

POINT SETS - DISTRIBUTIONS -

- DISTANCE METRIC - PCA etc.

[WHY? Histograms/distributions viewed as points in high-dim. space]

• "Affine Invariant Norm" for point sets:

→ Given:  $n$  points  $P_i = (x_i^1, x_i^2, \dots, x_i^k)^T$ ,  $i = 1 \dots n$ ,  
in  $k$ -dim. space

→ Norm ' $\|\cdot\|$ ' defines square of length of vector  
 $W = (x_1, \dots, x_k)^T$ :

$$\|W\|^2 = W^T Q W, \quad \text{where}$$

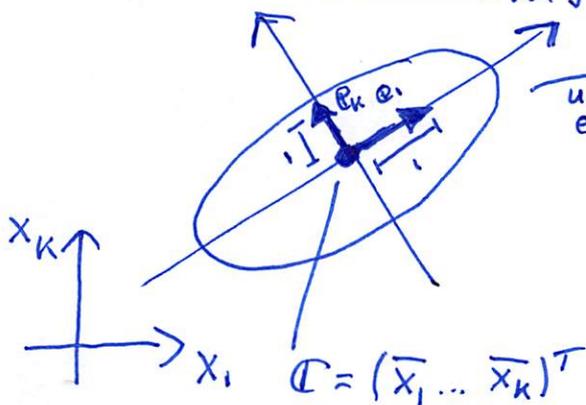
$$Q = n (D^T D)^{-1}, \quad \text{where}$$

$$D = \begin{pmatrix} x_1^1 - \bar{x}_1 & \dots & x_1^k - \bar{x}_k \\ \vdots & & \vdots \\ x_n^1 - \bar{x}_1 & \dots & x_n^k - \bar{x}_k \end{pmatrix}, \quad \text{where}$$

$$\bar{x}_j = \frac{1}{n} \sum_{i=1}^n x_j^i, \quad j = 1 \dots k$$

→  $Q$  has REAL eigenvalues  $\lambda_1, \dots, \lambda_k$

(and [normalized] corresponding eigenvectors  $e_1, \dots, e_k$ )



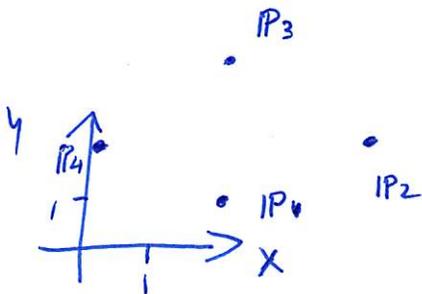
→ Condition for points  $p$  on  
UNIT ellipsoid:

$$p^T Q p = 1$$

$$l_1^2 = 1/\lambda_1, \dots, l_k^2 = 1/\lambda_k$$

are the squared lengths  
of ellipsoid's principal axes.

• Simple 2D example

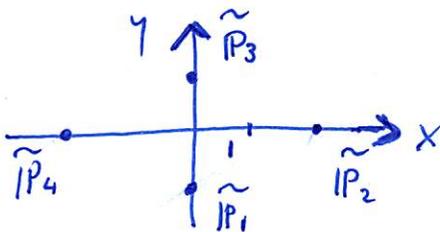


n=4:

$$P_1 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, P_2 = \begin{pmatrix} 4 \\ 2 \end{pmatrix}, P_3 = \begin{pmatrix} 2 \\ 3 \end{pmatrix}, P_4 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

(i) 
$$\underline{C} = \frac{1}{4} \sum_{i=1}^4 P_i = \frac{1}{4} \begin{pmatrix} 8 \\ 8 \end{pmatrix} = \underline{\underline{\begin{pmatrix} 2 \\ 2 \end{pmatrix}}}$$

subtract mean C



$$\underline{\tilde{P}_i = P_i - C}$$

(ii) Perform mean-subtraction

and compute D ( $P_i \mapsto \tilde{P}_i$ ):

$$\underline{D} = \begin{pmatrix} [ \tilde{P}_1 ] \\ [ \tilde{P}_2 ] \\ [ \tilde{P}_3 ] \\ [ \tilde{P}_4 ] \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 2 & 0 \\ 0 & 1 \\ -2 & 0 \end{pmatrix}$$

(iii) Compute Q:

$$D^T D = \begin{pmatrix} 0 & 2 & 0 & -2 \\ -1 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 2 & 0 \\ 0 & 1 \\ -2 & 0 \end{pmatrix} = \begin{pmatrix} 8 & 0 \\ 0 & 2 \end{pmatrix}$$

$$\Rightarrow (D^T D)^{-1} = \begin{pmatrix} 1/8 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$\Rightarrow \underline{Q} = n \cdot (D^T D)^{-1} = 4 \cdot \begin{pmatrix} 1/8 & 0 \\ 0 & 1/2 \end{pmatrix} = \underline{\underline{\begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix}}}$$

(iv) Eigenvalues & eigenvectors of Q:

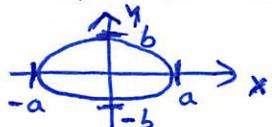
$$\begin{vmatrix} 1/2 - \lambda & 0 \\ 0 & 2 - \lambda \end{vmatrix} = 0 \Rightarrow \underline{\lambda_1 = 1/2}, \underline{\lambda_2 = 2}$$

$$\begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} e_x \\ e_y \end{pmatrix} = \frac{1}{2} \begin{pmatrix} e_x \\ e_y \end{pmatrix} \Rightarrow \underline{e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}}, \begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} e_x \\ e_y \end{pmatrix} = 2 \begin{pmatrix} e_x \\ e_y \end{pmatrix} \Rightarrow \underline{e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}}$$

(v) Length of ellipse's principal axes:

$$l_1^2 = 1/\lambda_1 = 2 \Rightarrow \underline{l_1 = \sqrt{2}}, l_2^2 = 1/\lambda_2 = 1/2 \Rightarrow \underline{l_2 = \sqrt{2}/2}$$

(vi) Ellipse:



$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 = 1$$

Here:  $a = \sqrt{2}$   
 $b = \sqrt{2}/2$



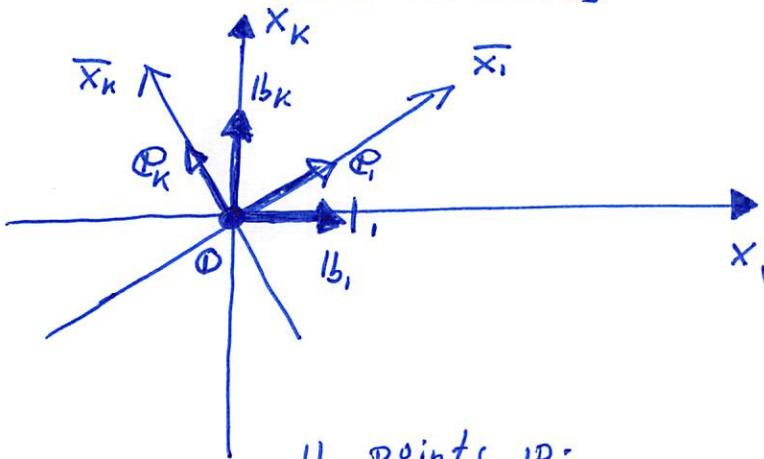
■ USING THE PCA-based EIGENDIRECTIONS

OF A POINT SET TO DEFINE "TIGHT" OBJECT

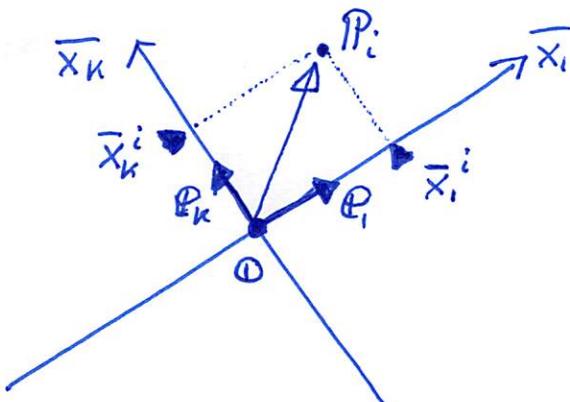
POINT SET-ALIGNED BOUNDING BOXES (PSABBs)

• ILLUSTRATION

[MEAN SUBTRACTION HAS ALREADY BEEN DONE..]



points  $P_i$  must be expressed w.r.t. eigen system; then the MINIMAL PSABB is computed.



