

ENM 3600: AI for Science and Engineering

Lecture #1: Primer on Linear Algebra and Scientific Computing



Lecture outline

Scientific computing



Linear algebra



Matrix/vector calculus/operations

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

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

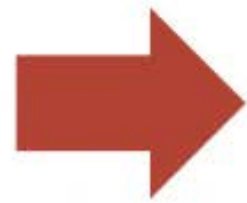
Useful resources:

- <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

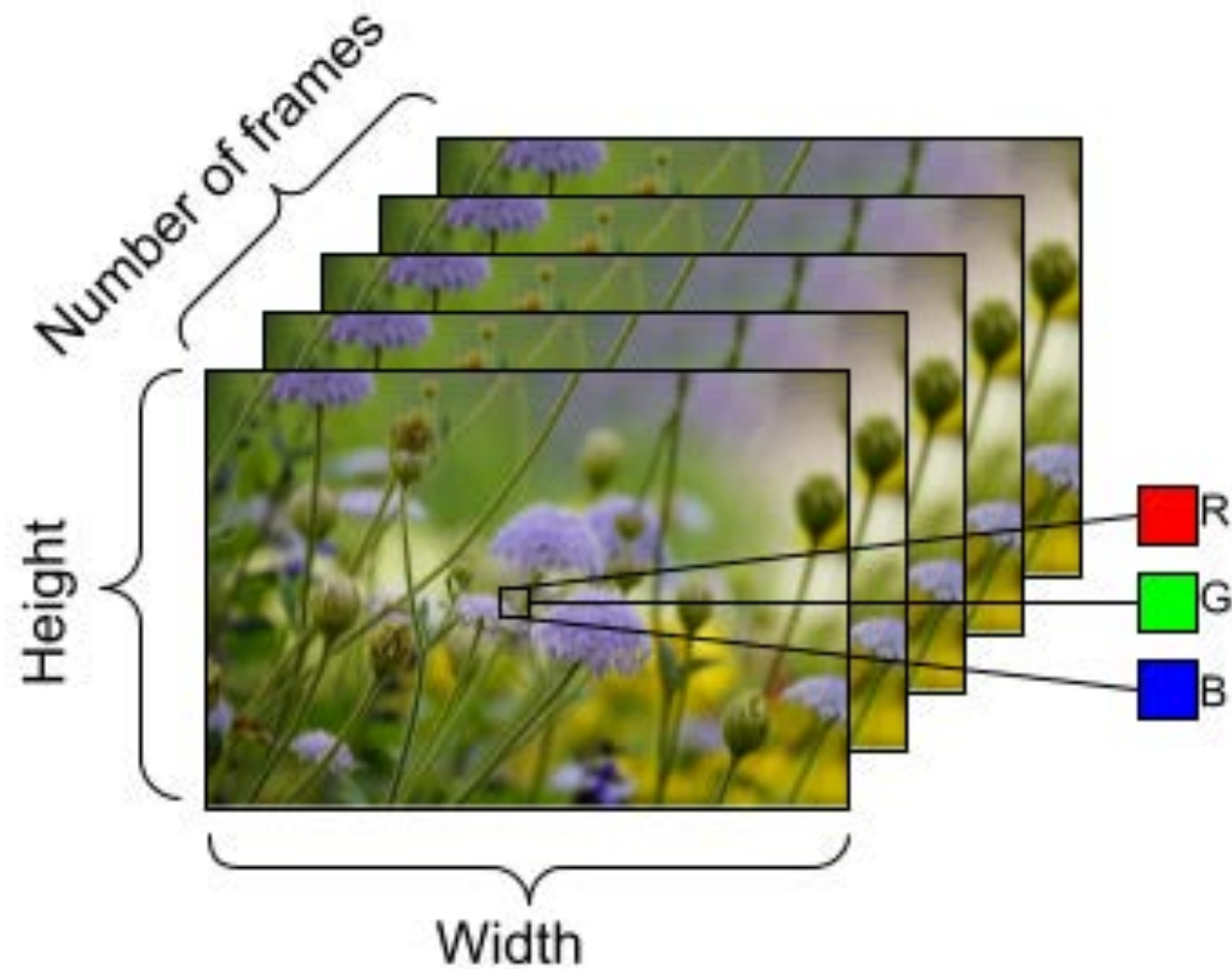


| | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 157 | 153 | 174 | 168 | 150 | 152 | 129 | 151 | 172 | 161 | 155 | 156 |
