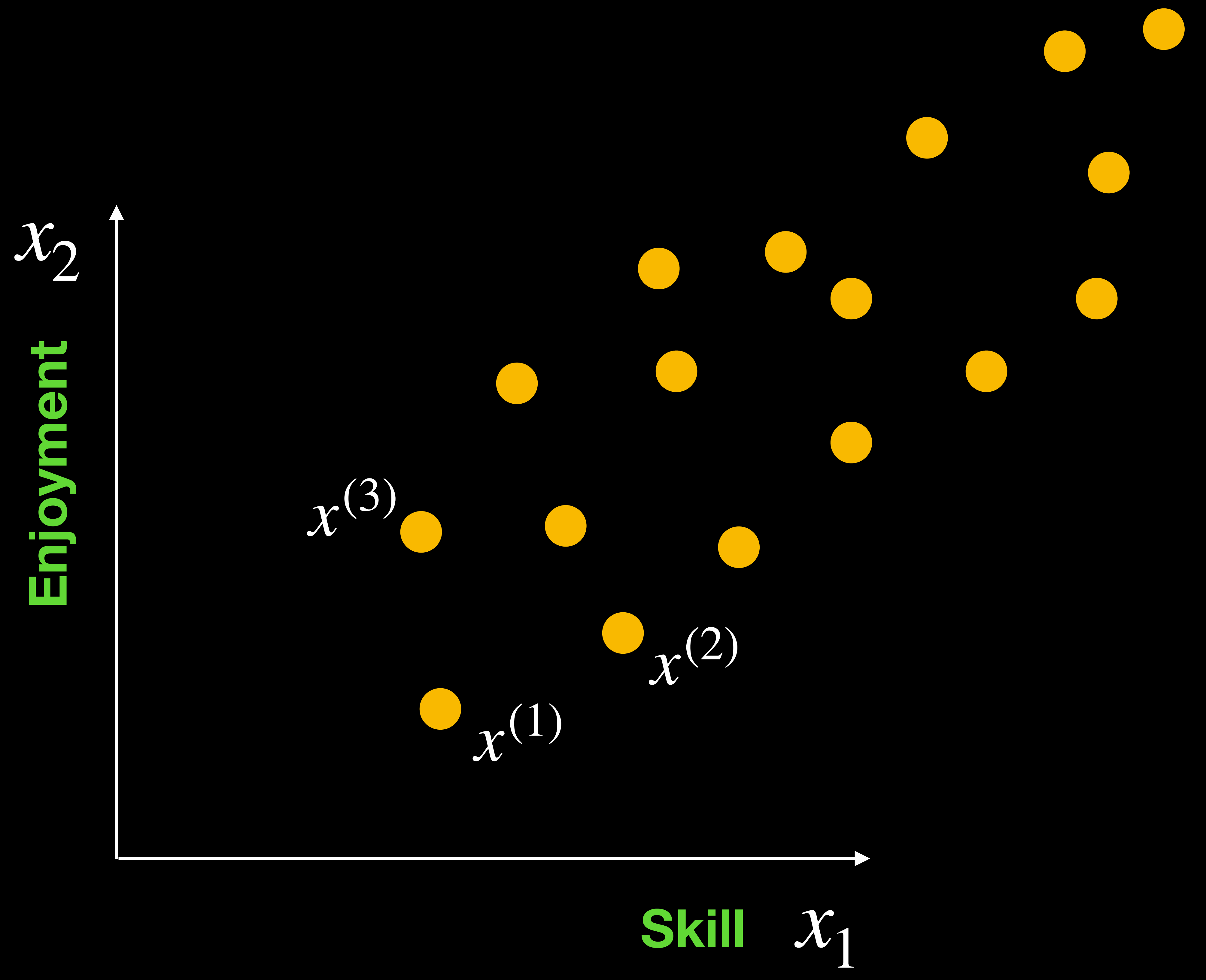
Principal Component Analysis

Principal Component Analysis

Dataset

x_1	x_2
1.2	1.2
3.2	5.4
4.3	6.4
3.2	5.4
…	…



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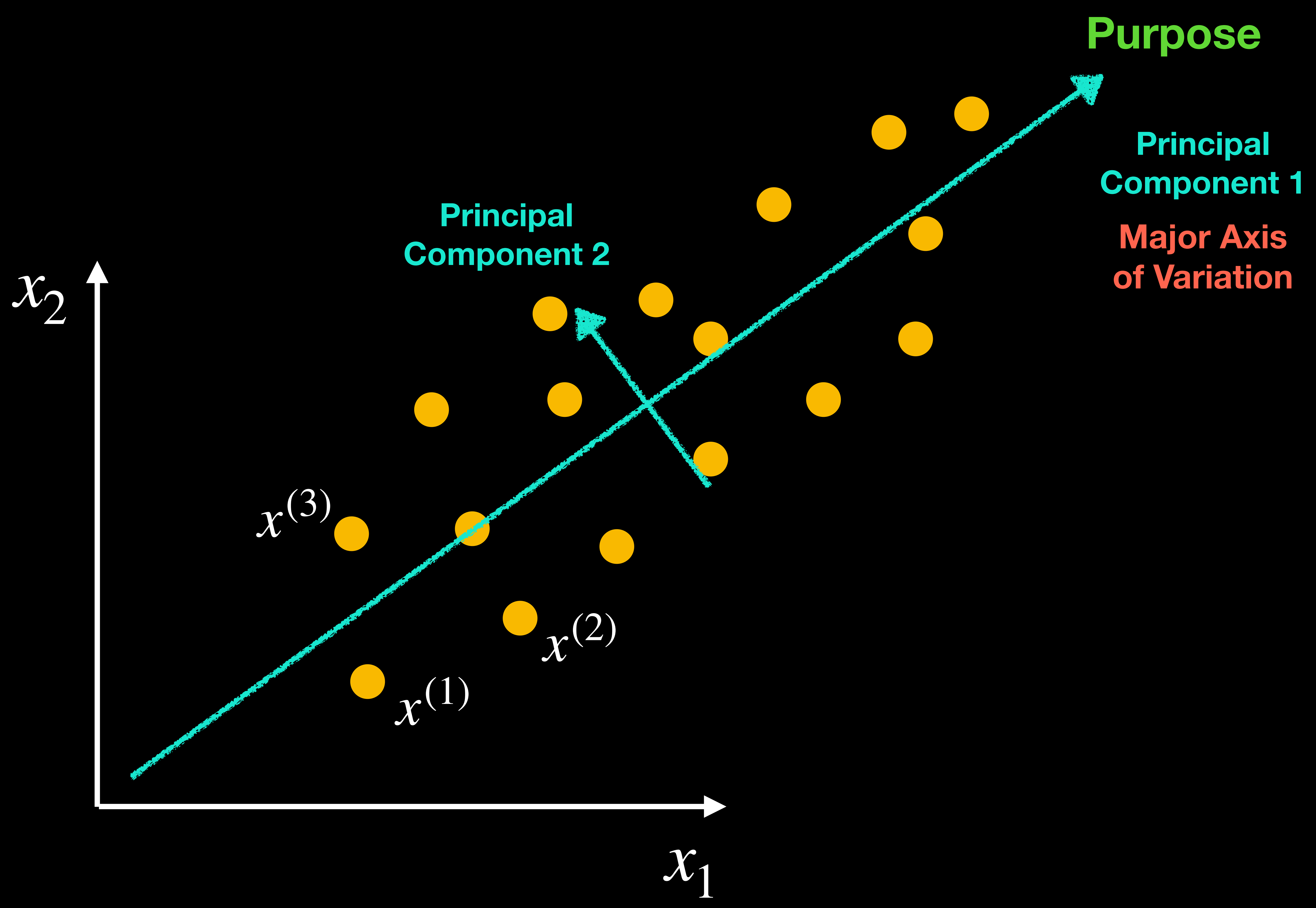

