

ENM 3600: AI for Science and Engineering

Lecture #2: Primer on Linear Algebra and Scientific Computing



Lecture outline

Scientific computing



Linear algebra



Matrix/vector calculus/operations

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

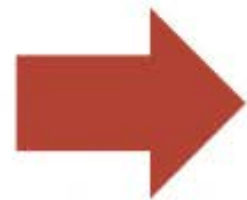
Useful resources:

- <https://pabloinsente.github.io/intro-linear-algebra>
- https://www.youtube.com/playlist?list=PLZHQQObOWTQDPD3MizzM2xVFitgF8hE_ab

Examples

Word  Vector

Vocabulary:
Man, woman, boy,
girl, prince,
princess, queen,
king, monarch



	1	2	3	4	5	6	7	8	9
man	1	0	0	0	0	0	0	0	0
woman	0	1	0	0	0	0	0	0	0
boy	0	0	1	0	0	0	0	0	0
girl	0	0	0	1	0	0	0	0	0
prince	0	0	0	0	1	0	0	0	0
princess	0	0	0	0	0	1	0	0	0
queen	0	0	0	0	0	0	1	0	0
king	0	0	0	0	0	0	0	1	0
monarch	0	0	0	0	0	0	0	0	1

Each word gets
a 1x9 vector
representation

Examples

Image  Matrix  Vector

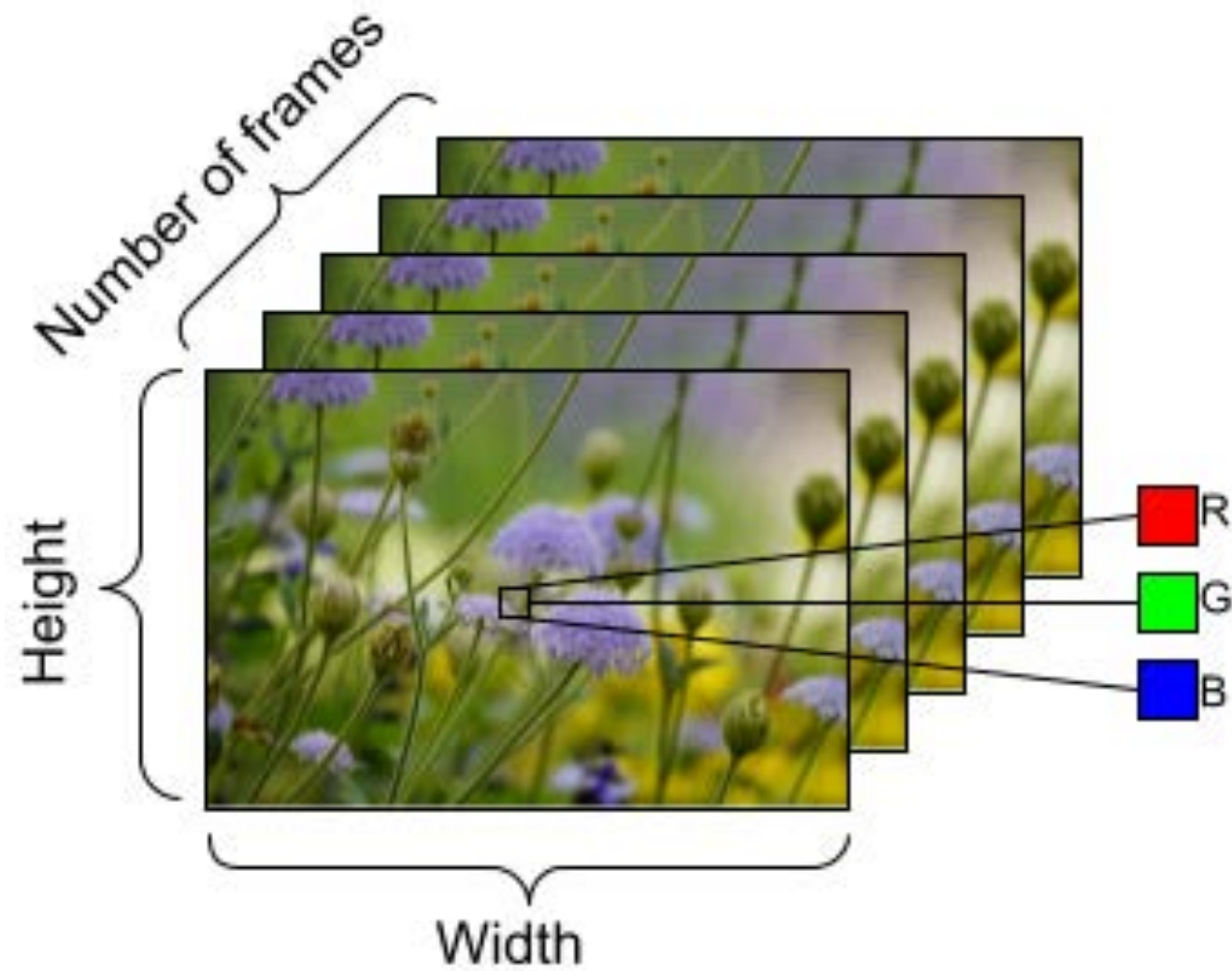


157	153	174	168	150	152	129	151	172	161	155	156
