

Chapter II: Background Mathematics

Information Retrieval & Data Mining
Universität des Saarlandes, Saarbrücken
Winter Semester 2013/14

Chapter II: Background Mathematics

1. Linear Algebra

Matrices, vectors, and related concepts

2. Probability Theory and Statistical Inference

Events, probabilities, random variables, and limit theorems; likelihoods and estimators

3. Confidence Intervals, Hypothesis Testing and Regression

Confidence intervals, statistical tests, linear regression

Chapter II.1: Linear Algebra

1. Matrices and vectors

1.1. Definitions

1.2. Basic algebraic operations

2. Basic concepts

2.1. Orthogonality and linear independence

2.2. Rank, invertibility, and pseudo-inverse

3. Fundamental decompositions

3.1. Eigendecomposition

3.2. Singular value decomposition

Matrices and vectors

- A **vector** is
 - a 1D array of numbers
 - a geometric entity with magnitude and direction
- The **norm** of the vector defines its magnitude
 - **Euclidean** (L_2) norm:
 - L_p norm ($1 \leq p \leq \infty$)
$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^n |x_i|^p\right)^{1/p}$$
- The direction is the angle

Matrices and vectors

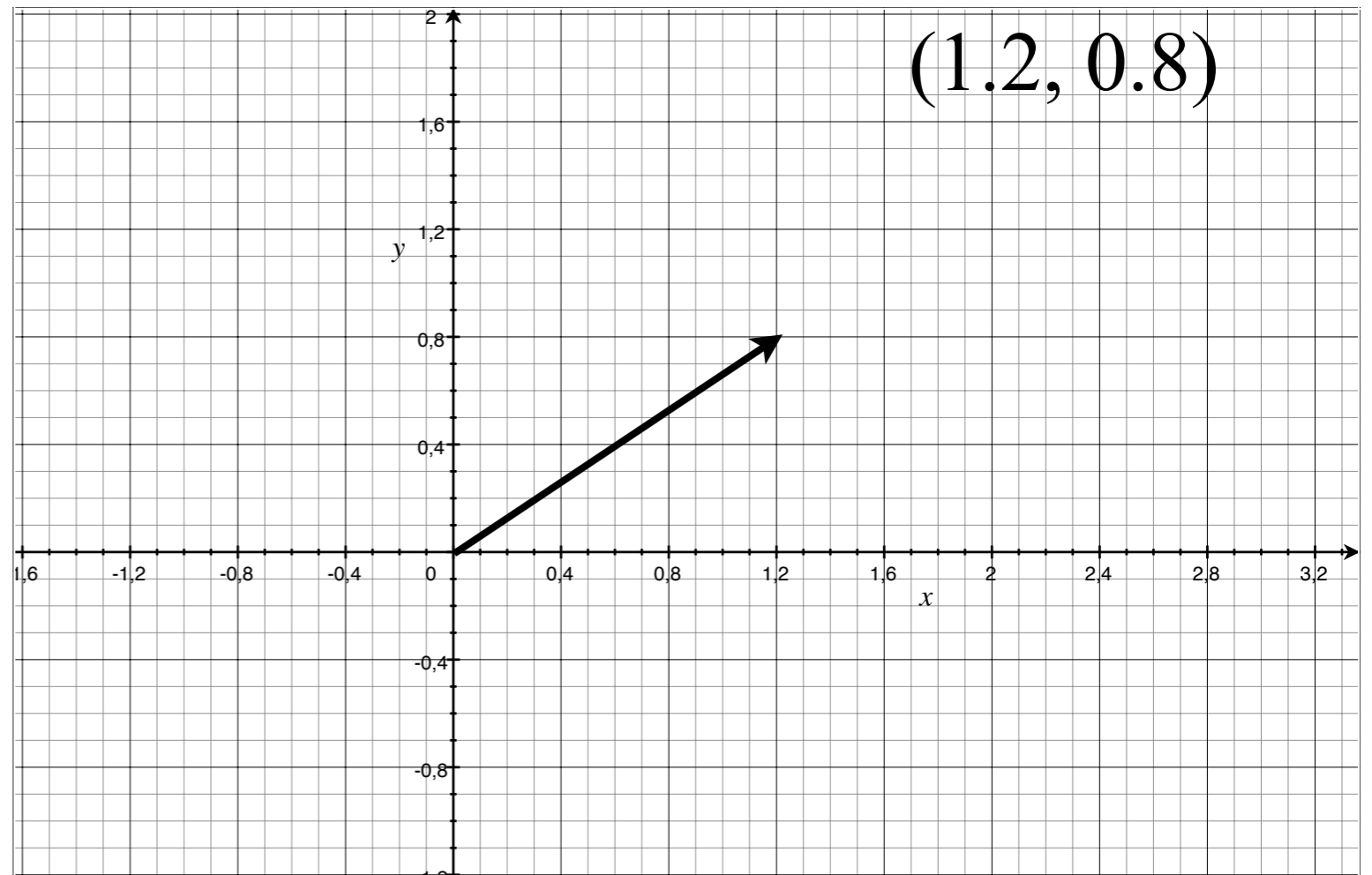
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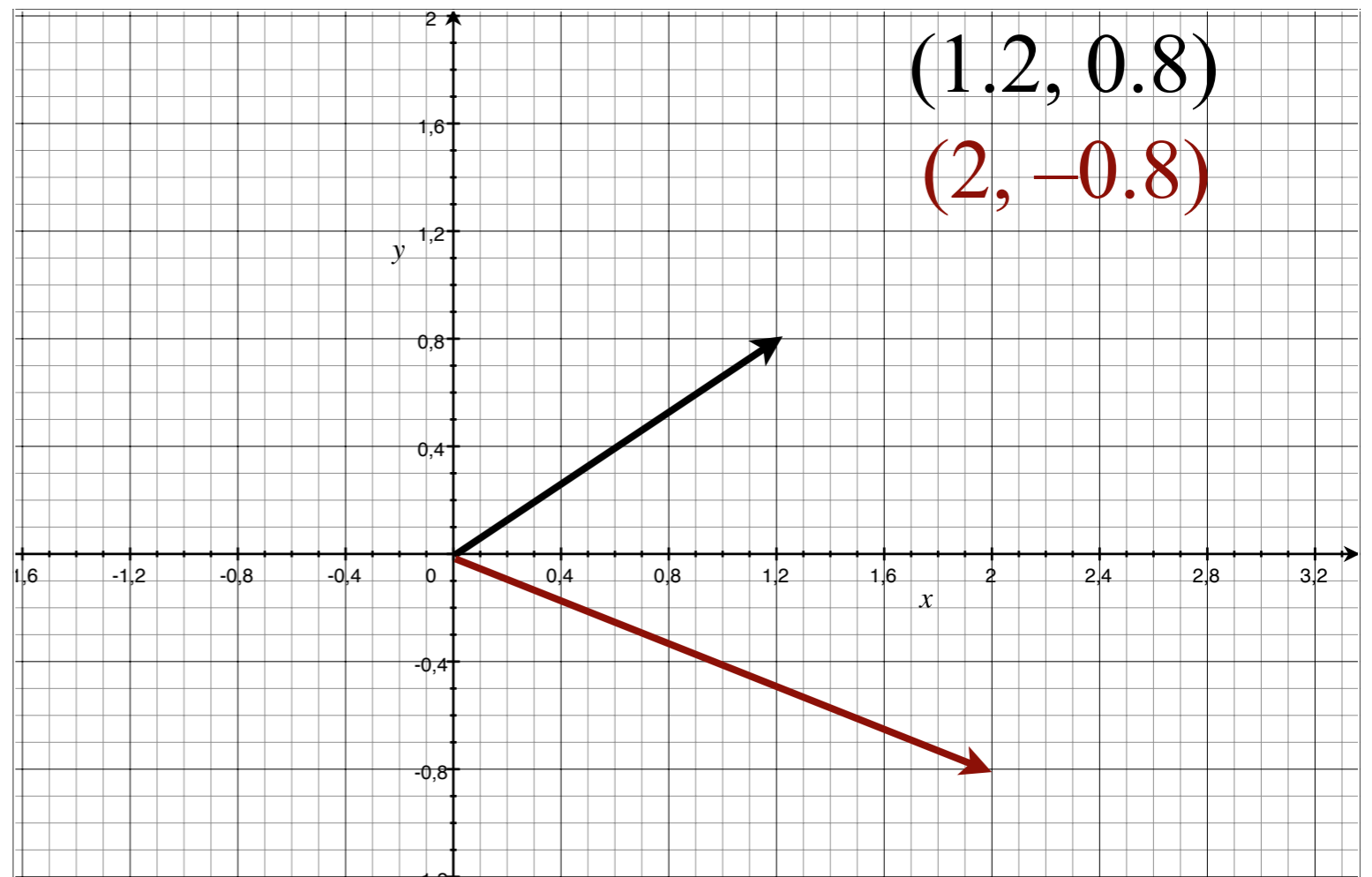
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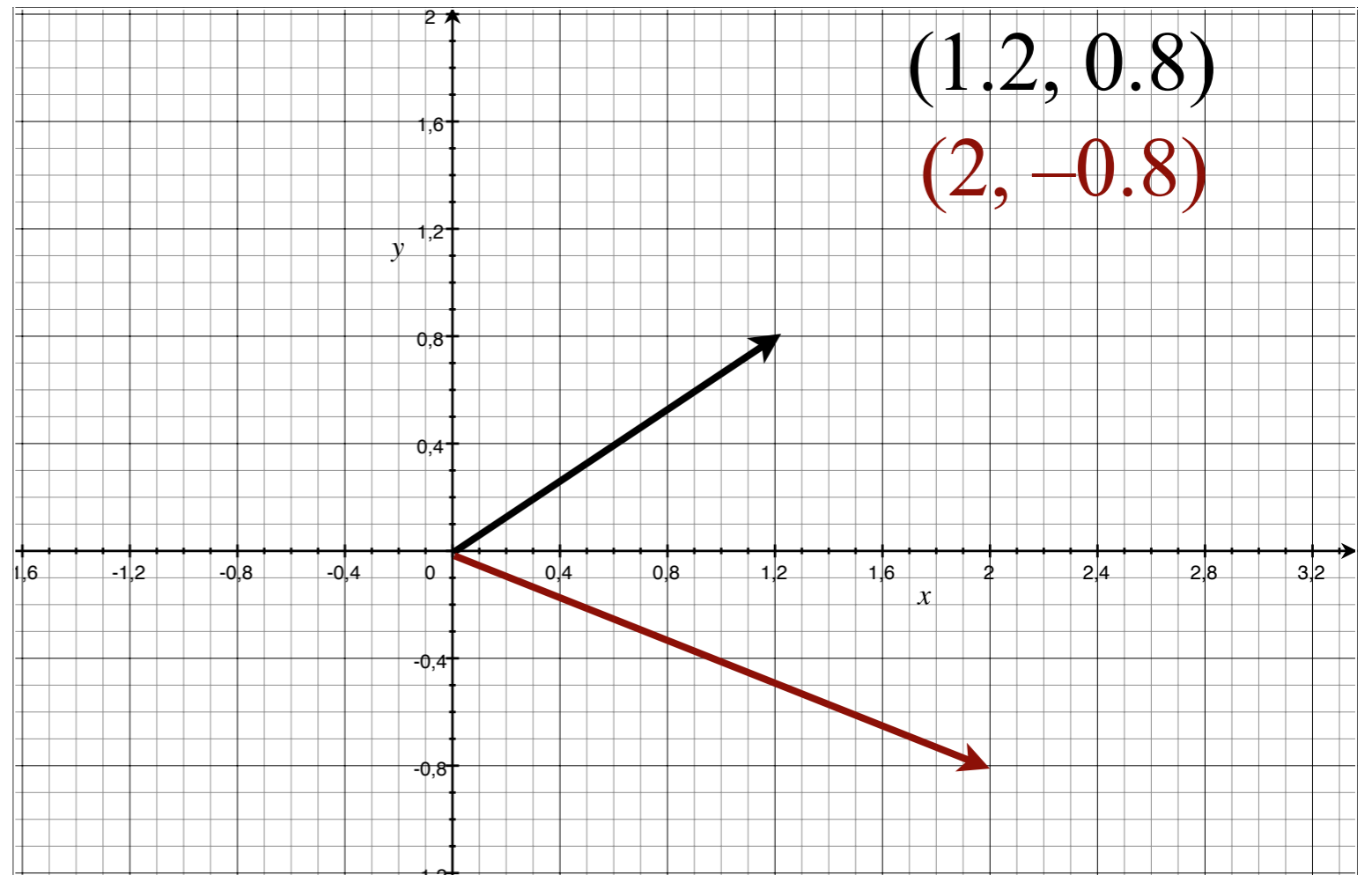
