CS 189/289

Today's lecture outline:

1. Finish Transformers
2. Unsupervised learning, dimensionality reduction
3. PCA

Assigned reading: 16.1 (PCA)

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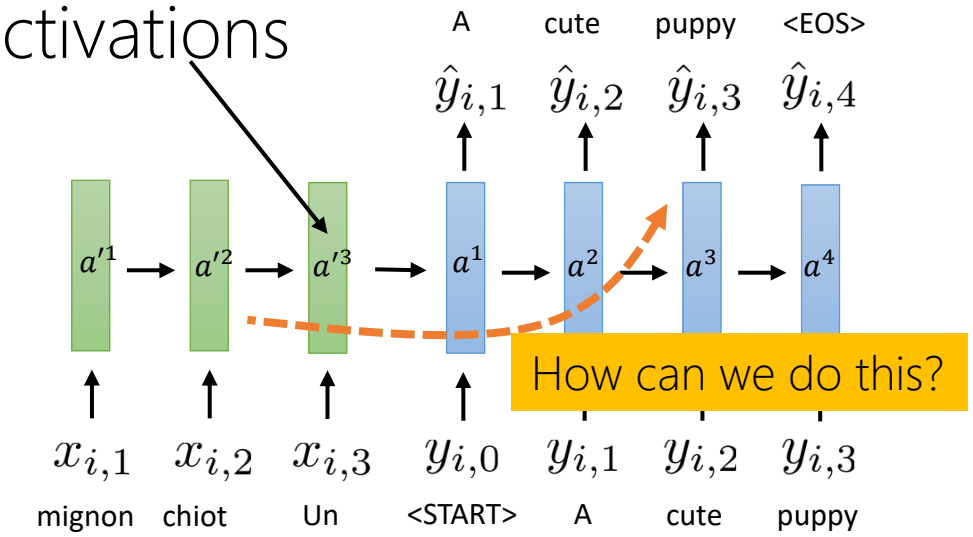
Recall: RNN bottleneck problem

all information about the conditioned sequence is contained in these activations



Idea: what if we could somehow "peek" at the source sentence while decoding?

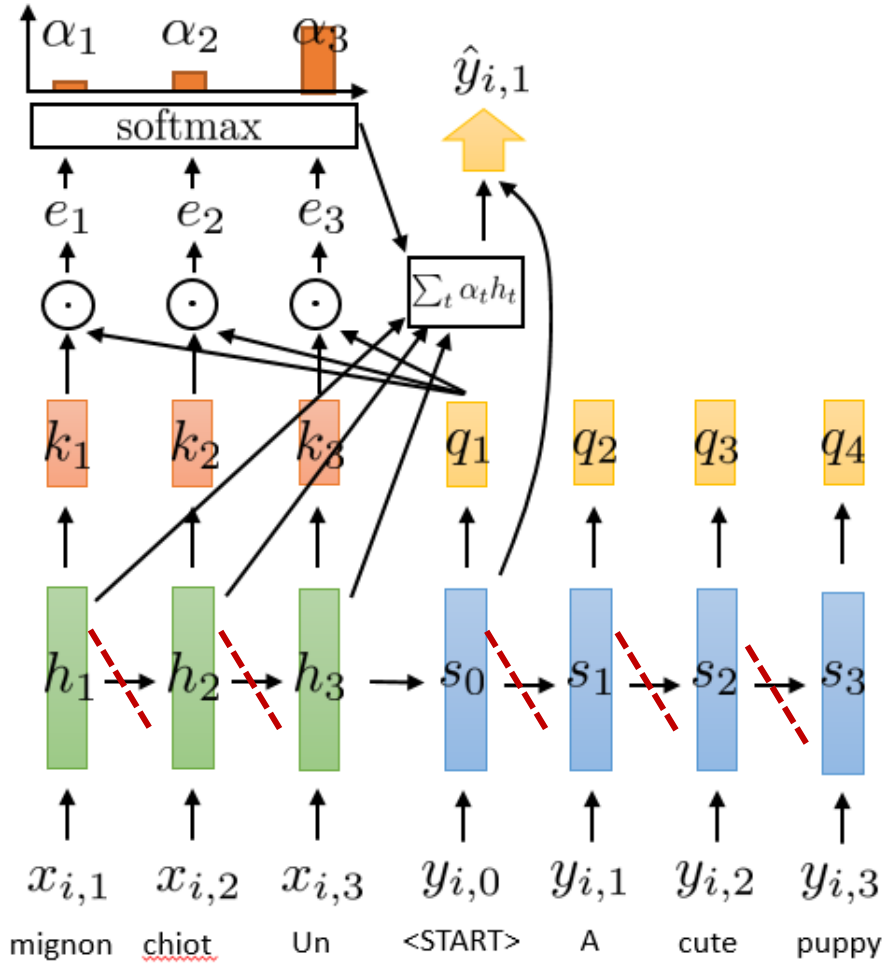
Attention to the rescue!

Recall: Is Attention All We Need?

- If we have **attention**, do we even need recurrent connections?
- Can we **transform** our RNN into a **purely attention-based** model?

This has a few issues we must overcome:

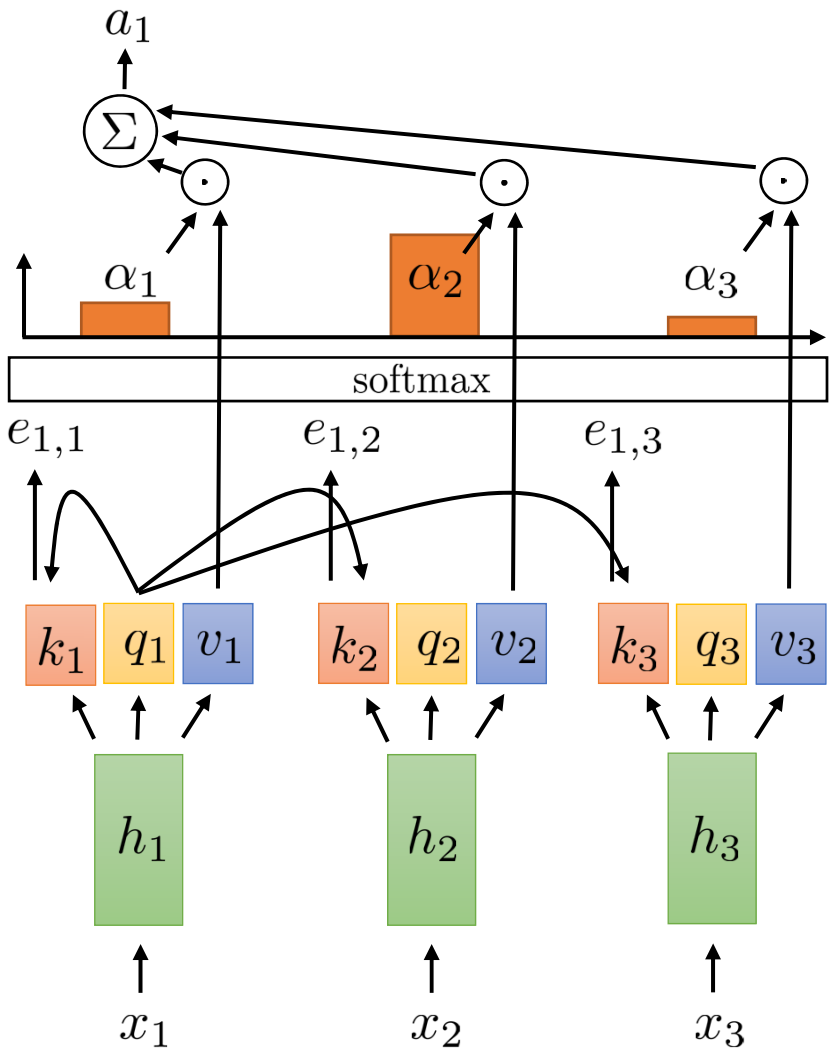
- Decoding position 3 can't access s_1 or s_0.
- Solution: self-attention.

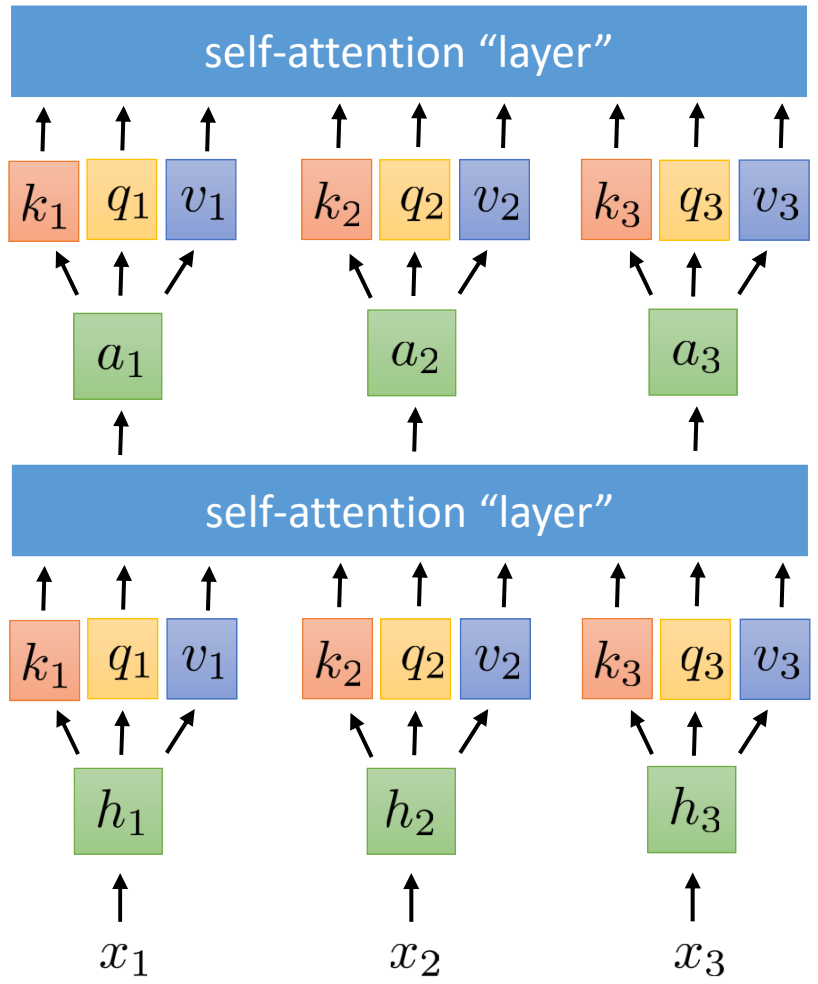


Recall: Self-Attention

keep repeating until we've processed this enough

then hand off to next part of overall model



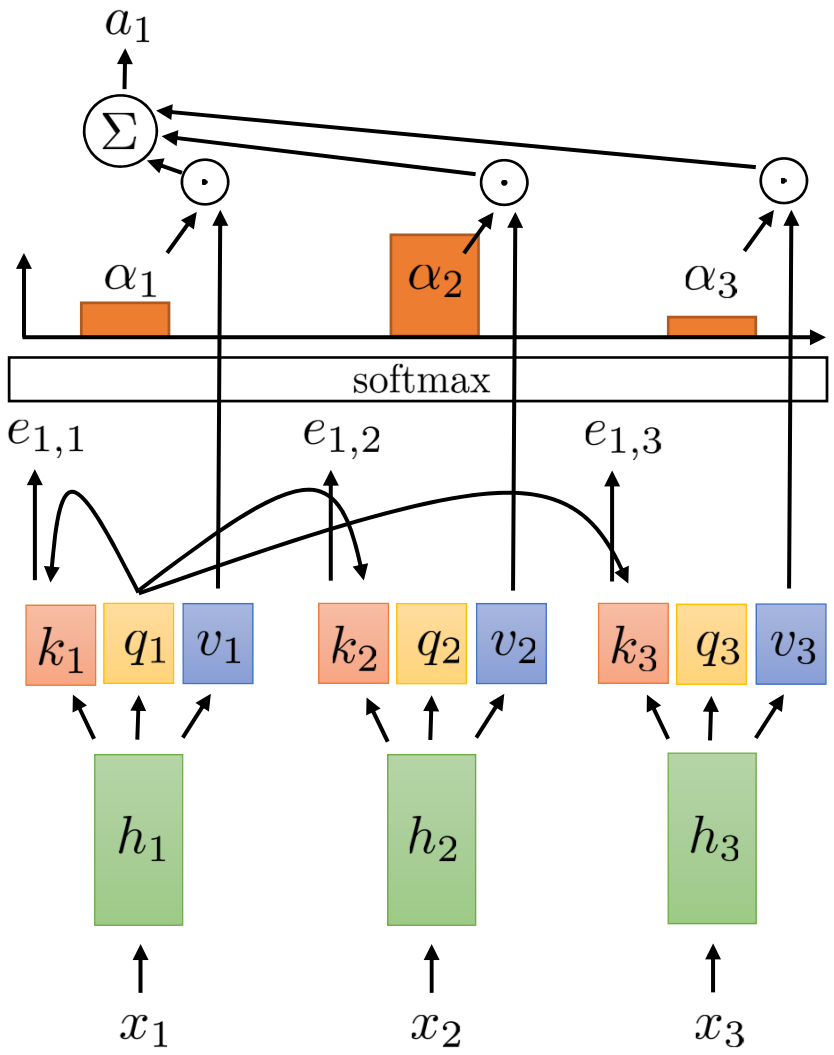


From Self-Attention to Transformers

- The basic concept of **self-attention** can be used to develop a very powerful type of sequence model, called a **transformer**
- But to make this actually work, we need to develop a few additional components to address some fundamental limitations

1. Positional encoding	addresses lack of sequence information
2. Multi-headed attention	allows querying multiple positions at each layer
3. Adding nonlinearities	so far, each successive layer is *linear* in the previous one
4. Masked decoding	how to prevent attention lookups into the future?

Self-Attention is **Linear**



$$k_t = W_k h_t \qquad q_t = W_q h_t \qquad v_t = W_v h_t$$

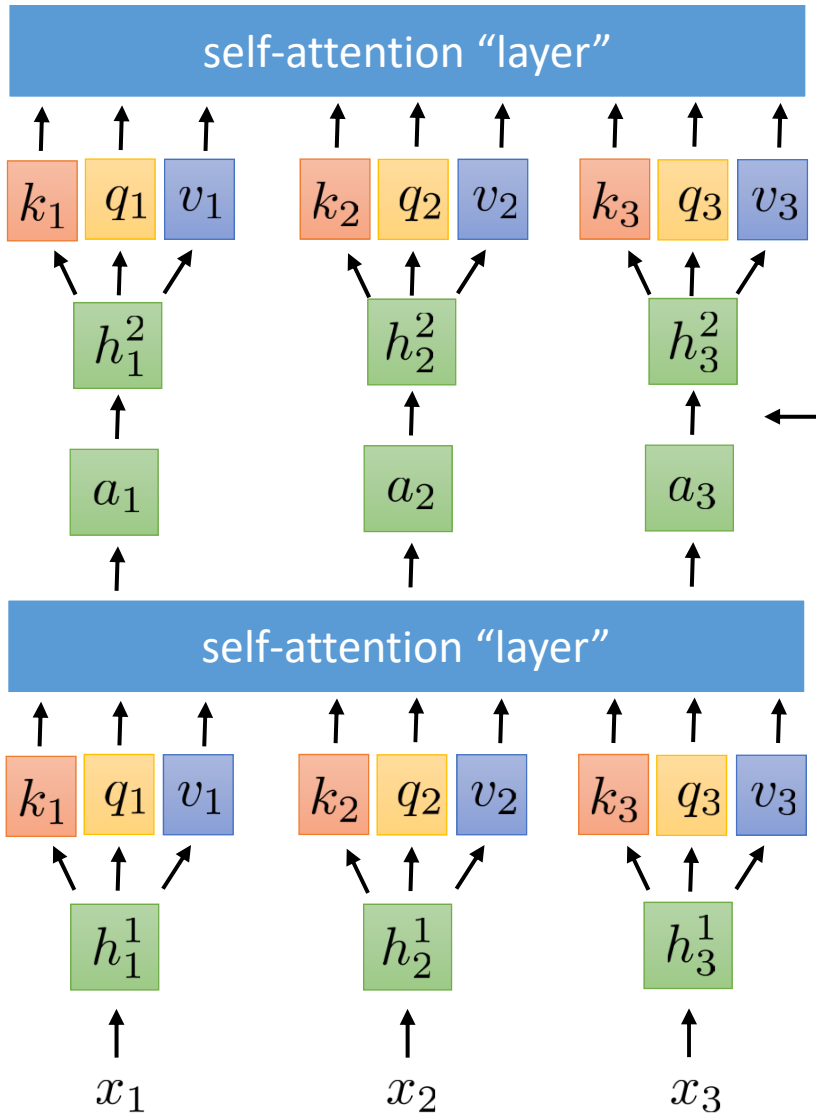
$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$

$$e_{l,t} = q_l \cdot k_t$$

$$a_l = \sum_t \alpha_{l,t} v_t = \sum_t \alpha_{l,t} W_v h_t = \boxed{W_v \sum_t \alpha_{l,t} h_t}$$

Every self-attention "layer" is a linear transformation of the previous layer

Alternating self-attention & non-linearity



some non-linear (learned) function

$$\text{e.g., } h_t^\ell = \sigma(W^\ell a_t^\ell + b^\ell)$$

just a simple neural net applied at every position after every self-attention layer

