

# Upper and Lower Bounds on the Quality of the PCA Bounding Boxes

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## Known algorithms that solve bounding box problem

$$\mathbb{R}^2$$

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- Heuristics

AABB (Axis Aligned Bounding Boxes)

*R*-tree

Packed *R*-tree [Rousopoulos, Leifker '85]

*R*<sup>+</sup>-tree [Sellis, Rousopoulos, Faloutsos '87]]

*R*<sup>\*</sup>-tree [Beckmann, Kriegel, Schneider, Seeger '90]

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$$O(n + \frac{1}{\epsilon^{4.5}})$$

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PCA-bounding box  $O(n), O(n \log n), O(n^{\lfloor \frac{d}{2} \rfloor + 1})$

OBB-tree [Gottchalk, Lin, Manocha, '96]

BOXTREE [Barequet, Chazelle, Guibas, Mitchell, Tal '96]

...

# Principal Component Analysis

$X = \{x_1, x_2, \dots, x_m\}$ ,     $x_i$  is a  $d$ -dimensional vector

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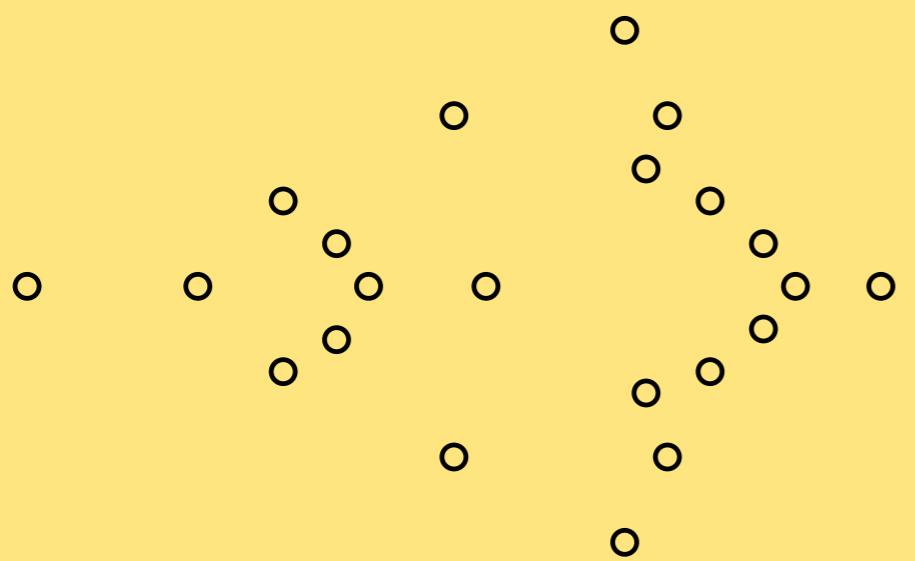
$\text{var}(X, v) = \langle Cv, v \rangle$  ,     $C_{ij} = \frac{1}{m} \sum_{k=1}^m (x_{ik} - c_i)(x_{jk} - c_j)$ .

## PCA

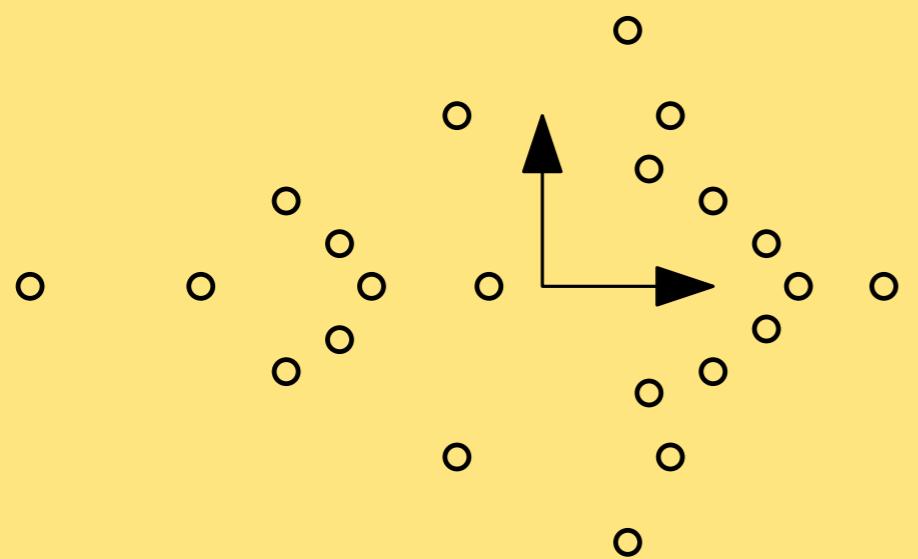
**Lemma 1.** For  $1 \leq j \leq d$ , let  $\lambda_j$  be the  $j$ -th largest eigenvalue of  $C$  and let  $v_j$  denote the unit eigenvector for  $\lambda_j$ . Let  $B_j = \{v_1, v_2, \dots, v_j\}$ ,  $sp(B_j)$  be the linear subspace spanned by  $B_j$ , and  $sp(B_j)^\perp$  be the orthogonal complement of  $sp(B_j)$ . Then  $\lambda_1 = \max\{var(X, v) : \text{unit vector } v \text{ in } \mathbb{R}^d\}$  and for any  $2 \leq j \leq d$ ,

- i)  $\lambda_j = \max\{var(X, v) : \text{unit vector } v \text{ in } sp(B_{j-1})^\perp\}.$
- ii)  $\lambda_j = \min\{var(X, v) : \text{unit vector } v \text{ in } sp(B_j)\}.$
- iii)  $var(X, B_j) \geq var(X, S)$  for any set  $S$  of  $j$  orthogonal unit vectors.