| 155 | 182 | 163 | 74 | 75 | 62 | 33 | 17 | 110 | 210 | 180 | 154 |
| 180 | 180 | 50 | 14 | 34 | 6 | 10 | 33 | 48 | 106 | 159 | 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 |

| | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 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 |

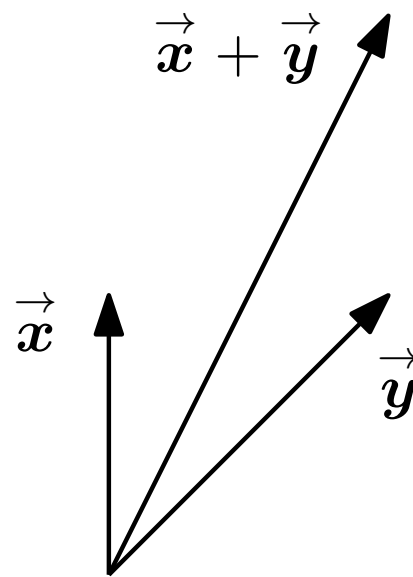
Timeseries

Image  Matrix  Vector

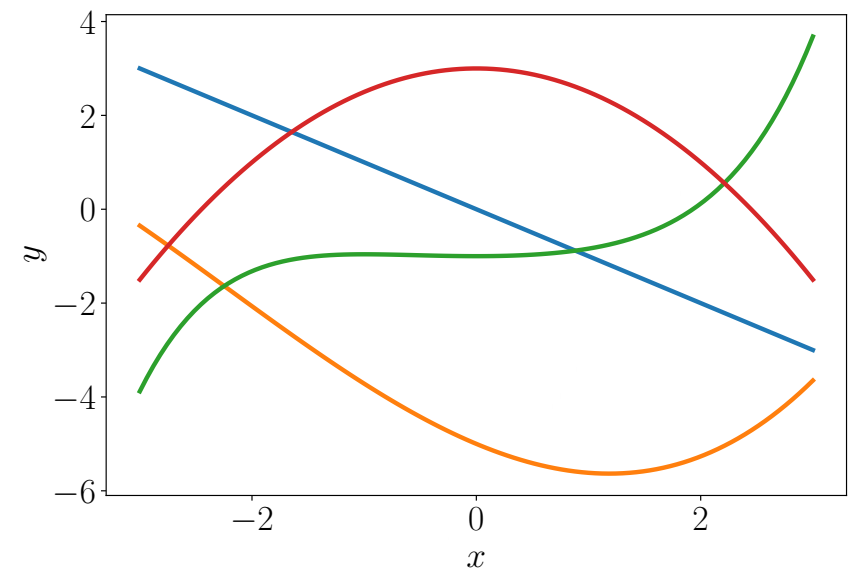


Vectors

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



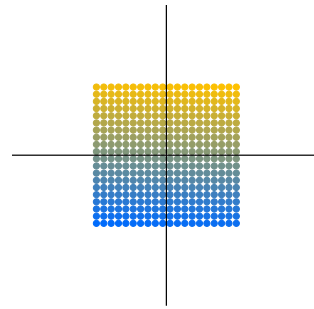
(a) Geometric vectors.



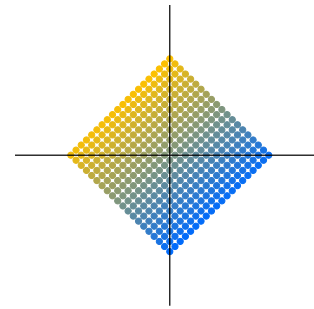
(b) Polynomials.

