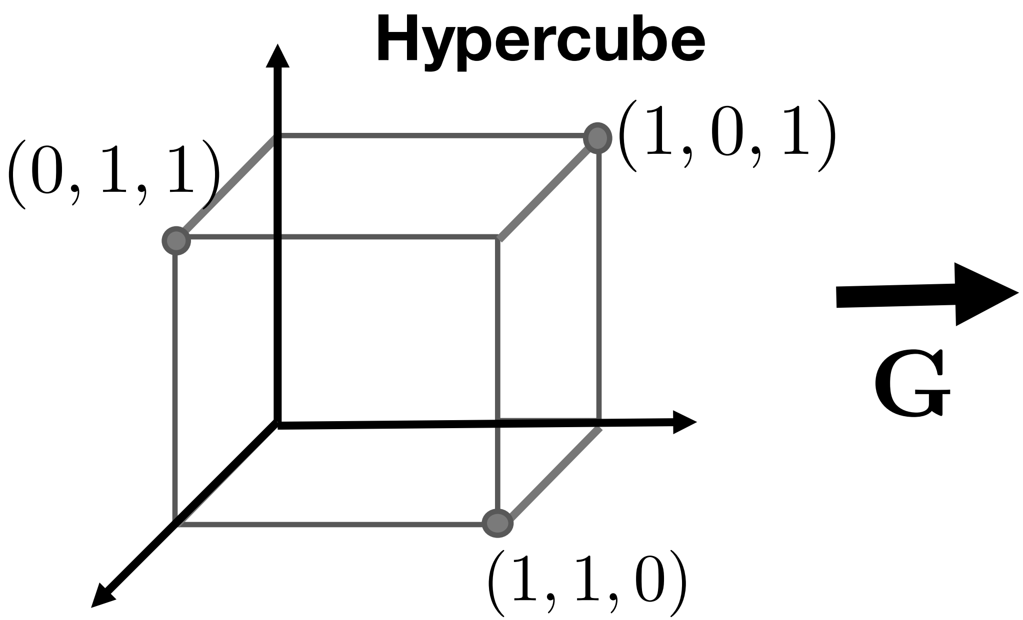
$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]^n\}$$



Zonotope: the linear projection of a hypercube into a lower dimensional space

$$\mathbf{G} \in \mathbb{R}^{d \times n}$$

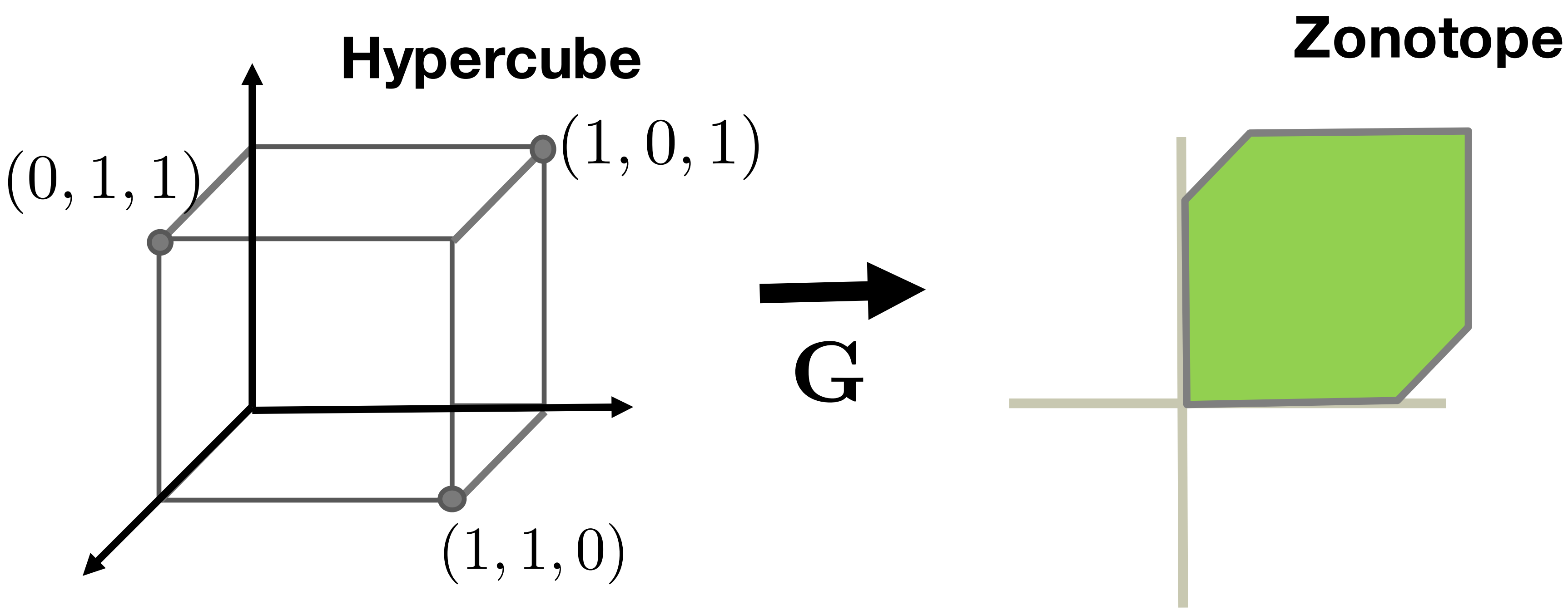
$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]^n\}$$



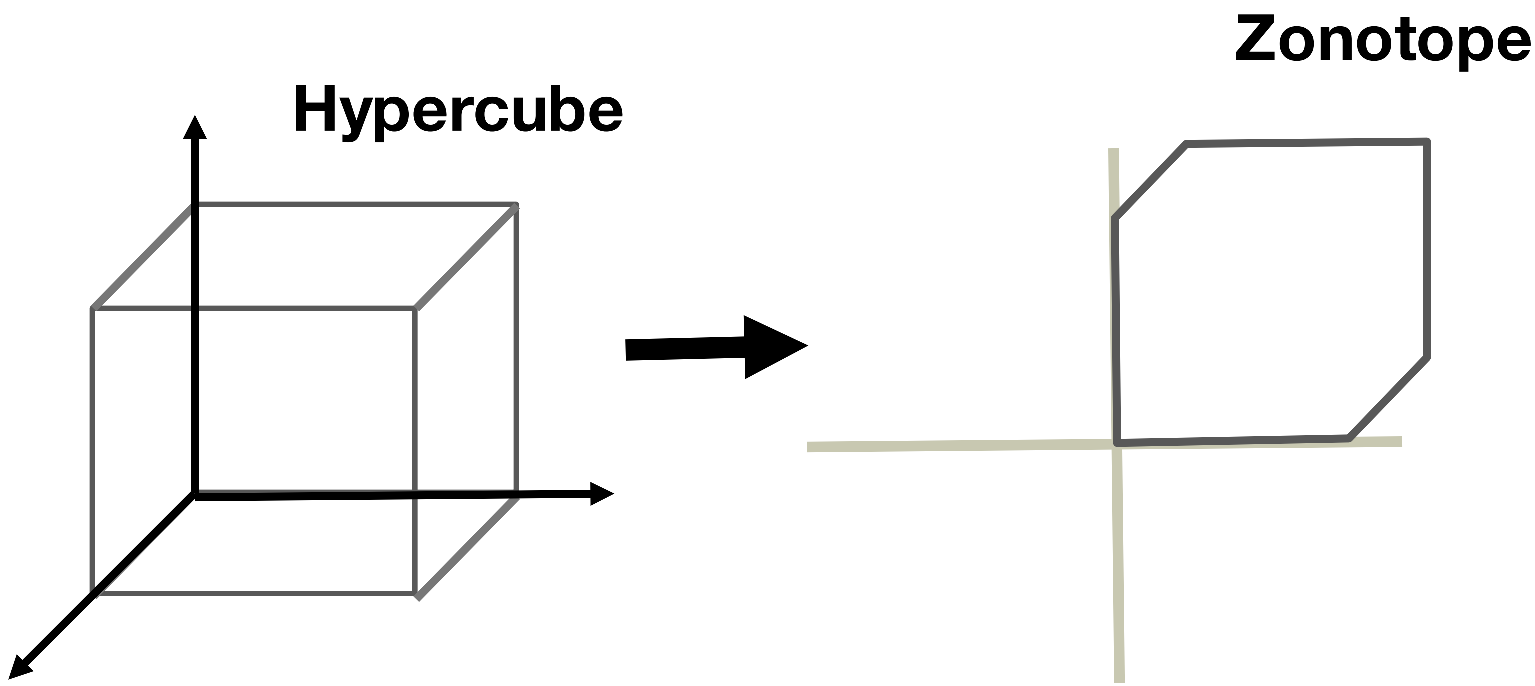
Zonotope: the linear projection of a hypercube into a lower dimensional space

$$\mathbf{G} \in \mathbb{R}^{d \times n}$$

$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]^n\}$$



Zonotope: the linear projection of a hypercube into a lower dimensional space

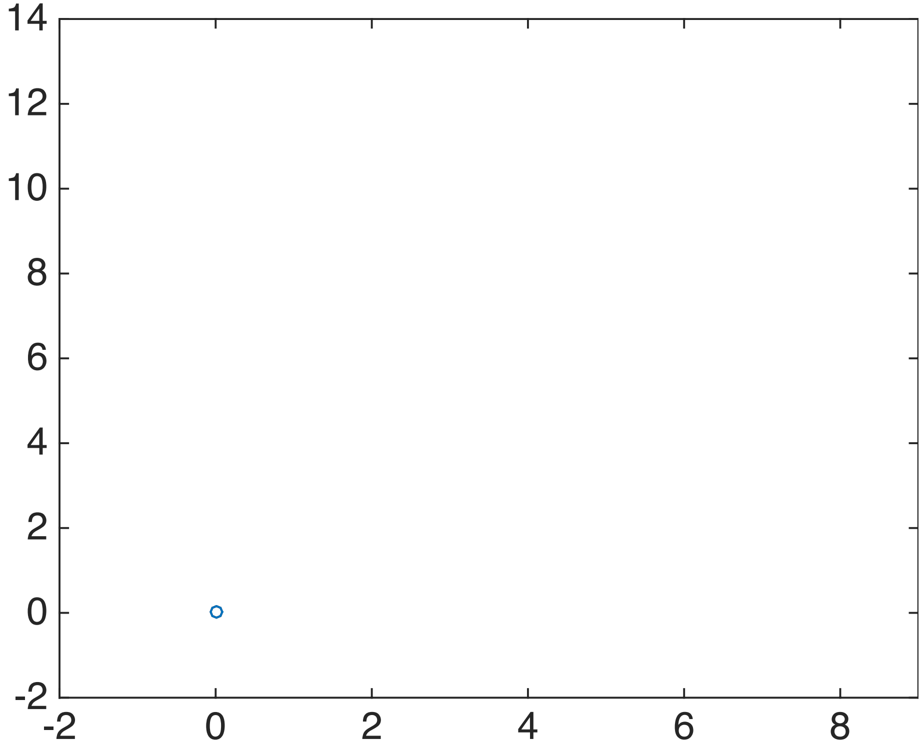


$$\mathbf{G} \in \mathbb{R}^{d \times n}$$

$$\mathcal{Z} = \mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]\}$$

Example of a 2D zonotope

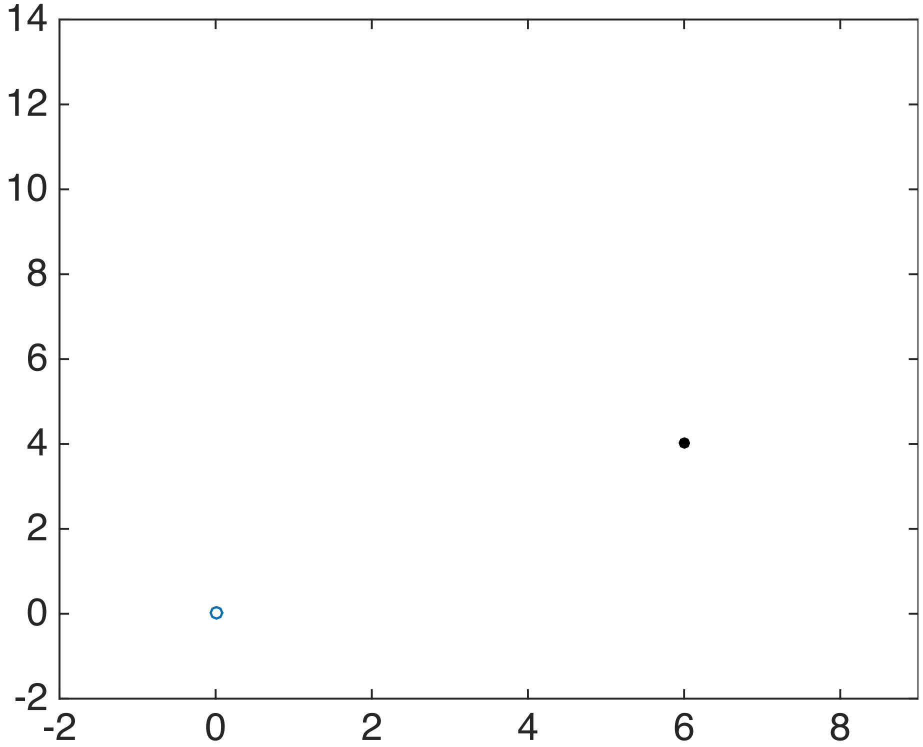
$$\mathbf{G} \begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix} \quad \mathbf{x} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$



$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \mid \mathbf{x} \in [0,1]\}$$

Example of a 2D zonotope

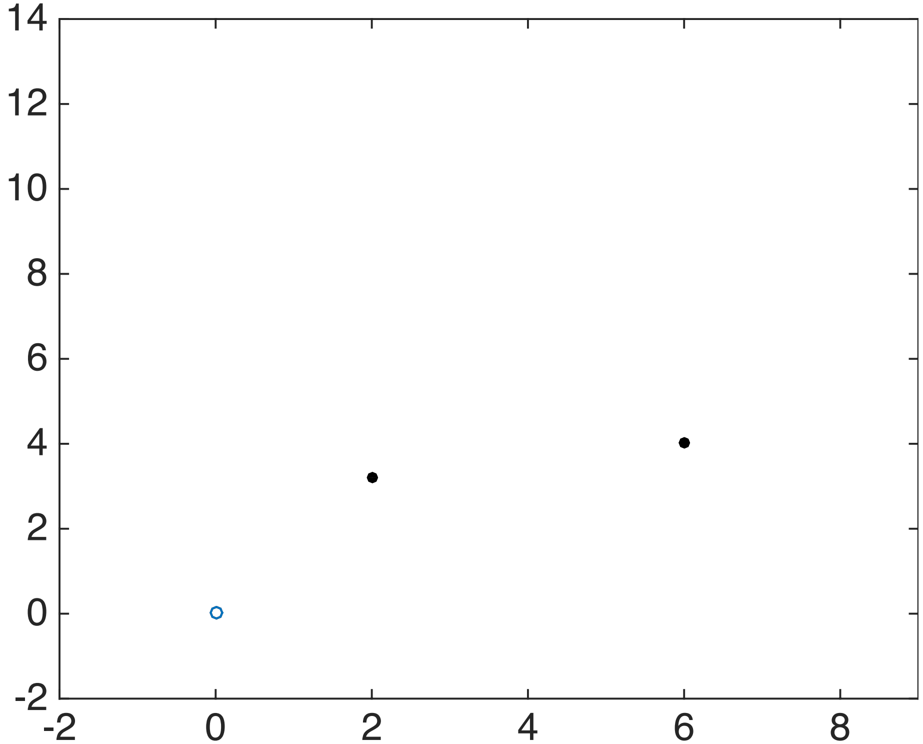
$$\mathbf{G} \begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix} \overset{\mathbf{x}}{\begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}} = \begin{bmatrix} 6 \\ 4 \end{bmatrix}$$



$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]\}$$

Example of a 2D zonotope

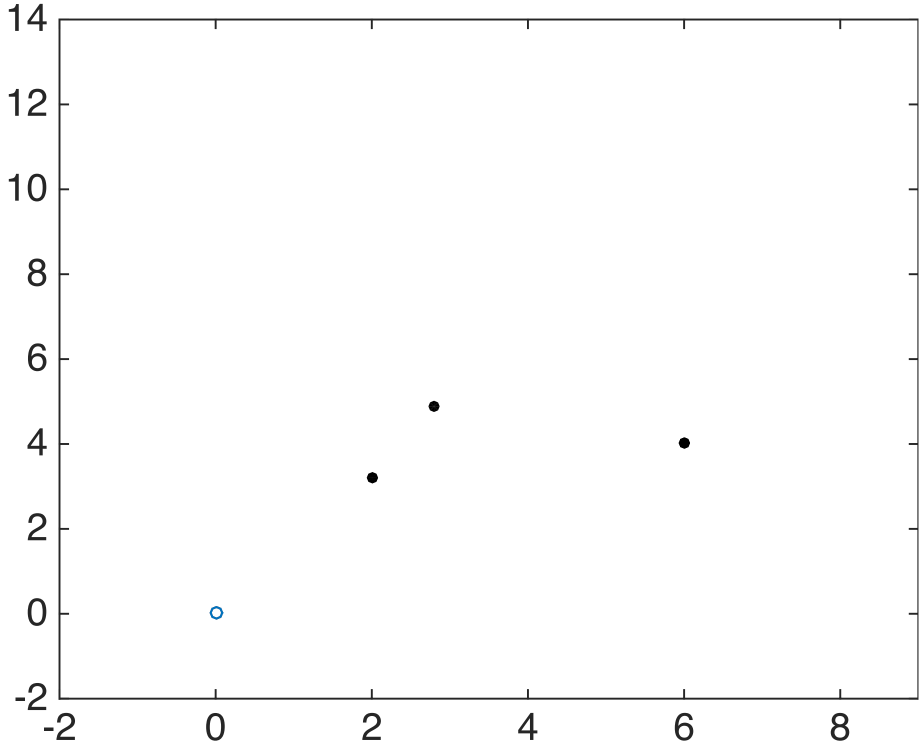
$$\begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix} \overset{\mathbf{x}}{\begin{bmatrix} .5 \\ .8 \\ .2 \\ .1 \end{bmatrix}} = \begin{bmatrix} 2 \\ 3.2 \end{bmatrix}$$



$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \mid \mathbf{x} \in [0,1]\}$$

Example of a 2D zonotope

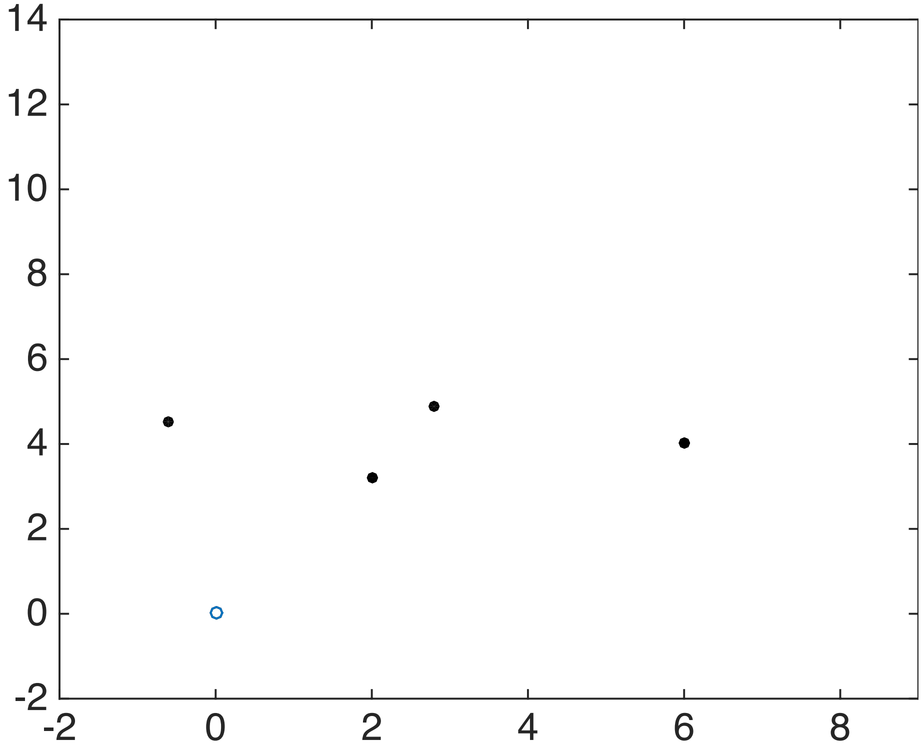
$$\begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix} \overset{\mathbf{x}}{\begin{bmatrix} .1 \\ 1 \\ 0 \\ .4 \end{bmatrix}} = \begin{bmatrix} 2.8 \\ 4.9 \end{bmatrix}$$



$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]\}$$

Example of a 2D zonotope

$$\begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix} \overset{\mathbf{x}}{\begin{bmatrix} 0 \\ 0 \\ 1 \\ .1 \end{bmatrix}} = \begin{bmatrix} -0.6 \\ 4.5 \end{bmatrix}$$

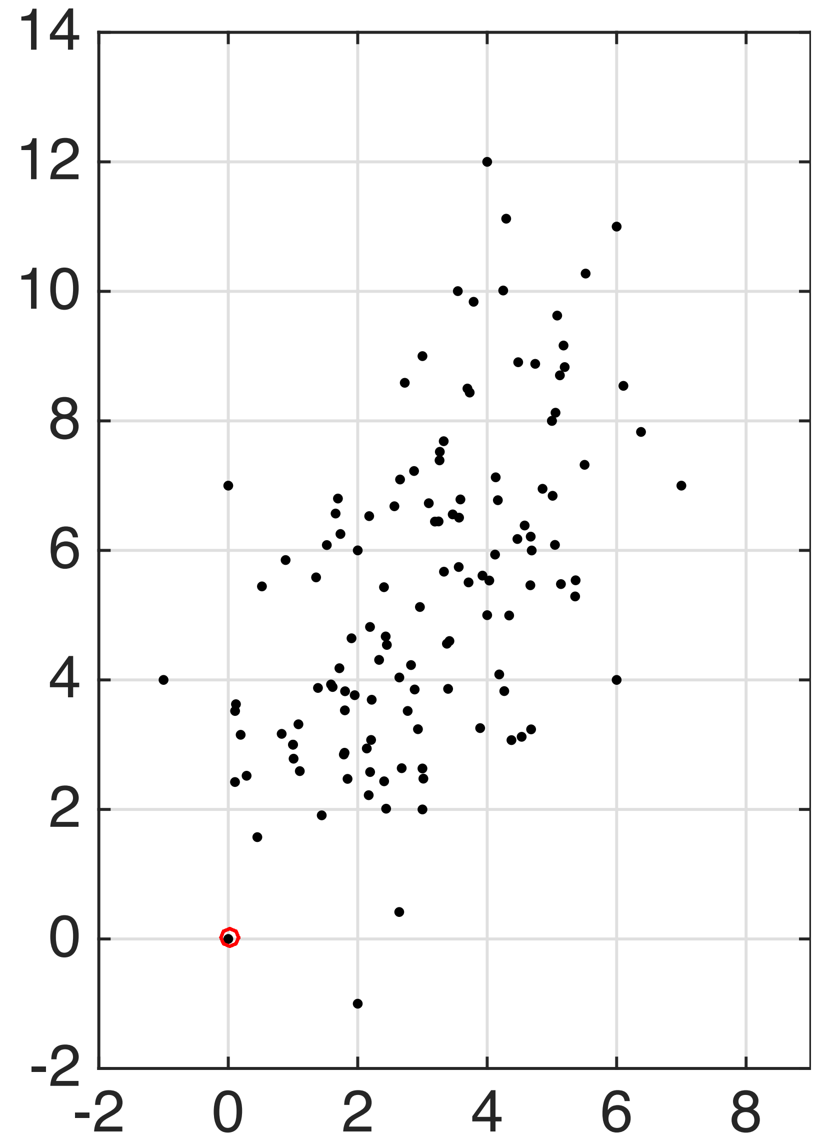


$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]\}$$

Example of a 2D zonotope

$$\mathbf{G}$$

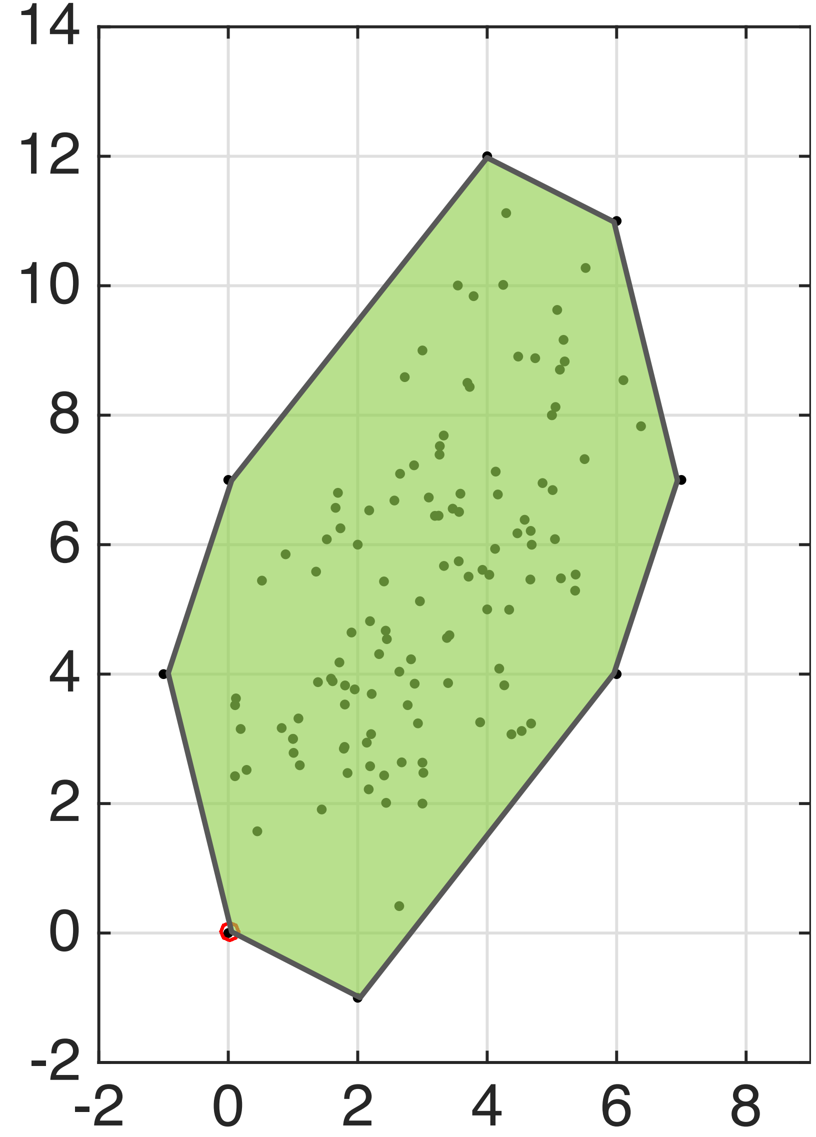
$$\begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix}$$