155	182	163	74	75	62	33	17	110	210	180	154
180	180	50	14	34	6	10	33	48	106	159	181
206	109	5	124	131	111	120	204	166	15	56	180
194	68	137	251	237	239	239	228	227	87	71	201
172	106	207	233	233	214	220	239	228	98	74	206
188	88	179	209	185	215	211	158	139	75	20	169
189	97	165	84	10	168	134	11	31	62	22	148
199	168	191	193	158	227	178	143	182	106	36	190
205	174	155	252	236	231	149	178	228	43	95	234
190	216	116	149	236	187	86	150	79	38	218	241
190	224	147	108	227	210	127	102	36	101	255	224
190	214	173	66	103	143	96	50	2	109	249	215
187	196	235	75	1	81	47	0	6	217	255	211
183	202	237	145	0	0	12	108	200	138	243	236
195	206	123	207	177	121	123	200	175	13	96	218

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199	168	191	193	158	227	178	143	182	106	36	190
205	174	155	252	236	231	149	178	228	43	95	234
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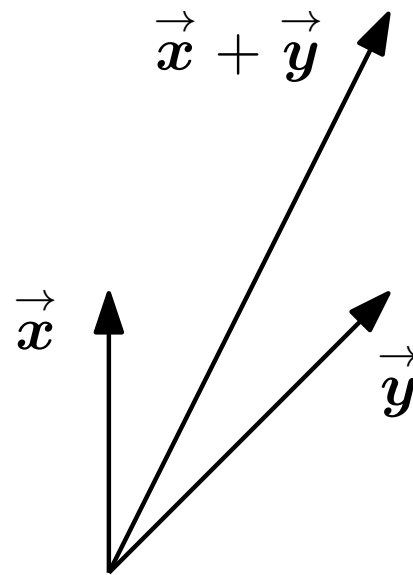
Timeseries

