From SVD to PCA

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- Now we drive SVD when the rank of $\mathbf{X}$ is $r < n$.

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- It is also known that $\lambda_i \geq 0$ (Homework: Verify it!). If the rank of $\mathbf{X}$ is r ($r \leq n$), there are exactly r positive eigenvalues, say

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- Then
$$\mathbf{X}^T\mathbf{u}_i = \sigma_i\mathbf{v}_i$$
$$\mathbf{X}\mathbf{v}_i = \sigma_i\mathbf{u}_i$$

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- Put in matrix notation:

$$\mathbf{X}[\mathbf{v}_1\ \mathbf{v}_2\ \cdots\ \mathbf{v}_r] = [\sigma_1\mathbf{u}_1\ \sigma_2\mathbf{u}_2\ \cdots\ \sigma_r\mathbf{u}_r]$$

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- Answer: Since the coefficient matrix $\mathbf{V}_1 := [\mathbf{v}_1\ \mathbf{v}_2\ \cdots\ \mathbf{v}_r]$ has rank r (Why?), the dimension of the solution space is $n - r$.

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- Answer: Since the coefficient matrix $\mathbf{V}_1 := [\mathbf{v}_1\ \mathbf{v}_2\ \cdots\ \mathbf{v}_r]$ has rank r (Why?), the dimension of the solution space is $n - r$.
- So, there are exactly $n - r$ orthogonal vectors $\mathbf{v}_{r+1}$, $\mathbf{v}_{r+2}$, ... , $\mathbf{v}_n$ such that $\mathbf{v}_1$, $\mathbf{v}_2$, ..., $\mathbf{v}_n$ form an orthogonal basis of $\mathbb{R}^n$.

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- Use the extended basis:

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- So, $\mathbf{XV} = [\mathbf{u}_1\ \mathbf{u}_2\ \cdots\ \mathbf{u}_r][D \vdots \mathbf{0}_{r\times(n-r)}]$. Thus

$$\mathbf{X} = [\mathbf{u}_1\ \mathbf{u}_2\ \cdots\ \mathbf{u}_r][D \vdots \mathbf{0}_{r\times(n-r)}]\mathbf{V}^T$$

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- Finally, to make the $\mathbf{u}_i$ matrix a square matrix, we extend it an orthogonal basis: $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_m$.

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- Define $U := [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_m]$ and fill 0's under $[D \vdots \mathbf{0}_{r\times(n-r)}]$:

$$\mathbf{X} = \mathbf{U} \begin{bmatrix} D \vdots \mathbf{0}_{r\times(n-r)} \\ \mathbf{0}_{m-r\times n} \end{bmatrix} \mathbf{V}^T$$

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- We are done!

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- Put **U** and **V** back to column vector form in SVD:

$$\mathbf{X} = \mathbf{U} \left[\begin{array}{c} D \vdots \mathbf{0}_{r\times(n-r)} \\ \mathbf{0}_{m-r\times n} \end{array} \right] \mathbf{V}^T$$

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- So,

$$\mathbf{X} = [\sigma_1 \mathbf{u}_1 \ \cdots \ \sigma_r \mathbf{u}_r \ \mathbf{0} \ \cdots \ \mathbf{0}] \begin{bmatrix} \mathbf{v}_1^T \\ \mathbf{v}_2^T \\ \vdots \\ \mathbf{v}_n^T \end{bmatrix} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

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- If we can do so, then

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for some coefficients f_{ij}'s.

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  for some coefficients f_{ij}'s.
- Note that $f_{ij} = \mathbf{a}_i^T \mathbf{u}_j$, the projection of $\mathbf{a}_i$ along the direction of $\mathbf{u}_j$.

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- So,

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- We have

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- Assume $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$. Then

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This is the largest eigenvalue of A.

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- Using the same idea, the second principal component is the direction: be orthogonal to the first and maximize the total projection:

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- Now you see the pattern:
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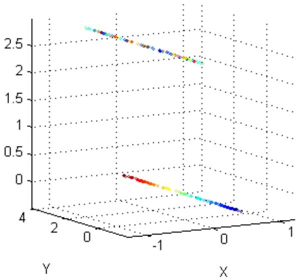

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- Form the $m \times n$ data matrix

$$X := [\tilde{\mathbf{I}}_1 \ \tilde{\mathbf{I}}_2 \ \cdots \ \tilde{\mathbf{I}}_n]$$