Linear Algebra Primer

Joshua Jung

Homogeneous system

- In general, a matrix multiplication lets us linearly combine components of a vector

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \times \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} ax + by \\ cx + dy \end{bmatrix}$$

  - This is sufficient for scale, rotate, skew transformations.
  - But notice, we can't add a constant! ☹

Homogeneous system

– The (somewhat hacky) solution? Stick a “1” at the end of every vector:

$$\begin{bmatrix} a & b & c \\ d & e & f \\ 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} ax + by + c \\ dx + ey + f \\ 1 \end{bmatrix}$$

– Now we can rotate, scale, and skew like before, AND translate (note how the multiplication works out, above)

– This is called “homogeneous coordinates”

Homogeneous system

– In homogeneous coordinates, the multiplication works out so the rightmost column of the matrix is a vector that gets added.

$$\begin{bmatrix} a & b & c \\ d & e & f \\ 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} ax + by + c \\ dx + ey + f \\ 1 \end{bmatrix}$$

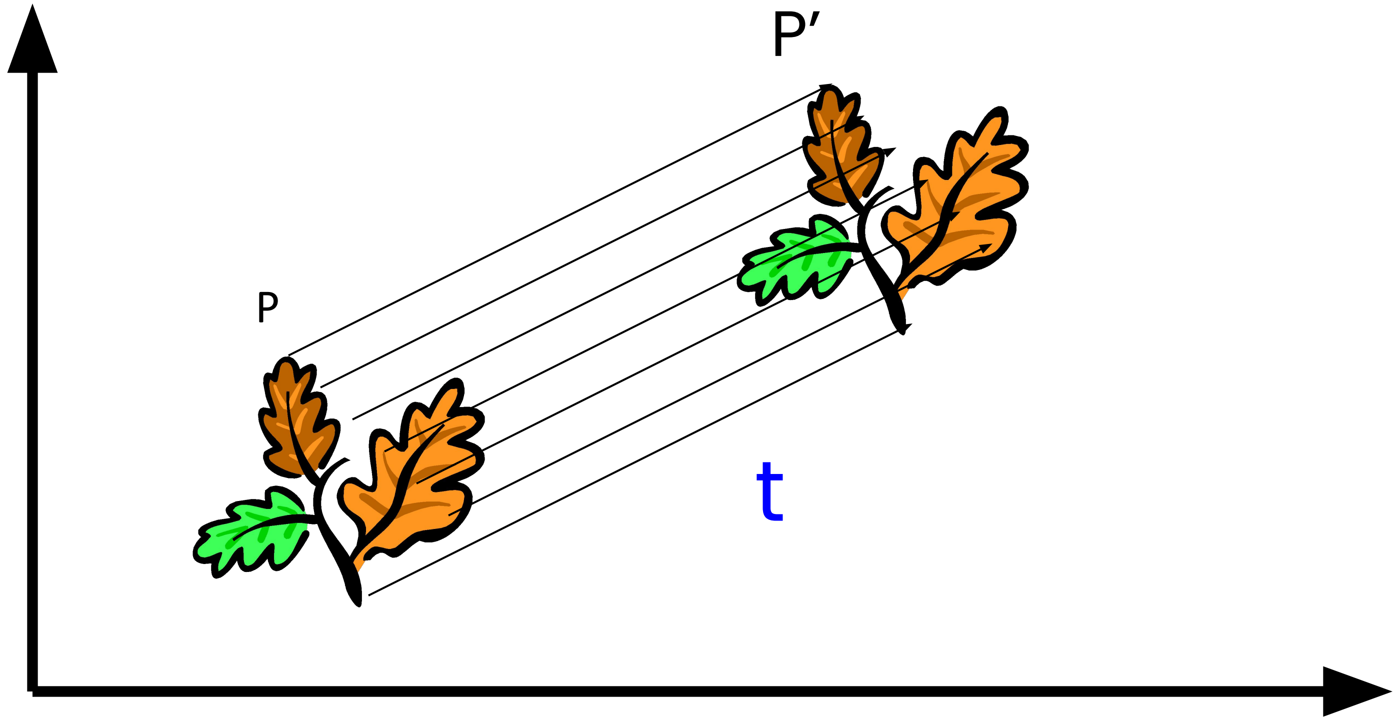
– Generally, a homogeneous transformation matrix will have a bottom row of [0 0 1], so that the result has a “1” at the bottom too.

Homogeneous system

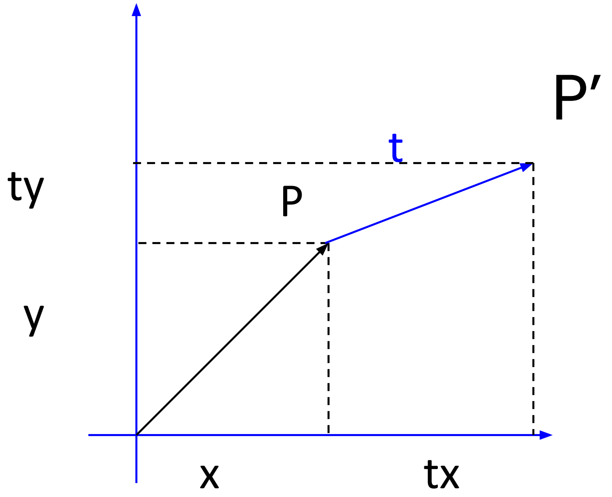
- One more thing we might want: to divide the result by something
  - For example, we may want to divide by a coordinate, to make things scale down as they get farther away in a camera image
  - Matrix multiplication can't actually divide
  - So, **by convention**, in homogeneous coordinates, we'll divide the result by its last coordinate after doing a matrix multiplication

$$\begin{bmatrix} x \\ y \\ 7 \end{bmatrix} \Rightarrow \begin{bmatrix} x/7 \\ y/7 \\ 1 \end{bmatrix}$$

2D Translation



2D Translation using Homogeneous Coordinates



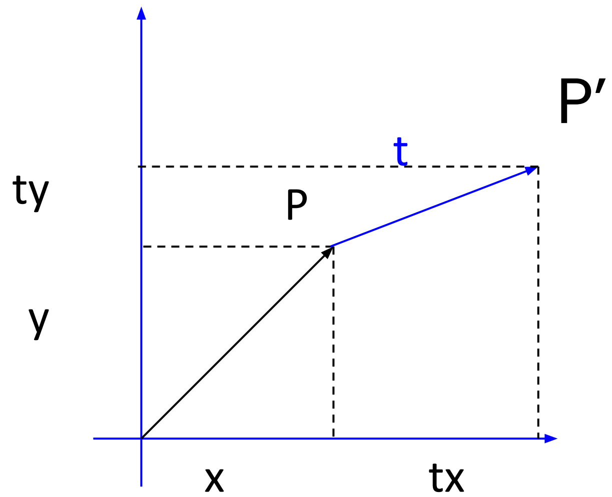
$$\mathbf{P} = (x, y) \rightarrow (x, y, 1)$$

$$\mathbf{t} = (t_x, t_y) \rightarrow (t_x, t_y, 1)$$

P

$$\mathbf{P'} \rightarrow \begin{bmatrix} x + t_x \\ y + t_y \\ 1 \end{bmatrix} = \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ 1 \end{bmatrix}$$

