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Statistical Machine Learning

Lecture 02: Linear Algebra Refresher

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Today's Objectives

- Make you remember Linear Algebra!
- I know this is mostly easy but some of you may have forgotten all of it...
- Covered Topics:
  - Vectors, Matrices
  - Linear Transformations

Outline

1. Vectors
2. Matrices
3. Operations and Linear Transformations
4. Wrap-Up

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Outline

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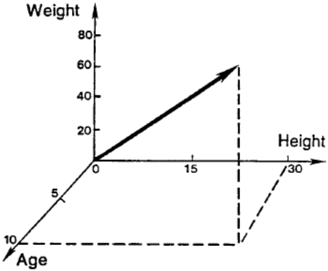
Vectors



$$\text{Joe} = \begin{bmatrix} 37 \\ 72 \\ 175 \end{bmatrix}, \text{Mary} = \begin{bmatrix} 10 \\ 30 \\ 61 \end{bmatrix}, \text{Carol} = \begin{bmatrix} 25 \\ 65 \\ 121 \end{bmatrix}, \text{Brad} = \begin{bmatrix} 66 \\ 67 \\ 155 \end{bmatrix}, \text{Joe} = \begin{bmatrix} 37 \\ 72 \\ 175 \\ 8 \\ 1946 \end{bmatrix}$$

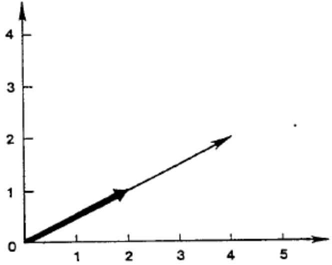
What can you do with vectors?

- Multiplication by a scalar $c\,\mathbf{v}$

$$2\begin{bmatrix}2\\1\end{bmatrix}=\begin{bmatrix}4\\2\end{bmatrix}$$

$$5\begin{bmatrix}-3\\4\\1\end{bmatrix}=\begin{bmatrix}-15\\20\\5\end{bmatrix}$$

$$c\,\mathbf{v}=c\begin{bmatrix}v_1\\\vdots\\v_n\end{bmatrix}=\begin{bmatrix}c\,v_1\\\vdots\\c\,v_n\end{bmatrix}$$



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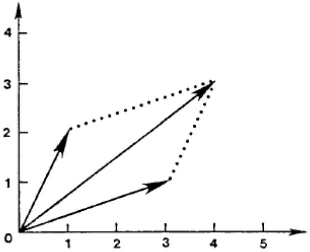
What can you do with vectors?

- Addition of vectors $\mathbf{v}_1 + \mathbf{v}_2$

$$\begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} + \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ 4 \end{bmatrix}$$

$$\begin{bmatrix} 2 \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} 3 \\ -3 \end{bmatrix} = \begin{bmatrix} 5 \\ -1 \end{bmatrix}$$

$$\begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} + \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} a_1 + b_1 \\ \vdots \\ a_n + b_n \end{bmatrix}$$



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Linear Combination of Vectors

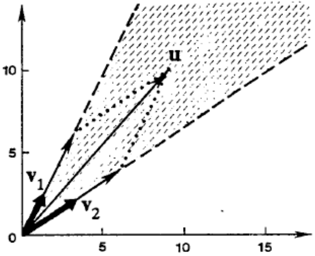
- By positive recombination we can obtain:
  - $\mathbf{u} = c_1\mathbf{v_1} + c_2\mathbf{v_2} + \ldots + c_n\mathbf{v_n}$
- Examples:

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} \text{ and } \begin{bmatrix} 2 \\ 2 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} \text{ and } \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ 1 \end{bmatrix} \text{ and } \begin{bmatrix} -1 \\ 3 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}, \begin{bmatrix} 3 \\ 2 \\ 0 \end{bmatrix} \text{ and } \begin{bmatrix} 9 \\ 10 \\ 0 \end{bmatrix}$$



Inner Product and Length of a Vector

- Inner Product
  - $\mathbf{v} = \begin{bmatrix} 3 \\ -1 \\ 2 \end{bmatrix}, \mathbf{w} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}$
  - $\mathbf{v} \cdot \mathbf{w} = \mathbf{v}^\intercal \mathbf{w} = (3 \cdot 1) + (-1 \cdot 2) + (2 \cdot 1) = 3$
- Length of a vector (Frobenius norm)
  - $\|\mathbf{v}\| = (\mathbf{v} \cdot \mathbf{v})^{1/2}$
  - $\|c\,\mathbf{v}\| = |c|\,\|\mathbf{v}\|$
  - $\|\mathbf{v}_1 + \mathbf{v}_2\| \leq \|\mathbf{v}_1\| + \|\mathbf{v}_2\|$ (triangle inequality)

