Review:

② Mean and variance and covariance:

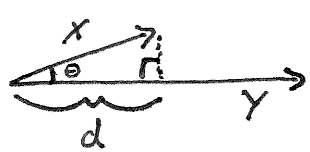
$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X^{(i)}$$

$$Var(X) = \frac{1}{n}\sum_{i=1}^{n}\left(X^{(i)} - \bar{X}\right)^2$$

$$Cov(X,Y) = \frac{1}{n}\sum_{i=1}^{n}(X^{(i)} - \bar{X})(Y^{(i)} - \bar{Y})$$

④ Dot product, orthogonal projections, ~~orthogonal~~ orthonormal basis, and orthogonal matrix.

$$X \cdot Y = \sum_{i=1}^{p} X_i Y_i$$



Recall:

$$\cos(\theta) = \frac{X \cdot Y}{|X||Y|}$$

$$\cos(\theta) = \frac{d}{|X|}$$

$$d = \frac{X \cdot Y}{|Y|} = X \cdot \hat{Y}$$

$$V = \begin{bmatrix} | & | & \\ v_1 & v_2 & \cdots \\ | & | & \end{bmatrix}_{p \times p}$$

Let V be an orthogonal basis. That means the cols of V are all orthogonal to one another and have unit length.

Note:

$$V^T V = I$$

$\therefore V^T = V^{-1}$

$\therefore V V^T = I$

Put an orthonormal basis into a matrix to make an orthogonal matrix

PCA method:

① Our dataset:
n samples
p features

$X^{(1)}, X^{(2)}, \ldots X^{(n)}$

$X^{(i)} \in \mathbb{R}^p$

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③ Step 1: Create the "centered design matrix" M.

$$M = \begin{bmatrix} — X^{(1)} - \bar{X} \\ — X^{(2)} - \bar{X} \\ \vdots \\ — X^{(n)} - \bar{X} \end{bmatrix}_{n \times p}$$

⑤ Step 2: Compute the covariance Matrix

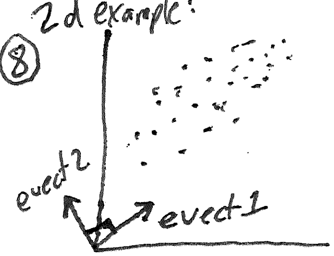
$$\Sigma = M^T M / n$$

⑦ Step 3: Compute the eigenvectors/values of Σ.

evals, evects = eig$(M^T M)$

The evect w/ the largest eval is the direction of most variance in the data.
... second most...

⑧ 2d example:



evect1 is the "first principal component"

all evects are orthogonal.

PCA derivation:

What will Σ look like?

... It is like there is a little covariance between all pairs, and some pair will have (possibly) a lot of covariance.

Crazy idea: Could we find a new orthogonal basis, project our data to it, and have no covariance?

Let's see...

$$(MV)^T(MV) = \begin{bmatrix} \lambda_1 & & \emptyset \\ & \lambda_2 & \\ \emptyset & & \ddots \; \lambda_p \end{bmatrix}$$

(no covariance)

$$(MV)^T(MV) = V^T M^T M V$$

$$V V^T M^T M V = V \begin{bmatrix} \lambda_1 & & \emptyset \\ & \lambda_2 & \\ \emptyset & & \ddots \; \lambda_p \end{bmatrix}$$

$$M^T M V = V \begin{bmatrix} \lambda_1 & \cdots & \emptyset \\ \emptyset & & \lambda_p \end{bmatrix}$$

$$\begin{bmatrix} M^T M \end{bmatrix} \begin{bmatrix} | & | & \\ v_1 & v_2 & \cdots \\ | & | & \end{bmatrix} = \begin{bmatrix} | & | & \\ v_1 & v_2 & \cdots \\ | & | & \end{bmatrix} \begin{bmatrix} \lambda_1 & \cdots & \emptyset \\ \emptyset & & \lambda_p \end{bmatrix}$$

consider only one column of result on each side

⑥

$$\begin{bmatrix} M^T M \end{bmatrix} \begin{bmatrix} | \\ v_i \\ | \end{bmatrix} = \begin{bmatrix} | \\ v_i \\ | \end{bmatrix} \lambda_i \rightarrow Ax = \lambda x$$

→ Eigenvectors!

(9) The relative size of the eigenvalues tell us the % explained variance of each eigenvector.

Let $\lambda_1, \lambda_2, \dots, \lambda_p$ be the decreasing list of eigenvalues. also called the "loadings".

total power $= \sum_{i=1}^{p} \lambda_i$

~~tota~~ power of k eigenvetors $= \dfrac{\sum_{i=1}^{k} \lambda_k}{\sum_{i=1}^{p} \lambda_p}$

Typically, set k s.t. 90% of the variance is explained.

(10) Keep k eigenvectors $\rightarrow$ let $U_{p\times k} = \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_k \\ | & | & & | \end{bmatrix}$ where u_i are the principal componets. i.e. $\text{eig}(M^T M)$

Edit: (I should have called this V.)

(11) Reduce the dims. by $R = MU$ i.e. $R_{n\times k} = M_{n\times p} U_{p\times k}$

↳ reduced to k dims.

(12) Reconstruct an estimate of M by "undoing" the dim reduction:

$$R = MU \rightarrow \tilde{M} = RU^{-1} = RU^T$$

Singular Value Decomposition (SVD)

① Every matrix M has a unique decomposition in the following form:

$$M = USV^T$$

where:

$M_{n \times p}$ is any matrix

$U_{n \times n}$ is an orthogonal matrix

$S_{n \times p}$ is a diagonal matrix with positive dec. real values on the diagonal
↳ these values are the "singular values" of M.

