COMP6237 Data Mining

Covariance, EVD, PCA & SVD

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Variance and Covariance

Random Variables and Expected Values

- Mathematicians talk variance (and covariance) in terms of *random variables* and *expected values*

- A random variable is a variable that takes on different values due to chance.

    - The set of sample values from a single dimension of a featurespace can be considered to be a random variable

- The expected value (denoted E[X]) is the most likely value a random variable will take.

    - If we **assume** that the values an element of a feature can take are all equally likely then expected value is thus just the **mean value**

Variance

$$\sigma^2(x) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

Variance (σ^2) is the mean squared difference from the mean (μ).

It's a measure of how spread-out the data is.

technically it's $E[(X - E[X])^2]$

Covariance

$$\sigma(x,y) = \frac{1}{n}\sum_{i=1}^{n}(x-\mu_x)(y-\mu_y)$$

Covariance ($\sigma(x,y)$) measures how two variables change together

technically it's E[(x - E[x])(y-E[y])]

Covariance

$$\sigma(x,y) = \frac{1}{n}\sum_{i=1}^{n}(x-\mu_x)(y-\mu_y)$$

The variance is the covariance when the two variables are the same ($\sigma(x,x)=\sigma^2(x)$)

Covariance

$$\sigma(x,y) = \frac{1}{n}\sum_{i=1}^{n}(x-\mu_x)(y-\mu_y)$$

A covariance of 0 means the variables are uncorrelated

(Covariance is related to Correlation… see notes)

Covariance Matrix

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma(X_1, X_1) & \sigma(X_1, X_2) & \dots & \sigma(X_1, X_n) \\ \sigma(X_2, X_1) & \sigma(X_2, X_2) & \dots & \sigma(X_2, X_n) \\ \vdots & \vdots & \ddots & \vdots \\ \sigma(X_n, X_1) & \sigma(X_n, X_2) & \dots & \sigma(X_n, X_n) \end{bmatrix}$$

A covariance matrix encodes how all possible pairs of dimensions in an *n*-dimensional dataset vary together

Covariance Matrix

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma(X_1, X_1) & \sigma(X_1, X_2) & \dots & \sigma(X_1, X_n) \\ \sigma(X_2, X_1) & \sigma(X_2, X_2) & \dots & \sigma(X_2, X_n) \\ \vdots & \vdots & \ddots & \vdots \\ \sigma(X_n, X_1) & \sigma(X_n, X_2) & \dots & \sigma(X_n, X_n) \end{bmatrix}$$

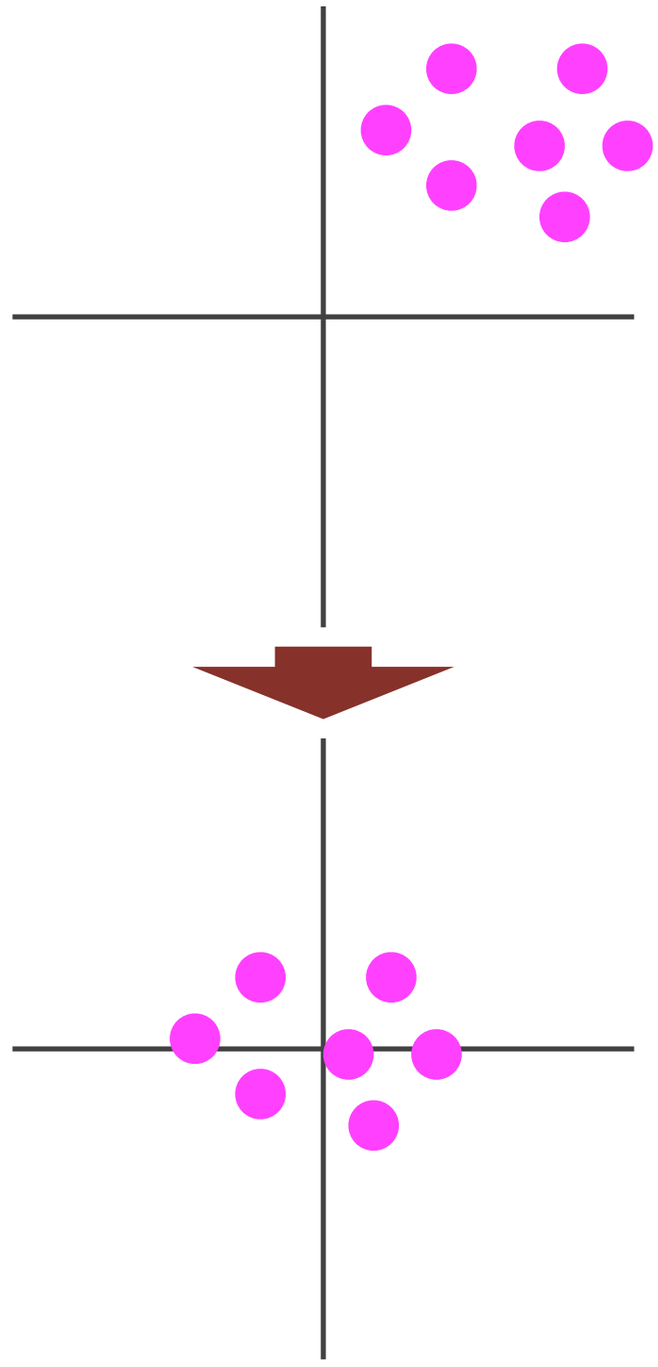
The covariance matrix is a **square symmetric matrix**

Demo: 2D covariance

Mean Centring

- Mean Centring is the process of computing the mean (across each dimension independently) of a set of vectors, and then subtracting the mean vector from every vector in the set.

- All the vectors will be translated so their average position is the origin



Covariance matrix again

$$\mathbf{Z} = \begin{bmatrix} v_{11} & v_{12} & v_{12} & \dots \\ v_{21} & v_{22} & v_{22} & \dots \\ v_{31} & v_{32} & v_{32} & \dots \\ v_{41} & v_{42} & v_{42} & \dots \end{bmatrix}$$