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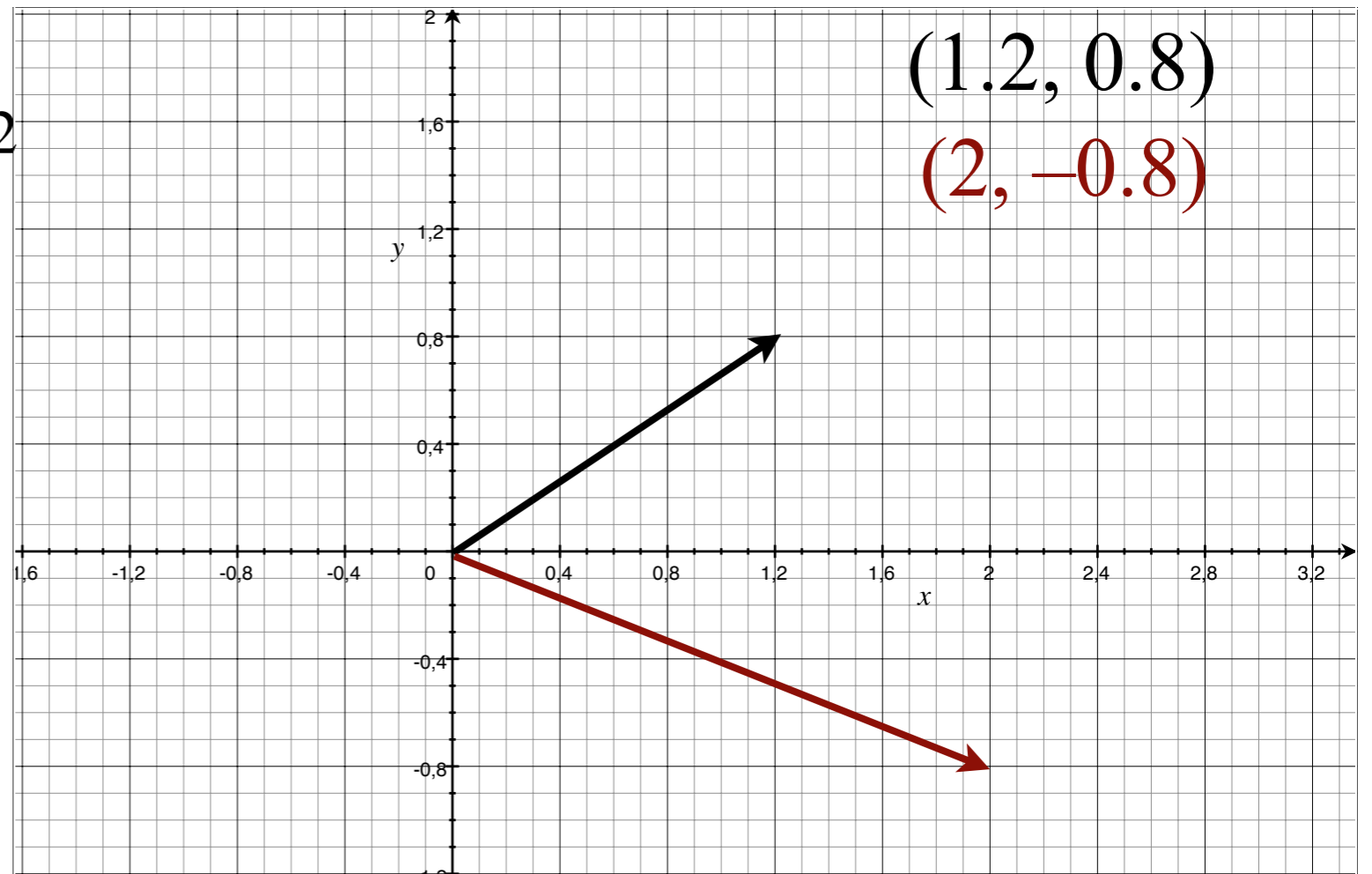
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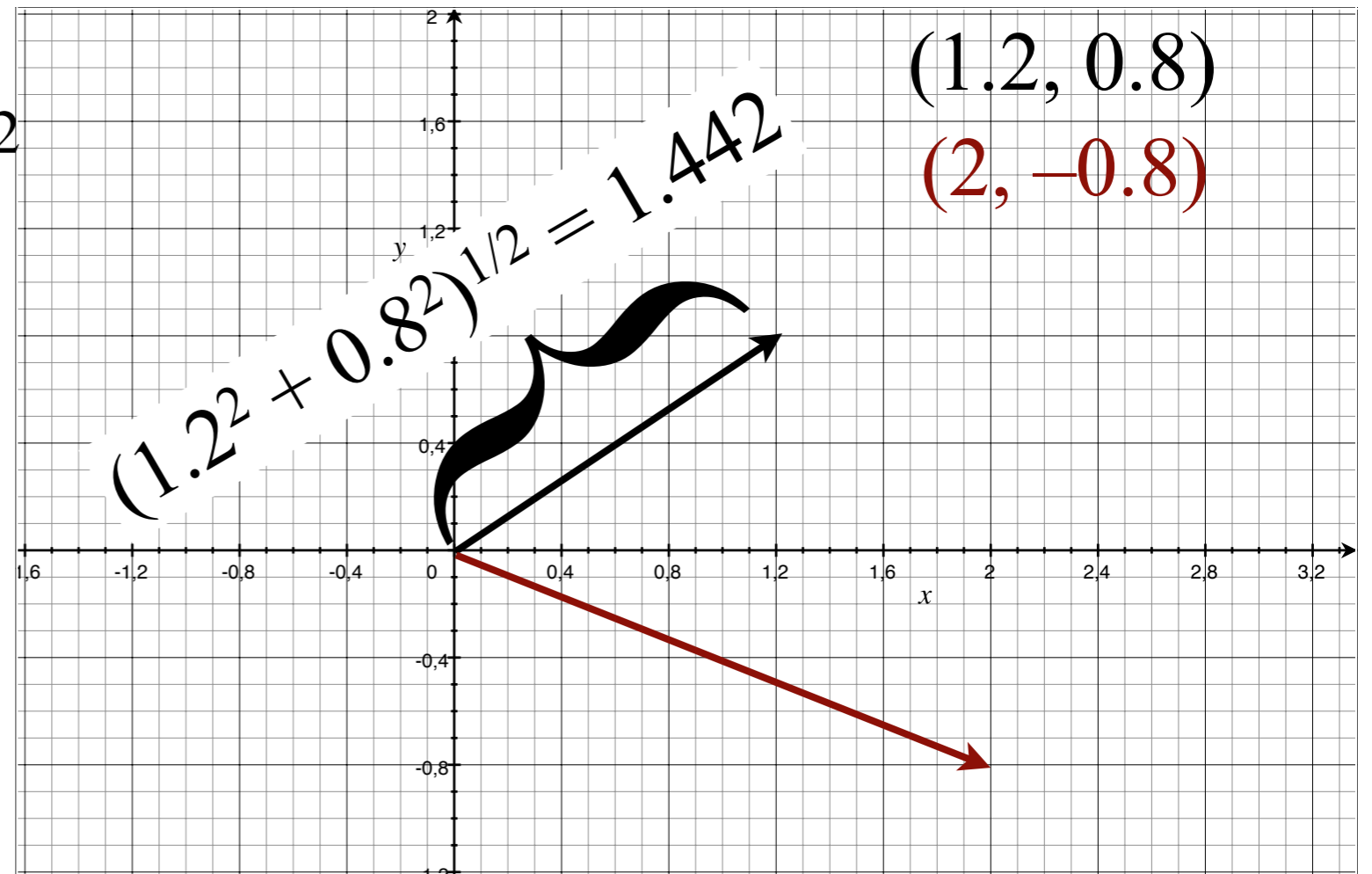
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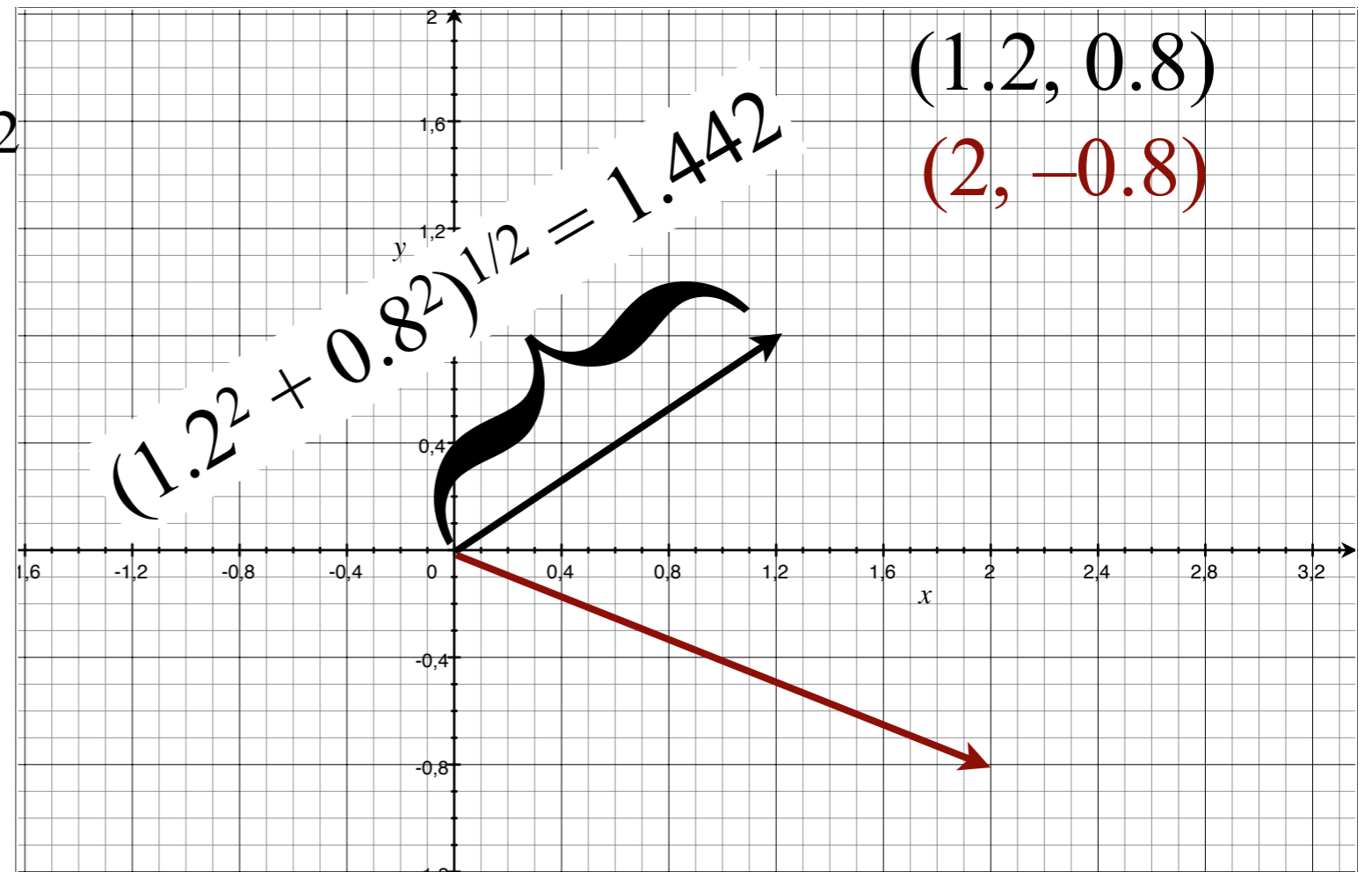
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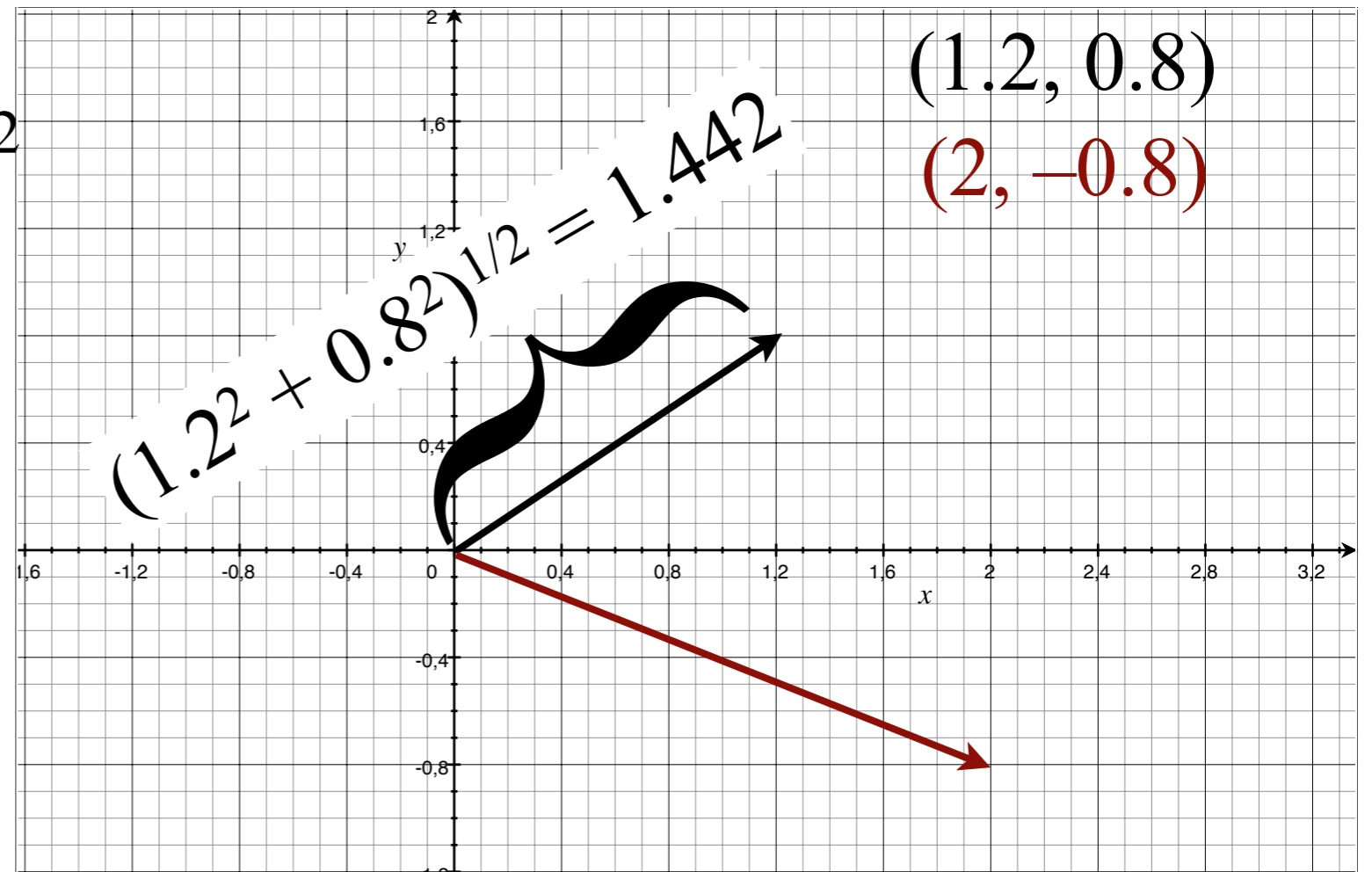
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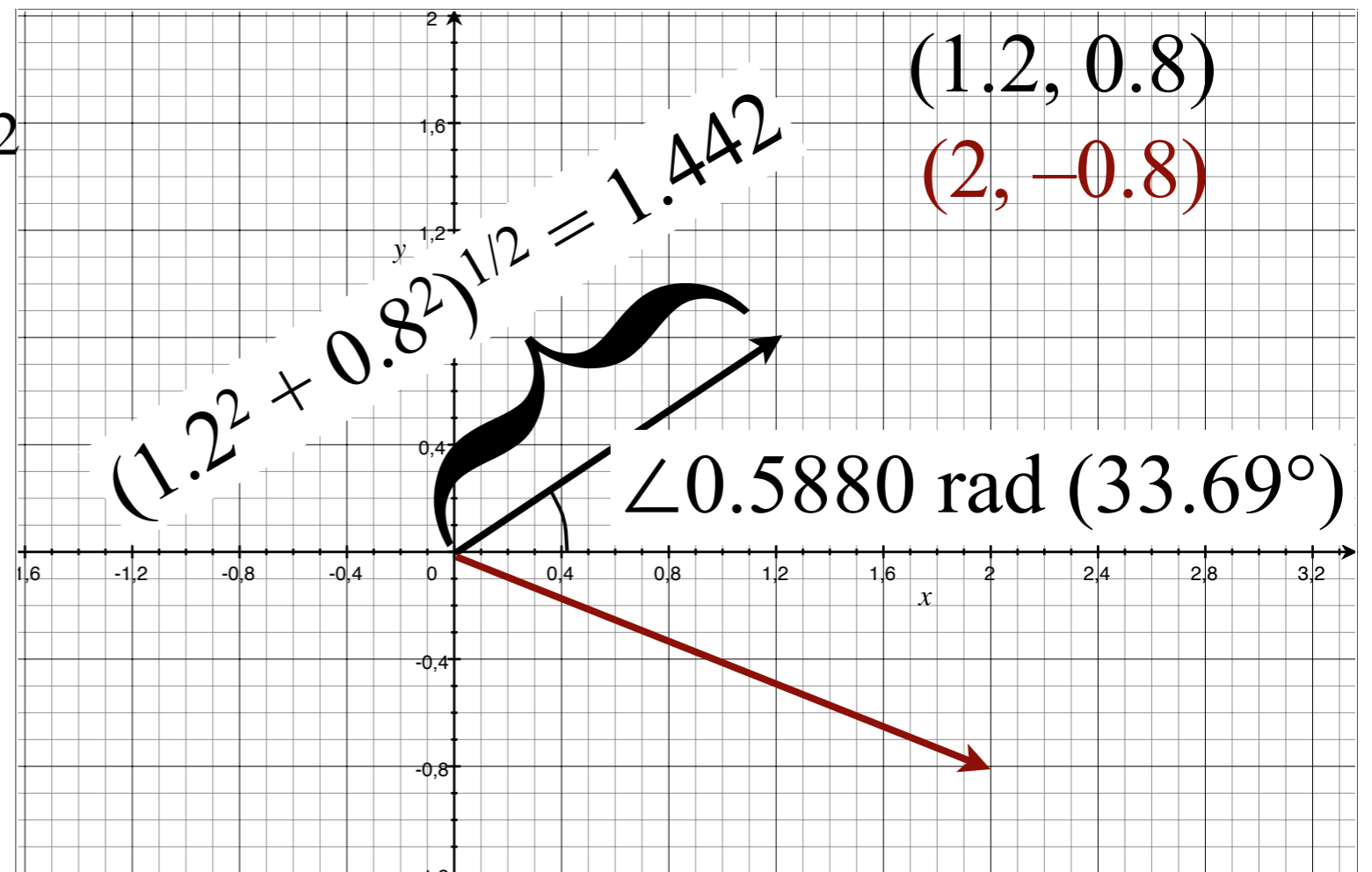
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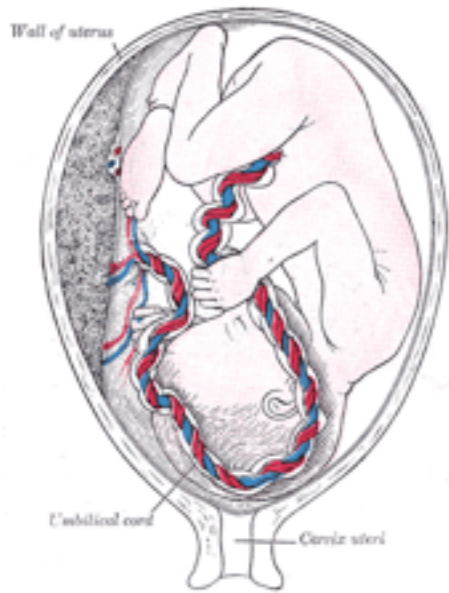
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What is a matrix?

