# Normal Distribution Covariance Matrix

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# Covariance
## Definition

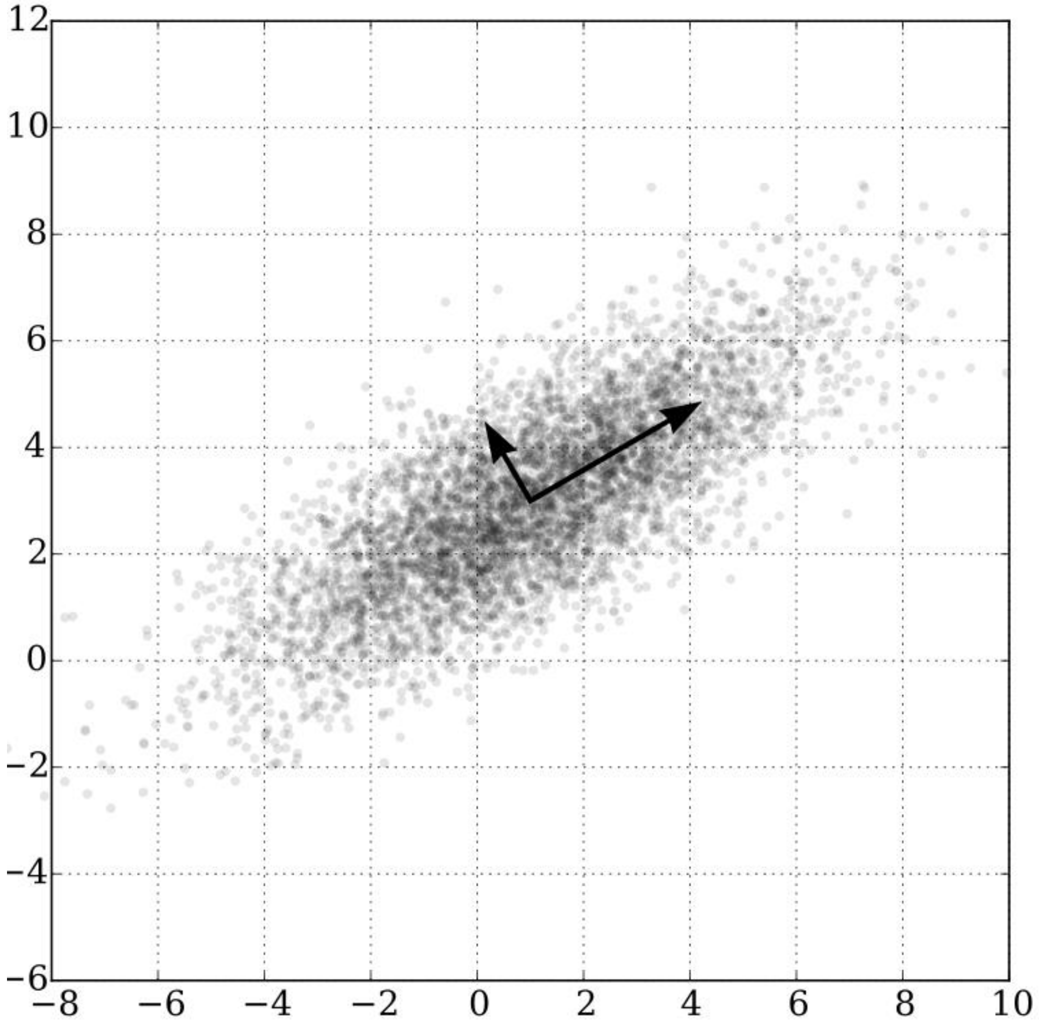
- Let $\boldsymbol{x} = (x_1 \quad x_2 \quad \cdots \quad x_n)^T$ be a random vector

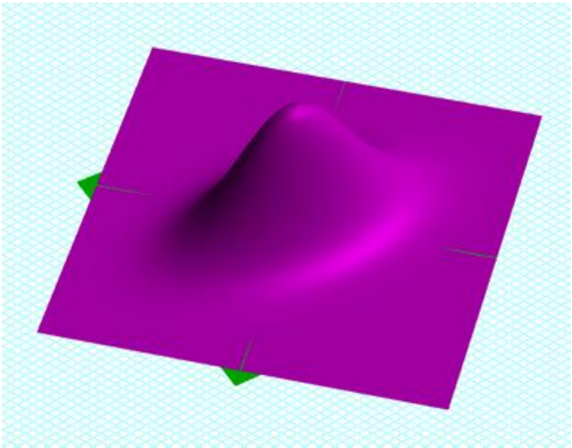
- We measure the coupling of the pair $x_i, x_j$ by the Covariance
$$\mathrm{Cov}(x_i, x_j) = E_x\left[(x_i - \overline{x_i})\left(x_j - \overline{x_j}\right)\right] \underset{\uparrow}{=} E_x[x_i x_j]$$
zero mean

- $\mathrm{Cov}(\boldsymbol{x}) = E_x[(\boldsymbol{x} - \overline{\boldsymbol{x}})(\boldsymbol{x} - \overline{\boldsymbol{x}})^T]$
$$= E[\boldsymbol{x} \cdot \boldsymbol{x}^T] - \overline{\boldsymbol{x}} \cdot \overline{\boldsymbol{x}}^T$$

$$\Sigma = \begin{bmatrix} \sigma_{11}^2 & E(x_1 x_2) & \cdots & \\ E(x_2 x_1) & \sigma_{22}^2 & & \\ \vdots & & \ddots & \\ & & & \sigma_{nn}^2 \end{bmatrix}$$

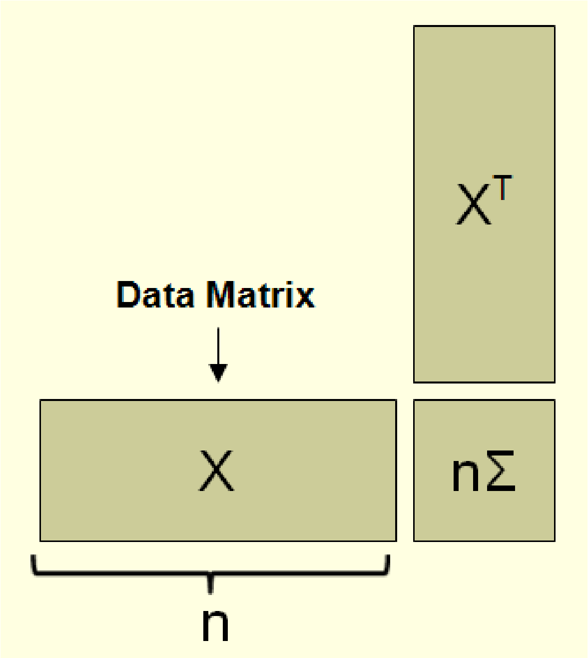
# Covariance
## Estimation



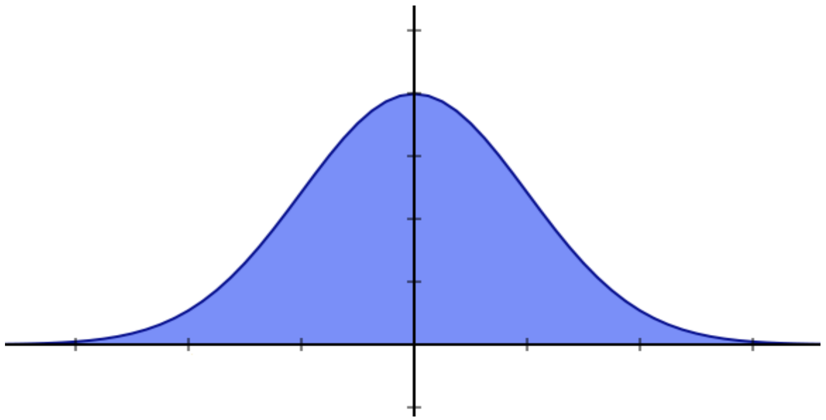



# Covariance
## Estimation

- $\Sigma = \frac{1}{n} X X^T$ is used as an approximation
  - $\Sigma = \frac{1}{n-1} X X^T$ may be better
- $\Sigma$ is symmetric and positive semidefinite
  - $v^T (X X^T) v = (X^T v)^T X^T v = \|X^T v\|^2 \geq 0$
- Every symmetric positive semidefinite matrix $\Sigma$ is a legal covariance matrix and can be expressed as $\Sigma = X X^T$