1) Original system:  
 $\{0, b_1, \dots, b_k\}$   
→ coordinates  $x_1, \dots, x_k$

2) "Eigen system":  
 $\{0, e_1, \dots, e_k\}$   
→ coordinates  $\bar{x}_1, \dots, \bar{x}_k$

3) Basis vectors  $b_i$  &  $e_i$  are all normalized.

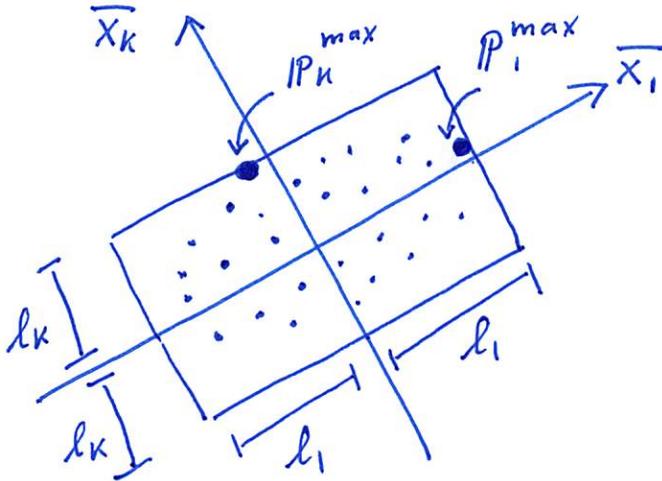
4) Coordinates of  $P_i$  w.r.t.  $e_1, \dots, e_k$ :

$$\bar{x}_1^i = P_i \cdot e_1$$

$$\bar{x}_k^i = P_i \cdot e_k$$

$$\Rightarrow \bar{x}_j^i = P_i \cdot e_j, \quad j=1 \dots k \quad !$$

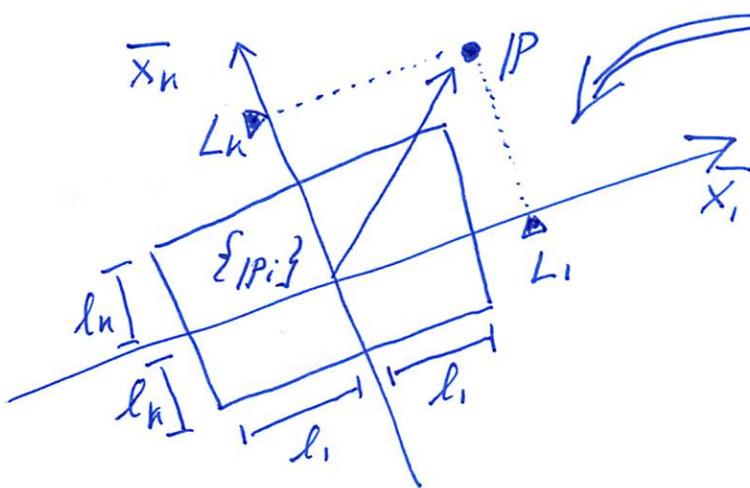
5) Establish minimal PSABB for set of  $\{P_i\}$ :



→ Determine the points  $P_i^{\max}, \dots, P_k^{\max}$  with maximal value for coordinate  $x_j$ : (absolute value!)

→ minimal PSABB's edge lengths can be computed; compute values for  $l_1, \dots, l_k$ .

6) Utilization: Can quickly determine whether a "new" point  $P$  (expressed relative to  $q_1, \dots, q_k$  - after mean subtraction) "is inside the point set  $\{P_i\}$  or not:



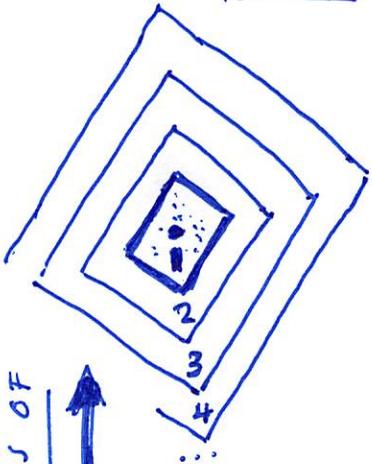
• here:  $|L_1| > l_1$   
 $\Rightarrow$  " $P \notin \{P_i\}$ "

• Can quickly "classify" point  $P$  as being of type  $\{P_i\}$  - or not.