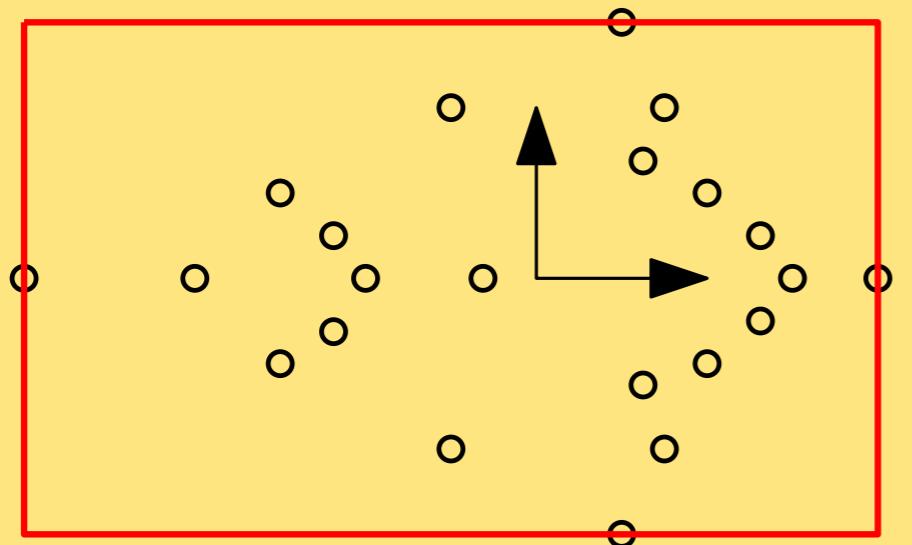
P



P

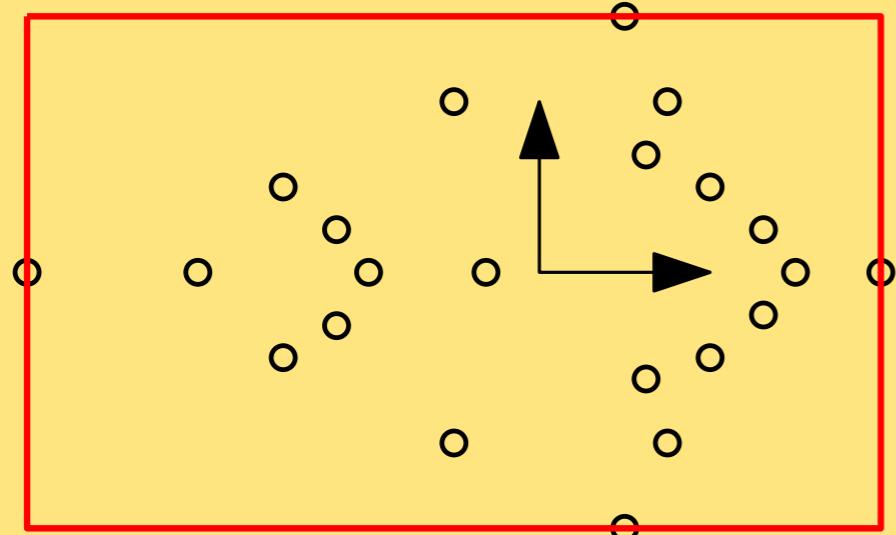


P



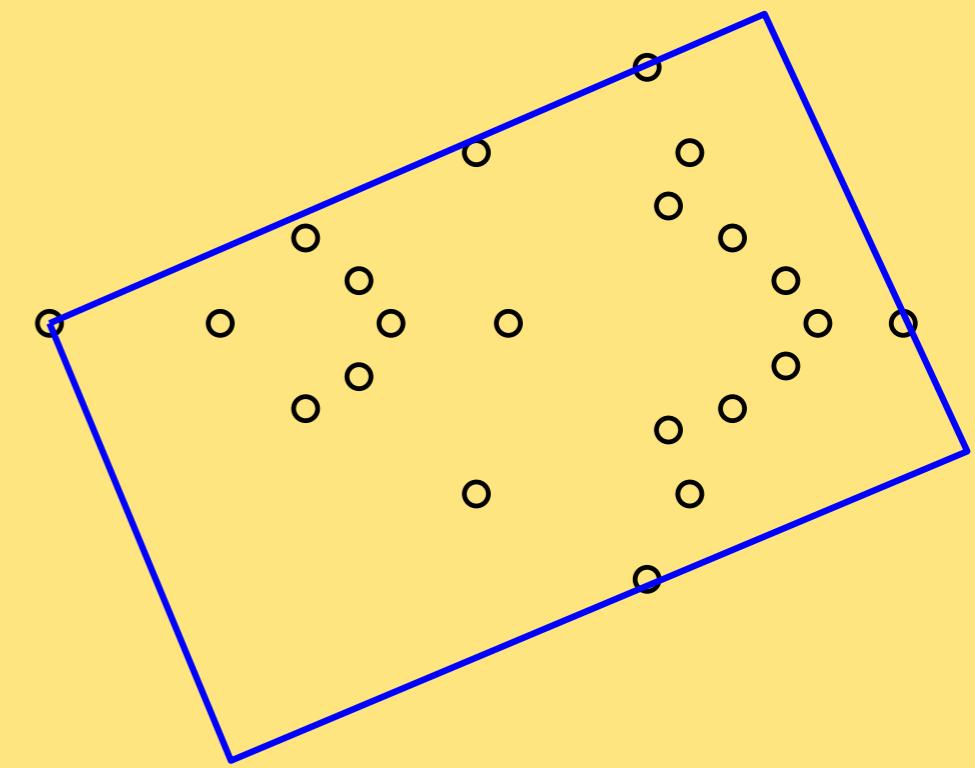
$BB_{pca}(P)$

P



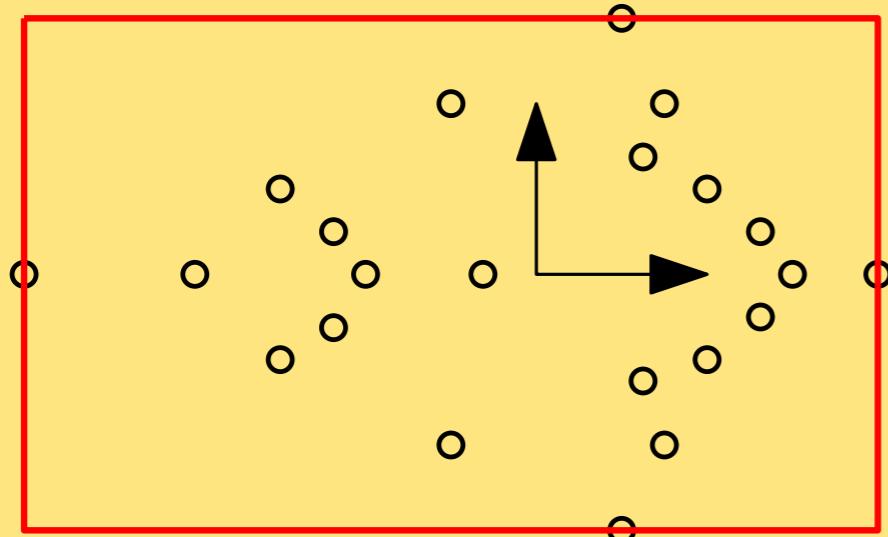
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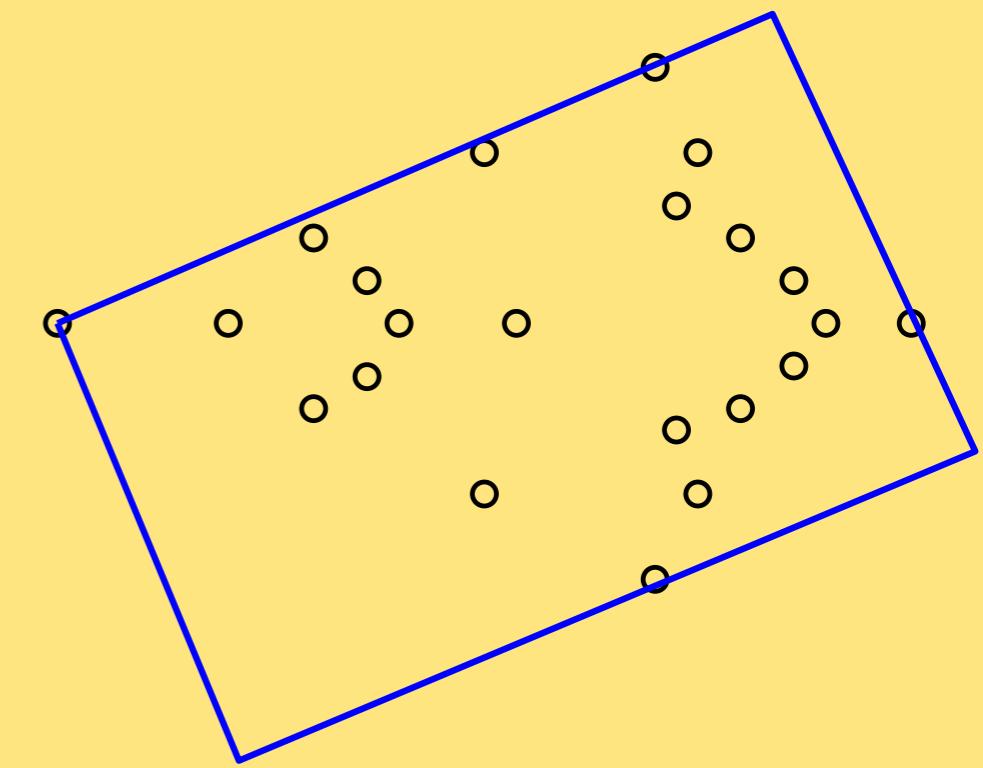
$BB_{opt}(P)$

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$BB_{pca}(P)$

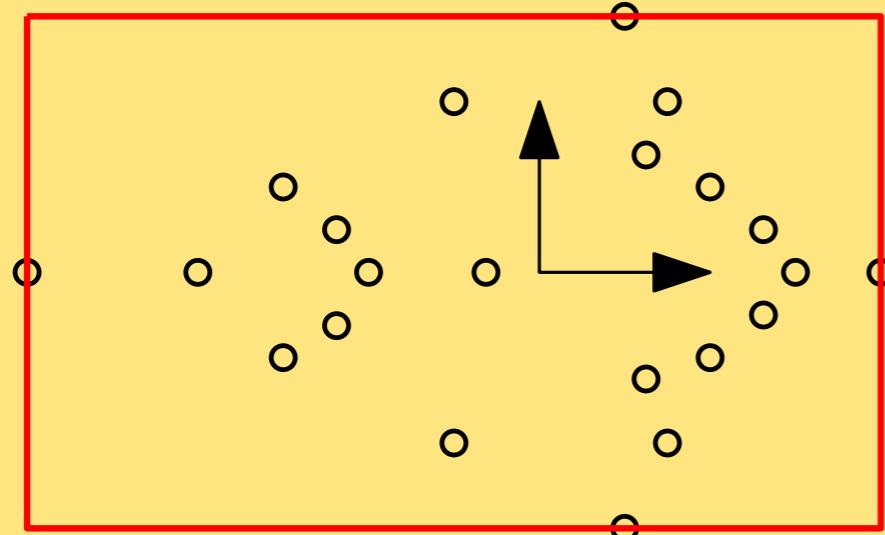
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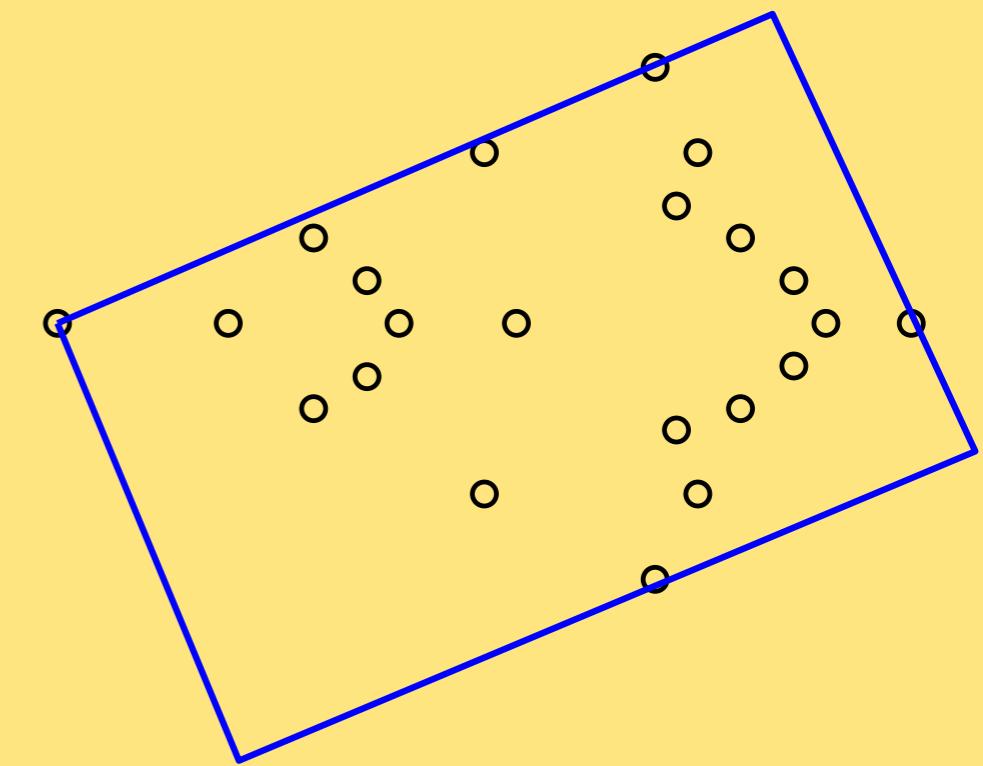
$$\lambda_d(P) = \frac{Vol(BB_{pca}(P))}{Vol(BB_{opt}(P))}$$

P



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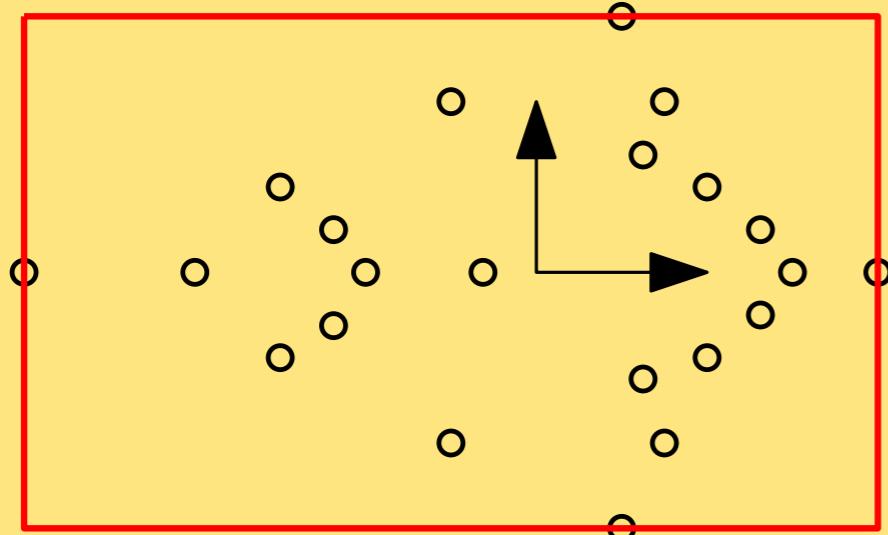