2D Translation using Homogeneous Coordinates



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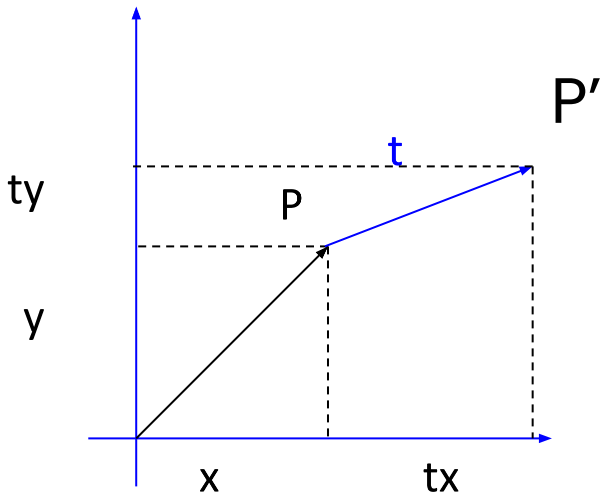

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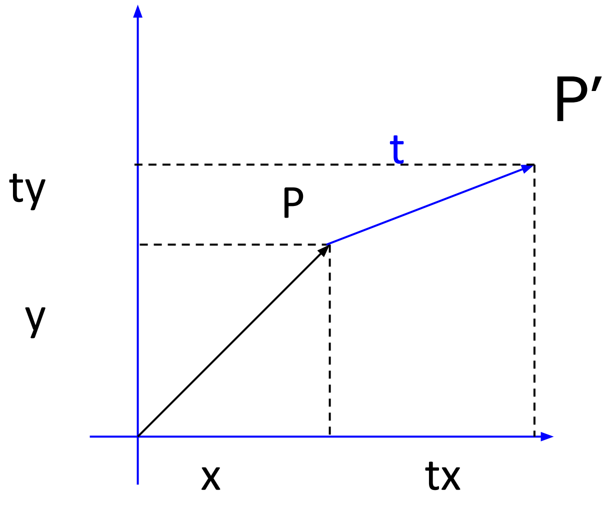
2D Translation using Homogeneous Coordinates



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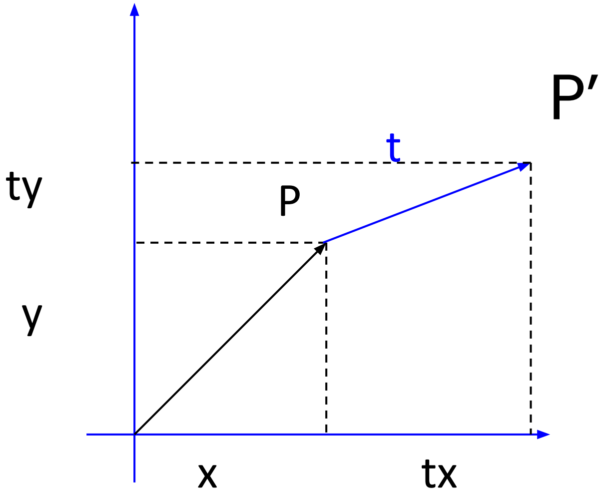
2D Translation using Homogeneous Coordinates