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Angles between Vectors

- The angle between vectors is defined by
  - $\cos\theta = \frac{\mathbf{v}\cdot\mathbf{w}}{\|\mathbf{v}\|\,\|\mathbf{w}\|} = \frac{\sum_{i=1}^{n} v_i w_i}{\left(\sum_{i=1}^{n} v_i^2\right)^{1/2}\left(\sum_{i=1}^{n} w_i^2\right)^{1/2}}$
- Example:
  - Find the angle between vectors $\mathbf{v}_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ and $\mathbf{v}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$
    - $\mathbf{v}_1 \cdot \mathbf{v}_2 = 1$, $\|\mathbf{v}_1\| = 1$, $\|\mathbf{v}_2\| = \sqrt{2}$
    - $\cos\theta = \frac{1}{1\sqrt{2}} = 0.707$, $\theta = \pi/4$

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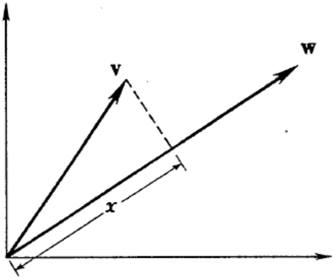
Projections of Vectors: Basic Idea

- What is a projection of $\mathbf{v}$ onto $\mathbf{w}$?
- Formally

$$\begin{aligned} x &= \|\mathbf{v}\| \cos\theta \\ &= \|\mathbf{v}\| \frac{\mathbf{v}\cdot\mathbf{w}}{\|\mathbf{v}\|\,\|\mathbf{w}\|} \\ &= \frac{\mathbf{v}\cdot\mathbf{w}}{\|\mathbf{w}\|} \end{aligned}$$



- Note that x is a **not** a vector!

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Vector Transpose, Inner and Outer Products

- Vector Transpose
  - $\mathbf{v} = \begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix}, \mathbf{v}^\intercal = \begin{bmatrix} 3 & 1 & 2 \end{bmatrix}$
- Inner Product
  - $\mathbf{v}^\intercal \mathbf{u} = \begin{bmatrix} 3 & 1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 4 \\ 1 \end{bmatrix} = \begin{bmatrix} 6 \end{bmatrix}$
- Outer Product
  - $\mathbf{w}\mathbf{v}^\intercal = \begin{bmatrix} 1 \\ 4 \\ 0 \end{bmatrix} \begin{bmatrix} 3 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 3 & 1 & 2 \\ 12 & 4 & 8 \\ 0 & 0 & 0 \end{bmatrix}$

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Outline

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Matrices

- Examples
  - $\mathbf{M} = \begin{bmatrix} 3 & 4 & 5 \\ 1 & 0 & 1 \end{bmatrix}$, 2x3 matrix
  - $\mathbf{N} = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 1 \end{bmatrix}$, 3x3 matrix
  - $\mathbf{P} = \begin{bmatrix} 10 & -1 \\ -1 & 27 \end{bmatrix}$, 2x2 matrix

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What can you do with Matrices?

- Multiplication by Scalars

$$3 \cdot \mathbf{M} = 3 \begin{bmatrix} 3 & 4 & 5 \\ 1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 9 & 12 & 15 \\ 3 & 0 & 3 \end{bmatrix}$$

- Addition of Matrices

$$\mathbf{M} + \mathbf{N} = \begin{bmatrix} 3 & 4 & 5 \\ 1 & 0 & 1 \end{bmatrix} + \begin{bmatrix} -1 & 0 & 2 \\ 4 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 2 & 4 & 7 \\ 5 & 1 & 0 \end{bmatrix}$$

  - Addition is only defined for matrices with the same dimensions.

- Transpose of a Matrix

$$\mathbf{M}^{\intercal} = \begin{bmatrix} 3 & 4 & 5 \\ 1 & 0 & 1 \end{bmatrix}^{\intercal} = \begin{bmatrix} 3 & 1 \\ 4 & 0 \\ 5 & 2 \end{bmatrix}$$

Matrix-Vector multiplication

- Multiplication of a Vector by a Matrix

$$\mathbf{u} = \mathbf{W}\mathbf{v} = \begin{bmatrix} 3 & 4 & 5 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} = \begin{bmatrix} 3 \cdot 1 + 4 \cdot 0 + 5 \cdot 2 \\ 1 \cdot 1 + 0 \cdot 0 + 1 \cdot 2 \end{bmatrix} = \begin{bmatrix} 13 \\ 3 \end{bmatrix}$$