Example of a 2D zonotope

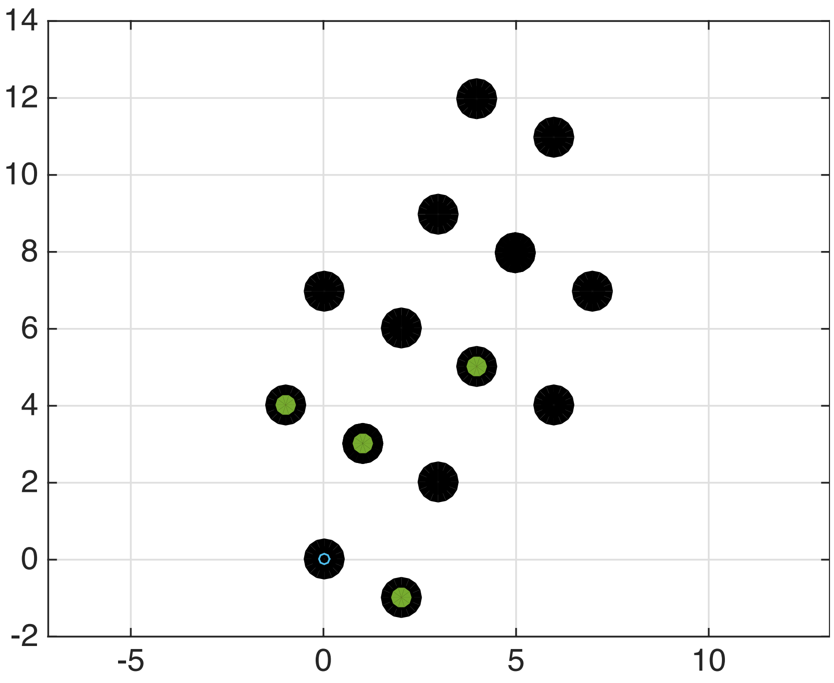
$$\mathbf{G}$$

$$\begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix}$$



Example of a 2D zonotope

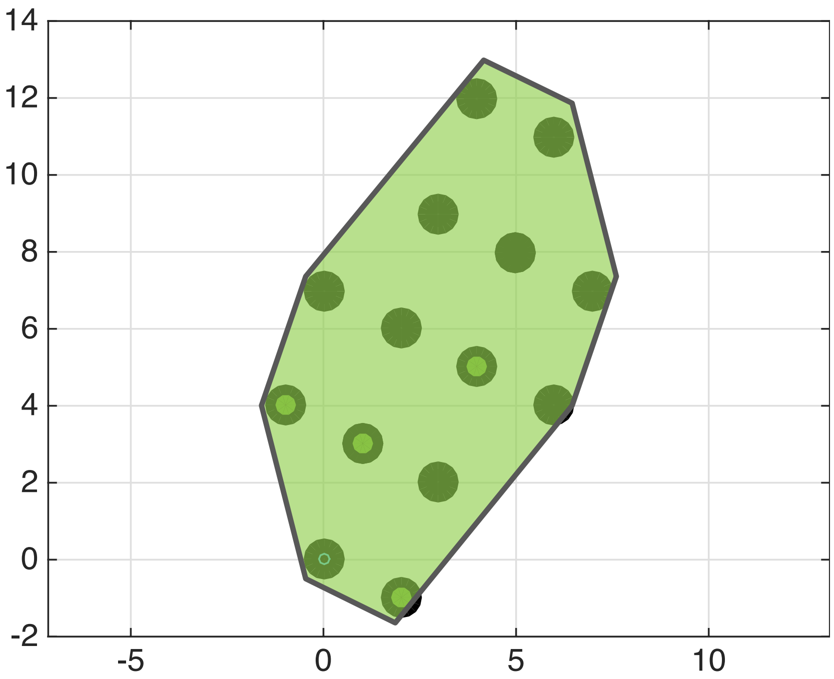
$$\mathbf{G}\begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix} \overset{\mathbf{x}}{\begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}} = \begin{bmatrix} 6 \\ 4 \end{bmatrix}$$



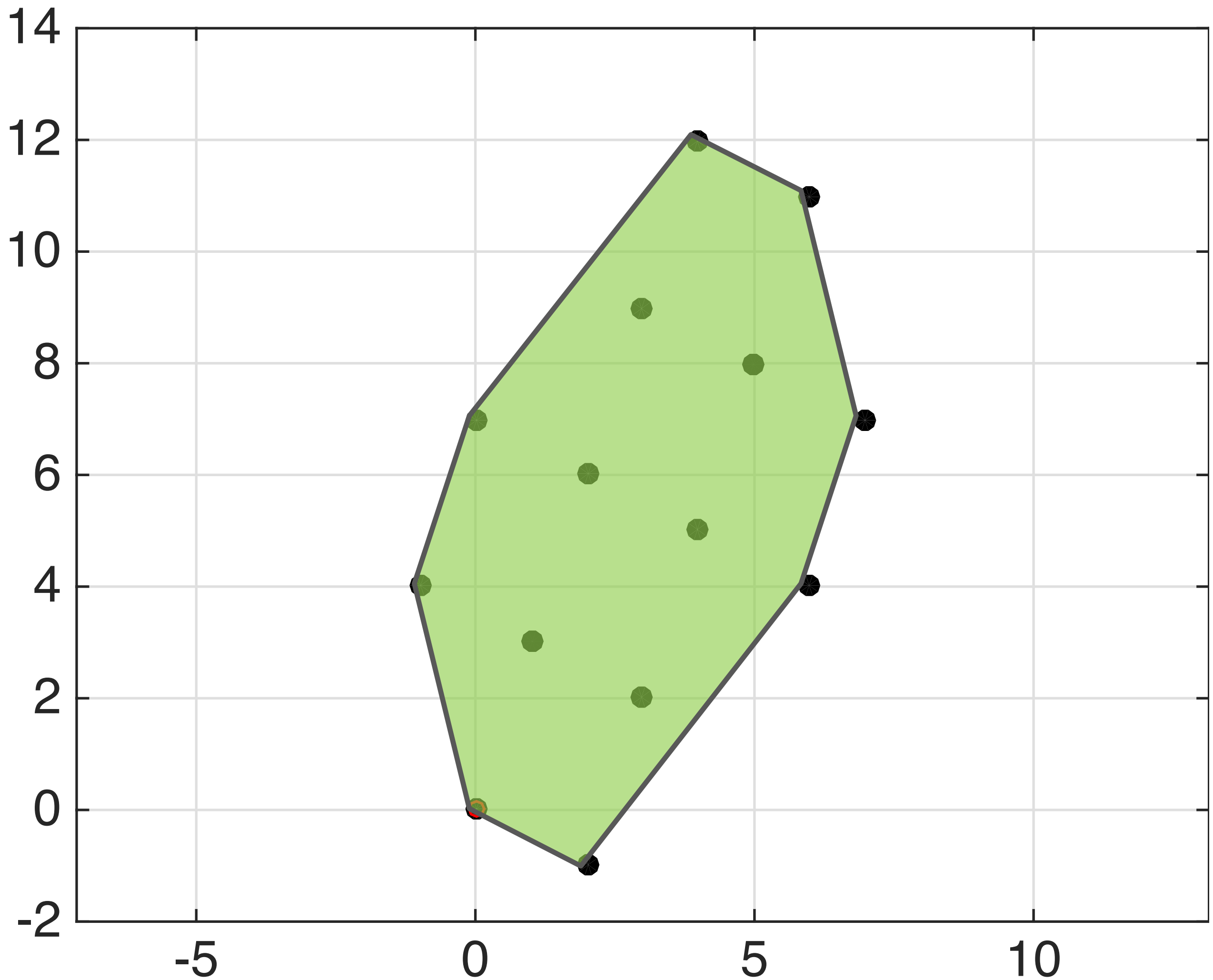
Just map the vertices of the hypercube and find the convex hull

Example of a 2D zonotope

$$\mathbf{G} \begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix} \overset{\mathbf{x}}{\begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}} = \begin{bmatrix} 6 \\ 4 \end{bmatrix}$$



Just map the vertices of the hypercube and find the convex hull



$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]^n\}$$

$$\mathcal{Z}(\mathbf{G}) = \mathbf{conv}\{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in \{0,1\}^n\}$$

A zonotope is a Minkowski Sum

Minkowski Sum of sets $P, Q \subset \mathbb{R}^d$:

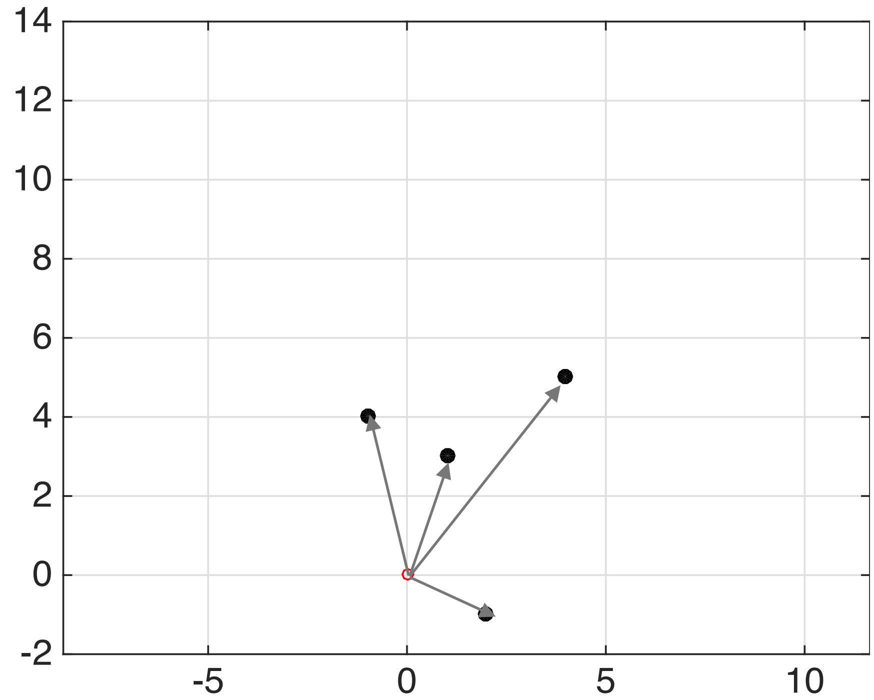
$$P \oplus Q = \{p + q \,|\, p \in P, q \in Q\}$$

A zonotope is a Minkowski Sum

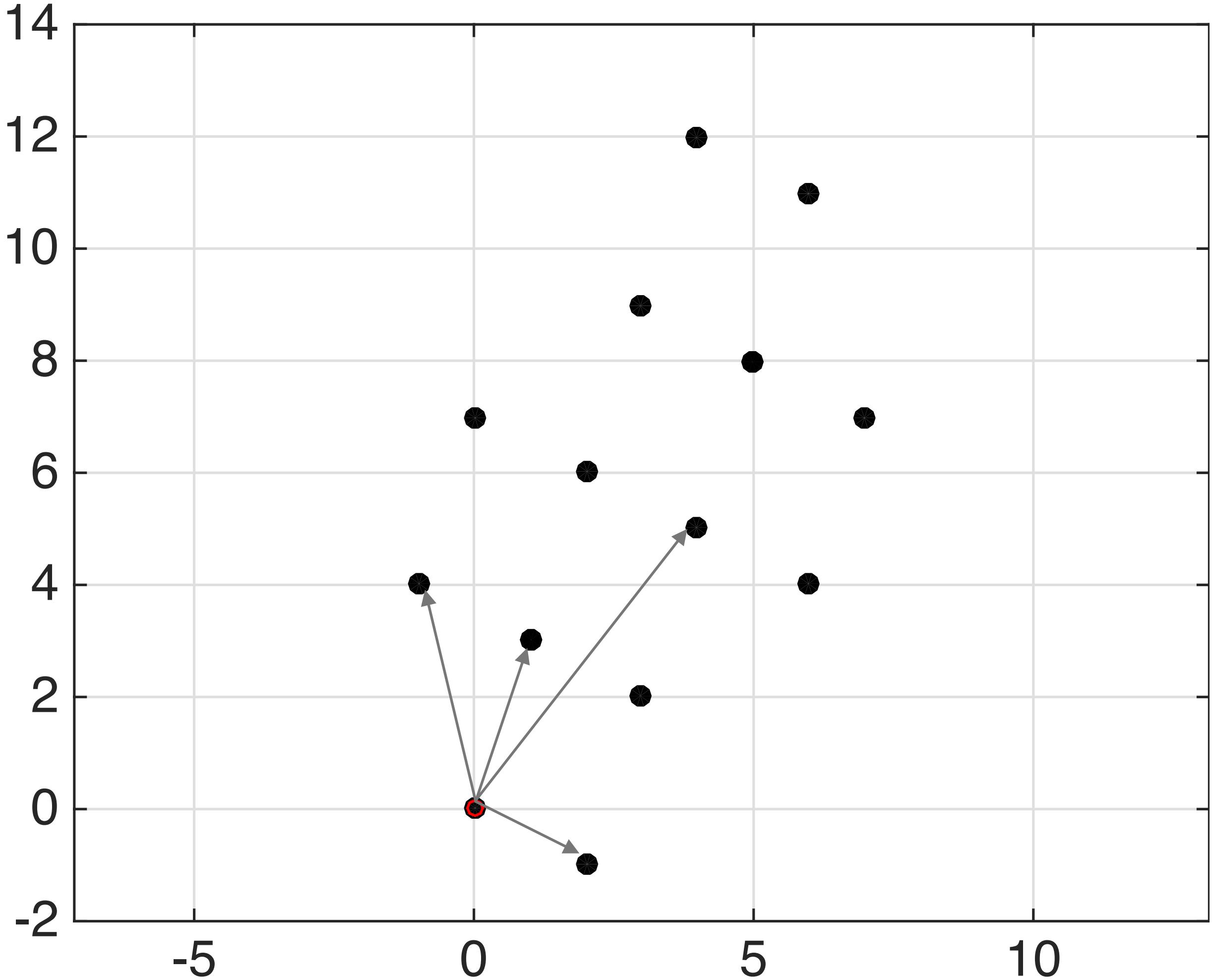
Minkowski Sum of sets $P, Q \subset \mathbb{R}^d$:

$$P \oplus Q = \{p + q \,|\, p \in P, q \in Q\}$$

$$\begin{array}{cccc} \begin{bmatrix} 2 & 1 & -1 & 4 \\ -1 & 3 & 4 & 5 \end{bmatrix} \\ g_1 \quad g_2 \quad g_3 \quad g_4 \end{array}$$

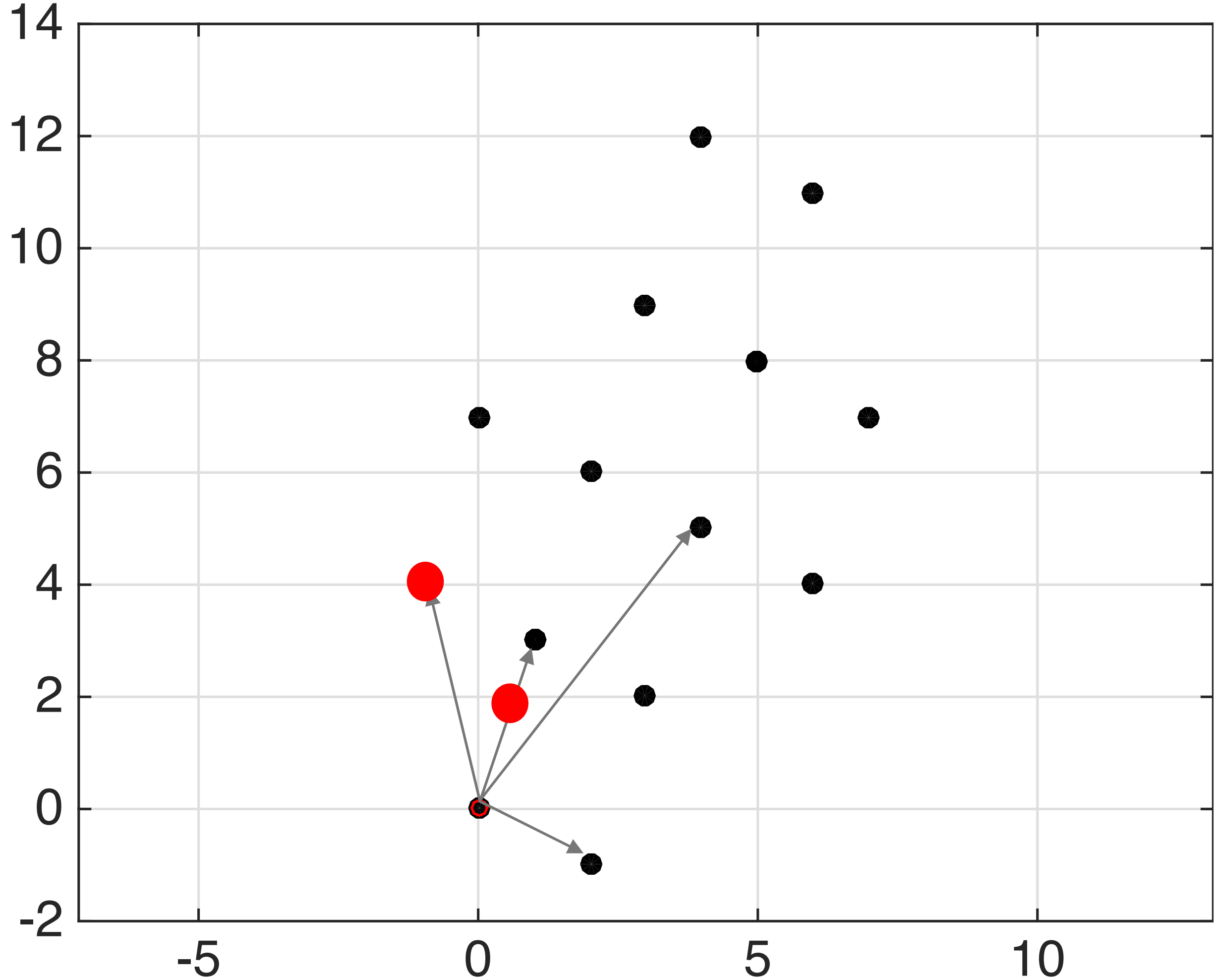


$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



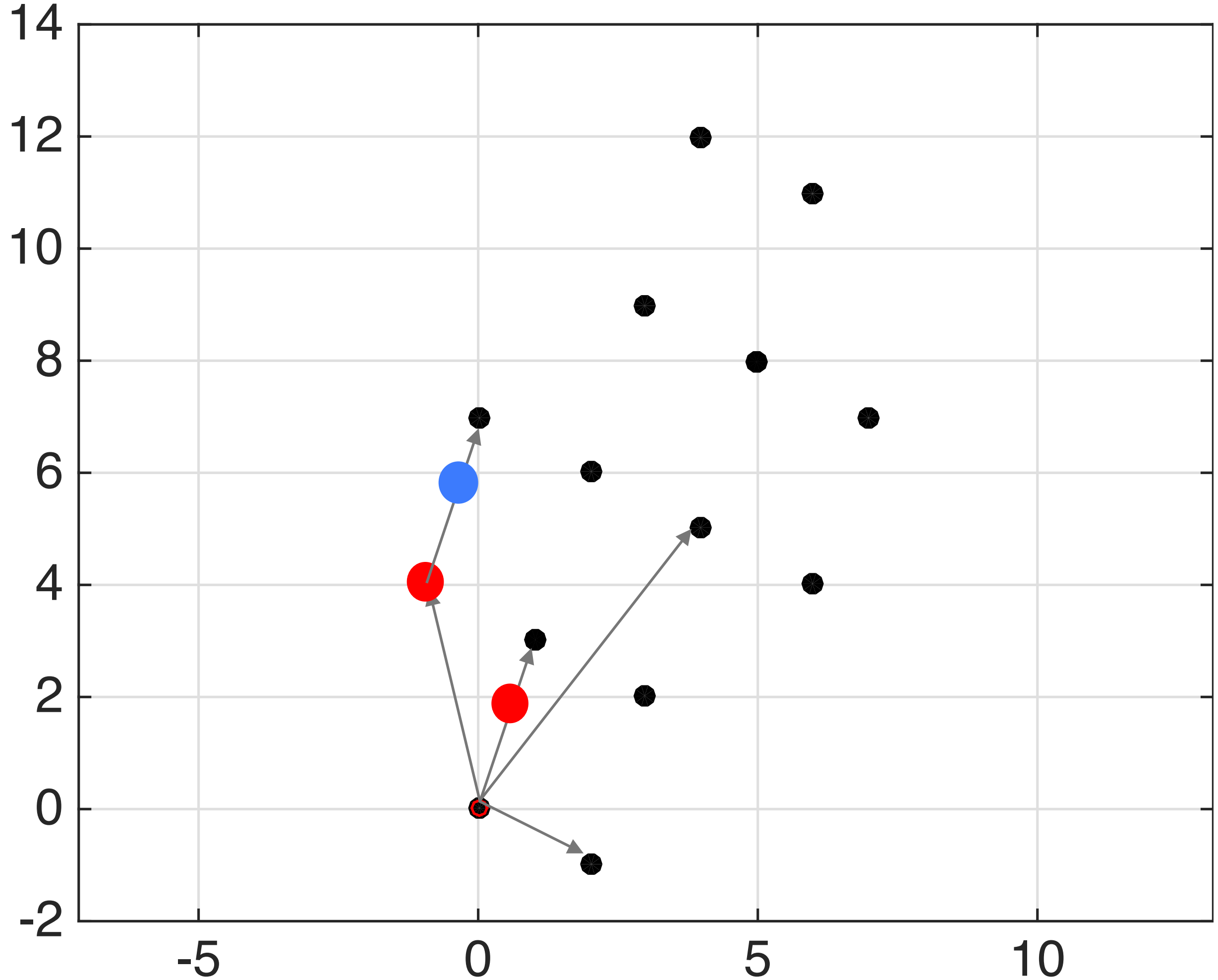
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



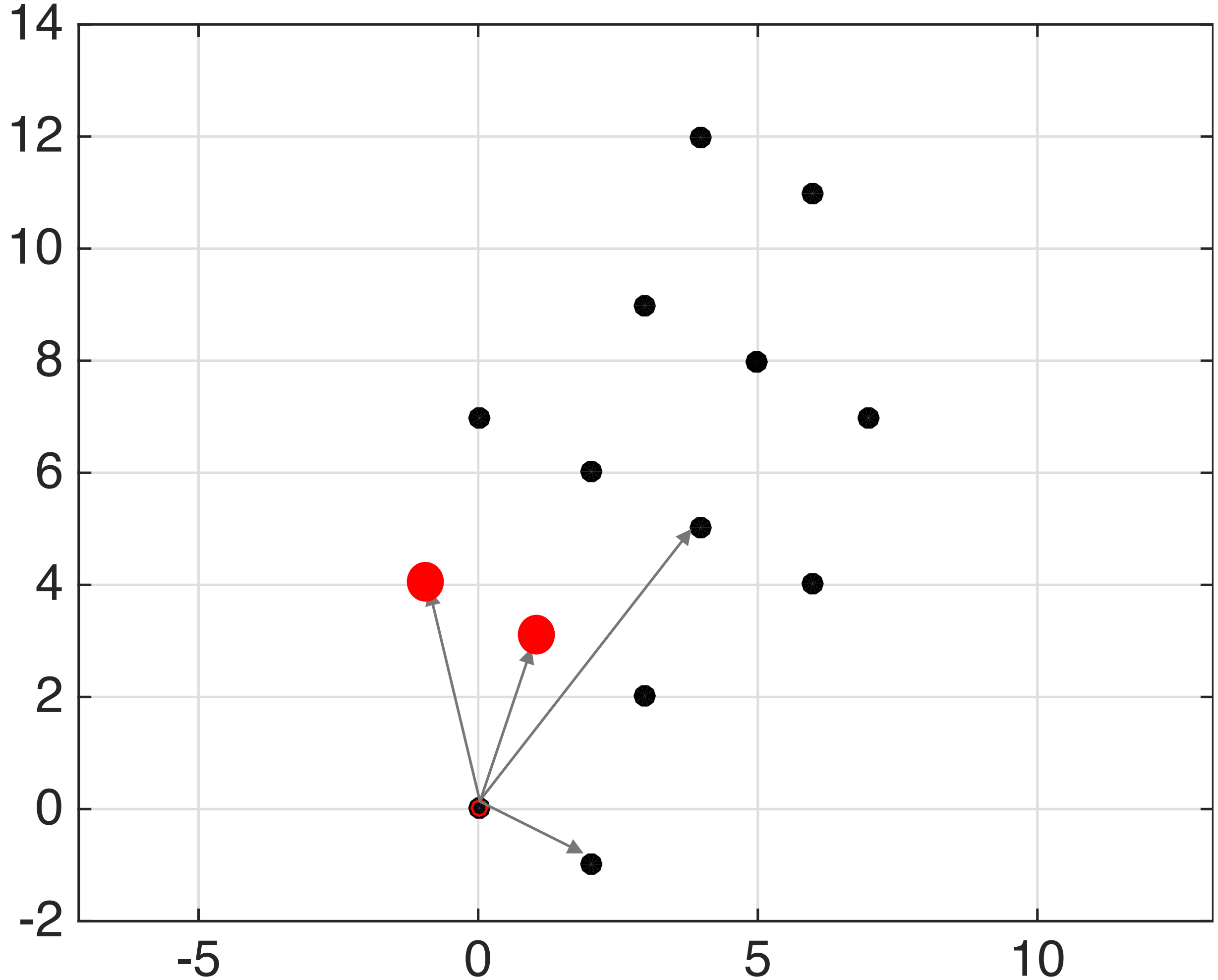
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