$$\mathbf{P} = (x, y) \rightarrow (x, y, 1)$$

$$\mathbf{t} = (t_x, t_y) \rightarrow (t_x, t_y, 1)$$

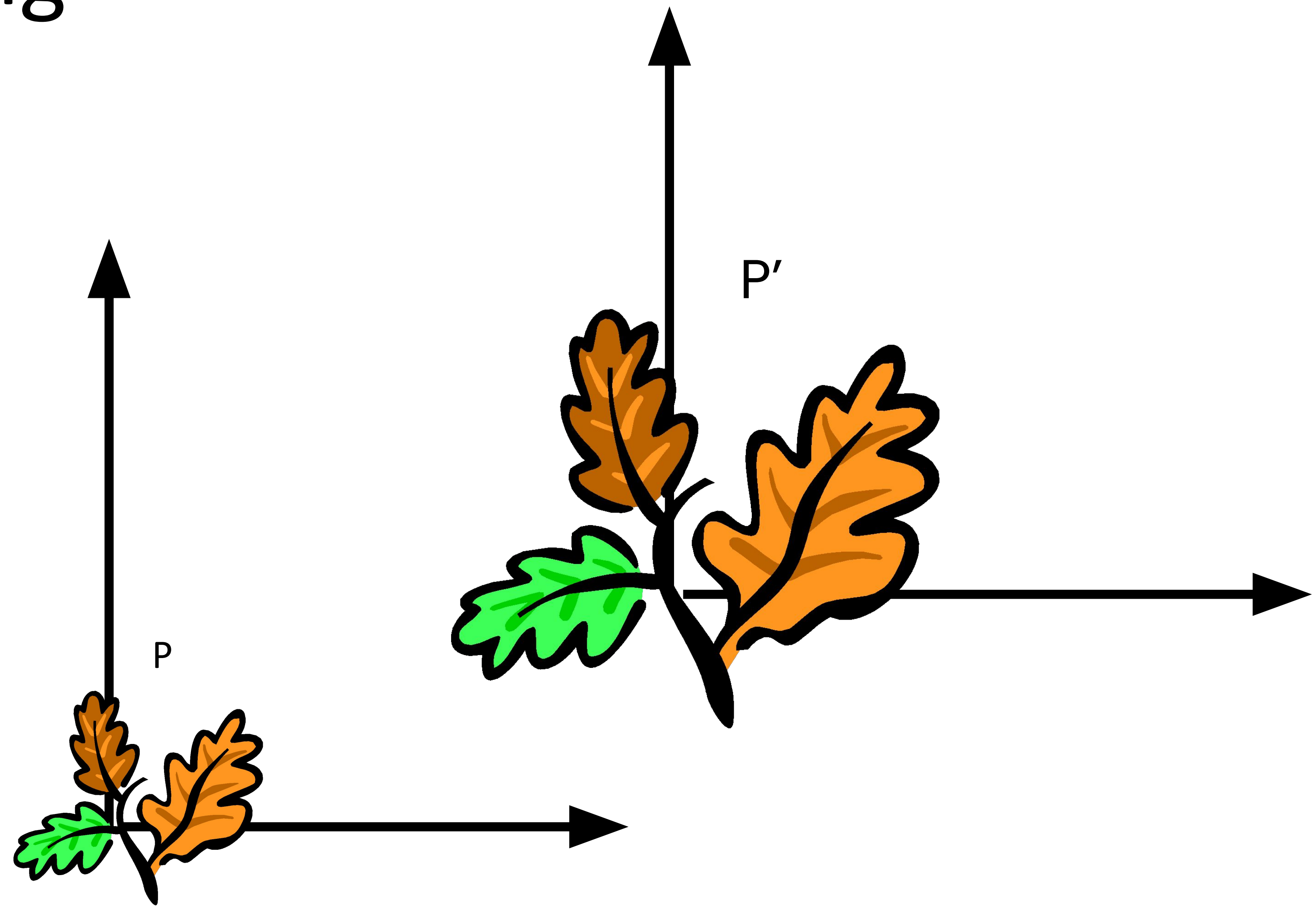
t

P

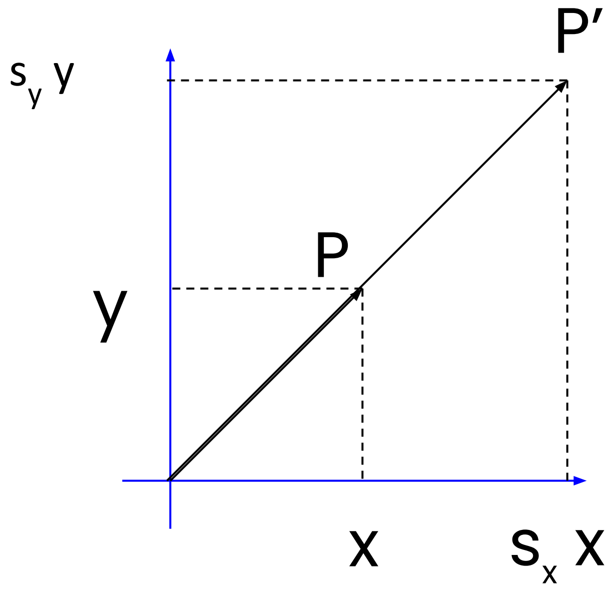
$$\mathbf{P'} \rightarrow \begin{bmatrix} x + t_x \\ y + t_y \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & t_x \\ 0 & 1 & t_y \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} \mathbf{I} & \mathbf{t} \\ 0 & 1 \end{bmatrix} \cdot \mathbf{P} = \mathbf{T} \cdot \mathbf{P}$$

Scaling



Scaling Equation



$$\mathbf{P} = (\mathrm{x}, \mathrm{y}) \rightarrow \mathbf{P}' = (\mathrm{s_x x}, \mathrm{s_y y})$$

$$\mathbf{P} = (x, y) \rightarrow (x, y, 1)$$

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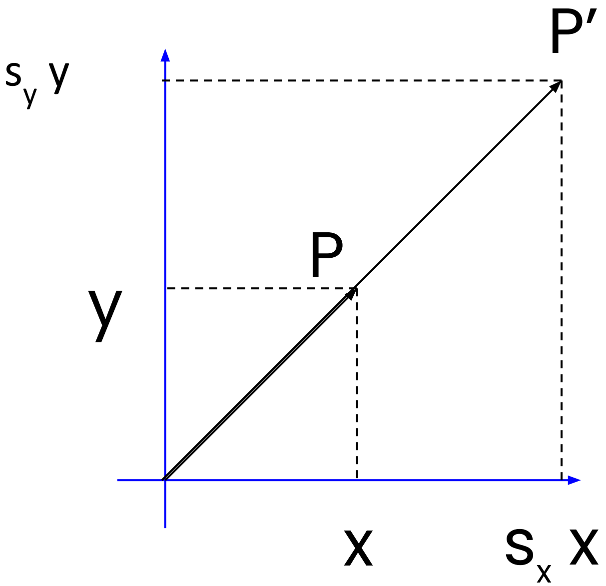
Scaling Equation



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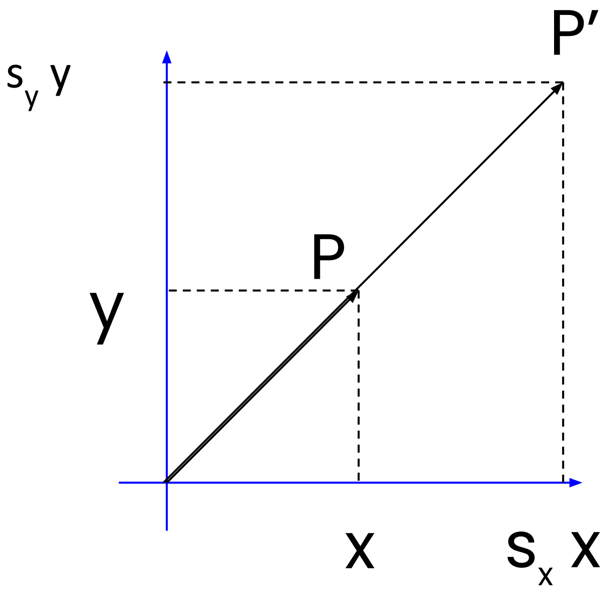
$$\mathbf{P}' \rightarrow \begin{bmatrix} s_x x \\ s_y y \\ 1 \end{bmatrix} = \begin{bmatrix} \quad & \quad & \quad \\ \quad & \quad & \quad \\ \quad & \quad & \quad \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ 1 \end{bmatrix}$$