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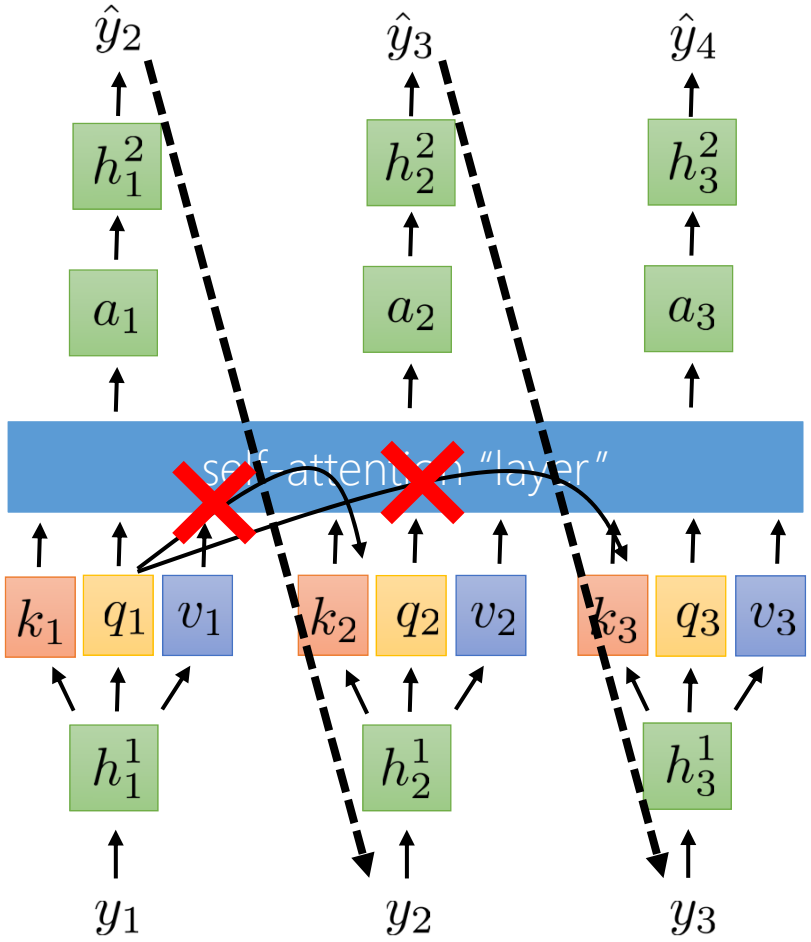
Self-attention can see the future!

$$a_l = \sum_t \alpha_{l,t} v_t$$
$$\alpha_{l,t} = \exp(e_{l,t}) / \sum_{t'} \exp(e_{l,t'})$$



Problem:

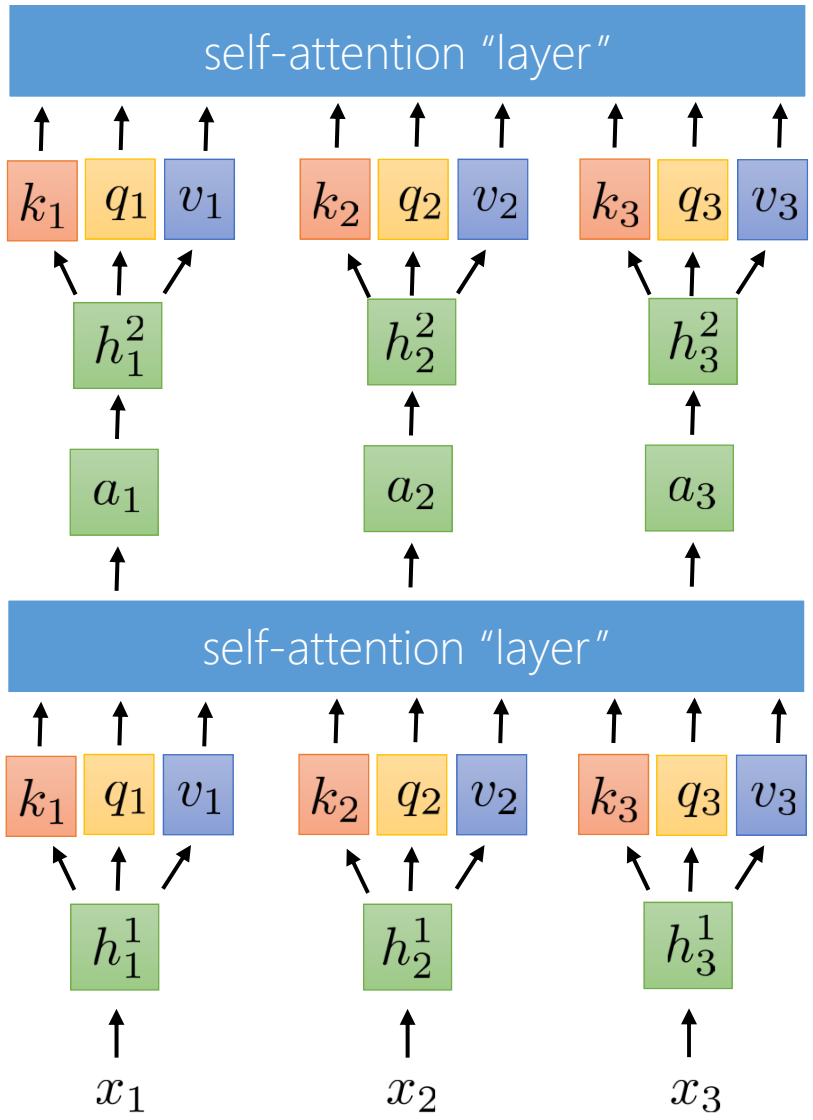
- Each position looks at future values.
- Also cyclic: output 1 depends on input 2 which depends on output 1.

Solution ("masked attention"):

$$e_{l,t} = \begin{cases} q_l \cdot k_t & \text{if } t \leq l \\ -\infty & \text{otherwise} \end{cases}$$

Now we are read for
The Transformer!

Sequence-to-sequence with self-attention

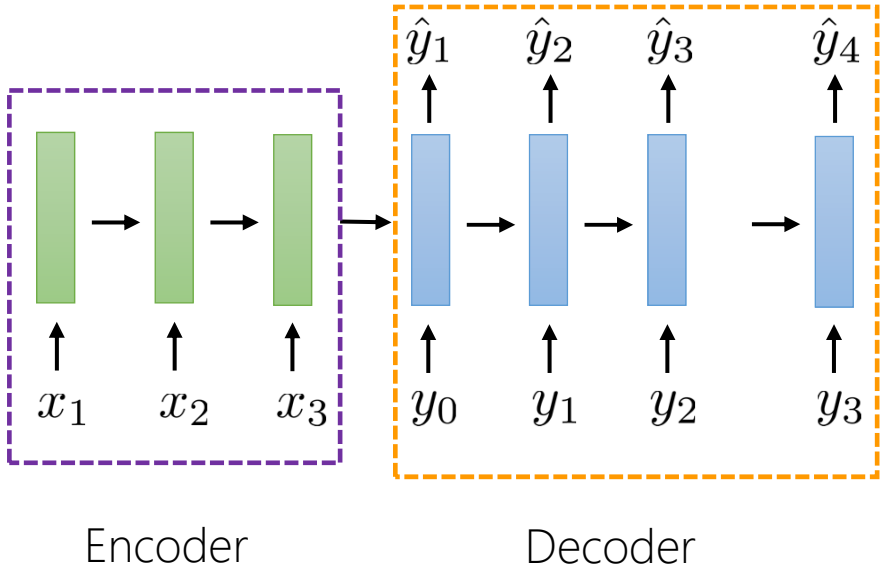


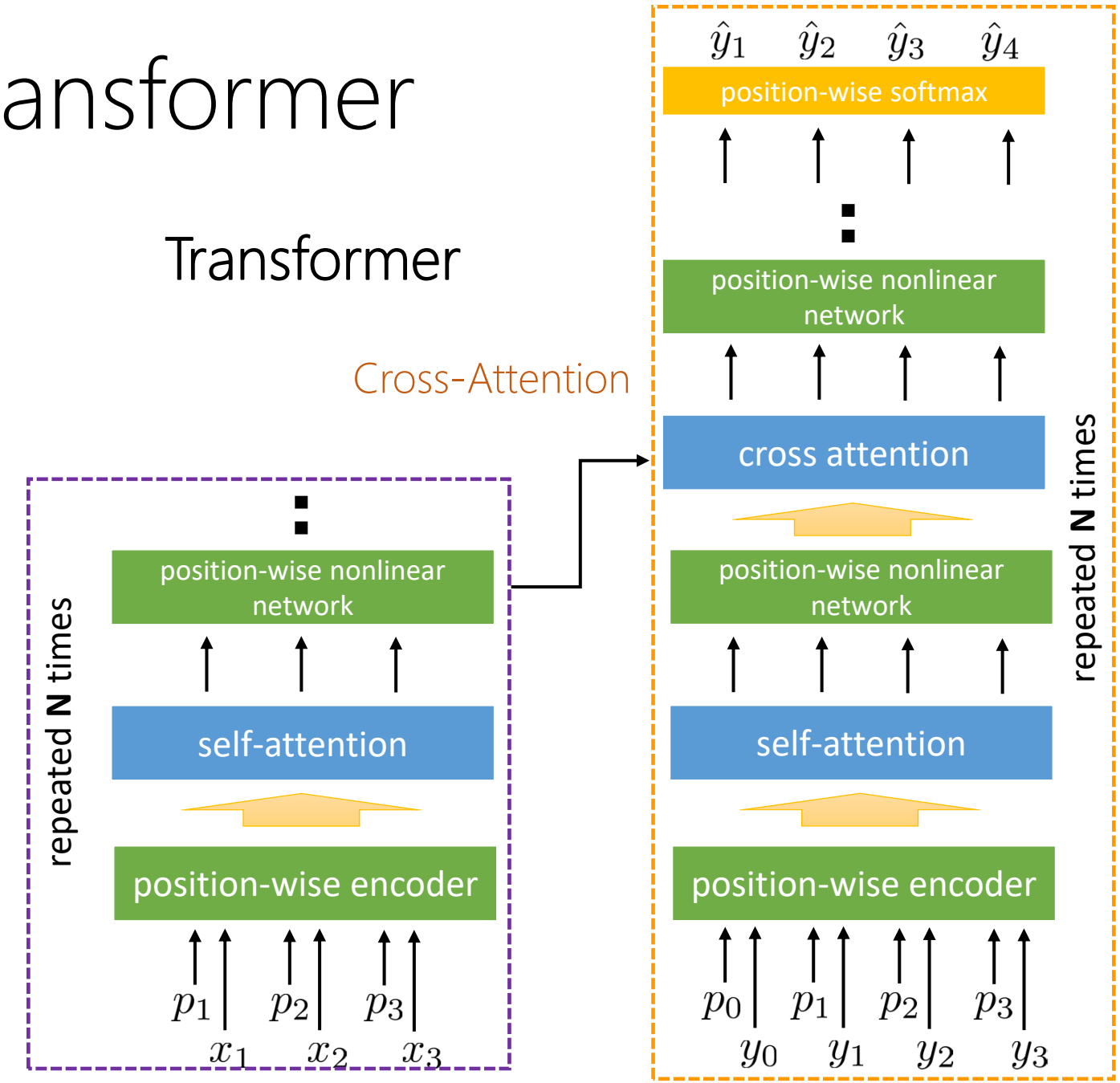
"*Transformer*" architecture:

- Stacked self-attention layers with position-wise nonlinearities.
- *Transform* one sequence into another at **each** layer.
- For sequence data.

[Vaswani et al. **Attention Is All You Need.** 2017]

Encoder-Decoder Transformer





Transformers pros and cons

Downsides:

- Attention computations are theoretically* $O(n^2)$.
- Slightly more complex to implement (positional encodings, etc.)

Benefits:

+ Better long-range connections (compared to RNN).
+ *Much easier to parallelize.
+ In practice, can make it much deeper (more layers) than RNN.

- Benefits often **vastly** outweigh the downsides.
- Transformers work **much** better than RNNs in general.
- One of the most important sequence modeling improvements of the past decade.
- Can use just encoder, or just decoder, or both.

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Unsupervised learning

So far: *supervised learning*, $\{(x_i, y_i)\}$ for $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$ or $y \in \mathbb{Z}$.

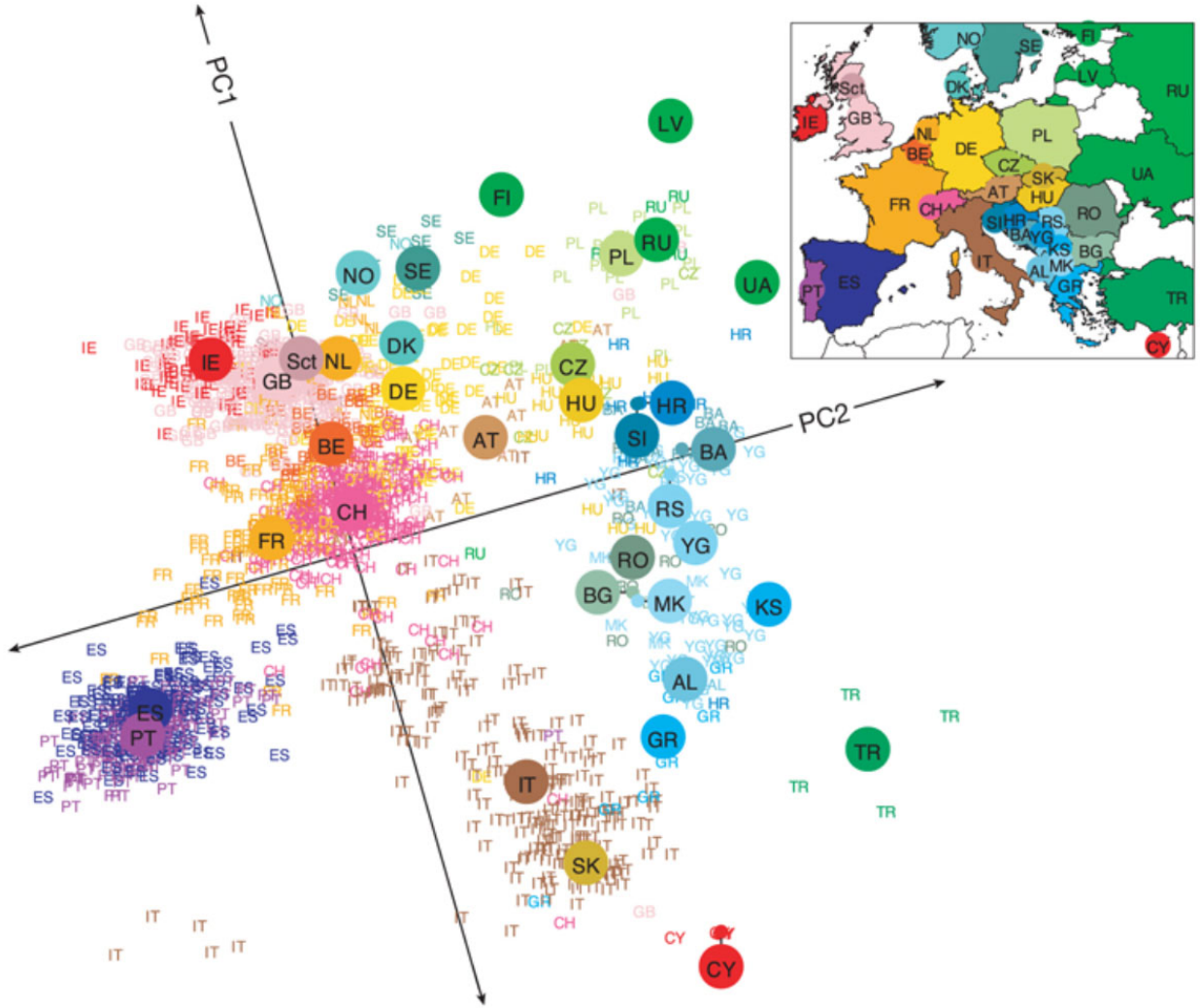
Often model just $\{x_i\}$: *unsupervised learning*, includes:

i. *Dimensionality reduction*, $z \in \mathbb{R}^m = f_\theta(x \in \mathbb{R}^d)$, $m \ll d$.
ii. *Clustering*, for each x_i, assign cluster label, $z_i \in \{1,2,3 \ldots K\}$
iii. *Representation learning*, $z \in \mathbb{R}^m$, $z = f_\theta(x)$, or $z \sim p_\theta(x)$.
iv. *Density estimation*, evaluate $p_\theta(x)$.
v. *"Generative" modeling*, $x \sim p_\theta(x)$