- Think of it as

$$\begin{bmatrix} | & & | \\ \mathbf{w}_1 & \dots & \mathbf{w}_n \\ | & & | \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} & | & \\ v_1\mathbf{w}_1 + & \dots & + v_n\mathbf{w}_n \\ & | & \end{bmatrix}$$

  - Dimensions: $\mathbf{W} \in \mathbb{R}^{\mathrm{M} \times \mathrm{N}}$, $\mathbf{v} \in \mathbb{R}^{\mathrm{N} \times 1}$, $\mathbf{u} \in \mathbb{R}^{\mathrm{M} \times 1}$

- Hence

$$\mathbf{u} = v_1\mathbf{w}_1 + v_2\mathbf{w}_2 + v_3\mathbf{w}_3 = 1 \begin{bmatrix} 3 \\ 1 \end{bmatrix} + 0 \begin{bmatrix} 4 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 5 \\ 1 \end{bmatrix} = \begin{bmatrix} 13 \\ 3 \end{bmatrix}$$

Matrix-Matrix multiplication

- Multiplication of a Matrix by a Matrix

$$\mathbf{C} = \mathbf{AB} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} =$$

$$\begin{bmatrix} 1 \cdot 1 + 2 \cdot 3 + 3 \cdot 5 & 1 \cdot 2 + 2 \cdot 4 + 3 \cdot 6 \\ 4 \cdot 1 + 5 \cdot 3 + 6 \cdot 5 & 4 \cdot 2 + 5 \cdot 4 + 6 \cdot 6 \end{bmatrix} = \begin{bmatrix} 22 & 28 \\ 49 & 64 \end{bmatrix}$$

- Dimensions: $\mathbf{A} \in \mathbb{R}^{M \times N}$, $\mathbf{B} \in \mathbb{R}^{N \times K}$, $\mathbf{C} \in \mathbb{R}^{M \times K}$

- Verifying the right dimensions is an important sanity checker when working with matrices

Matrix Inverse

- Definition for square matrices $\mathbf{W} \in \mathbb{R}^{n \times n}$

$$\mathbf{W}^{-1}\mathbf{W} = \mathbf{W}\mathbf{W}^{-\mathbf{1}} = \mathbf{I}$$

$$\mathbf{W}^{-1} = \frac{1}{\det \mathbf{W}}\mathbf{C}^{\mathsf{T}}$$

  where $\mathbf{C}$ is the cofactor matrix of $\mathbf{W}$.

- If $\mathbf{W}^{-1}$ exists, we say $\mathbf{W}$ is nonsingular.

Matrix Inverse

- A condition for invertibility is that the determinant has to be different than zero.
- For an intuition consider the following linear transformation matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \det \mathbf{A} = 0$$

- Applying this transformation to a vector gives

$$\mathbf{v}' = \mathbf{A}\mathbf{v} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = v_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + v_2 \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} v_1 \\ 0 \end{bmatrix} = \begin{bmatrix} v_1' \\ v_2' \end{bmatrix}$$

- This transformation removes one dimension from **v** and projects it as a point along the first dimension.

Matrix Inverse

- Can we from **A** and $\mathbf{v}' = \begin{bmatrix} v_1' & v_2' \end{bmatrix}^\intercal$ recover the initial vector **v**?
- We have the following linear system of equations

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} v_1' \\ v_2' \end{bmatrix} = \begin{bmatrix} v_1 \\ 0 \end{bmatrix}$$

- While there is only one solution for v_1, there are *infinitely many solutions* for v_2. This means we cannot recover the initial value of v_2.
- On the contrary, a nonsingular matrix, such as the identity matrix, admits one solution.

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Matrix Inverse

- Example

$$\mathbf{W} = \begin{bmatrix} 1 & 1/2 \\ -1 & 1 \end{bmatrix}, \mathbf{W}^{-1} = \begin{bmatrix} 2/3 & -1/3 \\ 2/3 & 2/3 \end{bmatrix}$$

- Verify it!

$$\mathbf{W}\mathbf{W}^{-1} = \begin{bmatrix} 1 & 1/2 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 2/3 & -1/3 \\ 2/3 & 2/3 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{W}^{-1}\mathbf{W} = \begin{bmatrix} 2/3 & -1/3 \\ 2/3 & 2/3 \end{bmatrix} \begin{bmatrix} 1 & 1/2 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Matrix Pseudoinverse

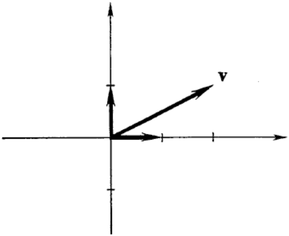
How can we invert a matrix $\mathbf{J} \in \mathbb{R}^{n \times m}$ that is not squared?