Scaling Equation



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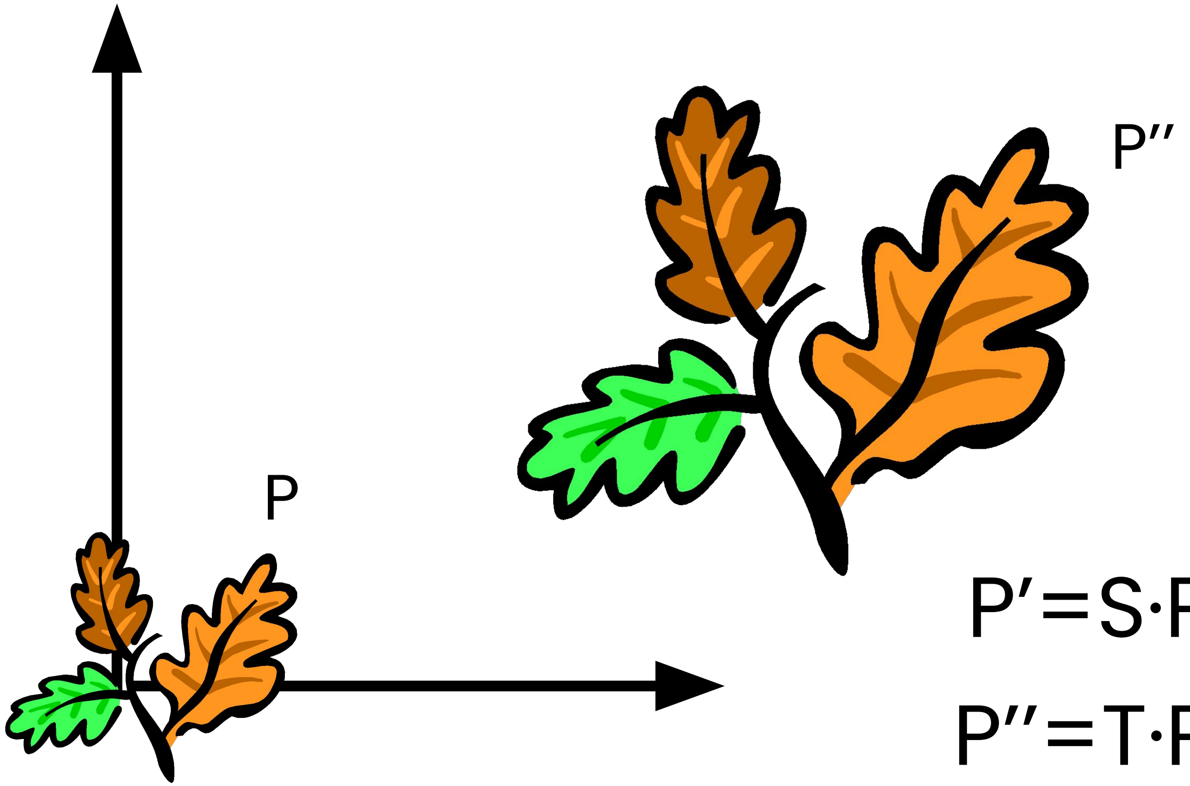
$$\mathbf{P'} \rightarrow \begin{bmatrix} s_x x \\ s_y y \\ 1 \end{bmatrix} = \underbrace{\begin{bmatrix} s_x & 0 & 0 \\ 0 & s_y & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\mathbf{S}} \cdot \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} \mathbf{S'} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{bmatrix} \cdot \mathbf{P} = \mathbf{S} \cdot \mathbf{P}$$

Scaling & Translating



$P' = S \cdot P$

$P'' = T \cdot P'$

$P'' = T \cdot P' = T \cdot (S \cdot P) = T \cdot S \cdot P$

Scaling & Translating

$$\mathbf{P}'' = \mathbf{T} \cdot \mathbf{S} \cdot \mathbf{P} = \begin{bmatrix} 1 & 0 & t_x \\ 0 & 1 & t_y \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} s_x & 0 & 0 \\ 0 & s_y & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix}$$

Scaling & Translating

$$\mathbf{P}'' = \mathbf{T} \cdot \mathbf{S} \cdot \mathbf{P} = \begin{bmatrix} 1 & 0 & t_x \\ 0 & 1 & t_y \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} s_x & 0 & 0 \\ 0 & s_y & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} =$$

$$= \begin{bmatrix} s_x & 0 & t_x \\ 0 & s_y & t_y \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} s_x x + t_x \\ s_y y + t_y \\ 1 \end{bmatrix} = \begin{bmatrix} S & t \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix}$$

Translating & Scaling != Scaling & Translating

$$\mathbf{P}''' = \mathbf{T} \cdot \mathbf{S} \cdot \mathbf{P} = \begin{bmatrix} 1 & 0 & t_x \\ 0 & 1 & t_y \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} s_x & 0 & 0 \\ 0 & s_y & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} s_x & 0 & t_x \\ 0 & s_y & t_y \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} s_x x + t_x \\ s_y y + t_y \\ 1 \end{bmatrix}$$

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Translating & Scaling != Scaling & Translating