Matrices

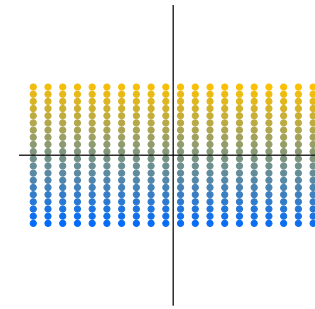
- Basic definitions
- Matrix operations (e.g. addition, subtraction, multiplication, etc.)
- Unit matrices, transposes, inverses
- Basic properties
- Norms
- Linear transformation of vectors
- Eigenvalues and eigenvectors
- Linear systems



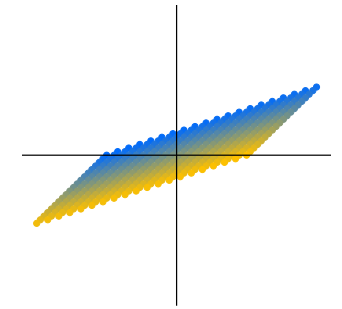
(a) Original data.



(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

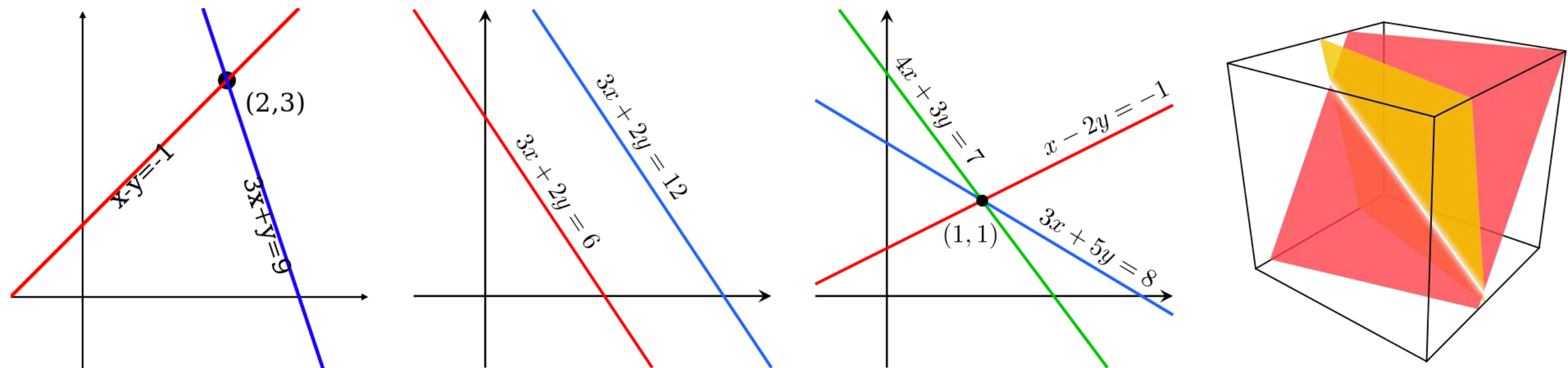
- Direct solvers:
 - Gauss elimination/LU decomposition
 - Cholesky decomposition (SPD matrices)
 - QR decomposition
 - SVD
- Iterative solvers:
 - Jacobi iterations
 - Gauss-Seidel
 - Successive over-relaxation (SOR)
 - Krylov subspace methods (conjugate gradients, etc.)