$V^T_{p \times p}$ is an orthogonal matrix

Some Properties:

The columns of U are the eigenvectors of MM^T

The columns of V are the eigenvectors of M^TM

If the rank of M is k, the SVD can look like this:

$$M_{n \times p} = U_{n \times k} S_{k \times k} V^T_{k \times p}$$

Note: $k \leq \min(n,p)$

② We can already see the SVD is computing the same thing as PCA from our description on the left: Both compute $\boxed{eig(M^TM)}$

Here's another way to see the same thing (that SVD and PCA are doing the same thing):

$\Lambda = \begin{bmatrix} \lambda_1 & & \emptyset \\ & \ddots & \\ \emptyset & & \lambda_p \end{bmatrix}$

Recall: (from PCA)

$(MV)^T MV = \Lambda$

$V^T M^T MV = \Lambda$

$M^T MV = V\Lambda$

$M^TM = V \Lambda V^T$

New: (in SVD world)

$M = USV^T$

$M^TM = (USV^T)^T USV^T$

$= VS^TU^TUSV^T$

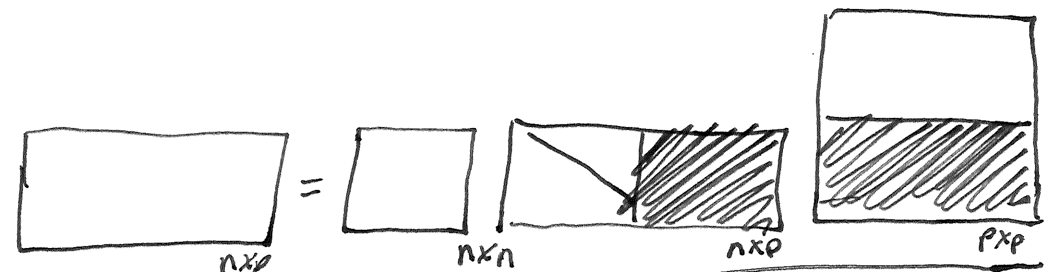
$= VS^TSV^T$

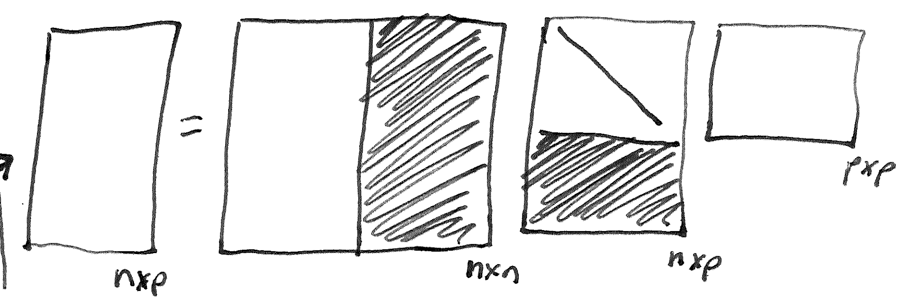
$M^TM = VS^2V^T$

In SVD world, V is the matrix where the cols are $eig(M^TM)$

$\Lambda = S^2$

↳ the evals are the squared singular vals.





So... SVD and PCA do the same thing... but there are two ways SVD wins.

SVD FTW #1:

(3) When we calculated eigenfaces...

M is $n \times p$ where

$n = 105$

$p = 320 \times 243 = 77{,}760$

$M^T M$ is $p \times p$...

... so $M^T M$ contains

6,046,617,600

real values (floats in python)

... a float is 8 bytes, so we need ~ 48 GB of RAM to store $M^T M$.

We can shortcut this with SVD.

SVD allows us to ~~calculate~~ compute $\text{eig}(M^T M)$ without actually ~~calculating~~ computing $M^T M$.

Using "compact SVD": $M_{n \times p} = U_{n \times r} S_{r \times r} V^T_{r \times p}$

where $r \leq n$ (r = rank of M)

SVD FTW #2:

(4) SVD can reveal "latent features" in your data. This can be used for "topic modeling" in datasets of user ratings.

... switch to IPython notebook because we don't want to be writing a ton of real values on the board...

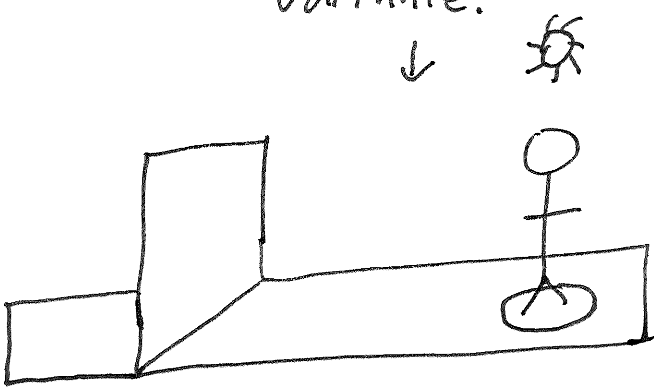
... we'll do a real example of this (w/ real numbers) in the notebook...

Takeaway: SVD is more computationally efficient than PCA when $n \ll p$.

PCA analogy to shadows cast by my body!

Projection from
3d to 2d via
the sun.

↳ Not in
the direction
of my body's most
variance.



In the direction
of my body's most
variance.