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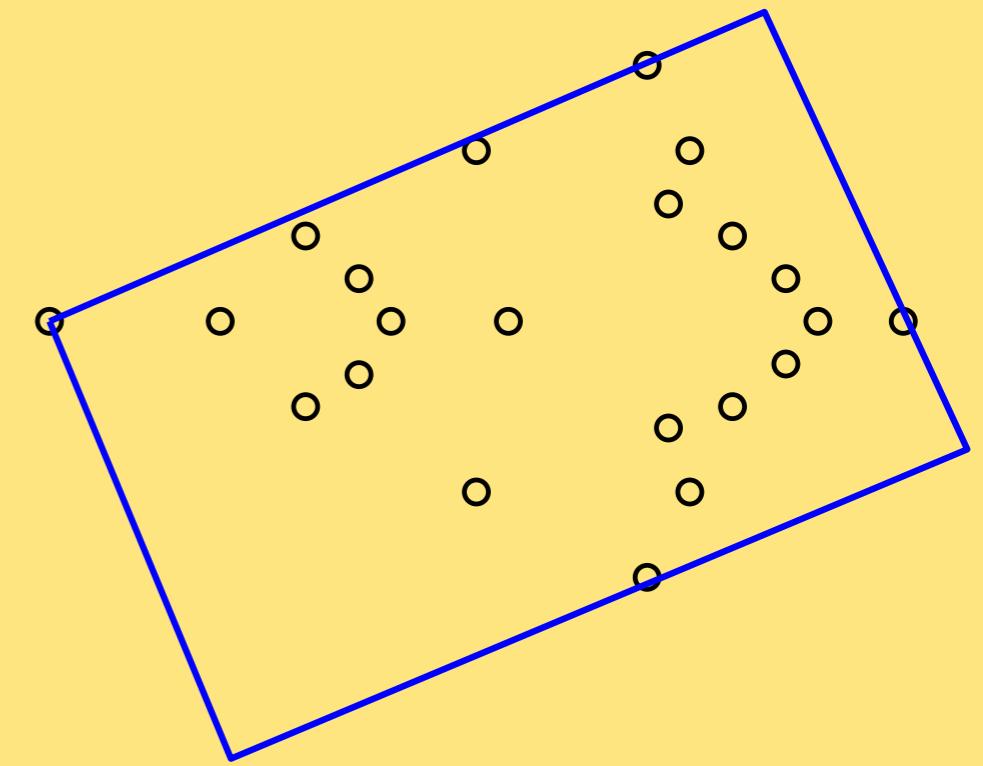
$$\lambda_d = \sup \left\{ \lambda_d(P) \mid P \subseteq \mathbb{R}^d, Vol(CH(P)) > 0 \right\}$$

P



$BB_{pca}(P)$

P



$BB_{opt}(P)$

$$\lambda_{d,i}(P) = \frac{Vol(BB_{pca(d,i)}(P))}{Vol(BB_{opt}(P))}$$

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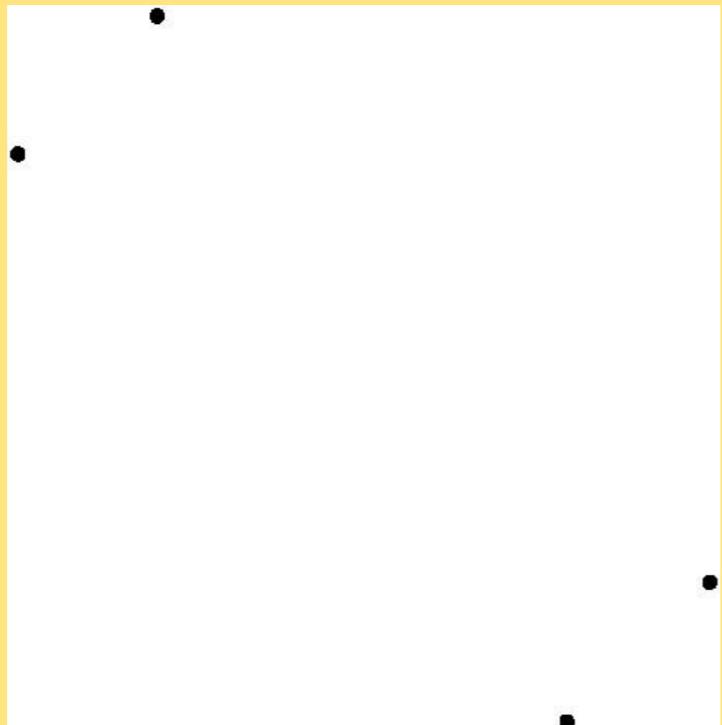
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**Proposition 1.**       $\lambda_{d,0} = \infty$     for any  $d \geq 2$ .