Each row is a **mean centred** featurevector

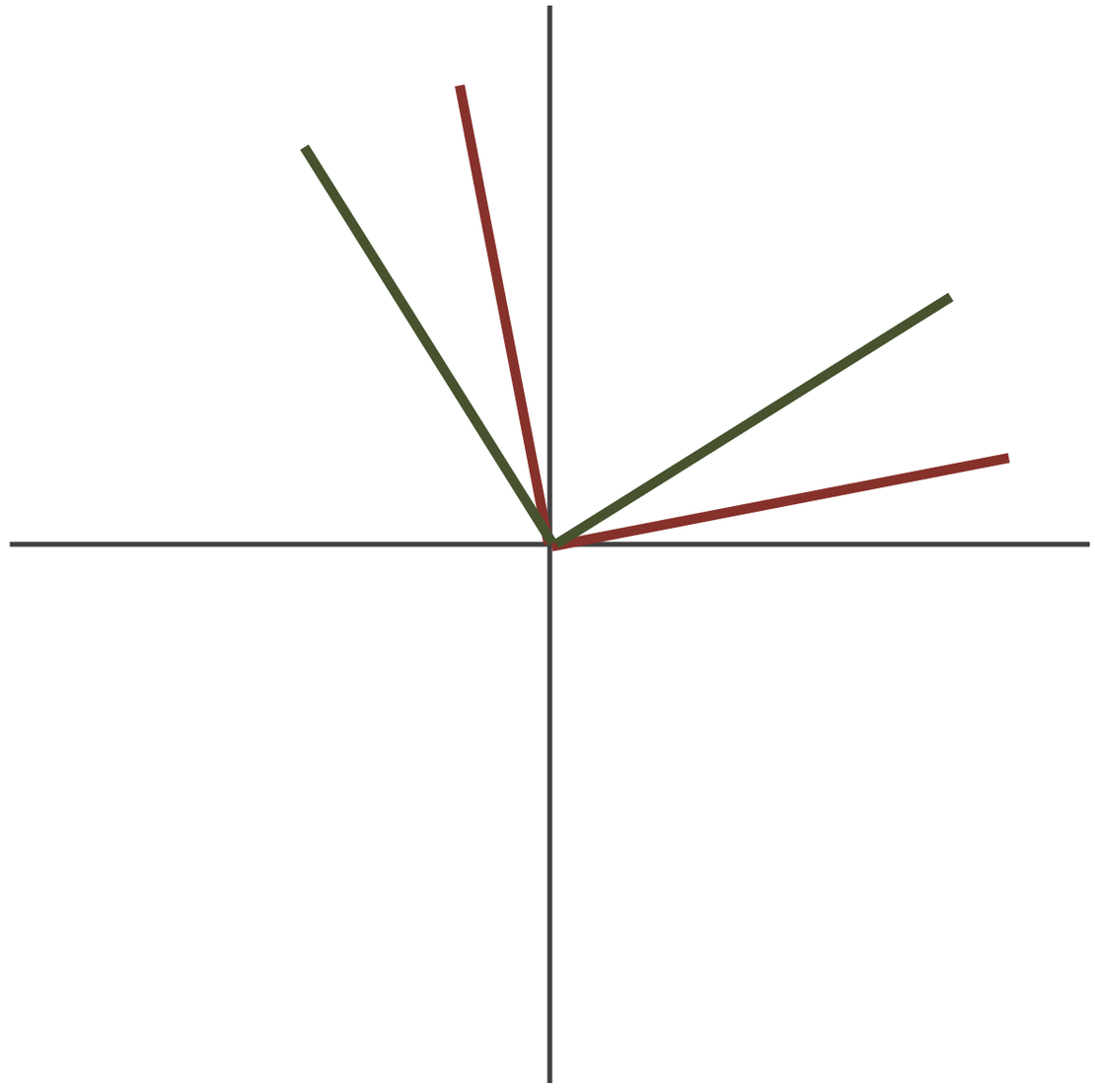
Then

$$\Sigma \propto \mathbf{Z}^T\mathbf{Z}$$

Principal axes of variation

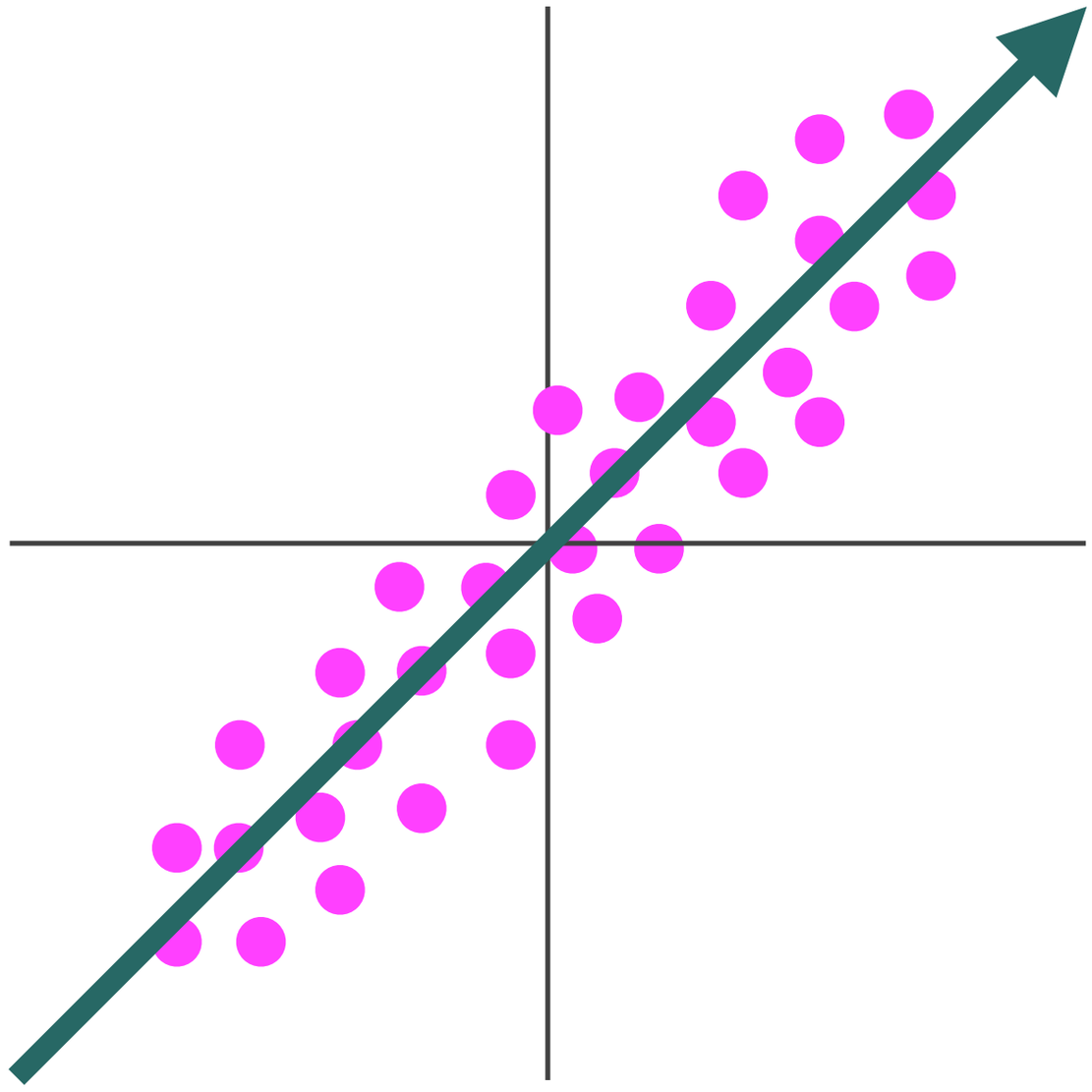
Basis

- A basis is a set of *n* **linearly independent** vectors in an *n* dimensional space
  - The vectors are **orthogonal**
  - They form a “coordinate system”
  - There are an infinite number of possible basis



