24. XI. 25

Goals

- principal component analysis
- data = point cloud
- variance & covariance
- orthogonal diagonalization

Suppose each trial of an experiment makes m real-valued measurements, and we run n trials. This produces

$$P = \underbrace{\{x_1, \dots, x_n\}}_{\text{point cloud}} \subseteq \mathbb{R}^m$$

The **mean** of P is $\mu := \frac{1}{n}(x_1 + \cdots + x_n)$.

The **recentering** of P is $B = \begin{pmatrix} | & | & & | \\ x_1 - \mu & x_2 - \mu & \cdots & x_n - \mu \\ | & | & & | \end{pmatrix} \in \mathbb{R}^{m \times n}$.

Note The mean of the columns of B is $\vec{0}$.

Defn The covariance matrix of P is the symmetric matrix.

$$S = \frac{1}{n-1} B B^T \in \mathbb{R}^{m \times m}$$

$$(BB^T)^T = (B^T)^T \cdot B^T = BB^T$$

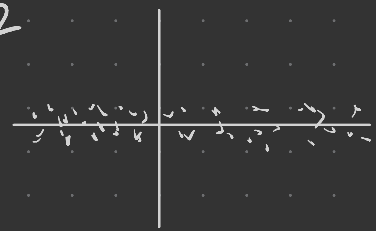
Note $$S_{ii} = \frac{1}{n-1} \sum_{j=1}^{n} (x_{ji} - \mu_i)^2$$ = variance of i-th measurement/variable

For $i \neq j$, $$S_{ij} = \frac{1}{n-1} \sum_{j=1}^{n} (x_{ji} - \mu_i)(x_{ij} - \mu_j)$$ = covariance of i-th, j-th variables

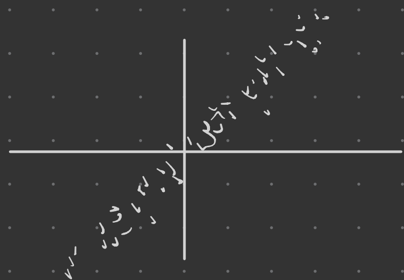
- Variance measures how much things differ from the mean. Its square root is standard deviation.
- Covariance measures how variables depend on each other.

Defn The <u>total</u> <u>variance</u> of P is $\operatorname{tr}(S) = \sum$ variance of variables.

E.g. $m=2$



$$S = \begin{pmatrix} 95 & 1 \\ 1 & 5 \end{pmatrix}$$



$$S = \begin{pmatrix} 50 & 40 \\ 40 & 50 \end{pmatrix}$$

Idea Use linear algebra to recognize the similarity of these data.

Spectral Thm If $A \in \mathbb{R}^{n\times n}$ and $A = A^T$, then $\exists\, \lambda_1, \dots, \lambda_n \in \mathbb{R}$ and orthonormal nonzero vectors $v_1, \dots, v_n$ such that $Av_i = \lambda v_i$.

Note • If $P = \begin{pmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{pmatrix}$ then $PP^T = I_n$ and

$$\mathrm{diag}(\lambda_1, \dots, \lambda_n) = P^{-1}AP.$$

• For $B \in \mathbb{R}^{m\times n}$, $BB^T = (BB^T)^T \in \mathbb{R}^{m\times m}$ and the spectral theorem applies.

Prop $\underbrace{BB^T}_{\mathbb{R}^{m\times m}}$ and $\underbrace{B^TB}_{\mathbb{R}^{n\times n}}$ share the same nonzero eigenvalues.

Pf Take v an eigenvector of B^TB with eigenvalue $\lambda \neq 0$, so

$$B^TBv = \lambda v$$

$\Rightarrow (BB^T)(Bv) = \lambda (Bv)$ [mult on left by B]

$\Rightarrow \lambda$ is an eigenvalue of BB^T with eigenvector Bv.

($Bv \neq 0$ b/c $B^TBv = \lambda v \neq 0$)

Similarly, $BB^Tw = \lambda w \Rightarrow B^TB(B^Tw) = \lambda(B^Tw)$, so BB^T, B^TB have the same nonzero eigenvalues. $\square$

Q How should we find eigenvalues when $B \in \mathbb{R}^{500\times 2}$?

A $BB^T \in \mathbb{R}^{500\times 500}$

$B^TB \in \mathbb{R}^{2\times 2}$ work on this $\chi_{B^TB}(x)$ quadratic polynomial

$\rightsquigarrow \lambda_1, \lambda_2$ eigenvals of B^TB

BB^T has eigenvalues $\lambda_1, \lambda_2, 0$.