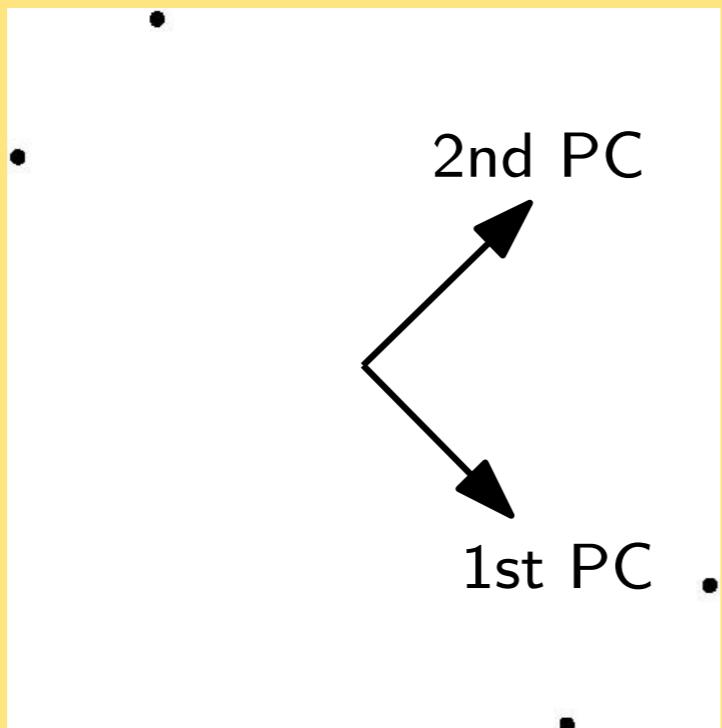
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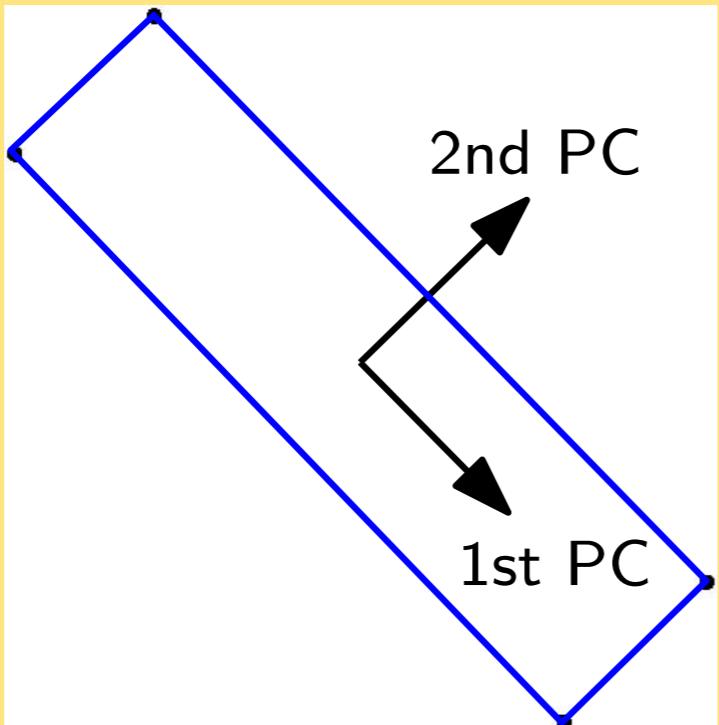
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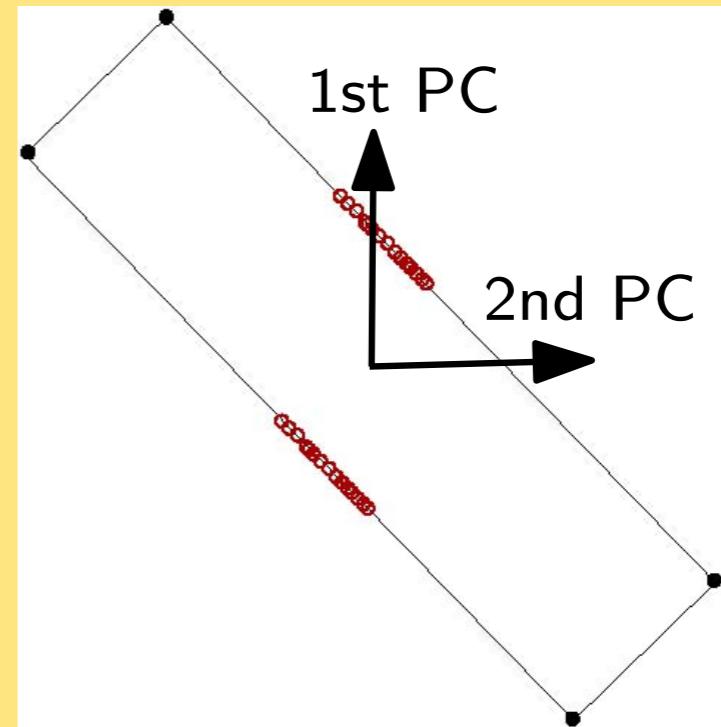
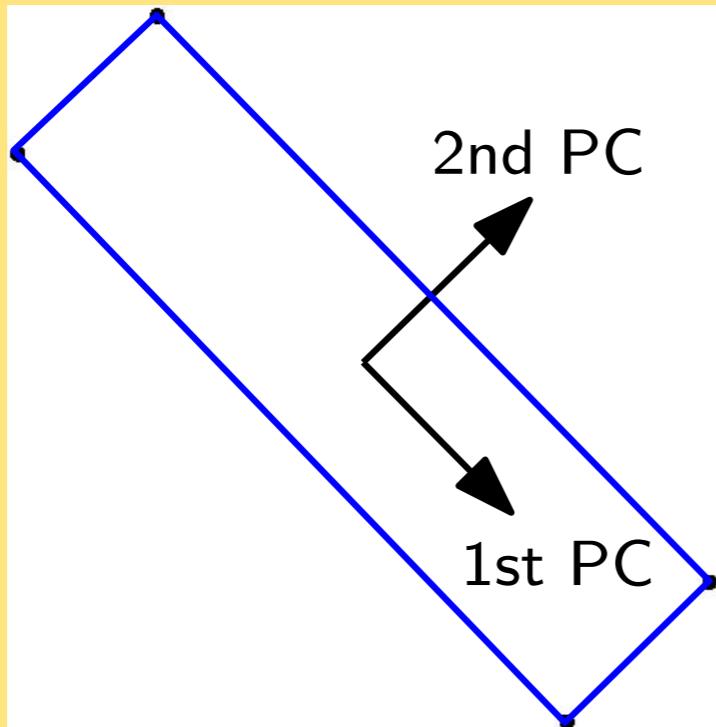
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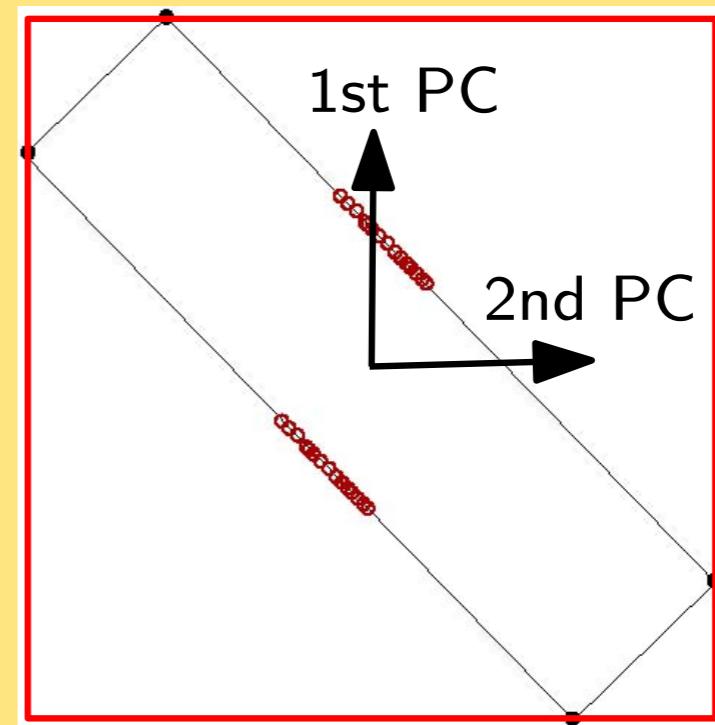
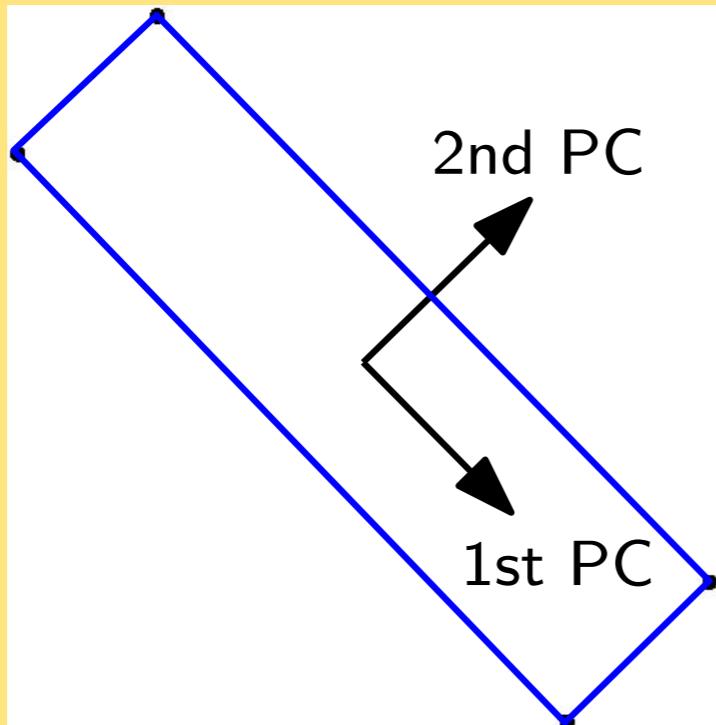
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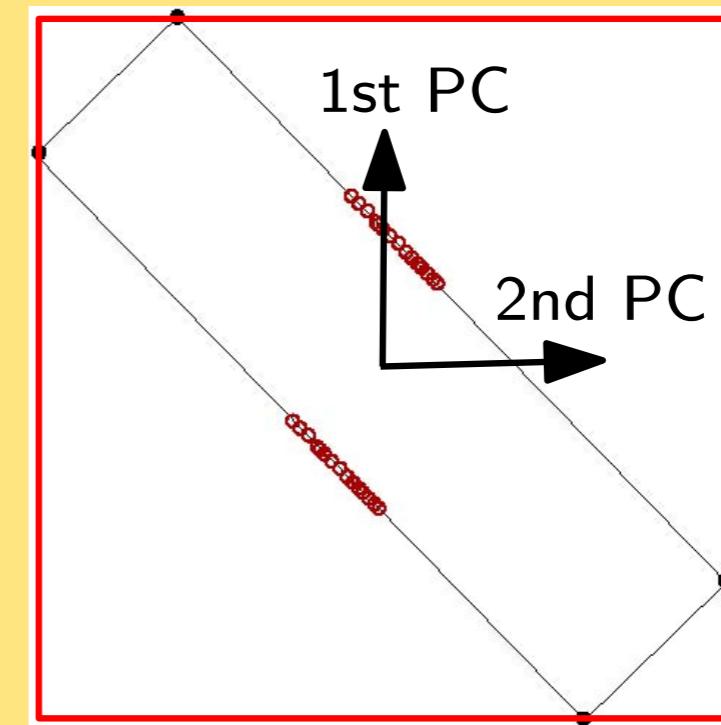
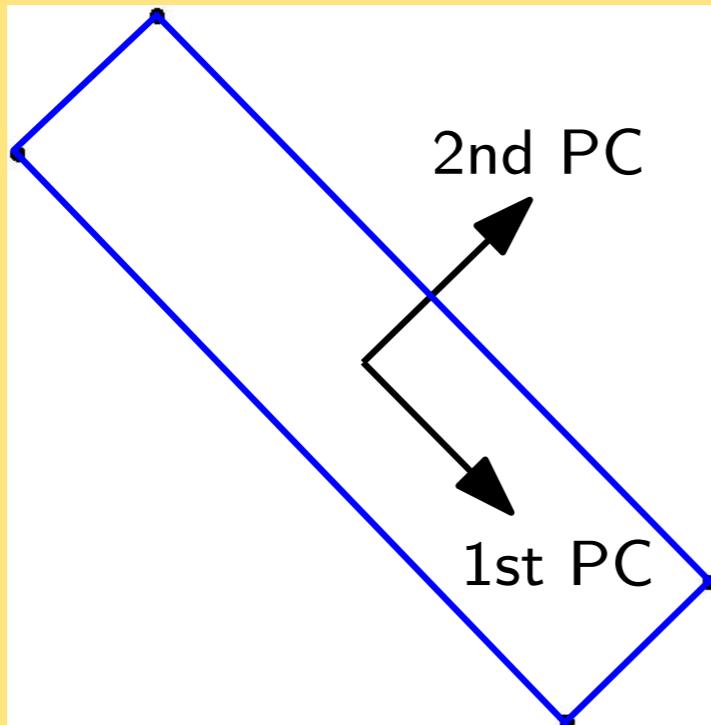
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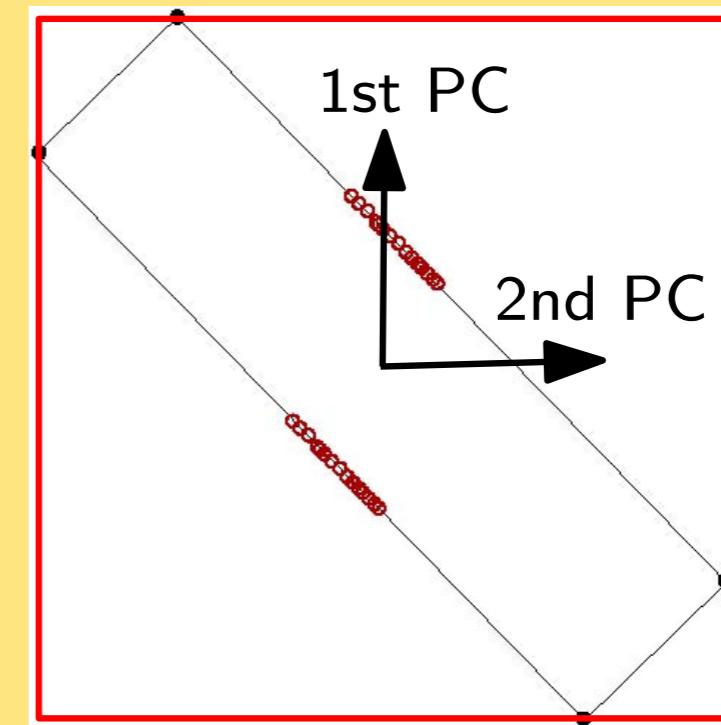
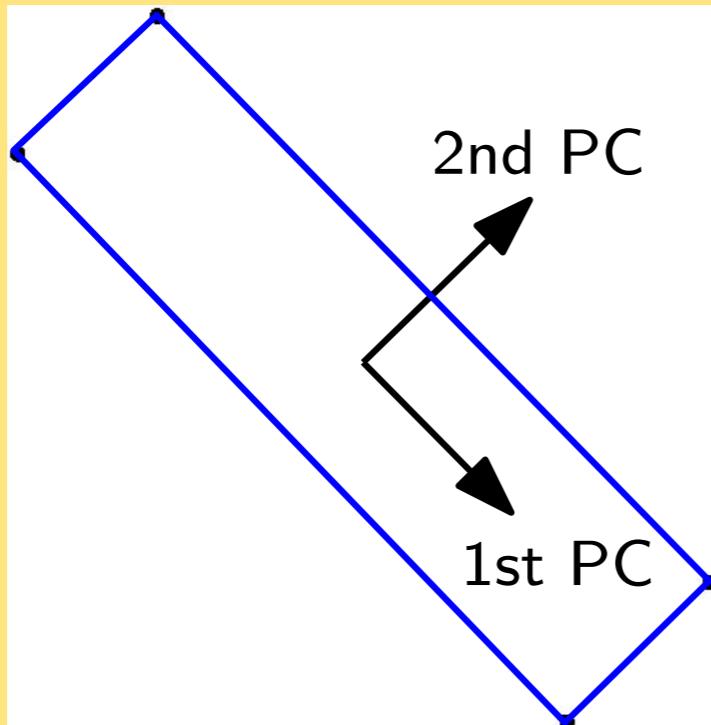
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$$\lambda_{d,d}, \quad \lambda_{d,d-1}$$