e.g. of Dimensionality reduction

ATGTTGAATCTG
AAAGTGAAATGT
TATTATACGAAG
AAGTATTTGCTA
GACCTCAAAACC
CTTCATCATAAC

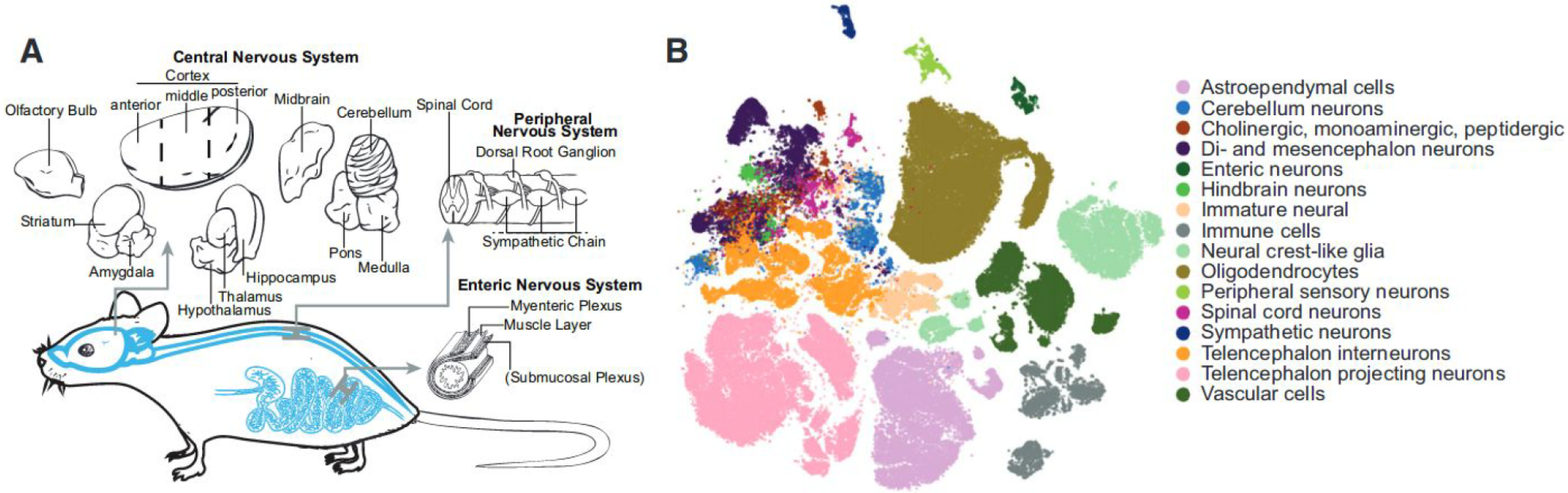
DNA from set of individuals



Novembre *et al Nature* 2008

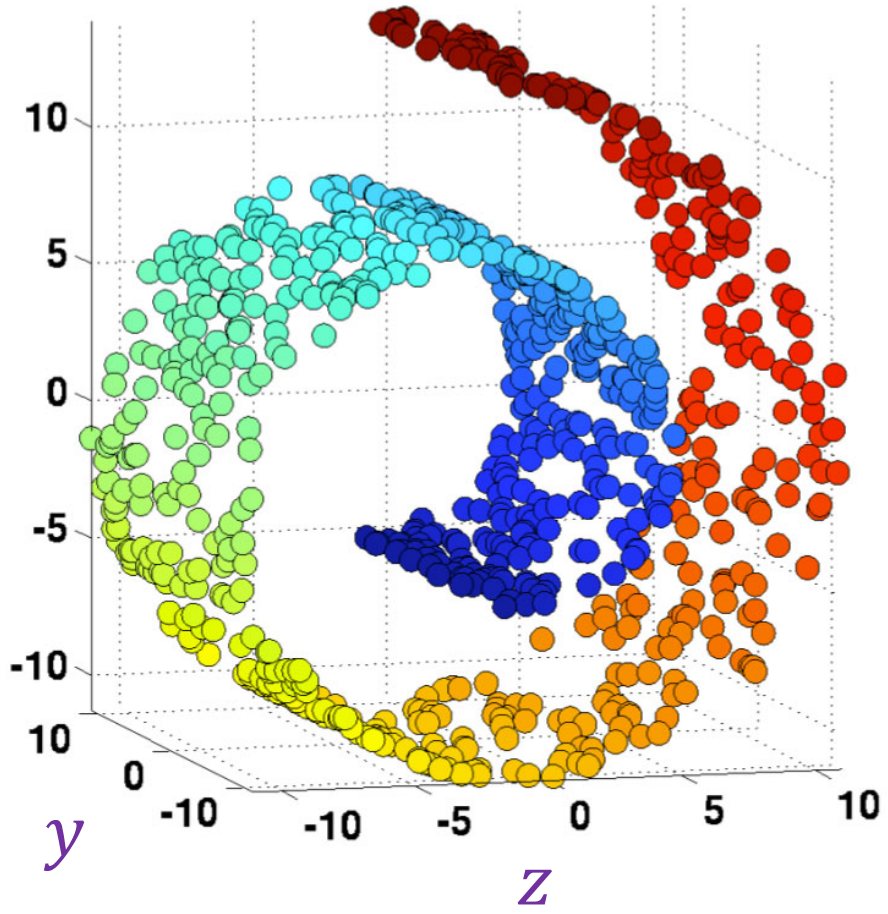
e.g. of dimensionality reduction+clustering

Single-cell transcriptomics (single-cell RNA sequencing): samples are cells, features are genes.



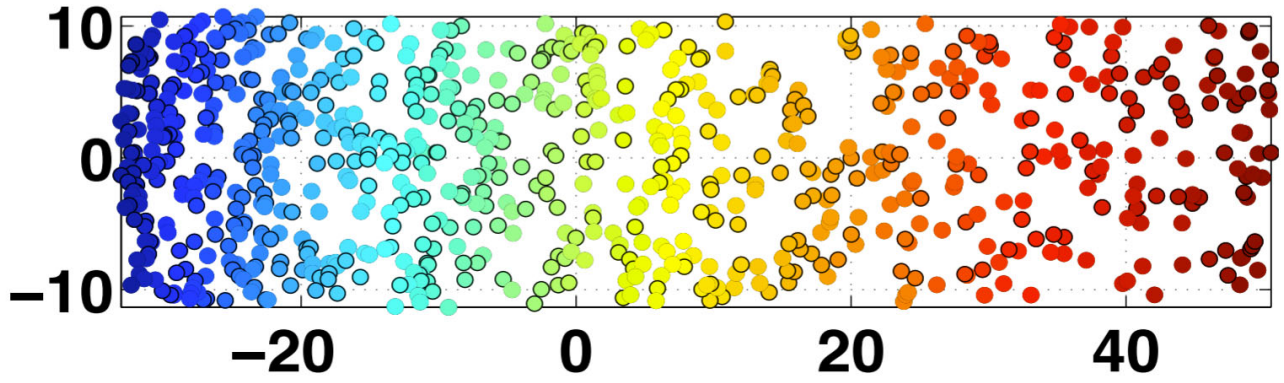
Zeisel et al. (2018)
$n \approx 500{,}000$

What dimensionality do these points live in?



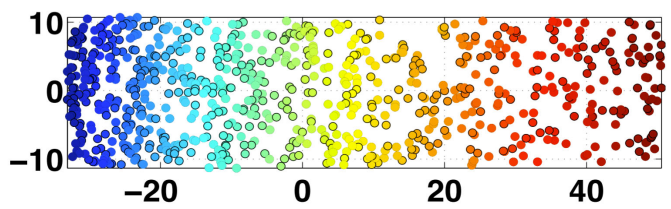
$x \in \mathbb{R}^3 = [x, y, z]$.

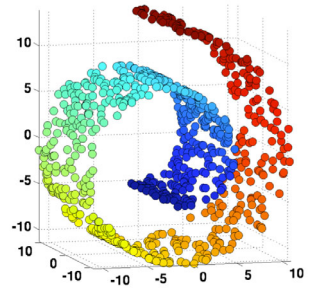
But could uniquely describe each point with just 2 *coordinates*.



Weinberger et al ICML 2004

The "manifold hypothesis"





- "*High dimensional data tend to lie in the vicinity of a low dimensional manifold*." e.g. [Fefferman 2013]
- Manifold: roughly speaking, a space that locally feels like a Euclidean space.
- For us: a manifold is a lower dimensional part of the observation space in which the data tend to lie.
- "*embedding* the data in a lower dimensional manifold", or "an *embedding* of the data".

What dimensionality do these points live in?

- 5000 faces, $\boldsymbol{x_i} \in \mathbb{R}^{\mathbf{32\times32=1024}}$
- How low a dimension do you think we can go and still "keep" the image?
- Turns out we can go down to $\sim\mathbf{100}$ from the "ambient" $\mathbf{1024}$ dimensions!
- Trick: carefully create 100 special "basis" images.
- Principal Components Analysis (PCA) will yield the PC basis vectors.

https://mikedusenberry.com/on-eigenfaces

What dimensionality do these points live in?

- 5000 f
- How l we can g
- Turns dimen
- Trick: asis" image
- Princip A) will tell us

PCA “basis” images, $x \in \mathbb{R}^{1024}$

https://mikedusenberry.com/on-eigenfaces

Representation with new truncated basis

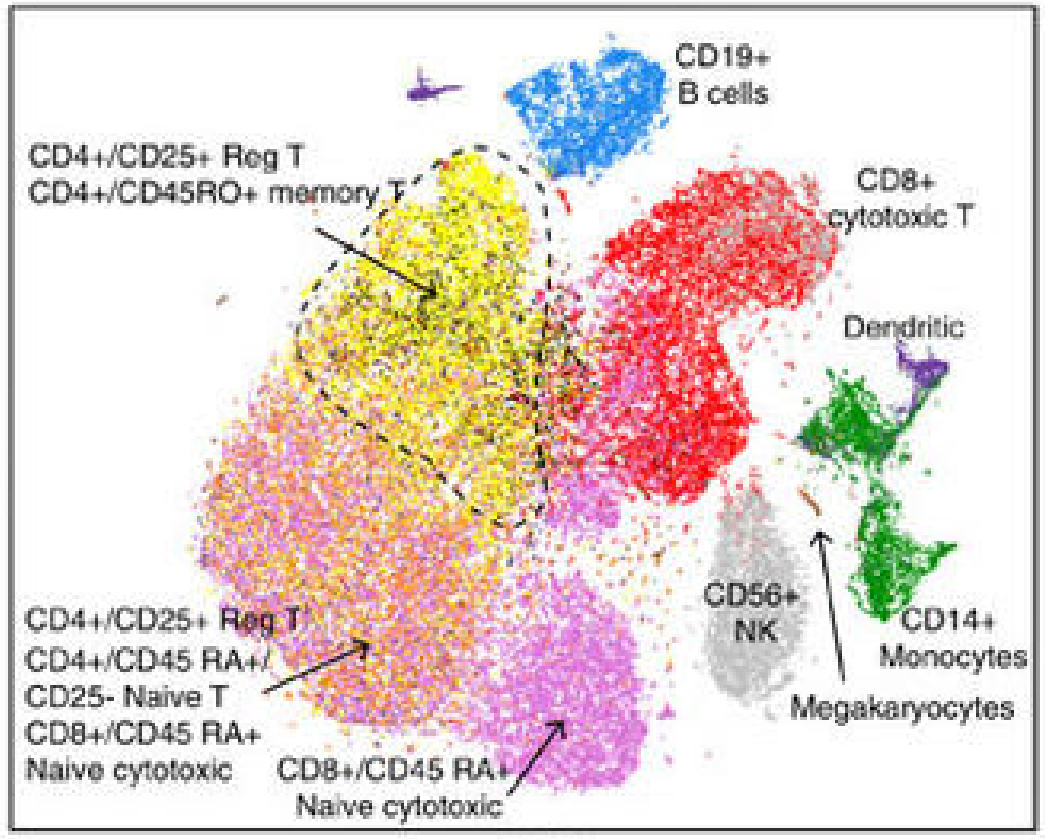
original faces, $x \in \mathbb{R}^{1024}$

approximate faces, $x' \in \mathbb{R}^{100}$

https://mikedusenberry.com/on-eigenfaces

Why might we want to reduce dimensionality?

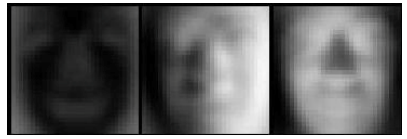
- Visualization, e.g. 2D plots.
- To denoise the data, or remove systematic artifacts (big one in biology).
- To compress the data (e.g. audio, images).
- To speed up supervised learning, or other analyses.



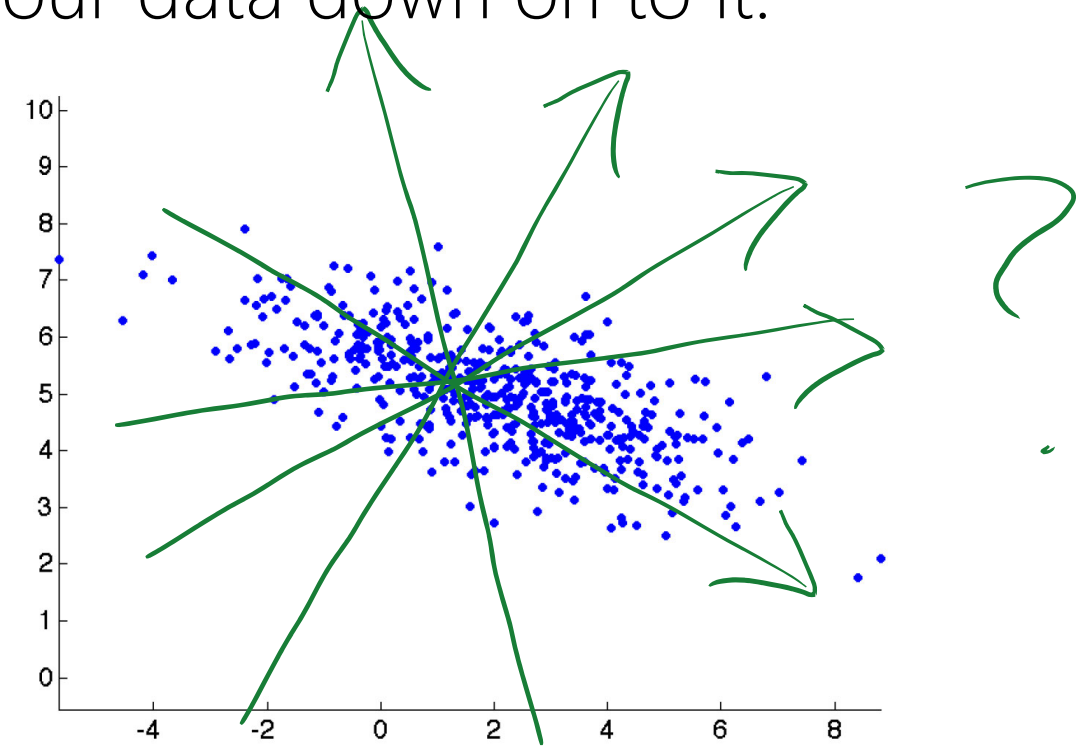
https://www.nature.com/articles/ncomms14049/figures/3

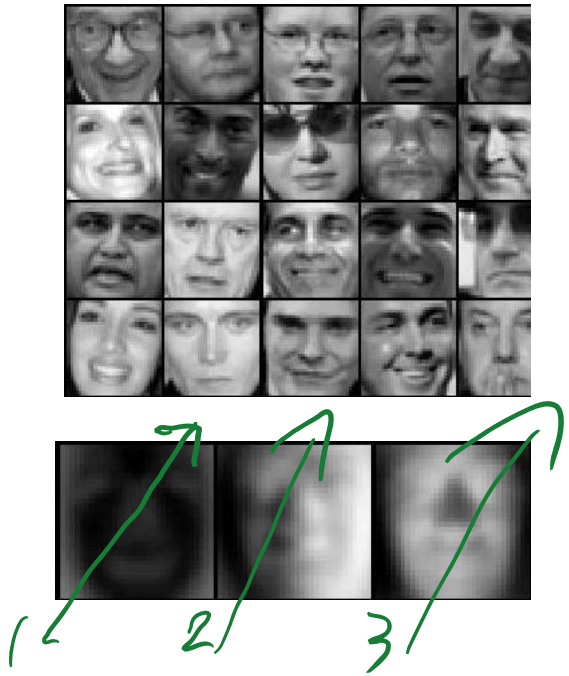
Principal Components Analysis (PCA)

- "eigenfaces" are the PCA basis



- Look for the direction in the original space that "retains most of the "information" if you project your data down on to it.





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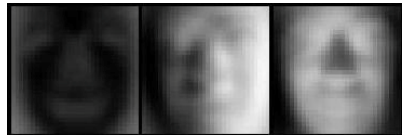

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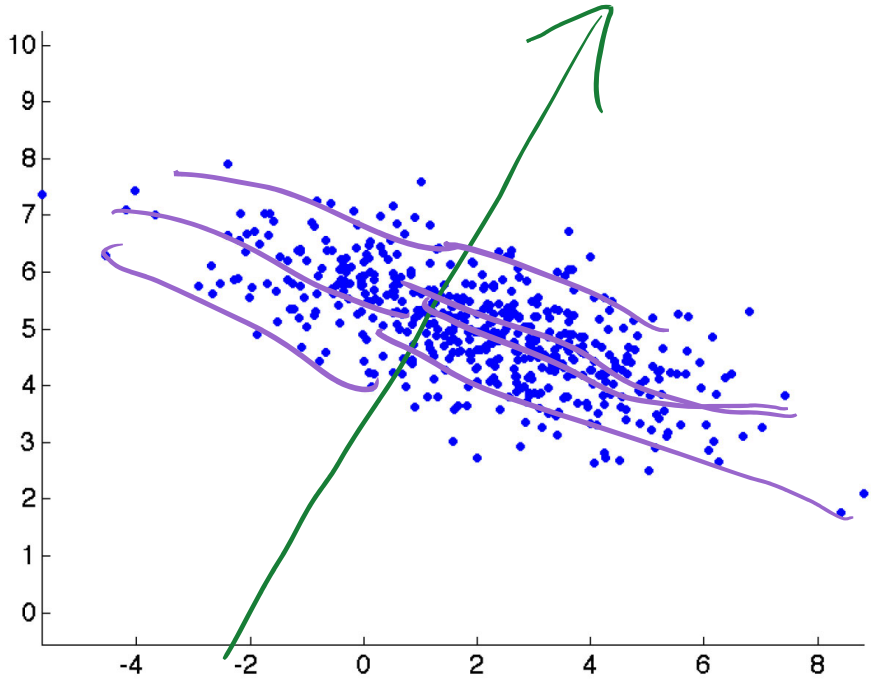
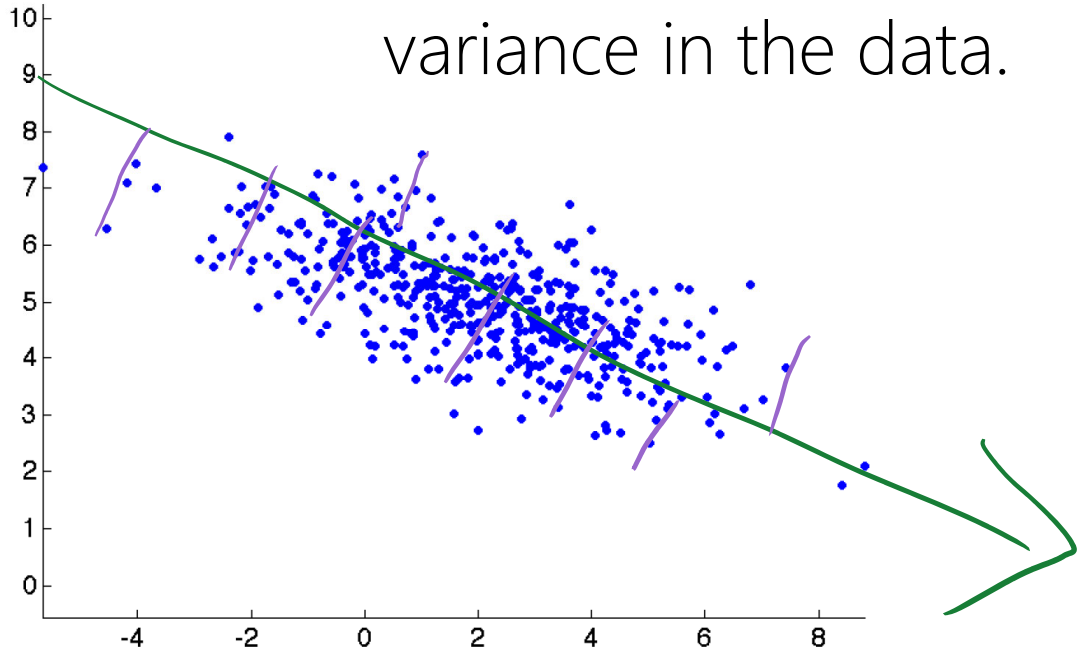


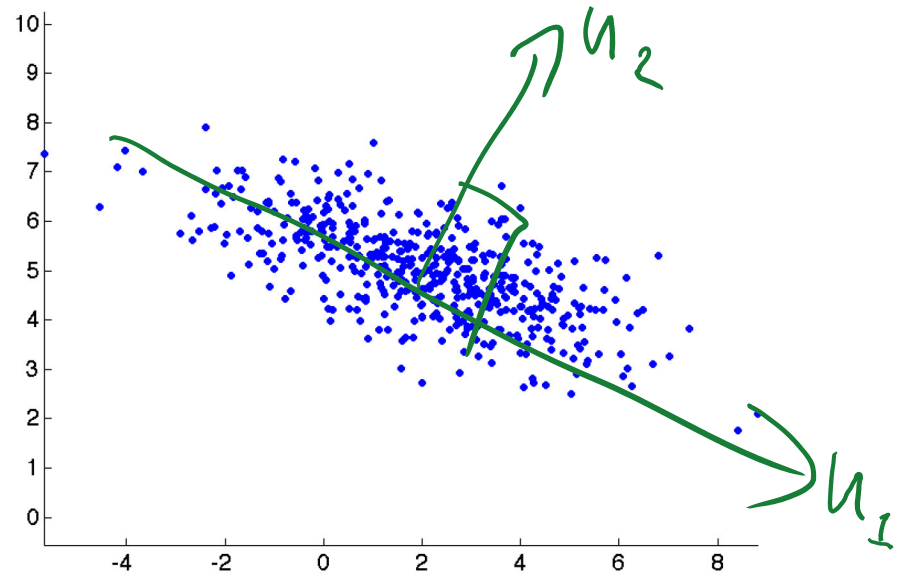
Direction with lowest *reconstruction loss*, is the direction with maximal variance in the data.