Image  Matrix  Vector

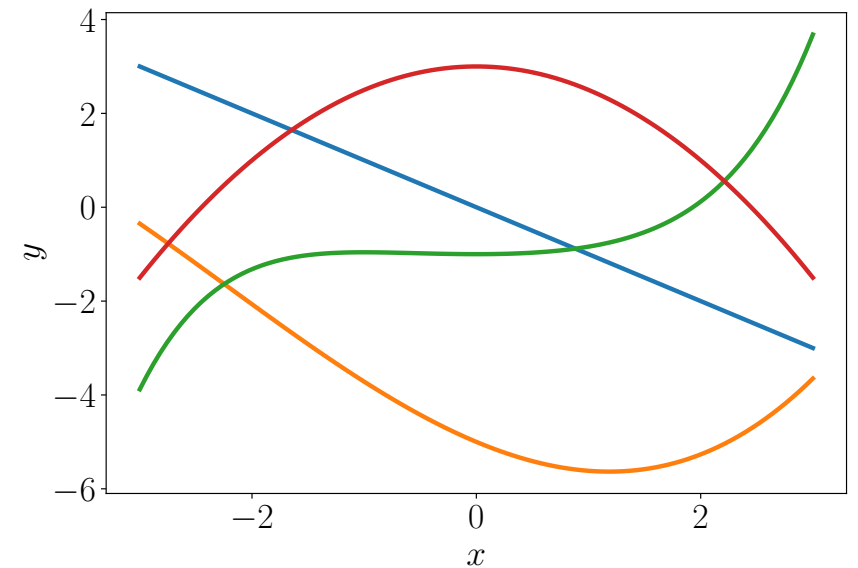


Vectors

- Basic definitions
- Vector operations (e.g. addition, subtraction, multiplication, etc.)
- Linear combinations
- Dot products
- Norms
- Vector/Linear spaces
- Linear (in)dependence
- Bases



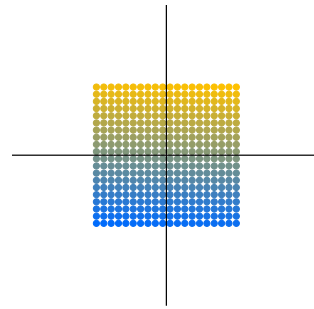
(a) Geometric vectors.



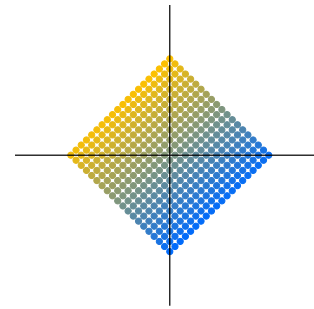
(b) Polynomials.

Matrices

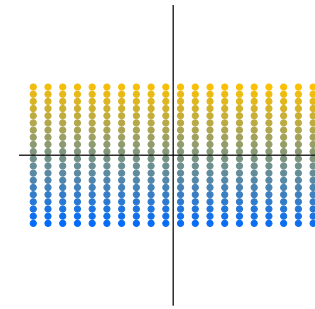
- Basic definitions
- Matrix operations (e.g. addition, subtraction, multiplication, etc.)
- Unit matrices, transposes, inverses
- Basic properties
- Norms
- Linear transformation of vectors
- Eigenvalues and eigenvectors
- Linear systems



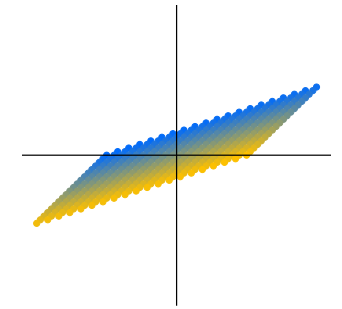
(a) Original data.



(b) Rotation by 45° .



(c) Stretch along the horizontal axis.



(d) General linear mapping.

$$\underbrace{\mathbf{A}}_{n \times k} \underbrace{\mathbf{B}}_{k \times m} = \underbrace{\mathbf{C}}_{n \times m}$$

For $\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{bmatrix} \in \mathbb{R}^{2 \times 3}$, $\mathbf{B} = \begin{bmatrix} 0 & 2 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \in \mathbb{R}^{3 \times 2}$, we obtain

$$\mathbf{AB} = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} 0 & 2 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 3 \\ 2 & 5 \end{bmatrix} \in \mathbb{R}^{2 \times 2},$$

$$2x_1 + 3x_2 + 5x_3 = 1$$

$$4x_1 - 2x_2 - 7x_3 = 8$$

$$9x_1 + 5x_2 - 3x_3 = 2$$

$$\begin{bmatrix} 2 & 3 & 5 \\ 4 & -2 & -7 \\ 9 & 5 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 8 \\ 2 \end{bmatrix}$$