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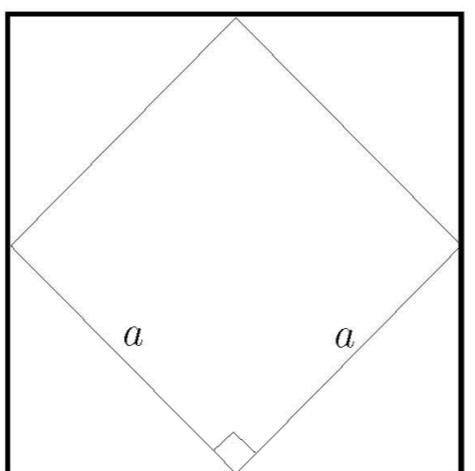
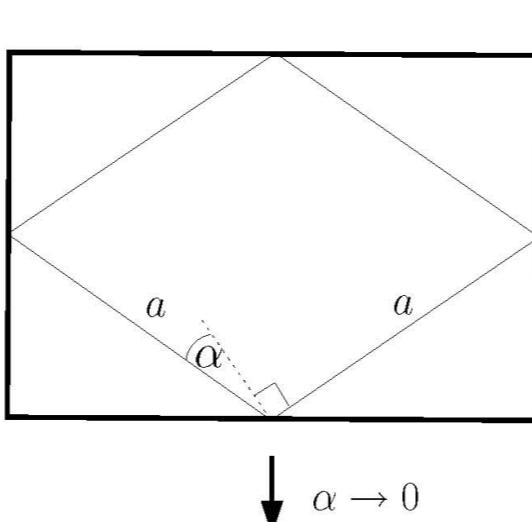
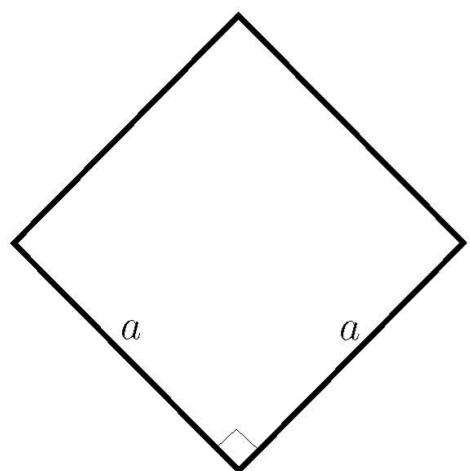
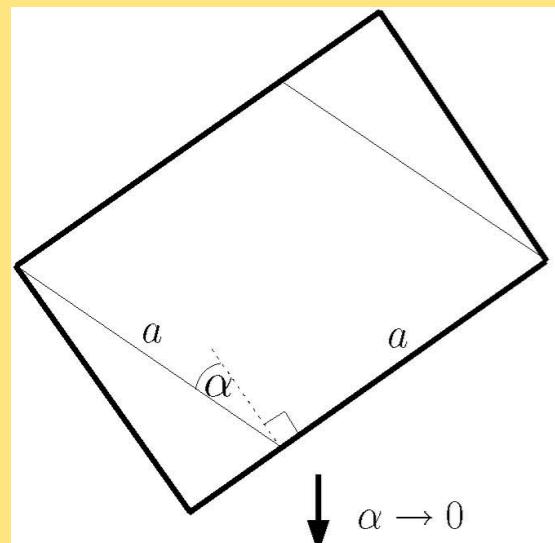
$$\lambda = C_{11} \quad e = (1, 0, \dots, 0)$$

Lower bounds  $\mathbb{R}^2$

**Theorem 2.**  $\lambda_{2,1} \geq 2$  and  $\lambda_{2,2} \geq 2$ .

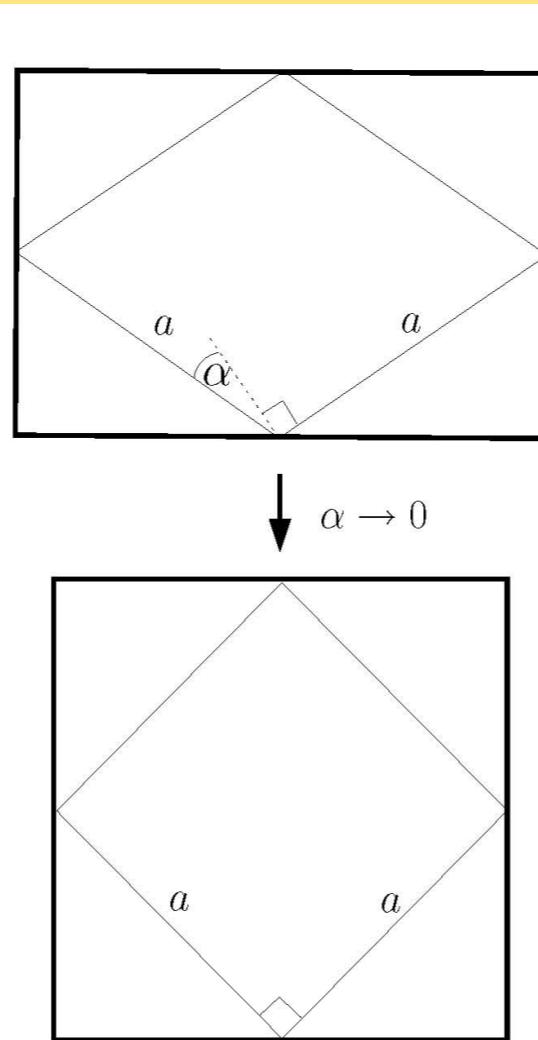
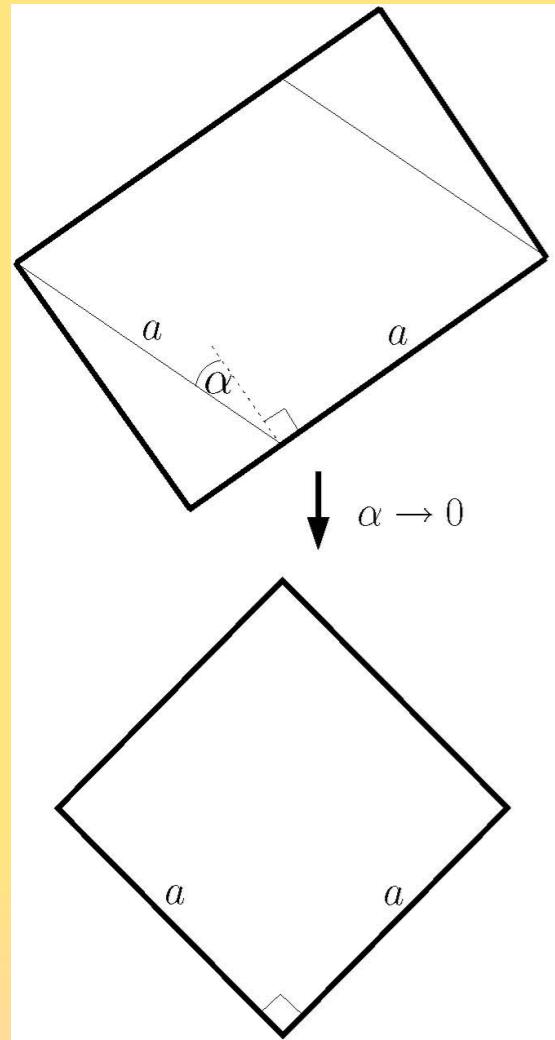
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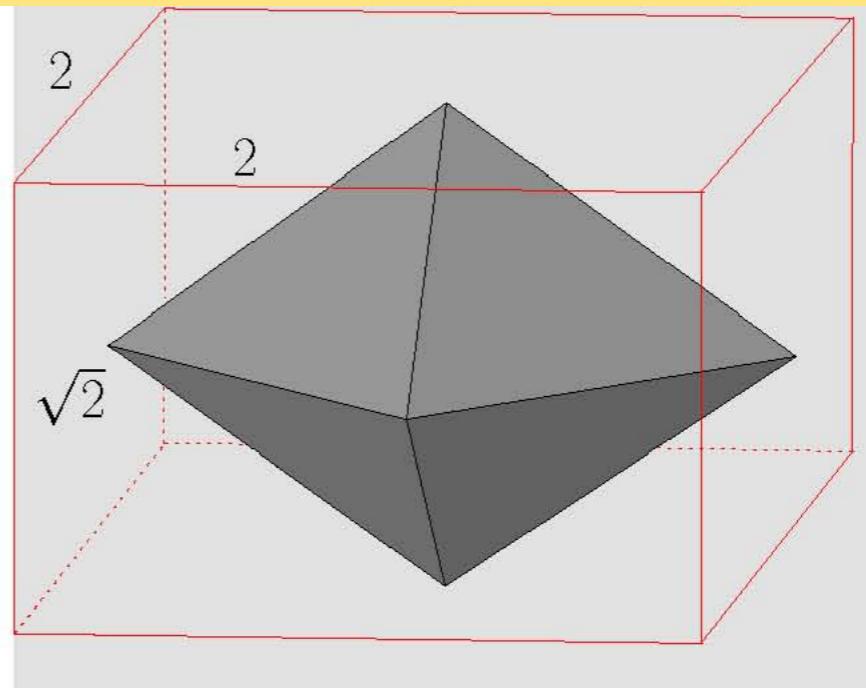
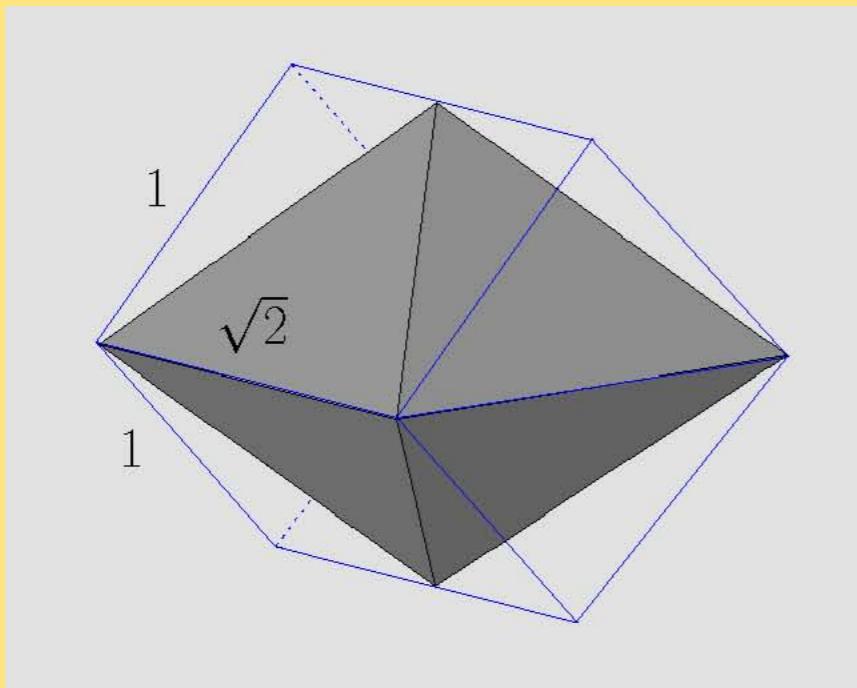
$$R_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Lower bounds  $\mathbb{R}^3$