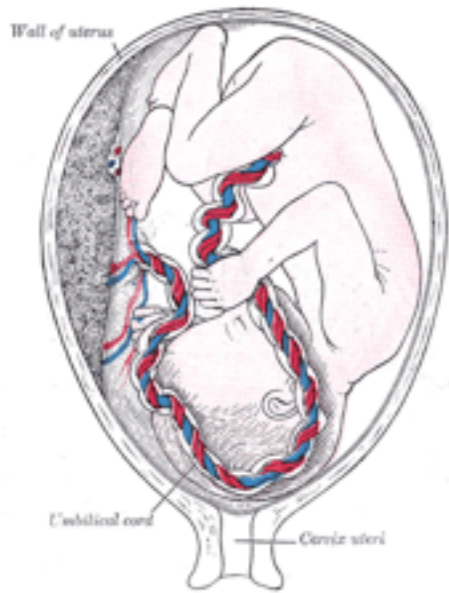
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A womb

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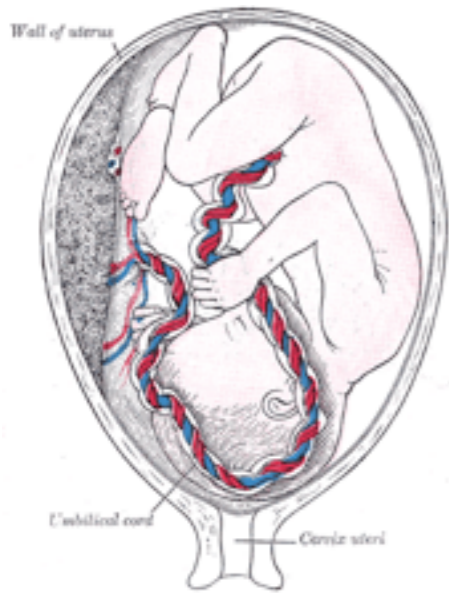