Useful resources:

- https://see.stanford.edu/materials/lsoeldsee263/Additional2-matrix_crimes.pdf

Linear systems

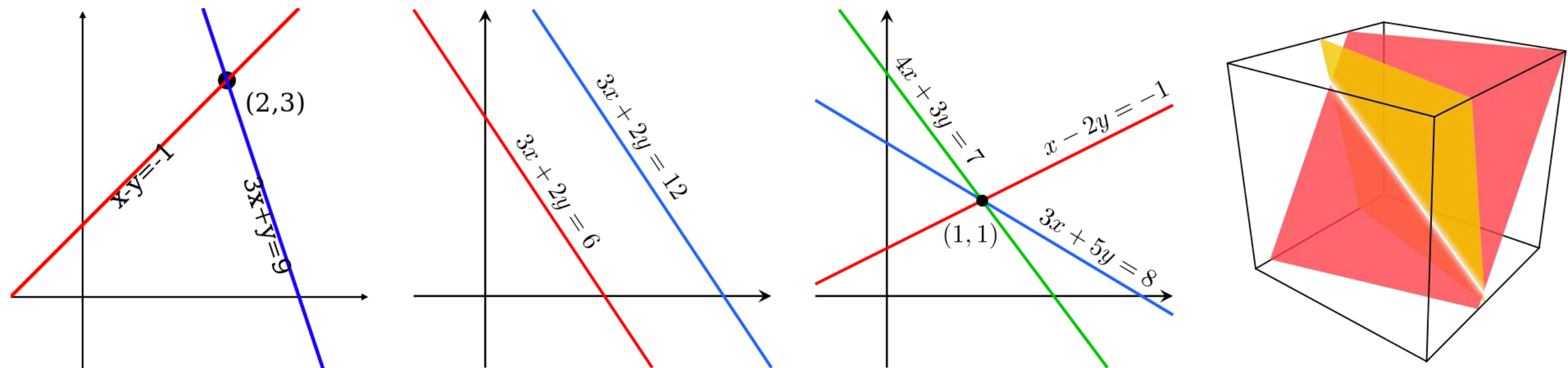
- Direct solvers:
 - Gauss elimination/LU decomposition
 - Cholesky decomposition (SPD matrices)
 - QR decomposition
 - SVD
- Iterative solvers:
 - Jacobi iterations
 - Gauss-Seidel
 - Successive over-relaxation (SOR)
 - Krylov subspace methods (conjugate gradients, etc.)

$$2x_1 + 3x_2 + 5x_3 = 1$$

$$4x_1 - 2x_2 - 7x_3 = 8$$

$$9x_1 + 5x_2 - 3x_3 = 2$$

$$\begin{bmatrix} 2 & 3 & 5 \\ 4 & -2 & -7 \\ 9 & 5 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 8 \\ 2 \end{bmatrix}$$



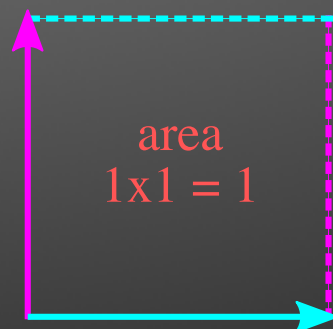
Useful resources:

- Gilbert Strang's lectures at MIT OCW: <https://ocw.mit.edu/courses/mathematics/18-06-linear-algebra-spring-2010/video-lectures/>
- Pavel Grinfeld's series on linear algebra: <https://www.youtube.com/playlist?list=PLIXfTHzgMRUKXD88ldzSI4F4NxAZudSmv>