**Theorem 3.**  $\lambda_{3,2} \geq 4$  and  $\lambda_{3,3} \geq 4$ .

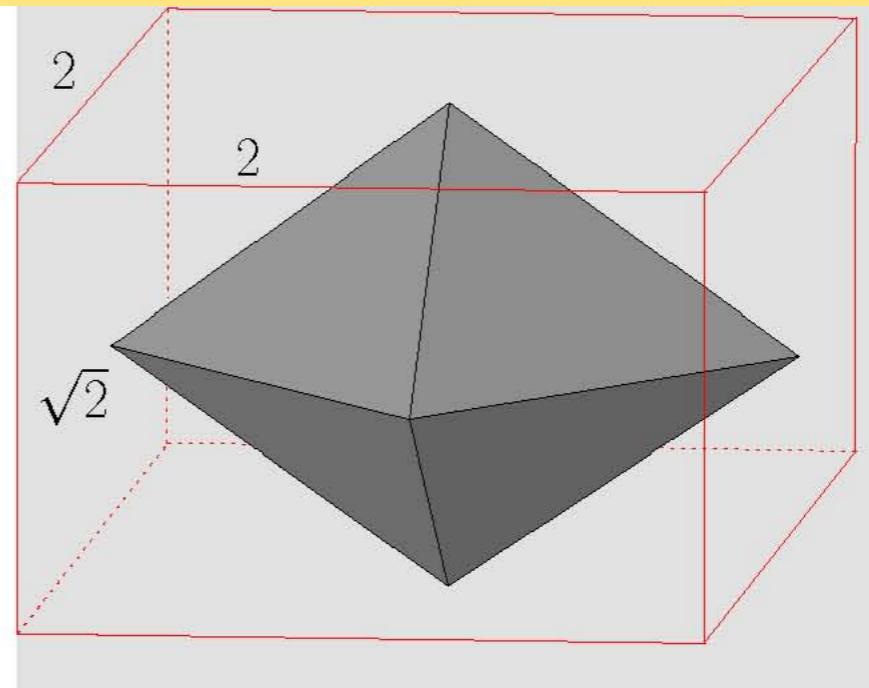
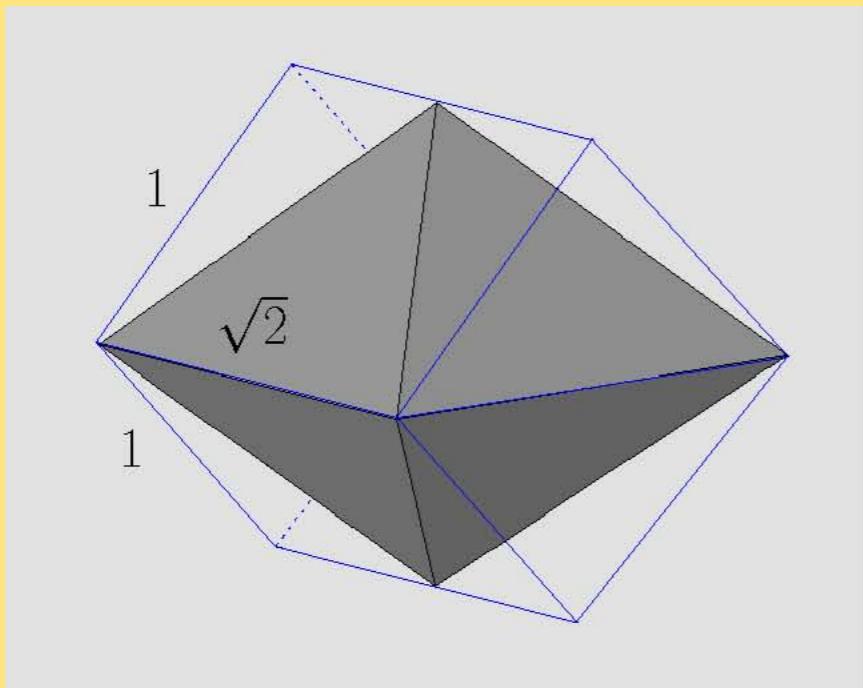
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$$R_3 = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

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 $a_{ii}$

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$$R_d = \frac{1}{\sqrt{2}} \left[ \begin{array}{c|c} R_{\frac{d}{2}} & R_{\frac{d}{2}} \\ \hline R_{\frac{d}{2}} & -R_{\frac{d}{2}} \end{array} \right]$$

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$$R_d = \frac{1}{\sqrt{2}} \left[ \begin{array}{c|c} R_{\frac{d}{2}} & R_{\frac{d}{2}} \\ \hline R_{\frac{d}{2}} & -R_{\frac{d}{2}} \end{array} \right] \quad R_2 = \frac{1}{\sqrt{2}} \left[ \begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right]$$

Lower bounds  $\mathbb{R}^d$

**Theorem 4.** If  $d$  is a power of two, then  $\lambda_{d,d-1} \geq \sqrt{d}^d$  and  $\lambda_{d,d} \geq \sqrt{d}^d$ .

$$a_i = (0, \dots, 0, \frac{\sqrt{d}}{2}, 0, \dots, 0), \quad \text{for } i = 1 \dots d$$



$$b_i = -a_i$$

convex polytop  $P_d$  with vertices:  $V = \{a_i, b_i | 1 \leq i \leq d\}$

unique PCs:  $a_{ii} := a_{ii} + \epsilon_i, \quad i = 1 \dots d, \quad \epsilon_1 > \dots > \epsilon_d$

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$R_d(P_d)$  fits into unit cube  $[-0.5, 0.5]^d$

Lower bounds  $\mathbb{R}^d$

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$\lambda_{d_1}$  is a lower bound in  $\mathbb{R}^{d_1}$

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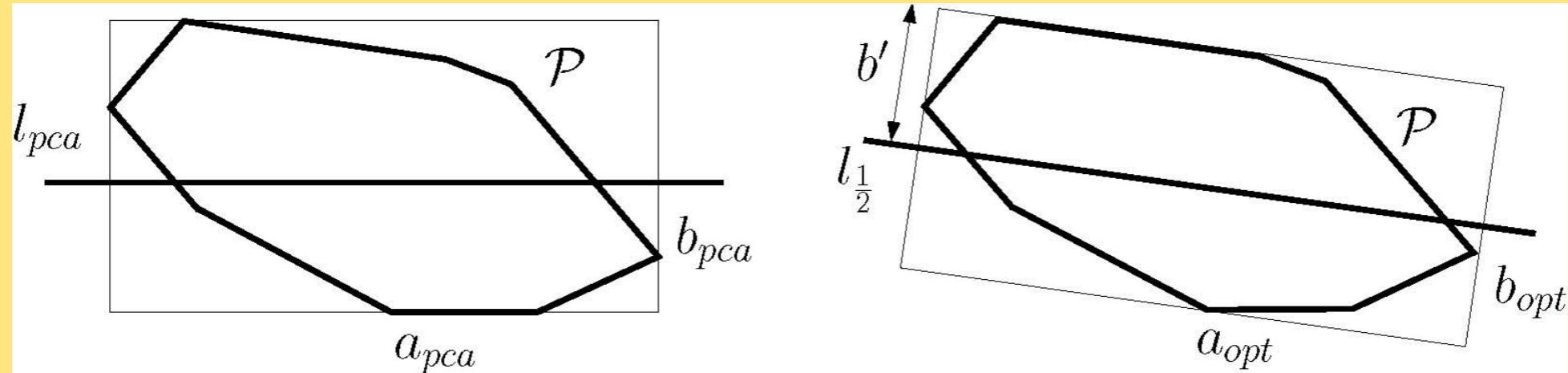
dimension	$\mathbb{R}$	$\mathbb{R}^2$	$\mathbb{R}^3$	$\mathbb{R}^4$	$\mathbb{R}^5$	$\mathbb{R}^6$	$\mathbb{R}^7$	$\mathbb{R}^8$	$\mathbb{R}^9$	$\mathbb{R}^{10}$
lower bound	1	2	4	16	16	32	64	4096	4096	8192

Upper bound  $\mathbb{R}^2$

**Theorem 5.**  $\lambda_{2,1} \leq 2.737$ .

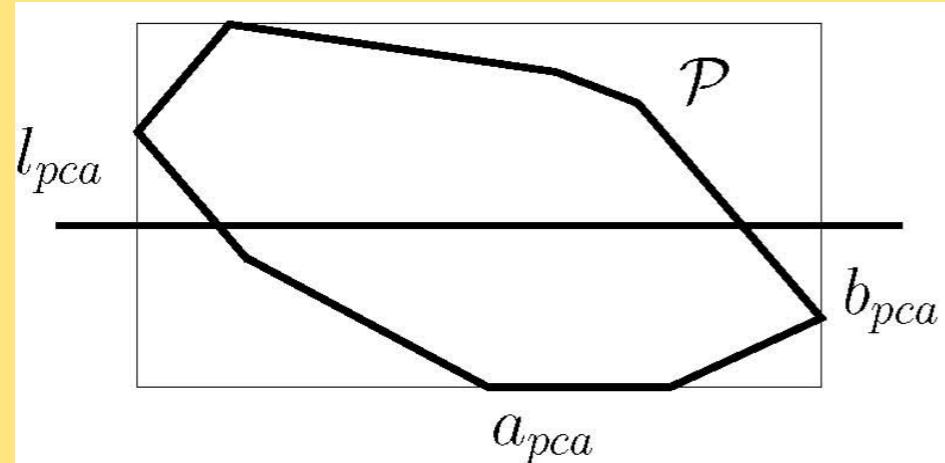
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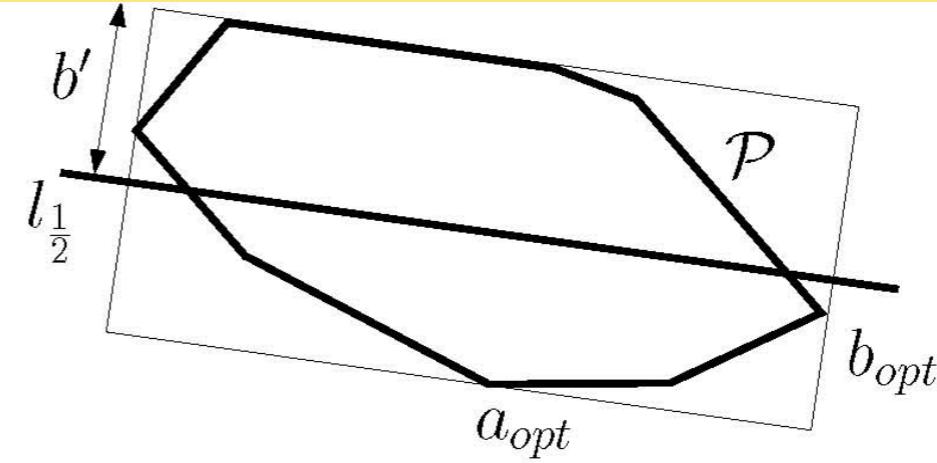