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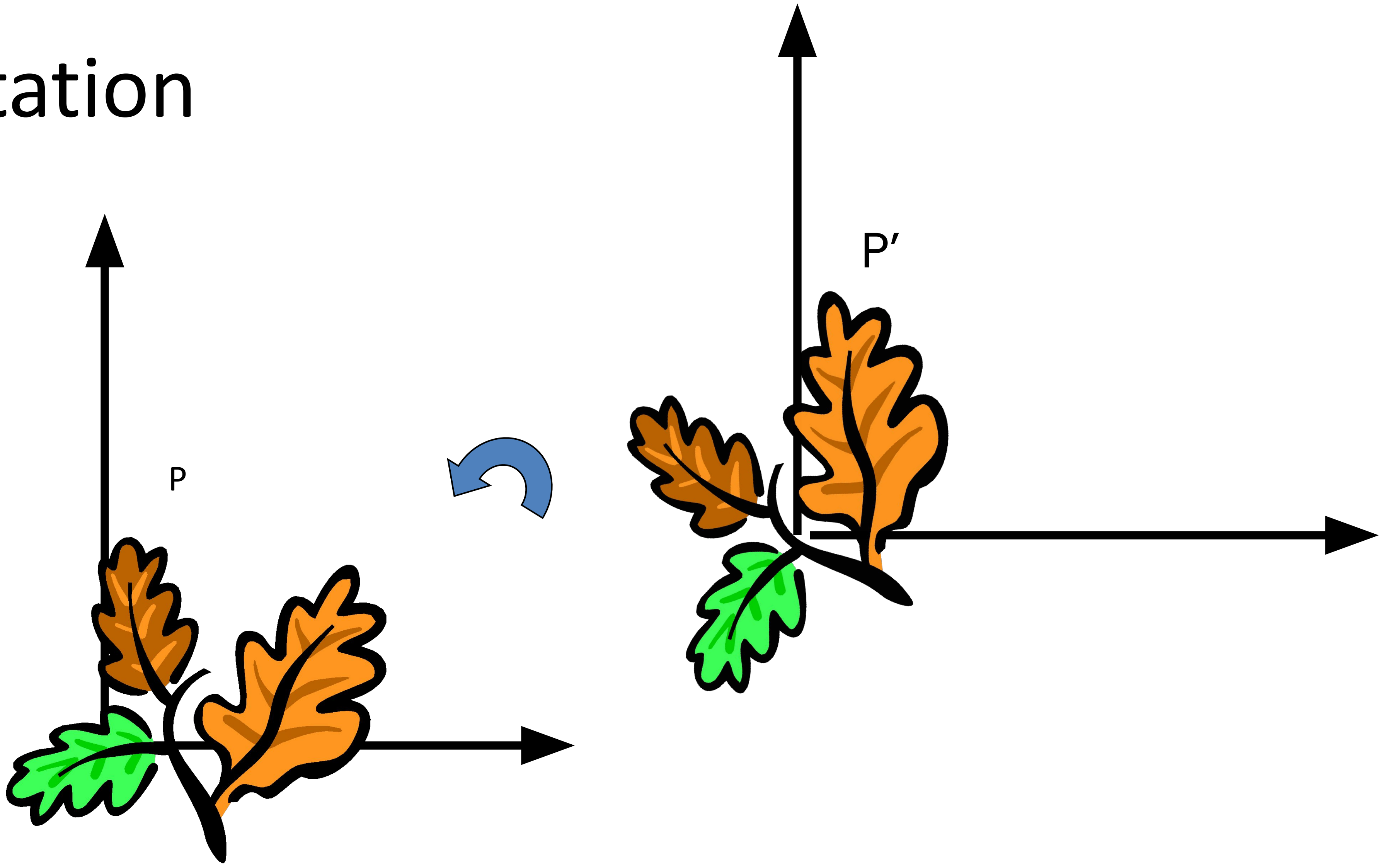
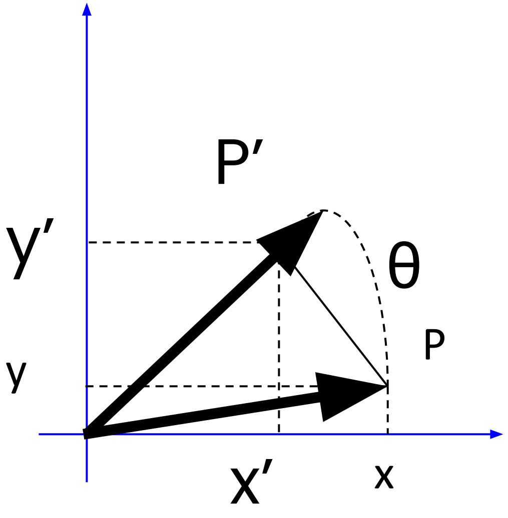
Rotation



Rotation Equations

Counter-clockwise rotation by an angle θ



$$x' = \cos\theta\, x - \sin\theta\, y$$

$$y' = \cos\theta\, y + \sin\theta\, x$$

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\mathbf{P'} = \mathbf{R}\ \mathbf{P}$$

Rotation Matrix Properties

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

A 2D rotation matrix is 2x2

Note: R belongs to the category of *normal* matrices
and satisfies many interesting properties:

$$\mathbf{R} \cdot \mathbf{R}^{\mathrm{T}} = \mathbf{R}^{\mathrm{T}} \cdot \mathbf{R} = \mathbf{I}$$

$$\det(\mathbf{R}) = 1$$

Rotation Matrix Properties

- Transpose of a rotation matrix produces a rotation in the opposite direction

$$\mathbf{R} \cdot \mathbf{R}^{\mathrm{T}} = \mathbf{R}^{\mathrm{T}} \cdot \mathbf{R} = \mathbf{I}$$

$$\det(\mathbf{R}) = 1$$

- The rows of a rotation matrix are always mutually perpendicular (a.k.a. orthogonal) unit vectors
  – (and so are its columns)

Scaling + Rotation + Translation

P'= (T R S) P

$$\mathbf{P'} = \mathbf{T} \cdot \mathrm{R} \cdot \mathbf{S} \cdot \mathbf{P} = \begin{bmatrix} 1 & 0 & t_x \\ 0 & 1 & t_y \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} s_x & 0 & 0 \\ 0 & s_y & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} =$$

$$= \begin{bmatrix} \cos\theta & -\sin\theta & t_x \\ \sin\theta & \cos\theta & t_y \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} s_x & 0 & 0 \\ 0 & s_y & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} =$$

$$= \begin{bmatrix} R & t \\ 0 & 1 \end{bmatrix} \begin{bmatrix} S & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} R\,S & t \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix}$$

This is the form of the general-purpose transformation matrix

Outline

- Vectors and matrices
  - Basic Matrix Operations
  - Determinants, norms, trace
  - Special Matrices
- Transformation Matrices
  - Homogeneous coordinates
  - Translation
- **Matrix inverse**
- Matrix rank
- Eigenvalues and Eigenvectors
- Matrix Calculate

The inverse of a transformation matrix reverses its effect

Inverse

- Given a matrix **A**, its inverse $\mathbf{A}^{-1}$ is a matrix such that $\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$
- E.g. $\begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{3} \end{bmatrix}$
- Inverse does not always exist. If $\mathbf{A}^{-1}$ exists, **A** is *invertible* or *non-singular*. Otherwise, it's *singular*.
- Useful identities, for matrices that are invertible:

$$(\mathbf{A}^{-1})^{-1} = \mathbf{A}$$

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$$

$$\mathbf{A}^{-T} \triangleq (\mathbf{A}^{T})^{-1} = (\mathbf{A}^{-1})^{T}$$

Matrix Operations

- Pseudoinverse
  - Fortunately, there are workarounds to solve AX=B in these situations. And python can do them!
  - Instead of taking an inverse, directly ask python to solve for X in AX=B, by typing **np.linalg.solve(A, B)**
  - Python will try several appropriate numerical methods (including the pseudoinverse if the inverse doesn't exist)
  - Python will return the value of X which solves the equation
    - If there is no exact solution, it will return the closest one
    - If there are many solutions, it will return the smallest one

Matrix Operations

- Python example:

$$AX = B$$

$$A = \begin{bmatrix} 2 & 2 \\ 3 & 4 \end{bmatrix}, B = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

```
>> import numpy as np
>> x = np.linalg.solve(A,B)
x =
     1.0000
    -0.5000
```

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The rank of a transformation matrix tells you how many dimensions it transforms a vector to.

