

Statistical Machine Learning

Lecture 1 a: 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

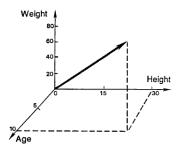


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Vectors





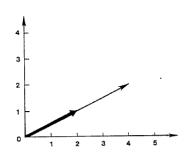
What can you do with vectors?

Multiplication by a scalar cv

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

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

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





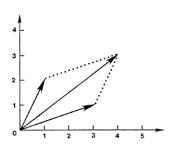
What can you do with vectors?

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

$$\left[\begin{array}{c}1\\2\\1\end{array}\right]+\left[\begin{array}{c}2\\1\\3\end{array}\right]=$$

$$\left[\begin{array}{c}2\\1\end{array}\right]+\left[\begin{array}{c}0\\1\end{array}\right]+\left[\begin{array}{c}3\\-3\end{array}\right]=$$

$$\left[\begin{array}{c} a_1 \\ \vdots \\ a_n \end{array}\right] + \left[\begin{array}{c} b_1 \\ \vdots \\ b_n \end{array}\right] = \left[\begin{array}{c} a_1 + b_1 \\ \vdots \\ a_n + b_n \end{array}\right]$$





Linear Combination of Vectors

By positive recombination we can obtain:

$$\blacksquare \mathbf{u} = c_1 \mathbf{v_1} + c_2 \mathbf{v_2} + \ldots + c_n \mathbf{v_n}$$

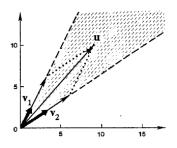
■ Examples:

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

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

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

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





Inner Product and Length of a Vector

■ Inner Product

$$\mathbf{v} = \begin{bmatrix} 3 \\ -1 \\ 2 \end{bmatrix}, \mathbf{w} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}$$

$$\mathbf{w} \cdot \mathbf{w} = \mathbf{v}^{\mathsf{T}} \mathbf{w} = (3 \cdot 1) + (-1 \cdot 2) + (2 \cdot 1) = 3$$

■ Length of a vector (Frobenius norm)

$$\|\mathbf{v}\| = (\mathbf{v} \cdot \mathbf{v})^{1/2}$$

$$\| \mathbf{v}_1 + \mathbf{v}_2 \| \le \| \mathbf{v}_1 \| + \| \mathbf{v}_2 \|$$
 (triangle inequality)



Angles between Vectors

■ The angle between vectors is defined by

$$\label{eq:theta_total} \blacksquare \; \cos \theta = \frac{\mathbf{v} \cdot \mathbf{w}}{\|\mathbf{v}\| \|\mathbf{w}\|} = \frac{\sum_{i=1}^n v_i w_i}{\left(\sum_{i=1}^n v_i^2\right)^{1/2} \left(\sum_{i=1}^n w_i^2\right)^{1/2}}$$

Example:

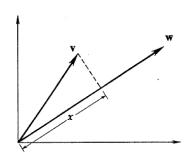
■ Find the angle between vectors
$$\mathbf{v}_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$
 and $\mathbf{v}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$
■ $\mathbf{v}_1 \cdot \mathbf{v}_2 = 1$, $\|\mathbf{v}_1\| = 1$, $\|\mathbf{v}_2\| = \sqrt{2}$
■ $\cos \theta = \frac{1}{1/2} = 0.707$, $\theta = \pi/4$



Projections of Vectors: Basic Idea

- What is a projection of v onto w?
- Formally

$$x = \|\mathbf{v}\| \cos \theta$$
$$= \|\mathbf{v}\| \frac{\mathbf{v} \cdot \mathbf{w}}{\|\mathbf{v}\| \|\mathbf{w}\|}$$
$$= \frac{\mathbf{v} \cdot \mathbf{w}}{\|\mathbf{w}\|}$$



Note that x is a not a vector!