Principal Components Analysis (PCA)

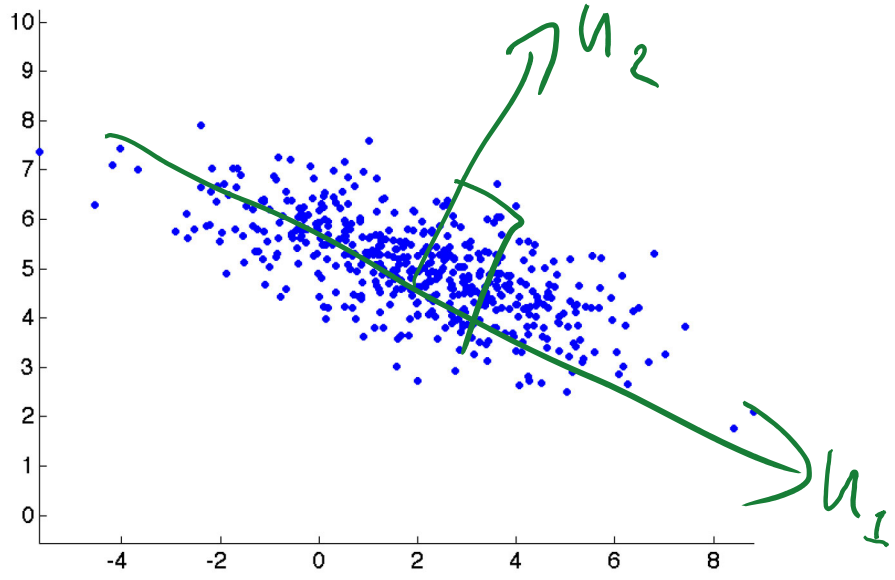
Recursively apply this idea to find 2nd best direction, then 3rd best:

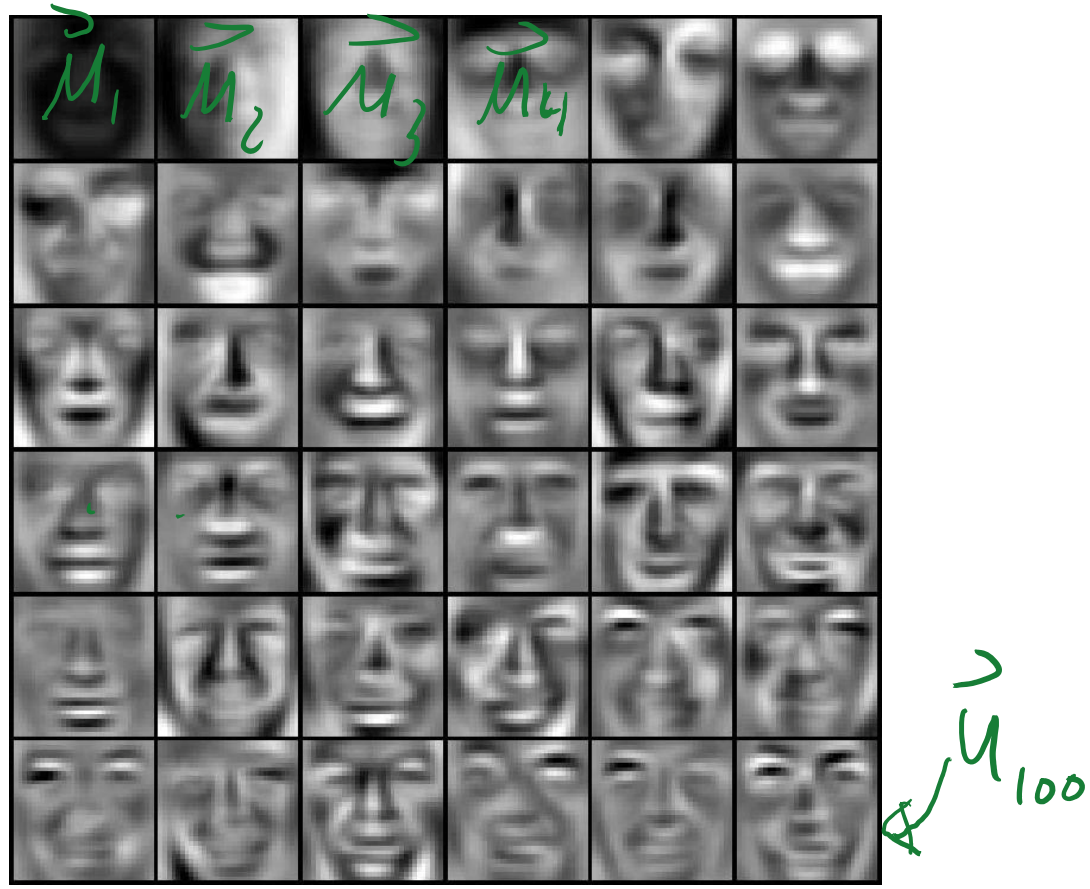
- 2nd direction should be orthogonal to the first… and…
- … be direction of most variance subject to that constraint.
- What's the maximum number of such directions we can find?



Principal Components Analysis (PCA)

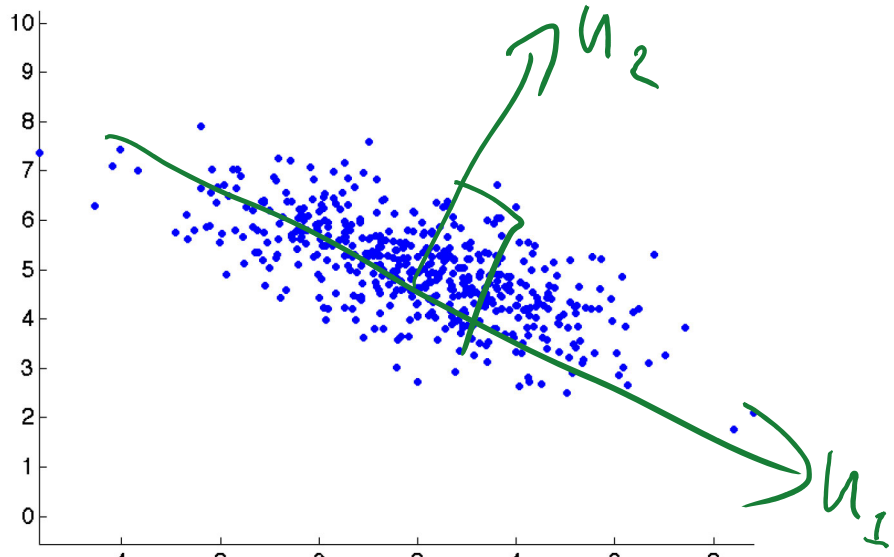
- Each of the 100 eigenfaces was one of these special directions in the original 1024-dimensional image space.





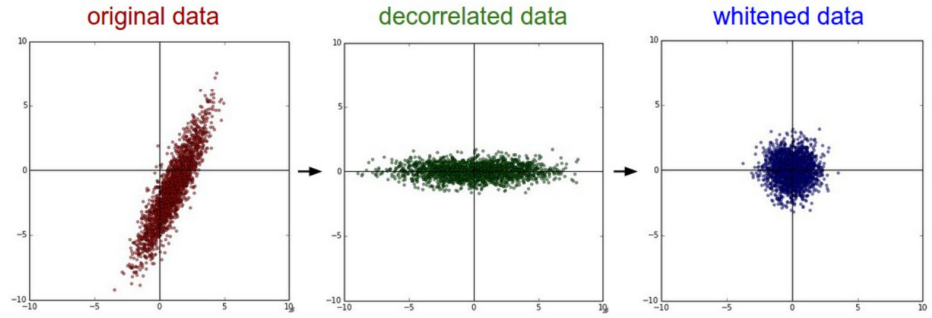
Principal Components Analysis (PCA)

Is this starting to remind you of anything?



Diagonalizing a MVG ("sphering")

- To sphere a MVG is to make all its contour lines be spheres (also called "whitening").
- Thus we need to make the ellipses look like spheres.
- To do this, we need to understand how to diagonalize a matrix.



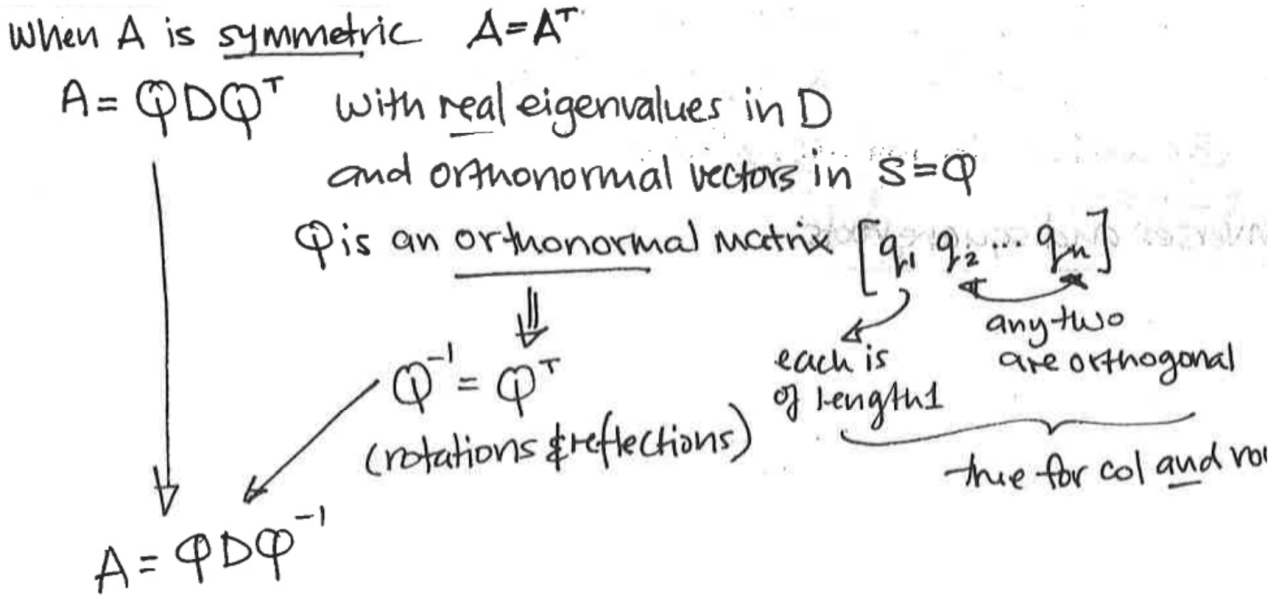
Can be derived (16.2.1-16.2.3) with MLE for params μ, W, assuming $p(x \in \mathbb{R}^d) = N(\mu + xW; I\sigma^2)$, for $\sigma^2 \to 0$ and $W \in \mathbb{R}^{d \times k}$.

Principal Components Analysis (PCA)

Recall: to diagonalize a MVG distribution, we made use of a special factorization of its covariance matrix, $A = QDQ^T$, an "eigen" or "spectral"-decomposition:

Linear Algebra: Diagonalizing a matrix

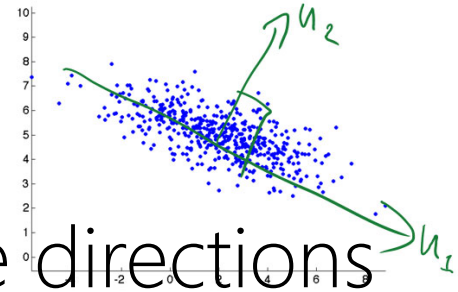
Spectral theorem:



Can use this to do PCA.

(Even if data are not Gaussian).

PCA overview



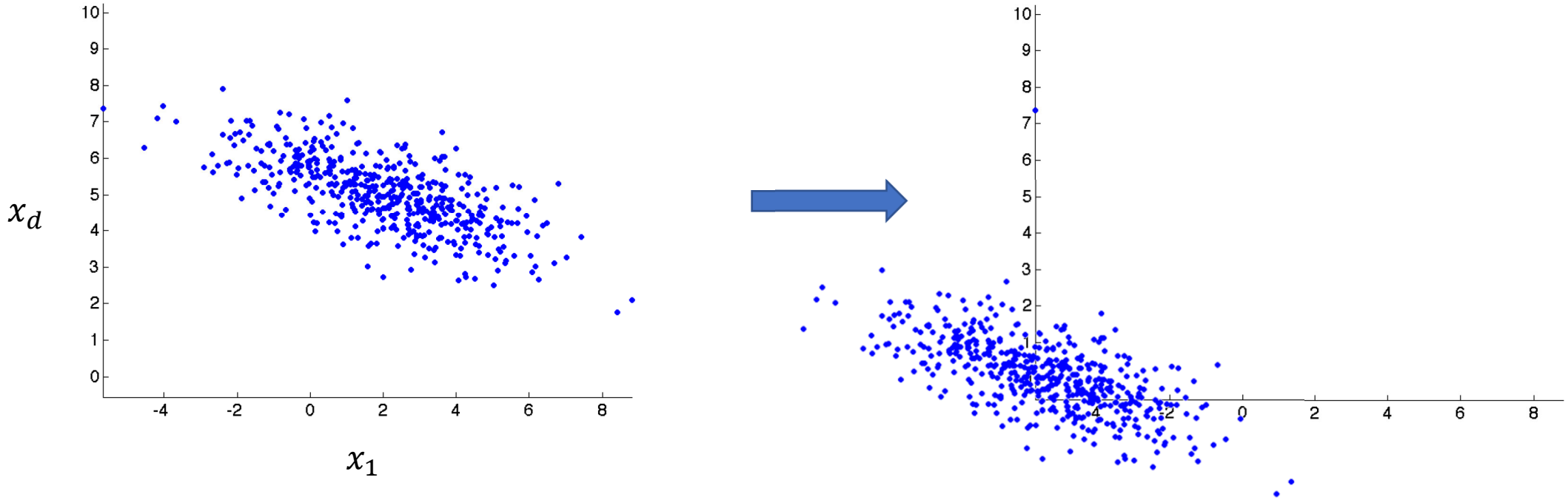
Compute covariance matrix of the data and pick off the directions with the top k eigenvalues (all $\lambda_i \geq 0$ because covariance is PSD):

- Given data matrix, $X \in \mathbb{R}^{n \times d}$.
- Construct, $X^T X \in \mathbb{R}^{d \times d}$ (after mean-centering each feature).
- Apply spectral theorem, $X^T X = QDQ^T$ to pick off k directions.
- Now approximate this covariance matrix with the "best" low rank approximation to it (rank k). (*Eckart-Young theorem*)
- Yields lowest "reconstruction loss", and highest variance directions.

PCA step-by-step

Given $\boldsymbol{n}$ data points of dimension $\boldsymbol{d}$, $\boldsymbol{X \in \mathbb{R}^{n \times d}}$, to perform PCA, we:

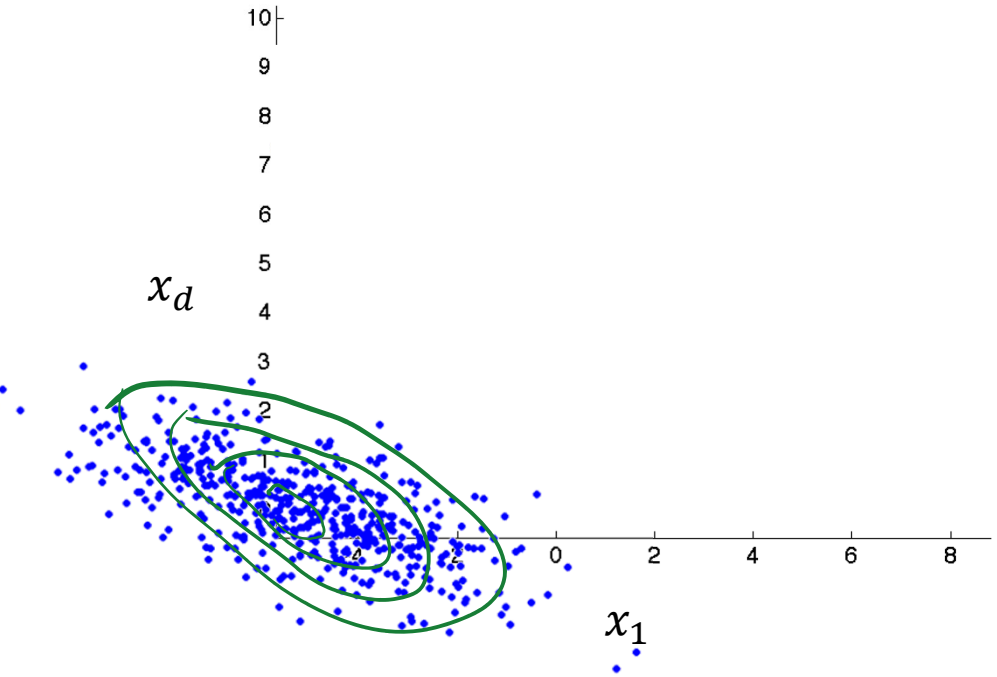
1. Center the data (make each feature zero mean), $\bar{X} = X - [\overline{x_1}, \ldots, \overline{x_d}]$. (We will continue on only with the matrix $\bar{X}$).



PCA step-by-step

Given $\boldsymbol{n}$ data points of dimension $\boldsymbol{d}$, $\boldsymbol{X} \in \mathbb{R}^{n \times d}$, to perform PCA, we:

2. Compute the covariance matrix, $\Sigma = \bar{X}^T \bar{X}$.



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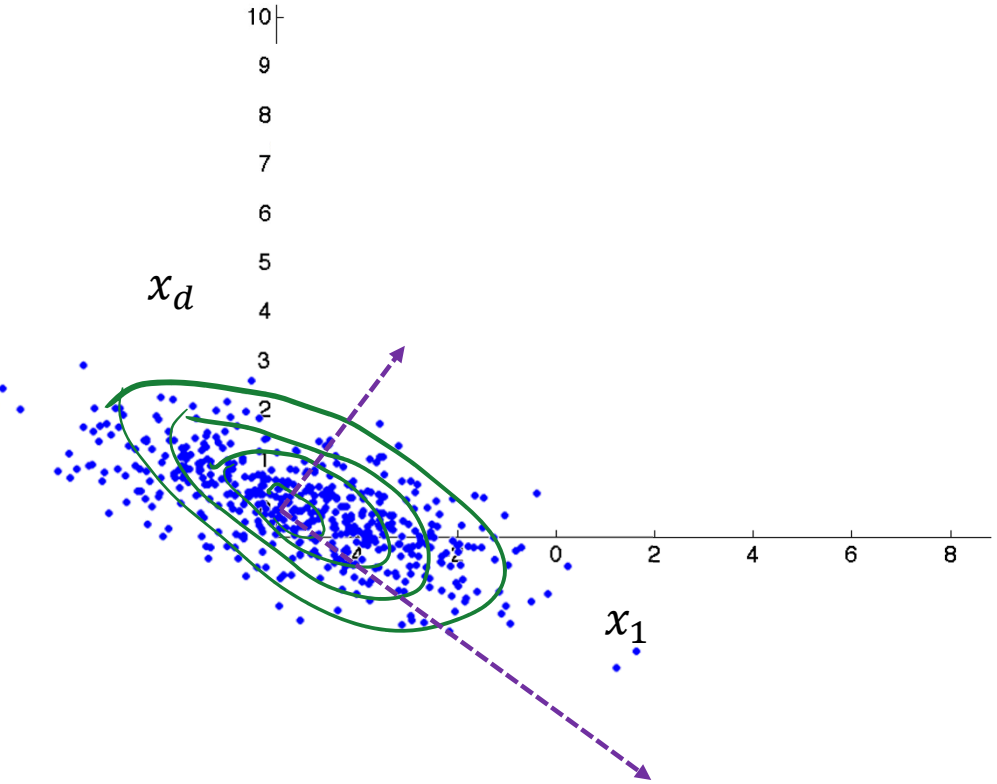
Given n data points of dimension d, $X \in \mathbb{R}^{n \times d}$, to perform PCA, we:

2. Compute the covariance matrix, $\Sigma = \bar{X}^T \bar{X}$.
3. Compute $\bar{X}^T \bar{X} = QDQ^T$ to get eigenvectors (aka *principal directions*).

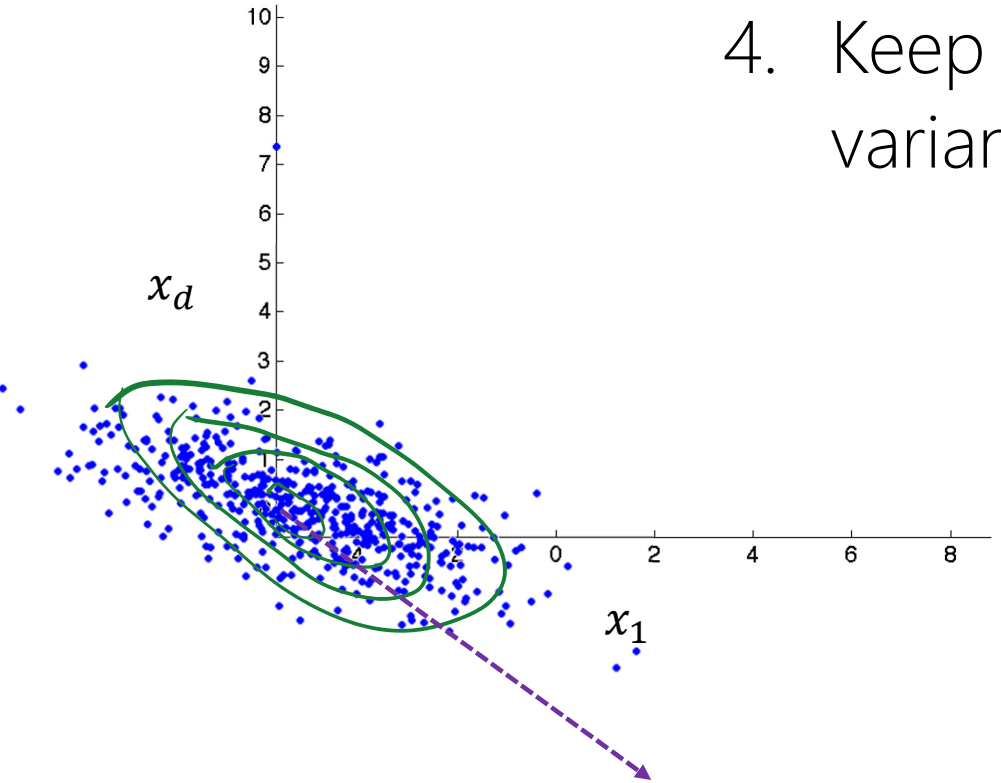


- *This decomposition is typically implemented with a call to "eig" function (linalg package in python), but can also be obtained from "svd".*
- *Are the same for PSD matrices, but svd may be more stable.*

PCA step-by-step

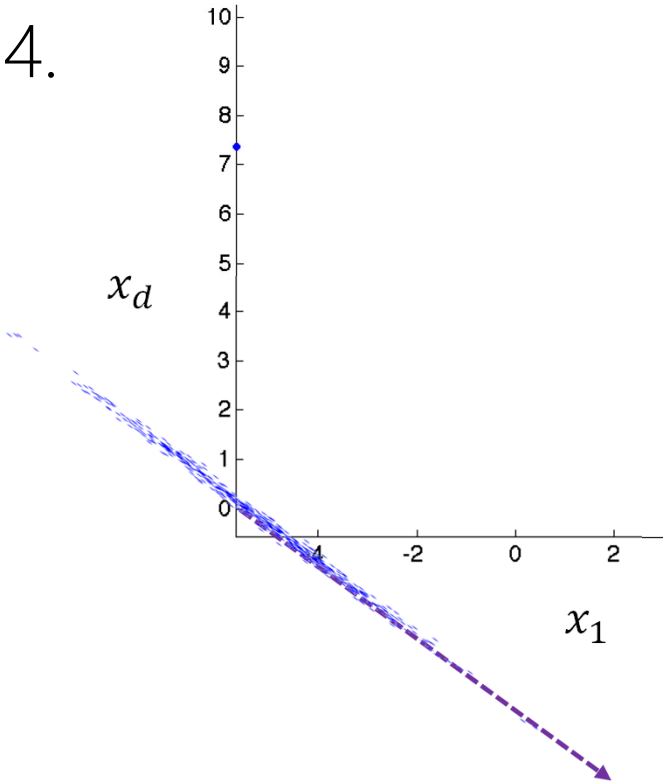
Given n data points of dimension d, $X \in \mathbb{R}^{n \times d}$, to perform PCA, we:

2. Compute the covariance matrix, $\Sigma = \bar{X}^T \bar{X}$.
3. Compute $\bar{X}^T \bar{X} = QDQ^T$ to get eigenvectors (aka *principal component axes*).
4. Keep the k eigenvectors, $Q_k \equiv Q_{:,1:k}$, with the most variance (highest eigenvalues in D).



PCA step-by-step

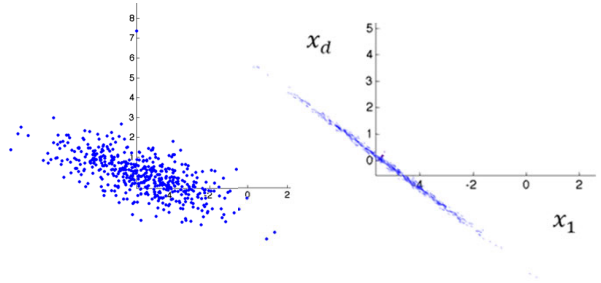
Given n data points of dimension d, $X \in \mathbb{R}^{n \times d}$, to perform PCA, we:

2. Compute the covariance matrix, $\Sigma = \bar{X}^T \bar{X}$.
3. Compute $\bar{X}^T \bar{X} = QDQ^T$ to get eigenvectors (aka *principal component axes*).
4. 

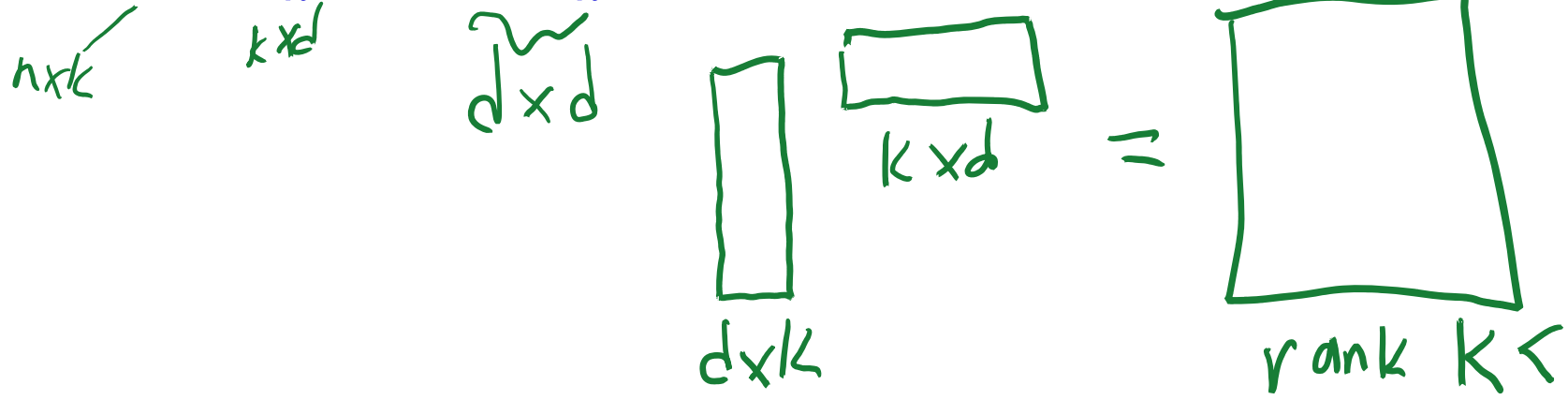
    4. Keep the k eigenvectors, $Q_k \equiv Q_{:,1:k} \in \mathbb{R}^{n \times k}$, with the most variance (highest eigenvalues in D).
    5. Project your points (original, or new ones) down to this subspace, $\bar{X}_k = \bar{X} Q_k \in \mathbb{R}^{n \times k}$, these are your *principal component scores*.

    Final, dimensionality-reduced data is.

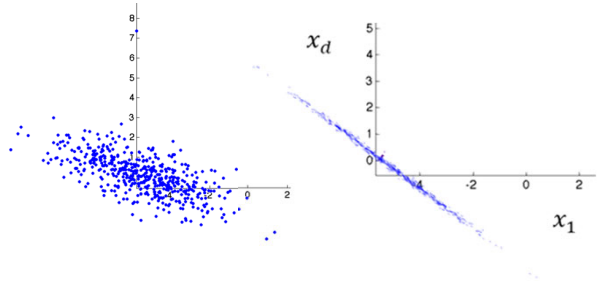
PCA step-by-step



- Final, dimensionality-reduced data is $\bar{X}_k = \bar{X}Q_k \in \mathbb{R}^{n\times k}$.
- What if we wanted our data in the original dimension (d), but with only the information retained from our PCA-k analysis? (e.g. reconstructed faces)
- We need to "reconstruct" the original points. We can do this by expanding back from PCA basis to original basis, but with only the first k PCA basis vectors, $\bar{X}_{recon-k} = \bar{X}_k Q_k^T = \bar{X}Q_k Q_k^T \in \mathbb{R}^{n\times d}$



PCA step-by-step



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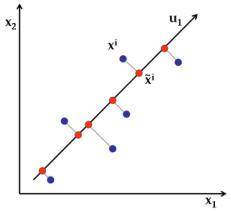
- Now we talk about the "reconstruction loss", as the difference between original and reconstructed data, $\|\bar{X}_{recon-k} - \bar{X}\|_{\mathbf{F}}$.



- The larger the reconstruction loss, the more information we have lost.

and Frobenius norm as

$$\|X\|_F = \sqrt{\sum_{ij} X_{ij}^2} = \sqrt{\operatorname{tr}(X^\top X)} = \sqrt{\sum s_i^2},$$

where s_i are singular values of X, i.e. diagonal

Original, and reconstructed faces

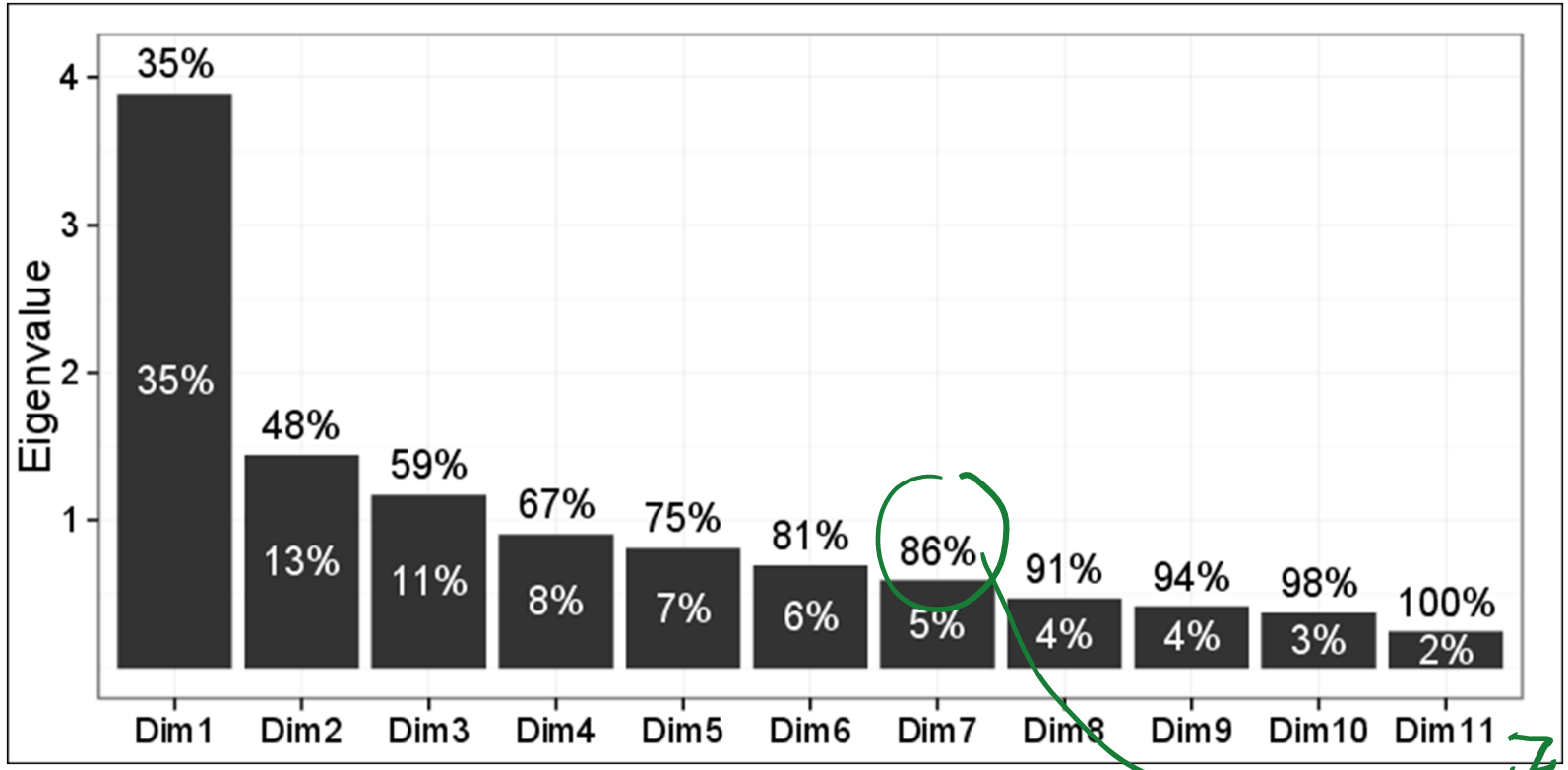
original faces, $x \in \mathbb{R}^{1024}$