Linear independence

- Suppose we have a set of vectors $\mathbf{v_1, \ldots, v_n}$
- If we can express $\mathbf{v}_1$ as a linear combination of the other vectors $\mathbf{v}_2 \ldots \mathbf{v}_n$, then $\mathbf{v}_1$ is linearly *dependent* on the other vectors.
  - The direction $\mathbf{v}_1$ can be expressed as a combination of the directions $\mathbf{v}_2 \ldots \mathbf{v}_n$. (E.g. $\mathbf{v}_1 = .7\ \mathbf{v}_2 - .7\ \mathbf{v}_4$)

Linear independence

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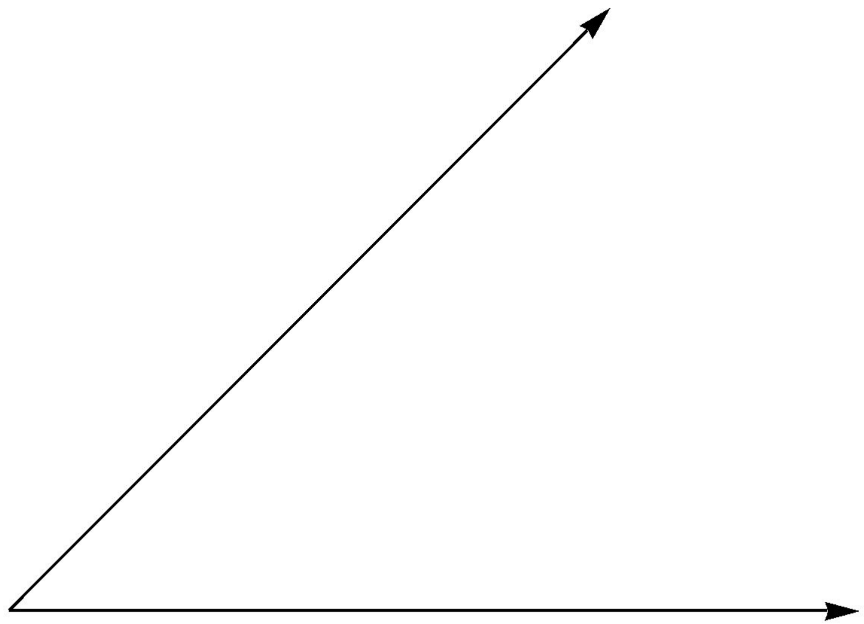
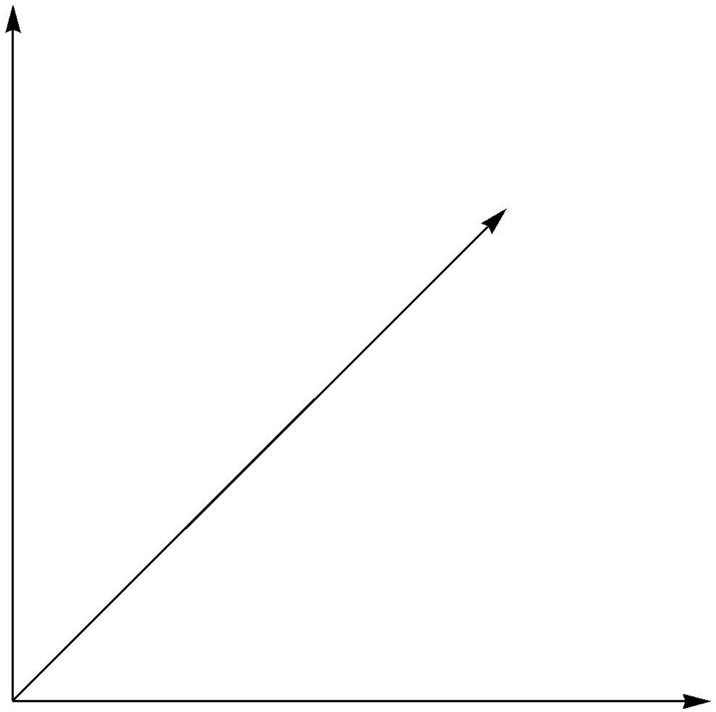
  - The direction $\mathbf{v}_1$ can be expressed as a combination of the directions $\mathbf{v}_2 \ldots \mathbf{v}_n$. (E.g. $\mathbf{v}_1 = .7\ \mathbf{v}_2 - .7\ \mathbf{v}_4$)
- If no vector is linearly dependent on the rest of the set, the set is linearly *independent*.
  - Common case: a set of vectors $\mathbf{v_1}, \ldots, \mathbf{v_n}$ is always linearly independent if each vector is perpendicular to every other vector (and non-zero)

Linear independence

Linearly independent set



Not linearly independent



Matrix rank

- Column/row rank

[redacted]

  – Column rank always equals row rank

- Matrix rank

$$\text{rank}(\mathbf{A}) \triangleq \text{col-rank}(\mathbf{A}) = \text{row-rank}(\mathbf{A})$$

Matrix rank

- For transformation matrices, the rank tells you the dimensions of the output
- E.g. if rank of **A** is 1, then the transformation

  p'=Ap

  maps points onto a line.
- Here's a matrix with rank 1:

$$\begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix} \times \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x + y \\ 2x + 2y \end{bmatrix}$$

← All points get mapped to the line y=2x

Matrix rank

- If an m x m matrix is rank m, we say it's "full rank"
  - Maps an m x 1 vector uniquely to another m x 1 vector
  - An inverse matrix can be found
- If rank < m, we say it's "singular"
  - At least one dimension is getting collapsed. No way to look at the result and tell what the input was
  - Inverse does not exist
- Inverse also doesn't exist for non-square matrices

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- Eigenvalues and Eigenvectors(SVD)
- Matrix Calculus

Eigenvector and Eigenvalue

- An eigenvector **x** of a linear transformation *A* is a non-zero vector that, when *A* is applied to it, does not change direction.

$$Ax = \lambda x, \quad x \neq 0.$$

Eigenvector and Eigenvalue

- An eigenvector **x** of a linear transformation *A* is a non-zero vector that, when *A* is applied to it, does not change direction.
- Applying *A* to the eigenvector only scales the eigenvector by the scalar value λ, called an eigenvalue.

$$Ax = \lambda x, \quad x \neq 0.$$

Eigenvector and Eigenvalue

- We want to find all the eigenvalues of A:

$$Ax = \lambda x, \quad x \neq 0.$$

- Which can we written as:

$$Ax = (\lambda I)x \quad x \neq 0.$$

- Therefore:

$$(\lambda I - A)x = 0, \quad x \neq 0.$$

Eigenvector and Eigenvalue

- We can solve for eigenvalues by solving:

$$(\lambda I - A)x = 0, \quad x \neq 0.$$

- Since we are looking for non-zero **x**, we can instead solve the above equation as:

$$|(\lambda I - A)| = 0.$$

Properties

- The trace of a A is equal to the sum of its eigenvalues:

$$\mathrm{tr}A = \sum_{i=1}^{n} \lambda_i.$$

- The determinant of A is equal to the product of its eigenvalues

$$|A| = \prod_{i=1}^{n} \lambda_i.$$

- The rank of A is equal to the number of non-zero eigenvalues of A.
- The eigenvalues of a diagonal matrix D = diag(d1, . . . dn) are just the diagonal entries d1, . . . dn