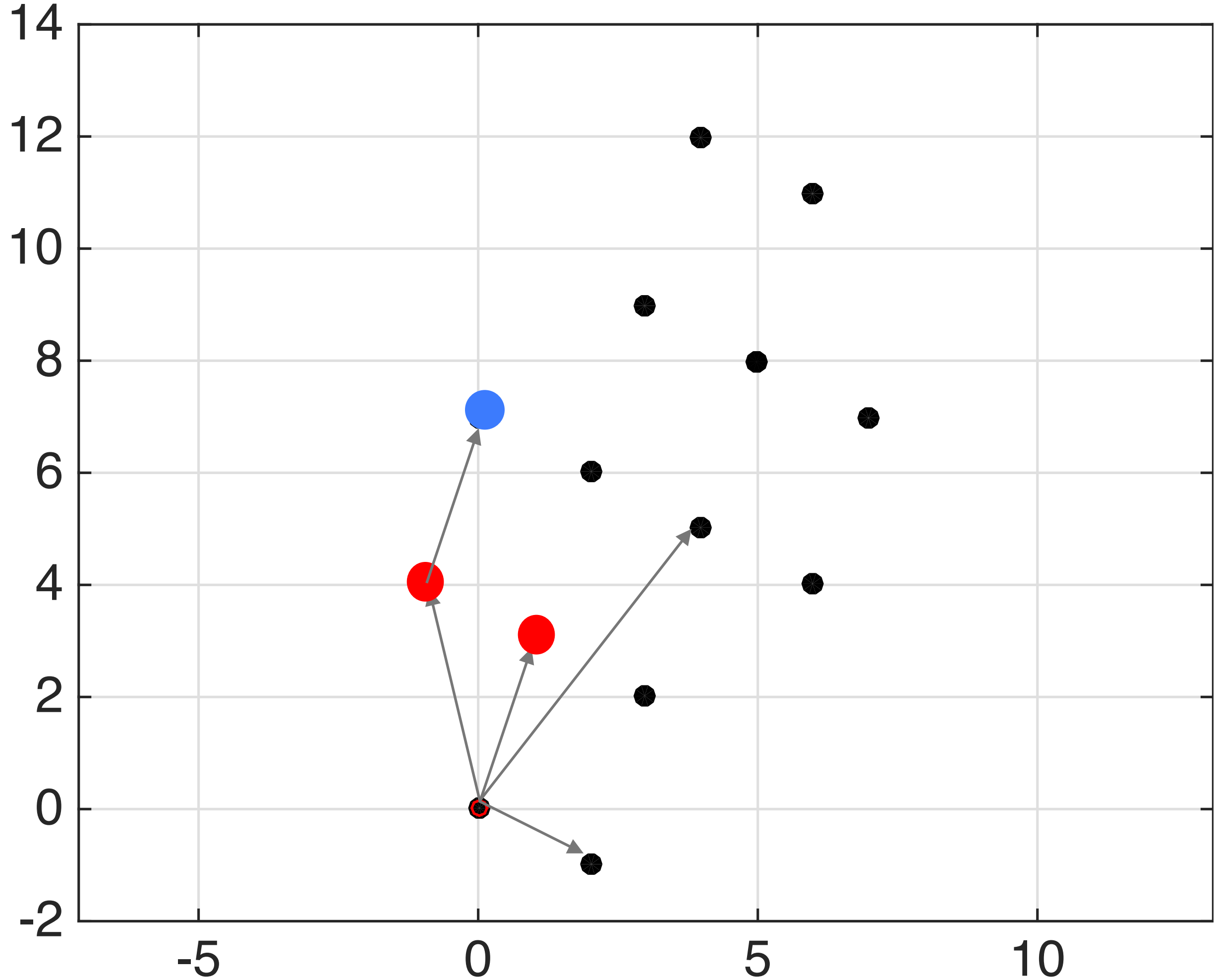
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



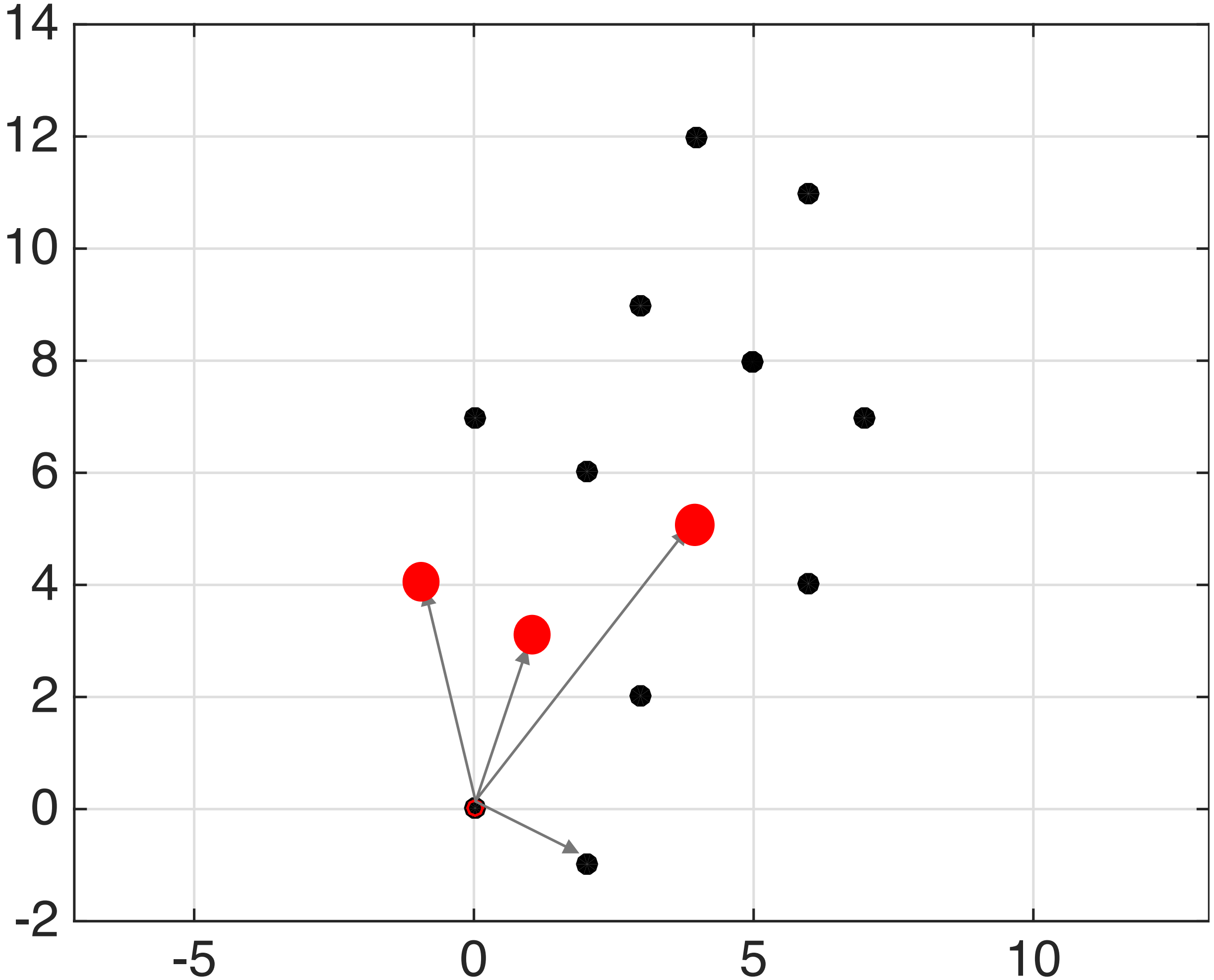
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



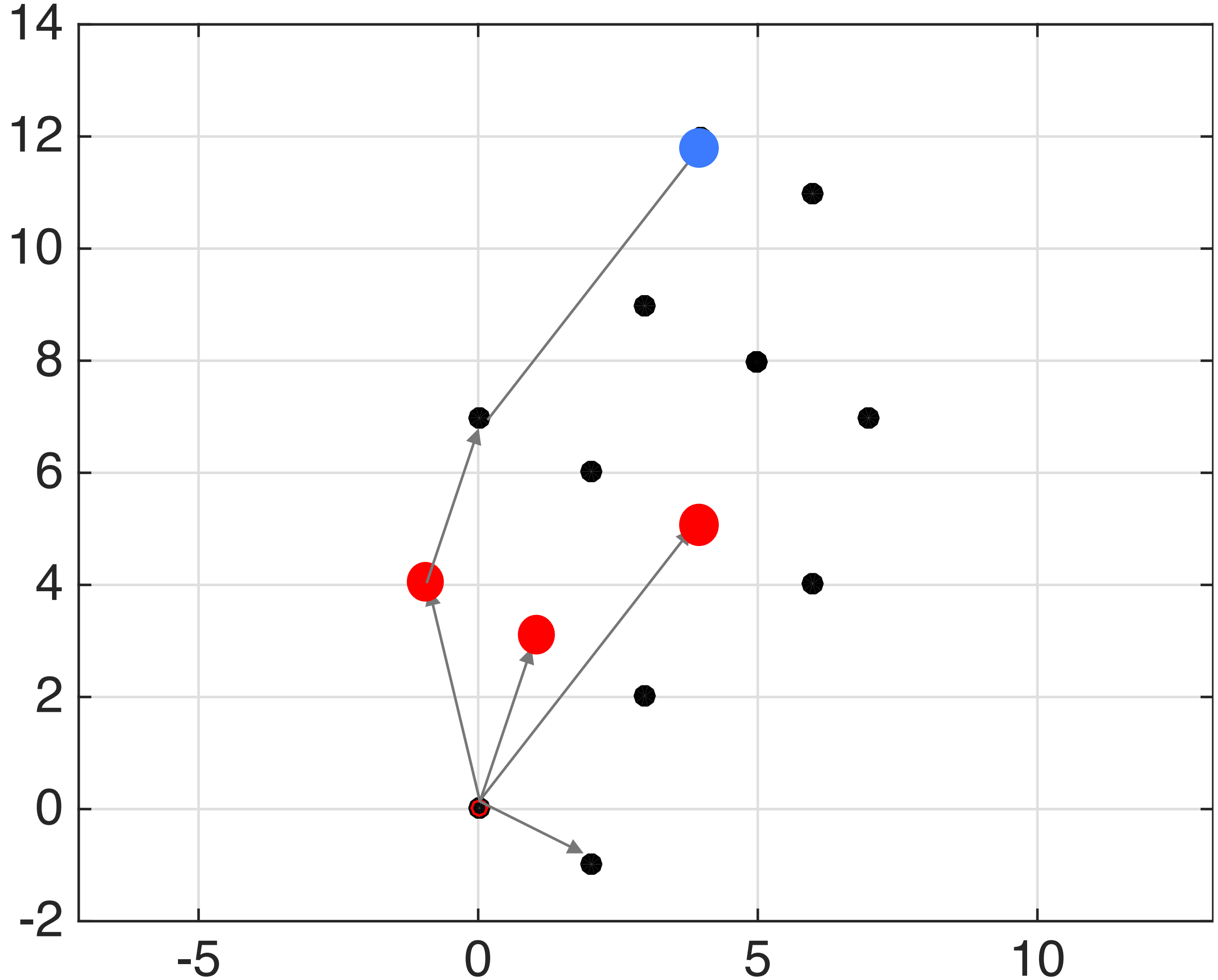
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



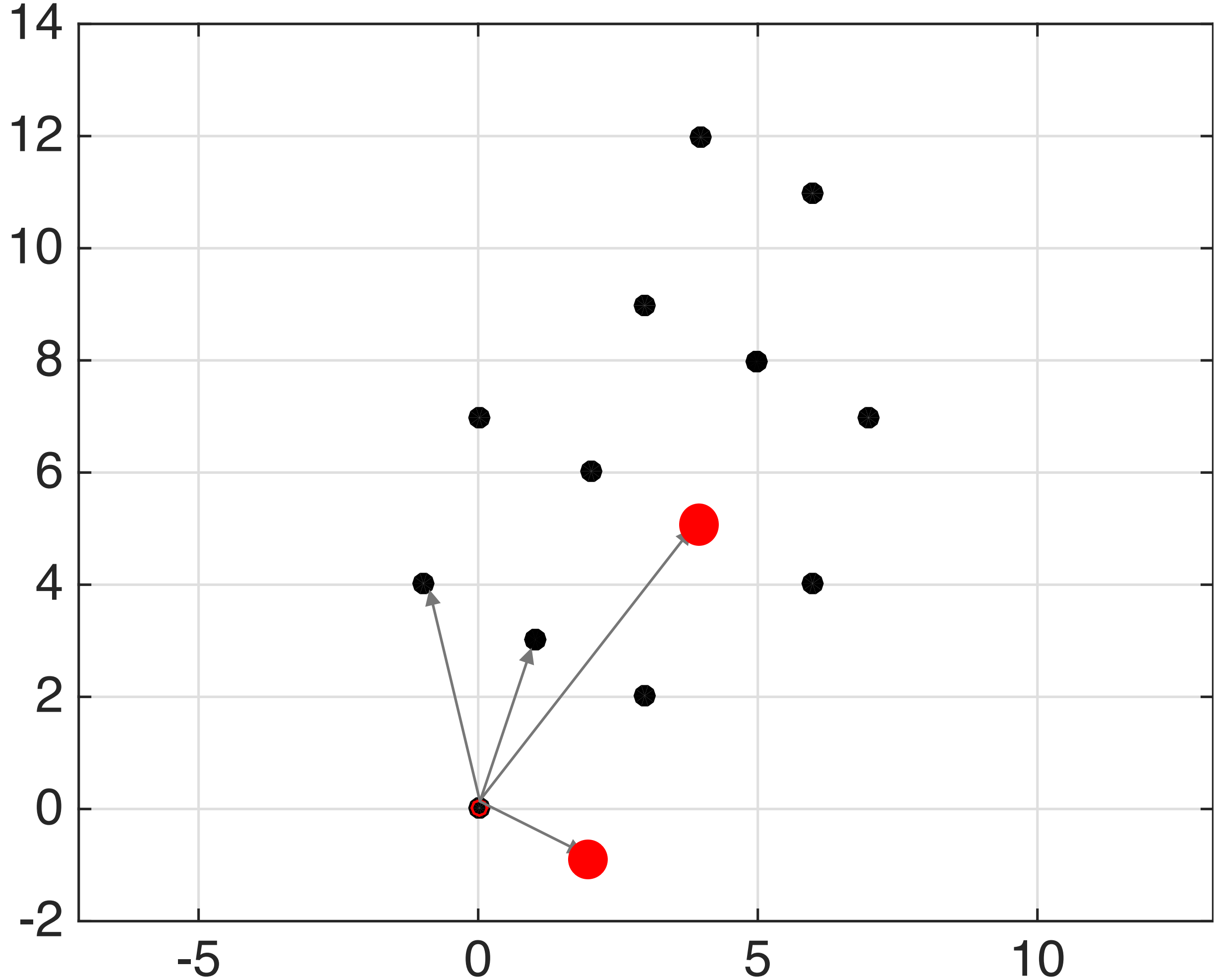
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



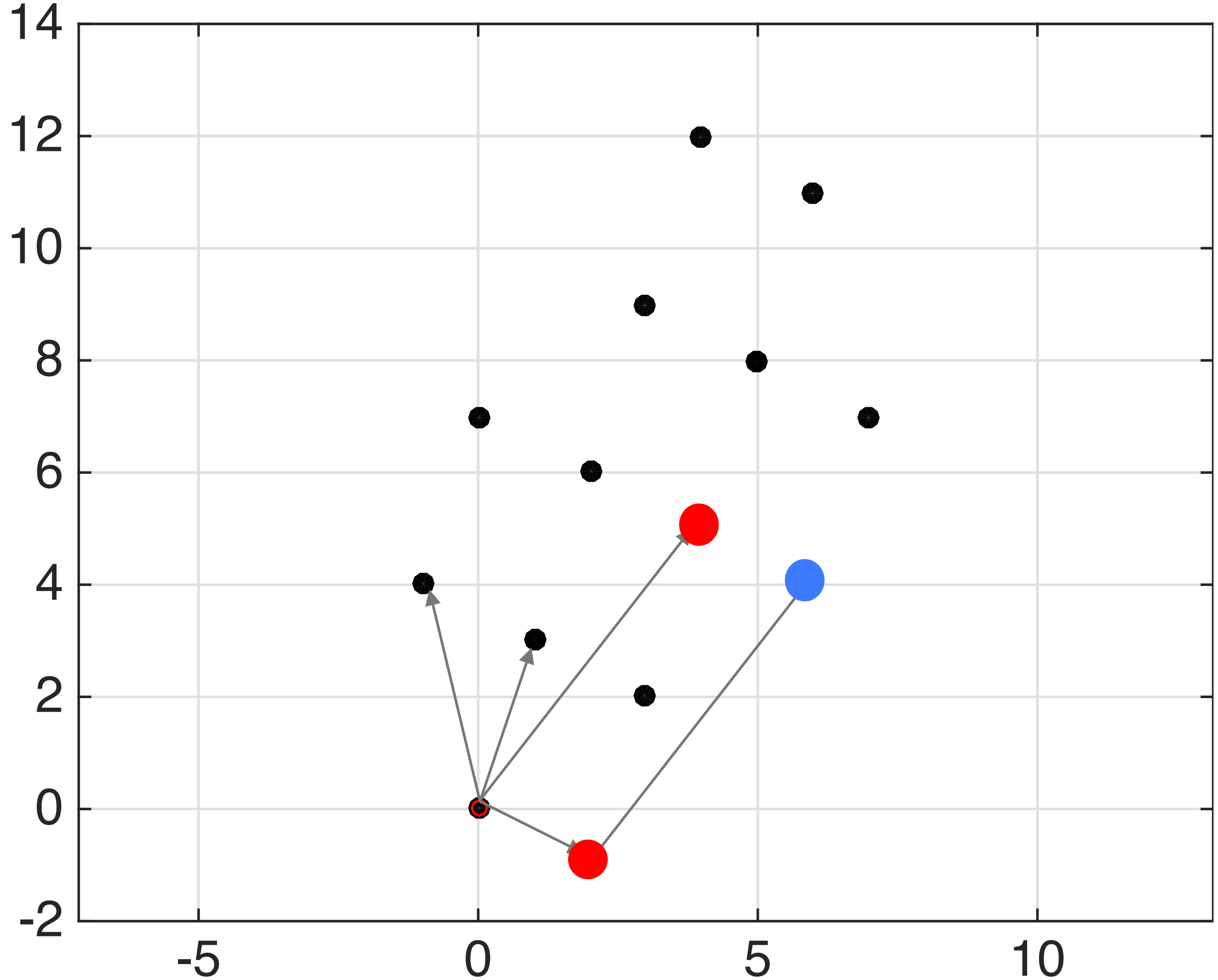
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



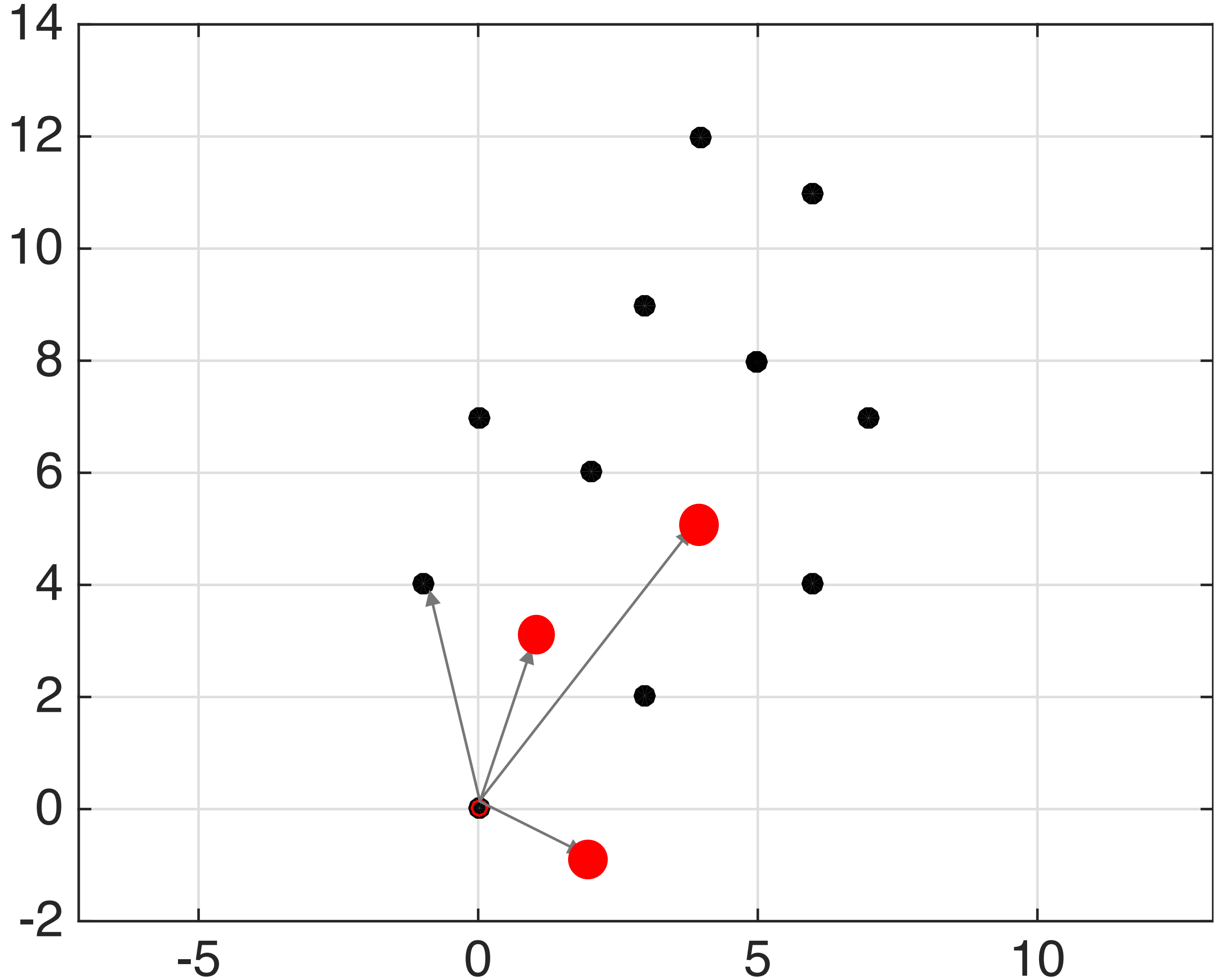
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



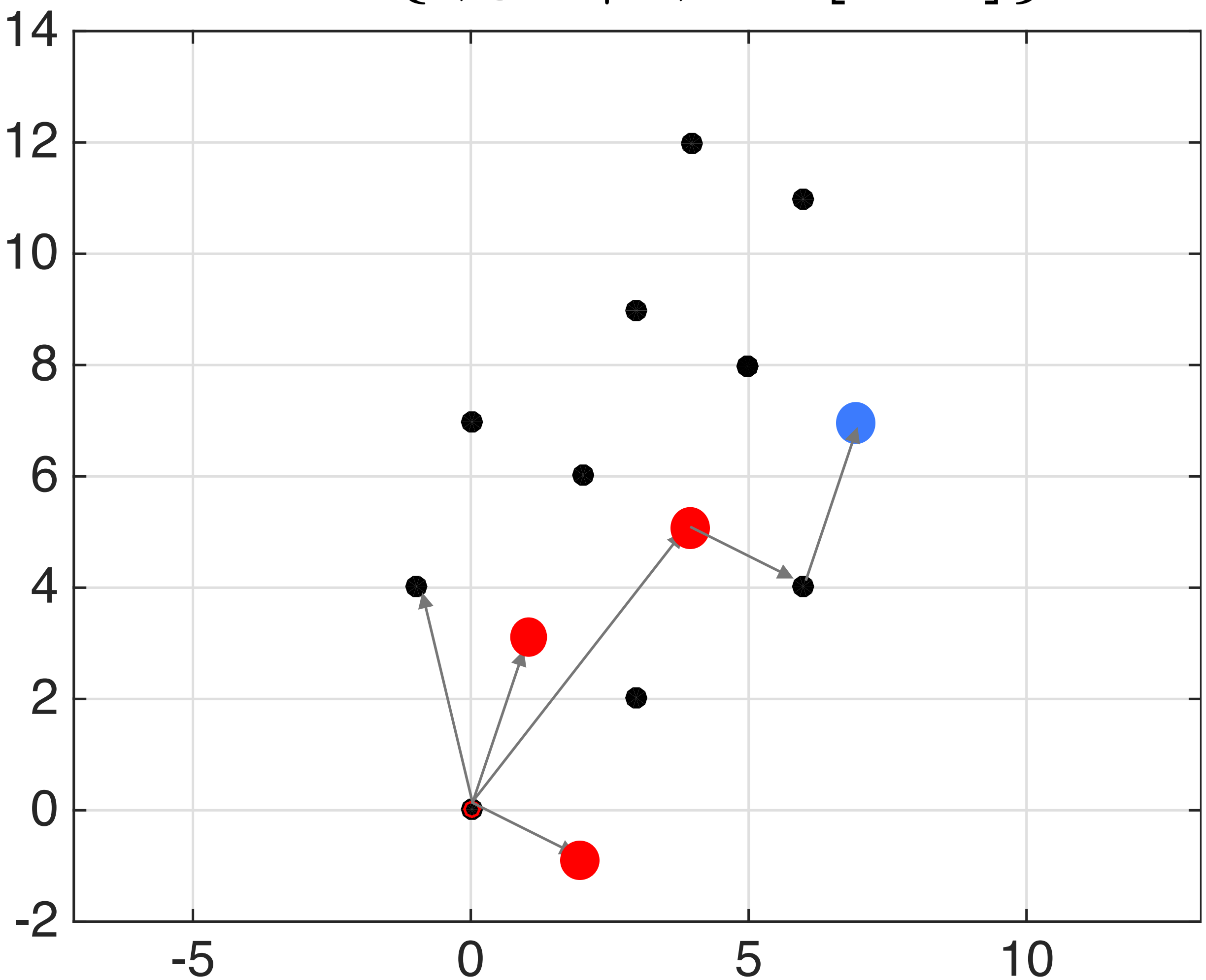
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0, 1]\}$$