Determinants

Determinants as scaling factors

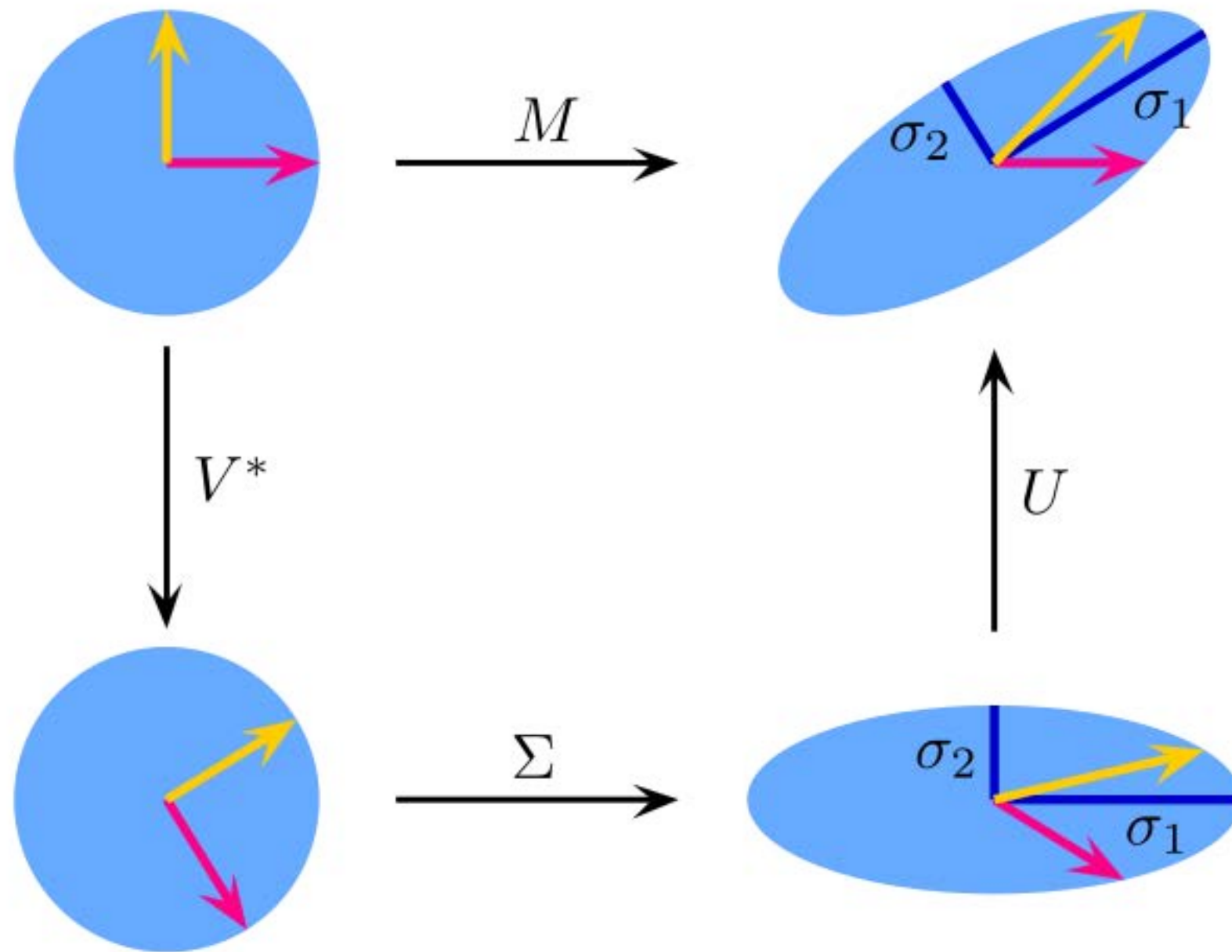
$$A\mathbf{x} = \begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ 3 \end{bmatrix}$$



$$\det(A) = 8$$



Singular Value Decomposition



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

Derivatives & Jacobians

		vector	
	scalar	x	\mathbf{x}
scalar	f	$\frac{\partial f}{\partial x}$	$\frac{\partial f}{\partial \mathbf{x}}$
vector	\mathbf{f}	$\frac{\partial \mathbf{f}}{\partial x}$	$\frac{\partial \mathbf{f}}{\partial \mathbf{x}}$