Prop The eigenvalues of BB^T, B^TB are all nonnegative.

Pf Take v an eigenvector of B^TB w/ eigenvalue λ. Then

$$\begin{aligned}
\|Bv\|^2 &= Bv \cdot Bv \\
&= (Bv)^T (Bv) \\
&= v^T (B^TB) v \\
&= v^T (\lambda v) \\
&= \lambda (v^T v) \\
&= \lambda \|v\|^2 .
\end{aligned}$$

Since $\|Bv\|^2 \geq 0$ and $\|v\|^2 > 0$, must have $\lambda \geq 0$. $\square$

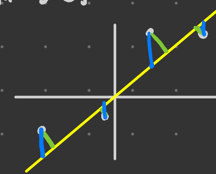
The covariance matrix $S = \frac{1}{n-1} BB^T$ thus has nonnegative real eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m \geq 0$.

Let $u_1, \dots, u_m$ be the corresponding orthonormal eigenvectors; these are the principal components of the data.

Note

- total variance $= \operatorname{tr}(S) = \lambda_1 + \cdots + \lambda_m =: T$
- The first principal component u_1 accounts for $\frac{\lambda_1}{T}$ of the total variance. In general, u_i accounts for $\frac{\lambda_i}{T}$ of the total variance.
- u_1 points in the "most significant" direction.
- Among $u_1^\perp$, u_2 points in the most significant direction. Etc.

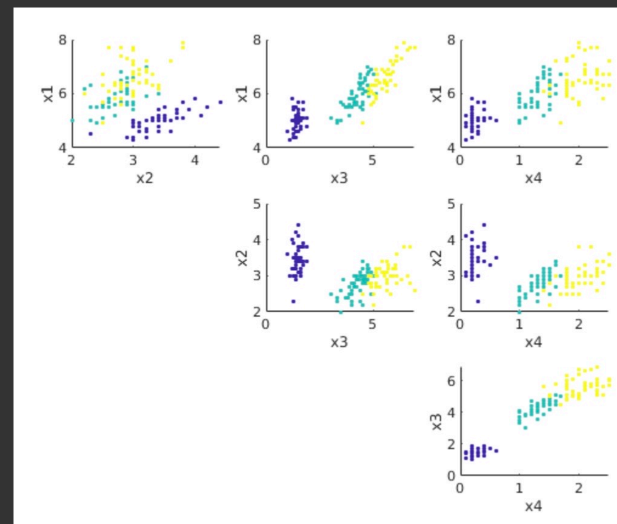
Fact span$\{u_1\}$ minimizes orthogonal distance from line to point cloud.

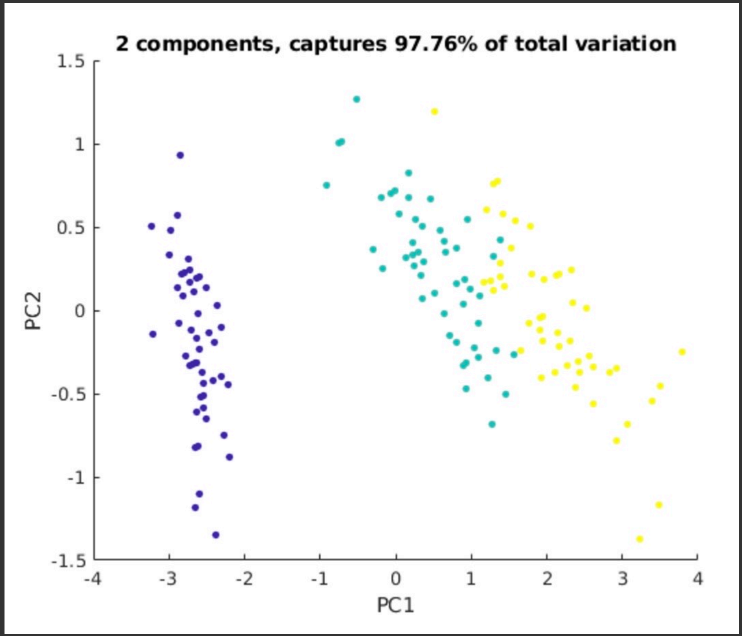


| least squares

\ PCA

E.g. 150 iris flowers measured by sepal and petal length/width




2 components, captures 97.76% of total variation
1.5
1
0.5
0
-0.5
-1
-1.5
PC2
-4
-3
-2
-1
0
1
2
3
4
PC1