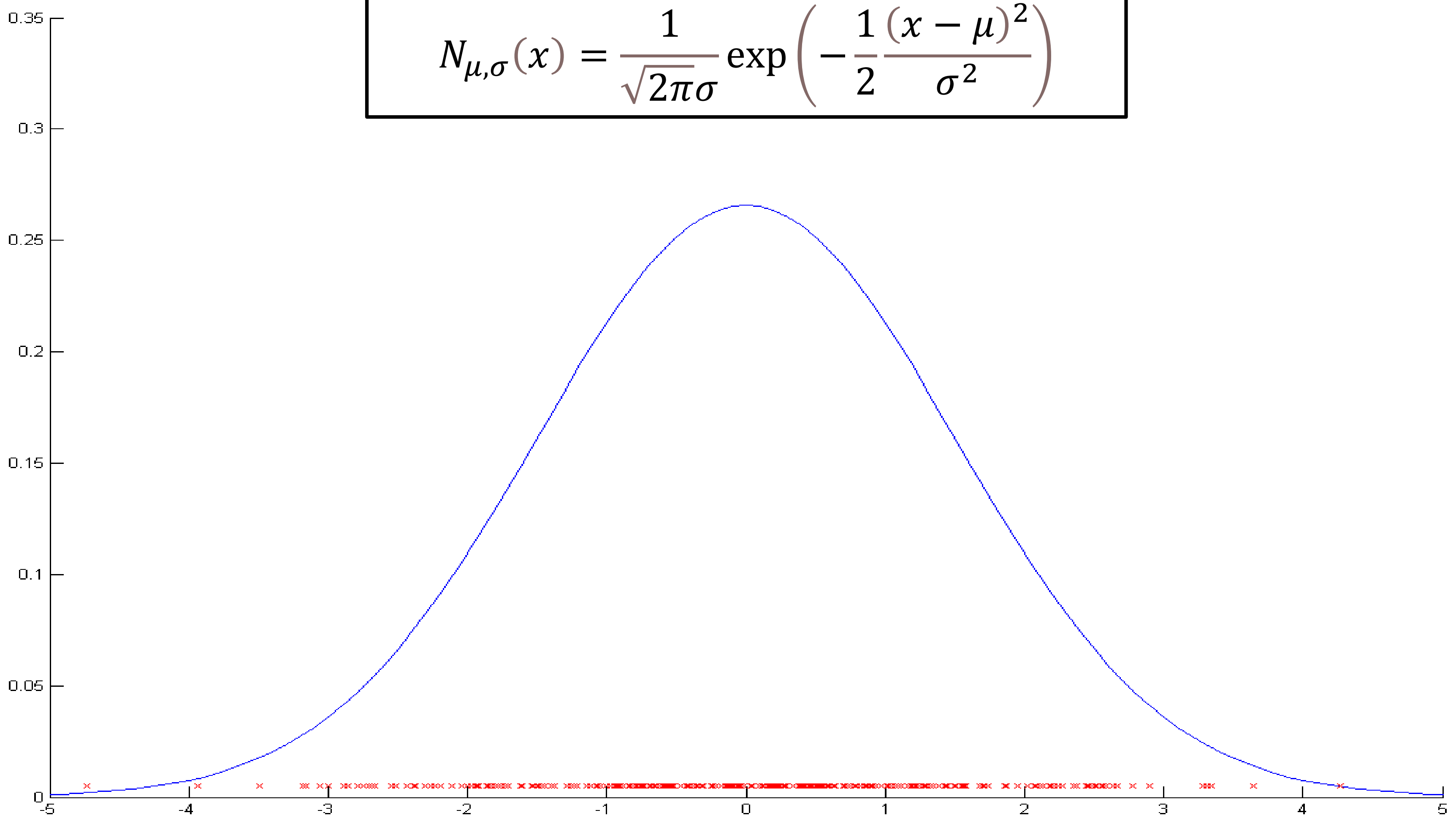
# Normal Distribution
## Overview



- The most prominent probability distribution
- Very tractable analytically
- Central limit theorem
  - The sum of many independent random variables has normal distribution
- In practice many observed random variables have bell shaped density function

# Normal Distribution
## 1D Gaussian

$$N_{\mu,\sigma}(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right)$$



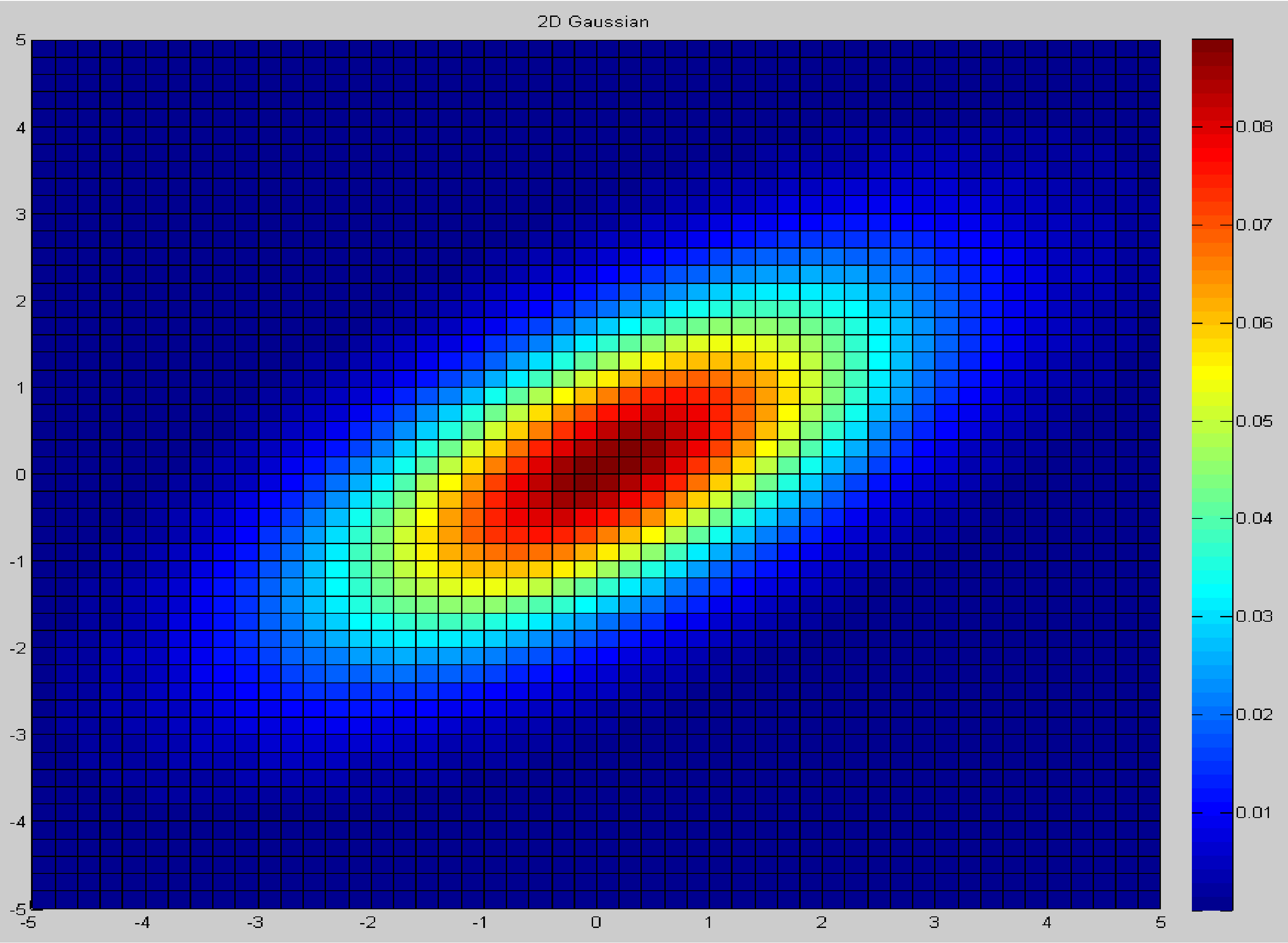
# Normal Distribution
## General Gaussian