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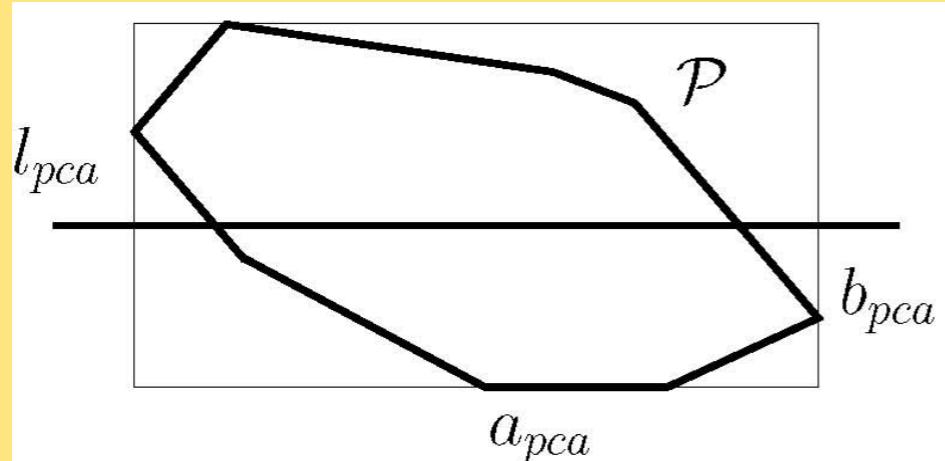
$$a_{pca}(P) \geq b_{pca}(P)$$



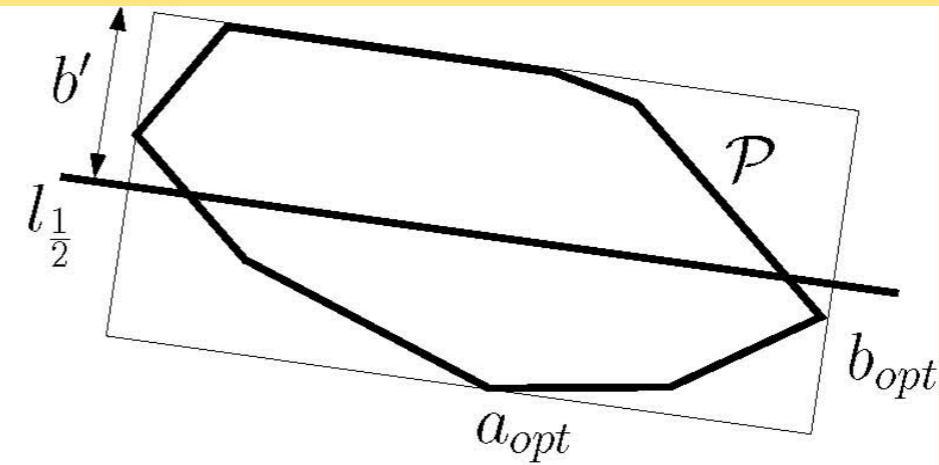
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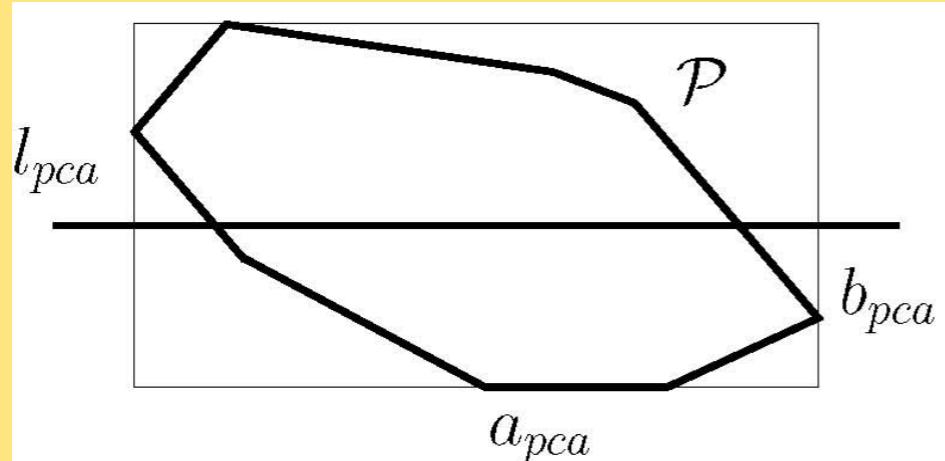


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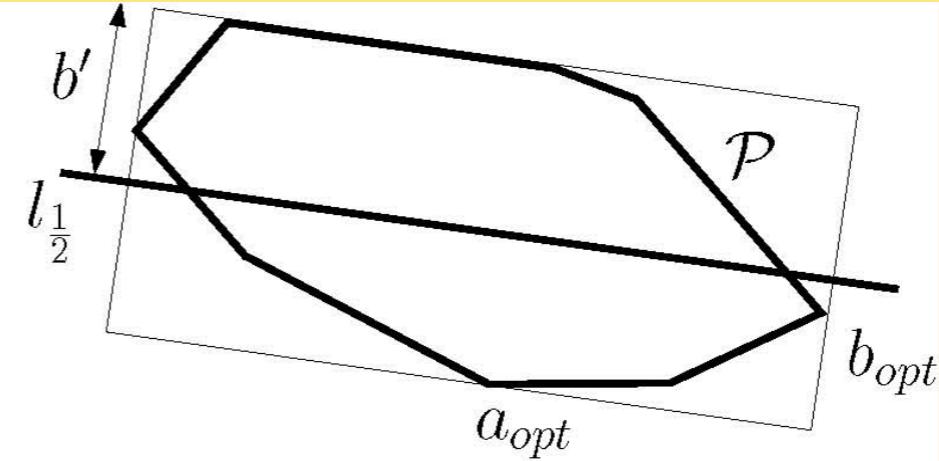
$$\alpha = \alpha(P) = \frac{a_{pca}(P)}{a_{opt}(P)}$$

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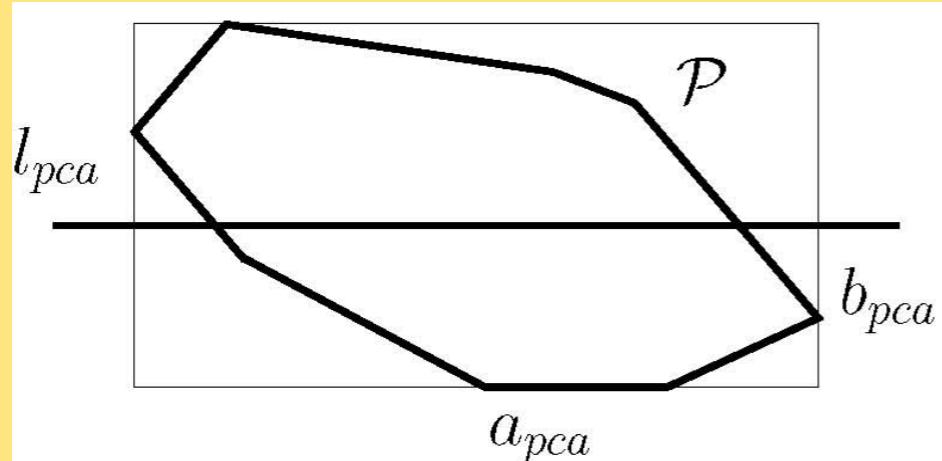
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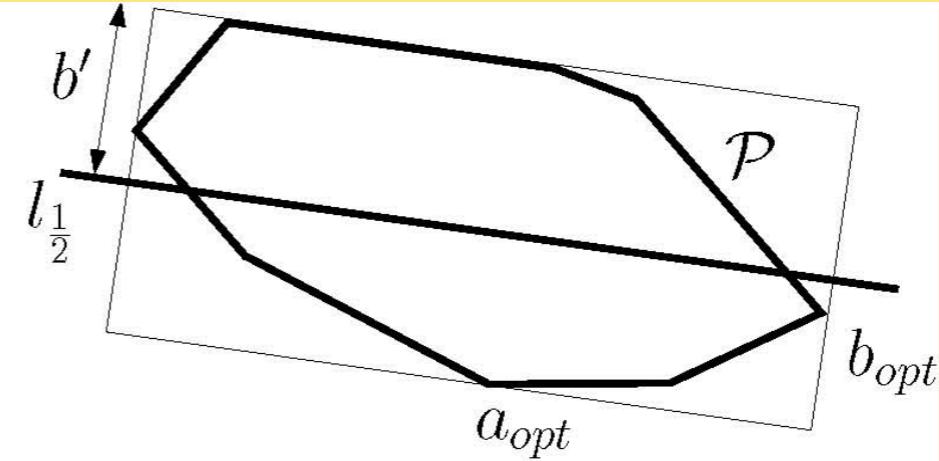
$$\beta = \beta(P) = \frac{b_{pca}(P)}{b_{opt}(P)}$$