Vector Transpose, Inner and Outer Products

■ Vector Transpose

$$\blacksquare \mathbf{v} = \begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix}, \mathbf{v}^{\mathsf{T}} = \begin{bmatrix} 3 & 1 & 2 \end{bmatrix}$$

■ Inner Product

$$\mathbf{v}^{\mathsf{T}}\mathbf{u} = \begin{bmatrix} 3 & 1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 4 \\ 1 \end{bmatrix} = 6$$

Outer Product



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Matrices

Examples

$$\blacksquare \mathbf{M} = \begin{bmatrix} 3 & 4 & 5 \\ 1 & 0 & 1 \end{bmatrix}, 2x3 \text{ matrix}$$

■
$$\mathbf{N} = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
, 3x3 matrix

$$\blacksquare \mathbf{P} = \begin{bmatrix} 10 & -1 \\ -1 & 27 \end{bmatrix}, 2x2 \text{ matrix}$$



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

Flip the rows and columns

$$\mathbf{M}^{\mathsf{T}} = \left[\begin{array}{ccc} 3 & 4 & 5 \\ 1 & 0 & 1 \end{array} \right]^{\mathsf{T}} = \left[\begin{array}{ccc} 3 & 1 \\ 4 & 0 \\ 5 & 1 \end{array} \right]$$

Properties of transposes:

$$\blacksquare (M^{\intercal})^{\intercal} = M$$

$$\blacksquare (MN)^{\intercal} = N^{\intercal}M^{\intercal}$$

$$\blacksquare (\mathbf{M} + \mathbf{N})^{\mathsf{T}} = \mathbf{M}^{\mathsf{T}} + \mathbf{N}^{\mathsf{T}}$$

If a squared matrix satisfies $\mathbf{M} = \mathbf{M}^{\mathsf{T}}$, it is called **symmetric**.



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

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

- 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

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Matrix Inverse

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

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

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

where **C** is the cofactor matrix of **W**.

- If \mathbf{W}^{-1} exists, we say \mathbf{W} is nonsingular.
- Properties of Inverses:

$$MM^{-1} = I = M^{-1}M$$

$$(MN)^{-1} = N^{-1}M^{-1}$$

$$\mathbf{m} \ (\mathbf{M} + \mathbf{N})^{-1} \neq \mathbf{M}^{-1} + \mathbf{N}^{-1}$$

If \mathbf{M} is invertible, then so is \mathbf{M}^{T} , and $(\mathbf{M}^{-1})^{\mathsf{T}} = (\mathbf{M}^{\mathsf{T}})^{-1}$



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

$$\mathbf{v}' = \mathbf{A}\mathbf{v} = \left[\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right] \left[\begin{array}{c} v_1 \\ v_2 \end{array}\right] = v_1 \left[\begin{array}{c} 1 \\ 0 \end{array}\right] + v_2 \left[\begin{array}{c} 0 \\ 0 \end{array}\right] = \left[\begin{array}{c} v_1 \\ 0 \end{array}\right] = \left[\begin{array}{c} v_1' \\ v_2' \end{array}\right]$$

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



Matrix Inverse

- Can we from **A** and $\mathbf{v}' = \begin{bmatrix} v_1' & v_2' \end{bmatrix}^\mathsf{T}$ recover the initial vector \mathbf{v} ?
- We have the following linear system of equations

$$\left[\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right] \left[\begin{array}{c} v_1 \\ v_2 \end{array}\right] = \left[\begin{array}{c} v_1' \\ v_2' \end{array}\right] = \left[\begin{array}{c} v_1 \\ 0 \end{array}\right]$$

- 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.



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!

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

$$\mathbf{W}^{-1}\mathbf{W} = \left[\begin{array}{cc} 2/3 & -1/3 \\ 2/3 & 2/3 \end{array} \right] \left[\begin{array}{cc} 1 & 1/2 \\ -1 & 1 \end{array} \right] = \left[\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right]$$



Matrix Pseudoinverse

How can we invert a matrix $J \in \mathbb{R}^{n \times m}$ 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 J has full column rank
- Right-Pseudo Inverse $\mathbf{JJ}^{\#} = \mathbf{J} \underbrace{\mathbf{J}^{\mathsf{T}}(\mathbf{JJ}^{\mathsf{T}})^{-1}}_{\text{right multiplied}} = \mathbf{I}_n$
 - Works if J has full row rank

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Vector spaces

Let a vector $\mathbf{v} \in \mathbb{R}^n$ be a point in an n-dimensional Euclidean space. A **vector space** is a collection of such vectors that can be **added together** and **scaled by scalars** to create new points.