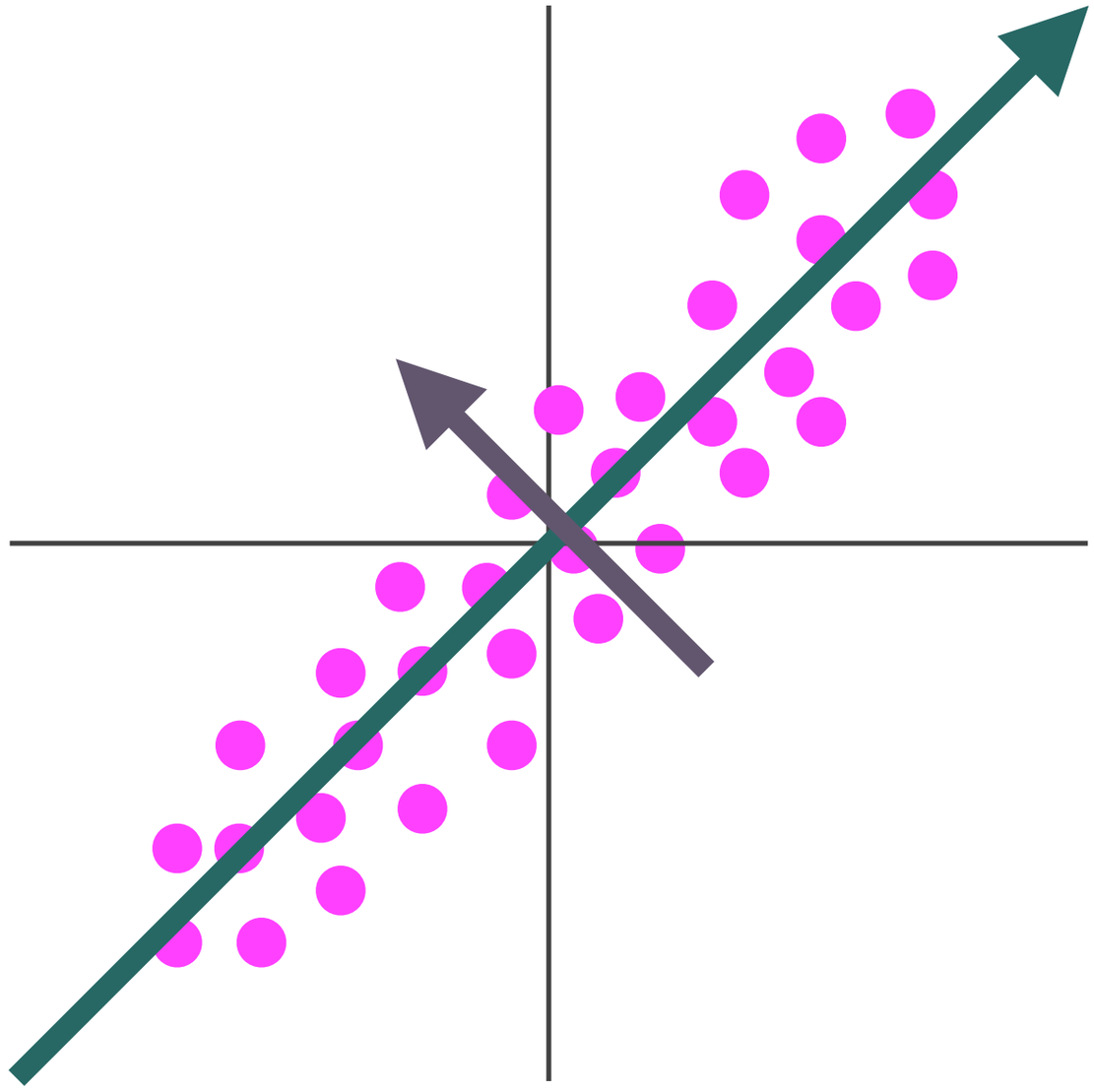
The first principal axis

- For a given set of *n* dimensional data, the ***first principle axis*** (or just ***principal axis***) is the vector that describes the direction of **greatest** variance.



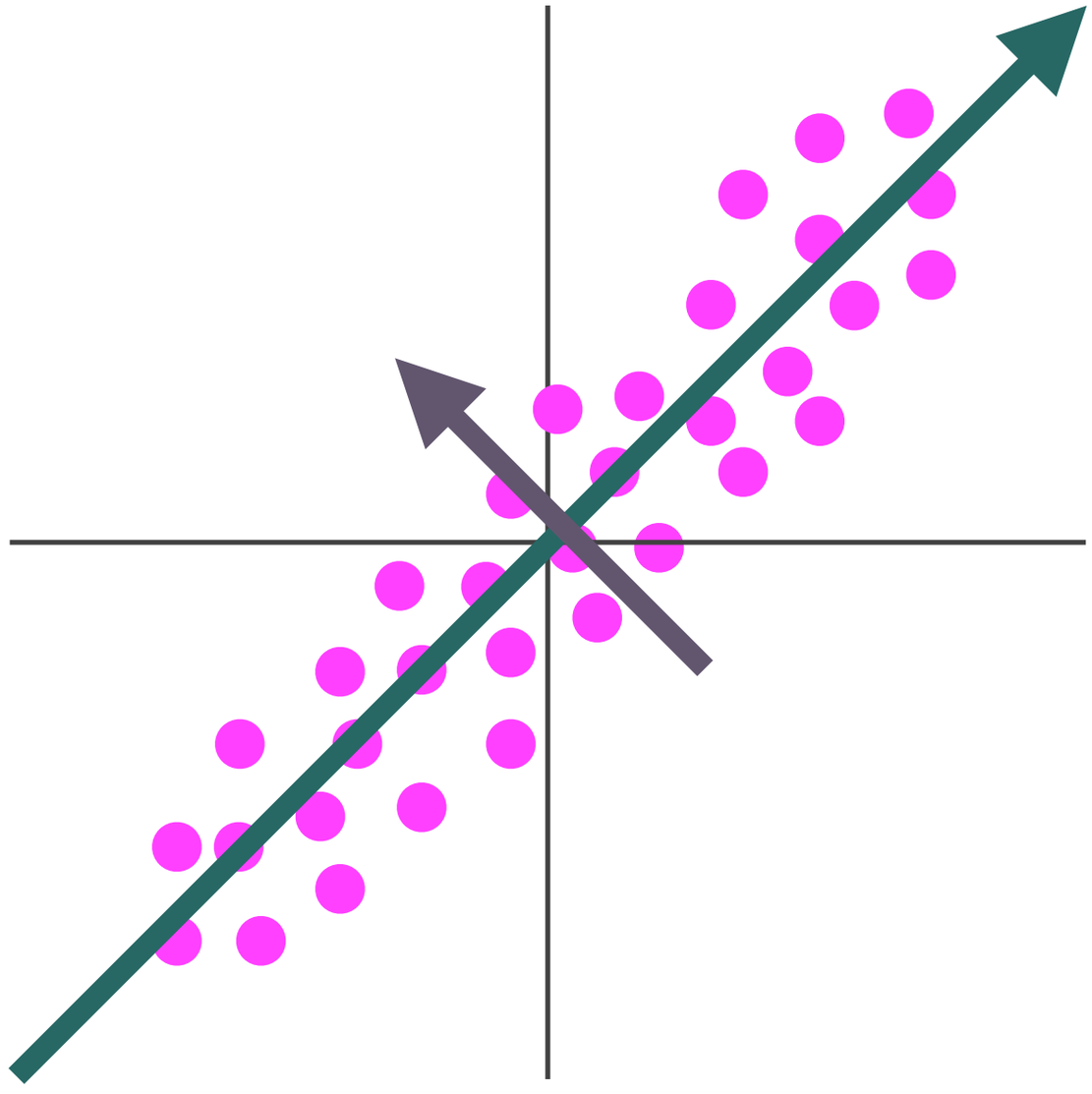
The second principal axis

- The **second principal axis** is a vector in the direction of greatest variance orthogonal (perpendicular) to the first major axis.



The third principal axis

- In a space with 3 or more dimensions, the third principal axis is the direction of greatest variance orthogonal to both the first and second principal axes.
  - The forth… … and so on…
- The set of *n* **principal axes** of an *n* dimensional space are a **basis**



Eigenvectors, Eigenvalues and Eigendecomposition

Eigenvectors and Eigenvalues

Very important equation!

$$\mathbf{A}v = \lambda v$$

Eigenvectors and Eigenvalues

a $n \times n$ square matrix

a scalar value, known as an **eigenvalue**

$$\mathbf{A}v = \lambda v$$

an n dimensional vector, known as an **eigenvector**

Eigenvectors and Eigenvalues

$$\mathbf{A}v = \lambda v$$

There are at most *n* eigenvector-eigenvalue pairs

If **A** is symmetric, then the set of eigenvectors is orthogonal

Can you see where this is going?

Eigenvectors and Eigenvalues

$$\mathbf{A}v = \lambda v$$

If **A** is a **covariance matrix**, then the eigenvectors are the **principal axes**.

The eigenvalues are proportional to the **variance** of the data along each eigenvector.

The eigenvector corresponding to the **largest** eigenvalue is the first P.C.

Finding the EVecs and EVals

- For small matrices ($n \leq 4$) there are algebraic solutions to finding all the eigenvector-eigenvalue pairs

- For larger matrices, numerical solutions to the **Eigendecomposition** must be sought.