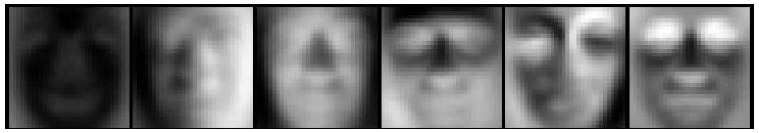
reconstructed faces

$x' \in \mathbb{R}^{100} \rightarrow x_k \in \mathbb{R}^{1024}$

https://mikedusenberry.com/on-eigenfaces

PCA: % variance explained to help pick hyper-parameter, k





$X^T X = Q D Q^T$

If you normalize the eigenvalues in D by their sum, then they correspond to % variance explained.

$$V_i \equiv \frac{D_{i,i}}{\sum_j D_{j,j}}$$

$$\sum_{j=1}^{7} V_j$$

https://stats.stackexchange.com/questions/133451/is-there-any-required-amount-of-variance-captured-by-pca-in-order-to-do-later-an

PCA: reconstruction loss and % variance

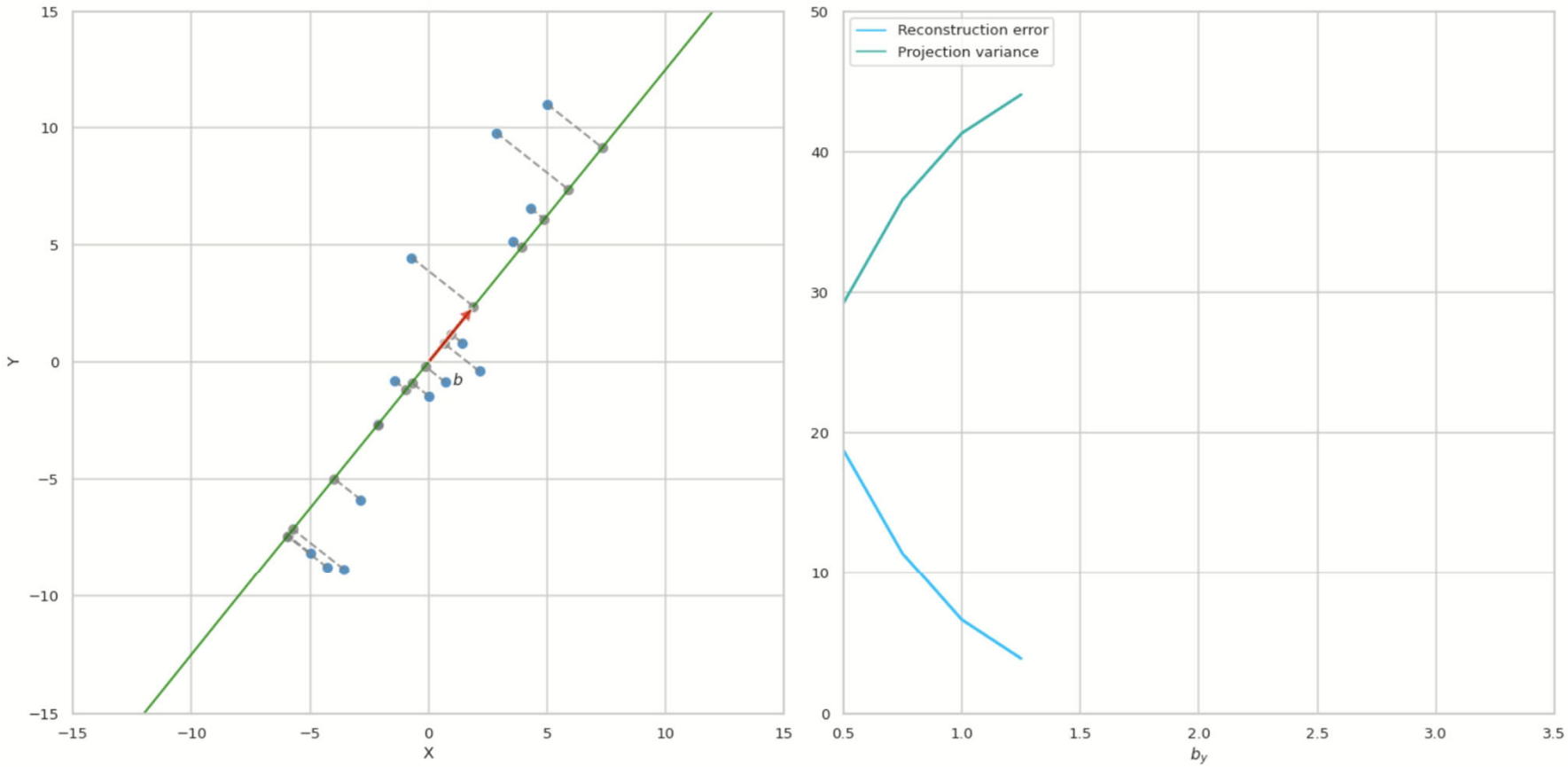


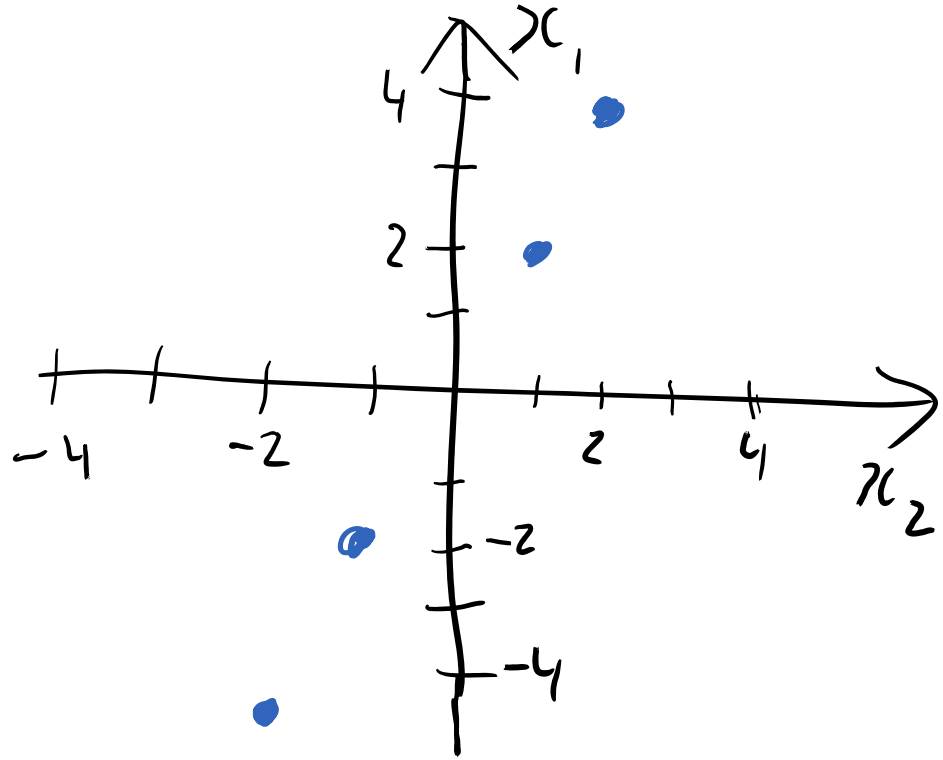
Fig.5. We rotate basis vector b and project data on corresponding subspace, then calculate reconstruction error L and projection variance Var(λ).

https://towardsdatascience.com/dimensionality-reduction-with-pca-from-basic-ideas-to-full-derivation-37921e13cae7

Example of PCA

$$X_{n \times d} = \begin{bmatrix} 1 & 2 \\ 2 & 4 \\ -1 & -2 \\ -2 & -4 \end{bmatrix} \qquad d = 2 \quad n = 4$$

x_1 x_2



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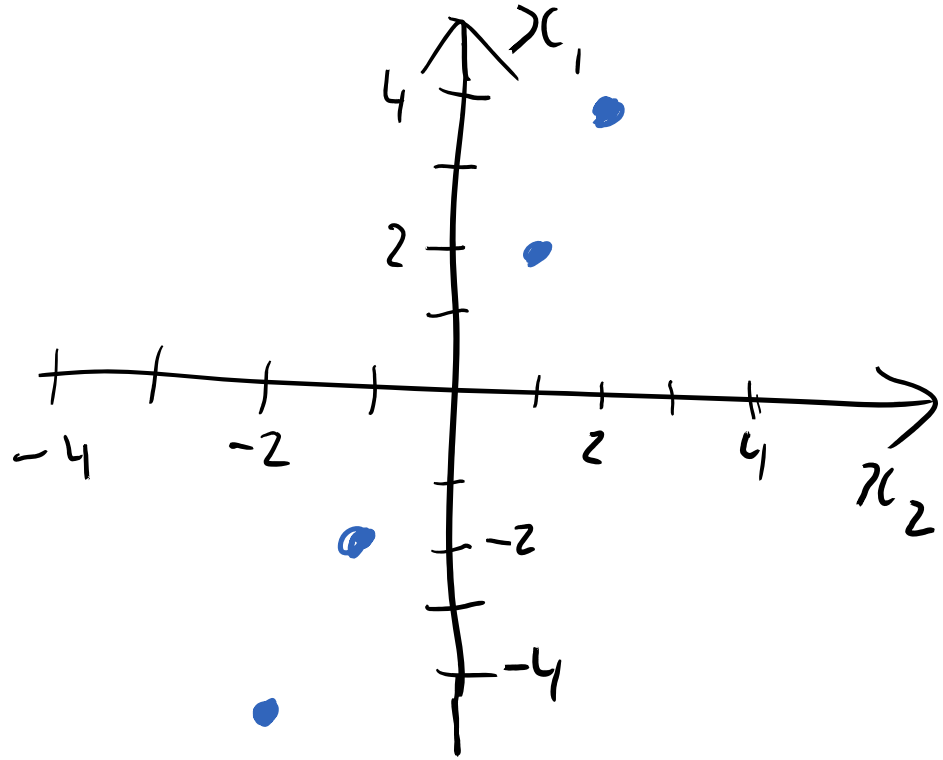
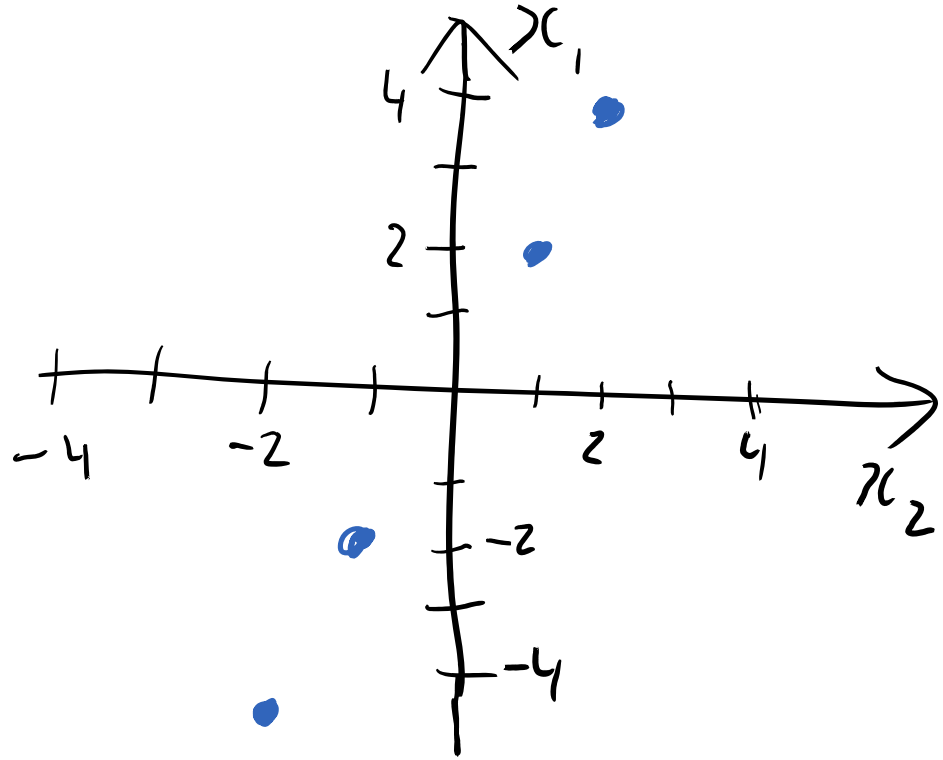


mean of each dimension $[0 \; 0] \Rightarrow \bar{X} = X$

Example of PCA

$$X = \underset{n \times d}{\begin{bmatrix} 1 & 2 \\ 2 & 4 \\ -1 & -2 \\ -2 & -4 \end{bmatrix}} \qquad d = 2 \quad n = 4$$

$x_1 \quad x_2$



$$X^T X = \underset{d \times d}{\begin{bmatrix} 1 & 2 & -1 & -2 \\ 2 & 4 & -2 & -4 \end{bmatrix}} \begin{bmatrix} 1 & 2 \\ 2 & 4 \\ -1 & -2 \\ -2 & -4 \end{bmatrix} = \begin{bmatrix} 10 & 20 \\ 20 & 40 \end{bmatrix}$$

Example of PCA

$$X = \underset{n \times d}{\begin{bmatrix} 1 & 2 \\ 2 & 4 \\ -1 & -2 \\ -2 & -4 \end{bmatrix}}$$

$x_1 \quad x_2$

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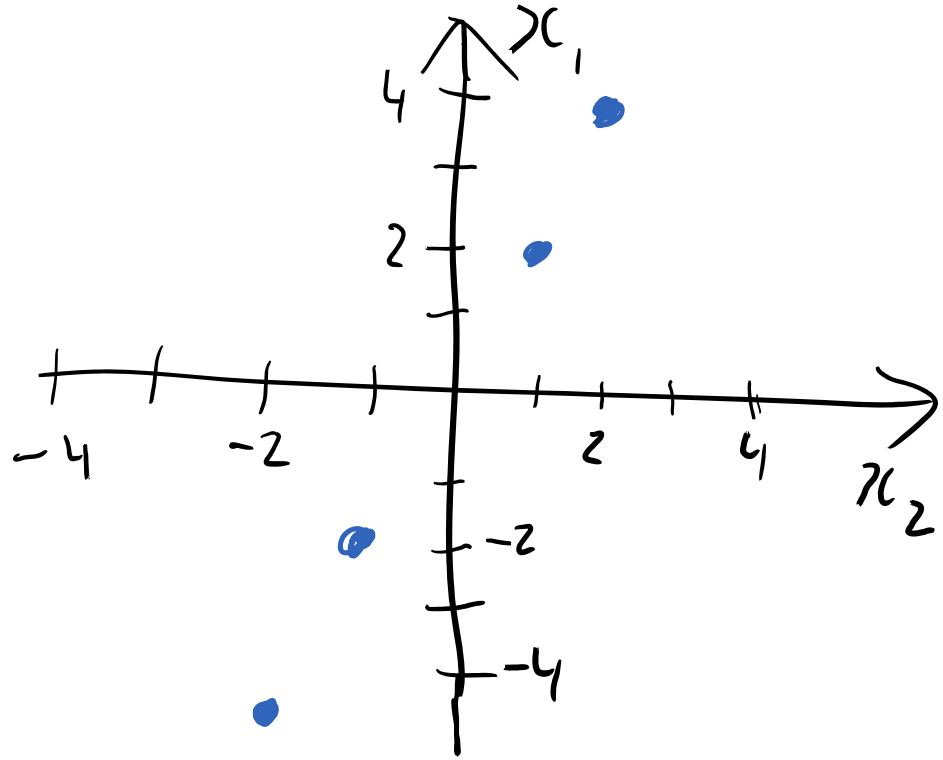

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linalg.eig($X^T X$)

$\Rightarrow$ eigenvalues [50 0]

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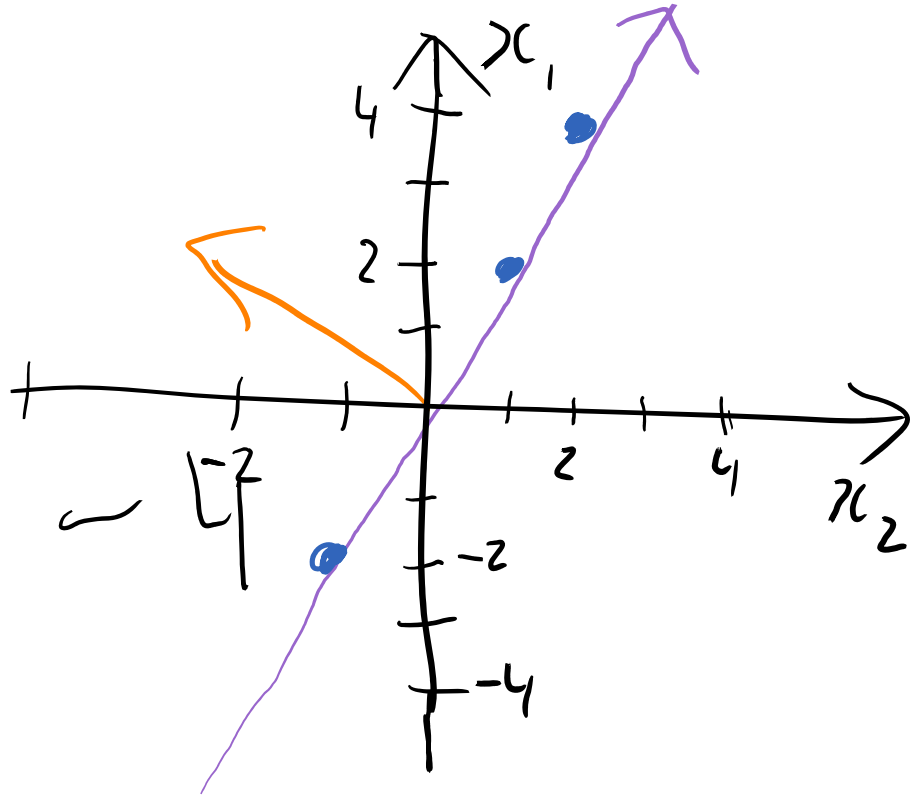