- Given $\mu \in M_{n\times 1}$ and $\Sigma \in M_{n\times n}$ the PDF is given by:

$$\boxed{N_{\mu,\Sigma}(z) = \frac{1}{\sqrt{(2\pi)^n|\Sigma|}} \exp\left(-\frac{1}{2}(z-\mu)^T\Sigma^{-1}(z-\mu)\right)}$$

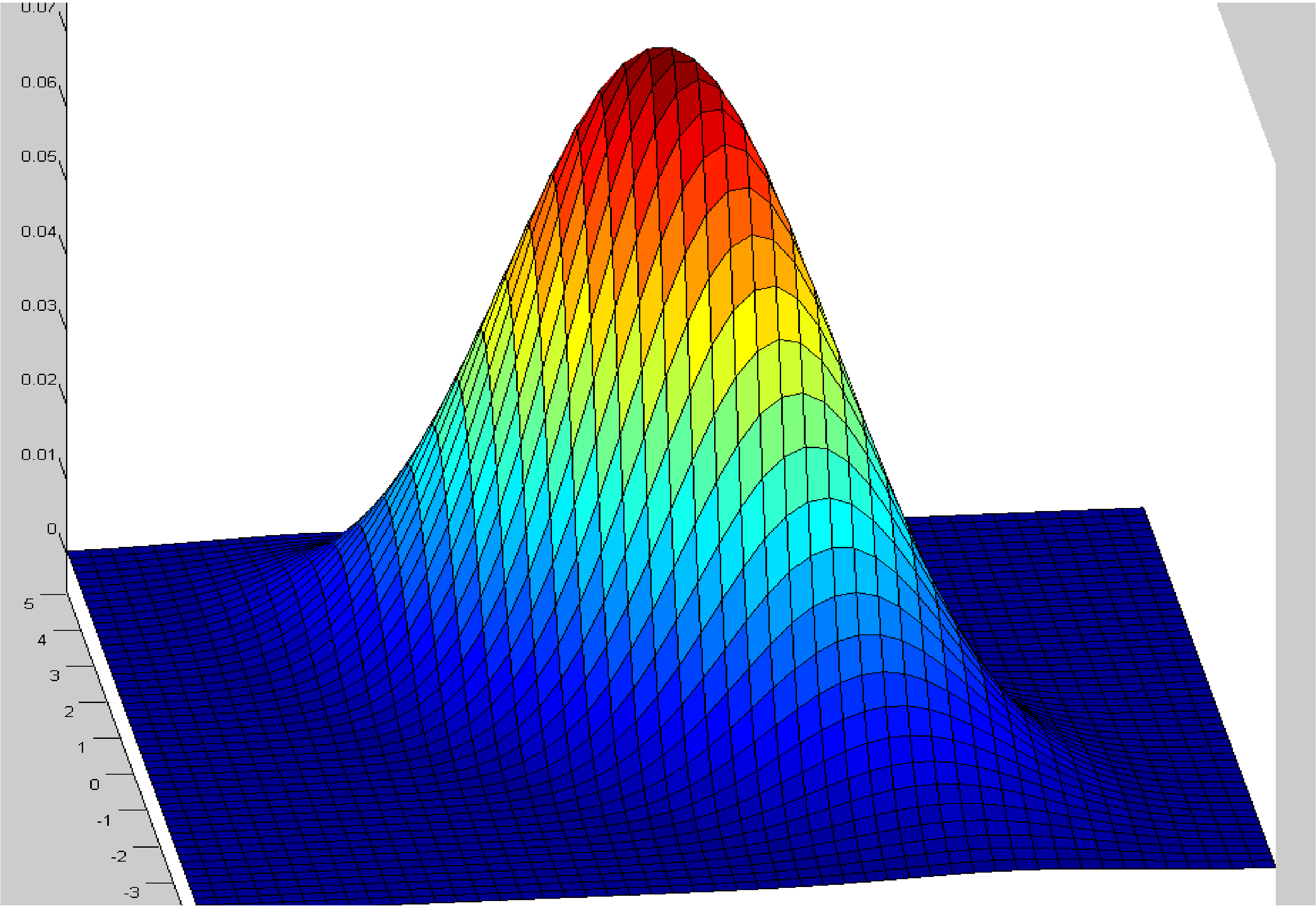
- Visualization in higher dimensions
  (especially higher than 3) is more challenging

# Gaussian 2D



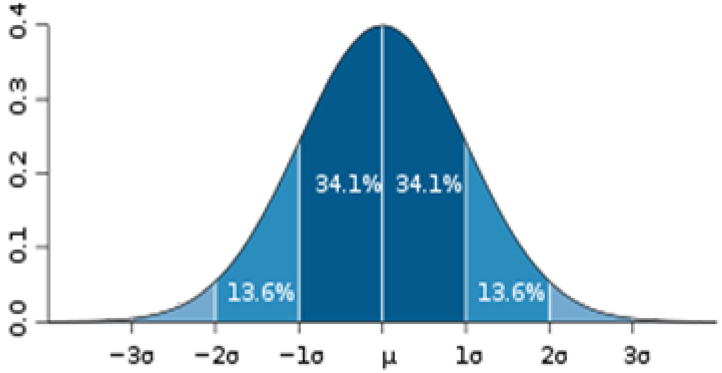
2D Gaussian
5
4
3
2
1
0
-1
-2
-3
-4
-5
-5
-4
-3
-2
-1
0
1
2
3
4
5
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01

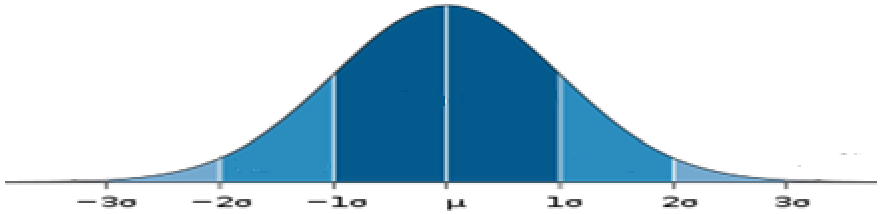
# Gaussian 2D



# Mahalanobis Distance

- Mahalanobis distance: $r = \dfrac{|x-\mu|}{\sigma}$
- 68-95-99.7 rule:




- For general dimensions: $r^2 = (z-\mu)^T\Sigma^{-1}(z-\mu)$ $\qquad \|z-\mu\|_\Sigma^2$

- Intuitively, measures the distance from the mean in standard deviation units.

# Cholesky Decomposition

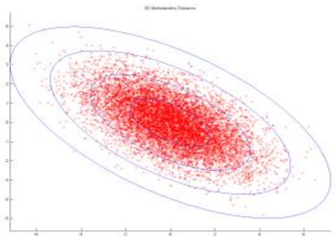
- $\Sigma = C^T C$ is the Cholesky decomposition of $\Sigma$ if $C$ is upper triangular
  - Every symmetric positive semidefinite matrix has a Cholesky decomposition.