Eigendecomposition (aka EVD)

columns of **Q** are the eigenvectors

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{-1}$$

diagonal eigenvalue matrix ($\mathbf{\Lambda}_{ii} = \lambda_i$)

Eigendecomposition

$$\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{-1}$$

If **A** is *real symmetric* (i.e. a covariance matrix), then $\mathbf{Q}^{-1} = \mathbf{Q}^{\mathrm{T}}$ (i.e. eigenvectors are orthogonal), so:

$$\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\mathrm{T}}$$

Eigendecomposition

In summary, the Eigendecomposition of a covariance matrix **A**:

$$\mathbf{A} = \mathbf{Q} \Lambda \mathbf{Q}^{\top}$$

Gives you the principal axes and their relative magnitudes

Ordering

- Standard Eigendecomposition implementations will order the eigenvectors (columns of $\mathbf{Q}$) such that the eigenvalues (in the diagonal of $\mathbf{\Lambda}$) are sorted in order of decreasing value.

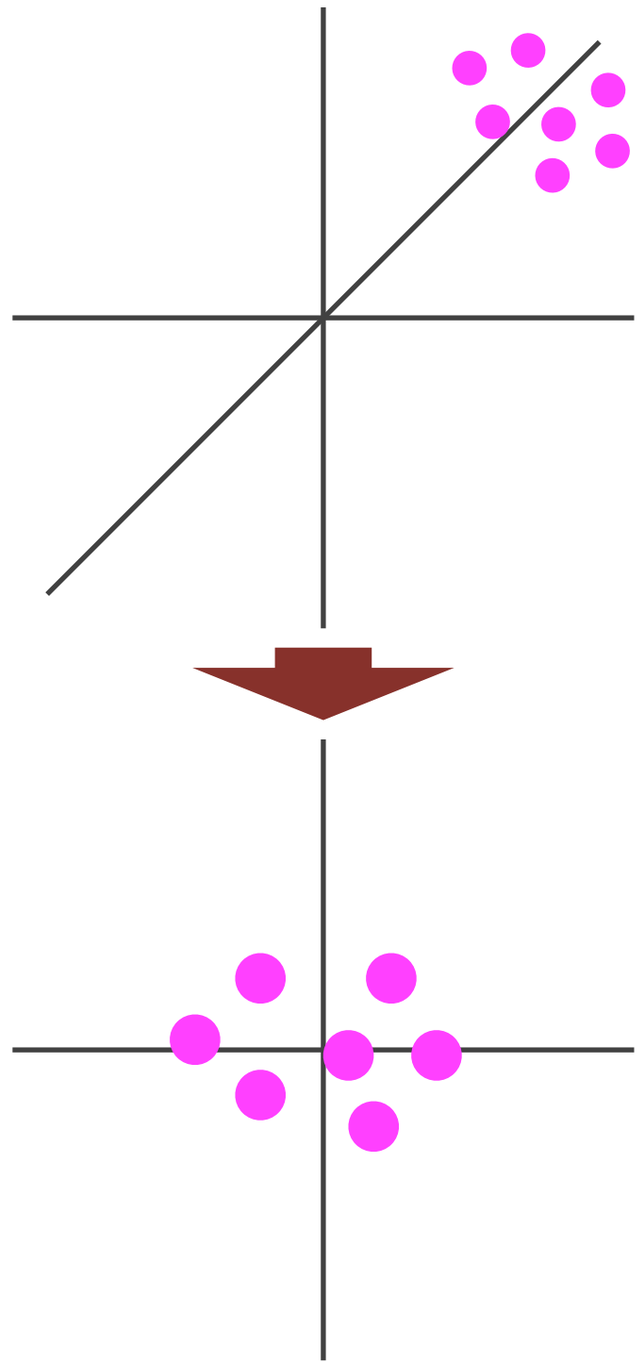
- Some solvers are optimised to only find the top *k* eigenvalues and corresponding eigenvectors, rather than all of them.

Demo: Covariance, Eigendecomposition and principal axes

Principal Component Analysis

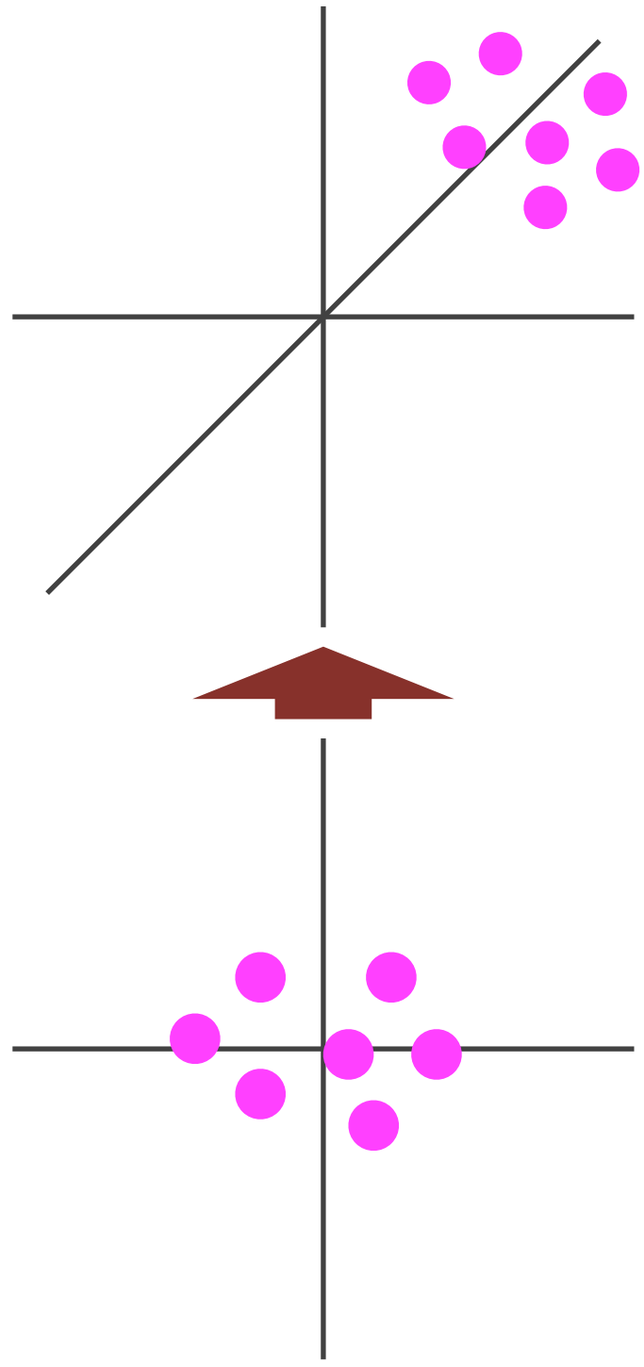
Linear Transform

- A linear transform **W** projects data from one space into another:
  - **T** = **ZW**
    - Original data stored in the rows of **Z**
- **T** can have fewer dimensions than **Z**.



Linear Transforms

- The effects of a linear transform can be reversed if **W** is **invertible**:
  - $\mathbf{Z} = \mathbf{T}\mathbf{W}^{-1}$
    - A lossy process if the dimensionality of the spaces is different



PCA

- PCA is an **Orthogonal Linear Transform** that maps data from its original space to a space defined by the principal axes of the data.

  - The transform matrix **W** is just the eigenvector matrix **Q** from the Eigendecomposition of the covariance matrix of the data.

- Dimensionality reduction can be achieved by removing the eigenvectors with low eigenvalues from **Q** (i.e. keeping the first *L* columns of **Q** assuming the eigenvectors are sorted by decreasing eigenvalue).