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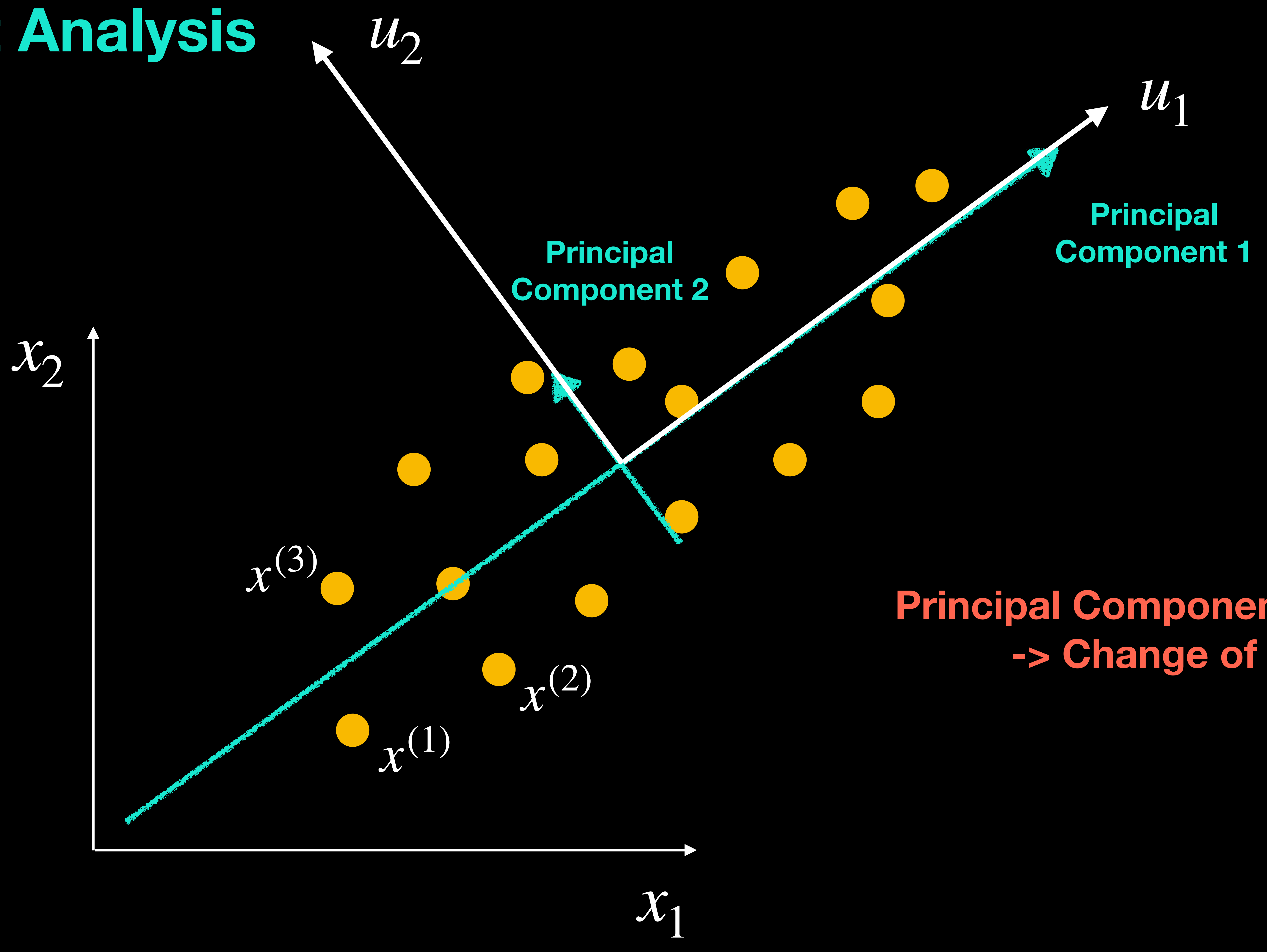

Principal Components Are Orthogonal
-> Change of Coordinates

Principal Component Analysis

Mean

$$\mu_j = \frac{1}{n}\sum_{i=1}^{n} x_j^{(i)}$$

Center the data

$$x_j^{(i)} \leftarrow x_j^{(i)} - \mu_j$$

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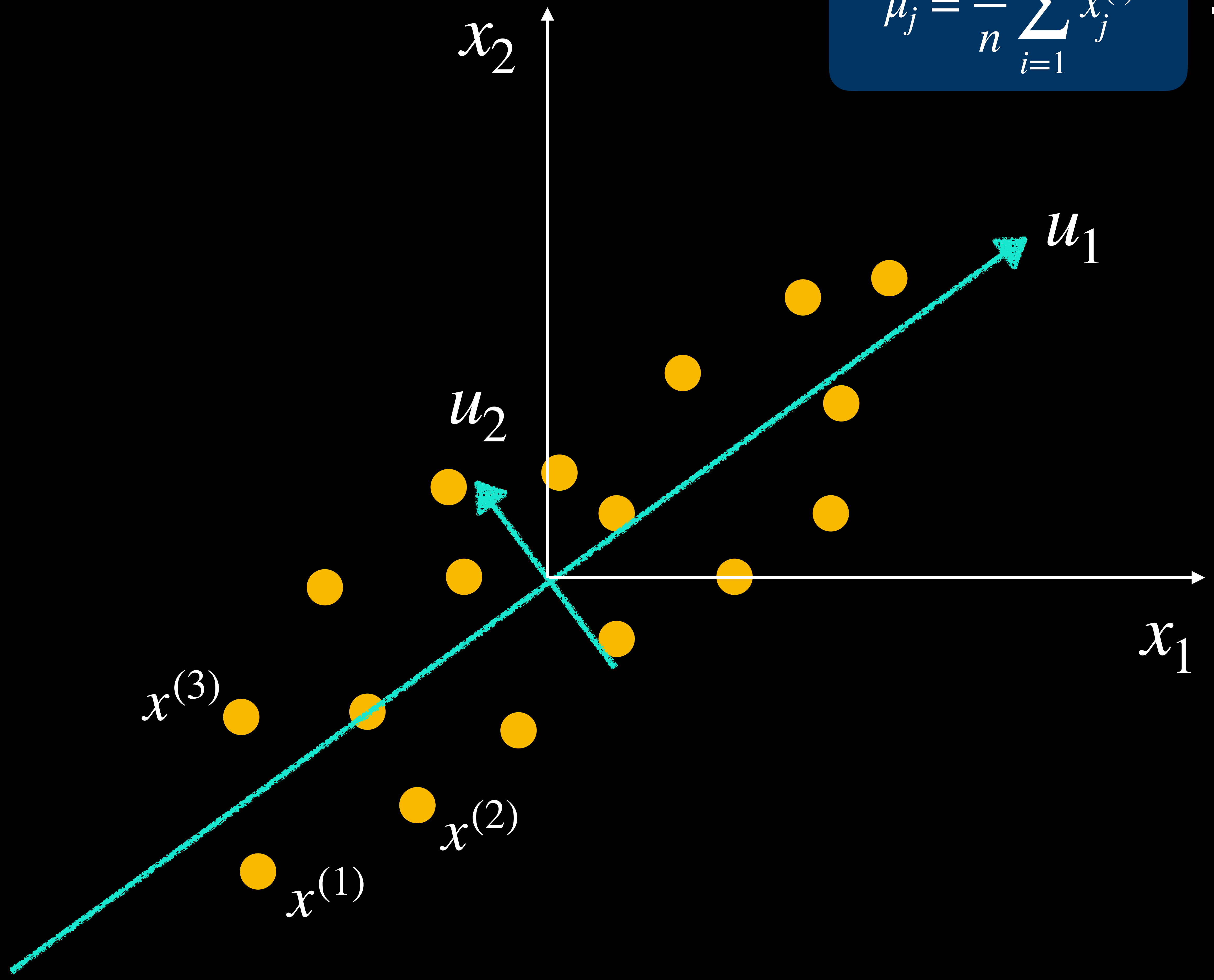

Principal Component Analysis

Variance

$$\sigma_j^2 = \frac{1}{n}\sum_{i=1}^{n}\left(x_j^{(i)} - \mu_j\right)^2$$

Normalize the data

$$x_j^{(i)} \leftarrow x_j^{(i)}/\sigma_j$$

Dataset

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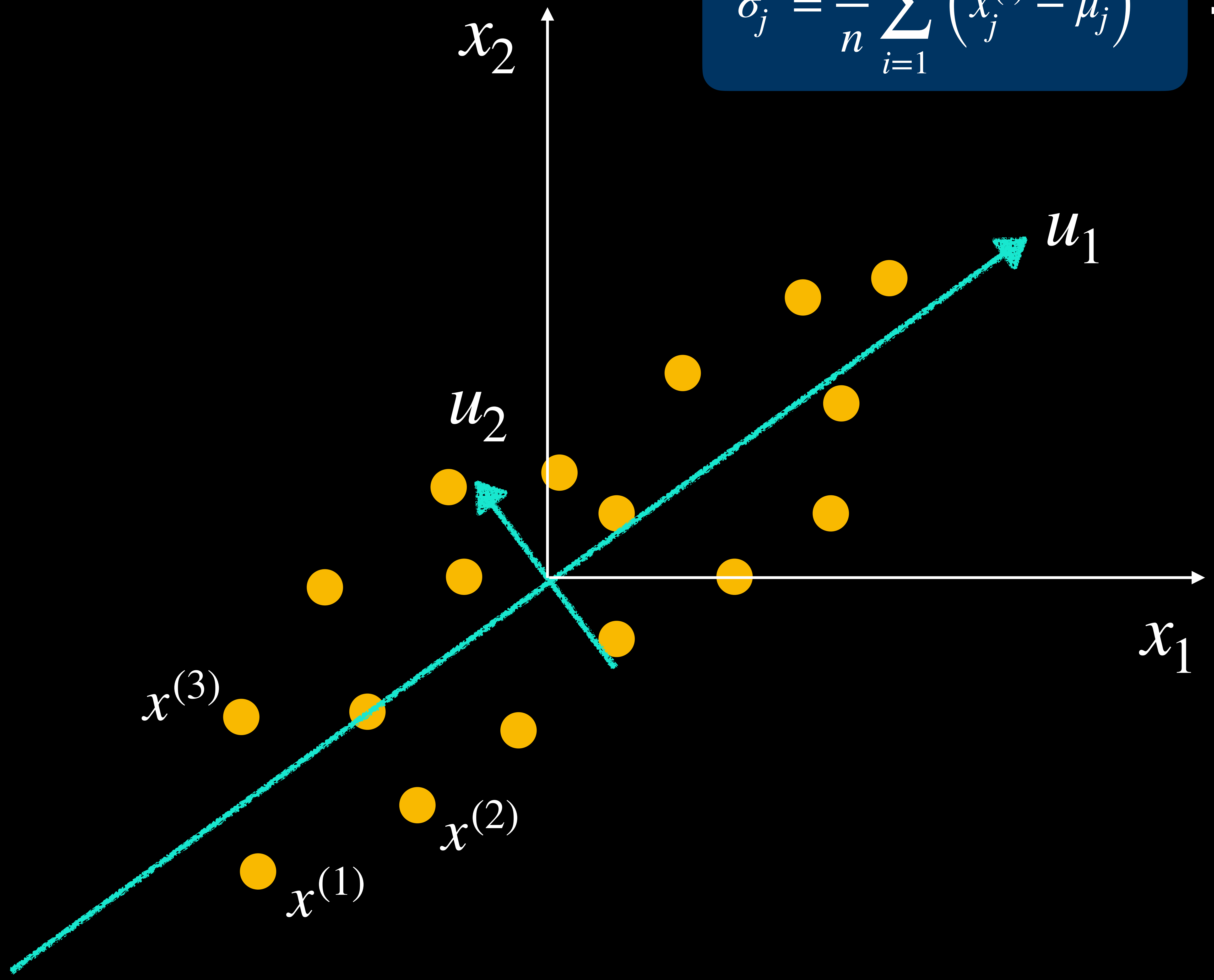
...	...



Principal Component Analysis

Data can be **projected**

On axis of highest variation: u_1

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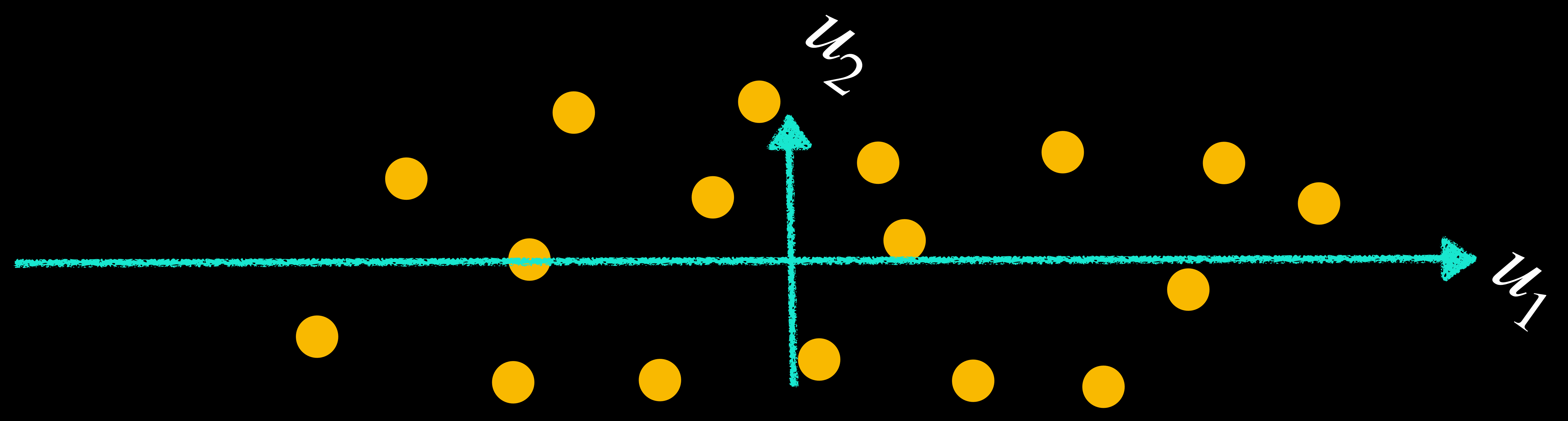

Principal Component Analysis

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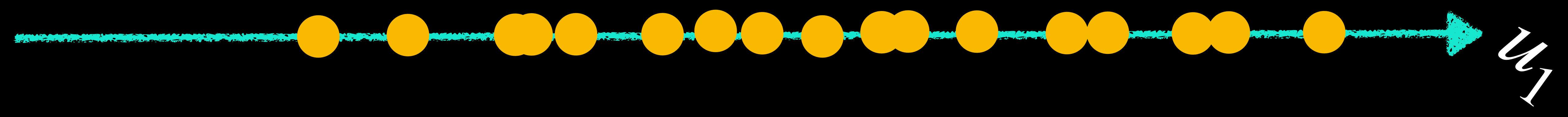

Principal Component Analysis

Error can be computed from distances in direction of u_2

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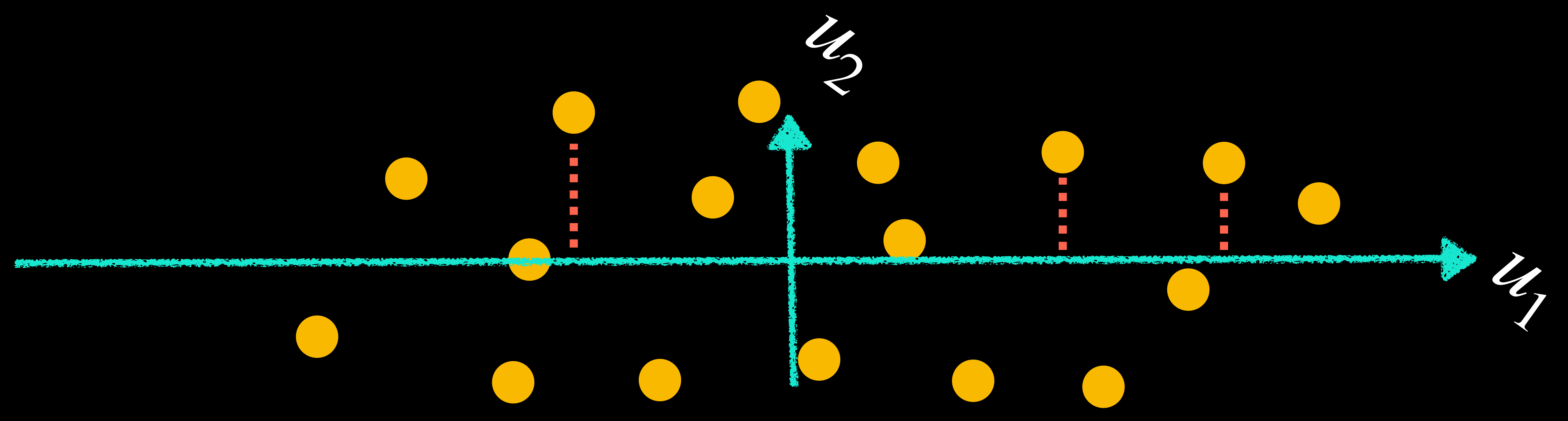
…	…



How do we find u_1 and u_2?

```
U, S, Vt = np.linalg.svd(data_centered)
```

Principal Component Analysis

What's the Major Axis (Direction) of Variation?

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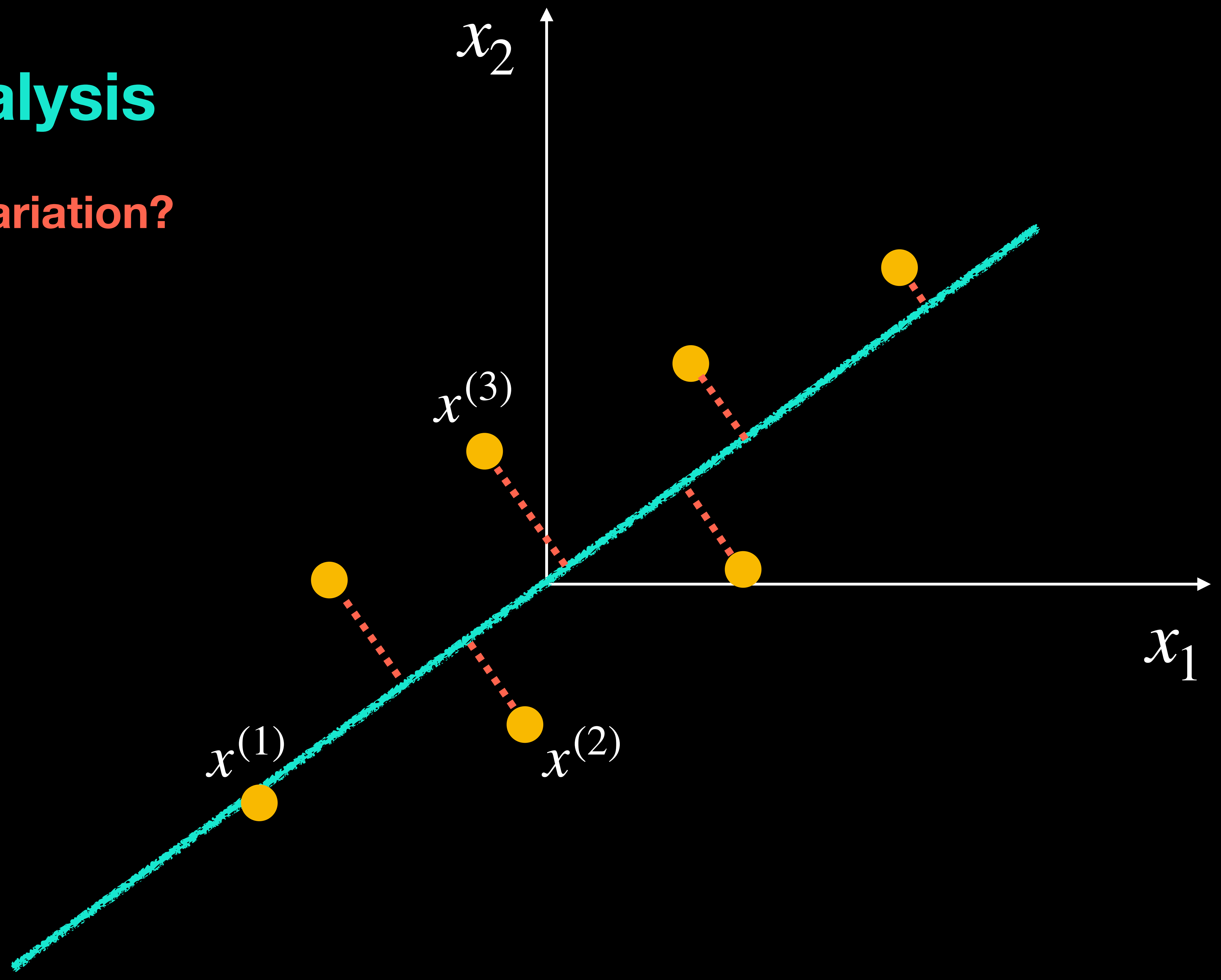

Principal Component Analysis

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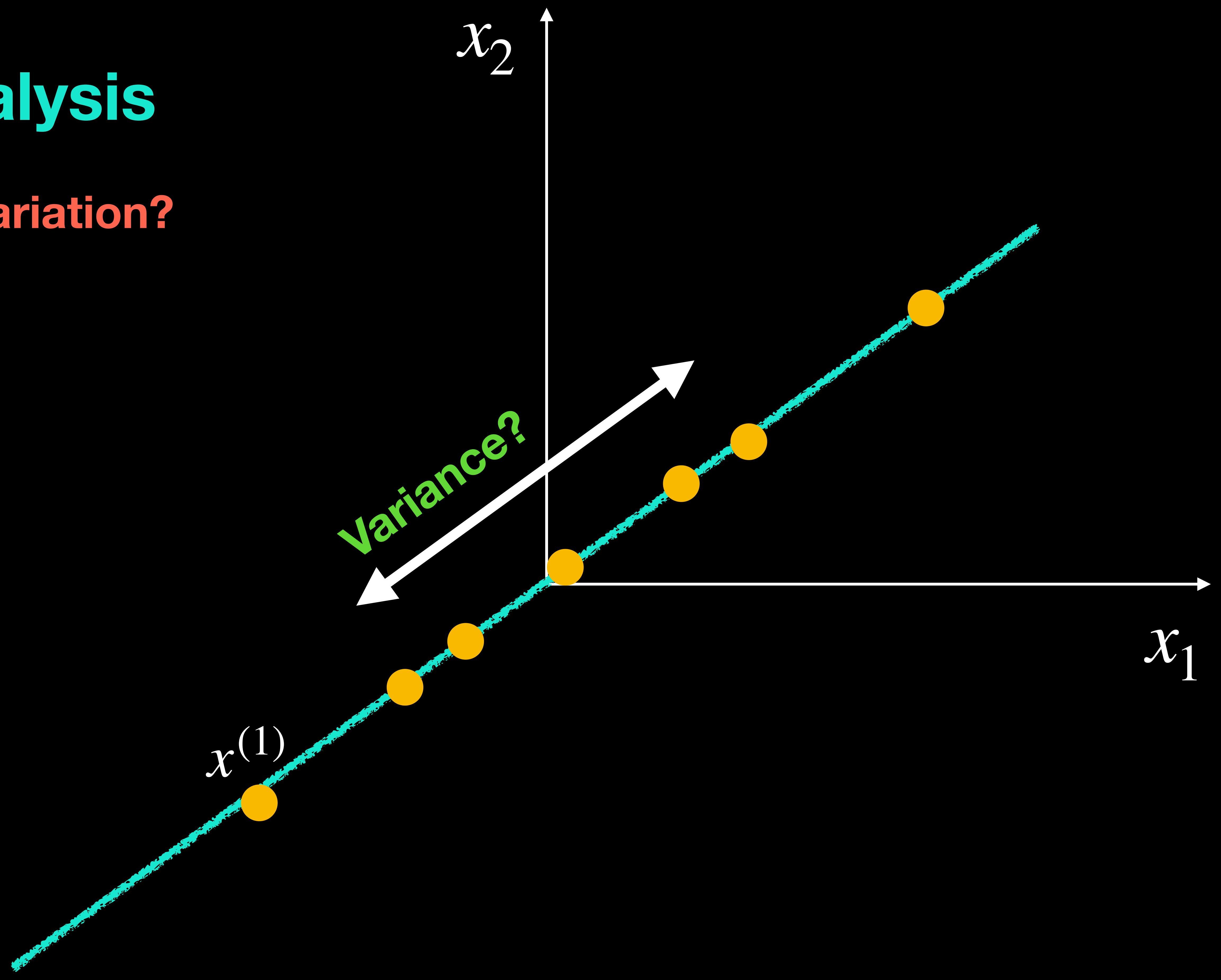

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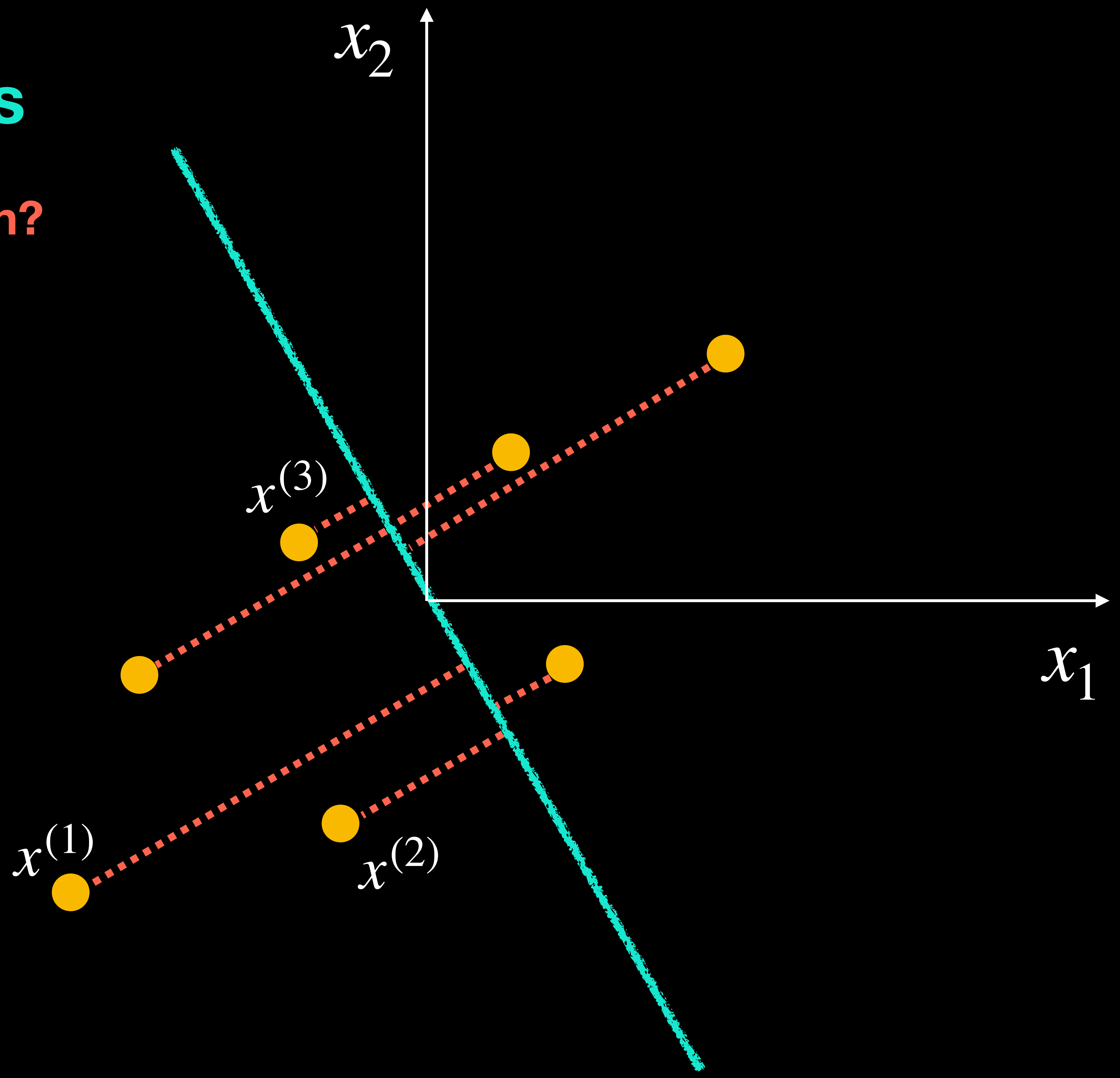

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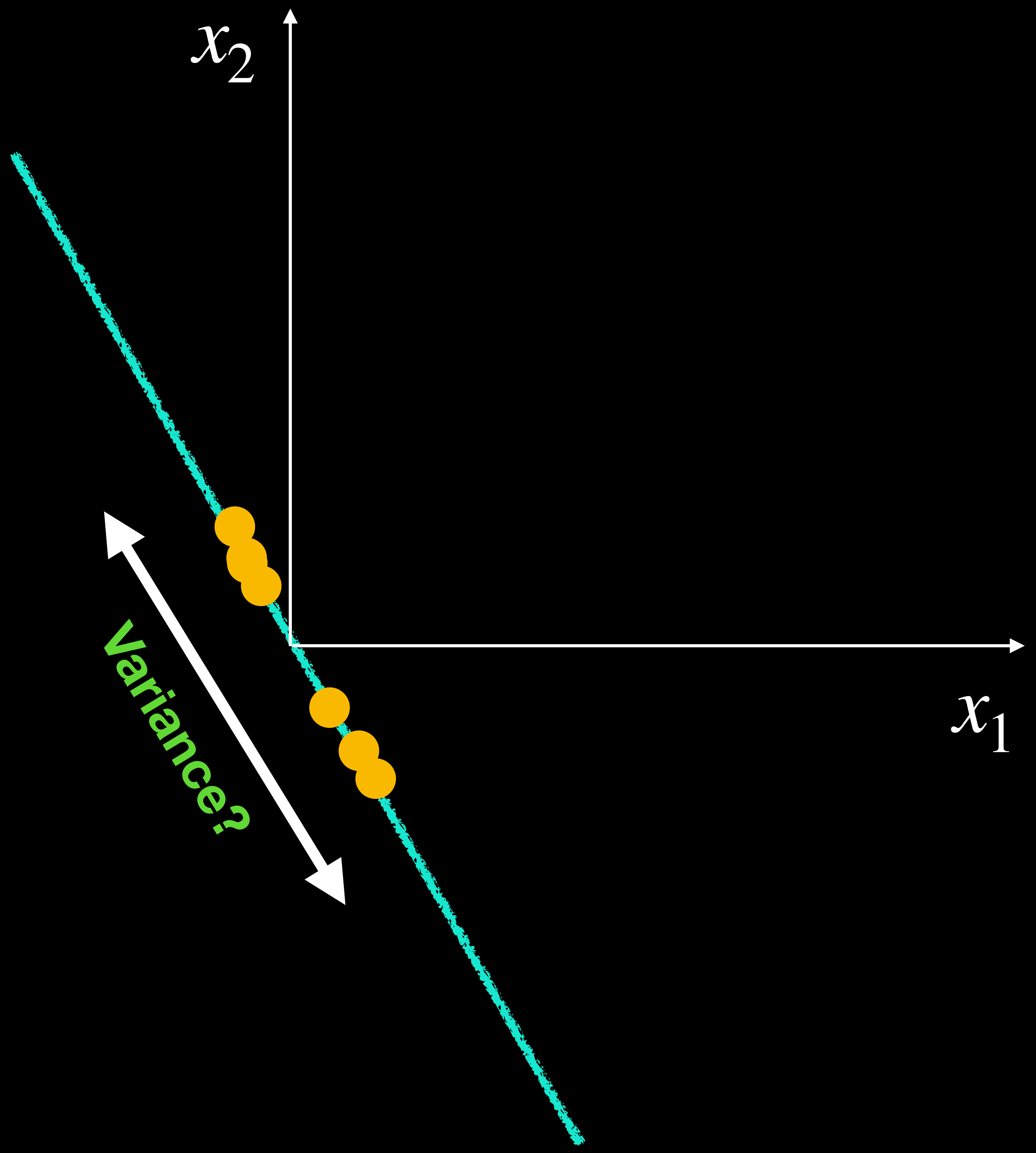

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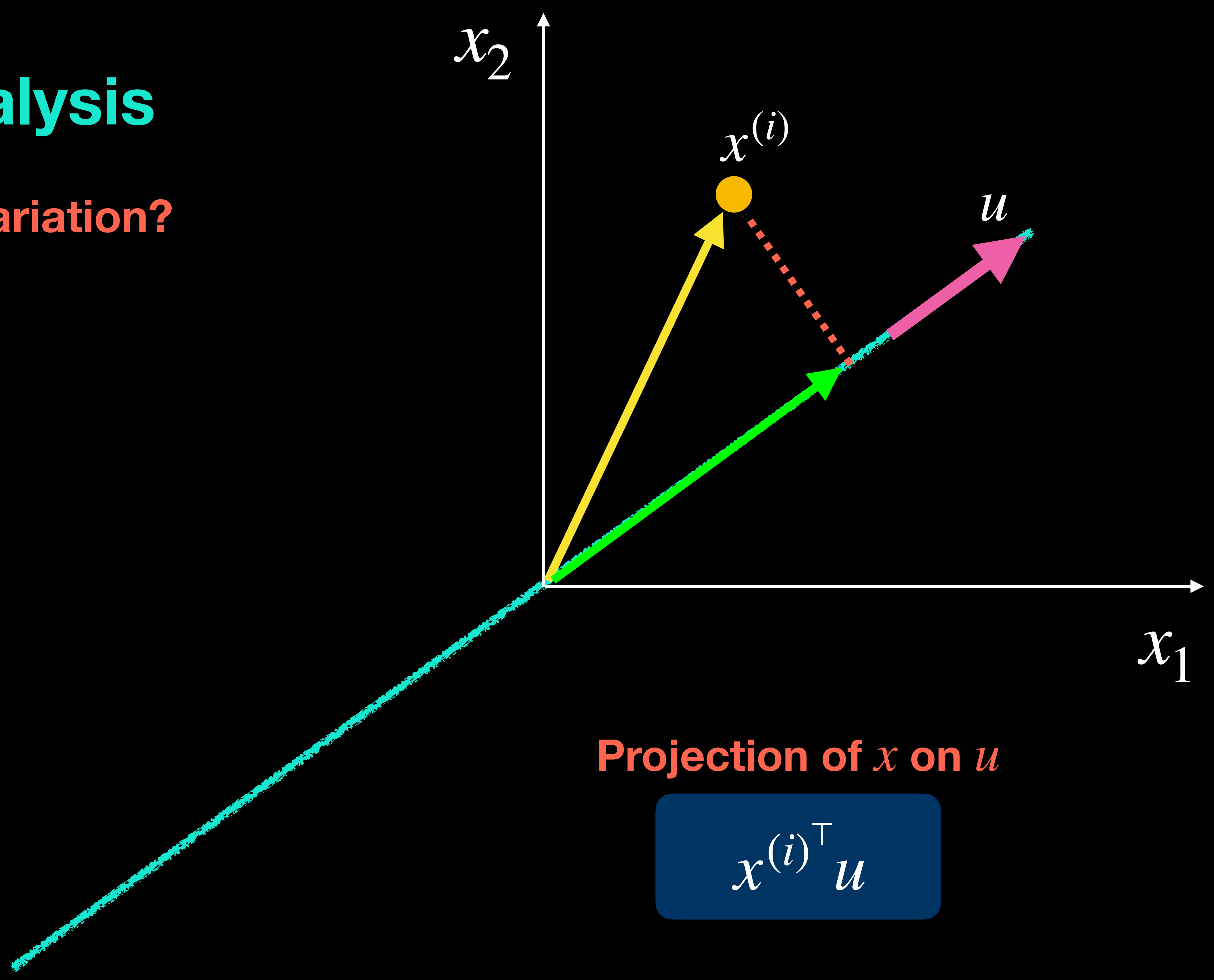


Projection of x on u

$$x^{(i)^\top} u$$

Principal Component Analysis

Maximize Variance of Projections

Maximize $\frac{1}{n}\sum_{i=1}^{n}\left(x^{(i)^\top}u\right)^2$

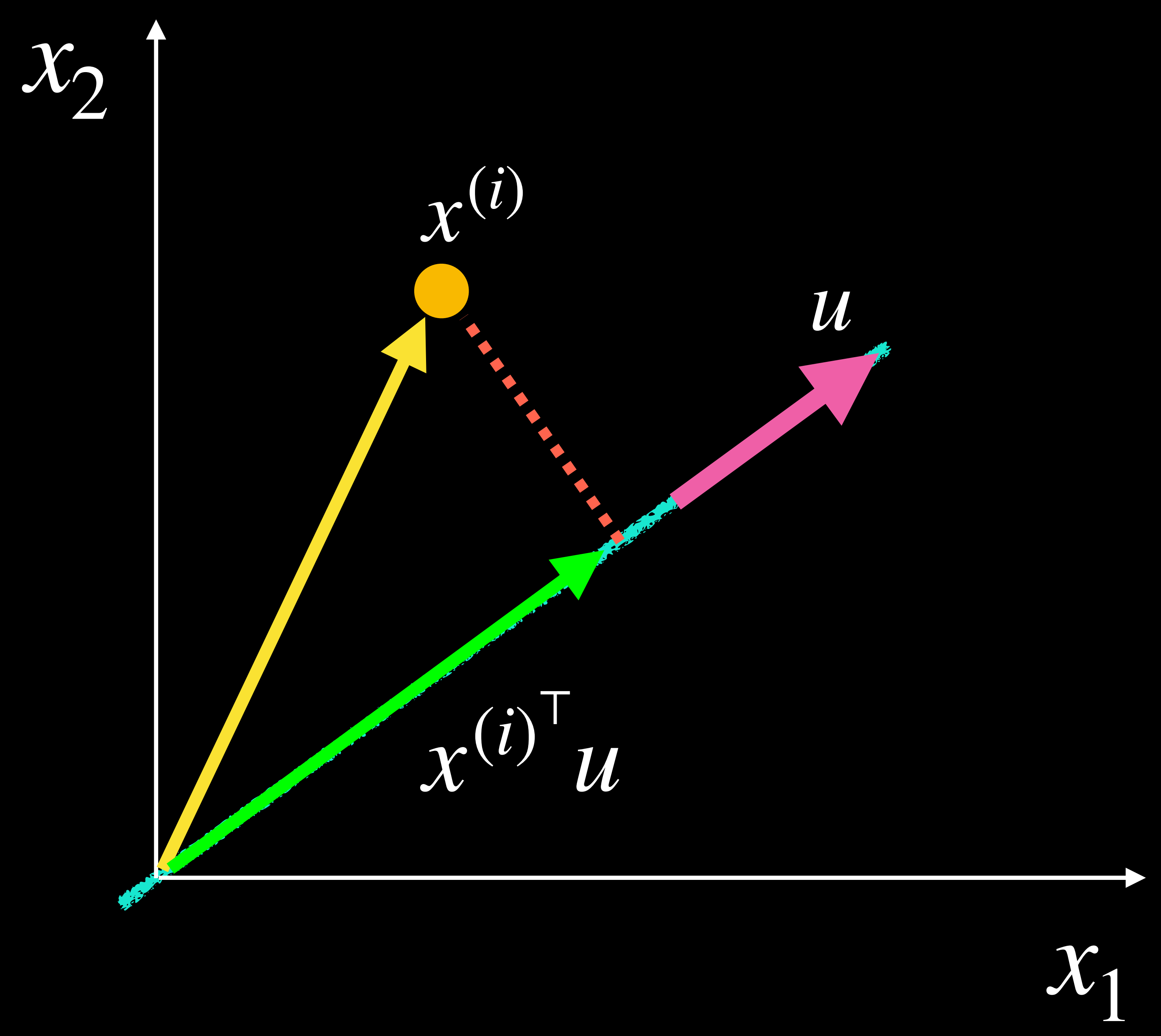
s.t. $\|u\|_2 = 1$

$$= \frac{1}{n}\sum_{i=1}^{n} u^T x^{(i)} x^{(i)T} u$$

$$= u^T \left(\frac{1}{n}\sum_{i=1}^{n} x^{(i)} x^{(i)T}\right) u\,.$$

Covariance Matrix

$$\max_{\|u\|=1} u^T \Sigma u$$



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Lagrange Multipliers

$$L(u, \lambda) = u^T \Sigma u - \lambda(u^T u - 1)$$

$$\frac{\partial L}{\partial u} = 2\Sigma u - 2\lambda u = 0$$

$$\Sigma u = \lambda u$$

Principal Component Analysis

To Maximize Variance of Projections

Solve

$$\boxed{\Sigma u = \lambda u}$$

Eigenvalue problem

$x \in R^d$

$\Sigma \in \mathbb{R}^{d \times d}$

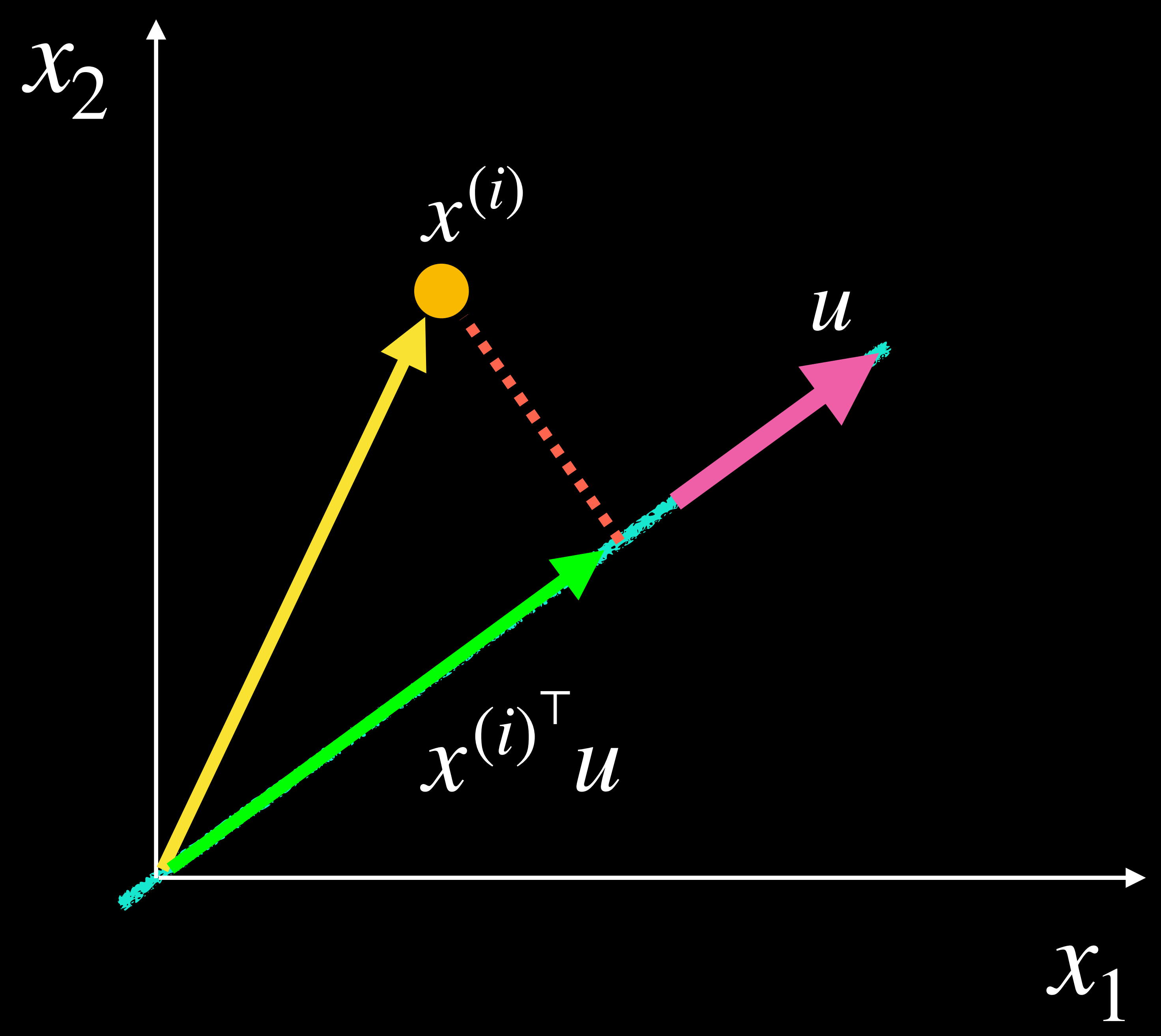
$\downarrow$

$$u_1, u_2, \ldots, u_d \in \mathbb{R}^d$$

$$\lambda_1, \lambda_2, \ldots, \lambda_d \in \mathbb{R}$$

```
# Compute the covariance matrix
Sigma = X_centered.T @ X_centered

# Find eigenvalues and eigenvectors of the covariance matrix
eigenvalues, eigenvectors = np.linalg.eig(Sigma)
```



Dataset

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...	...

Projection to k dimensions

$$y^{(i)} = \begin{bmatrix} u_1^\top x^{(i)} \\ u_2^\top x^{(i)} \\ \vdots \\ u_k^\top x^{(i)} \end{bmatrix} \in \mathbb{R}^k$$

Principal Component Analysis

To Maximize Variance of Projections

Solve

$$\boxed{\Sigma u = \lambda u}$$

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$x \in R^d$

$\Sigma \in \mathbb{R}^{d \times d}$

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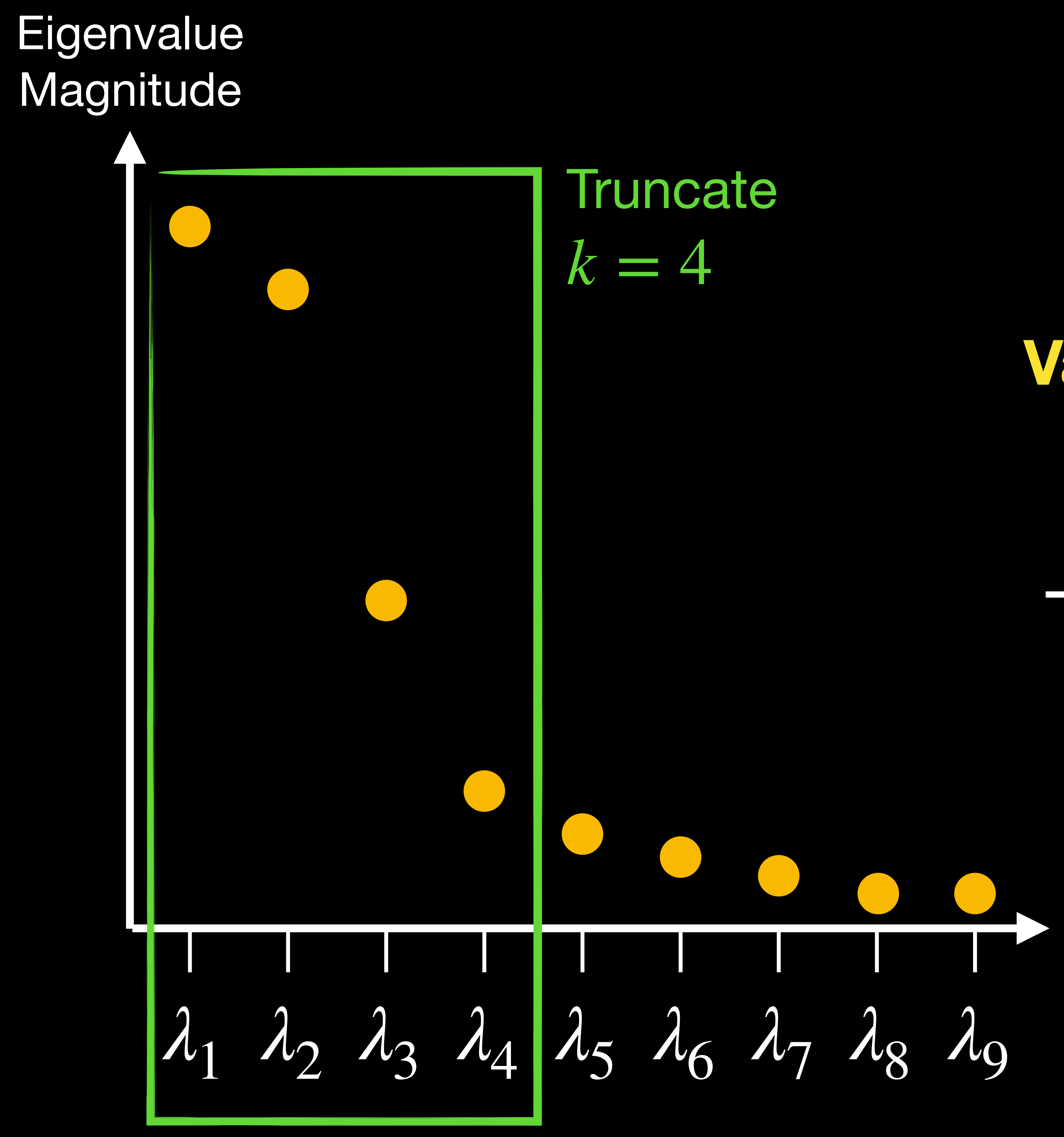


Percentage of Variance Preserved

$$\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i} \times 100$$

What are the dimensions of x, Σ and u in this case?

Principal Component Analysis

Typically, eigenvalues and eigenvectors

Solve

$$\Sigma v = \lambda v$$

naming eigenvectors v

More efficient $\longrightarrow$

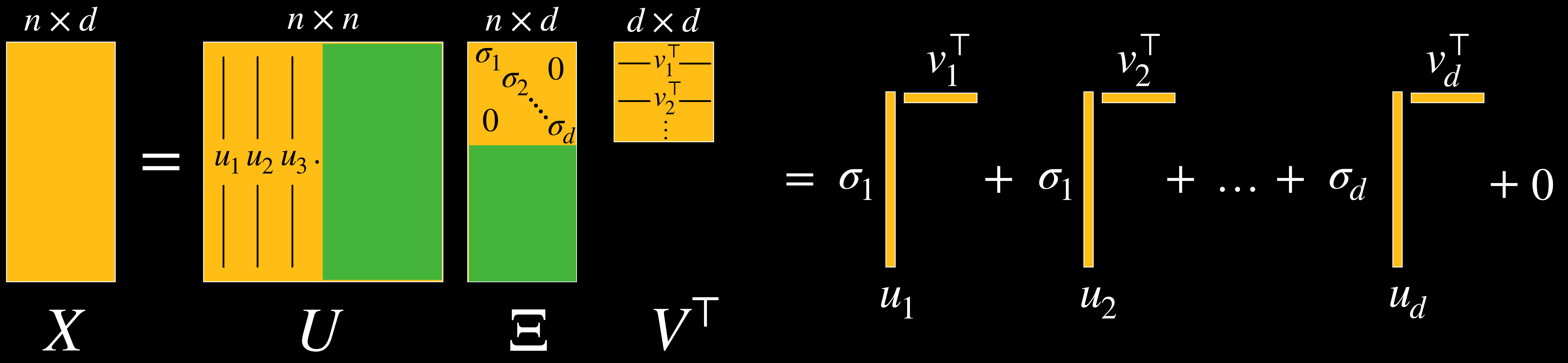
Solve

$$X = U \Xi V^\top$$

Singular Value Decomposition

U and V are unary

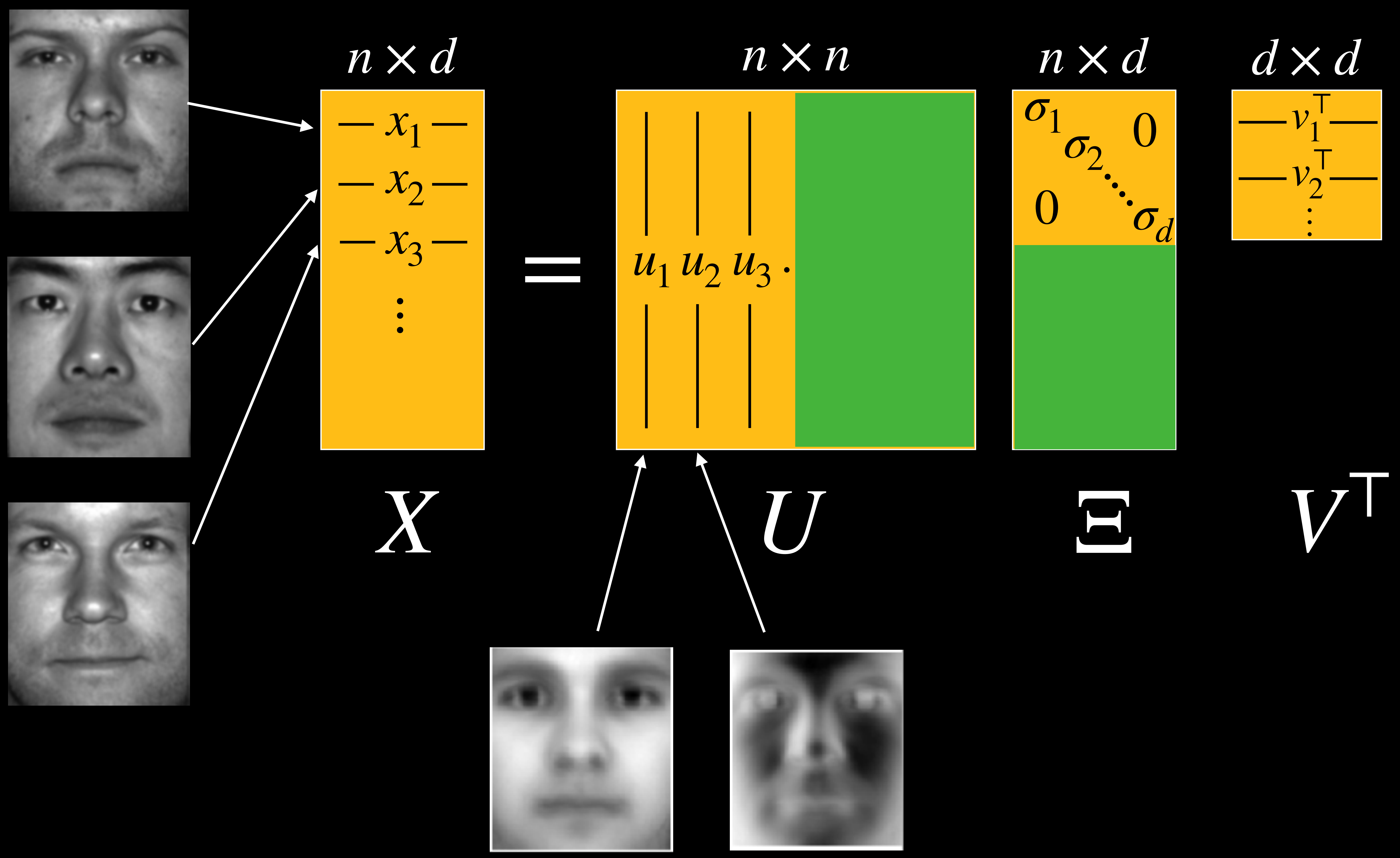
$$U^T U = U U^T = I$$
$$V^T V = V V^T = I$$



Singular Value Decomposition

$$X = U\Xi V^{\top}$$

A Dataset of Faces



“Eigen-faces”

U and V are unary

$$U^T U = UU^T = I$$
$$V^T V = VV^T = I$$