Spectral theory

- We call an eigenvalue λ and an associated eigenvector an **eigenpair**.
- The space of vectors where (A − λI) = 0 is often called the **eigenspace** of A associated with the eigenvalue λ.
- The set of all eigenvalues of A is called its **spectrum**:

$$\sigma(A) = \{\lambda \in \mathbb{C} : \lambda I - A \text{ is singular}\}.$$

Spectral theory

- The magnitude of the largest eigenvalue (in magnitude) is called the spectral radius

$$\rho(A) = \max\{|\lambda_1|, \ldots, |\lambda_n|\}$$

  - Where C is the space of all eigenvalues of A

Spectral theory

- The spectral radius is bounded by infinity norm of a matrix: $$\rho(A) = \lim_{k\to\infty} \|A^k\|^{1/k}$$
- Proof: Turn to a partner and prove this!

Spectral theory

- The spectral radius is bounded by infinity norm of a matrix: $$\rho(A) = \lim_{k\to\infty} \|A^k\|^{1/k}$$
- Proof: Let λ and v be an eigenpair of A:

$$|\lambda|^k \|\mathbf{v}\| = \|\lambda^k \mathbf{v}\| = \|A^k \mathbf{v}\| \le \|A^k\| \cdot \|\mathbf{v}\|$$

and since $\mathbf{v} \neq 0$ we have

$$|\lambda|^k \le \|A^k\|$$

and therefore

$$\rho(A) \le \|A^k\|^{\frac{1}{k}}.$$

Diagonalization

- An $n \times n$ matrix A is diagonalizable if it has n linearly independent eigenvectors.
- Most square matrices (in a sense that can be made mathematically rigorous) are diagonalizable:
  - Normal matrices are diagonalizable
  - Matrices with n distinct eigenvalues are diagonalizable

Lemma: Eigenvectors associated with distinct eigenvalues are linearly independent.

Diagonalization

- An $n \times n$ matrix A is diagonalizable if it has n linearly independent eigenvectors.
- Most square matrices are diagonalizable:
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Lemma: Eigenvectors associated with distinct eigenvalues are linearly independent.

Diagonalization

- Eigenvalue equation:

$$AV = VD$$
$$A = VDV^{-1}$$

  - Where D is a diagonal matrix of the eigenvalues

$$\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$$

Diagonalization

- Eigenvalue equation:

$$AV = VD$$

$$A = VDV^{-1}$$

- Assuming all λ_i's are unique:

$$A = VDV^T$$

  - Remember that the inverse of an orthogonal matrix is just its transpose and the eigenvectors are orthogonal

Symmetric matrices

- Properties:
  - For a symmetric matrix A, all the eigenvalues are real.
  - The eigenvectors of A are orthonormal.

$$A = VDV^T$$

Symmetric matrices

- Therefore:

$$x^T A x = x^T V D V^T x = y^T D y \; = \sum_{i=1}^{n} \lambda_i y_i^2$$

  – where $y = V^T x$

- So, what can you say about the vector x that satisfies the following optimization? $\max_{x \in \mathbb{R}^n} \; x^T A x \quad \text{subject to } \|x\|_2^2 = 1$

Symmetric matrices

- Therefore:

$$x^T A x = x^T V D V^T x = y^T D y = \sum_{i=1}^{n} \lambda_i y_i^2$$

  – where $y = V^T x$

- So, what can you say about the vector x that satisfies the following optimization? $\max_{x \in \mathbb{R}^n} \; x^T A x \quad \text{subject to } \|x\|_2^2 = 1$
  – Is the same as finding the eigenvector that corresponds to the largest eigenvalue of A.

Some applications of Eigenvalues

- PageRank
- Schrodinger’s equation
- PCA

- We are going to use it to compress images in future classes

Outline

- Vectors and matrices
  - Basic Matrix Operations
  - Determinants, norms, trace
  - Special Matrices
- Transformation Matrices
  - Homogeneous coordinates
  - Translation
- Matrix inverse
- Matrix rank
- Eigenvalues and Eigenvectors(SVD)
- Matrix Calculus

Matrix Calculus – The Gradient

- Let a function $f : \mathbb{R}^{m \times n} \to \mathbb{R}$ take as input a matrix A of size m × n and return a real value.
- Then the **gradient** of **f:**

$$\nabla_A f(A) \in \mathbb{R}^{m \times n} = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \cdots & \frac{\partial f(A)}{\partial A_{1n}} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \cdots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix}$$

Matrix Calculus – The Gradient

- Every entry in the matrix is: $\nabla_A f(A))_{ij} = \frac{\partial f(A)}{\partial A_{ij}}.$
- the size of $\nabla_A f(A)$ is always the same as the size of A. So if A is just a vector x:

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$$

Exercise

- Example:

For $x \in \mathbb{R}^n$, let $f(x) = b^T x$ for some known vector $b \in \mathbb{R}^n$

$$f(x) = \begin{bmatrix} b_1 & b_2 & \dots & b_n \end{bmatrix}^T \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- Find:

$$\frac{\partial f(x)}{\partial x_k} = ?$$

$$\nabla_x f(x) = ?$$

Exercise

- Example:

For $x \in \mathbb{R}^n$, let $f(x) = b^T x$ for some known vector $b \in \mathbb{R}^n$

$$f(x) = \sum_{i=1}^{n} b_i x_i$$

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} b_i x_i = b_k.$$

- From this we can conclude that: $\nabla_x b^T x = b.$

Matrix Calculus – The Gradient

- Properties

  - $\nabla_x(f(x) + g(x)) = \nabla_x f(x) + \nabla_x g(x)$.
  - For $t \in \mathbb{R}$, $\nabla_x(t\ f(x)) = t\nabla_x f(x)$.

Matrix Calculus – The Hessian

- The Hessian matrix with respect to x, written $\nabla_x^2 f(x)$ or simply as H:

$$\nabla_x^2 f(x) \in \mathbb{R}^{n\times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}$$

- The Hessian of n-dimensional vector is the n × n matrix.