PCA Algorithm

1. Mean-centre the data vectors

2. Form the vectors into a matrix $\mathbf{Z}$, such that each row corresponds to a vector

3. Perform the Eigendecomposition of the matrix $\mathbf{Z}^T\mathbf{Z}$, to recover the eigenvector matrix $\mathbf{Q}$ and diagonal eigenvalue matrix $\mathbf{\Lambda}$: $\mathbf{Z}^T\mathbf{Z} = \mathbf{Q\Lambda Q}^T$

4. Sort the columns of $\mathbf{Q}$ and corresponding diagonal values of $\mathbf{\Lambda}$ so that the eigenvalues are decreasing.

5. Select the L largest eigenvectors of $\mathbf{Q}$ (the first L columns) to create the transform matrix Q_L.

6. Project the original vectors into a lower dimensional space, $\mathbf{T}_L$: $\mathbf{T}_L = \mathbf{ZQ}_L$

Demo: PCA

Singular Value Decomposition

Singular Value Decomposition

(Complex Valued M)

Conjugate Transpose

$$\mathbf{M=U\Sigma V}^{*}$$

Note that this is a different $\mathbf{\Sigma}$ *to the one used earlier*

(Real Valued M)

$$\mathbf{M=U\Sigma V}^{\mathsf{T}}$$

(Real) Singular Value Decomposition

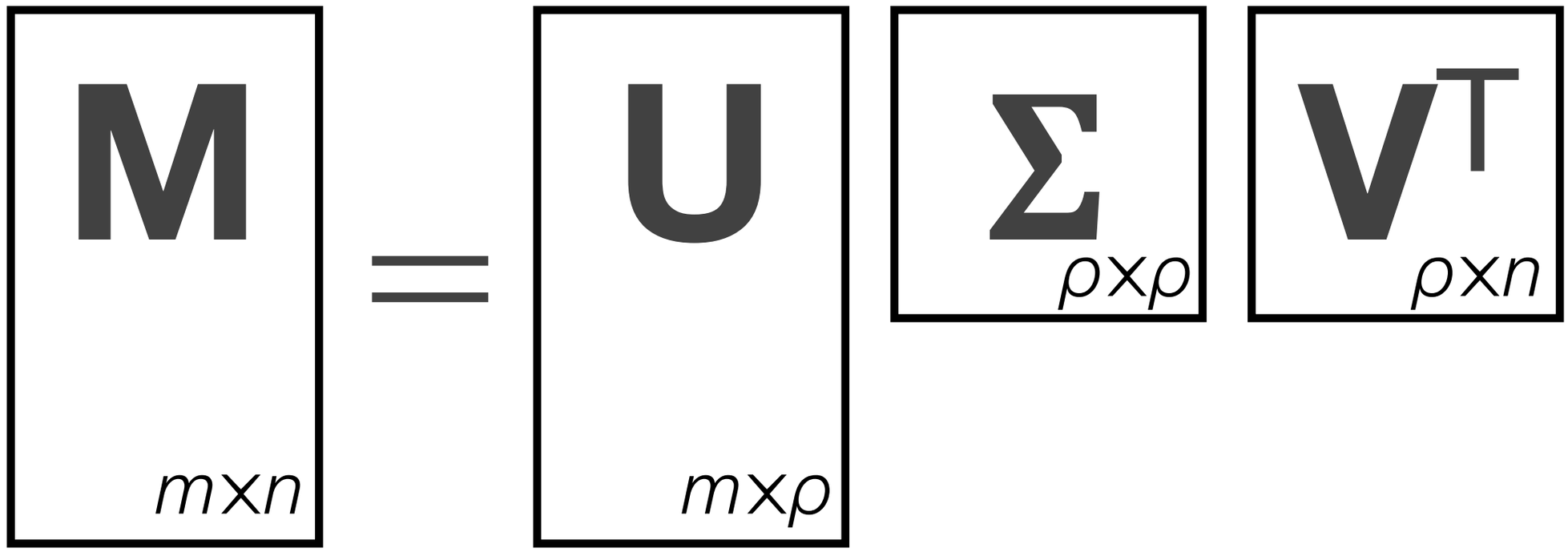
Orthogonal matrix:
$\boldsymbol{U^TU=UU^T=I}$