A womb

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

A rectangular array
of numbers

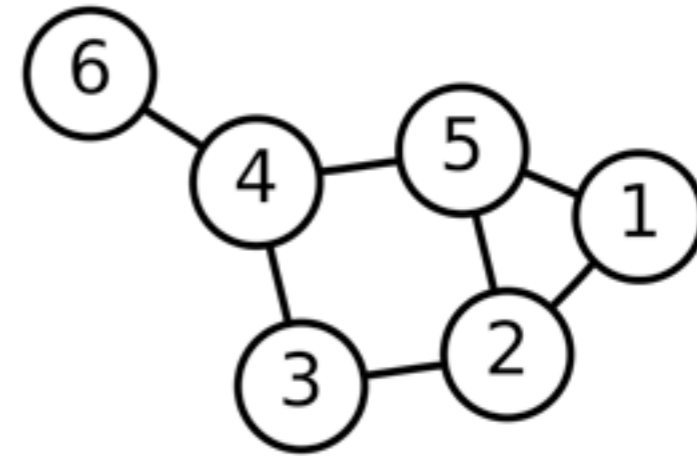
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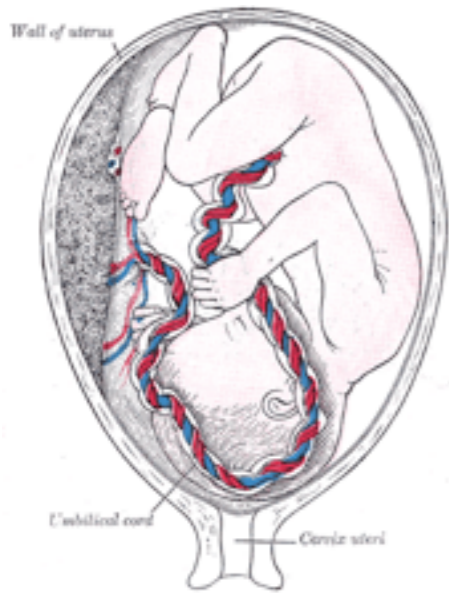
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A graph

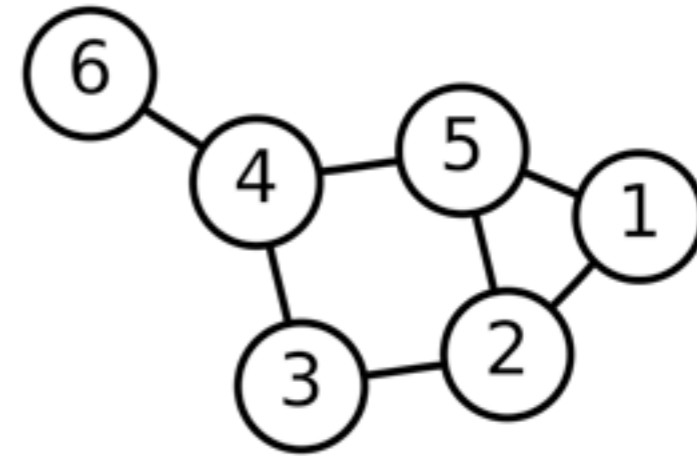
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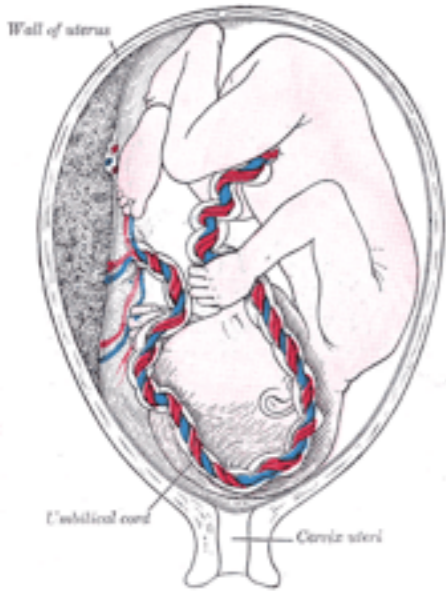
$$3x + 2y + z = 39$$

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$$x + 2y + 3z = 26$$

A system of
linear equations

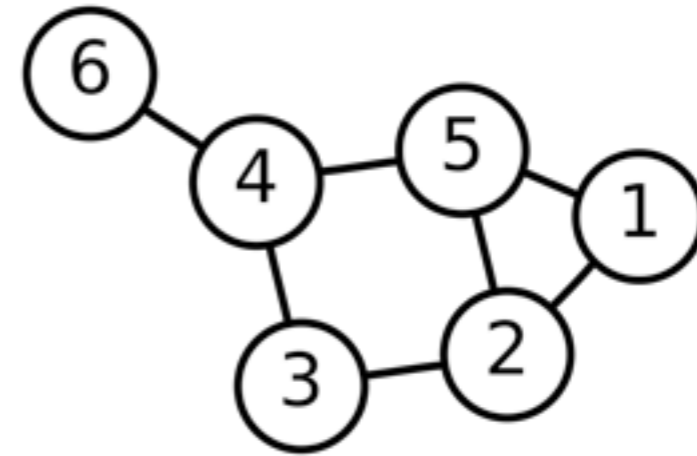
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A system of linear equations

$$f_1(x, y, z) = 3x + 2y + z$$

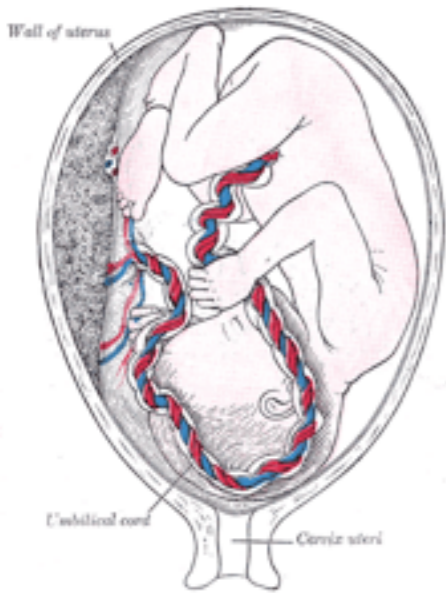
$$f_2(x, y, z) = 2x + 3y + z$$

$$f_3(x, y, z) = x + 2y + 3z$$

$$f_4(x, y, z) = x$$

A linear mapping

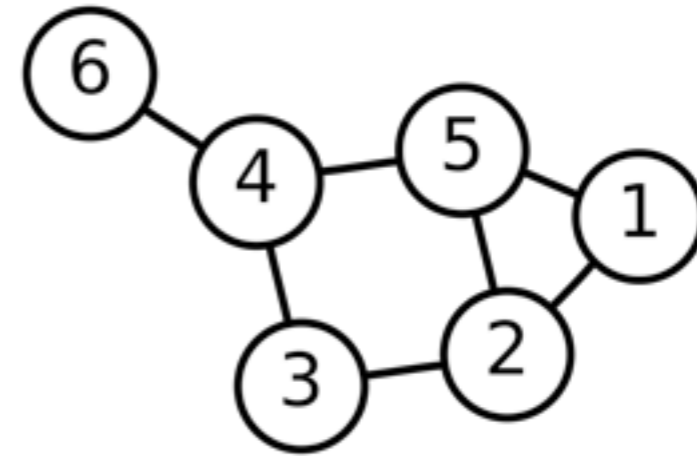
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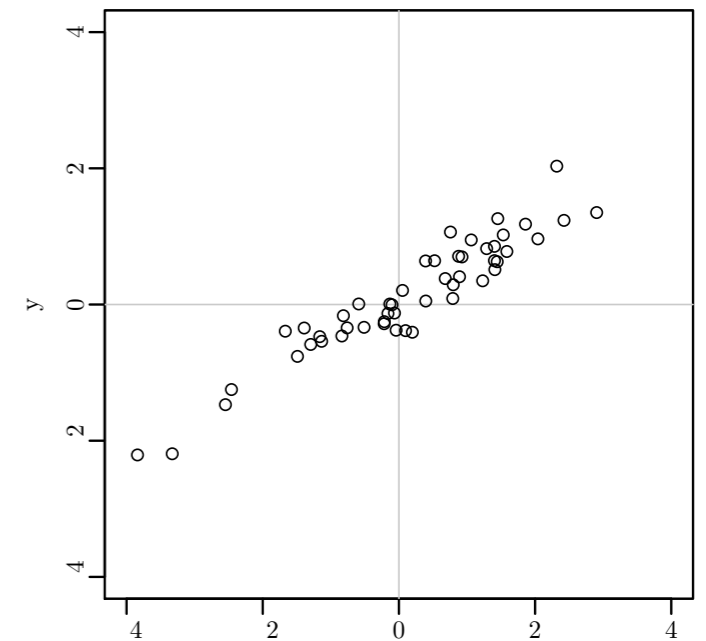
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A linear mapping



A set of data points

Vectors in IR&DM

- All above meanings of matrices and vectors (and more) are important ways to understand them
 - Different intuitions provide different insights
- In IR&DM, the most important one is the **vector space model**
 - A document in a vocabulary of n terms is represented as an n -dimensional vector
 - A customer transaction in a supermarket selling n items is represented as an n -dimensional vector

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Data
Star
Trek
Google
Information
(5, 0, 0, 1, 3, ...)