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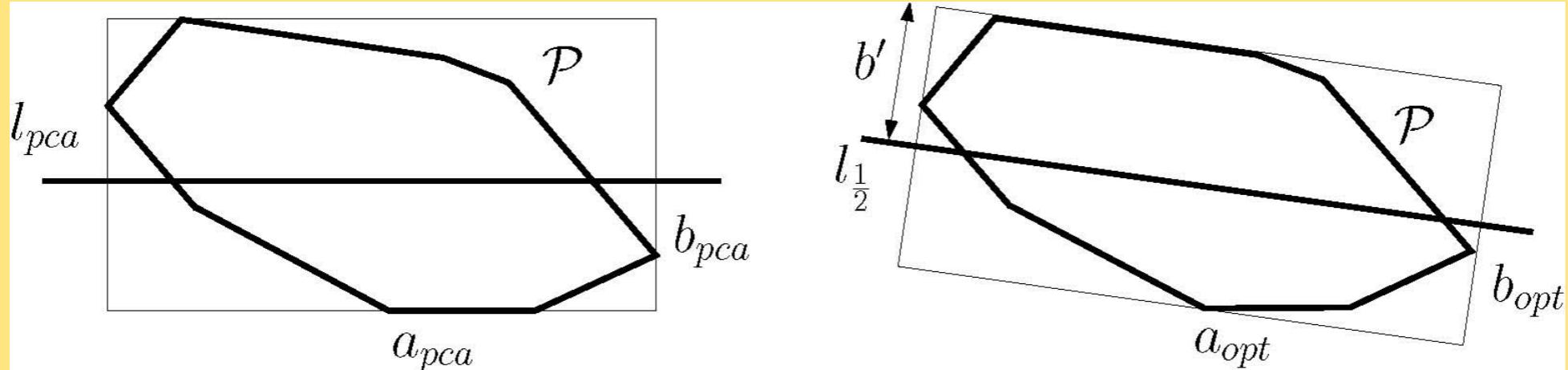
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$$\lambda_{2,1}(P) = \alpha(P) \cdot \beta(P)$$

Upper bound  $\mathbb{R}^2$

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$$\lambda_{2,1}(P) = \alpha(P) \cdot \beta(P)$$

$$\eta(P) = a_{opt}(P)/b_{opt}(P)$$

Upper bound  $\mathbb{R}^2$

**Theorem 5.**  $\lambda_{2,1} \leq 2.737$ .

Upper bound  $\mathbb{R}^2$

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**Lemma 2.**  $\lambda_{2,1}(P) \leq \eta + \frac{1}{\eta}$  and  $\lambda_{2,2}(P) \leq \eta + \frac{1}{\eta}$  for any point set  $P$  with fixed aspect ratio  $\eta(P) = \eta$ .

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**Lemma 3.**  $\lambda_{2,1}(P) \leq \sqrt{\frac{6\eta+2}{\eta}} \sqrt{1 + \frac{1}{\eta^2}}$  for any point set  $P$  with fixed aspect ratio  $\eta(P) = \eta$ .

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$$\lambda_{2,1} \leq \sup_{\eta \geq 1} \left\{ \min \left( \eta + \frac{1}{\eta}, \sqrt{\frac{6\eta+2}{\eta}} \sqrt{1 + \frac{1}{\eta^2}} \right) \right\}$$

Upper bound  $\mathbb{R}^2$

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$$b_{pca} \leq a_{pca} \leq diam(P)$$

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$$\alpha\beta \leq \eta \left( \sqrt{1 + \frac{1}{\eta^2}} \right)^2 = \eta + \frac{1}{\eta}$$

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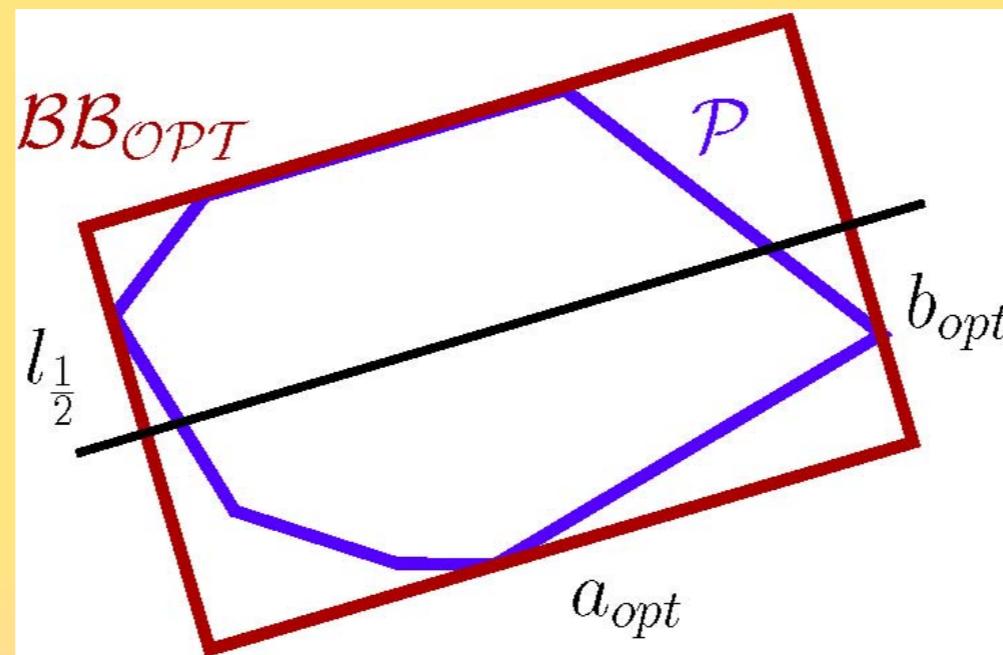
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Upper bound  $\mathbb{R}^2$

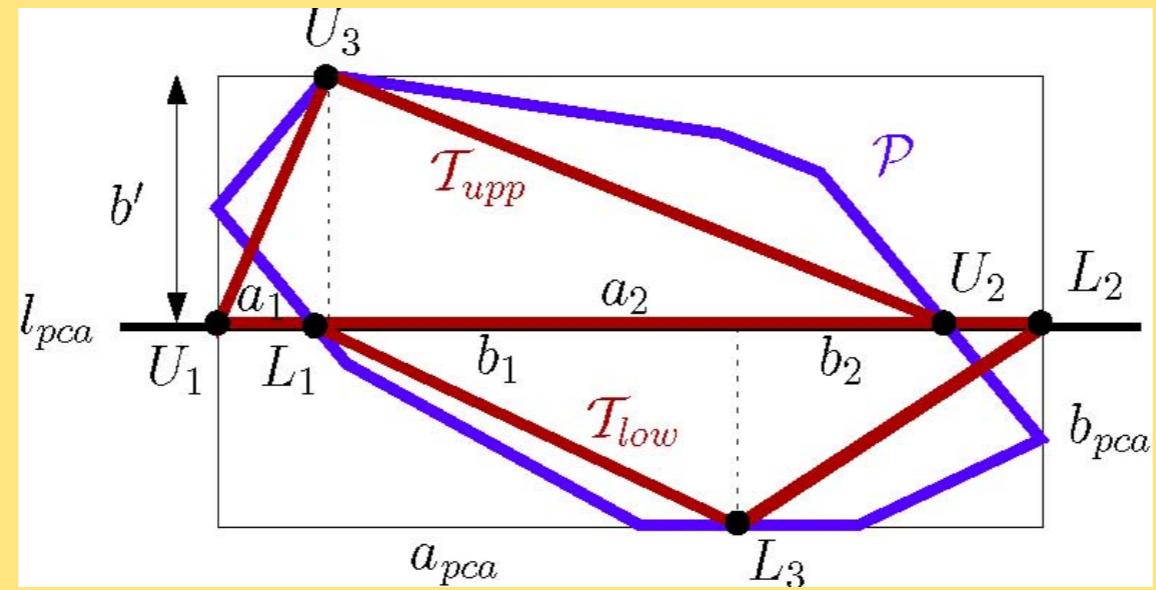
**Lemma 4.**  $d^2(\mathcal{P}, l_{\frac{1}{2}}) \leq d^2(\mathcal{BB}_{OPT}, l_{\frac{1}{2}}) \quad (= \frac{{b_{opt}}^2 a_{opt}}{2} + \frac{{b_{opt}}^3}{6})$

Upper bound  $\mathbb{R}^2$

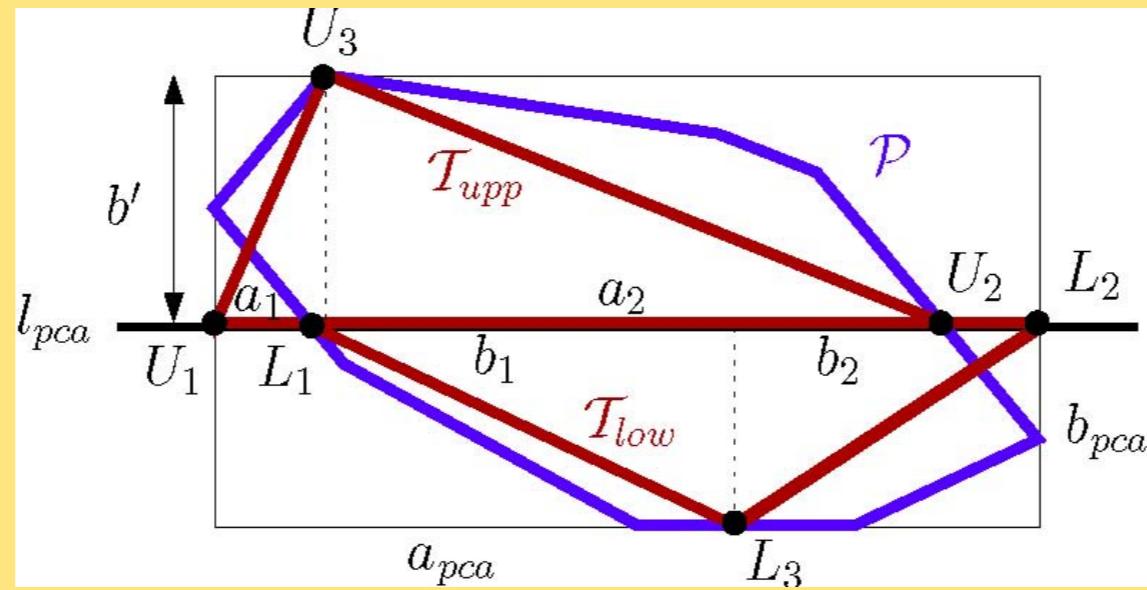
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Upper bound  $\mathbb{R}^2$



Upper bound  $\mathbb{R}^2$



**Lemma 5.**

$$\begin{aligned}
 d^2(\mathcal{P}, l_{pca}) &\geq d^2(\mathcal{T}_{upp}, l_{pca}) + d^2(\mathcal{T}_{low}, l_{pca}) \\
 &\geq \frac{b_{pca}^2}{12} \sqrt{a_{pca}^2 + 4b_{pca}^2}.
 \end{aligned}$$

## Future work and open problems

- Improving the upper bound in  $\mathbb{R}^2$
- Upper bound in  $\mathbb{R}^3$
- Upper bounds for an approximation factor in arbitrary dimension

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