- A set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_n\}$ is linearly independent if no vector can be represented as a linear combination of the remaining vectors
- The **span** of a set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_n\}$
- A basis is a set of linearly independent vectors that span the whole space
- A linear map or linear transformation is any function $f: \mathcal{V} \to \mathcal{W}$ such that $f(\mathbf{v} + \mathbf{w}) = f(\mathbf{v}) + f(\mathbf{w})$ and $f(\alpha \mathbf{v}) = \alpha f(\mathbf{v})$ for all $\mathbf{v}, \mathbf{w} \in \mathcal{V}$



Range and nullspace of a matrix

Let's consider a matrix $\mathbf{A} \in \mathbf{R}^{m \times n}$ as a set of m vectors in \mathbb{R}^n .

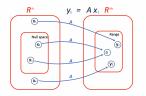
■ The **range** or (**column space**) of **A** is the span of its columns:

$$\mathsf{range}(\mathbf{A}) \triangleq \{\mathbf{v} \in \mathbb{R}^m : \mathbf{v} = \mathbf{A}\mathbf{x}, \mathbf{x} \in \mathbb{R}^n\}$$

i.e., the set of vectors generated by ${\bf A}$

■ The **nullspace** of **A** is the set of all vectors that get mapped to the **null vector** when multiplied by **A**, i.e.,

$$\operatorname{nullspace}(\mathbf{A}) \triangleq \{\mathbf{x} \in \mathbb{R}^n : \mathbf{A}\mathbf{x} = \mathbf{0}\}$$

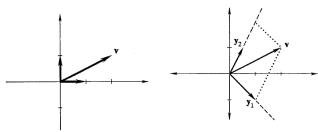


Source: Kevin P. Murphy, "Probabilistic Machine Learning: an Introduction", 2021 (online)



Change of Basis

Basis as Unit Vectors New Basis (vectors y₁ and y₂)



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

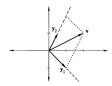
$$\mathbf{v} = c_1 \mathbf{y}_1 + \ldots + c_n \mathbf{y}_n = \mathbf{Y} \mathbf{v}^*$$

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

$$\mathbf{v}^* = \mathbf{Y}^{-1}\mathbf{v}$$



Change of Basis - Example



We have

$$\mathbf{y}_1 = \left[\begin{array}{c} 1 \\ -1 \end{array} \right], \, \mathbf{y}_2 = \left[\begin{array}{c} 1/2 \\ 1 \end{array} \right]$$

Thus

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

v* holds the coordinates in the new basis



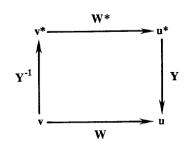
Change of Basis for a Linear Transformation

We know

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

Plugging these together

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

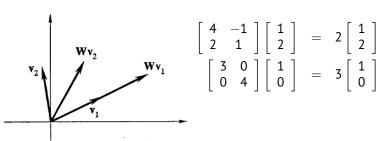


- \blacksquare To apply a transformation **W** to the vector \mathbf{v}^* in the new basis:
 - 1. Convert it to the unit basis: Y v*
 - 2. Apply the transformation: $\mathbf{W}(\mathbf{Y} \mathbf{v}^*)$
 - 3. Convert the result back to the new basis space: $Y^{-1}(W(Y v^*))$



Eigenvectors and Eigenvalues

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



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



Eigenvectors form a basis

■ Let us assume there are *n* Eigenvectors and corresponding Eigenvalues

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

$$\lambda_1, \lambda_2, \dots, \lambda_n$$

Theorem

- For an $n \times n$ matrix with eigenvectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n$, if they correspond to *distinct* eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, then the set $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n\}$ 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

lacktriangle This means that a transformation lacktriangle applied to a vector lacktriangle can be seen as a linear combination of eigenvectors

$$\mathbf{u} = \mathbf{W} \mathbf{v}$$

$$= \mathbf{W} (c_1 \mathbf{v}_1 + \ldots + c_n \mathbf{v}_n)$$

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

$$= c_1 \lambda_1 \mathbf{v}_1 + \ldots + c_n \lambda_n \mathbf{v}_n$$



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

$$WY = Y\Lambda$$

■ 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 **A**, is a symmetric matrix iff

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

 $\mathbf{A} = \mathbf{A}^{\mathsf{T}}$

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



Positive (semi-)Definite Matrix

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

$$\mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{x} > 0$$

- Or **positive semidefinite** if $\mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{x} \geq 0$
- These matrices are important in optimization and machine learning. For instance the covariance matrix is always positive semidefinite.

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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



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?

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References

- Reading material for this lecture: Murphy, Chapter 7
- 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