Orthogonal matrix:
$\boldsymbol{V^TV=VV^T=I}$

$$\mathbf{M=U\Sigma V^T}$$

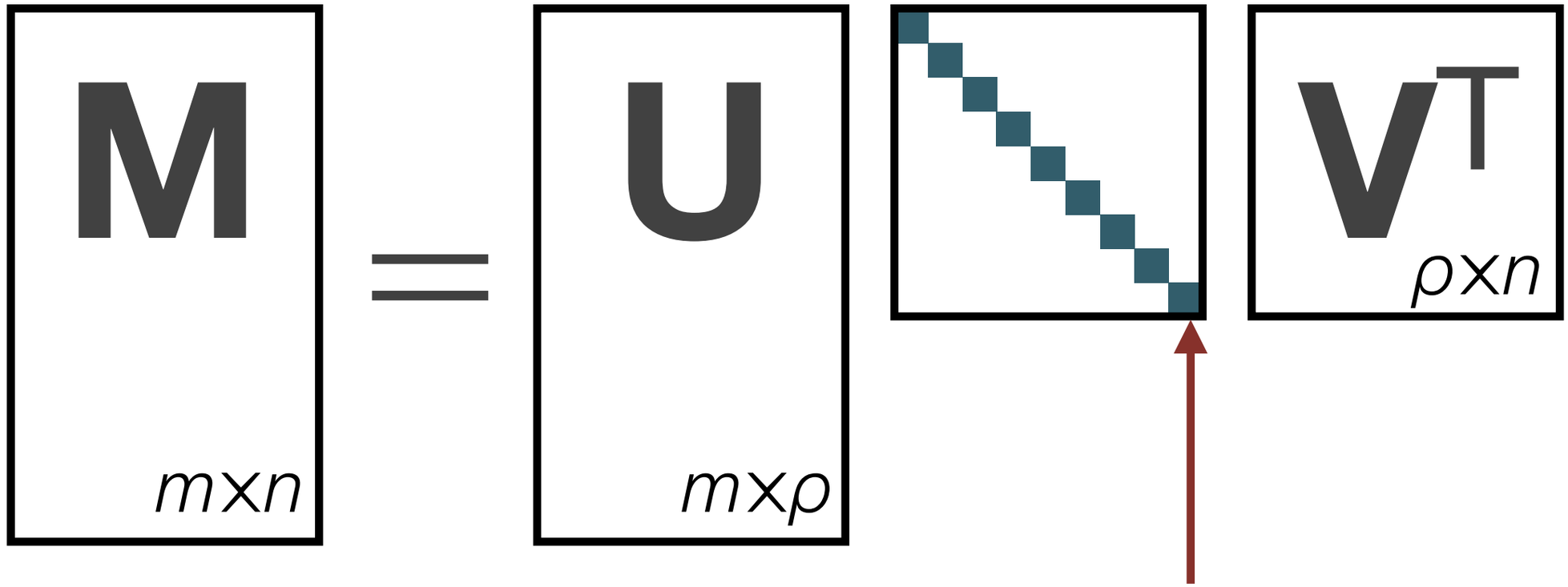
Real Diagonal Matrix

Singular Value Decomposition



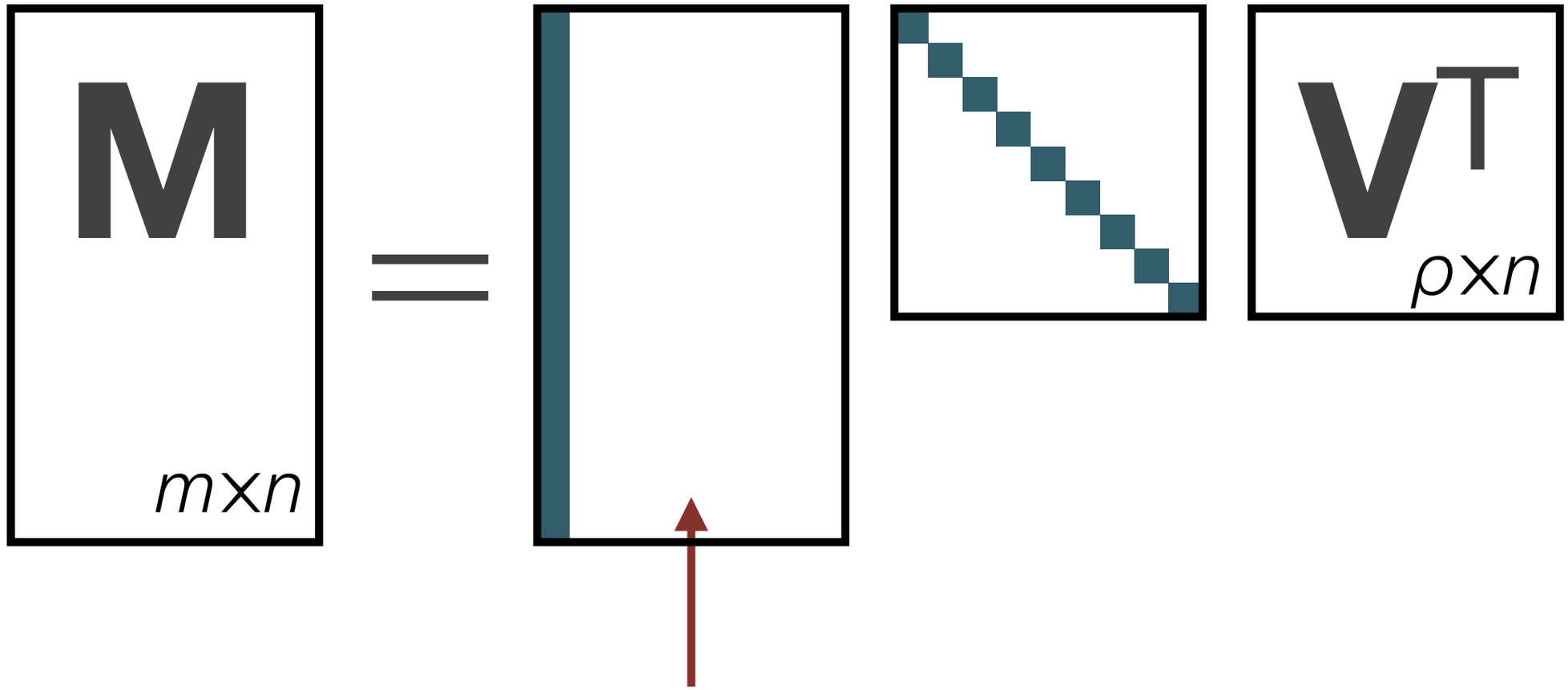
where ρ is the rank of **M**
(i.e. the number of linearly independent rows or columns)

Singular Value Decomposition



"Singular Values"
(Usually organised/computed so they monotonically decrease)

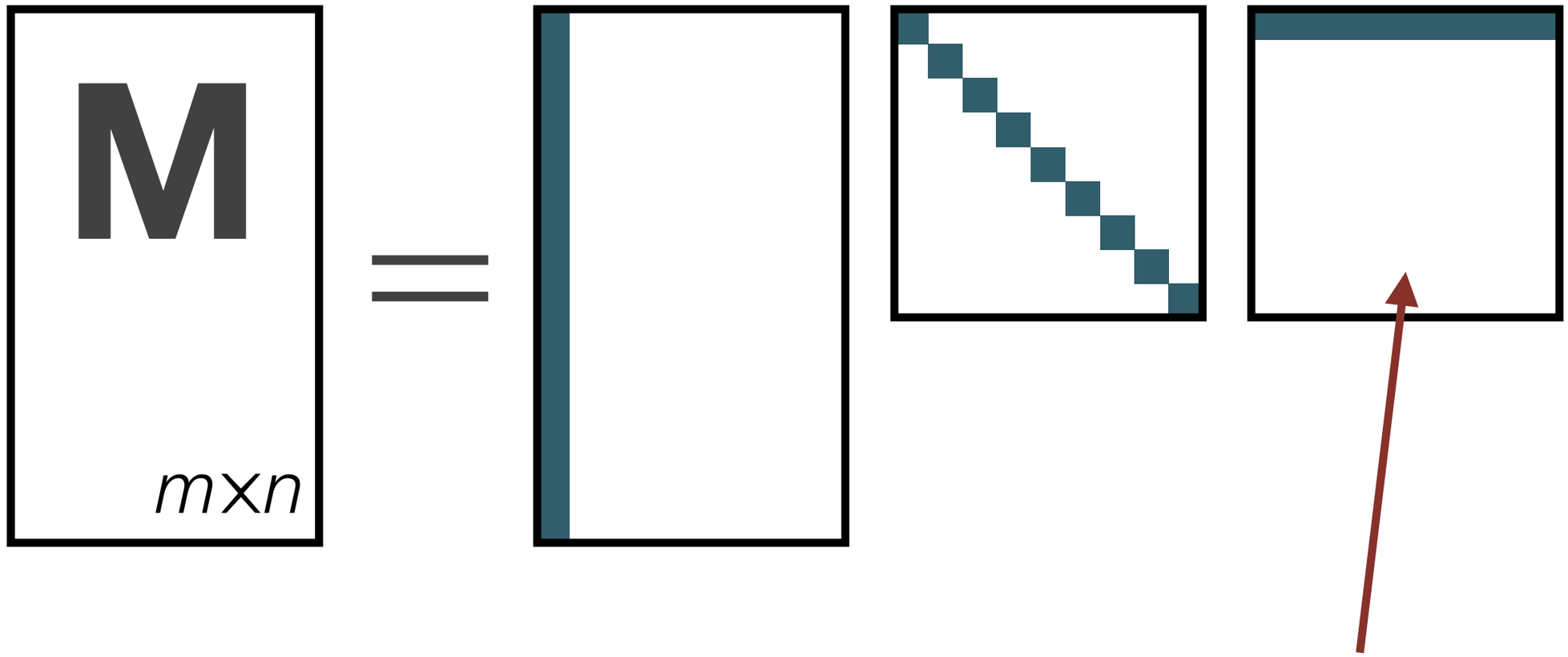
Singular Value Decomposition



Columns of **U** *are called the "left singular vectors"*

The left singular vectors are the eigenvectors of $\mathbf{MM}^T$

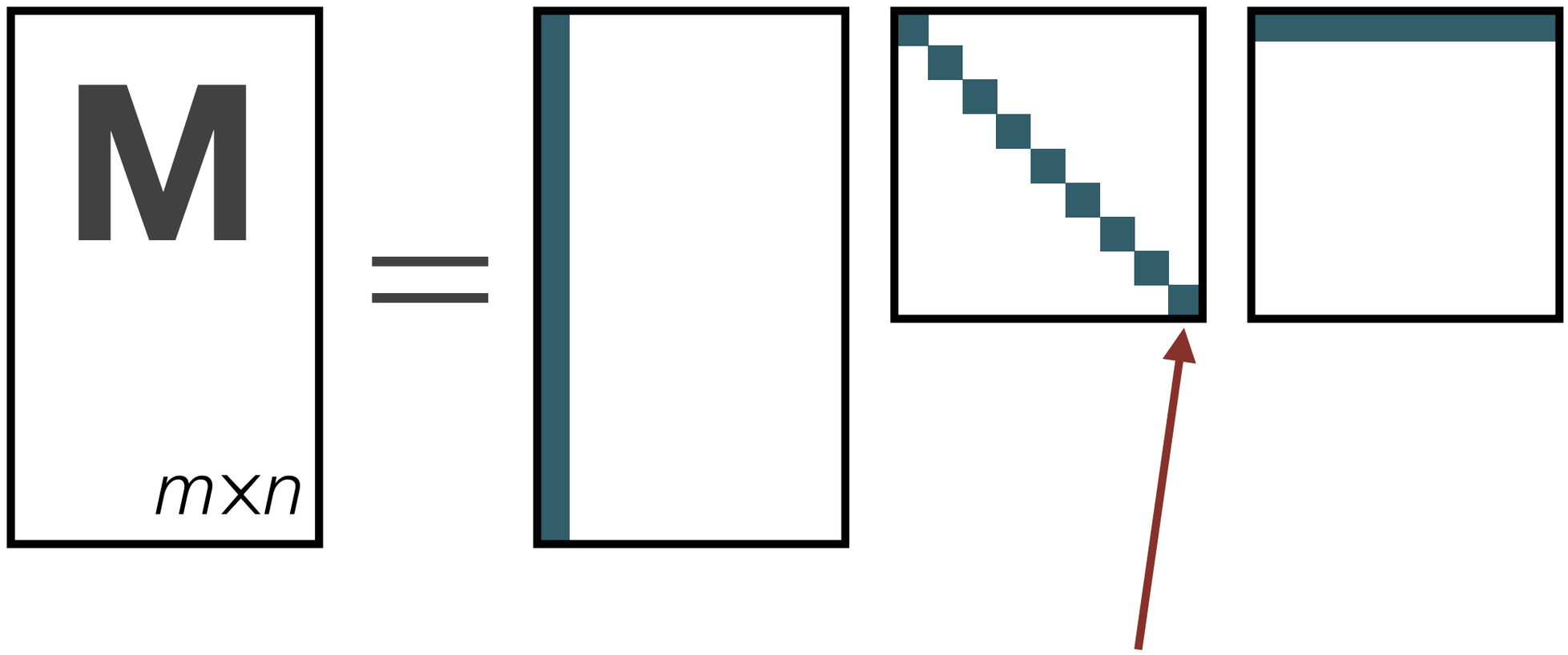
Singular Value Decomposition



Rows of $\mathbf{V}^T$ *(columns of* $\mathbf{V}$*) are called the "right singular vectors"*

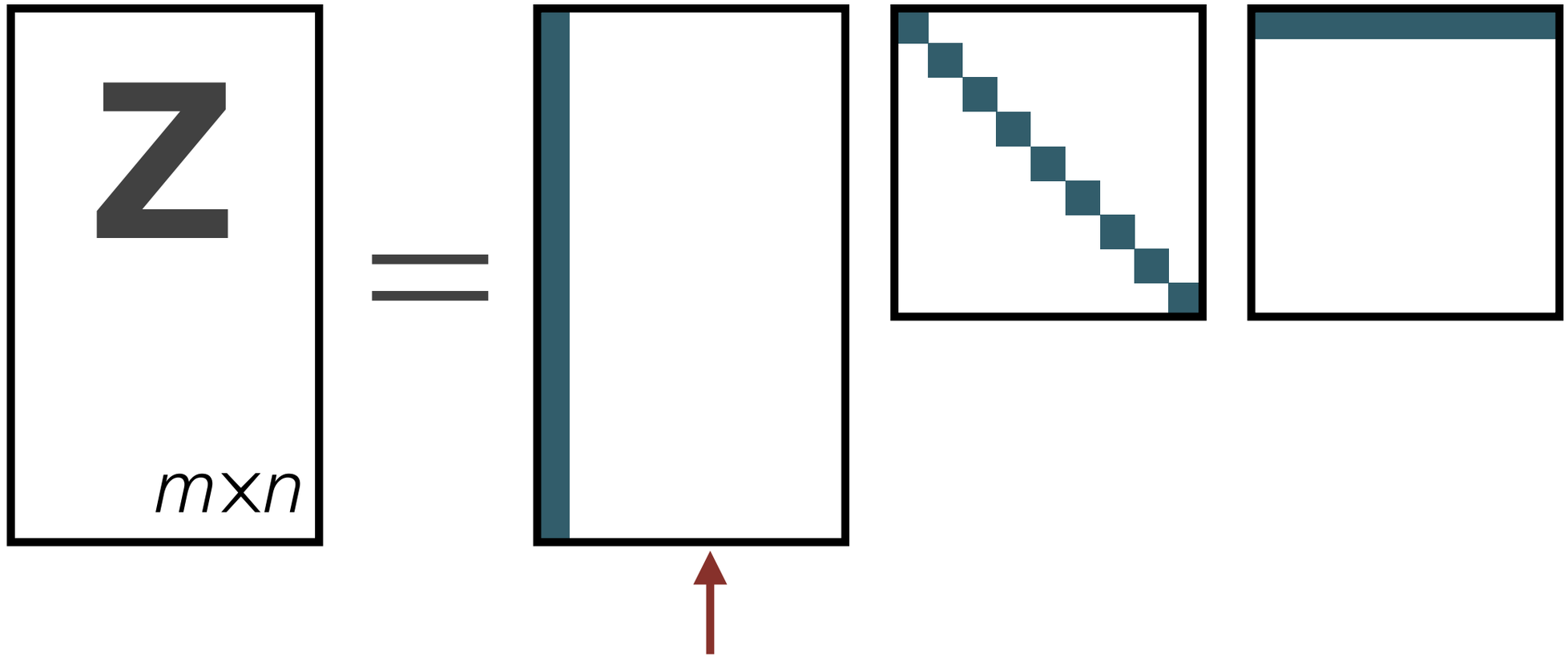
The right singular vectors are the eigenvectors of $\mathbf{M}^T\mathbf{M}$

Singular Value Decomposition



The singular values are the square roots of the eigenvalues of the corresponding eigenvectors of $\mathbf{M}^T\mathbf{M}$ and $\mathbf{M}\mathbf{M}^T$

Singular Value Decomposition



If **Z** *is the matrix of mean centred featurevectors that we introduced earlier, then the columns of* **U** *are the eigenvalues of* $\mathbf{ZZ}^T$ *- that is they are the* ***principle components of Z****!*

SVD-based PCA Algorithm

1. Mean-centre the data vectors

2. Form the vectors into a matrix $\mathbf{Z}$, such that each row corresponds to a vector

3. Perform the SVD of the matrix $\mathbf{Z}$, to recover the left singular vector matrix $\mathbf{U}$ and diagonal singular value matrix $\mathbf{\Sigma}$: $\mathbf{Z} = \mathbf{U\Sigma V}^{\mathsf{T}}$

4. Sort the columns of $\mathbf{U}$ and corresponding diagonal values of $\mathbf{\Sigma}$ so that the singular values are decreasing.

5. Select the first L left singular vectors from $\mathbf{U}$ (the first L columns) to create the transform matrix $\mathbf{Q}_L$.