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x_1 x_2

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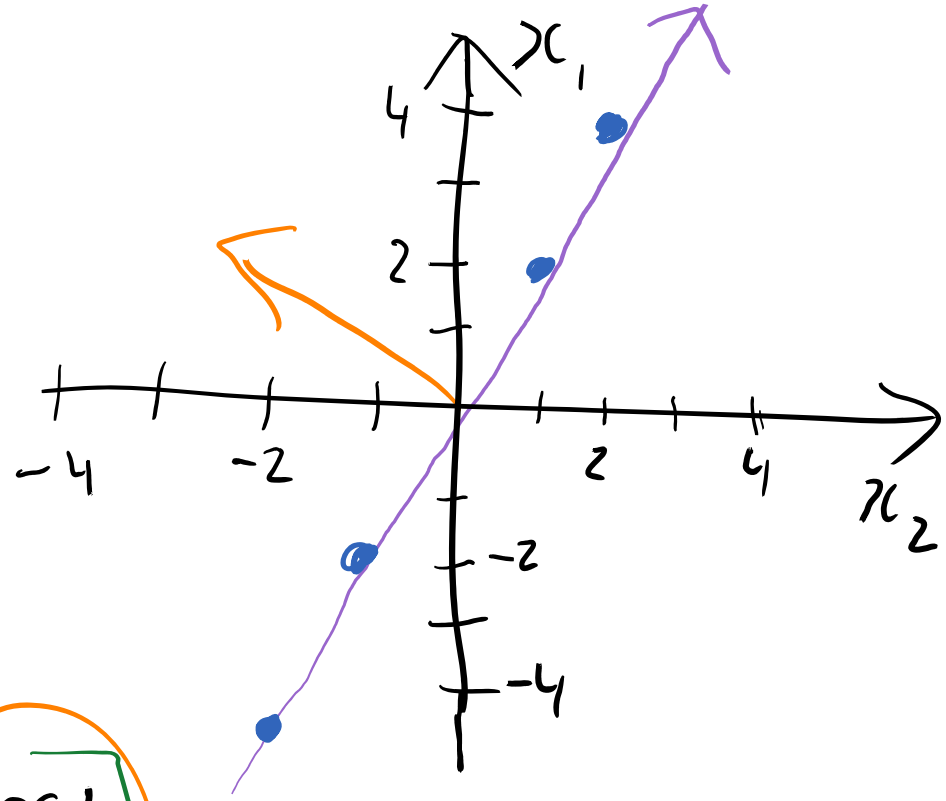
$\Rightarrow$ eigenvalues [50 0]

& eigenvectors

$$X^T X = \underset{d \times d}{\begin{bmatrix} 10 & 20 \\ 20 & 40 \end{bmatrix}}$$

$$\begin{bmatrix} 0.447 & -0.894 \\ 0.894 & 0.447 \end{bmatrix}$$



Example of PCA (take 2, noisy data)

$X = \underset{n \times d}{\begin{bmatrix} 1.07 & 2.16 \\ 2.05 & 4.1 \\ -0.93 & -2.03 \\ -1.97 & -4.09 \end{bmatrix}}$

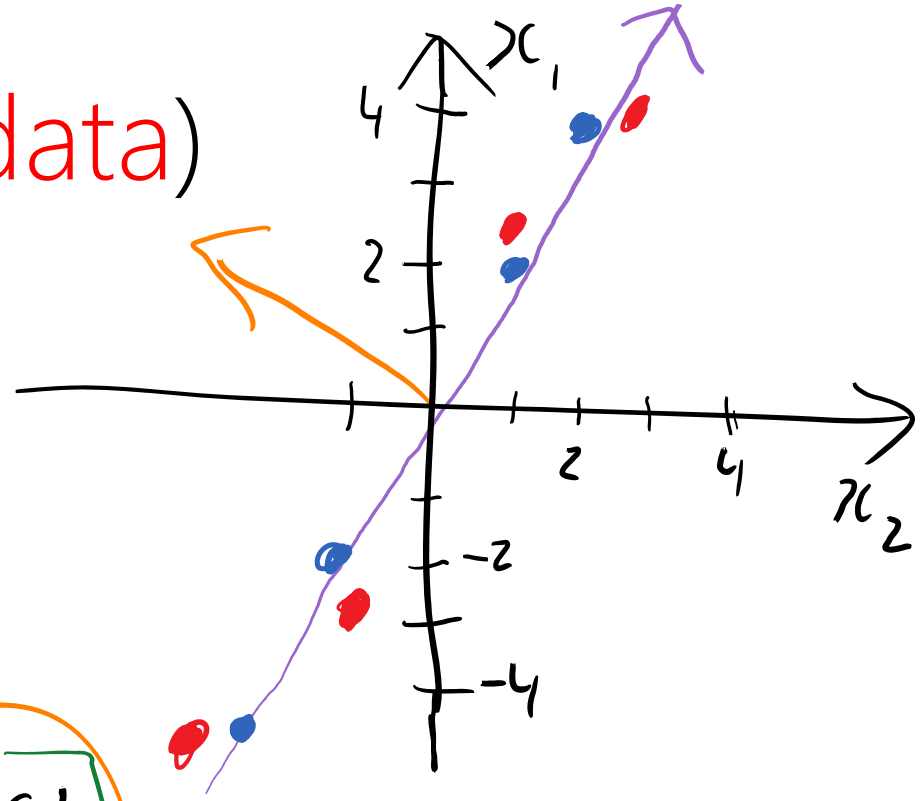
x_1 x_2

linalg.eig($X^T X$)

$\Rightarrow$ eigenvalues $\begin{bmatrix} 50 & 0 \end{bmatrix}$

& eigenvectors

$$\begin{bmatrix} 0.447 & -0.894 \\ 0.894 & 0.447 \end{bmatrix}$$



Example of PCA (take 2, noisy data)

$X =$ (nxd)

x_1	x_2
1.07	2.16
2.05	4.1
-0.93	-2.03
-1.97	-4.09

linalg.eig($X^T X$)

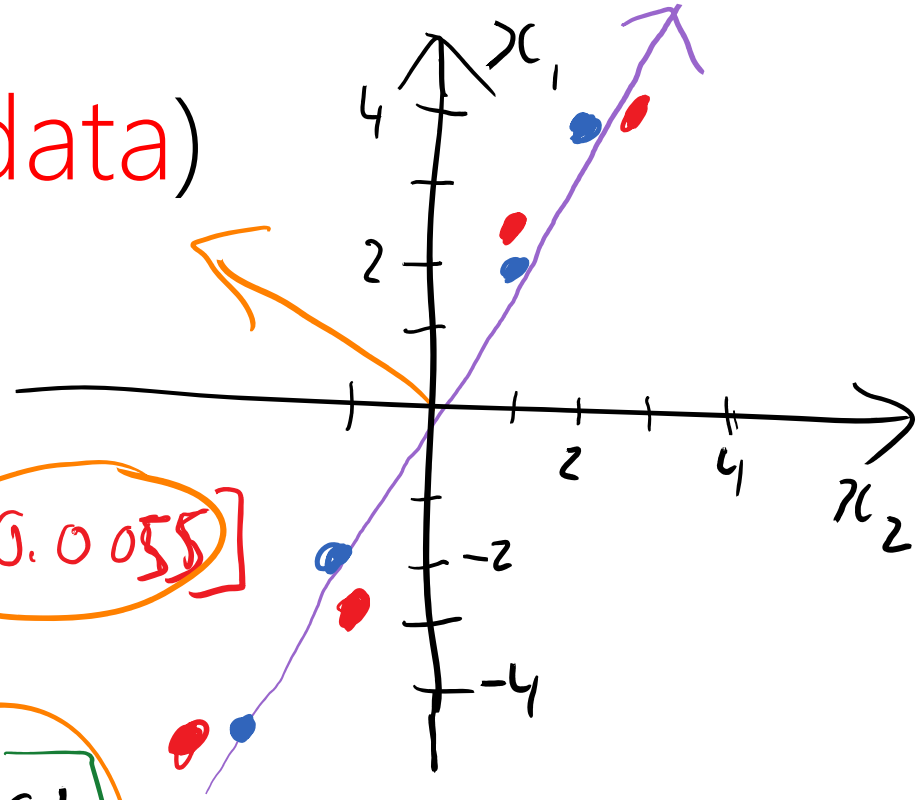
$\Rightarrow$ eigenvalues $\begin{bmatrix} 50 & 0 \end{bmatrix}$

& eigenvectors

$\begin{bmatrix} 52.3 & 0.0055 \end{bmatrix}$

$\begin{bmatrix} 0.439 & -0.898 \\ 0.898 & 0.439 \end{bmatrix}$

$\begin{bmatrix} 0.447 & -0.894 \\ 0.894 & 0.447 \end{bmatrix}$

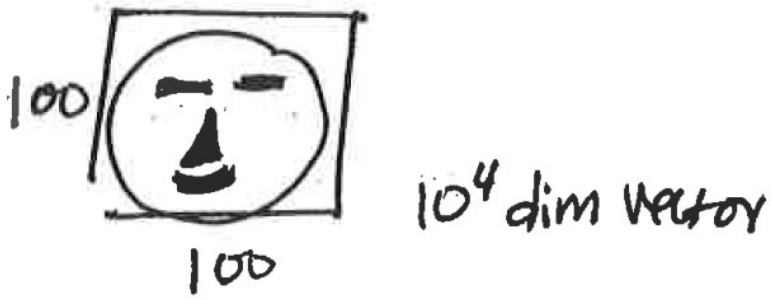


Linear algebra for PCA

$\bar{X} \in \mathbb{R}^{n \times d}$

- Need to compute the principal axes, Q, of $\bar{X}^T \bar{X} = QDQ^T \in \mathbb{R}^{d \times d}$.
- This is an *eigendecomposition* of the matrix $\bar{X}^T \bar{X}$.

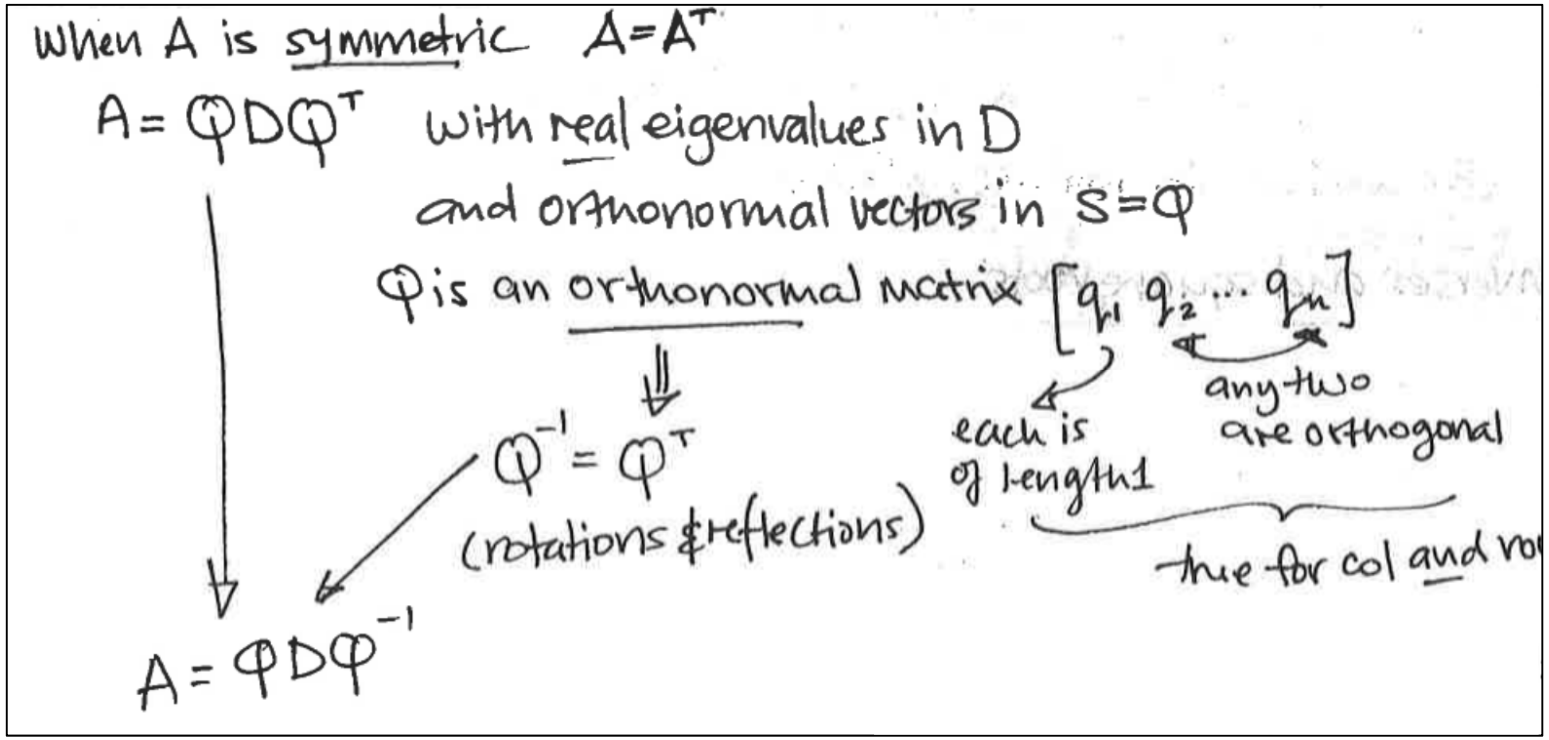
- Computing its eigendecomposition has time complexity $O(d^3)$.
- What if $d \gg n$? *e.g.*, images of $\mathbf{d = 100 \times 100 = 10^4}$ pixels, and $n = \mathbf{1{,}000}$ images.
- Could we do something cheaper?
- Yes. Need to understand the SVD.



Linear algebra for PCA

$\bar{X} \in \mathbb{R}^{n \times d}$

Recall the spectral theorem (principal axis theorem) from MVG lecture, which gives a *spectral (eigen) decomposition*:.

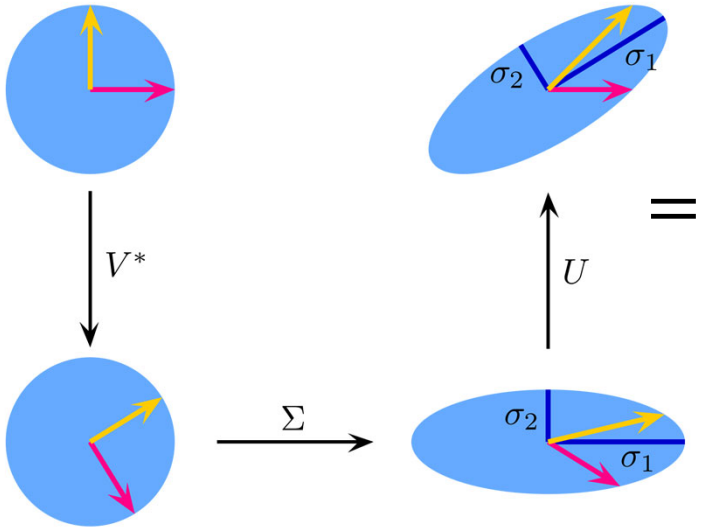


- The covariance matrix for PCA, $\bar{X}^T \bar{X}$, is symmetric (and PSD).
- It turns out, there is a generalization of the spectral decomposition, for non-symmetric and non-square matrices, the SVD that will be helpful.

Singular Value Decomposition (SVD)

Can think of M as linear transformation broken down into three steps, by looking at its effect on the unit disc and the two canonical unit vectors e_1 and e_2:

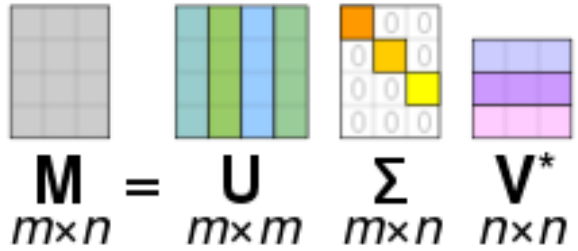
1. **Left:** $\boldsymbol{V^T}$ rotates the disc and unit vectors.
2. **Bottom: Σ** stretches scales axes by $\sigma_i = \Sigma_{i,i}$ (singular values).
3. **Right: U** performs another rotation.



$$= M \begin{bmatrix} e_2 \\ e_1 \end{bmatrix} = U\Sigma V^* \begin{bmatrix} e_2 \\ e_1 \end{bmatrix}$$

$$M = U \cdot \Sigma \cdot V^*$$

Can be applied to any matrix M.



$$Mv_1 = \Sigma_{1,1}u_1$$
$$Mv_2 = \Sigma_{2,2}u_2$$
$$\dots$$
$$Mv_r = \Sigma_{r,r}u_r$$

$$r = rank(M) \leq \min(m, n)$$

https://en.wikipedia.org/wiki/Singular_value_decomposition

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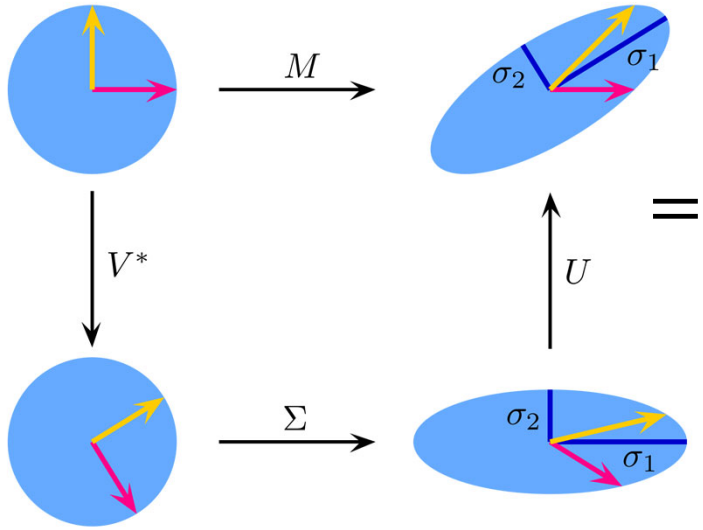

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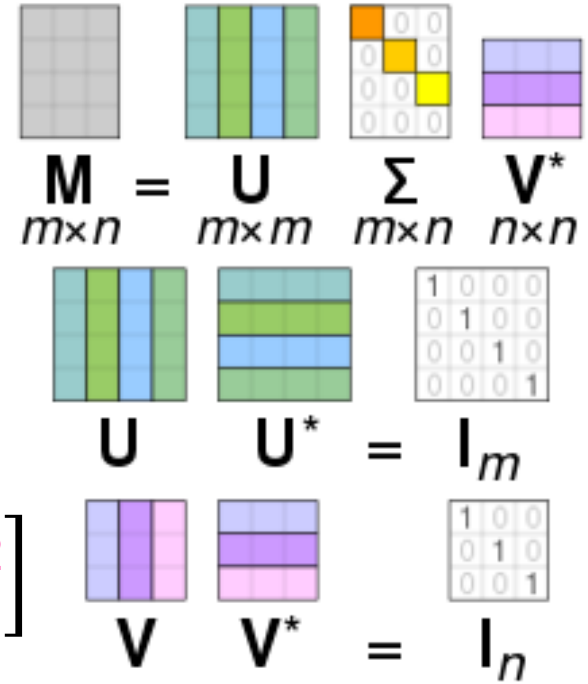


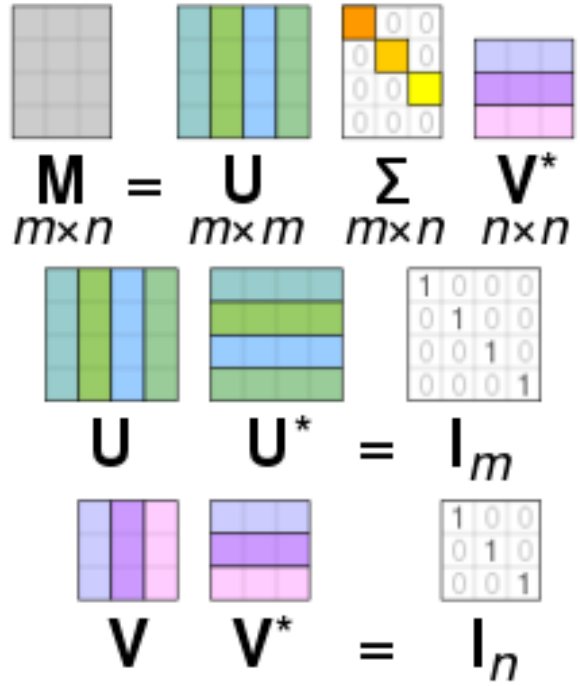
- *Has time complexity* $O(\min(m^2n, mn^2))$.
- *Σ is unique (if in descending order), but V and U are generally not: e.g. sign flips.*
- *(Eigendecomposition is unique if all eigenvalues are unique)*
- *If M is square+symmetric, yields the spectral decomposition.*

https://en.wikipedia.org/wiki/Singular_value_decomposition

Singular Value Decomposition (SVD)

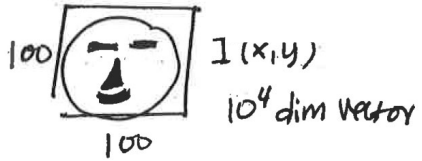
- Columns in U are the eigenvectors of MM^T, called the *left singular vectors of M* ($MM^T = U\Sigma V^T V\Sigma^T U^T = U\Sigma^2 U^T$).
- Columns in V are the eigenvectors of $M^T M$, called the *right singular vectors of M* ($M^T M = V\Sigma^T U^T U\Sigma V^T = V\Sigma^2 V^T$).
- Both spectral decompositions at once!
- Eigenvalues are the same, given by $\lambda_i = \Sigma_{i,i}^2$ ($\Sigma_{i,i}$ are the *singular values* of M).

Can be applied to any matrix M.

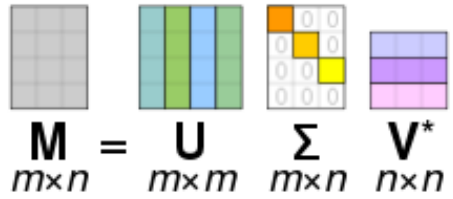


Singular Value Decomposition (SVD)

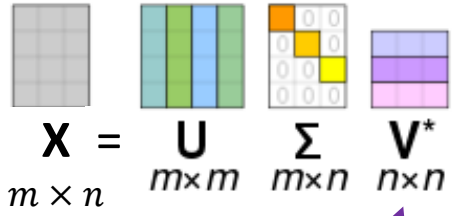
$X \in \mathbb{R}^{n \times d}$



- Recall this example with $d \gg n$,e.g. $d = 10^4$ pixels, $n = 1000$ images.
- How can we make use of what we just learned to do PCA faster than the eigendecomposition $O(d^3)$?
- Instead of spectral decomposition of $X^T X$…
- …directly use SVD of the data matrix: $SVD(X) = U\Sigma V^T$
- This SVD has time complexity $O(dn^2)$.
- $V \in \mathbb{R}^{d \times d}$ are the needed eigenvectors for $X^T X \in \mathbb{R}^{d \times d}$.
- $\lambda_i = \Sigma_{i,i}^2$ are needed eigenvalues.



Singular Value Decomposition (SVD)

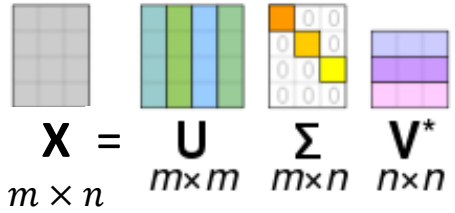


For PCA we want projections onto top k PCs.

- When we used a spectral decomposition, $X^T X = QDQ^T$, we compute: $X_k = XQ_k \in \mathbb{R}^{n \times k}$ (Q are eigvecs of $X^T X$).
- When using the SVD of X, we can instead get this from:
- $X_k = XV_{:,1:k}$

columns V are eigenvectors of $X^T X$

Singular Value Decomposition (SVD)



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- When using the SVD of X, we can instead get this from:
- $X_k = XV_{:,1:k} = U_{:,1:k}\Sigma_{1:k,1:k} \in \mathbb{R}^{n \times k}$ ("scores" in PCA basis).
- $X_{k-recon} = XV_{:,1:k}(V_{:,1:k})^T = U_{:,1:k}\Sigma_{1:k,1:k}(V_{:,1:k})^T$
- We don't need to compute covariance matrix, or do the projections, we just need $SVD(X)$!

$$Xv_i = \Sigma_{i,i}u_i$$

"Eckart Young theorem" 1936

- The SVD "k-reconstruction" produces the best $\boldsymbol{k}$-rank approximation by the matrix norm, $\|X - X_{recon-k}\|_F$.
- First proven by Schmidt (of Gram-Schmidt fame) in 1907 for Froebenius norm.
- Later rediscovered by Eckart & Young 1936, also generalized to other norms..
- Thus, PCA provides the best low rank approximation to the data matrix.

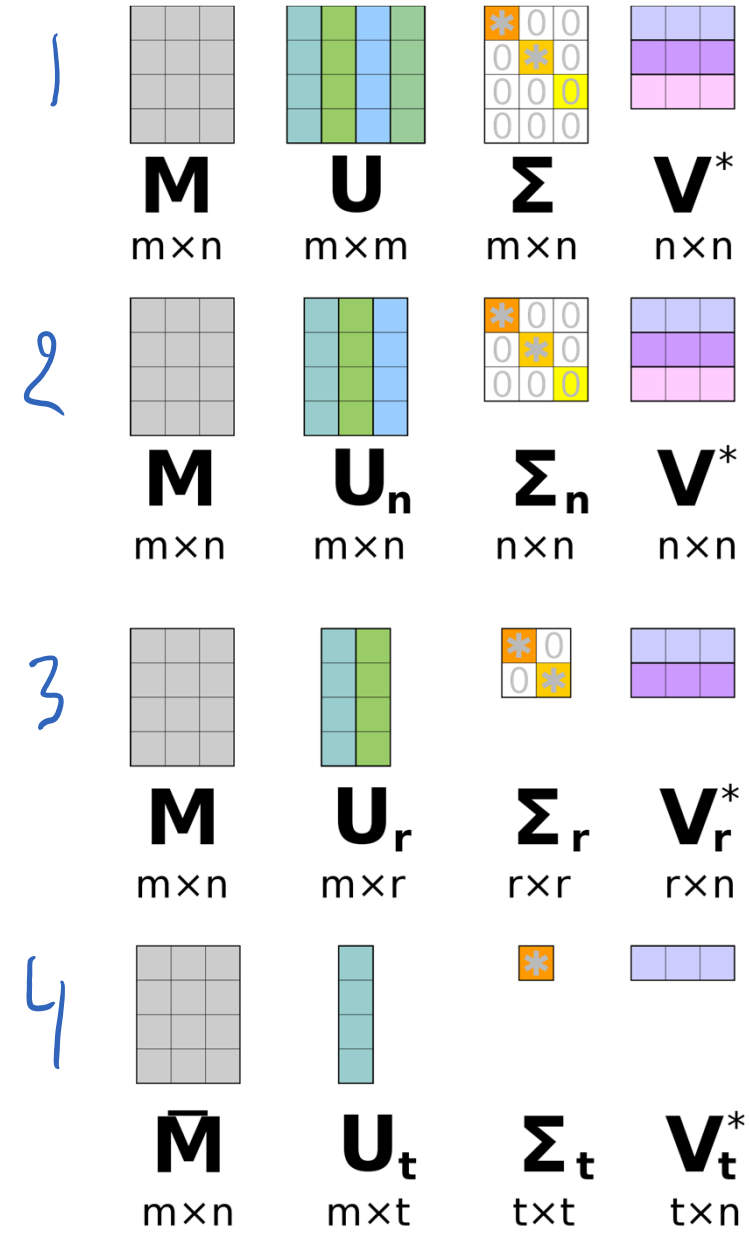
$$\|\mathbf{A}\|_F \equiv \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}|a_{ij}|^2}$$

https://en.wikipedia.org/wiki/Low-rank_approximation#Proof_of_Eckart%E2%80%93Young%E2%80%93Mirsky_theorem_(for_spectral_norm)

Practicalities: Reduced SVDs

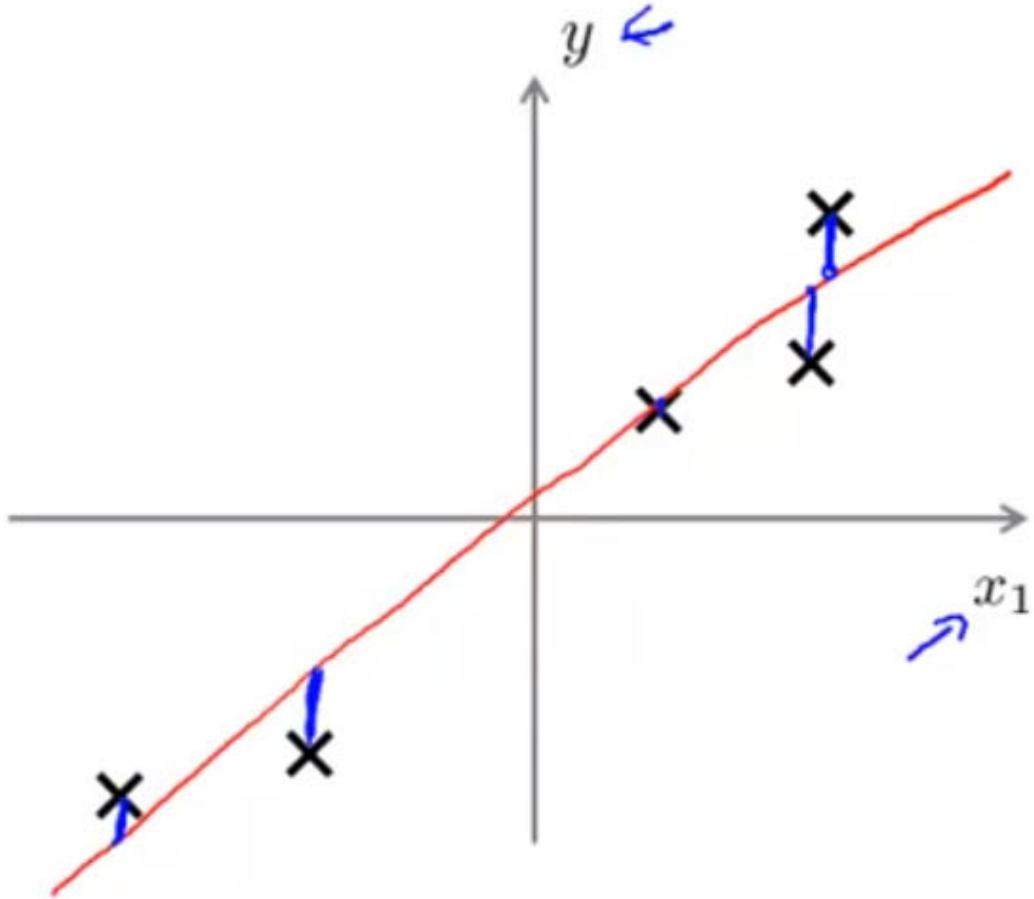
For PCA and other applications, don't need the entire SVD, and can make do with "trimmed down" versions:

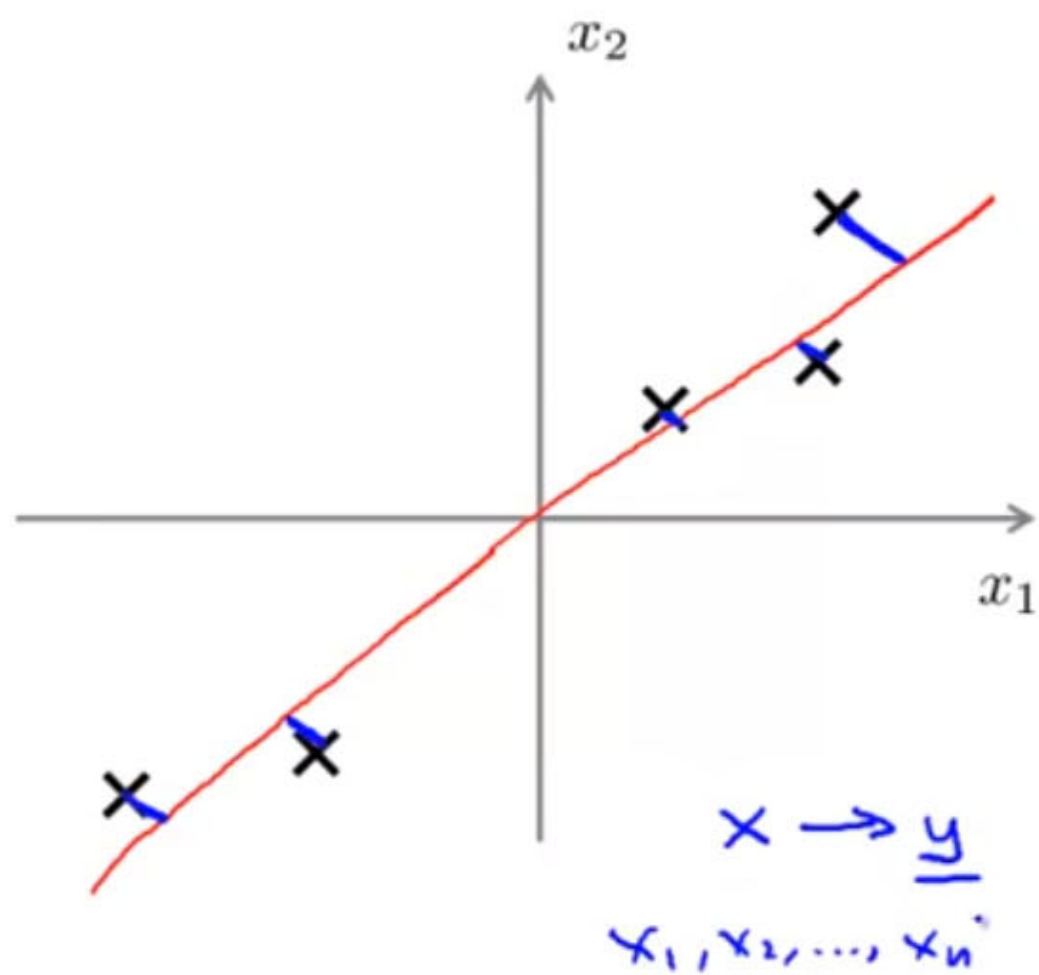
1. Full SVD
2. Thin SVD (remove columns of U not corresponding to rows of V*)
3. Compact SVD (remove vanishing singular values and corresponding columns/rows in U and V*),
4. Truncated SVD (keep only largest t singular values and corresponding columns/rows in U and V*)



https://en.wikipedia.org/wiki/Singular_value_decomposition

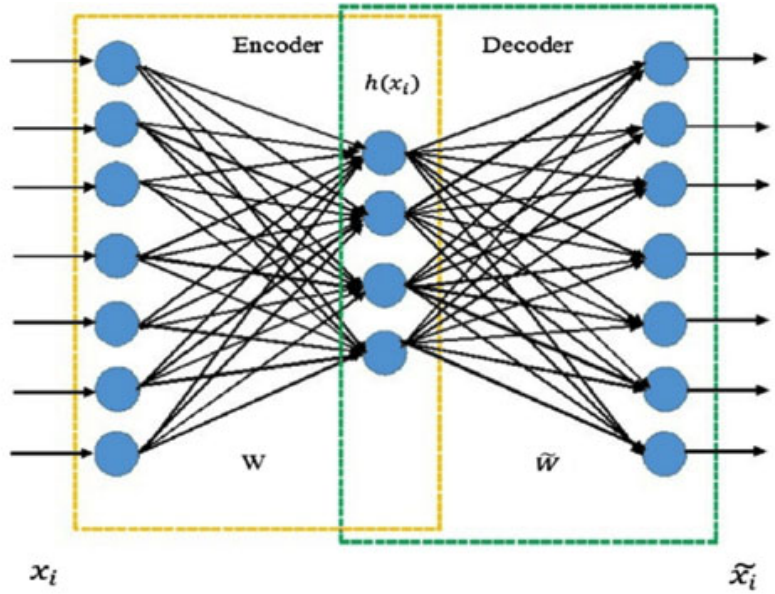
PCA is not linear regression





PCA from neural networks!

- Special kind of neural network, called an *autoencoder* recovers the same subspace as PC-k.
- Autoencoder tries to compress a data set by trying to predict itself back after going through a bottleneck.



- For a linear autoencoder with one hidden layer containing k nodes, using squared loss, the hidden layer representation is equivalent to that found from PCA-k (although W may correspond to different eigenvectors that span the same space).
- Can generalize by making non-linear transfers, and more layers, etc.

https://towardsdatascience.com/understanding-pca-autoencoders-algorithms-everyone-can-understand-28ee89b570e2