Matrix Calculus – The Hessian

- Each entry can be written as: $$\nabla_x^2 f(x))_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}.$$

- Exercise: Why is the Hessian always symmetric?

Matrix Calculus – The Hessian

- Each entry can be written as: $$\nabla_x^2 f(x))_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}.$$
- The Hessian is always symmetric, because
$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} = \frac{\partial^2 f(x)}{\partial x_j \partial x_i}.$$
- This is known as Schwarz's theorem: The order of partial derivatives don’t matter as long as the second derivative exists and is continuous.

Matrix Calculus – The Hessian

- Note that the hessian is not the gradient of whole gradient of a vector (this is not defined). It is actually the gradient of **every entry** of the gradient of the vector.

$$\nabla_x^2 f(x) \in \mathbb{R}^{n\times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}$$

Matrix Calculus – The Hessian

- Eg, the first column is the gradient of $\frac{\partial f(x)}{\partial x_1}$

$$\nabla_x^2 f(x) \in \mathbb{R}^{n\times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}$$

Exercise

- Example:

consider the quadratic function $f(x) = x^T Ax$

$$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

Exercise

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

Exercise

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k}\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}x_ix_j$$

$$= \frac{\partial}{\partial x_k}\left[\sum_{i\neq k}\sum_{j\neq k} A_{ij}x_ix_j + \sum_{i\neq k} A_{ik}x_ix_k + \sum_{j\neq k} A_{kj}x_kx_j + A_{kk}x_k^2\right]$$

Divide the summation into 3 parts depending on whether:

- i == k or
- j == k

Exercise

$$
\begin{aligned}
\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \\
&= \frac{\partial}{\partial x_k} \left[\sum_{i \neq k} \sum_{j \neq k} A_{ij} x_i x_j + \sum_{i \neq k} A_{ik} x_i x_k + \sum_{j \neq k} A_{kj} x_k x_j + A_{kk} x_k^2 \right] \\
&= \sum_{i \neq k} A_{ik} x_i + \sum_{j \neq k} A_{kj} x_j + 2 A_{kk} x_k
\end{aligned}
$$

Exercise

$$\begin{aligned}
\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \\
&= \frac{\partial}{\partial x_k} \left[\sum_{i \neq k} \sum_{j \neq k} A_{ij} x_i x_j + \boxed{\sum_{i \neq k} A_{ik} x_i x_k} + \sum_{j \neq k} A_{kj} x_k x_j + A_{kk} x_k^2 \right] \\
&= \boxed{\sum_{i \neq k} A_{ik} x_i} + \sum_{j \neq k} A_{kj} x_j + 2 A_{kk} x_k
\end{aligned}$$

Exercise

$$\begin{aligned}
\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \\
&= \frac{\partial}{\partial x_k} \left[\sum_{i \neq k} \sum_{j \neq k} A_{ij} x_i x_j + \sum_{i \neq k} A_{ik} x_i x_k + \boxed{\sum_{j \neq k} A_{kj} x_k x_j} + A_{kk} x_k^2 \right] \\
&= \sum_{i \neq k} A_{ik} x_i + \boxed{\sum_{j \neq k} A_{kj} x_j} + 2 A_{kk} x_k
\end{aligned}$$

Exercise

$$\begin{aligned}
\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k}\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}x_i x_j \\
&= \frac{\partial}{\partial x_k}\left[\sum_{i\neq k}\sum_{j\neq k} A_{ij}x_i x_j + \sum_{i\neq k} A_{ik}x_i x_k + \sum_{j\neq k} A_{kj}x_k x_j + \boxed{A_{kk}x_k^2}\right] \\
&= \sum_{i\neq k} A_{ik}x_i + \sum_{j\neq k} A_{kj}x_j + \boxed{2A_{kk}x_k}
\end{aligned}$$

Exercise

$$
\begin{aligned}
\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \\
&= \frac{\partial}{\partial x_k} \left[\sum_{i \neq k} \sum_{j \neq k} A_{ij} x_i x_j + \sum_{i \neq k} A_{ik} x_i x_k + \sum_{j \neq k} A_{kj} x_k x_j + A_{kk} x_k^2 \right] \\
&= \sum_{i \neq k} A_{ik} x_i + \sum_{j \neq k} A_{kj} x_j + 2 A_{kk} x_k
\end{aligned}
$$

Exercise

$$
\begin{aligned}
\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \\
&= \frac{\partial}{\partial x_k} \left[\sum_{i \neq k} \sum_{j \neq k} A_{ij} x_i x_j + \sum_{i \neq k} A_{ik} x_i x_k + \sum_{j \neq k} A_{kj} x_k x_j + A_{kk} x_k^2 \right] \\
&= \sum_{i \neq k} A_{ik} x_i + \sum_{j \neq k} A_{kj} x_j + 2 A_{kk} x_k \\
&= \sum_{i=1}^{n} A_{ik} x_i + \sum_{j=1}^{n} A_{kj} x_j = 2 \sum_{i=1}^{n} A_{ki} x_i,
\end{aligned}
$$

Exercise

$$f(x) = x^T A x$$

$$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

$$\frac{\partial^2 f(x)}{\partial x_k \partial x_\ell} = \frac{\partial}{\partial x_k} \left[\frac{\partial f(x)}{\partial x_\ell} \right] = \frac{\partial}{\partial x_k} \left[\sum_{i=1}^{n} 2 A_{\ell i} x_i \right]$$

Exercise

$$f(x) = x^T A x$$

$$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

$$\frac{\partial^2 f(x)}{\partial x_k \partial x_\ell} = \frac{\partial}{\partial x_k}\left[\frac{\partial f(x)}{\partial x_\ell}\right] = \frac{\partial}{\partial x_k}\left[\sum_{i=1}^{n} 2A_{\ell i} x_i\right]$$

$$= 2A_{\ell k} = 2A_{k\ell}.$$

Exercise

$$f(x) = x^T A x$$

$$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

$$\frac{\partial^2 f(x)}{\partial x_k \partial x_\ell} = \frac{\partial}{\partial x_k} \left[\frac{\partial f(x)}{\partial x_\ell} \right] = \frac{\partial}{\partial x_k} \left[\sum_{i=1}^{n} 2 A_{\ell i} x_i \right]$$

$$= 2A_{\ell k} = 2A_{k\ell}.$$

$$\nabla_x^2 f(x) = 2A$$

What we have learned

- Vectors and matrices
  - Basic Matrix Operations
  - Special Matrices
- Transformation Matrices
  - Homogeneous coordinates
  - Translation
- Matrix inverse
- Matrix rank
- Eigenvalues and Eigenvectors
- Matrix Calculate