Matrices in IR&DM

	Bread	Butter	Beer
Anna	1	1	0
Bob	1	1	1
Charlie	0	1	1

Customer transactions

	Data	Matrix	Mining
Book 1	5	0	3
Book 2	0	0	7
Book 3	4	6	5

Document-term matrix

	Avatar	The Matrix	Up
Alice		4	2
Bob	3	2	
Charlie	5		3

Incomplete rating matrix

	Jan	Jun	Sep
Saarbrücken	1	11	10
Helsinki	6.5	10.9	8.7
Cape Town	15.7	7.8	8.7

Cities and monthly temperatures

Basic operations on vectors

- A **transpose** \mathbf{v}^T transposes a row vector into a column vector and vice versa
- If $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$, $\mathbf{v} + \mathbf{w}$ is a vector with $(\mathbf{v} + \mathbf{w})_i = v_i + w_i$
- For vector \mathbf{v} and scalar α , $(\alpha\mathbf{v})_i = \alpha v_i$
- A **dot product** of two vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$ is

$$\mathbf{v} \cdot \mathbf{w} = \sum_{i=1}^n v_i w_i$$

- A.k.a. **scalar product** or **inner product**
- Alternative notations: $\langle \mathbf{v}, \mathbf{w} \rangle$, $\mathbf{v}^T \mathbf{w}$ (for column vectors), $\mathbf{v} \mathbf{w}^T$ (for row vectors)
- In Euclidean space $\mathbf{v} \cdot \mathbf{w} = \|\mathbf{v}\| \|\mathbf{w}\| \cos \theta$

Basic operations on matrices

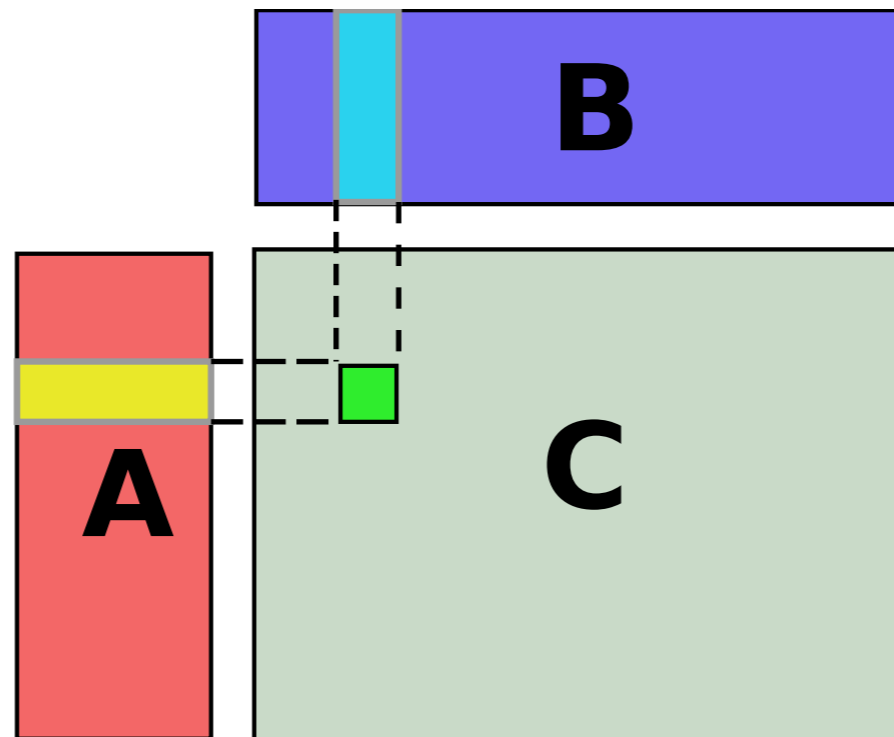
- Matrix transpose A^T has the rows of A as its columns
- If A and B are n -by- m matrices, then $A + B$ is an n -by- m matrix with $(A + B)_{ij} = m_{ij} + n_{ij}$
- If A is n -by- k and B is k -by- m , then AB is an n -by- m matrix with

$$(AB)_{ij} = \sum_{\ell=1}^k a_{i\ell} b_{\ell j}$$

- The inner dimension (k) must agree
- **Vector outer product** $\mathbf{v}\mathbf{w}^T$ (for column vectors) is the matrix product of n -by-1 and 1-by- m matrices

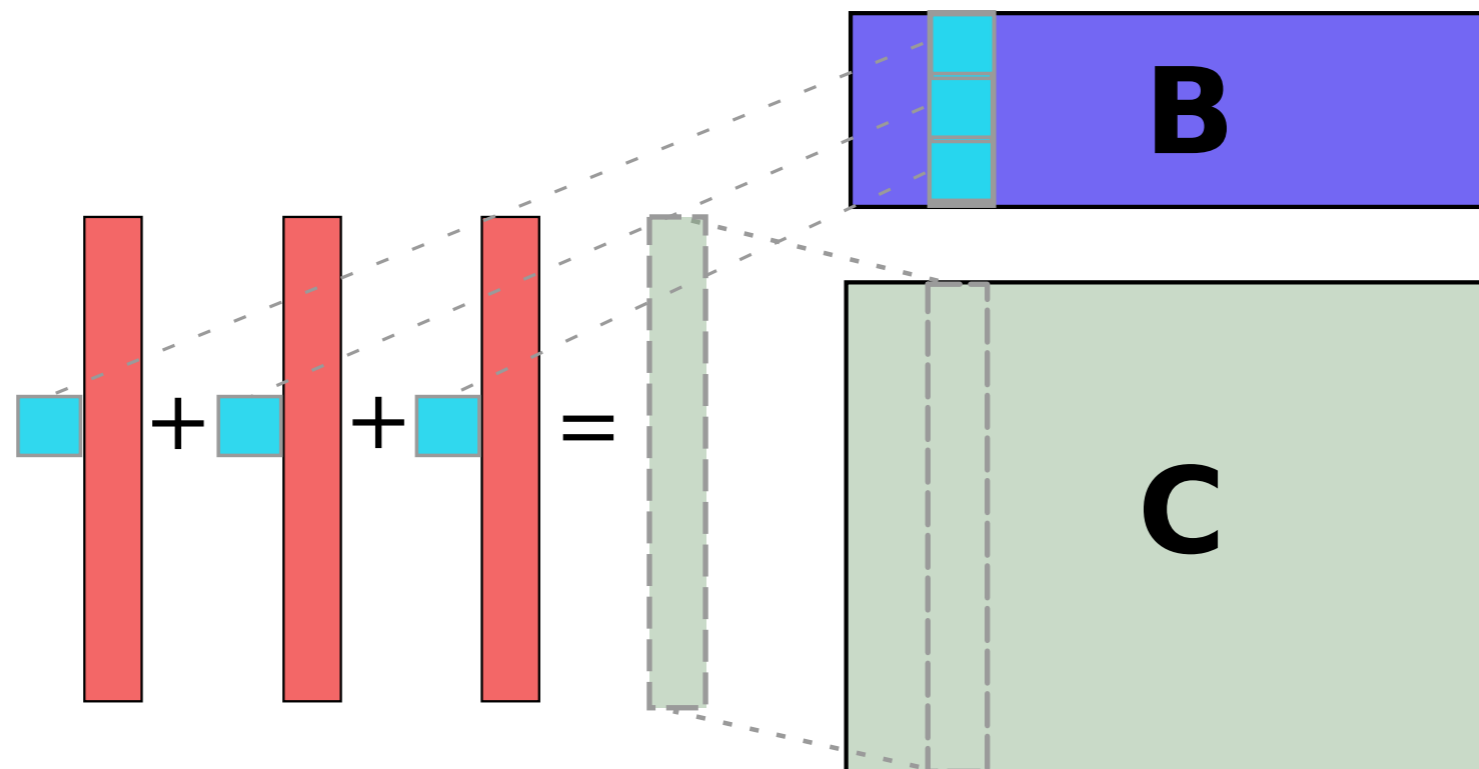
Intuition for matrix multiplication

- Element $(AB)_{ij}$ is the inner product of row i of A and column j of B



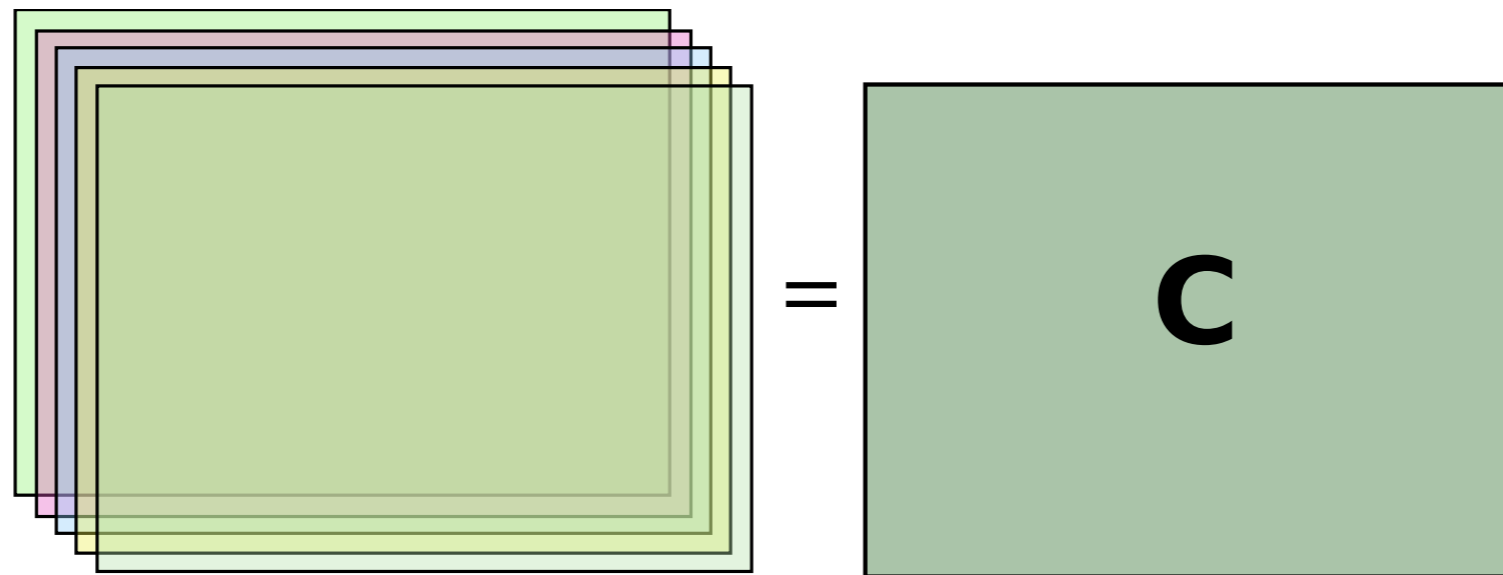
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Intuition for matrix multiplication

- Element $(AB)_{ij}$ is the inner product of row i of A and column j of B
- Column j of AB is the linear combination of columns of A with the coefficients coming from column j of B
- Matrix AB is a sum of k matrices $\mathbf{a}_l \mathbf{b}_l^T$ obtained by multiplying the l -th column of A with the l -th row of B



Ring of n -by- n matrices

- Square matrices of same size form a **ring**
 - Operations are addition, subtraction, and multiplication
 - The identity for addition and subtraction (0) is the all-zeros matrix $\mathbf{0}$
 - Multiplication doesn't always have an inverse (division)
 - Multiplication isn't commutative ($\mathbf{AB} \neq \mathbf{BA}$ in general)
 - The identity for multiplication is the **identity matrix \mathbf{I}** with 1s on the main diagonal and 0s elsewhere
 - $(\mathbf{I})_{ij} = 1$ iff $i = j$; $(\mathbf{I})_{ij} = 0$ otherwise
- With these limitations, we can do algebra on matrices as with real numbers

Matrices as linear mappings

- An n -by- m matrix A is a linear mapping from m -dimensional vector space to n -dimensional vector space
 - $A(\mathbf{x}) = A\mathbf{x}$, $(A\mathbf{x})_i = \sum_{j=1}^m a_{ij}x_j$
 - The transpose A^T is a mapping from n -dimensional to m -dimensional vector space
 - Typically it does **not** hold that if $\mathbf{y} = A\mathbf{x}$, then $\mathbf{x} = A^T\mathbf{y}$
- If A is n -by- m and B is m -by- k , then for the concatenated product $(A \circ B)(\mathbf{x}) = A(B\mathbf{x}) = (AB)\mathbf{x}$

Types of matrices

- Diagonal n -by- n matrix
 - Identity matrix I_n is a diagonal n -by- n matrix with 1s in diagonal

$$\begin{pmatrix} x_{1,1} & 0 & 0 & \dots & 0 \\ 0 & x_{2,2} & 0 & \dots & 0 \\ 0 & 0 & x_{3,3} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & x_{n,n} \end{pmatrix}$$

- Upper triangular matrix
 - Lower triangular is the transpose
 - If diagonal is full of 0s, matrix is *strictly triangular*

$$\begin{pmatrix} x_{1,1} & x_{1,2} & x_{1,3} & \dots & x_{1,n} \\ 0 & x_{2,2} & x_{2,3} & \dots & x_{2,n} \\ 0 & 0 & x_{3,3} & \dots & x_{3,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & x_{n,n} \end{pmatrix}$$

- Permutation matrix
 - Each row and column has exactly one 1, rest are 0
- Symmetric matrix: $M = M^T$

Matrix distances and norms

- Frobenius norm $\|\mathbf{X}\|_F = (\sum_{i,j} x_{ij}^2)^{1/2}$
 - Corresponds to Euclidean norm of vectors
- Sum of absolute values $|\mathbf{X}| = \sum_{i,j} |x_{ij}|$
 - Corresponds to L_1 -norm of vectors
- The above elementwise norms are sometimes (imprecisely) called L_2 and L_1 norms
 - Matrix L_1 and L_2 norms are something different altogether
- Operator norm $\|\mathbf{X}\|_p = \max_{\mathbf{y} \neq 0} \|\mathbf{X}\mathbf{y}\|_p / \|\mathbf{y}\|_p$
 - Largest norm of an image of a unit norm vector
 - $\|\mathbf{X}\|_2 \leq \|\mathbf{X}\|_F \leq \sqrt{\text{rank}(\mathbf{X})} \|\mathbf{X}\|_2$

Basic concepts

- Two vectors \mathbf{x} and \mathbf{y} are **orthogonal** if their inner product $\langle \mathbf{x}, \mathbf{y} \rangle$ is 0
 - Vectors are **orthonormal** if they have unit norm, $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$
 - In Euclidean space, this means that $\|\mathbf{x}\| \|\mathbf{y}\| \cos \theta = 0$ which happens iff $\cos \theta = 0$ which means \mathbf{x} and \mathbf{y} are perpendicular to each other
- A square matrix X is **orthogonal** if its rows and columns are orthonormal
 - An n -by- m matrix X is row-orthogonal if $n < m$ and its rows are orthogonal and column-orthogonal if $n > m$ and its columns are orthogonal

Linear independency

- Vector $\mathbf{v} \in \mathbb{R}^n$ is **linearly dependent** from a set of vectors $W = \{\mathbf{w}_i \in \mathbb{R}^n : i = 1, \dots, m\}$ if there exists a set of coefficients α_i such that $\mathbf{v} = \sum_{i=1}^m \alpha_i \mathbf{w}_i$
 - If \mathbf{v} is not linearly dependent, it is **linearly independent**
 - That is, \mathbf{v} can't be expressed as a linear combination of the vectors in W
- A set of vectors $V = \{\mathbf{v}_i \in \mathbb{R}^n : i = 1, \dots, m\}$ is **linearly independent** if \mathbf{v}_i is linearly independent from $V \setminus \{\mathbf{v}_i\}$ for all i

Matrix rank

- The **column rank** of an n -by- m matrix M is the number of linearly independent columns of M
- The **row rank** is the number of linearly independent rows of M
- The **Schein rank** of M is the least integer k such that $M = AB$ for some n -by- k matrix A and k -by- m matrix B
 - Equivalently, the least k such that M is a sum of k vector outer products
- *All these ranks are equivalent!*

The matrix inverse

- The **inverse** of a matrix M is the unique matrix N for which $MN = NM = I$
 - The inverse is denoted by M^{-1}
- M has an inverse (is invertible) iff
 - M is square (n -by- n)
 - The rank of M is n (full rank)
- Non-square matrices can have left or right inverses
 - $MR = I$ or $LA = I$
- If M is orthogonal, then (and only then) $M^{-1} = M^T$
 - That is, $MM^T = M^T M = I$

The matrix pseudo-inverse

- The Moore–Penrose **pseudo-inverse** of an n -by- m matrix M is an m -by- n matrix M^+ for which
 - $MM^+M = M$ (MM^+ doesn't have to be identity)
 - $M^+MM^+ = M^+$ (M^+M doesn't have to be identity)
 - $(MM^+)^T = MM^+$ (MM^+ is symmetric)
 - $(M^+M)^T = M^+M$ (M^+M is symmetric)
- If the rank of M is m (full column rank, $n \geq m$), then
$$M^+ = (M^T M)^{-1} M^T$$
 - If the rank of M is n ($n \leq m$), then $M^+ = M^T (M M^T)^{-1}$

Fundamental decompositions

- A **matrix decomposition** (or **factorization**) presents an n -by- m matrix A as a product of two (or more) **factor matrices**
 - $A = BC$
- For approximate decompositions, $A \approx BC$
- The size of the decomposition is the inner dimension of B and C
 - Number of columns in B and number of rows in C
 - For exact decompositions, the size is no less than the rank of the matrix

Eigenvalues and eigenvectors

- If X is an n -by- n matrix and \mathbf{v} is a vector such that $X\mathbf{v} = \lambda\mathbf{v}$ for some scalar λ , then
 - λ is an **eigenvalue** of X
 - \mathbf{v} is an **eigenvector** of X associated to λ
- That is, eigenvectors are those vectors \mathbf{v} for which $X\mathbf{v}$ only changes their magnitude, not direction
 - It is possible to exactly reverse the direction
 - The change in magnitude is the eigenvalue
- If \mathbf{v} is an eigenvector of X and α is a scalar, then $\alpha\mathbf{v}$ is also an eigenvector with the same eigenvalue

Properties of eigenvalues

- Multiple linearly independent eigenvectors can be associated with the same eigenvalue
 - The **algebraic multiplicity** of the eigenvalue
- Every n -by- n matrix has n eigenvectors and n eigenvalues (counting the multiplicity)
 - But some of these can be complex numbers
- If a matrix is symmetric, then all its eigenvalues are real
- Matrix is invertible iff all its eigenvalues are non-zero

Eigendecomposition

- The (real-valued) **eigendecomposition** of an n -by- n matrix X is $X = Q\Lambda Q^{-1}$
 - Λ is a diagonal matrix with eigenvalues in the diagonal
 - Columns of Q are the eigenvectors associated with the eigenvalues in Λ
- Matrix X has to be diagonalizable
 - PXP^{-1} is a diagonal matrix for some invertible matrix P
- Matrix X has to have n real eigenvalues (counting multiplicity)

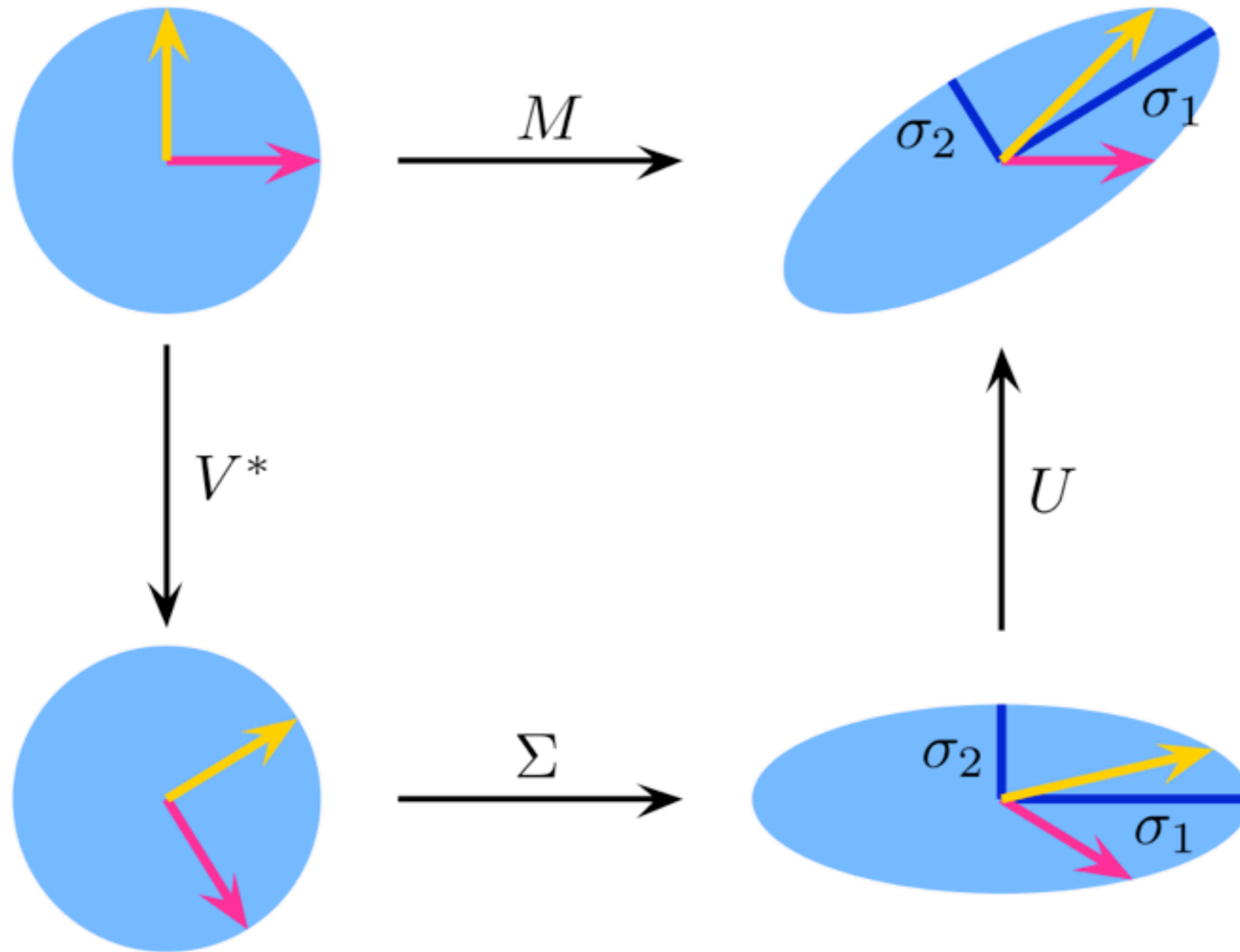
Some useful facts

- Not all matrices have eigendecomposition
 - Not all invertible matrices have eigendecomposition
 - Not all matrices that have eigendecomposition are invertible
 - If X is invertible and has eigendecomposition, then
$$X^{-1} = Q\Lambda^{-1}Q^{-1}$$
- If X is symmetric and invertible (and real), then X has eigendecomposition $X = Q\Lambda Q^T$

Singular value decomposition (SVD)

- Not every matrix has eigendecomposition, but:
Theorem. If X is n -by- m real matrix, there exists n -by- n orthogonal matrix U and m -by- m orthogonal matrix V such that $U^T X V$ is n -by- m matrix Σ with values $\sigma_1, \sigma_2, \dots, \sigma_{\min(n,m)}, \sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{\min(n,m)} \geq 0$, in its diagonal.
 - In other words, $X = U \Sigma V^T$
 - Values σ_i are the **singular values** of X
 - Columns of U are the **left singular vectors** and columns of V the **right singular vectors** of X

Example



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

Rank and SVD

- $\text{rank}(X) = r$ iff X has exactly r non-zero singular values
 - $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > \sigma_{r+1} = \dots = \sigma_{\min(n,m)} = 0$
 - A method to compute the rank of a matrix
- A **truncated SVD** of rank k is obtained by setting all but the first k singular values to 0
 - Typically denoted as $U_k \Sigma_k V_k^T$
 - For the product, we can ignore the columns of U and V corresponding to the zero singular values
 - U_k is n -by- k , V_k is m -by- k , and Σ_k is k -by- k

Properties of SVD

- If X is rank- r , then $X = \sum_{i=1}^r \sigma_i u_i v_i^T$
 - X is a sum of r rank-1 matrices scaled with singular values
- $\|X\|_F^2 = \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_{\min(n,m)}^2$
- $\|X\|_2 = \sigma_1$
- **Eckart–Young theorem.** Let X be of rank- r and let $U\Sigma V^T$ be its SVD. Denote by U_k the first k columns of U , by V_k the first k columns of V and by Σ_k the upper-left k -by- k corner of Σ . Then $X_k = U_k \Sigma_k V_k^T$ is the best rank- k approximation of X in the sense that $\|X - X_k\|_F \leq \|X - Y\|_F$ and $\|X - X_k\|_2 \leq \|X - Y\|_2$ for any rank- k matrix Y .

SVD and pseudo-inverse

- Recall that if X is n -by- m with $\text{rank}(X) = m \leq n$, the *pseudo-inverse* of X is $X^+ = (X^T X)^{-1} X^T$
- If $\text{rank}(X) = r$ and $X = U \Sigma V^T$, then we can define $X^+ = V \Sigma^+ U^T$
 - Σ^+ is a diagonal matrix with $1/\sigma_i$ in its i th position (or 0 if $\sigma_i = 0$)
 - More general than the above definition
- This gives the least-squares solution to the following problem: given A and X , find Y s.t. $\|A - XY\|_F^2$ is minimized
 - Setting $Y = X^+ A$ minimizes the squared Frobenius norm

SVD and eigendecomposition

- Let X be n -by- m and $X = U\Sigma V^T$ its SVD
- The **Gram matrix** of the columns of X is $X^T X$
 - For the rows it is XX^T
- Now $X^T X = (U\Sigma V^T)^T (U\Sigma V^T) = V\Sigma^T U^T U\Sigma V^T$
 $= V\Sigma^T \Sigma V^T = V\Sigma_m^2 V^T$
 - Σ_m^2 is an m -by- m diagonal matrix with σ_i^2 in its i th position
- Similarly $XX^T = U\Sigma_n^2 U^T$
- Therefore
 - Columns of U are the eigenvectors of XX^T
 - Columns of V are the eigenvectors of $X^T X$
 - Singular values are square roots of the associated eigenvalues