■ CAN USE POINT DENSITY & PCA-based METRIC  
OF DEFINED BY THE DISTINCT CLUSTERS TO ALSO  
DETERMINE TO WHAT POINT CLUSTER A NEW POINT  
P IS CLOSER TO:

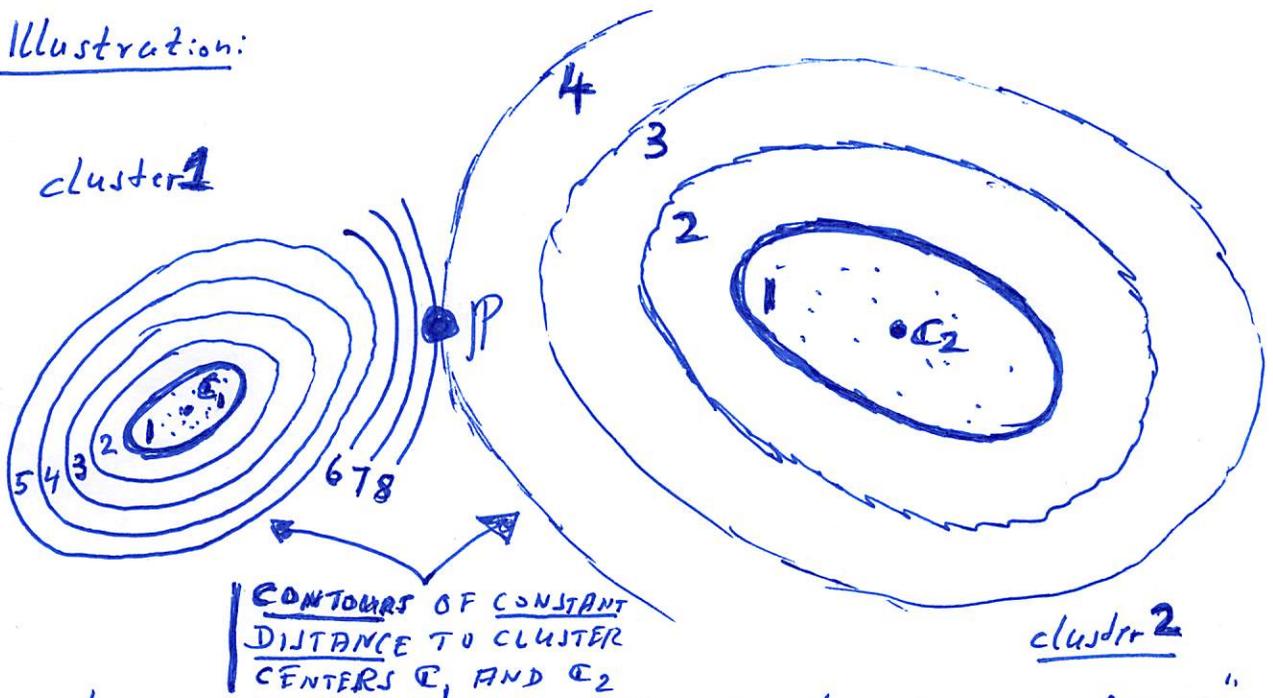
- Idea: The eigenvalues & eigenvectors associated with a cluster define cluster-specific off-sets (or contours of 'distance from cluster center') - that can be used to define a point P's distance to various clusters / cluster centers:

[SEE REF: Louis Feng, Ingrid Hote, Bernd Hamann, Ken Joy - "Anisotropic Noise Samples"]



EFFICIENT APPROXIMATION: PSABBS  
 USE OFF-SETS OF PSABBS

- Illustration:



here: " P is 8 units away from  $C_1$ , 4 units away from  $C_2$  ;  
 ⇒ P is closer to cluster 2 !!!