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

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

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

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



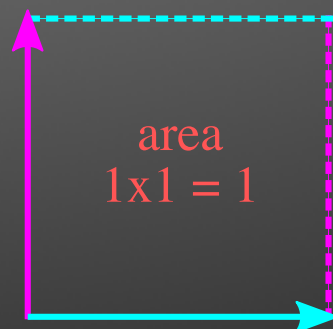
Useful resources:

- 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

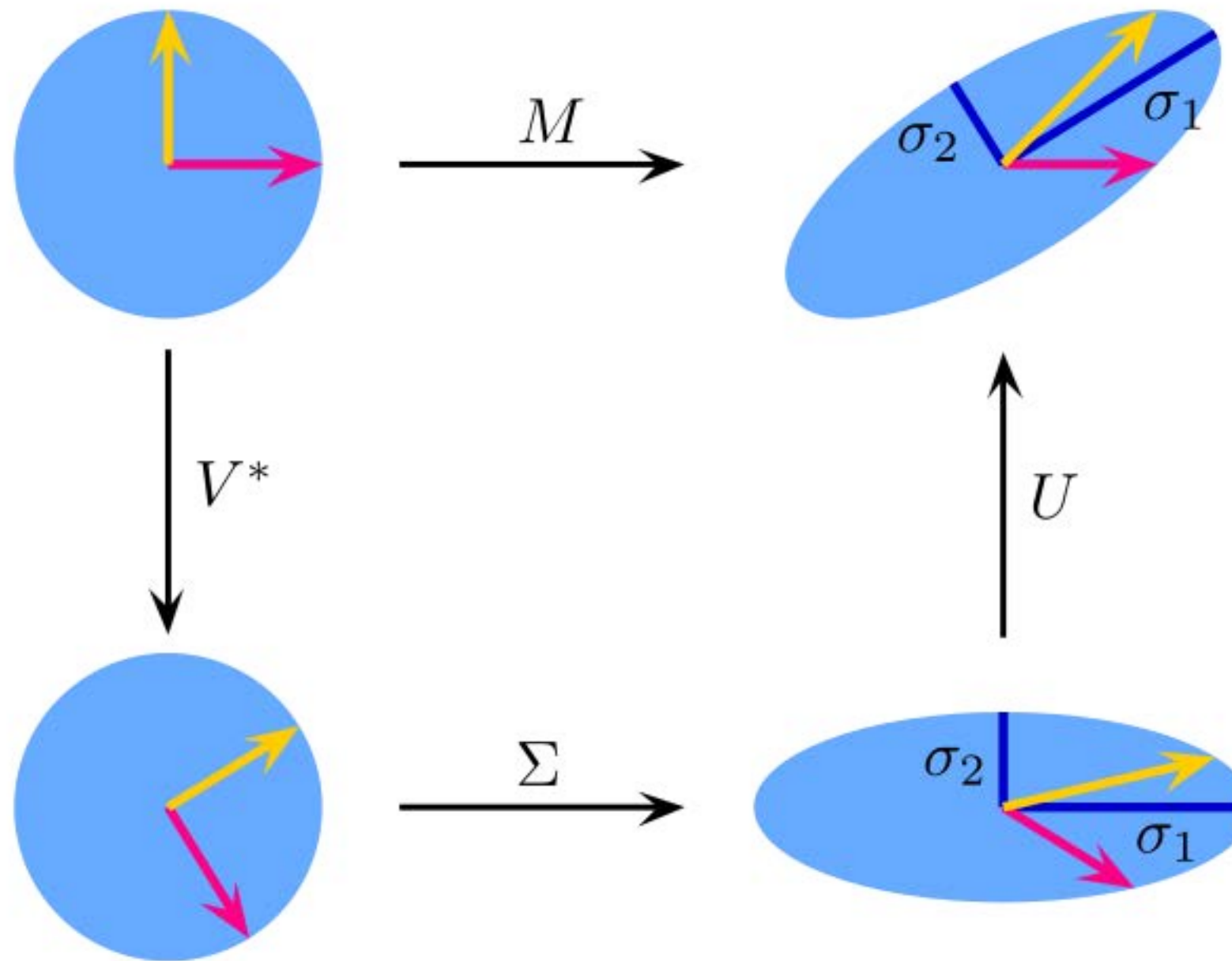
$$A\mathbf{x} = \begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ 3 \end{bmatrix}$$



$$\det(A) = 8$$



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} | $\frac{\partial \mathbf{f}}{\partial x}$ | $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}$ |