6. Project the original vectors into a lower dimensional space, $\mathbf{T}_L$: $\mathbf{T}_L = \mathbf{ZQ}_L$

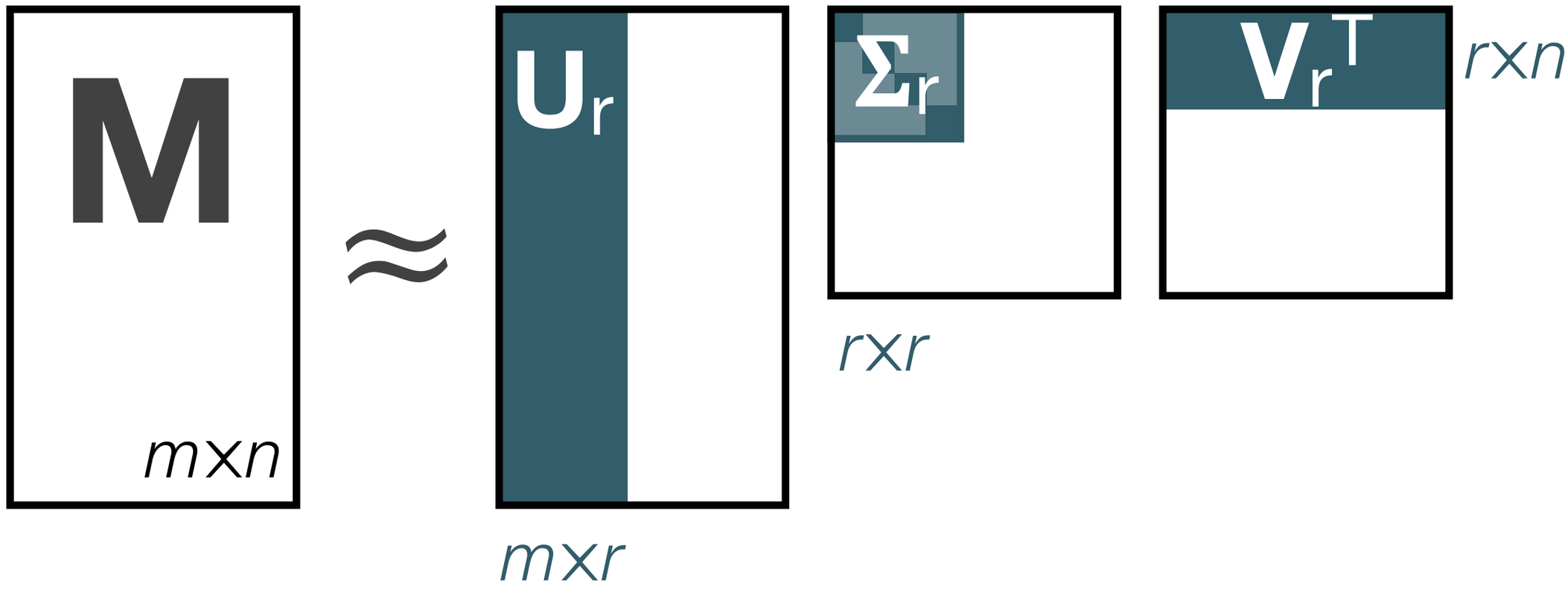
Why SVD-based PCA

- Numerical stability
  - Computing the covariance matrix might be disastrous - e.g. consider the Läuchli Matrix:

$$\begin{pmatrix} 1 & 1 & 1 \\ \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{pmatrix}^\top$$

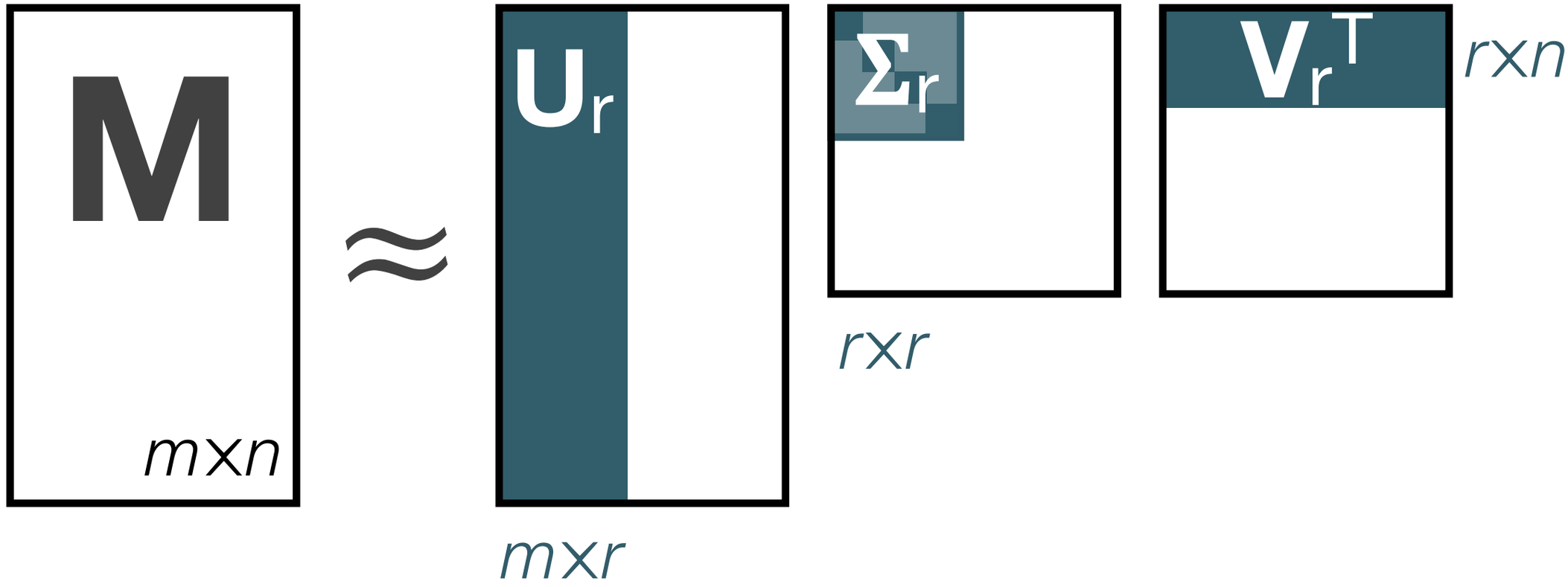
- Performance
  - SVD *can* be faster than computing covariance followed by EVD

Truncated Singular Value Decomposition



*Truncated SVD considers only the **largest** r singular values (and corresponding left & right vectors)*

Low Rank Approximation



It can be shown that $\acute{\mathbf{M}}=\mathbf{U}_r\mathbf{\Sigma}_r\mathbf{V}_r^T$ *is the "best" possible rank-r approximation to* **M** *in the sense that it minimises the Frobenius Norm* $||\acute{\mathbf{M}}-\mathbf{M}||_F$

(Frobenius Norm of **A** is just the square root of the sum of all the elements of **A** squared)

What else is SVD good for?

- Pseudoinverse
  - $\mathbf{A}^{+}=\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^{T}$
    - use to solve $\mathbf{A}x=b$ for x where $||\mathbf{A}x-b||_2$ *is minimised*: $x=\mathbf{A}^{+}b$ (i.e. solve least squares regression!)
- Solving homogeneous linear equations
  - $\mathbf{A}x=0$
- Data mining
  - e.g. model based CF recommender systems, latent factors, …
    - We'll see lots more in coming lectures

Computation of EVD and SVD

Classical EVD/SVD algorithms I

- All general E.V. algorithms are iterative
  - "Power Iteration"
    - Iterative process to find the biggest E.V.
    - Repeated for each E.V. by rotating and truncating the input to remove the effect of the previous E.V.

$$b_{k+1} = \frac{Ab_k}{\|Ab_k\|}$$

- "Arnoldi Iteration" and the "Lanczos Algorithm"
  - Move efficient variants of Power Iteration
    - use the "Gram-Schmidt" process to find the orthonormal basis of the top-r E.Vs

Classical EVD/SVD algorithms II

- Those algorithms are good for finding the **largest *r* E.V.s or S.V.s**
    - Lots of standard efficient implementations in LAPACK/ARPACK
        - including for relatively large, sparse matrices
            - **but not really massive matrices…**
- Variations exist for finding the **smallest non-zero E.V.s**

Summary

- Covariance measures the “shape” of data by measuring how different dimensions change together.!

- The principle axes are a basis, aligned such they describe most directions of greatest variance.!

- The Eigendecomposition of the covariance matrix produces pairs of eigenvectors (corresponding to the principal axes) and eigenvalues (proportional to the variance along the respective axis).!

- PCA aligns data with its principal axes, and allows dimensionally reduction by discounting axes with low variance.

- SVD is a general matrix factorisation tool with lots of uses