- The locus of points with Mahalanobis distance $r$ is $\boxed{\left\{ rC^T u \middle| \|u\| = 1 \right\}}$

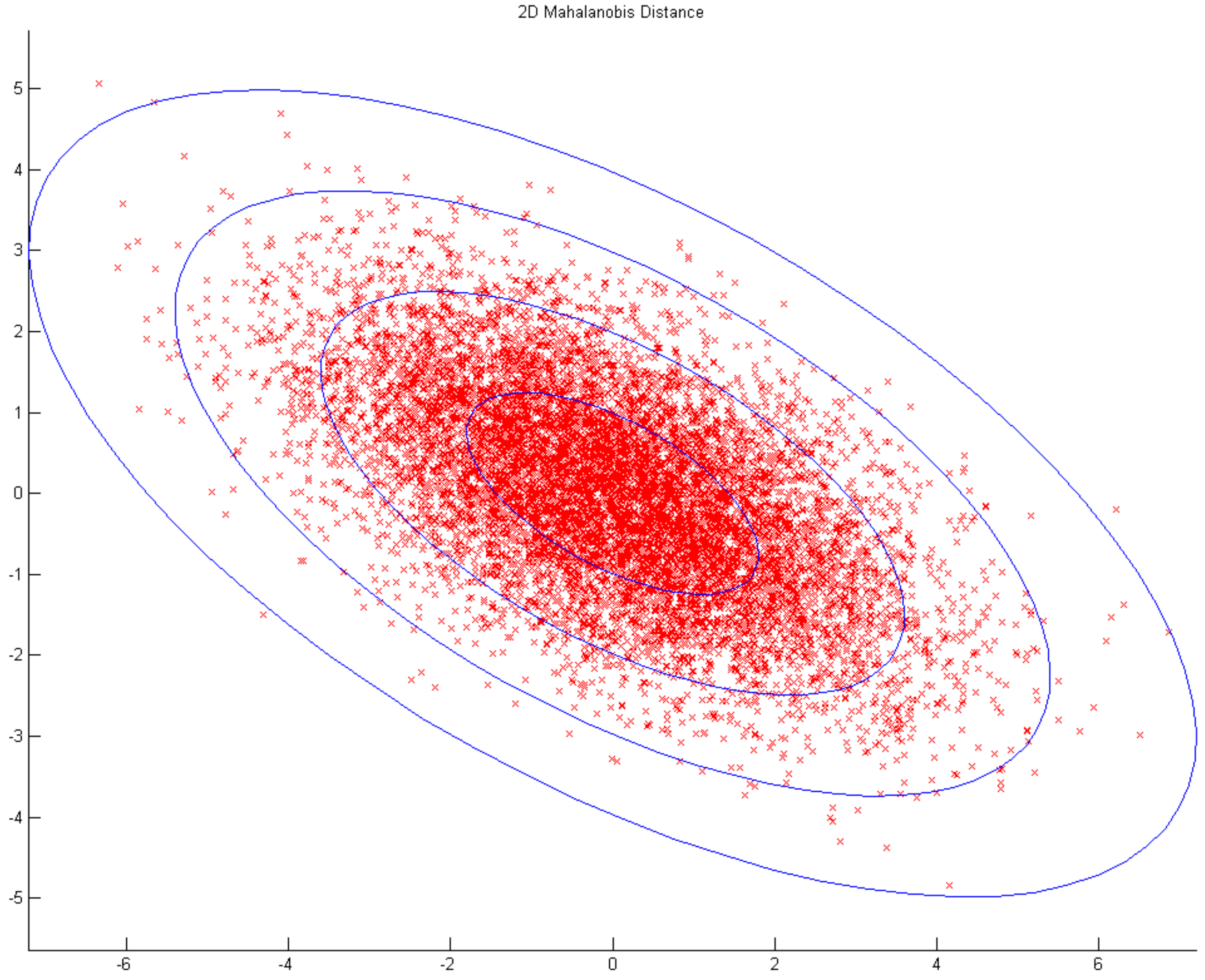
$$(rC^T u)^T \Sigma^{-1} (rC^T u) = r^2 u^T C (C^{-1} C^{-T}) C^T u = r^2 u^T u = r^2$$

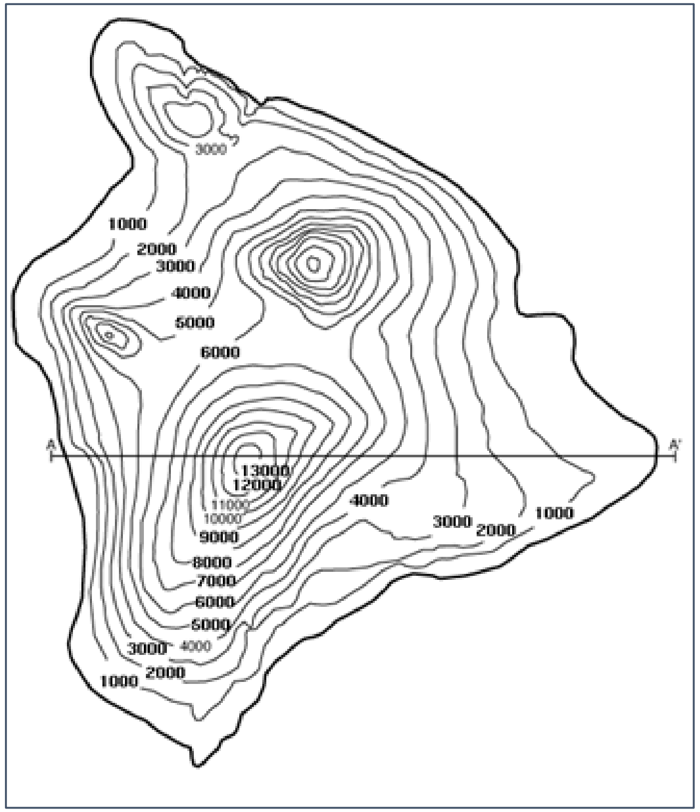
$\boxed{\Sigma^{-1} = C^{-1} C^{-T}}$

- Used as an intuitive visualization of the covariance matrix.



# Mahalanobis Distance
## Gaussian 2D Visualization

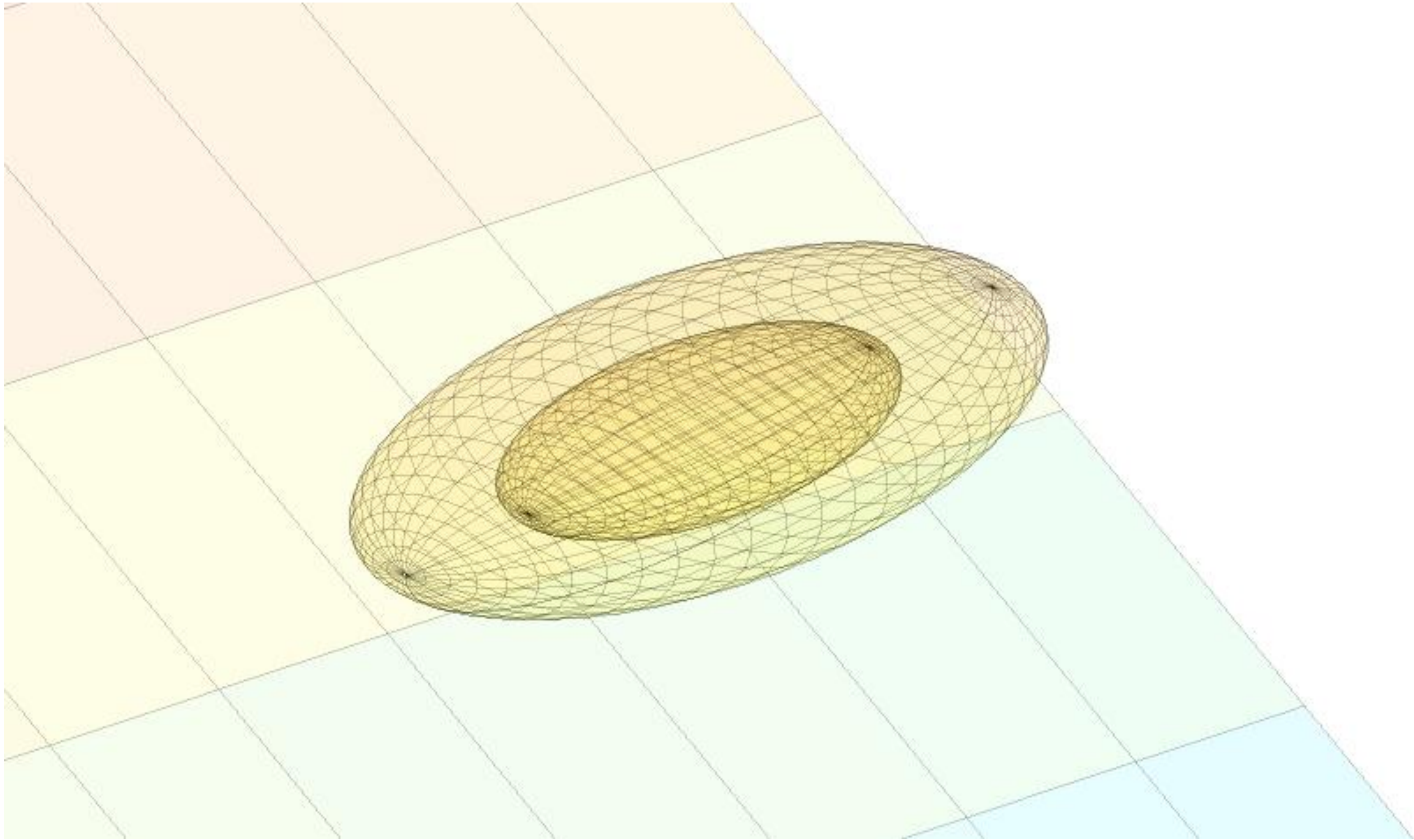


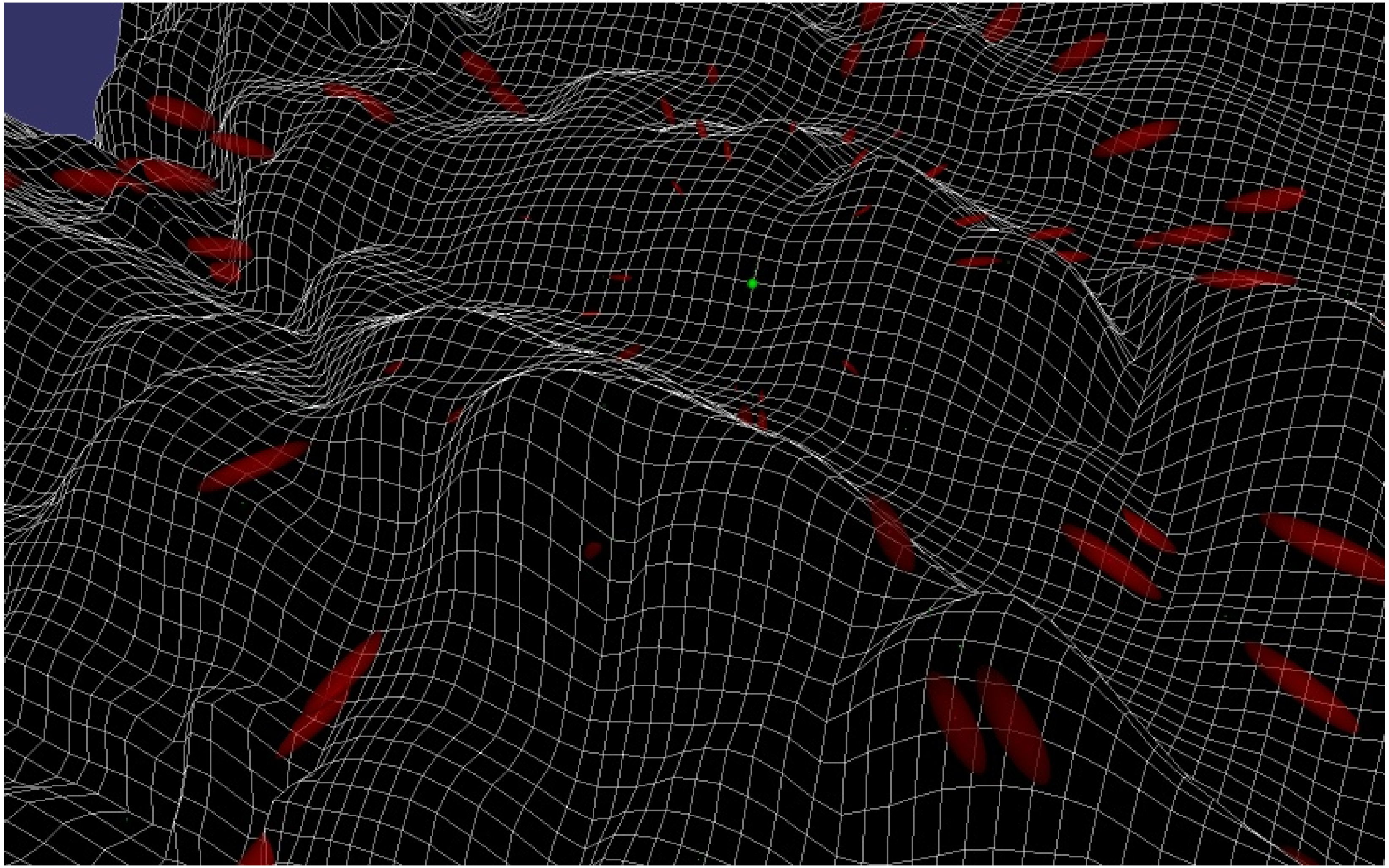

Courtesy of GIS3015 Map Blog Andrea Davis

# Mahalanobis Distance

## Gaussian 3D Visualization

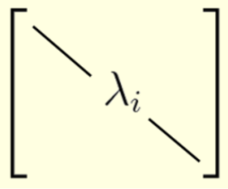


# Gaussian 3D Visualization

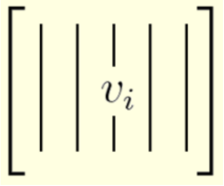


# SVD
## Singular Value Decomposition

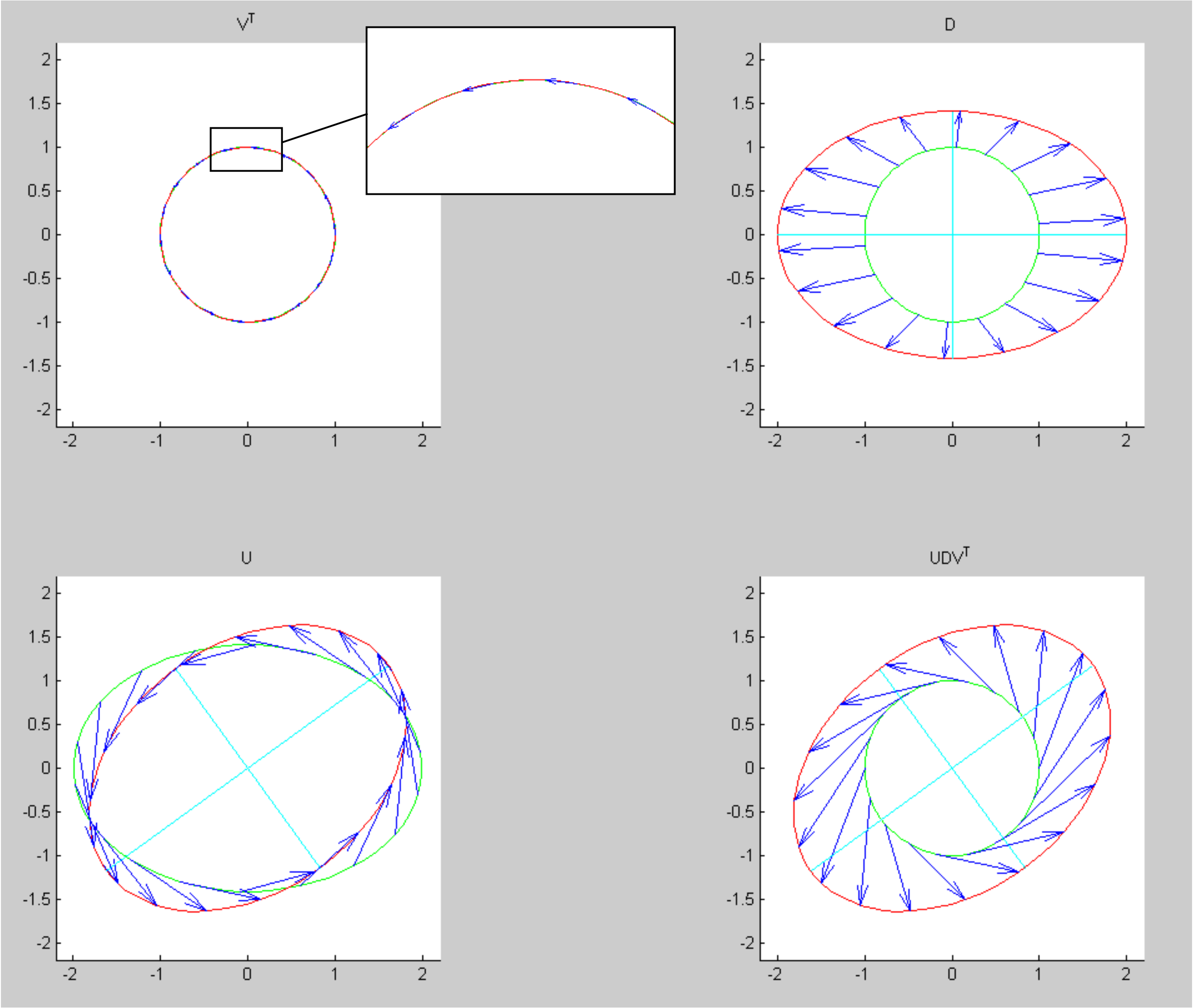
- $A = UDV^T$ is the SVD of $A$ if:
  - $U \in M_{m\times m}$ Orthonormal $(U^TU = I_{m\times m})$
  - $V \in M_{n\times n}$ Orthonormal $(V^TV = I_{n\times n})$
  - $D \in M_{m\times n}$ Diagonal with non-negative entries ordered in descending order.
- $D$ diagonal entries are:
  - called **singular values** of $A$
  - square root of the **eigenvalues** of $A^TA$




- $V$ columns are the **eigenvectors** of $A^TA$



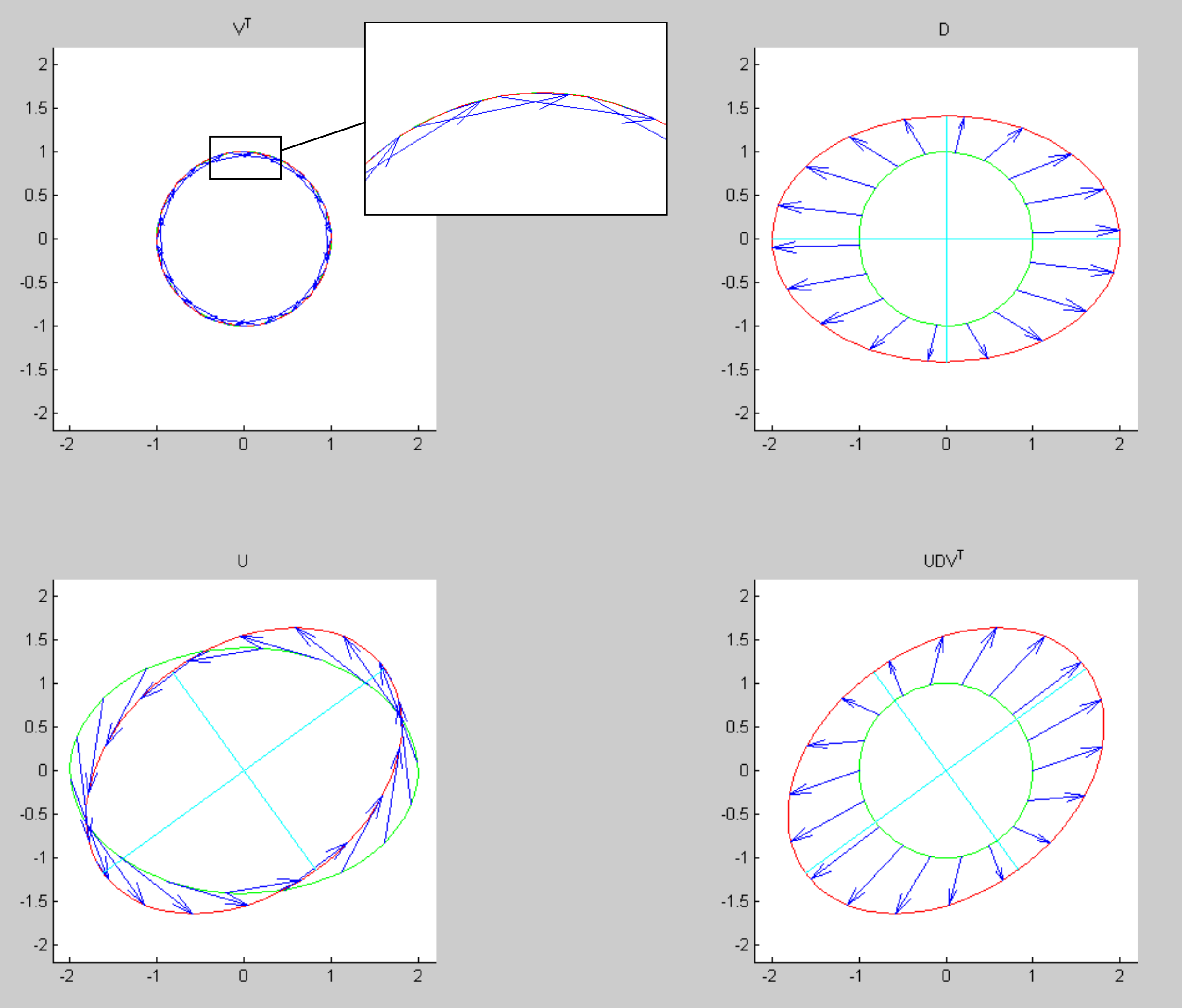
# SVD: $A = UDV^T$



# Covariance
## SVD

- Covariance matrix SVD properties
  - $\Sigma\ = UDU^T$ (i.e. $V = U$)
  - Since $\Sigma$ is symmetric (hermitian) the spectral theorem holds
  - $\Sigma = XX^T = (USV^T)(USV^T)^T = USV^TVSU^T = US^2U^T$
- $D$ diagonal entries are the eigenvalues of $\Sigma$
- $U$ columns are the eigenvectors of $\Sigma$

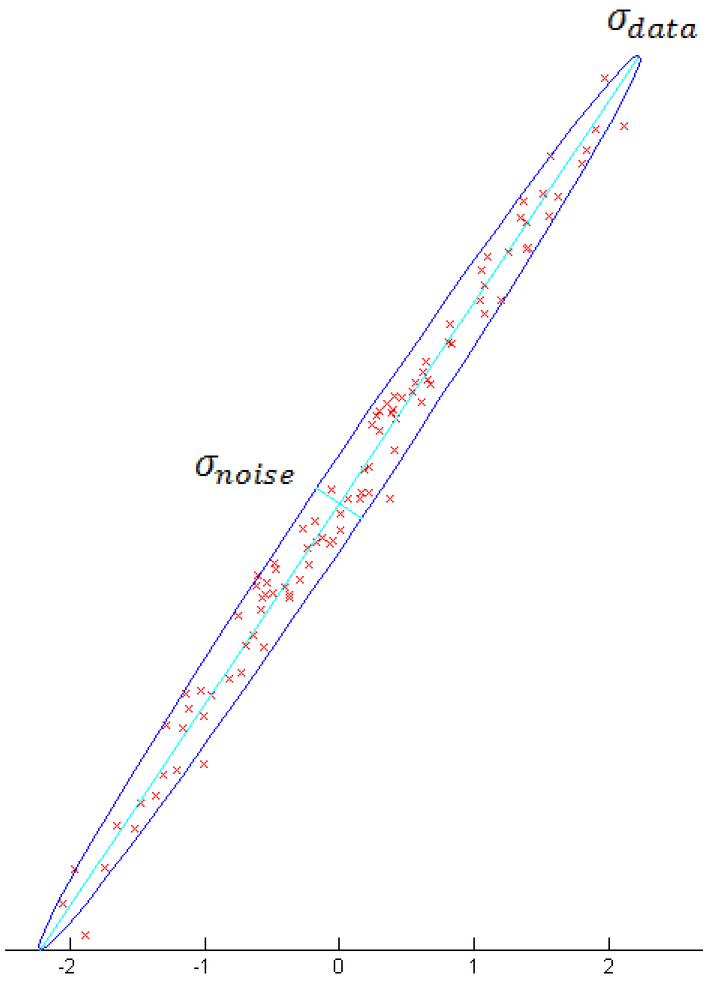
# SVD
## Covariance Matrix

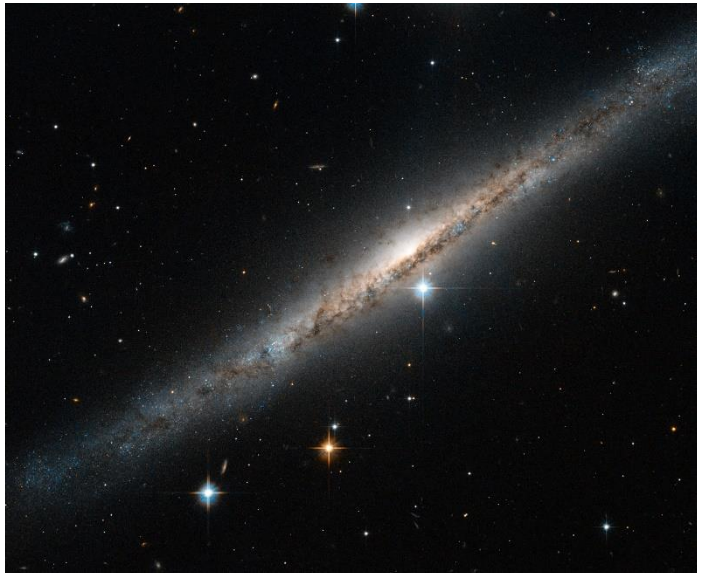


# Covariance
## Semantics

- How can we recognize the directions with small variance?

- How can we remove the noise from the data?



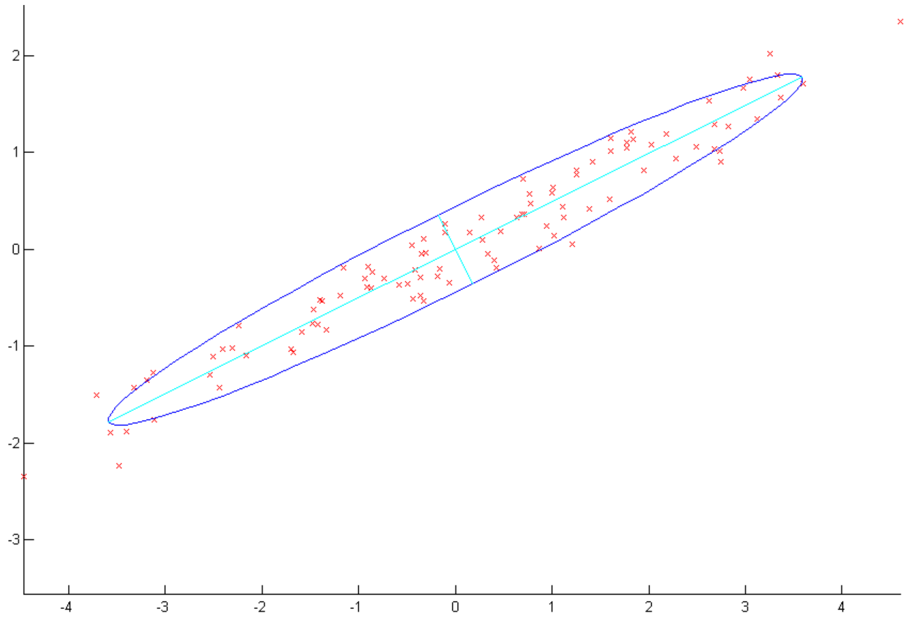



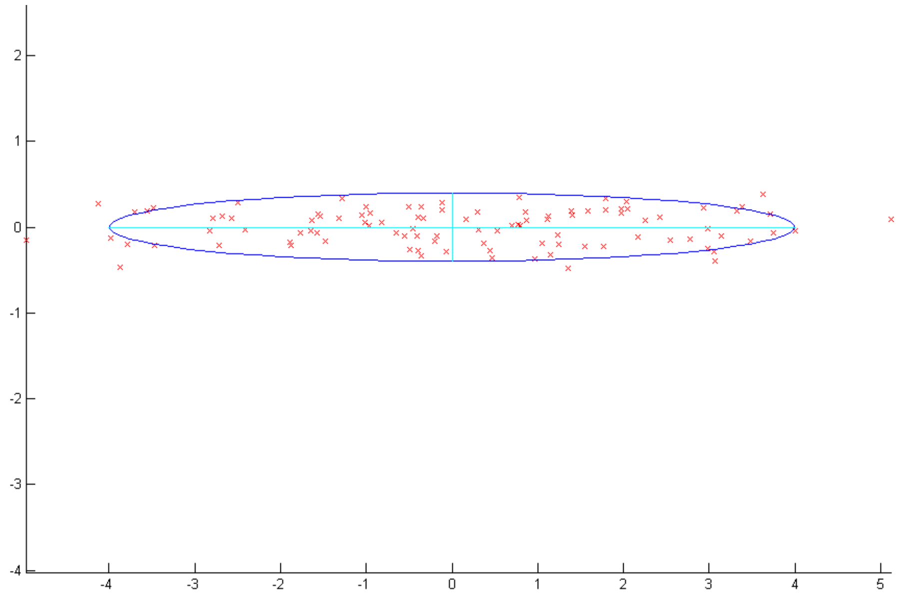
Courtesy of ESA/Hubble & NASA

# Covariance
## Principal Components

- $\frac{1}{n} X X^T = \Sigma = U D U^T \quad \rightarrow \quad nD = (U^T X)(U^T X)^T$
  - $U^T X$ is decorrelated.
  - $D$ diagonal holds the variance of $U^T X$ on each axis.
  - $U$ columns are called the *principal components* of $X$

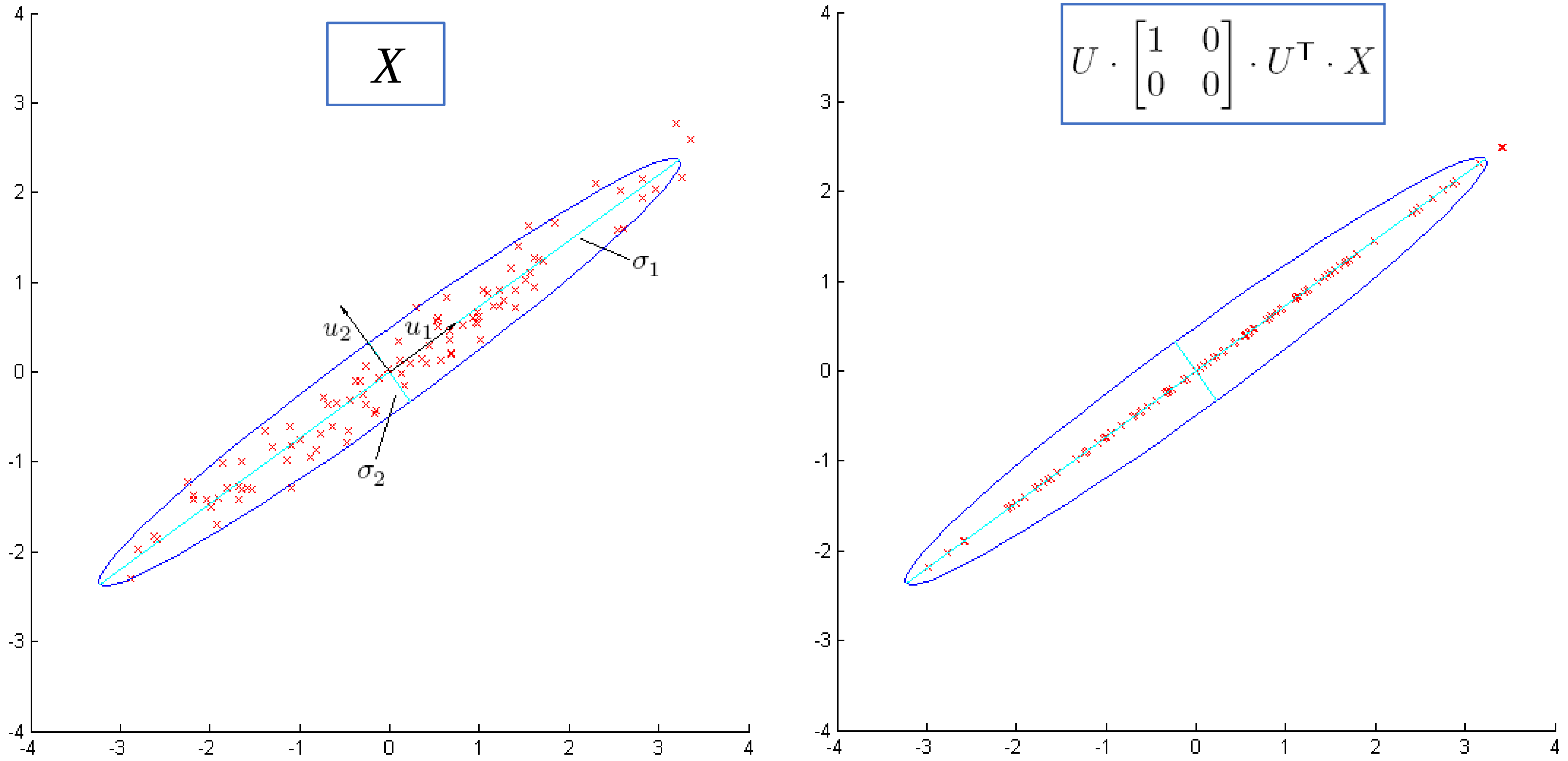
$\boxed{X} \longrightarrow \boxed{U^T X}$



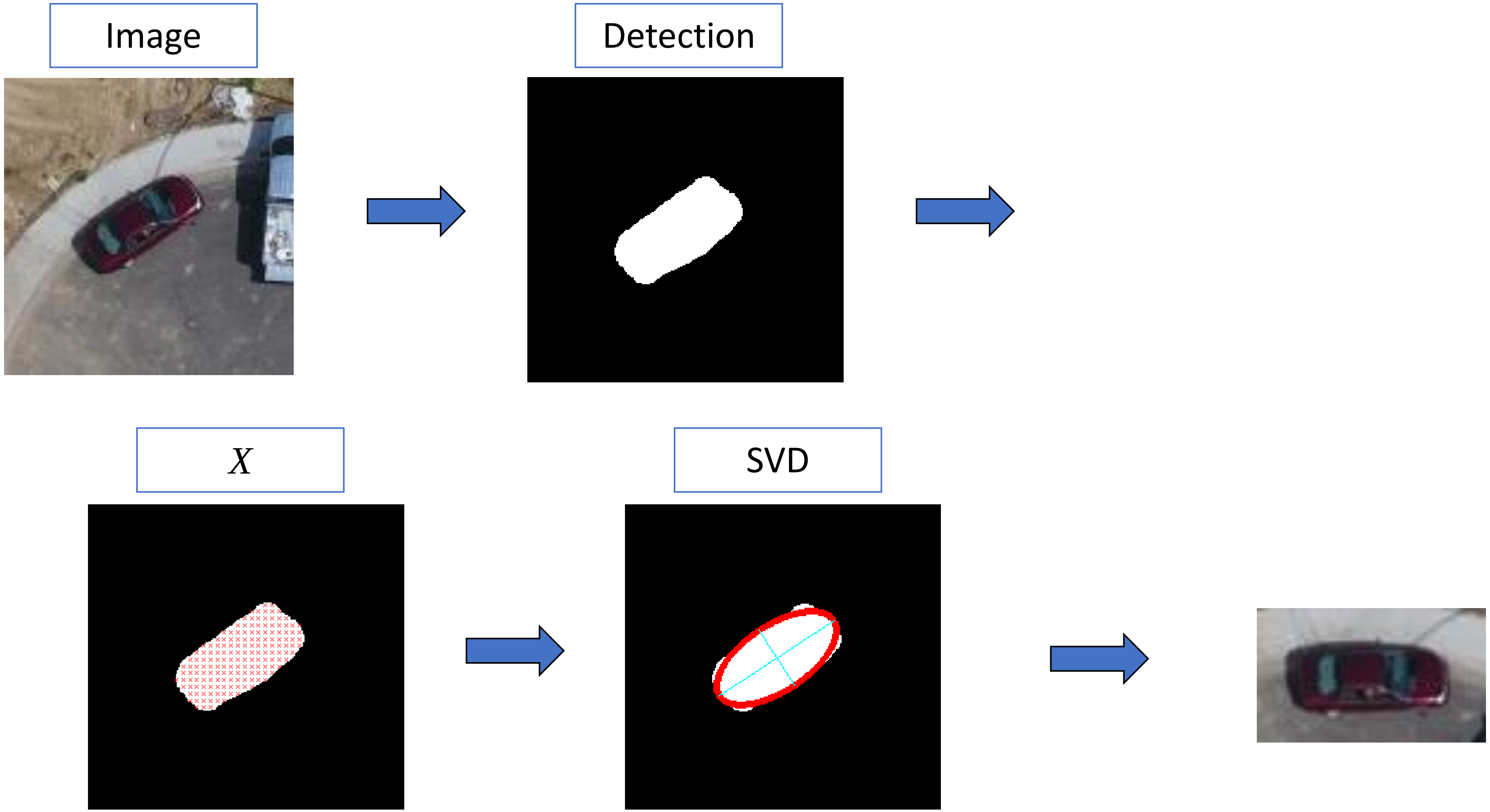



# Covariance
## Principal Components

- $\frac{1}{n}XX^T = \Sigma = UDU^T = \begin{bmatrix} | & | \\ u_1 & u_2 \\ | & | \end{bmatrix} \cdot \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix} \cdot \begin{bmatrix} — u_1 — \\ — u_2 — \end{bmatrix}$



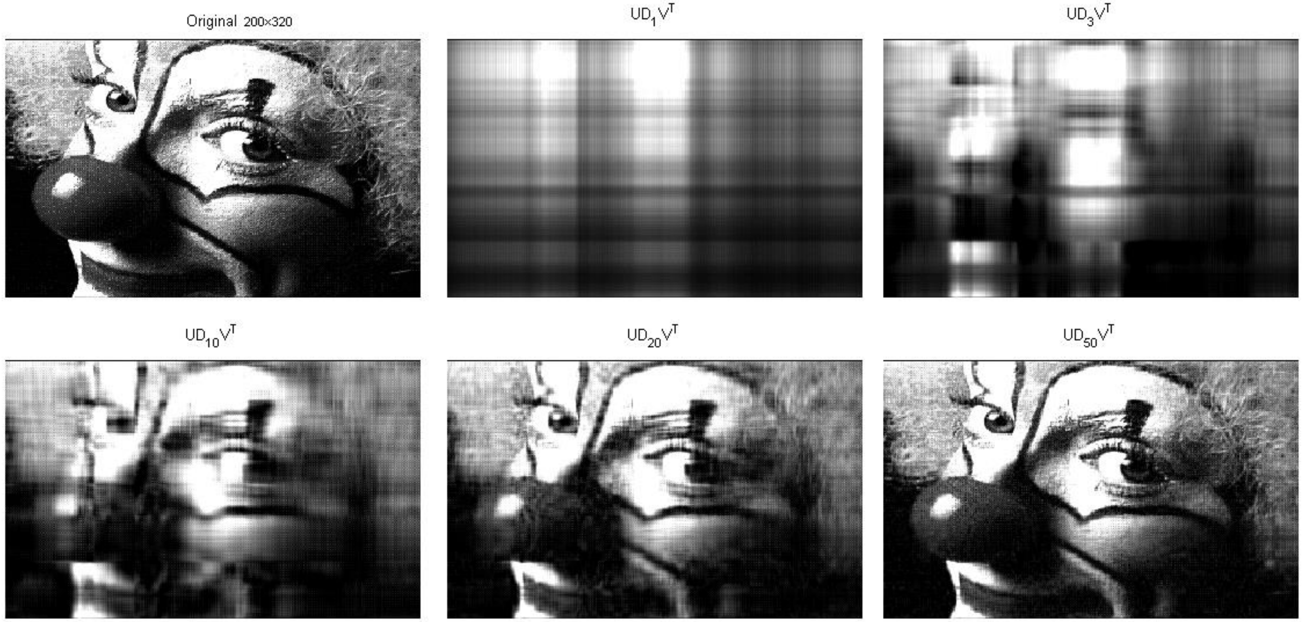
# **Covariance**
# Principal Components



# Matrix rank reduction

- Given SVD $X = UDV^T$
  - The rank $k<n$ matrix that is closest (in norm) to $X$

is $X_k = UD_kV^T$ with $D_k = \begin{bmatrix} \lambda_1 & & & & & \\ & \ddots & & & & \\ & & \lambda_k & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{bmatrix}$



# 2D Covariance