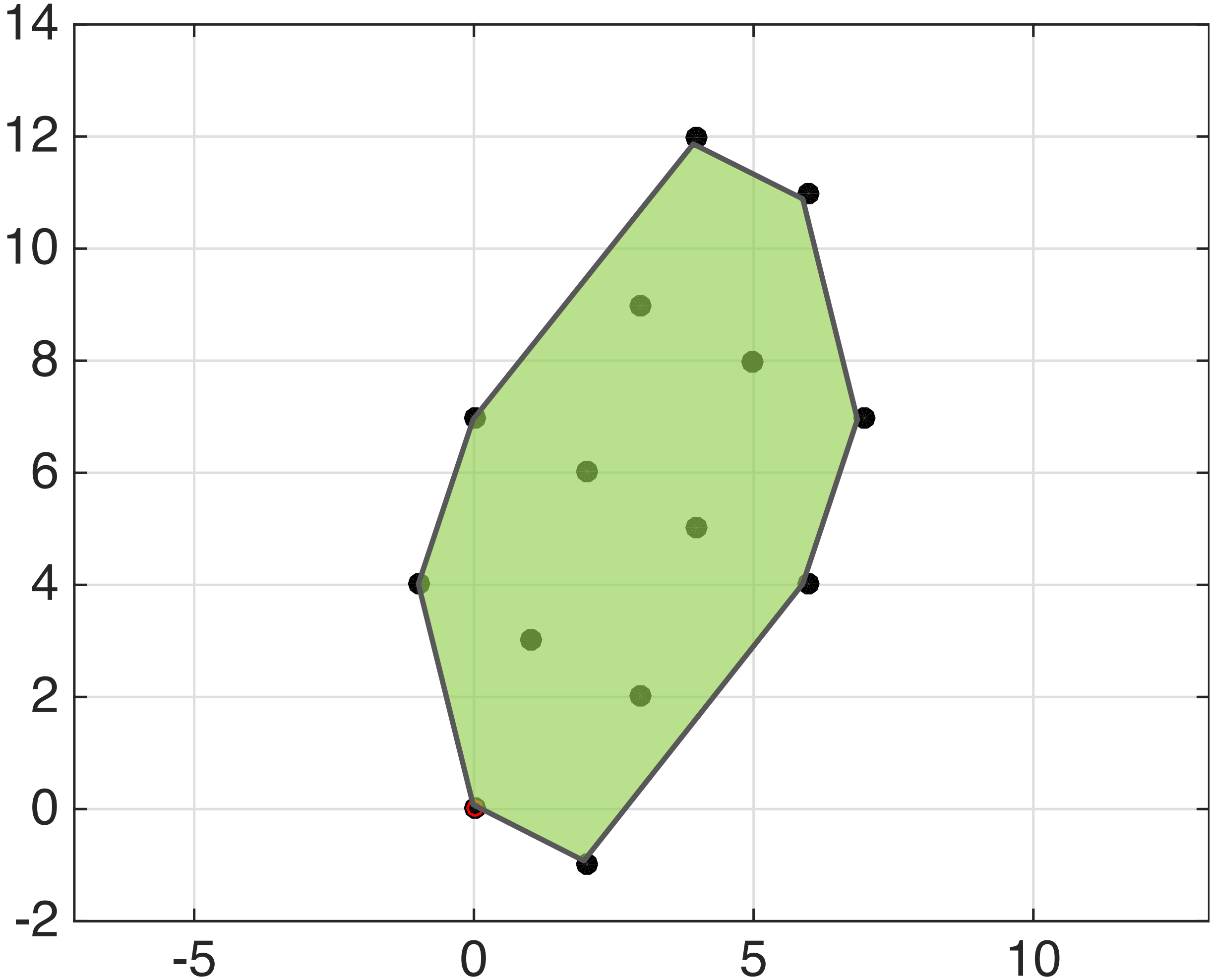
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0,1]\}$$



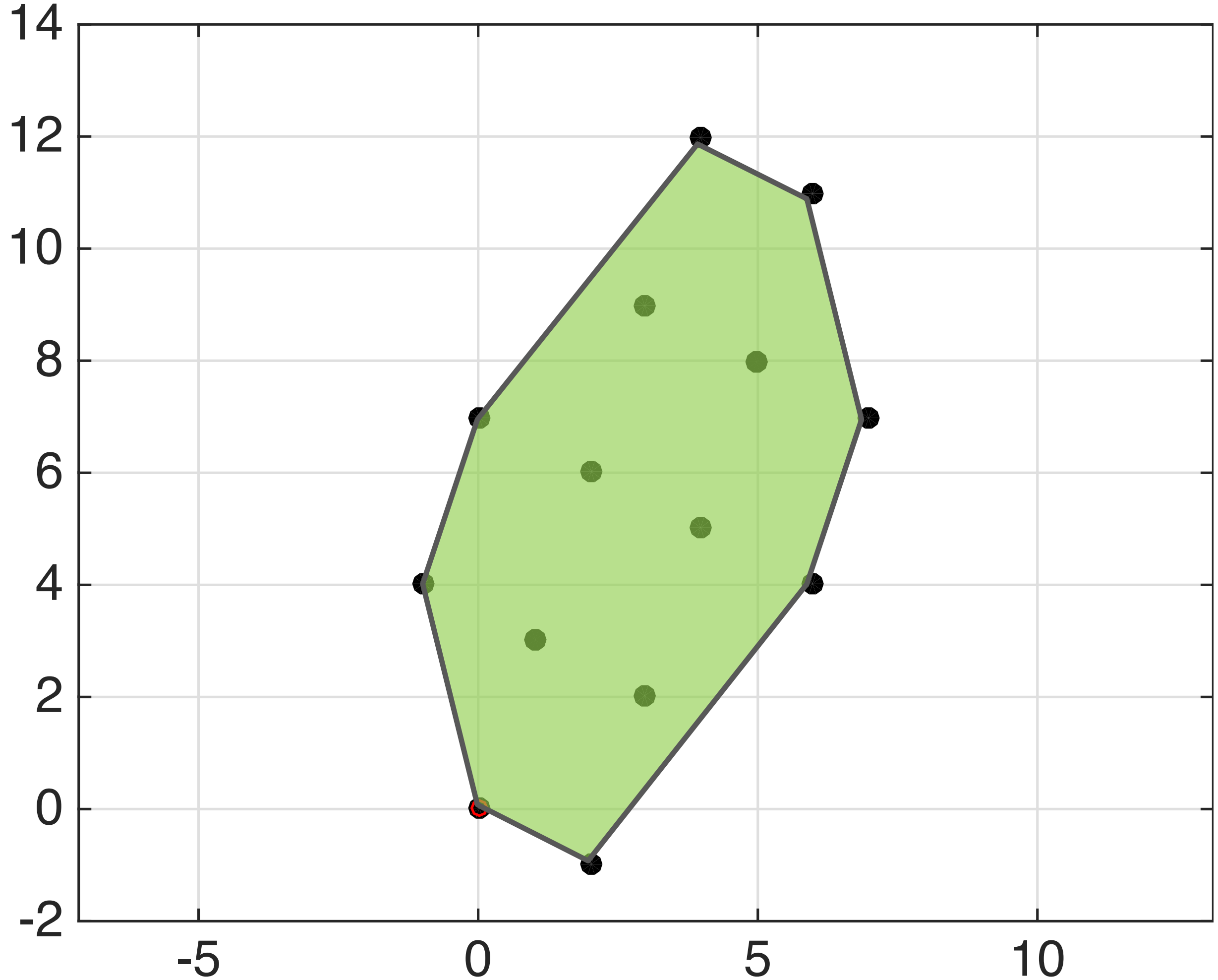
$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

$$\mathbf{G}_i = \{\gamma g_i \mid \gamma \in [0, 1]\}$$



$$\mathbf{G} = \begin{bmatrix} g_1 & g_2 & \cdots & g_n \end{bmatrix}$$

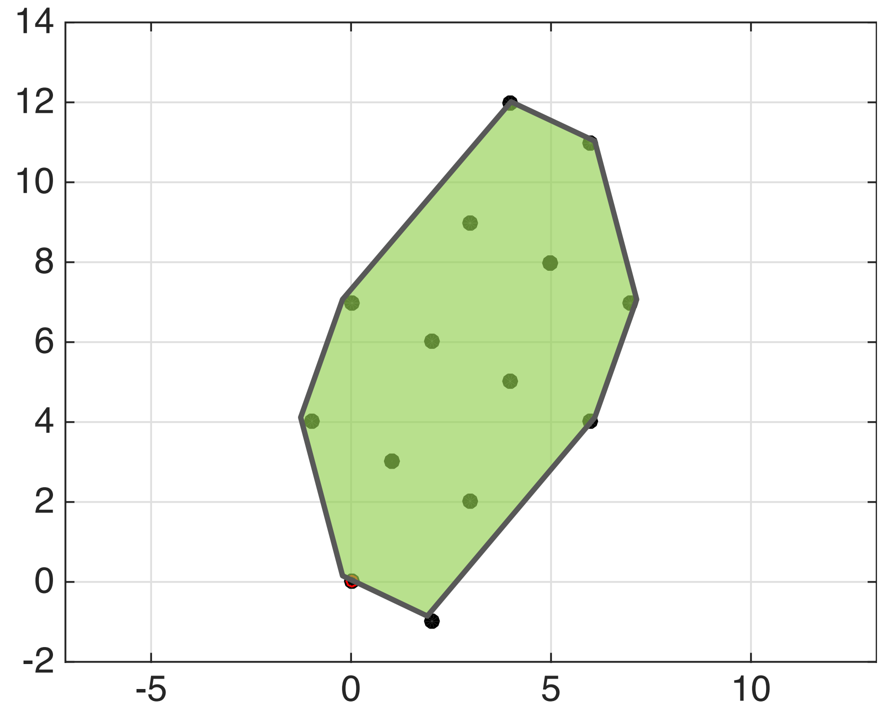
Zonotope: a minkowski sum of line segments



$$\mathcal{Z} = G_1 \oplus G_2 \oplus \cdots \oplus G_n$$

Zonotope Properties

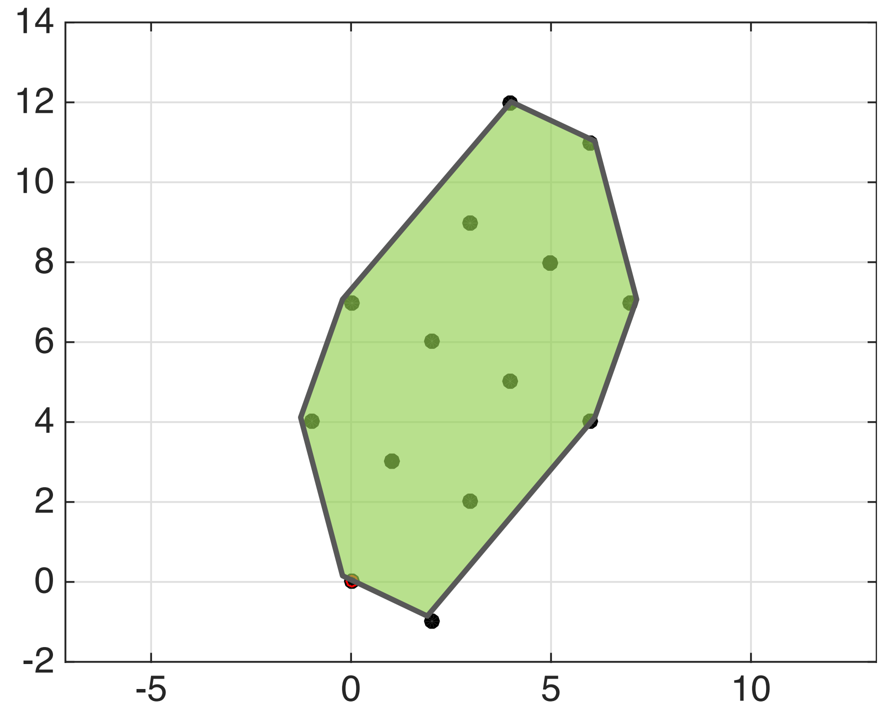
- Convex
- Centrally-symmetric
- $O(n^{d-1})$ vertices



$$\mathcal{Z}(\mathbf{G}) = \mathbf{conv}\{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in \{0,1\}^n\}$$

Zonotope Properties

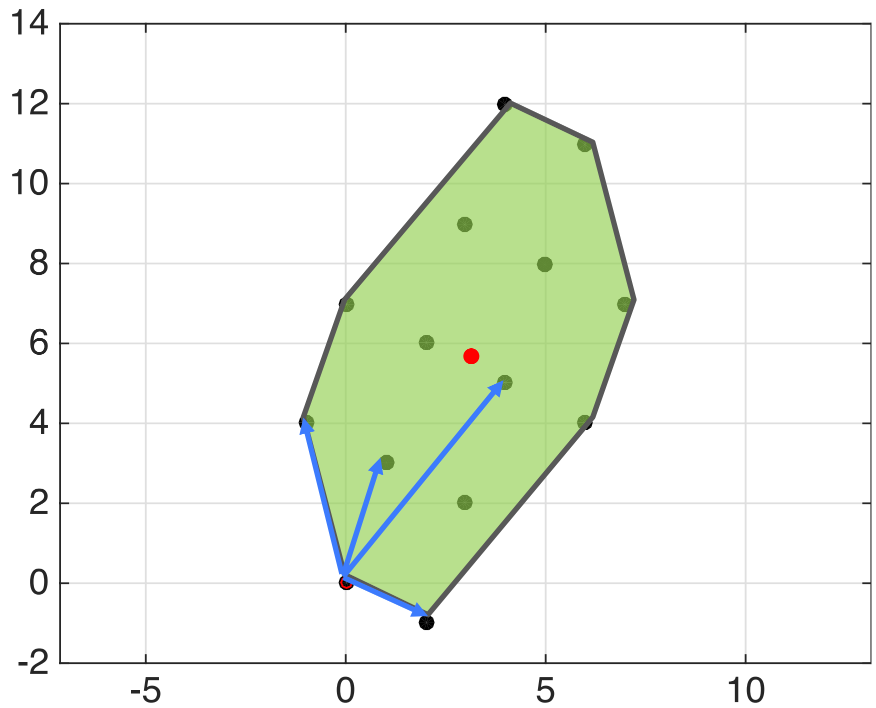
- Convex
- Centrally-symmetric
- $O(n^{d-1})$ vertices



Zonotope Properties

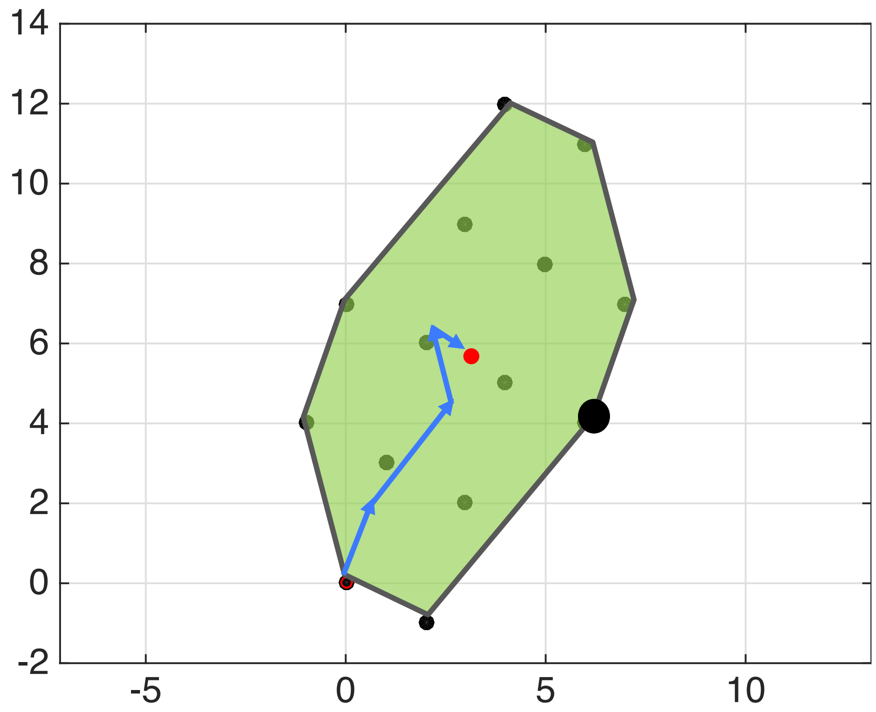
- Convex
- Centrally-symmetric
- $O(n^{d-1})$ vertices

$$\text{Center} = \frac{1}{2}\sum_{i}^{n} g_i$$



Zonotope Properties

- Convex
- Centrally-symmetric
- $O(n^{d-1})$ vertices

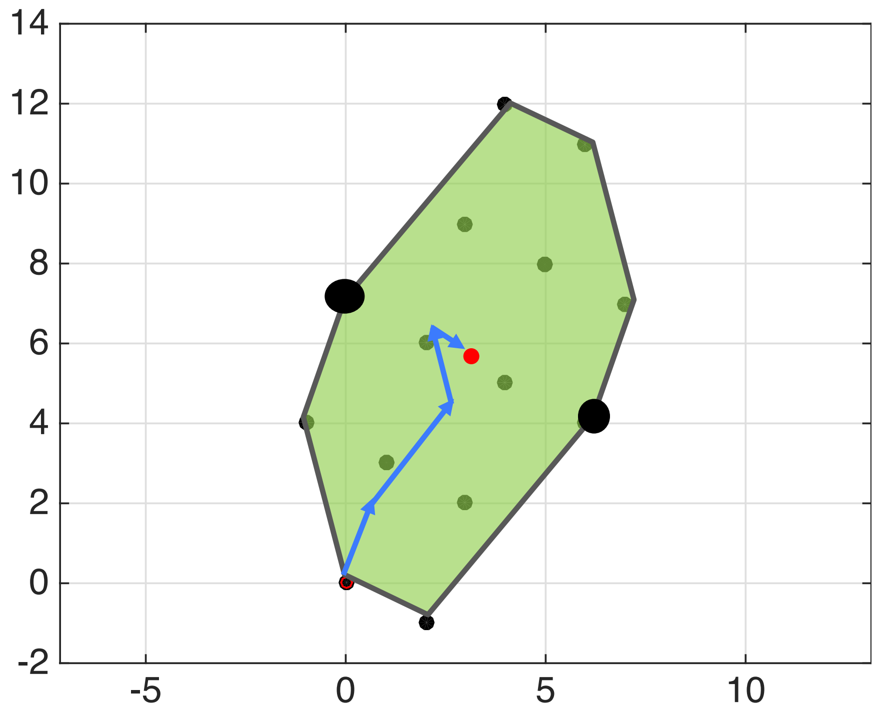


$$\text{Center} = \frac{1}{2}\sum_{i}^{n} g_i$$

$$\text{Both } (1, 0, 0, 1)$$

Zonotope Properties

- Convex
- Centrally-symmetric
- O(n^{d-1}) vertices

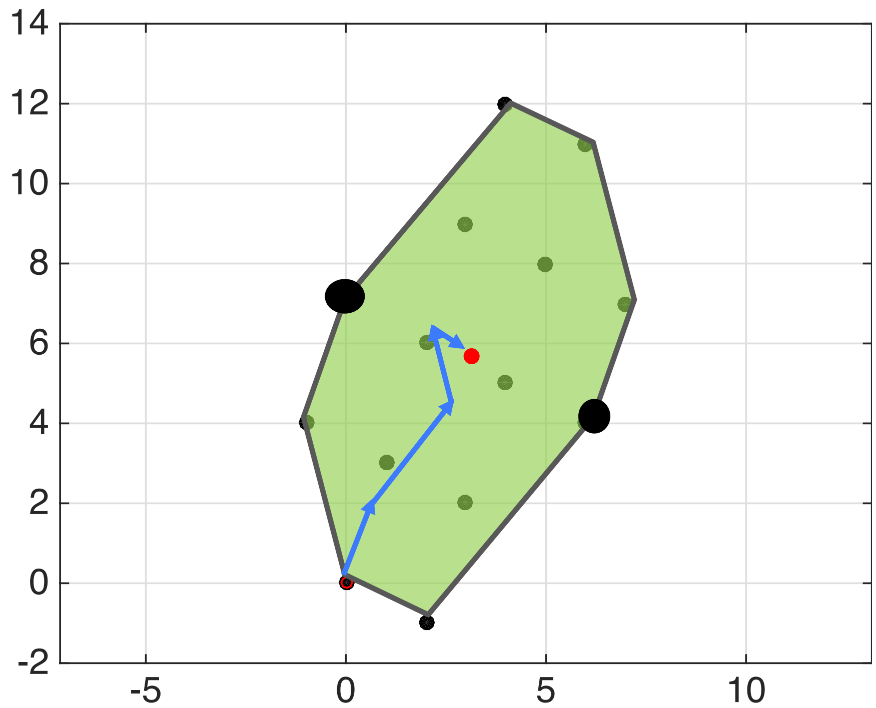


$$\text{Center } = \frac{1}{2}\sum_{i}^{n} g_i$$

Both $(1,0,0,1)$ and $(0,1,1,0)$ are inputs

Zonotope Properties

- Convex
- Centrally-symmetric
- $O(n^{d-1})$ vertices



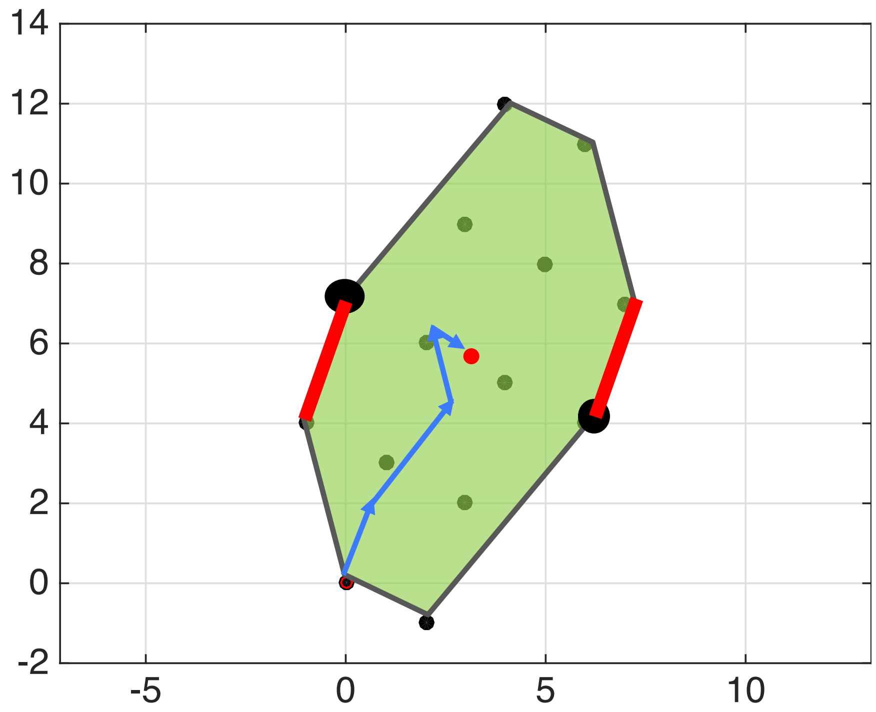
$$\text{Center } = \frac{1}{2}\sum_{i}^{n} g_i$$

Both $(1,0,0,1)$ and $(0,1,1,0)$ are inputs

The zonotope has parallel faces

Zonotope Properties

- Convex
- Centrally-symmetric
- $O(n^{d-1})$ vertices

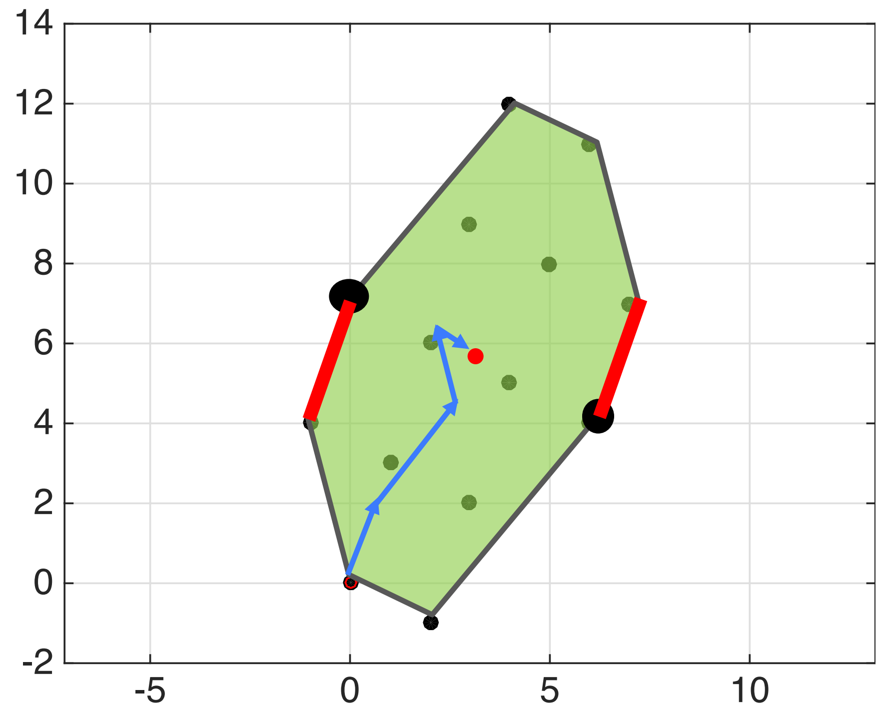


$$\text{Center} = \frac{1}{2}\sum_{i}^{n} g_i$$

Both $(1,0,0,1)$ and $(0,1,1,0)$ are inputs

The zonotope has parallel faces

Zonotope Properties

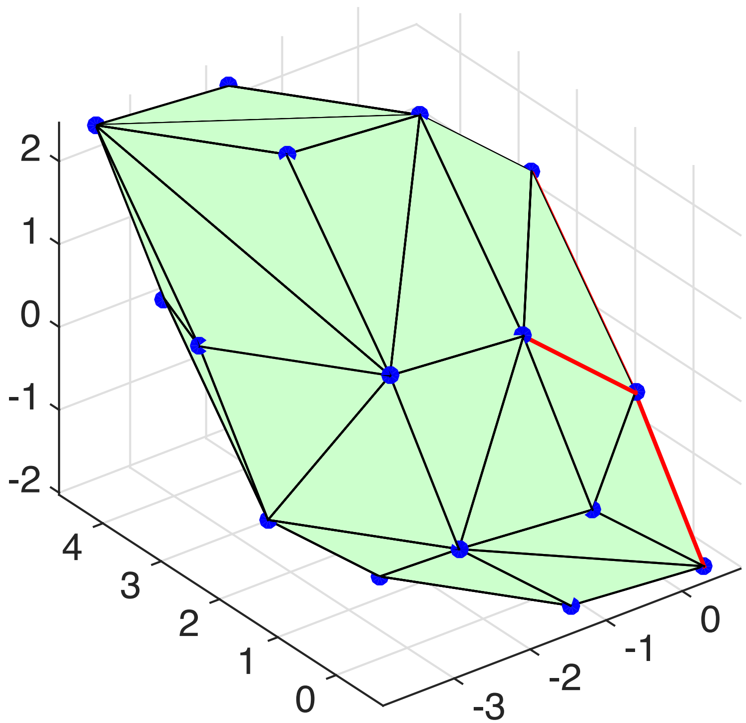


- Convex
- Centrally-symmetric
- $O(n^{d-1})$ vertices

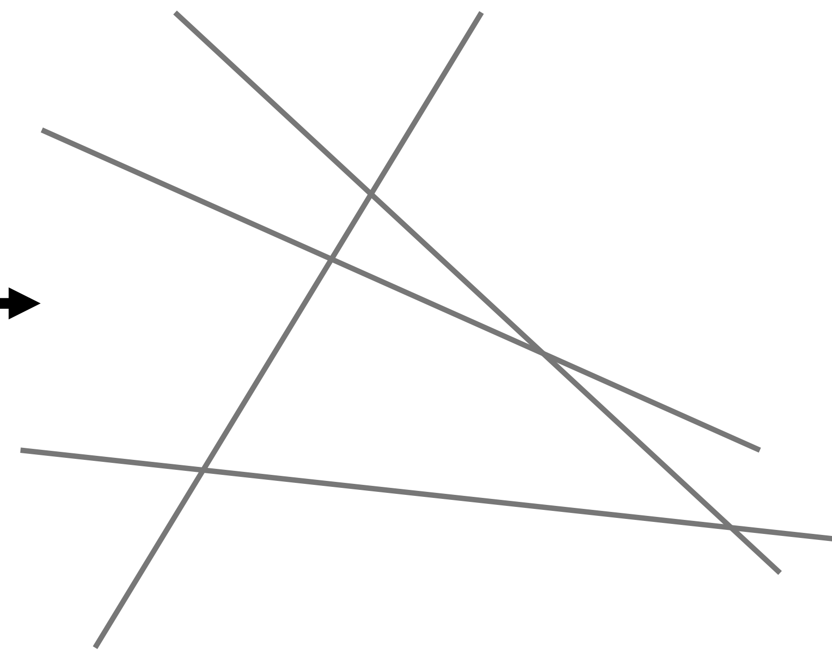
Theorem:

$$|\mathrm{vert}(\mathcal{Z}(\mathbf{G}))| \leq 2 \sum_{i=0}^{d-1} \binom{n-1}{i} = O(n^{d-1})$$