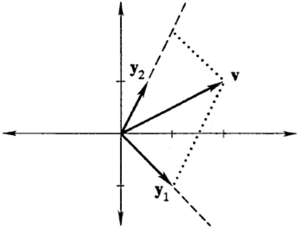
- Left-Pseudo Inverse $\mathbf{J}^{\#}\mathbf{J} = \underbrace{(\mathbf{J}^T\mathbf{J})^{-1}\mathbf{J}^T}_{\text{left multiplied}} \mathbf{J} = \mathbf{I}_m$
  - Works if $\mathbf{J}$ has full column rank
- Right-Pseudo Inverse $\mathbf{J}\mathbf{J}^{\#} = \mathbf{J} \underbrace{\mathbf{J}^T(\mathbf{J}\mathbf{J}^T)^{-1}}_{\text{right multiplied}} = \mathbf{I}_n$
  - Works if $\mathbf{J}$ has full row rank

Outline

Change of Basis

- Basis as **Unit Vectors**
- New Basis (vectors $\mathbf{y}_1$ and $\mathbf{y}_2$)



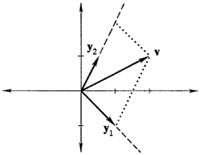


- Coordinates of vector **v** in the original coordinate system (with unit basis vectors)

$$\mathbf{v} = c_1\mathbf{y}_1 + \ldots + c_n\mathbf{y}_n = \mathbf{Y}\mathbf{v}^*$$

  - Where $\mathbf{v}^*$ holds the coordinates in the **new** coordinate system.
- To get the coordinates of $\mathbf{v}^*$ (in the new basis) we just apply the inverse transformation

Change of Basis - Example



- We have

$$\mathbf{y}_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \mathbf{y}_2 = \begin{bmatrix} 1/2 \\ 1 \end{bmatrix}$$

- Thus

$$\mathbf{Y} = \begin{bmatrix} 1 & 1/2 \\ -1 & 1 \end{bmatrix}, \mathbf{Y}^{-1} = \begin{bmatrix} 2/3 & -1/3 \\ 2/3 & 2/3 \end{bmatrix}$$

$$\mathbf{v}^* = \mathbf{Y}^{-1}\mathbf{v} = \begin{bmatrix} 2/3 & -1/3 \\ 2/3 & 2/3 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = 2 \begin{bmatrix} 2/3 \\ 2/3 \end{bmatrix} + 1 \begin{bmatrix} -1/3 \\ 2/3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

  - $\mathbf{v}^*$ holds the **coordinates** in the **new basis**

Change of Basis for a Linear Transformation

- We know

$$\mathbf{v} = \mathbf{Y}\,\mathbf{v}^* \qquad \mathbf{u} = \mathbf{W}\,\mathbf{v} \qquad \mathbf{u}^* = \mathbf{Y}^{-1}\mathbf{u}$$

$$\begin{tikzcd}
\mathbf{v}^* \arrow[r, "\mathbf{W}^*"] & \mathbf{u}^* \arrow[d, "\mathbf{Y}"] \\
\mathbf{v} \arrow[u, "\mathbf{Y}^{-1}"] \arrow[r, "\mathbf{W}"'] & \mathbf{u}
\end{tikzcd}$$

- Plugging these together

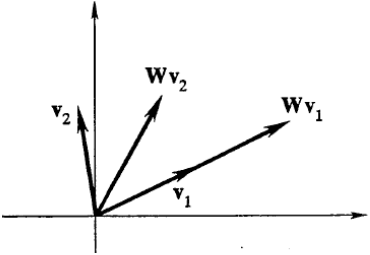
$$\begin{aligned}
\mathbf{u}^* &= \mathbf{Y}^{-1}\mathbf{u} \\
&= \mathbf{Y}^{-1}\mathbf{W}\,\mathbf{v} \\
&= \mathbf{Y}^{-1}\mathbf{W}\,\mathbf{Y}\,\mathbf{v}^* \\
&= \mathbf{W}^*\mathbf{v}^*
\end{aligned}$$

$$\mathbf{W}^* = \mathbf{Y}^{-1}\mathbf{W}\,\mathbf{Y}$$

- To apply a transformation $\mathbf{W}$ to the vector $\mathbf{v}^*$ in the new basis:
  1. Convert it to the unit basis: $\mathbf{Y}\,\mathbf{v}^*$
  2. Apply the transformation: $\mathbf{W}(\mathbf{Y}\,\mathbf{v}^*)$
  3. Convert the result back to the new basis space: $\mathbf{Y}^{-1}(\mathbf{W}(\mathbf{Y}\,\mathbf{v}^*))$