Dual Problem: Enumerating Cells of a Hyperplane Arrangement



A zonotope in 3D with 5 generators



A hyperplane arrangement in 2D with 4 hyperplanes

Solving 01BQ for low-rank, PSD matrices

$$\boxed{\begin{aligned} &\max \ \mathbf{x}^T \mathbf{A} \mathbf{x} \\ &\text{s.t. } \ \mathbf{x} \in \{0,1\}^n \end{aligned}}$$

$$\text{where} \quad \mathbf{A} = \mathbf{G}^T \mathbf{G}$$

$$\text{for } \mathbf{G} \in \mathbb{R}^{d \times n}$$

$$\text{since} \quad \mathbf{x}^T \mathbf{A} \mathbf{x} = \mathbf{x}^T \mathbf{G}^T \mathbf{G} \mathbf{x}$$
$$= ||\mathbf{G}\mathbf{x}||_2^2$$

$$\text{since} \quad \mathbf{x}^T\mathbf{A}\mathbf{x} = \mathbf{x}^T\mathbf{G}^T\mathbf{G}\mathbf{x}$$
$$= ||\mathbf{G}\mathbf{x}||_2^2$$

by convexity: $\mathbf{x} \in \{0,1\}^n \to \mathbf{x} \in [0,1]^n$

$$\text{since} \quad \mathbf{x}^T \mathbf{A} \mathbf{x} = \mathbf{x}^T \mathbf{G}^T \mathbf{G} \mathbf{x}$$
$$= ||\mathbf{G}\mathbf{x}||_2^2$$

$$\text{by convexity: } \mathbf{x} \in \{0,1\}^n \rightarrow \mathbf{x} \in [0,1]^n$$

The problem is equivalent to:

$$\max \, ||\mathbf{z}||_2^2$$

$$\text{s.t. } \mathbf{z} \in \mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]^n\}$$

$$\text{since} \quad \mathbf{x}^T \mathbf{A} \mathbf{x} = \mathbf{x}^T \mathbf{G}^T \mathbf{G} \mathbf{x}$$
$$= ||\mathbf{G}\mathbf{x}||_2^2$$

$$\boxed{\text{by convexity: } \mathbf{x} \in \{0,1\}^n \rightarrow \mathbf{x} \in [0,1]^n}$$

The problem is equivalent to:

$$\max \; ||\mathbf{z}||_2^2$$

$$\text{s.t. } \; \mathbf{z} \in \mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [0,1]^n\}$$

Theorem: the maximum of a convex function *f* over a convex polytope S will be attained at a vertex *v* of the S

$$\max_{x \in S} \; f(x)$$

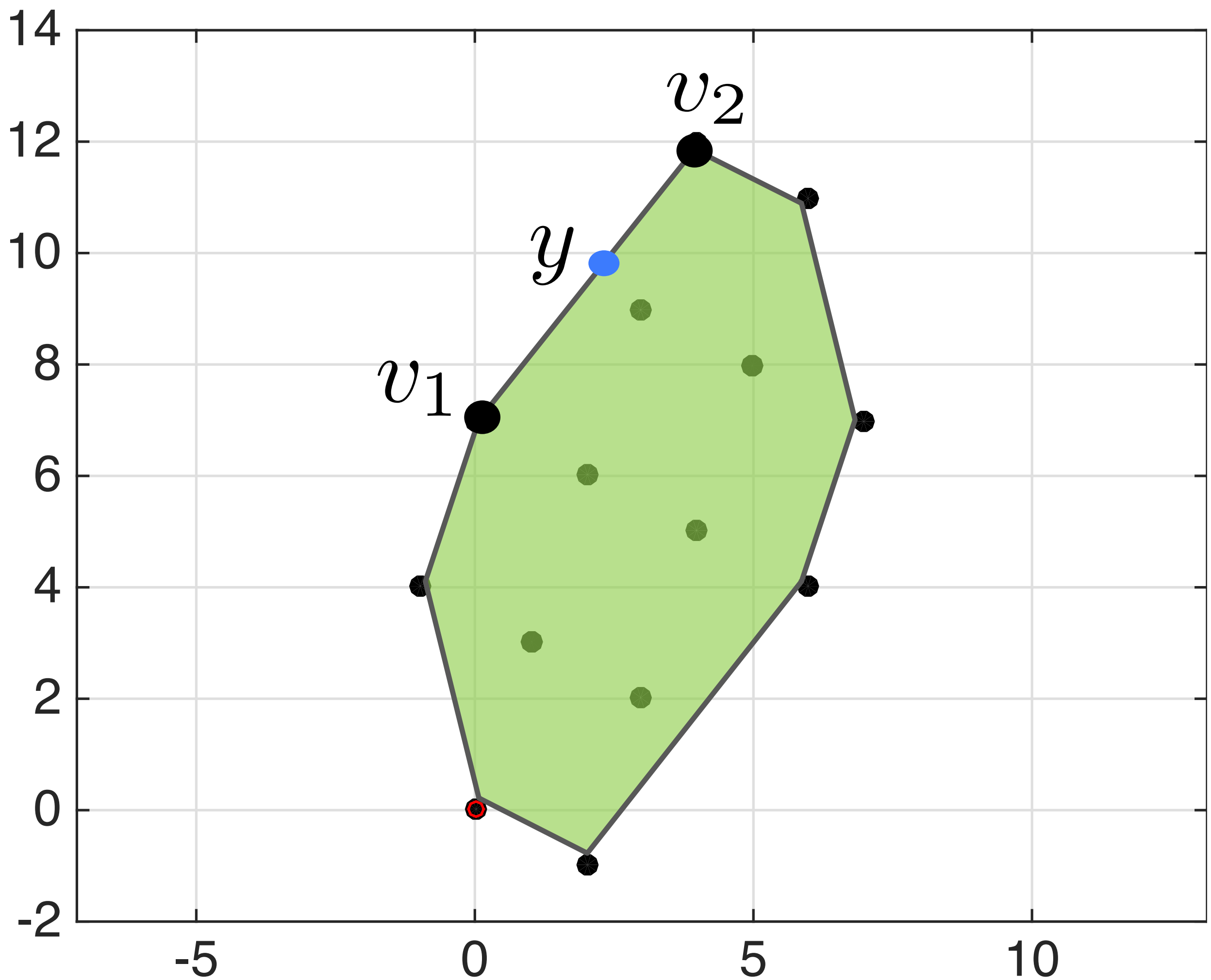
$$\text{where } S = \left\{ \sum_{i=1}^{k} \alpha_i v_i \; : \; \sum \alpha_i = 1, \alpha_i \geq 0 \right\}$$

Proof

$$\text{Let } y = \sum_{i=1}^{k} \alpha_i v_i$$

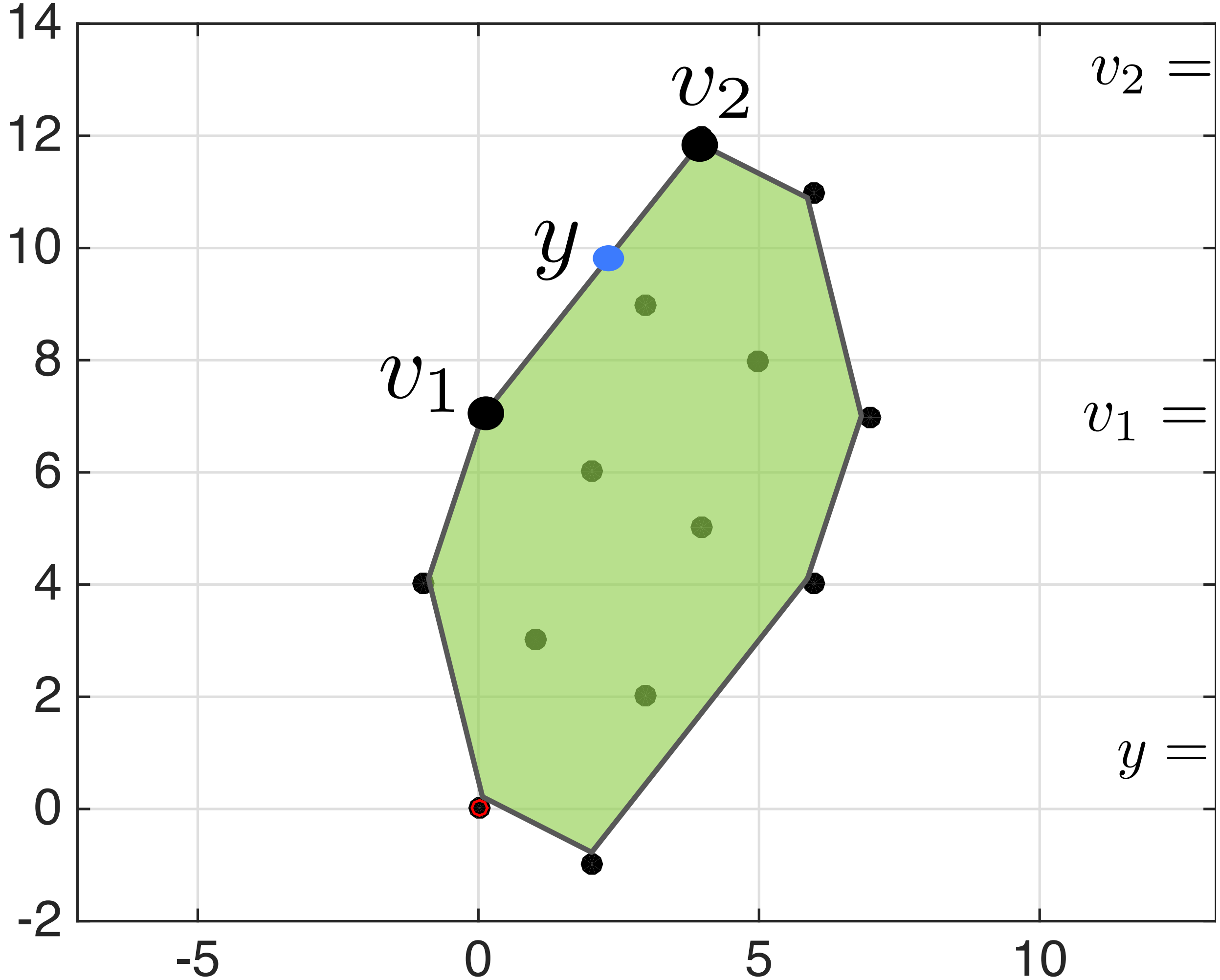
$$\begin{aligned} f(y) &= f\left(\sum_{i=1}^{k} \alpha_i v_i\right) \\ &\leq \sum_{i=1}^{k} \alpha_i f(v_i) \\ &\leq f(v_j) \quad \text{for some } j \end{aligned}$$

Proof



$$f(y) = f(\alpha v_1 + (1-\alpha)v_2) \leq \alpha f(v_1) + (1-\alpha) f(v_2) \leq f(v_i)$$

Proof



$$v_2 = \mathbf{G} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$v_1 = \mathbf{G} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$

$$y = \mathbf{G} \begin{bmatrix} 0 \\ 1 \\ 1 \\ .5 \end{bmatrix}$$

$$f(y) = f(\alpha v_1 + (1-\alpha) v_2) \leq \alpha f(v_1) + (1-\alpha) f(v_2) \leq f(v_i)$$

Solving Low-Rank, PSD Binary QP

$$\max \ ||\mathbf{z}||_2^2$$

$$\text{s.t. } \mathbf{z} \in \mathcal{Z}(\mathbf{G})$$

The max will be obtained at one of the $O(n^{d-1})$ vertices of the zonotope generated by $\mathbf{G}$

Solving Low-Rank, PSD Binary QP

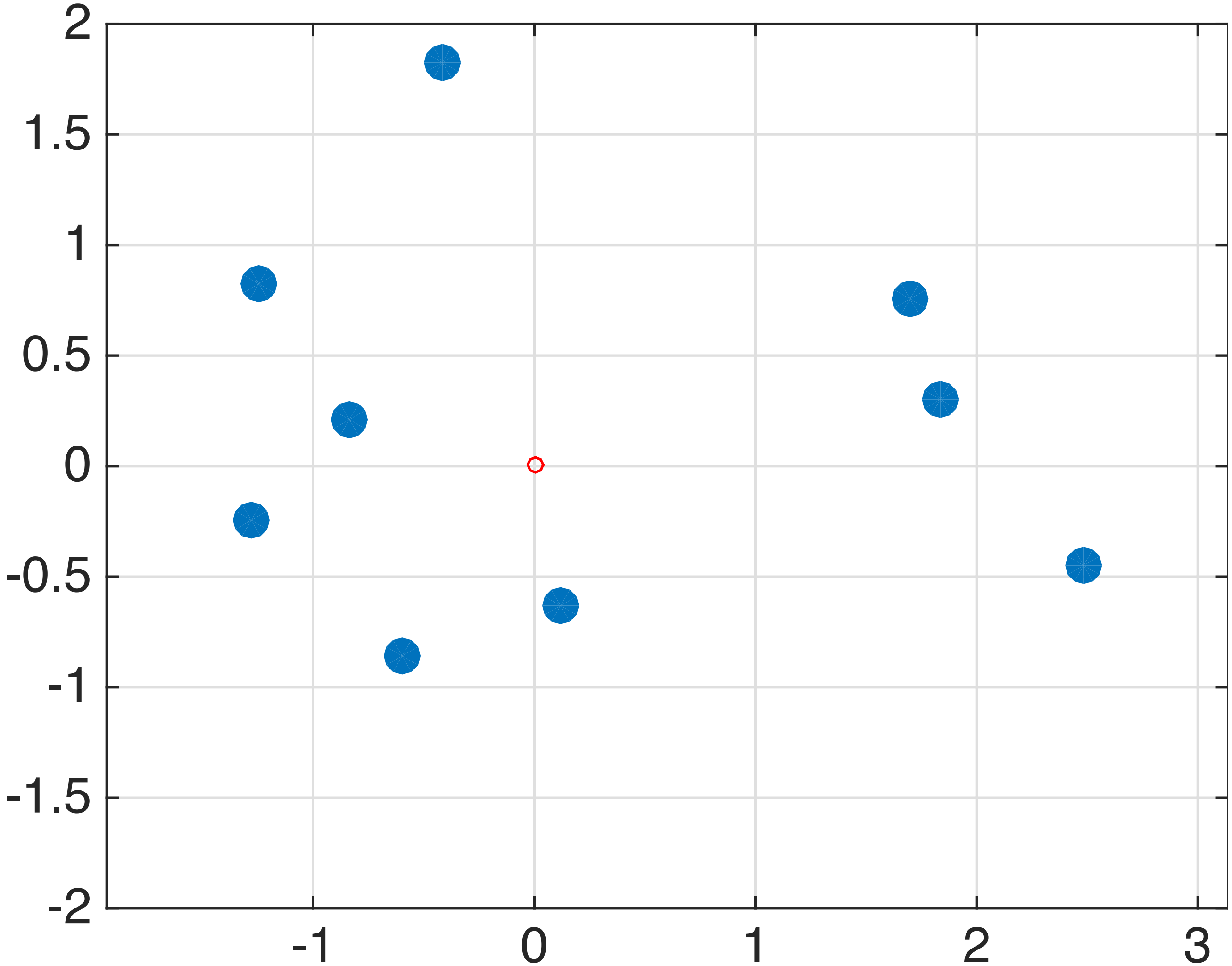
$$\max \ ||\mathbf{z}||_2^2$$

$$\text{s.t. } \ \mathbf{z} \in \mathcal{Z}(\mathbf{G})$$

The max will be obtained at one of the $O(n^{d-1})$ vertices of the zonotope generated by $\mathbf{G}$

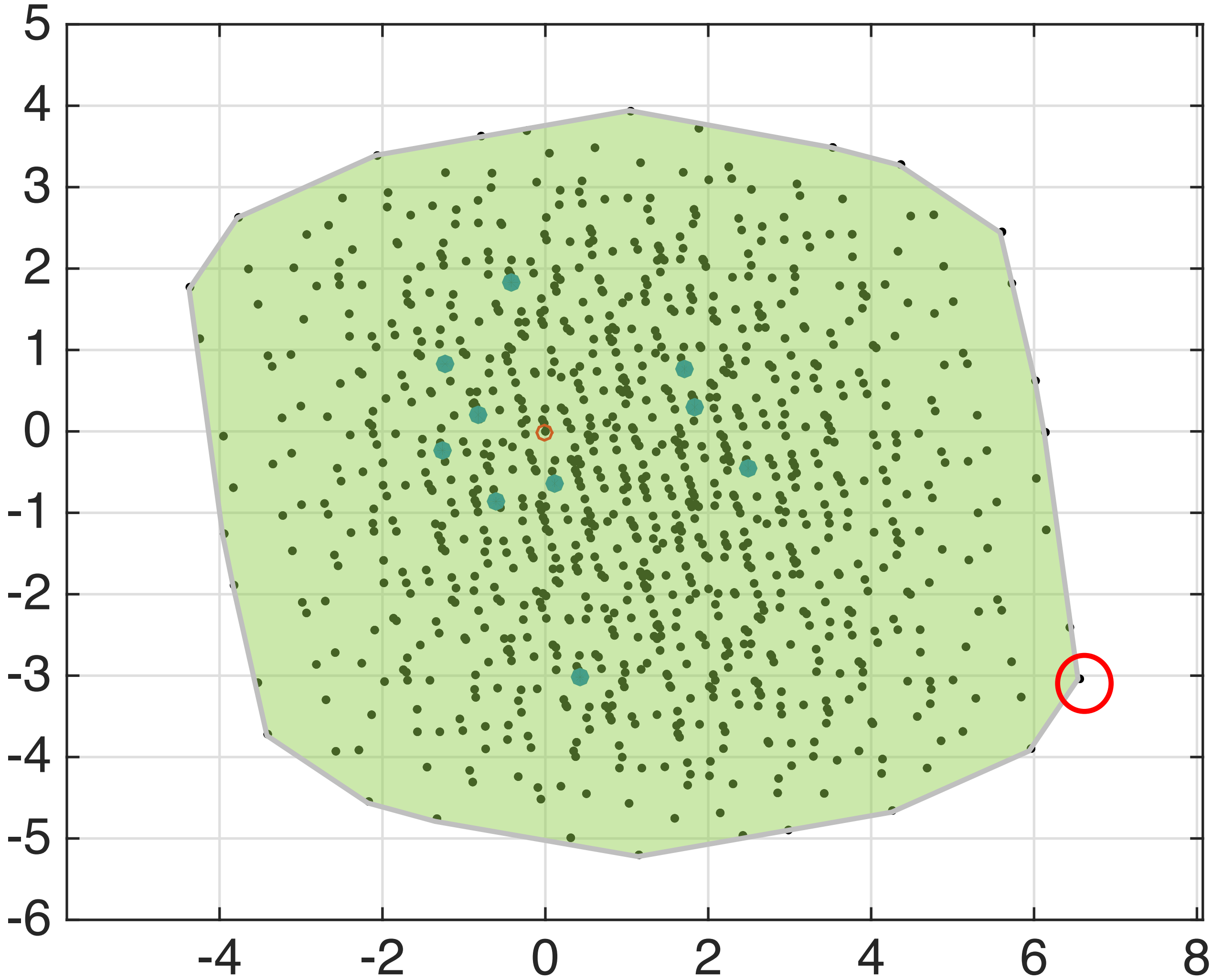
By exploring the vertices of the zonotope we solve the problem in polynomial time.

Example where n = 10, d = 2



Column vectors for a matrix G

Zonotope, with optimal vertex



What about if the binary variables are {-1,1}?

$$\max \ \mathbf{x}^T \mathbf{A} \mathbf{x}$$

$$\text{s.t.} \ \mathbf{x} \in \{-1, 1\}^n$$

$$\mathbf{A} = \mathbf{G}^T \mathbf{G}$$

What about if the binary variables are {-1,1}?

$$\max \quad ||\mathbf{G}\mathbf{x}||_2^2$$

$$\text{s.t.} \quad \mathbf{x} \in \{-1, 1\}^n$$

What about if the binary variables are {-1,1}?

$$\max \; ||\mathbf{G}\mathbf{x}||_2^2$$

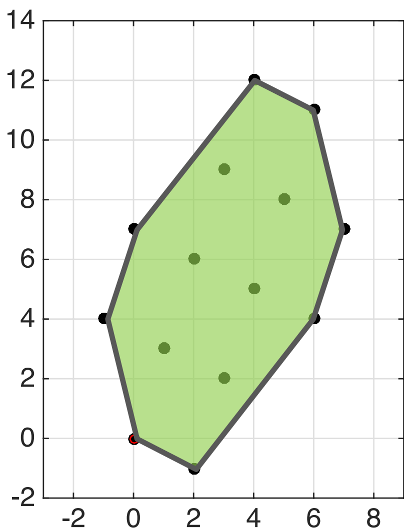
$$\text{s.t. } \mathbf{x} \in \{-1, 1\}^n$$

Project from the $[-1,1]^n$ hypercube

(rather than the $[0,1]^n$ hypercube)

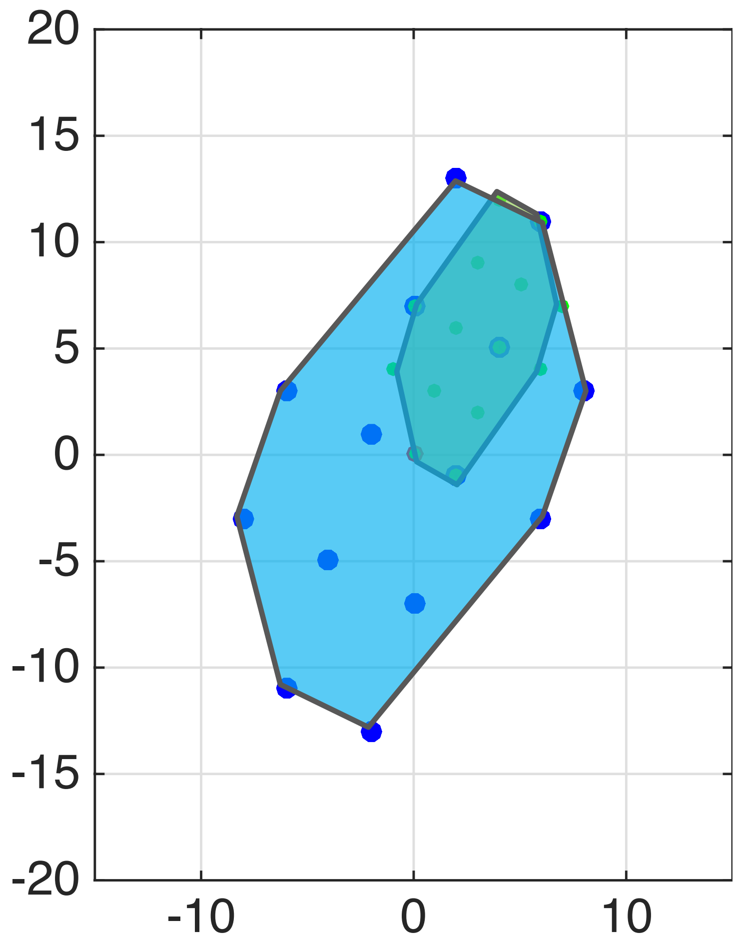
$$\mathcal{Z}(\mathbf{G}) = \{\mathbf{G}\mathbf{x} \,|\, \mathbf{x} \in [-1, 1]^n\}$$

Relationship between zonotopes



$$\mathbf{x} \in \{0, 1\}^n$$

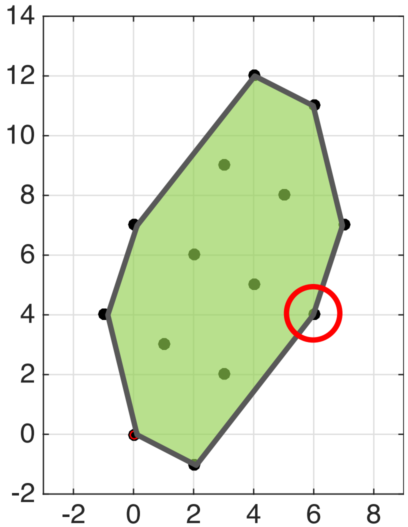
$$\text{Center } = \frac{1}{2}\sum_{i}^{n} g_i$$



$$\mathbf{x} \in \{-1, 1\}^n$$

$$\text{Center } = (0{,}0)$$

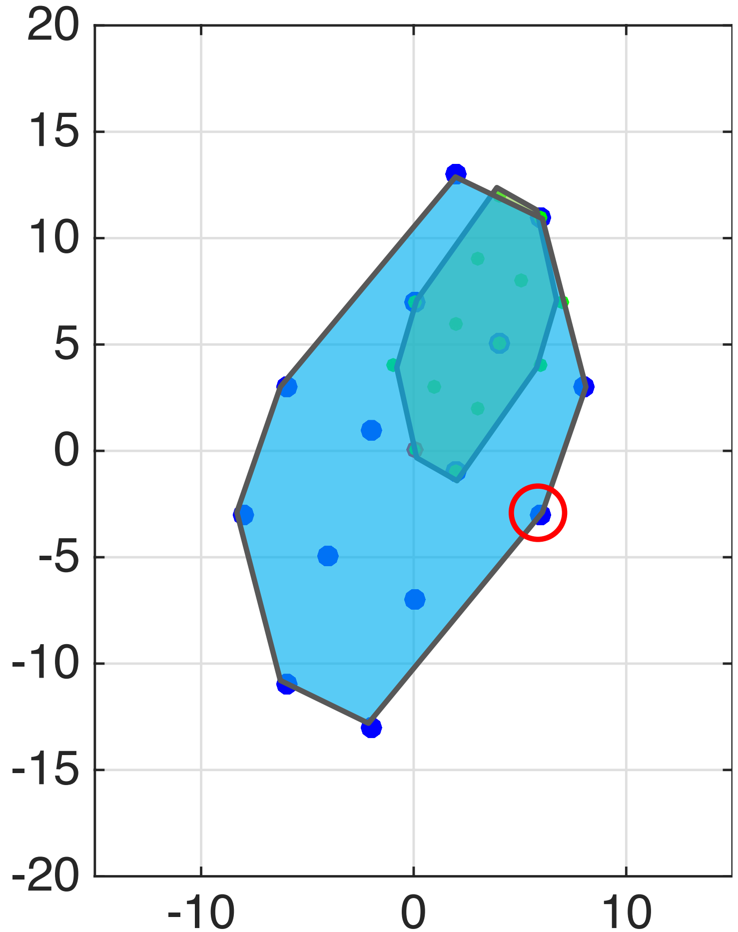
Relationship between zonotopes



$$\begin{bmatrix}1\\0\\0\\1\end{bmatrix}$$

$$\mathbf{x} \in \{0,1\}^n$$

$$\text{Center } = \frac{1}{2}\sum_i^n g_i$$

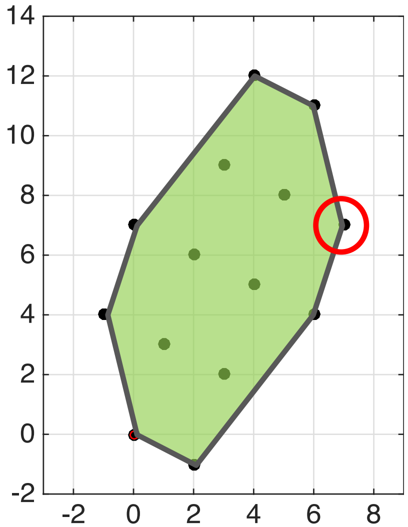


$$\begin{bmatrix}+1\\-1\\-1\\+1\end{bmatrix}$$

$$\mathbf{x} \in \{-1,1\}^n$$

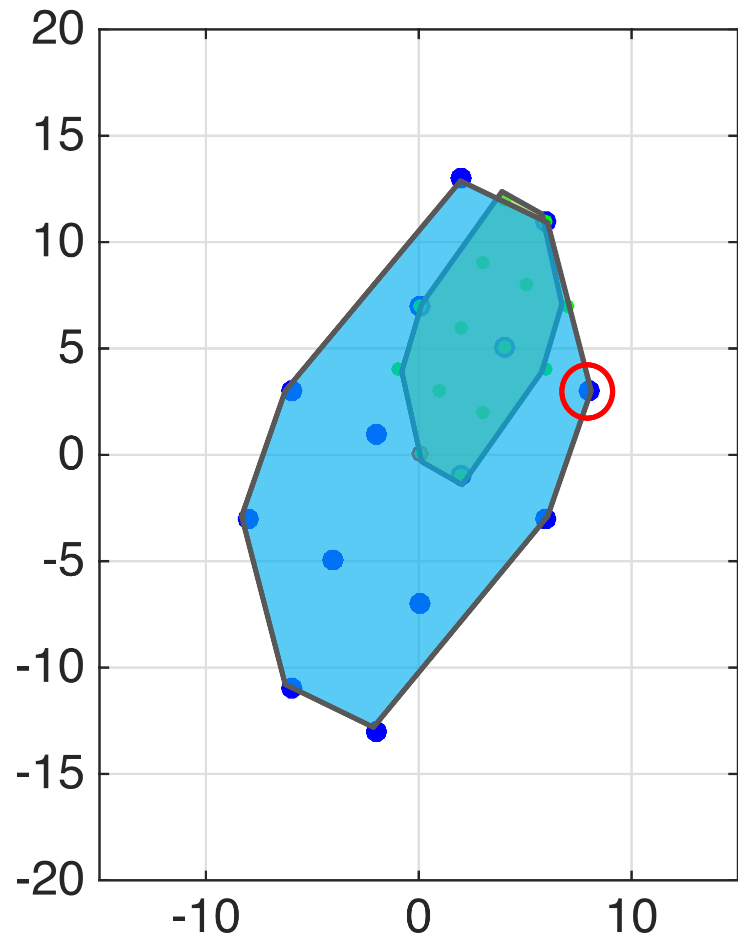
$$\text{Center } = (0{,}0)$$

Relationship between zonotopes



$$\mathbf{x} \in \{0, 1\}^n$$

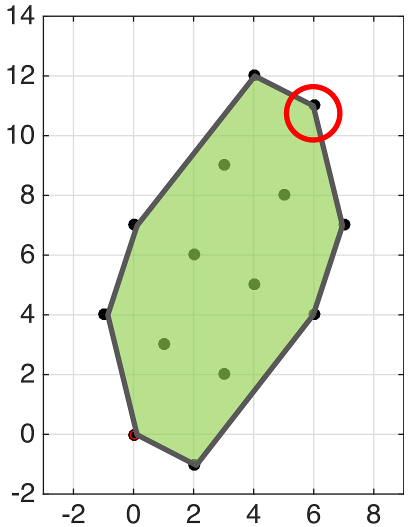
$$\text{Center } = \frac{1}{2}\sum_{i}^{n} g_i$$



$$\mathbf{x} \in \{-1, 1\}^n$$

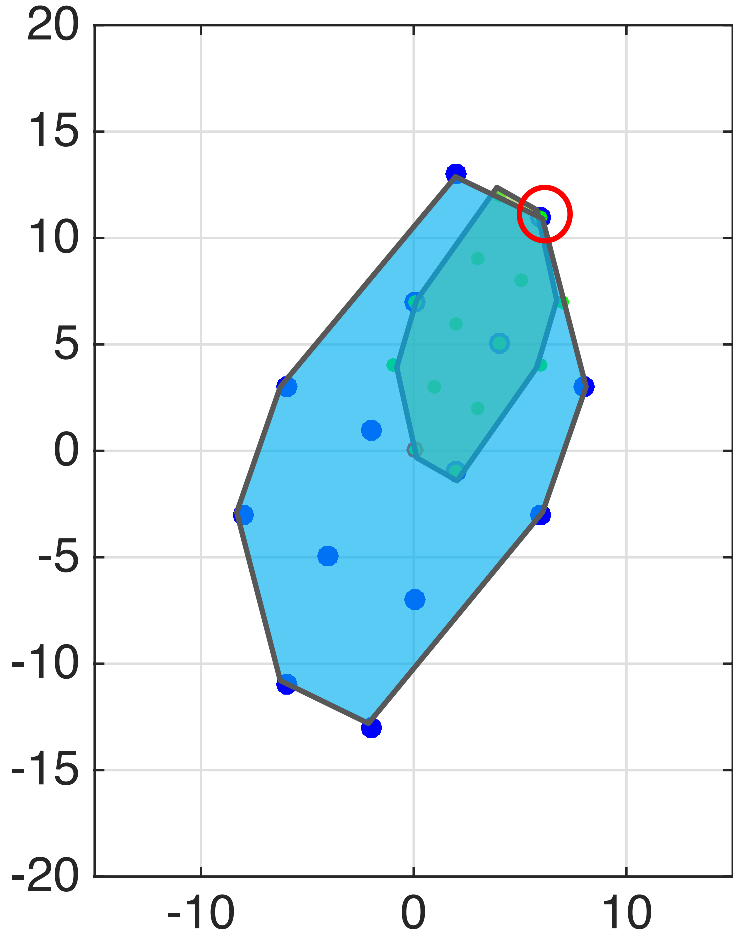
$$\text{Center } = (0,0)$$

Relationship between zonotopes



$$\mathbf{x} \in \{0, 1\}^n$$

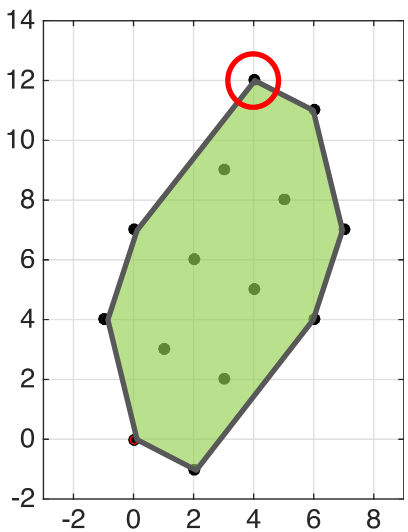
$$\text{Center} = \frac{1}{2}\sum_{i}^{n} g_i$$



$$\mathbf{x} \in \{-1, 1\}^n$$

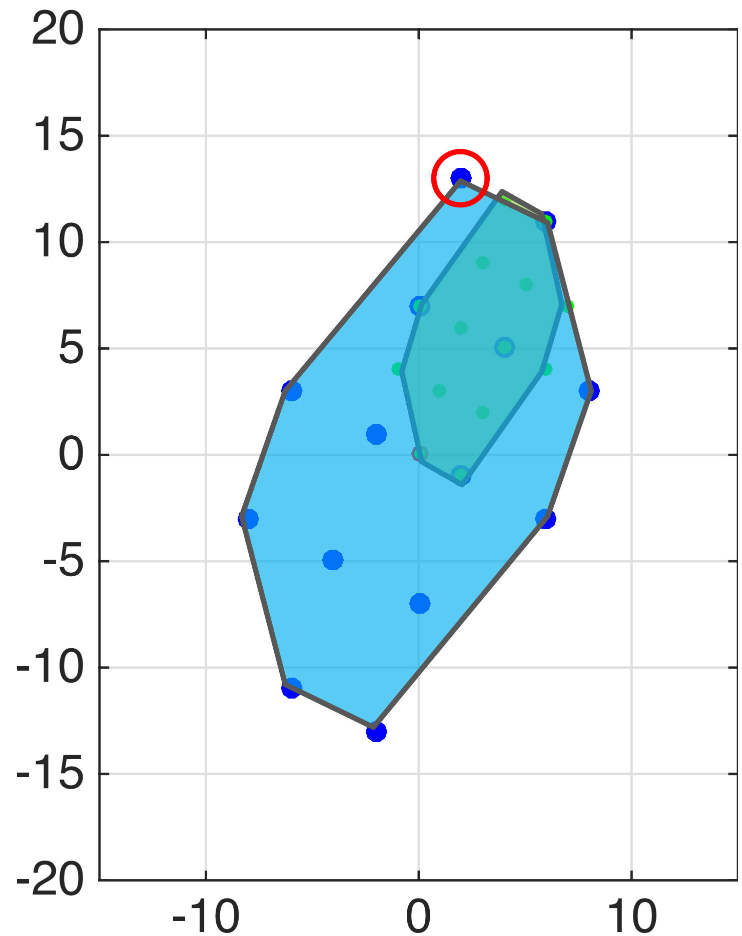
$$\text{Center} = (0{,}0)$$

Relationship between zonotopes



$$\mathbf{x} \in \{0, 1\}^n$$

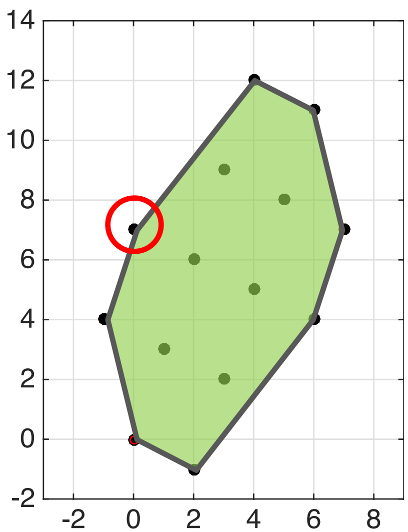
$$\text{Center } = \frac{1}{2}\sum_i^n g_i$$



$$\mathbf{x} \in \{-1, 1\}^n$$

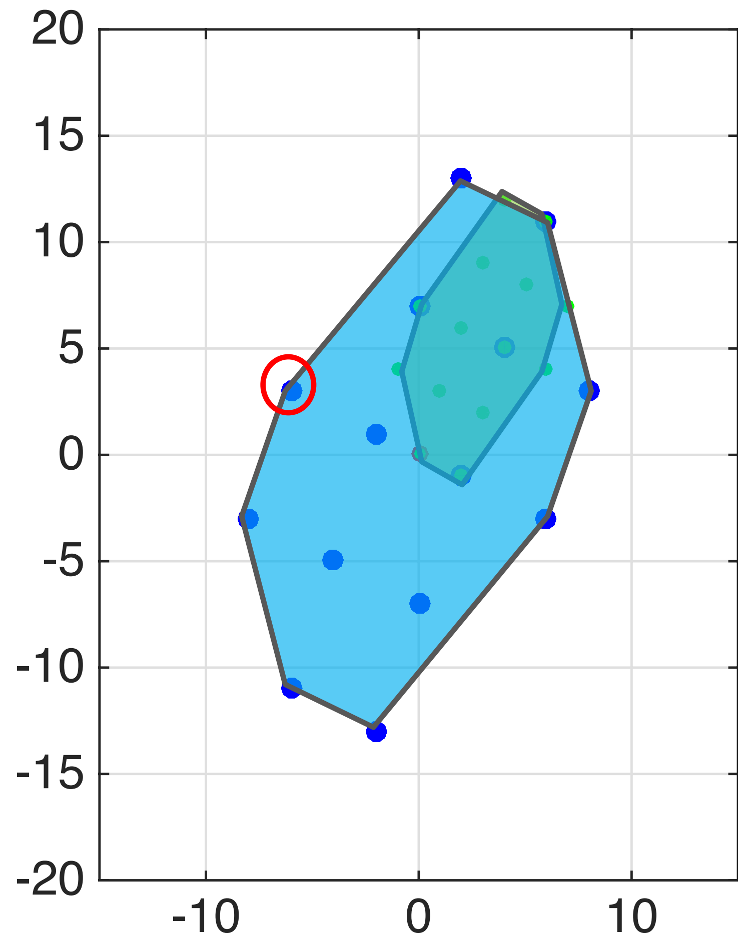
$$\text{Center } = (0{,}0)$$

Relationship between zonotopes



$$\mathbf{x} \in \{0,1\}^n$$

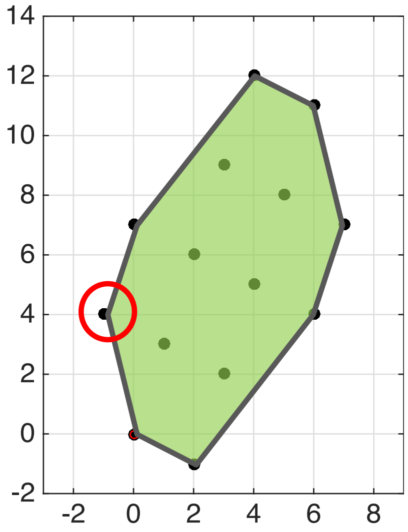
$$\text{Center } = \frac{1}{2}\sum_i^n g_i$$



$$\mathbf{x} \in \{-1,1\}^n$$

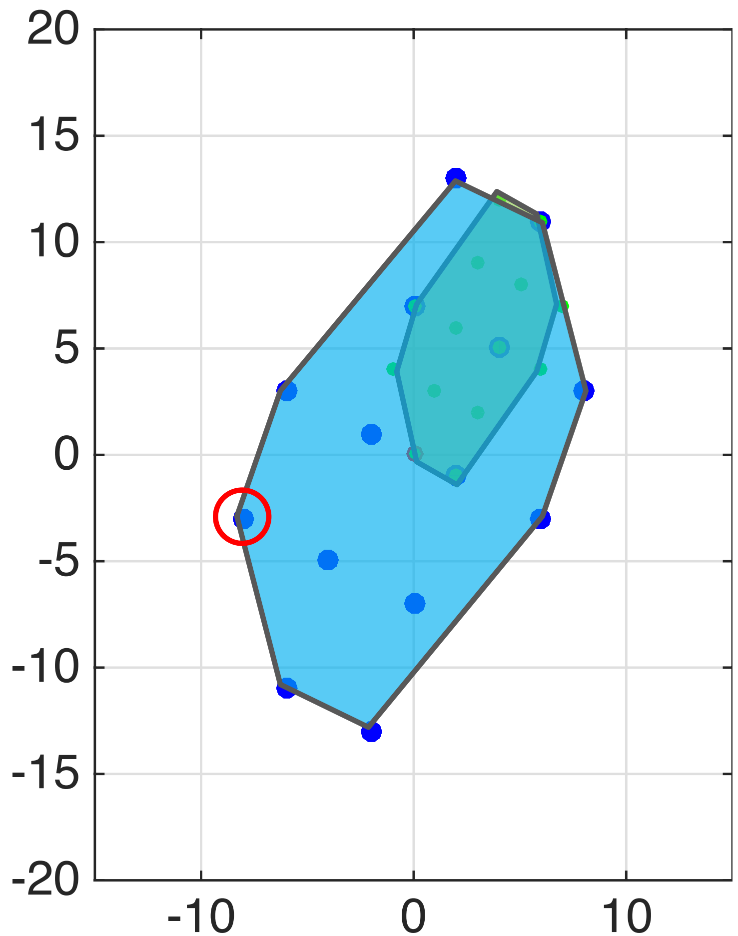
$$\text{Center } = (0{,}0)$$

Relationship between zonotopes



$$\mathbf{x} \in \{0, 1\}^n$$

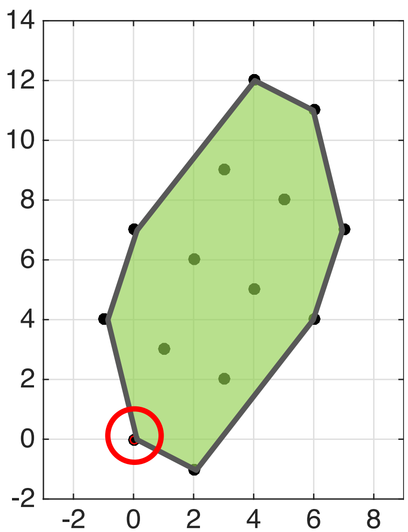
$$\text{Center } = \frac{1}{2}\sum_{i}^{n} g_i$$



$$\mathbf{x} \in \{-1, 1\}^n$$

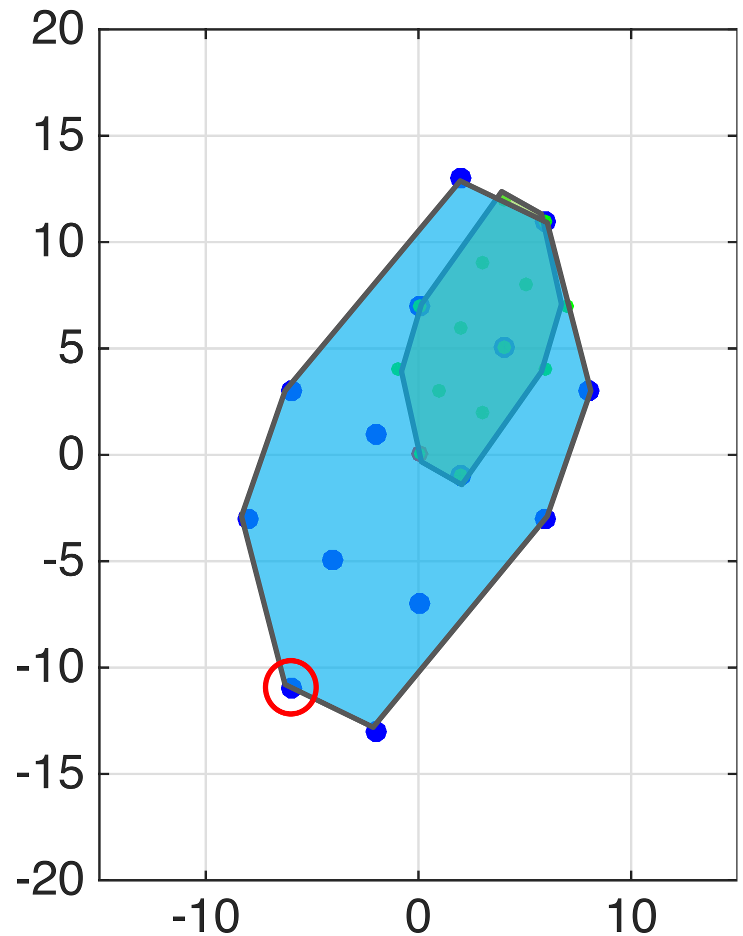
$$\text{Center } = (0{,}0)$$

Relationship between zonotopes



$$\mathbf{x} \in \{0,1\}^n$$

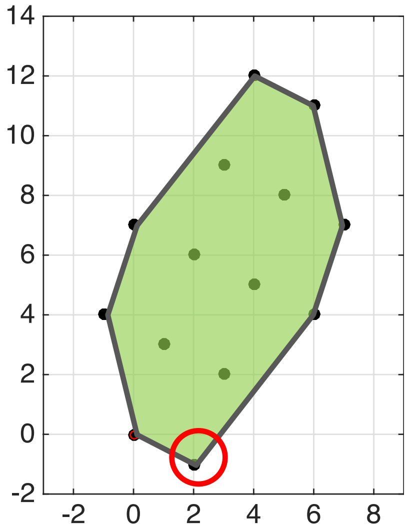
$$\text{Center } = \frac{1}{2}\sum_i^n g_i$$



$$\mathbf{x} \in \{-1,1\}^n$$

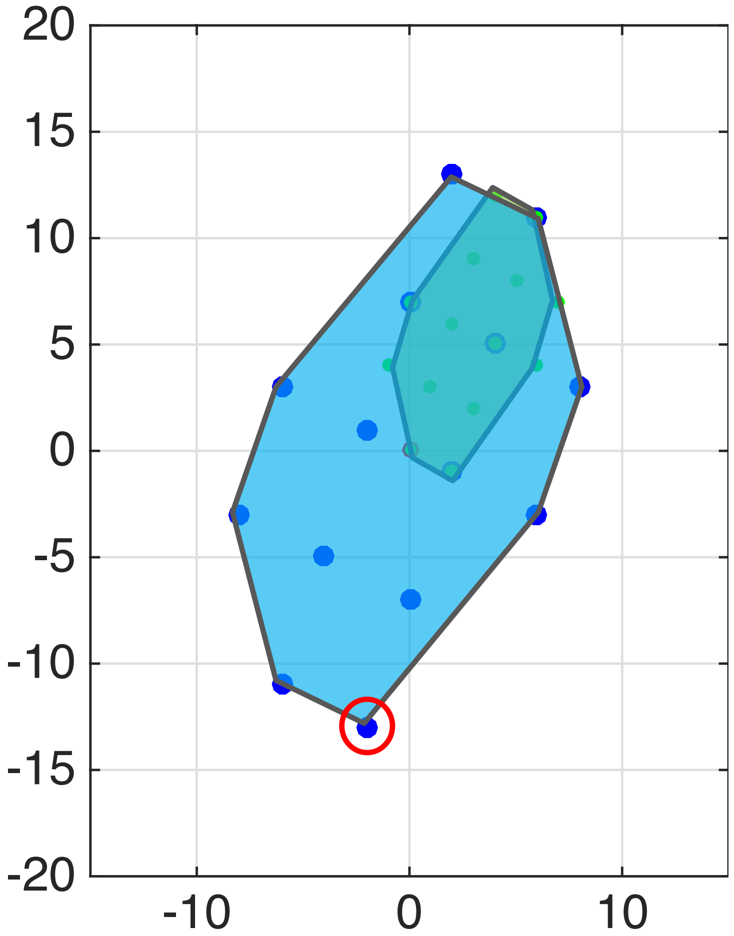
$$\text{Center } = (0,0)$$

Relationship between zonotopes



$$\mathbf{x} \in \{0, 1\}^n$$

$$\text{Center } = \frac{1}{2} \sum_i^n g_i$$



$$\mathbf{x} \in \{-1, 1\}^n$$

$$\text{Center } = (0{,}0)$$

Methods for vertex enumeration

Theorem:

Given **G**, there exists an $O(n^{d-1})$-time algorithm to enumerate all extremal binary input vectors **x** corresponding to vertices of the zonotope

Gritzmann, Sturmfels. Minkowski addition of polytopes: computational complexity and applications to Gröbner bases. *SIAM J. Disc. Math* 1993

Methods for vertex enumeration

1. Incremental strategy

Get vertices for k of the generators, and then update with one more generator.

Time Complexity:	$O(n^{d-1})$
Memory:	$O(n^{d-1})$

Edelsbrunner, Algorithms in Combinatorial Geometry, *Springer*, 1987

Methods for vertex enumeration

2. Reverse Search Enumeration

Use an "adjacency oracle" (returns a vertex's neighbors) and a "finite local search function" (maps a vertex to an adjacent vertex), to iterate through vertices of a zonotope.

Time Complexity: $O(n\ LP(n,d)\ |V|)$
Memory: $O(nd)$

Methods for vertex enumeration

2. Reverse Search Enumeration

Use an "adjacency oracle" (returns a vertex's neighbors) and a "finite local search function" (maps a vertex to an adjacent vertex), to iterate through vertices of a zonotope.

Time Complexity: $O(n\ LP(n,d)\ |V|)$
Memory: $O(nd)$

Ferrez, Fukuda, Libeling. Solving the fixed rank convex quadratic maximization in binary variable by a parallel zonotope construction algorithm.

Methods for vertex enumeration

3. Random vertex enumeration

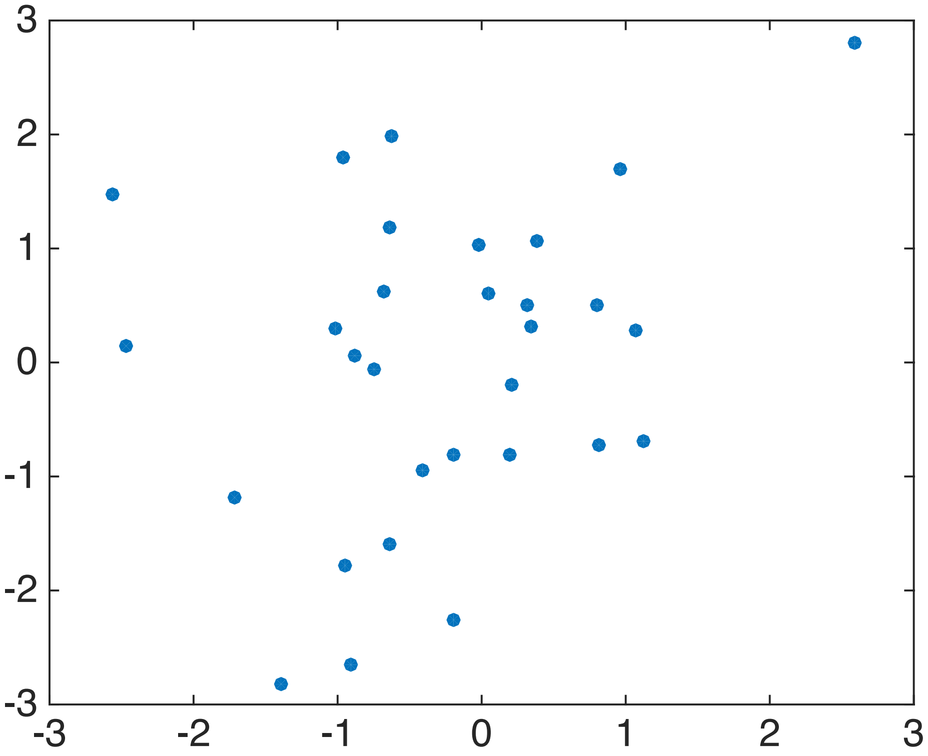
$$\text{For } \mathbf{x} \in \mathbb{R}^n \text{ s.t. } \mathbf{G}\mathbf{x} \neq 0,$$
$$\mathbf{v} = \mathbf{G}\,\mathrm{sign}(\mathbf{G}\mathbf{x}) \text{ is a vertex of } \mathcal{Z}(\mathbf{G})$$

Stinson, Gleich, Constantine. A randomized algorithm for enumerating zonotope vertices, *arXiv:1602.06620* 2016

Vector Partition Problem

Let $v_1, v_2, \ldots, v_n$ be n vectors in $\mathbb{R}^d$

$f : \mathbb{R}^{d \times p} \to \mathbb{R},$ convex objective function



$$\max \; f(S)$$

$$\mathbf{S} = \begin{bmatrix} s_1 & s_2 & \cdots & s_p \end{bmatrix}$$

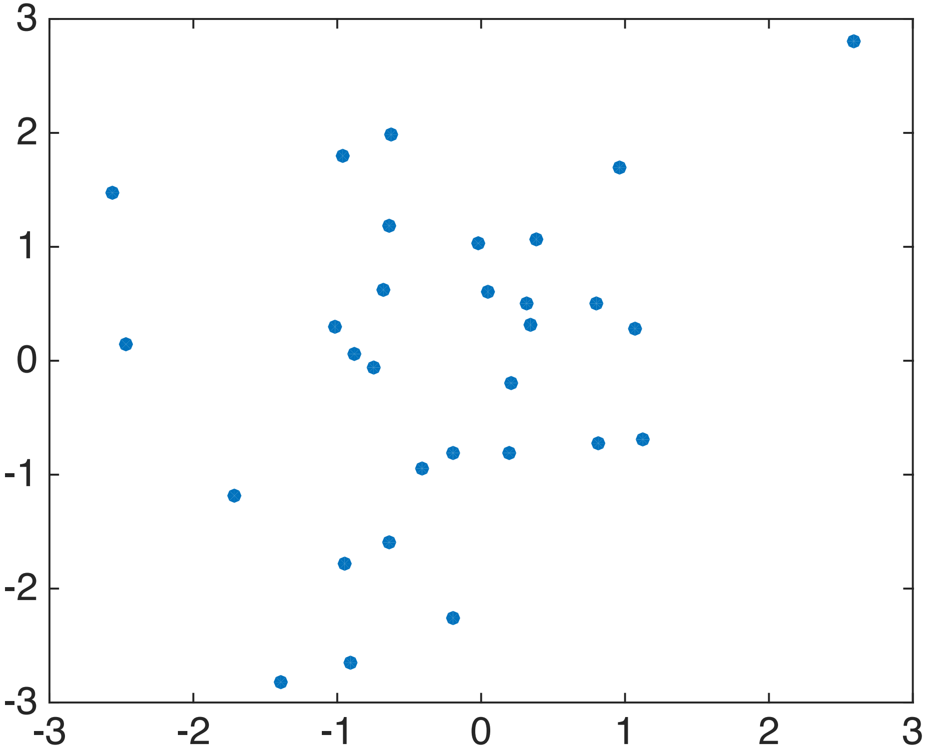
$$s_i = \sum_{v \in \text{ cluster } i} v \in \mathbb{R}^d$$

Goal: Cluster the n vectors into p disjoint sets to maximize a convex functional on the sum of vectors in each cluster.

Vector Partition Problem

Let $v_1, v_2, \ldots, v_n$ be n vectors in $\mathbb{R}^d$

$f : \mathbb{R}^{d \times p} \to \mathbb{R}$, convex objective function



$$\max \; f(S)$$

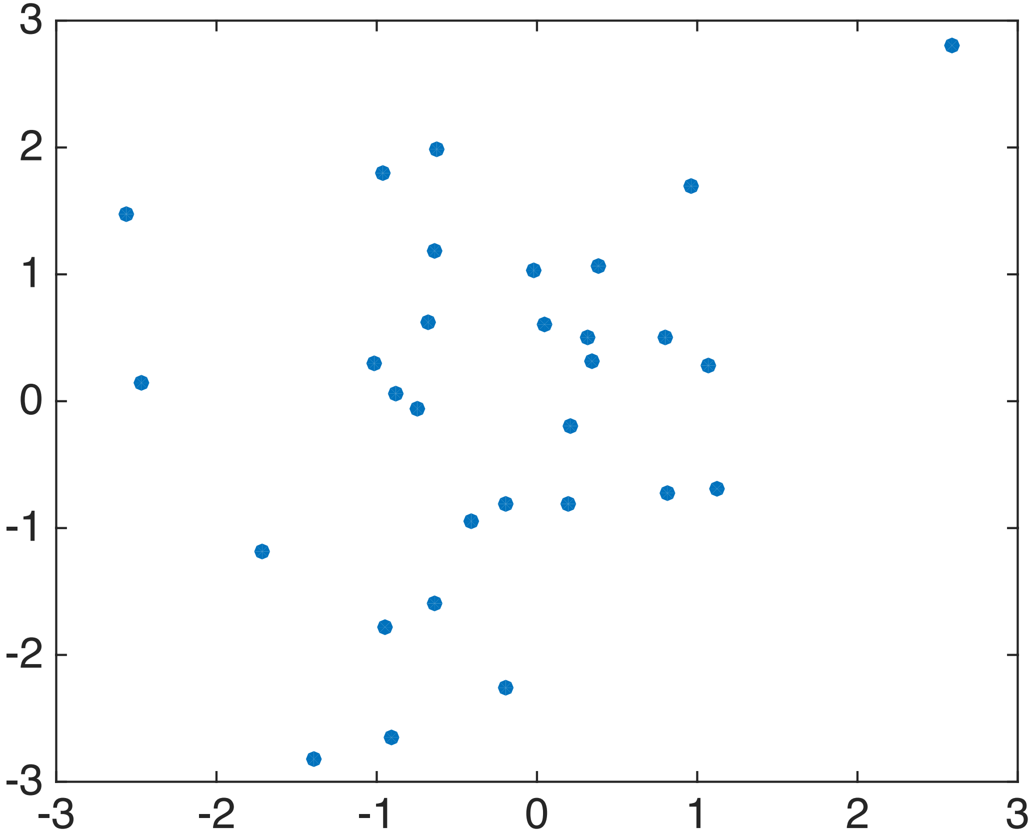
$$\mathbf{S} = \begin{bmatrix} s_1 & s_2 & \cdots & s_p \end{bmatrix}$$

$$s_i = \sum_{v \in \text{ cluster } i} v \in \mathbb{R}^d$$

Onn, Schulman. The Vector Partition Problem for Convex Objective Functions *Mathematics of Operations Research*. 2001

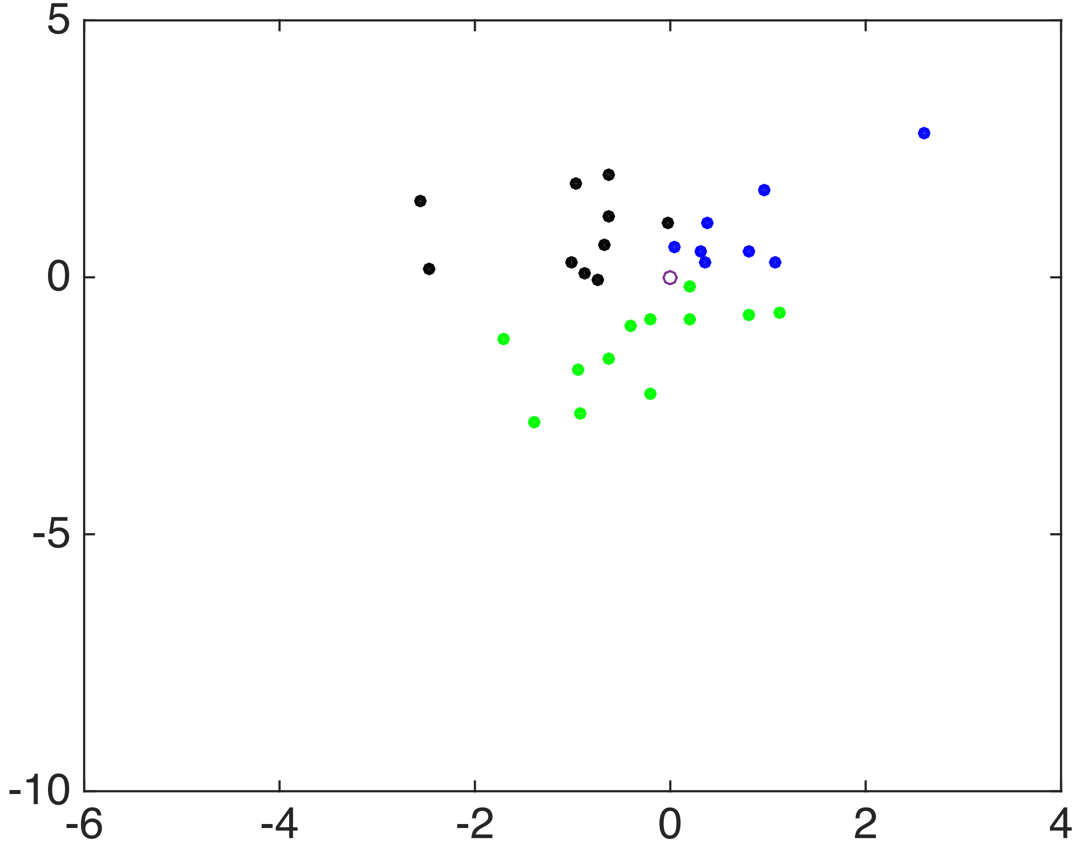
Vector Partition Problem

$$\max \ f(S)$$



Vector Partition Problem

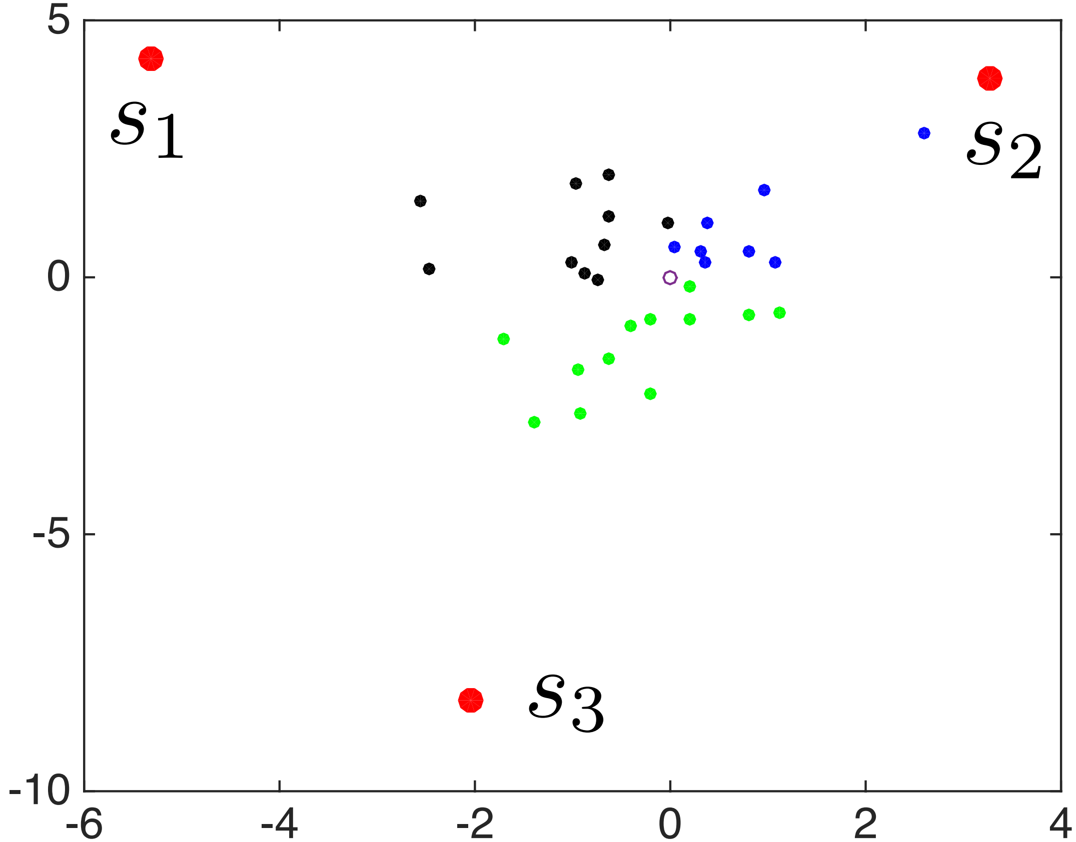
$$\max \ f(S)$$



Get a clustering of $v_1, v_2, \ldots, v_n$

Vector Partition Problem

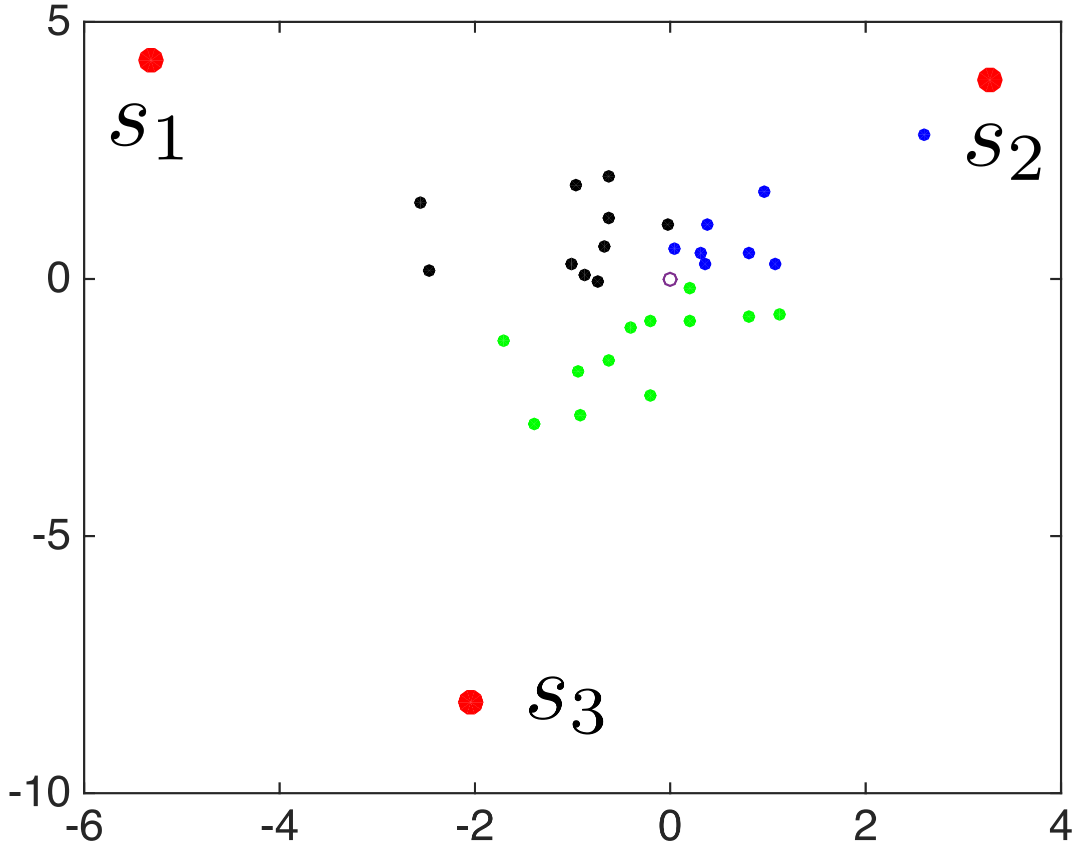
$$\max \ f(S)$$



Sum up vectors in each cluster to get $s_1, s_2, \ldots, s_p$

Vector Partition Problem

$$\max \ f(S)$$



$$\text{Form} \ \ \mathbf{S} = \begin{bmatrix} s_1 & s_2 & \cdots & s_p \end{bmatrix}$$

Vector Partition Problem

$$\max \ f(S)$$

$$\mathbf{S} = \begin{bmatrix} s_1 & s_2 & \cdots & s_p \end{bmatrix}$$

$$s_i = \sum_{v \in \text{ cluster } i} v \in \mathbb{R}^d$$

The set of all S matrices is *not* a zonotope.

The problem is solved by exploring the *signing zonotope*

Let $\sigma = (\sigma^i_{r,s}) \in \{-1, 1\}^M$, where

- i is the index of a vector v_i
- r, s are indices of distinct clusters
- $M = \binom{p}{2} n$

$$\sigma = (\sigma^i_{r,s}) \in \{-1,1\}^M$$

Associate with σ a matrix $\mathbf{A}_\sigma$:

$$\mathbf{A}_\sigma = \sum_{i=1}^{n} \sum_{1 \le r < s \le p} \sigma^i_{r,s} v_i \cdot (e_r - e_s)^T \in \mathbb{R}^{d \times p}$$

This is a ± 1 combination of matrices

$$W^i_{r,s} = v_i \cdot (e_r - e_s)^T \in \mathbb{R}^{d \times p}$$

Fact: $W^i_{r,s}$ have zero row sum.

Example: let $d = 2, p = 3, r = 1, s = 3,\ v = (1, 3)$

$$W^i_{r,s} = v_i \cdot (e_r - e_s)^T = \begin{bmatrix}1\\3\end{bmatrix}\left(\begin{bmatrix}1\\0\\0\end{bmatrix} - \begin{bmatrix}0\\0\\1\end{bmatrix}\right)^T$$

$$= \begin{bmatrix}1\\3\end{bmatrix}\left(\begin{bmatrix}1 & 0 & -1\end{bmatrix}\right) = \begin{bmatrix}1 & 0 & -1\\3 & 0 & -3\end{bmatrix}$$

Define a $d(p-1)$ dimensional vector by stacking columns

$$\rightarrow w(i, r, s) = \begin{bmatrix}1 & 3 & 0 & 0\end{bmatrix}^T$$

Given $\sigma \in \{-1,1\}^M$:

$$\mathbf{A}_\sigma = \sum_{i=1}^{n} \sum_{1 \le r < s \le p} \sigma^i_{r,s} W^i_{r,s} \in \mathbb{R}^{d \times p}$$

$\mathbf{A}_\sigma$ also has zero row sum, so associate σ with a $d(p-1)$ dimensional vector Z_σ by stacking columns.

Definition: The signing zonotope is the convex hull of vectors Z_σ:

$$\mathcal{Z} = \mathbf{conv}\{Z_\sigma : \sigma \in \{-1,1\}^M\}$$

Equivalently: $\mathcal{Z}$ is the zonotope generated by vectors $w(i,r,s)$.

VPP is solvable in polynomial time

Definition: An *extremal signing* σ is a signing that corresponds to a vertex of $\mathcal{Z}$.

Theorem (Onn, Schulman 2001)

- Every vertex of $\mathcal{Z}$ maps to a clustering of the n vectors
- There is some vertex of $\mathcal{Z}$ that maps to the optimal clustering
- $\mathcal{Z}$ has $O(n^{d(p-1)-1})$ vertices

By exploring the polynomially many vertices of $\mathcal{Z}$ we find the optimal clustering of the n input vectors.

VPP is solvable in polynomial time

Definition: An *extremal signing* σ is a signing that corresponds to a vertex of $\mathcal{Z}$.

Theorem (Onn, Schulman 2001)

- Every vertex of $\mathcal{Z}$ maps to a clustering of the n vectors
- There is some vertex of $\mathcal{Z}$ that maps to the optimal clustering
- $\mathcal{Z}$ has $O(n^{d(p-1)-1})$ vertices

Onn, Schulman. The Vector Partition Problem for Convex Objective Functions *Mathematics of Operations Research*. 2001

Intuition for mapping signings to clusterings

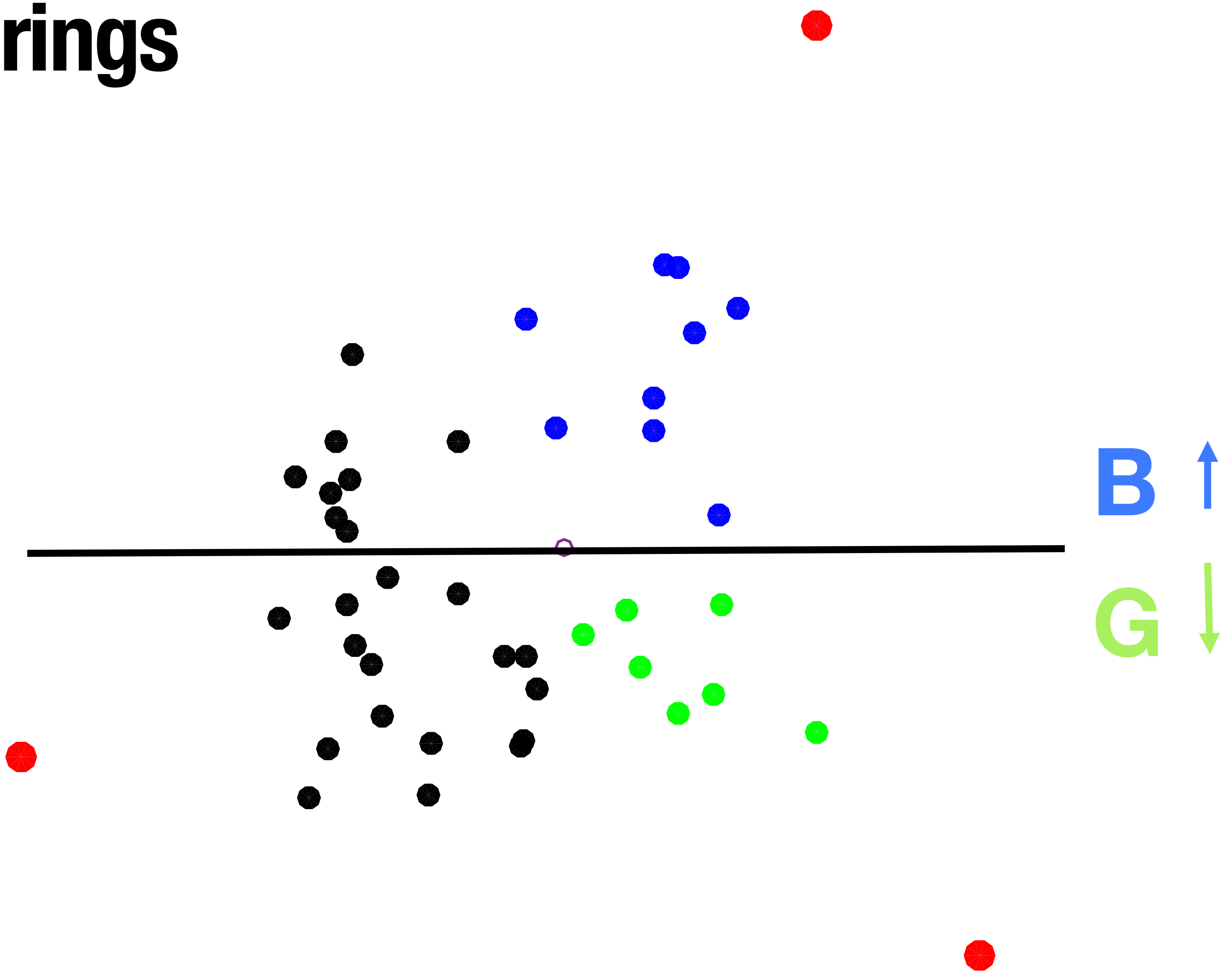
Every extremal signing σ encodes "separation" information:

$$\sigma^i_{r,s} = \begin{cases} +1 \text{ if } i \text{ could be in cluster } r\text{, but not } s \\ -1 \text{ if } i \text{ could be in cluster } s\text{, but not } r \end{cases}$$

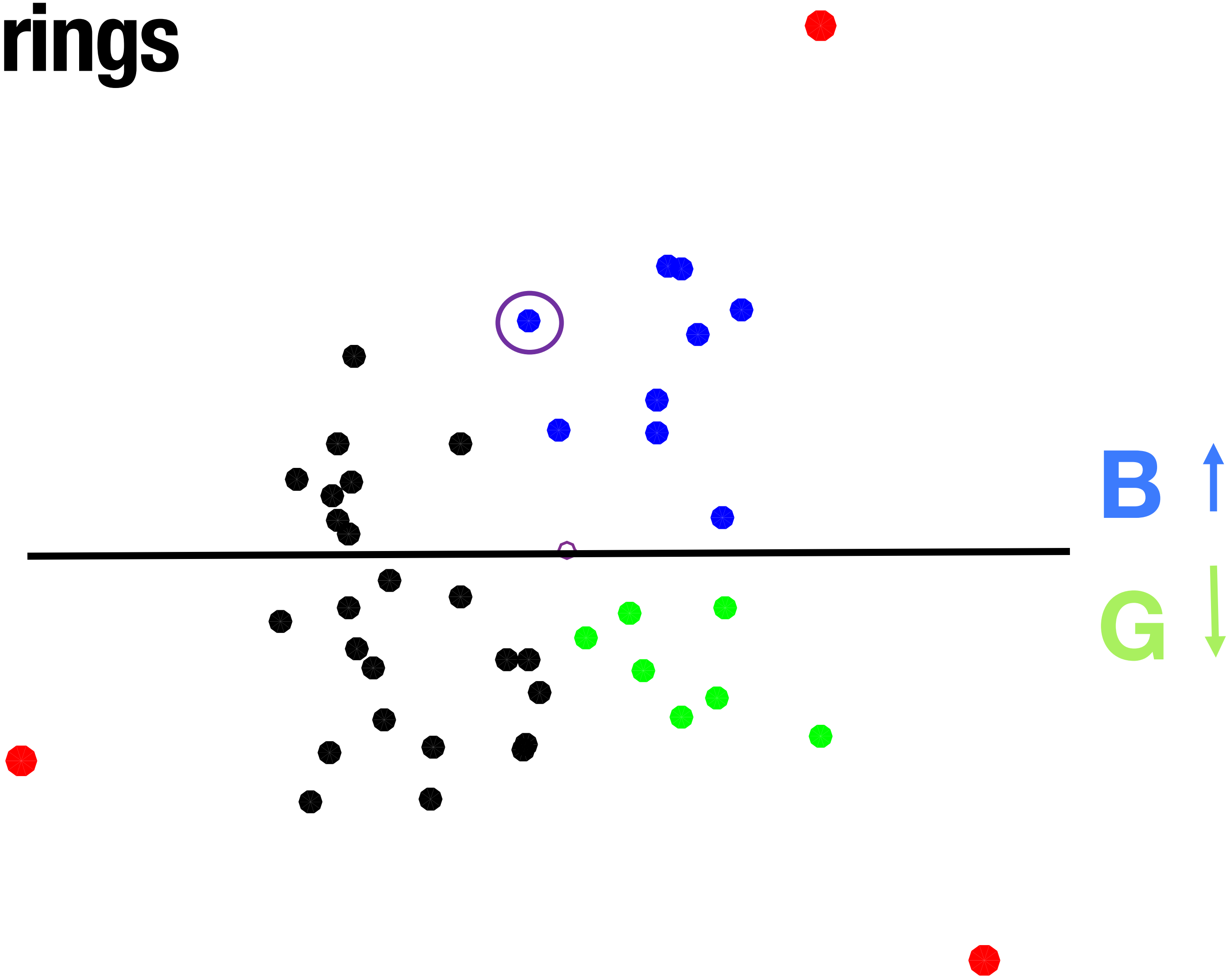
If we can obtain an extremal signing σ, we can figure out where each vector v_i belongs.

Onn, Schulman. The Vector Partition Problem for Convex Objective Functions *Mathematics of Operations Research*. 2001

Intuition for mapping signings to clusterings

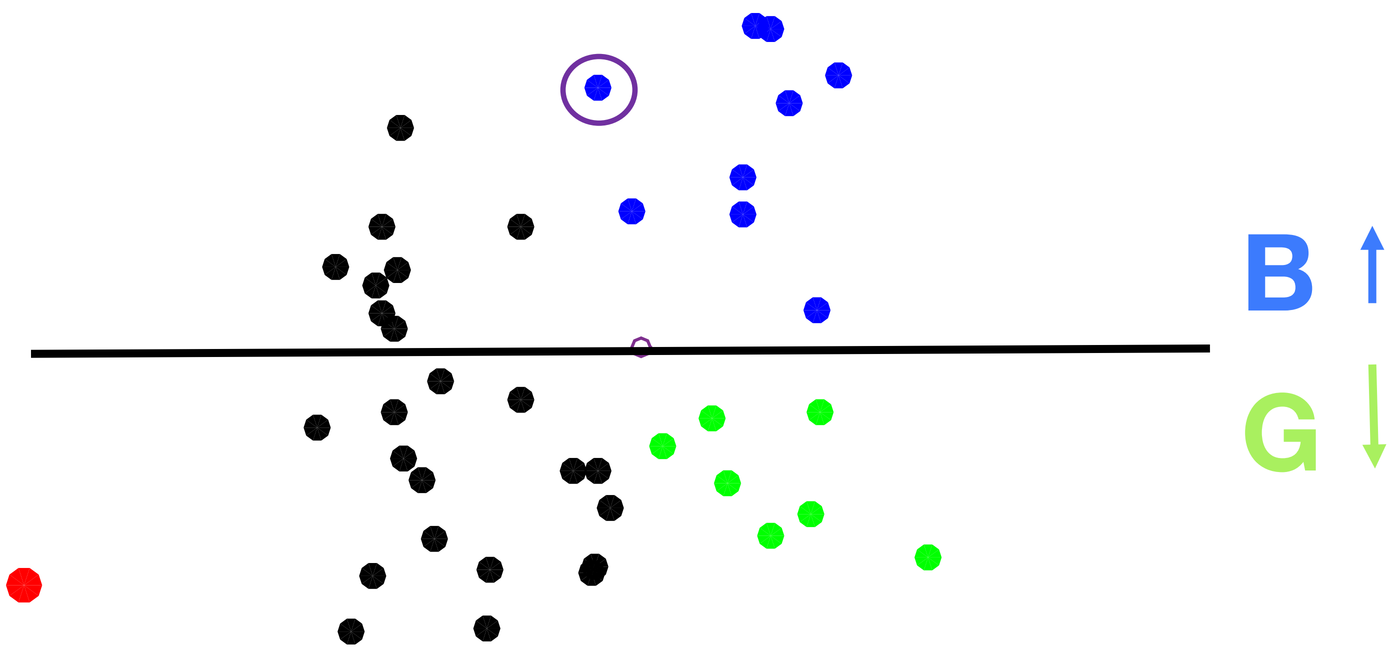


Intuition for mapping signings to clusterings

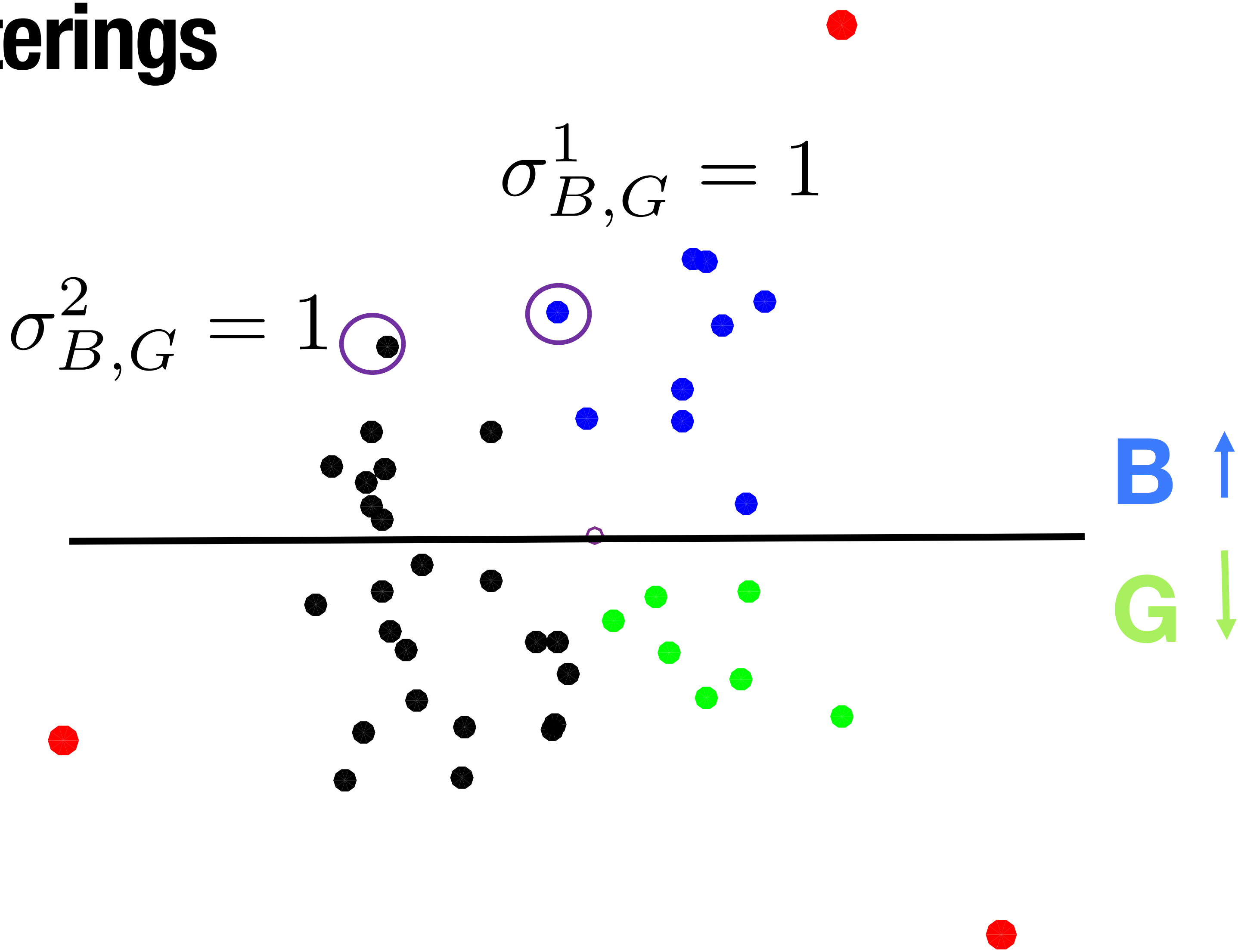


Intuition for mapping signings to clusterings

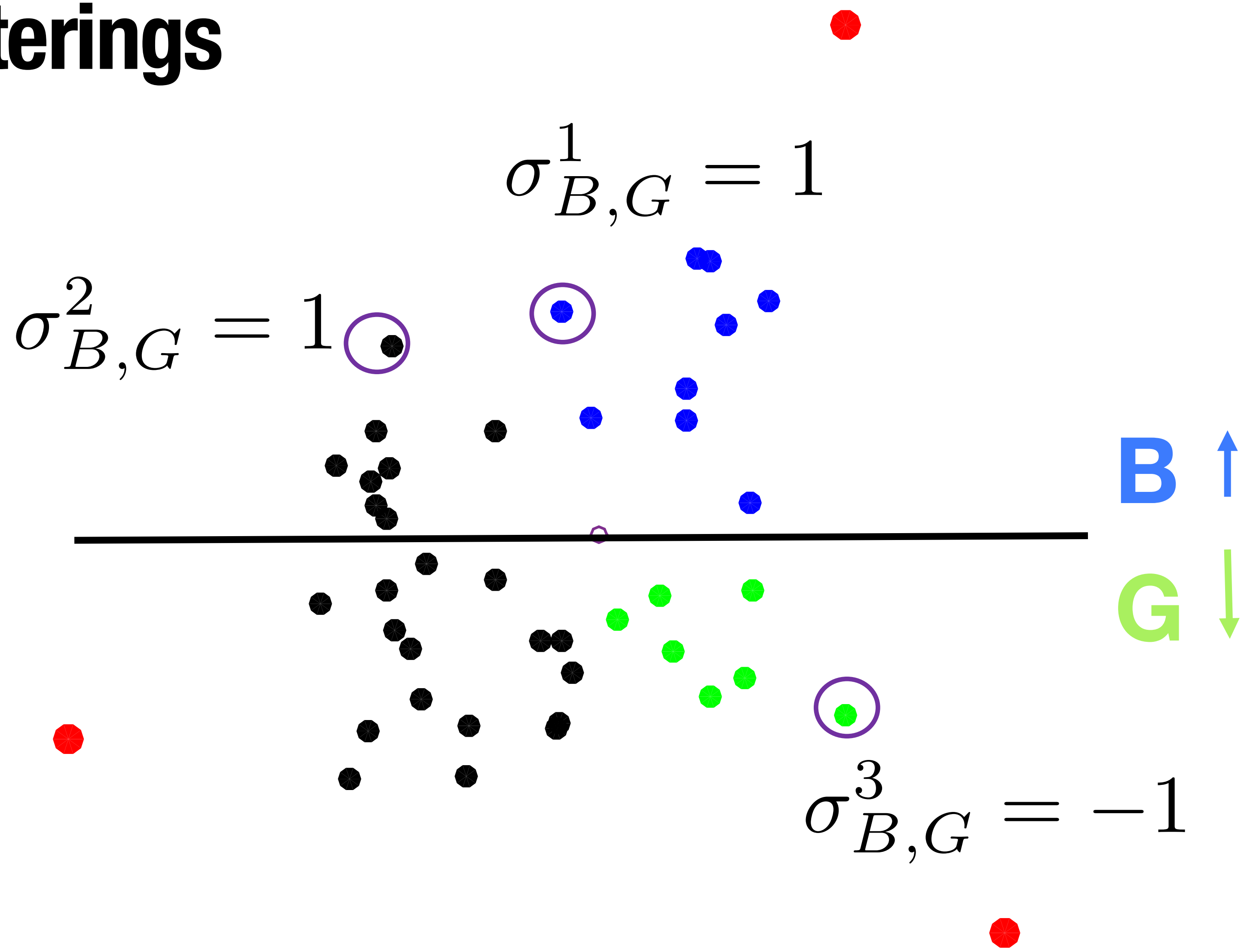
$$\sigma^1_{B,G} = 1$$



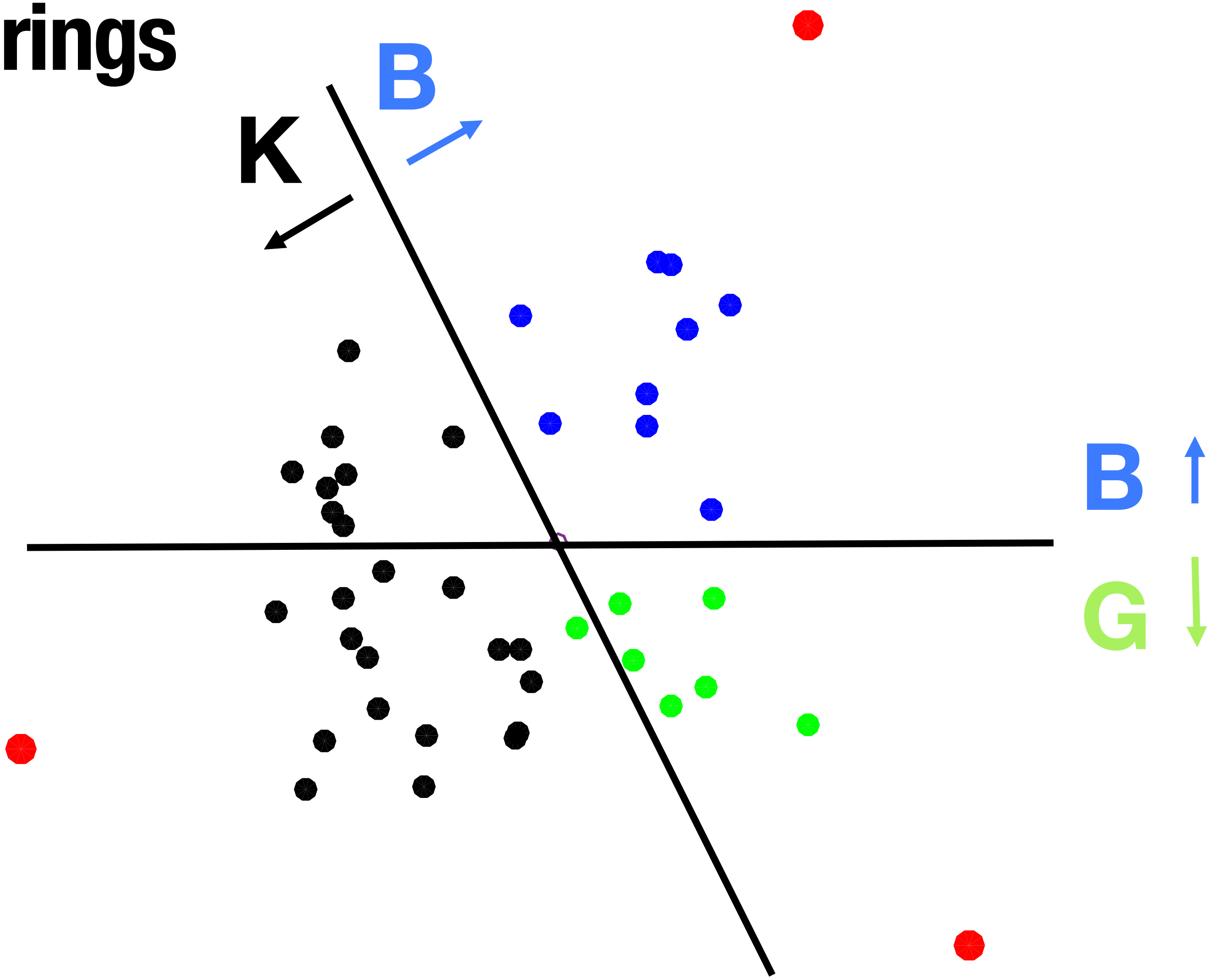
Intuition for mapping signings to clusterings



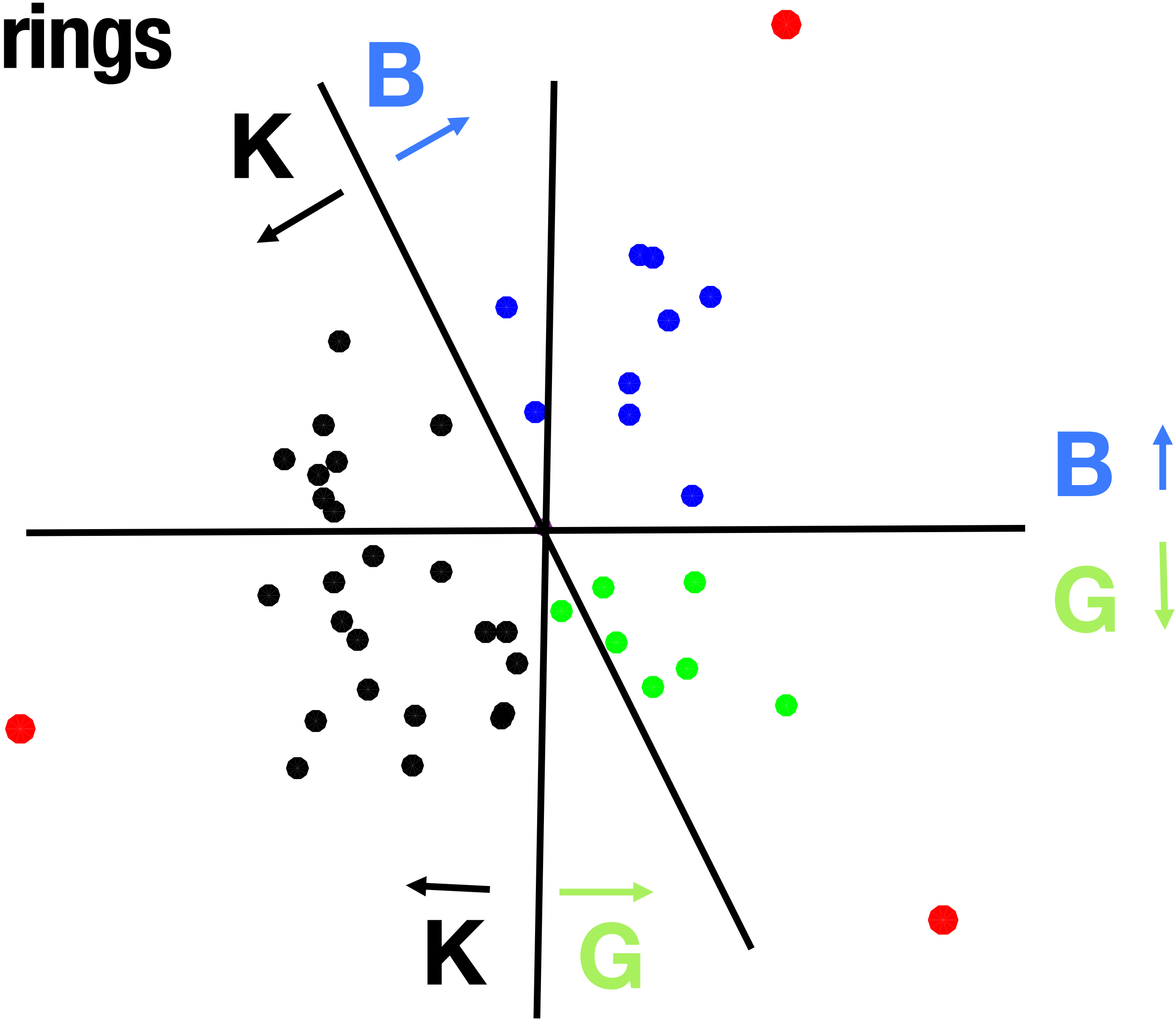
Intuition for mapping signings to clusterings



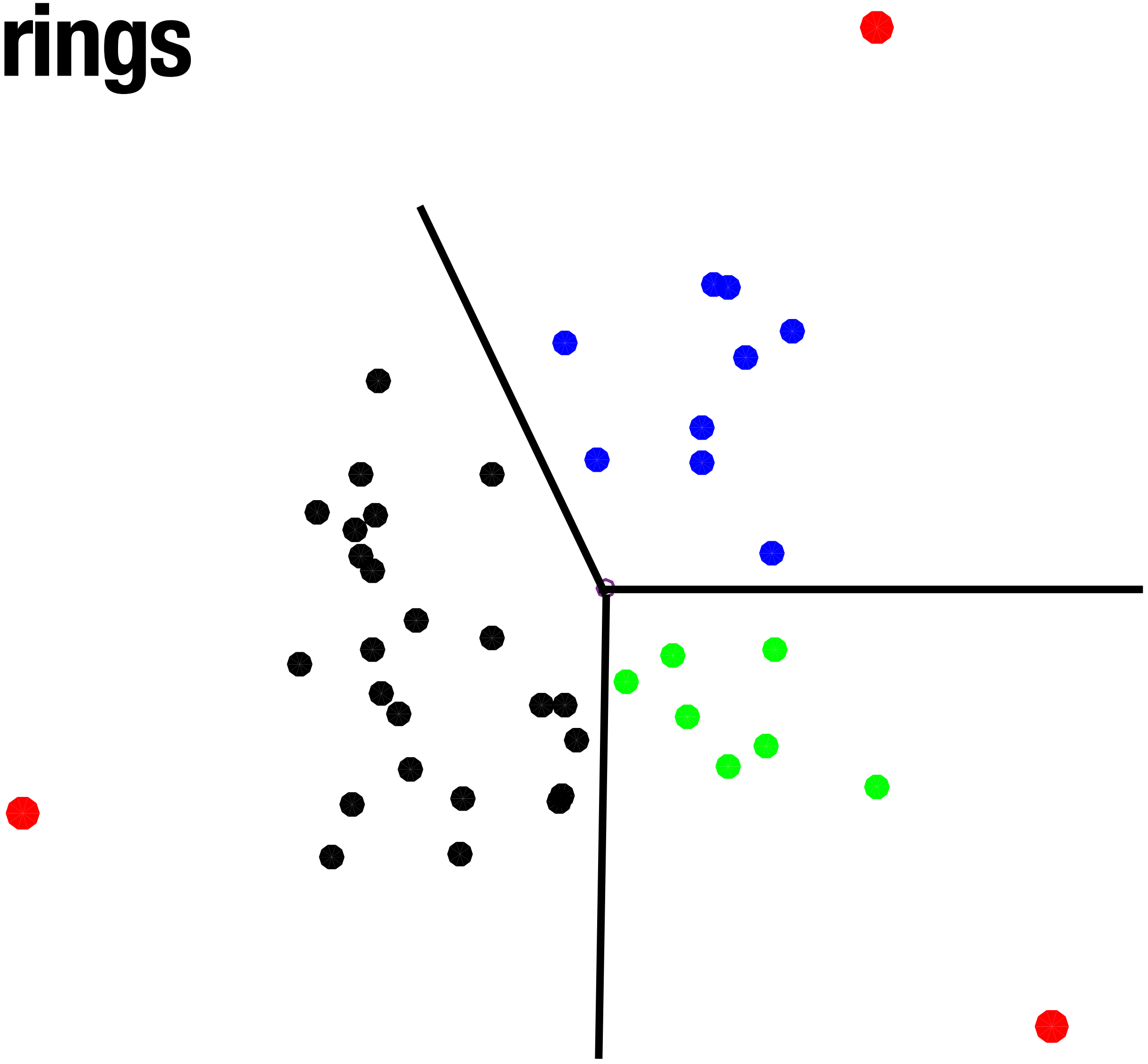
Intuition for mapping signings to clusterings



Intuition for mapping signings to clusterings



Intuition for mapping signings to clusterings



Thanks!