Eigenvectors and Eigenvalues

- Some vectors **v** change only their length when multiplied by a matrix **W**



$$\begin{bmatrix} 4 & -1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = 2 \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

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

- These vectors are called **eigenvectors** and the scaling factor is called **eigenvalues**.
- They obey the relation $\mathbf{W}\,\mathbf{v} = \lambda\,\mathbf{v}$
- Eigenvectors are defined for a particular transformation matrix **W**.

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Eigenvectors form a basis

- Let us assume there are n Eigenvectors and corresponding Eigenvalues

$$\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$$

$$\lambda_1, \lambda_2, \ldots, \lambda_n$$

- **Theorem**
  - For an $n \times n$ matrix with eigenvectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$, if they correspond to *distinct* eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, then the set $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ is linearly independent.
  - Hence, any vector can be expressed as a linear combination of eigenvectors

$$\mathbf{v} = c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \ldots + c_n\mathbf{v}_n$$

Eigenvectors form a basis

- This means that a transformation $\mathbf{W}$ applied to a vector $\mathbf{v}$ can be seen as a linear combination of eigenvectors

$$
\begin{aligned}
\mathbf{u} &= \mathbf{W}\,\mathbf{v} \\
&= \mathbf{W}(c_1\mathbf{v}_1 + \ldots + c_n\mathbf{v}_n) \\
&= c_1\mathbf{W}\mathbf{v}_1 + \ldots + c_n\mathbf{W}\mathbf{v}_n \\
&= c_1\lambda_1\mathbf{v}_1 + \ldots + c_n\lambda_n\mathbf{v}_n
\end{aligned}
$$

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Linear transformations in Eigen-Basis

- For each eigenvector $\mathbf{y}_i$, we have

$$\mathbf{W}\,\mathbf{y}_i = \lambda_i\,\mathbf{y}_i$$

- We can summarize them in one equation

$$\mathbf{W}\,\mathbf{Y} = \mathbf{Y}\,\mathbf{\Lambda}$$

- In this case, if we apply **W** we just stretch

$$\mathbf{W}^* = \mathbf{Y}^{-1}\mathbf{W}\,\mathbf{Y} = \mathbf{\Lambda}$$

- It is just a reformulation, but nice!

Symmetric Matrix

- Definition
  - A **squared** $n \times n$ matrix $\mathbf{A}$, is a **symmetric** matrix iff

$$\forall i, j \quad a_{ij} = a_{ji}$$

$$\mathbf{A} = \mathbf{A}^\intercal$$

- Some properties
  - The inverse $\mathbf{A}^{-1}$ is also symmetric.
  - $\mathbf{A}$ can be decomposed into $\mathbf{A} = \mathbf{Q}\mathbf{D}\mathbf{Q}^\intercal$, where the columns of $\mathbf{Q}$ are the eigenvectors of $\mathbf{A}$, and $\mathbf{D}$ is a diagonal matrix where the entries are the corresponding eigenvalues.

Positive (semi-)Definite Matrix

- Definition
  - A **squared symmetric** $n \times n$ matrix $\mathbf{A}$, is a **positive definite matrix** if for any vector $\mathbf{x} \in \mathbb{R}^n$

$$\mathbf{x}^\intercal \mathbf{A} \mathbf{x} > 0$$

  - Or **positive semidefinite** if $\mathbf{x}^\intercal \mathbf{A} \mathbf{x} \geq 0$

- These matrices are important in optimization and machine learning. For instance the covariance matrix is always positive semidefinite.

Outline

4. Wrap-Up

You know now:

- What vectors and matrices represent
- Which operations you can do with vectors and matrices
- What eigenvectors and eigenvalues are
- How to perform a linear transformation

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Self-Test Questions

- Remember vectors and what you can do with them
- Remember matrices and what you can do with them
- What is a projection? How do you use it?
- How to compute the inverse of a matrix?
- What are Eigenvectors and Eigenvalues?
- What is a change of basis? What is a linear transformation? Are they the same?

Homework

- Reading Assignment for next lecture
  - Bishop ch. 2
  - Murphy ch. 2
  - MacKay ch. 1, 2

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References

- If you want to grasp better the intuition behind Linear Algebra concepts
  - Essence of Linear Algebra by 3Blue1Brown: https://goo.gl/9wFTgS
- The Matrix Cookbook
  - https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf