Introduction to Deep Learning

Overview of Linear Algebra

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Scalars

- **A scalar is a single number**
- **It can be real, integer, etc.**
- **Typically it will be denoted using lowercase italics:** a, x, n
- **Example:**
  - **Let $s \in \mathbb{R}$ be the slope of the line**
  - **Let $n \in \mathbb{N}$ be the number of units**

Vectors

- It is an array of numbers (eg. scalars) and arranged in order

- Typically it will be denoted using lowercase bold font: $x = \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_n \end{bmatrix}$

- Need to specify what kind of numbers are stored
- If each element is in $\mathbb{R}$ then the vector lies in $\mathbb{R}^n$ (Cartesian product n times)
- Identify points in space, each element giving the coordinate along different axis
- A set of elements, x_1, x_3, x_5 can be specified as x_S where $S = 1, 3, 5$
- x_{-2} is a vector containing all elements except x_2

Matrices

- **A matrix is a 2D array of numbers** $X = [x_{i,j}] = \begin{bmatrix} x_{1,1} & x_{1,2} & \ldots & x_{1,n} \\ \vdots & \vdots & \vdots & \vdots \\ x_{m,1} & x_{m,2} & \ldots & x_{m,n} \end{bmatrix}$

- **Example notation for type and shape** $X \in \mathbb{R}^{m \times n}$

- **The jth column will be denoted as** x_j **or** $X_{:,j}$ **—** $X = \begin{bmatrix} | & | & \ldots & | \\ \mathsf{x}_1 & \mathsf{x}_2 & \ldots & \mathsf{x}_n \\ | & | & \ldots & | \end{bmatrix}$

- **n-dimensional vector can be represented as n rows and 1 column** $\mathsf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$

Tensors

- **A tensor is an array of numbers that may have**
  - **Zero dimensions, and be a scalar**
  - **One dimension, and be a vector**
  - **Two dimensions, and be a matrix**
  - **Or, more dimensions.**

Matrix transpose

- **Rows and columns are interchanged that is** $X^T = [x_{i,j}]^T = [x_{j,i}]$

- **For example,** $X = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \end{bmatrix}$ $X^T = \begin{bmatrix} x_{1,1} & x_{2,1} \\ x_{1,2} & x_{2,2} \\ x_{1,3} & x_{2,3} \end{bmatrix}$

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- $(AB)^T = B^T \times A^T$

Matrix manipulation

- **Matrix addition** $C = A + B \Rightarrow C_{i,j} = A_{i,j} + B_{i,j}$

- **Matrix multiplication** $C = A \times B \Rightarrow C_{i,j} = \sum_k A_{i,k} \times B_{k,j}$

- **Multiplication and addition are associative:**

$$(AB)C = A(BC)$$
$$(A + B) + C = A + (B + C)$$

- **Multiplication is distributive:** $A \times (B + C) = AB + AC$

- **Multiplication is not commutative (in general):** $AB \neq BA$

image source: Data Science Design Manual
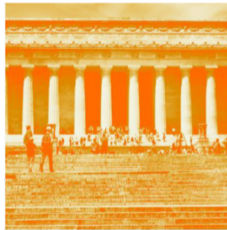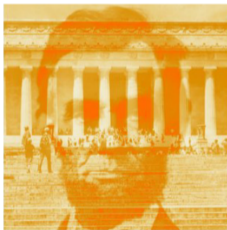
Matrix Dot Product

- Let us assume $Z = X \times Y$, where $X \in R^{m \times n}$ and $Y \in R^{n \times p}$

- Number of columns in X should be equal to number of rows in Y

- $z_{ij} = \sum\limits_{k=1}^{n} x_{ik} \times y_{kj}$

Identity matrix

- **All elements are 0 except for diagonal elements which are 1**

- **Example,** $I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

- $\forall x \in \mathbb{R}^n, I_n x = x$

Covariance matrix

- Multiplication by transpose matrix is common ie. $A \cdot A^T$
- Both $A \cdot A^T$ and $A^T \cdot A$ are compatible for multiplications
- Let $A_{n \times d}$ be a feature matrix, each row represents an item and each column denotes a feature

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- $D = A^T A$ **is a** $d \times d$ **dot products in syncness among the features**
  - D_{ij} **represents the similarity between feature** i **and feature** j

- $A,\ A \cdot A^T,\ A^T \cdot A$

image source: Data Science Design Manual
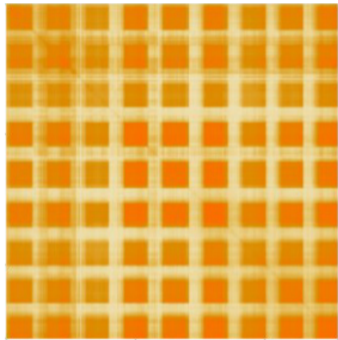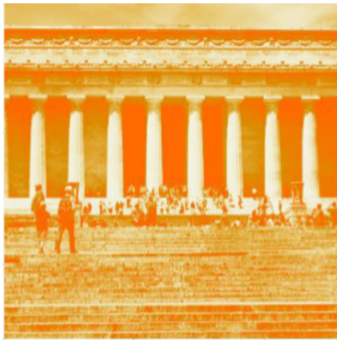
Systems of equations

- **Consider following equations:**

$$\begin{array}{rcrcr} 4x_1 & - & 5x_2 & = & -13 \\ -2x_1 & + & 3x_2 & = & 9 \end{array}$$
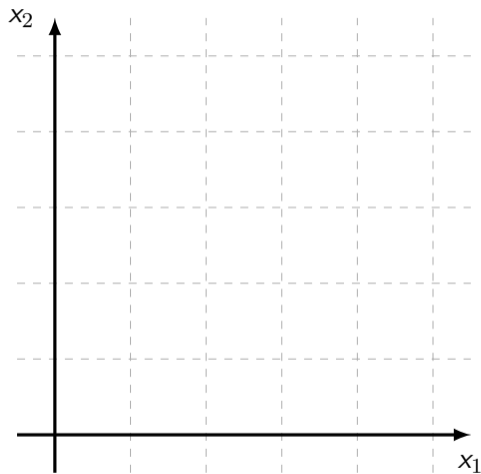
- **This can be expressed in the form $\mathrm{A}x = b$ where**

$$\mathrm{A} \;=\; \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix} \qquad b \;=\; \begin{bmatrix} -13 \\ 9 \end{bmatrix}$$

- $\mathrm{A}_{1,:}x = b_1, \mathrm{A}_{2,:}x = b_2, \ldots$
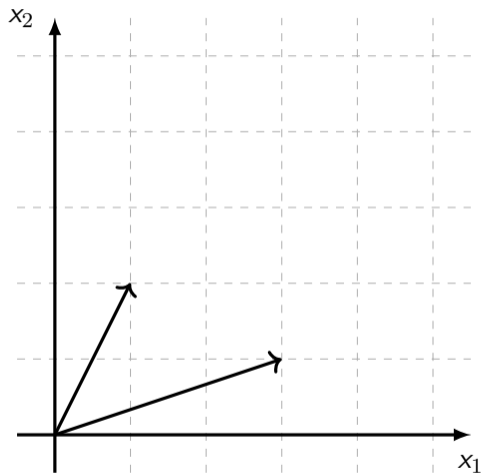- **A linear system of equations can have:**
  - **No solution**
  - **Many solutions**
  - **Exactly one solution: this means multiplication by the matrix is an invertible function**

x_2

x_1

$$A = \begin{bmatrix} 1 & 3 \\ 2 & 1 \end{bmatrix} \quad x = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

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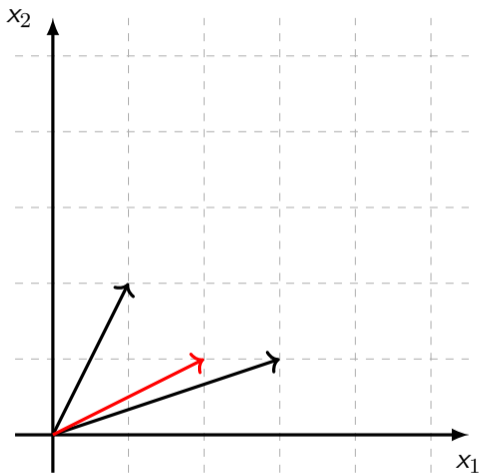
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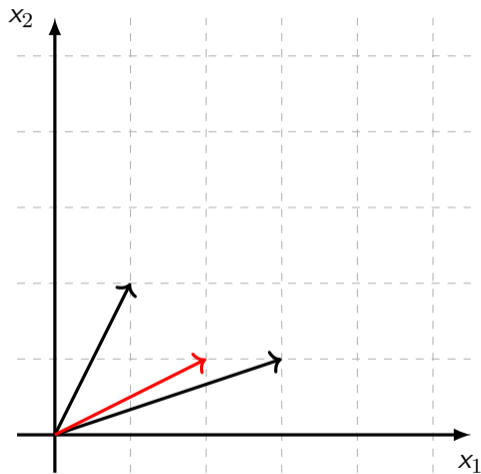
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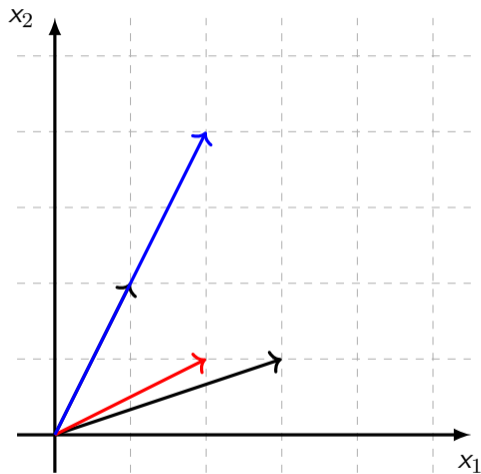
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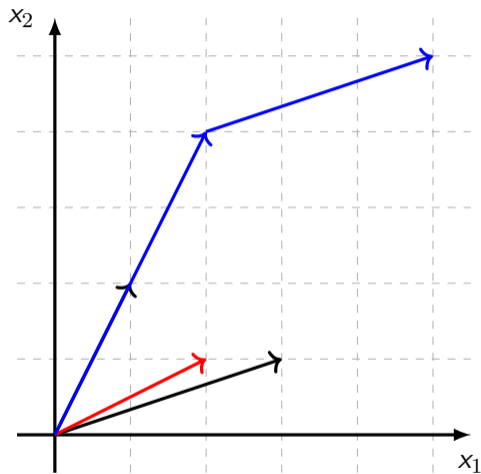
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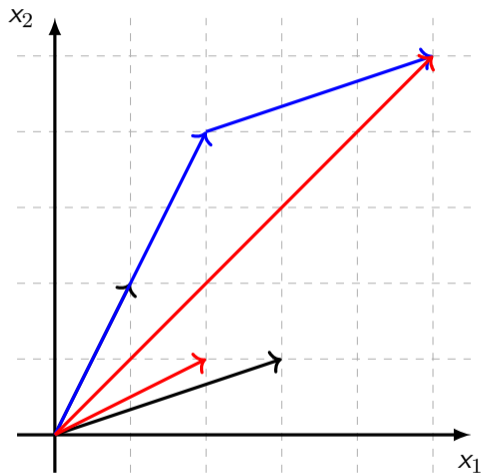
Matrix inversion

- $A^{-1} \times A = I_n$
- **Solving a system of equations using inverse**

$$
\begin{aligned}
Ax &= b \\
A^{-1}Ax &= A^{-1}b \\
I_n x &= A^{-1}b \\
x &= A^{-1}b
\end{aligned}
$$

- **Numerically unstable, but useful for abstract analysis**
- **Matrix cannot be inverted if**
  - **More rows than columns**
  - **More columns than rows**
  - **Redundant rows/columns ("linearly dependent","low rank")**

Inversion Example

- **Inverse of Lincoln image and** $M \cdot M^{-1}$
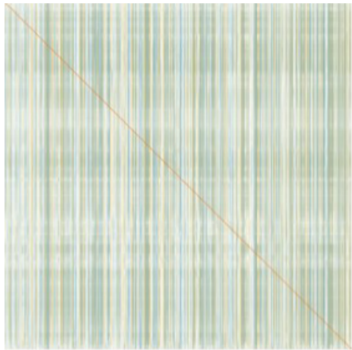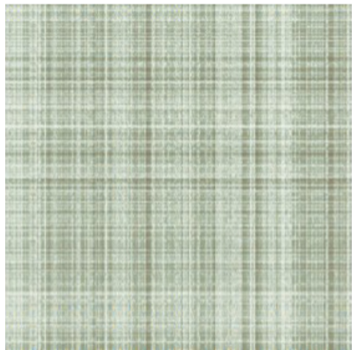
Linear Independence

- **Column can be thought of as specifying direction from origin**
- **Each element of x specify how far we should move in each of these direction ie, $Ax = \sum x_i A_{:,i}$**
- **Formally, this is a linear combination of the set of vectors**
- **Span of set of vectors is the set of all points obtainable by linear combination of the original vectors**
- **Solution of $Ax = b \Rightarrow$ Testing whether b is in span of column of A**
  - **Span is known as column space or range of A**

- $Ax = b$ to have solution for all $b \in \mathbb{R}^m$, column space of A must be $\mathbb{R}^m$
  - A must have at least m column ie. $n \geq m$
  - Consider A has size 3×2 and b is 3D point
    - x will be 2D point
    - It traces out 2D plane within $\mathbb{R}^3$
    - Equation will have solution if b lies in that plane
- $n \geq m$ is a necessary condition
  - Consider a 2×2 matrix where both columns are the same
  - Column space is just a line in $\mathbb{R}^2$

Linear Independence (contd.)

- **A set of vectors is linearly independent if no vectors in the set is a linear combination of other vectors**
  - **No new points will be added if linear combination of vectors are added in the set**
- **Suppose column space is $\mathbb{R}^m$**
  - **Need to have exactly m linearly independent column**
  - **No set of m dimensional vectors can have more than m mutually linearly independent column**
- **A square matrix with linearly dependent columns is known as singular**
- **A matrix to have inverse, $Ax = b$ has at most one solution for each value of b**
- **A is not square but singular, it is still possible to solve $Ax = b$. However, matrix inversion method cannot be used**

Norms

- **Measure the size of vector. It is defined as**

$$L^P = \|x\|_p = \left(\sum_i |x_i|^P \right)^{1/p} \qquad p \in \mathbb{R}, p \geq 1$$

- **Intuitive meaning: distance of x from the origin**
- **Norm is any function f that satisfies**
  - $f(x) = 0$

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Norms (contd)

- L^2 **norm is known as Euclidean norm**
  - **It is often denoted as $\|x\|$ instead of $\|x\|_2$**
  - **Squared L^2 norm can be determined by $x^T x$. This is very often used**
    - **Derivative of the squared L^2 norm depend only on the corresponding element**
      $$\frac{\partial(x^T x)}{\partial x_i} = \frac{\partial(x_1^2 + \ldots + x_m^2)}{\partial x_i}$$
    - **Derivative of L^2 depend on entire vector**
      $$\frac{\partial\sqrt{(x^T x)}}{\partial x_i} = \frac{\partial\sqrt{(x_1^2 + \ldots + x_m^2)}}{\partial x_i}$$
  - **Squared L^2 norm is undesirable as it increases very slowly at the origin**

Norms (contd)

- **Need to identify elements that are zero and elements that are non-zero but small**
  - **Need a function that grows at the same rate in all locations** $L^1 = \|x\| = \sum_i |x_i|$

  - L^1 **can be used to differentiate zero and non-zero elements**
- L^∞ **(max norm) - Absolute value of the elements with the largest magnitude in the vector** $\|x\|_\infty = \max_i |x_i|$
- **Frobenius norm**

$$\|A\|_F = \sqrt{\sum_{i,j} A_{i,j}^2}$$

  - **This is analogous to** L^2 **norm of vector**

Special matrices

- **Diagonal matrices — Non-zero diagonal elements and rests are zero. Formally $D_{i,j} = 0, i \neq j$**
  - **Identity matrix**
  - **diag(v) — vectors using diagonal elements**
  - **diag(v)x — x_i is scaled by v_i**
  - **Inversion is easy diag(v)$^{-1}$=diag($[1/v_1, 1/v_2, \ldots, 1/v_n]^T$)**
- **Not all diagonal matrix be square**
  - **Rectangular diagonal matrix is possible**
  - **Dx — Scaling each element of x**
    - **Concatenate some zero if D is taller**
    - **Discard some last elements if D is wider**
- **Symmetric matrix — Arises when the entries are generated by a function of two arguments that does not depend on order**
  - **Distance matrix $A_{i,j} = A_{j,i}$**

Special vectors & matrices

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- **In R^n, at most n vectors may be mutually orthogonal with non-zero norm**
- **Vectors orthogonal and have unit norm is known as orthonormal**
- **Orthogonal matrix** — **Square matrix, rows are mutually orthonormal, columns are mutually orthonormal**
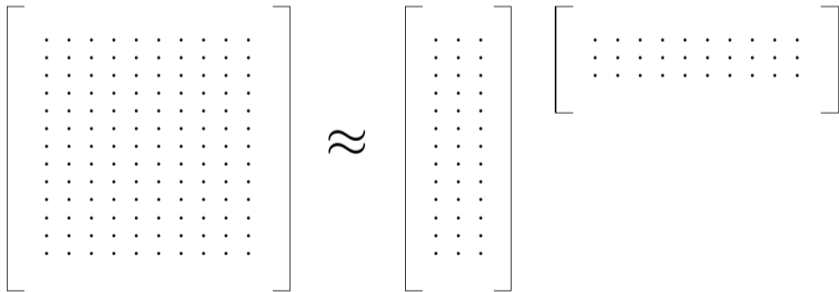 - $A^T A =$

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- **Orthogonal matrix — Square matrix, rows are mutually orthonormal, columns are mutually orthonormal**
  - $A^T A = A A^T = I \Rightarrow A^T = A^{-1}$
  - **Orthonormal matrices are of interest as inverse computation is easy**

Factoring matrices

- **Factoring matrix A into matrices in B and C represents particular aspect of division**
  - **Non-singular matrix has an inverse $I = M \cdot M^{-1}$**
- **Matrix factorization is an important abstraction in data science, leading to feature representation in a compact way**
- **Suppose matrix A can be factored as $A \approx BC$ where the size of A is $n \times m$, $B - n \times k$, $C - k \times m$ where $k < \min(n, m)$**

image source: Data Science Design Manual
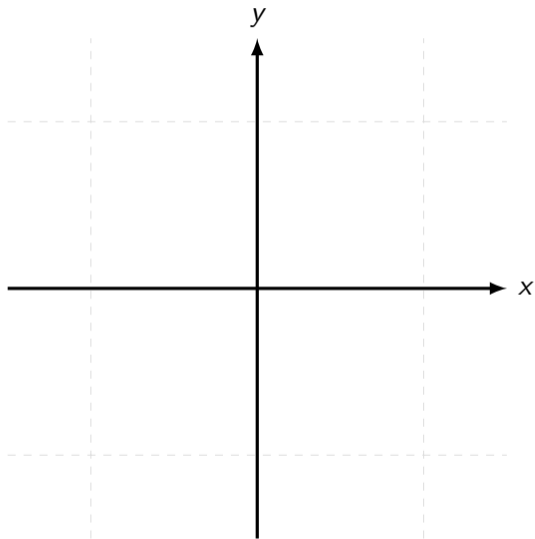
Eigen decomposition

- **Similar to prime factorization of integer**
  - $12 = 2 \times 2 \times 3$
  - **12 is not divisible by 5**
- **Eigen vector of square matrix A is a non-zero vector such that $Av = \lambda v$**
  - λ **is a scalar and known as eigen value**
  - **Mostly right eigen vector is considered**
  - **If v is eigen vector, then so is sv**
    - **Usually we look for unit eigen vector**
- **Suppose A has n linearly independent eigen vector $\{v^1, v^2 \ldots, v^n\}$ with corresponding eigen value $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$**
  - **Concatenate all eigen vector, one per column $V = [v^1, v^2 \ldots, v^n]$, similarly for $\lambda = [\lambda_1, \lambda_2, \ldots, \lambda_n]$**
    - **Eigen decomposition $AV = V\lambda$**

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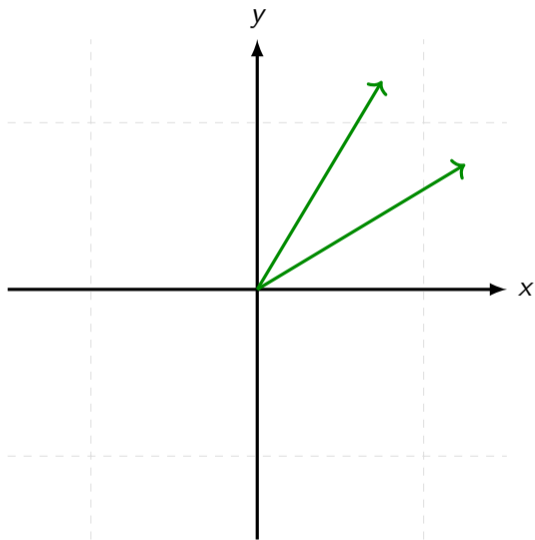   - **Eigen decomposition $AV = V\boldsymbol{\lambda} \Rightarrow A = V\text{diag}(\boldsymbol{\lambda})V^{-1}$**

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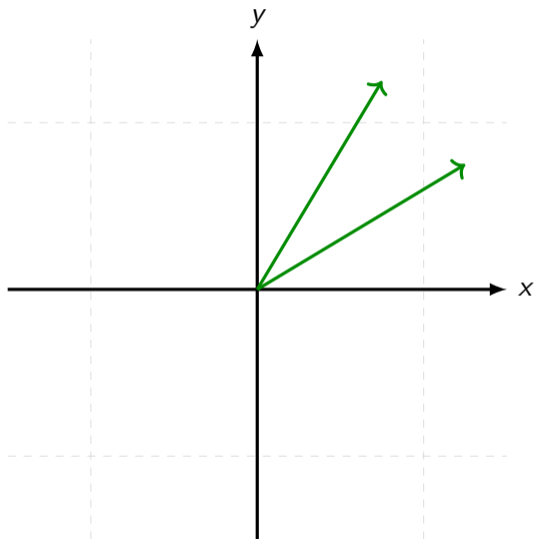
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$$v_1 = \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix}, \lambda_1 = 2.0$$

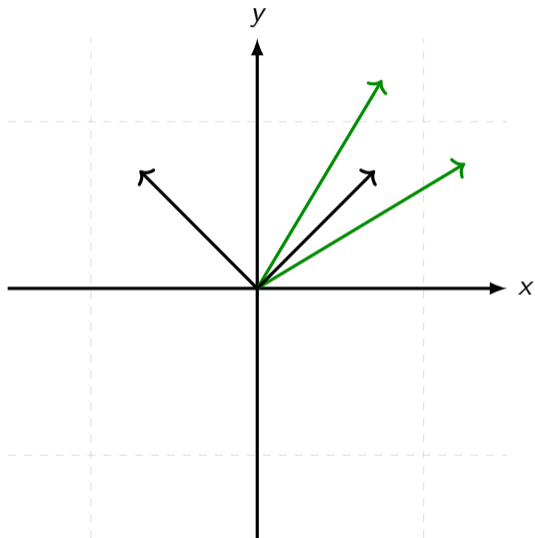$$v_2 = \begin{bmatrix} -0.707 \\ 0.707 \end{bmatrix}, \lambda_2 = 0.5$$

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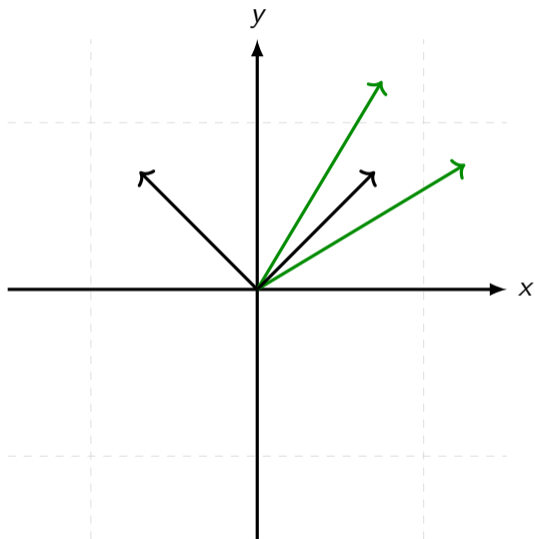$$Av_1 = \begin{bmatrix} 1.414 \\ 1.414 \end{bmatrix}$$

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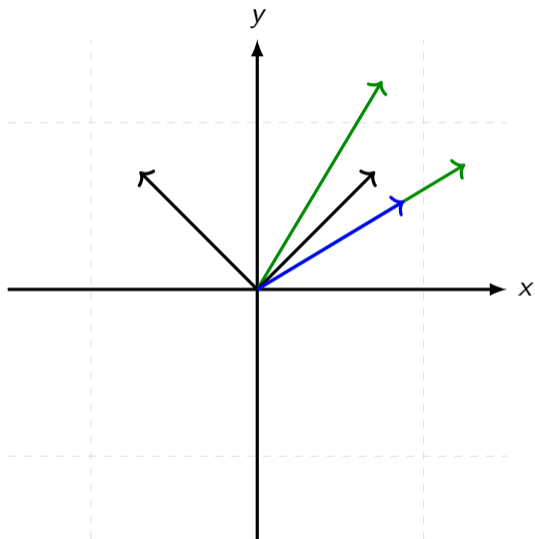$$Av_1 = \begin{bmatrix} 1.414 \\ 1.414 \end{bmatrix}$$

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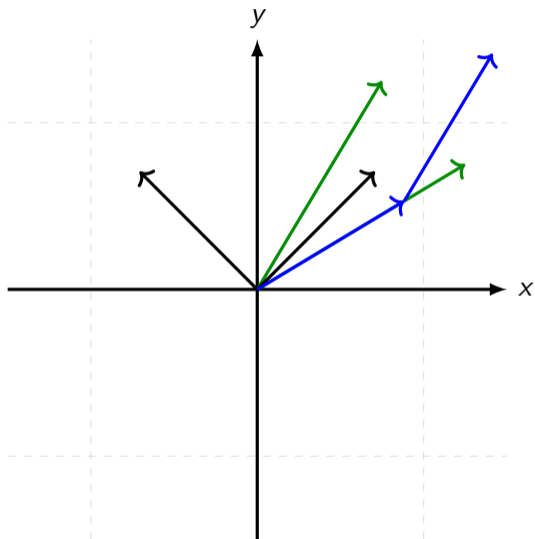$$Av_1 = \begin{bmatrix} 1.414 \\ 1.414 \end{bmatrix}$$

Example

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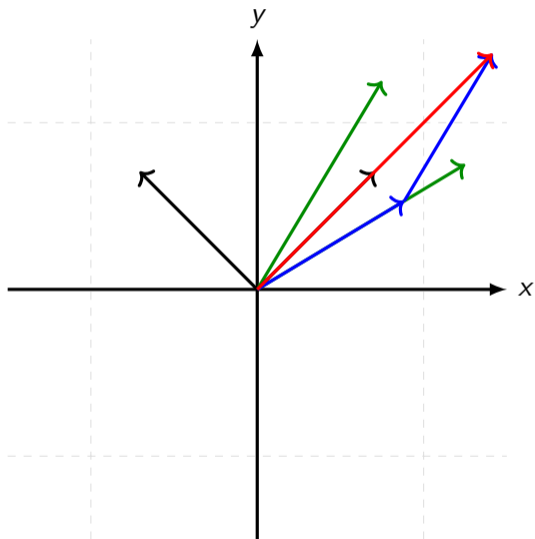
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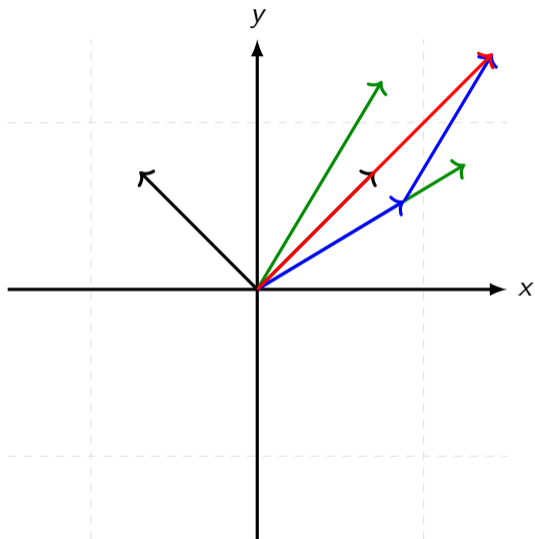
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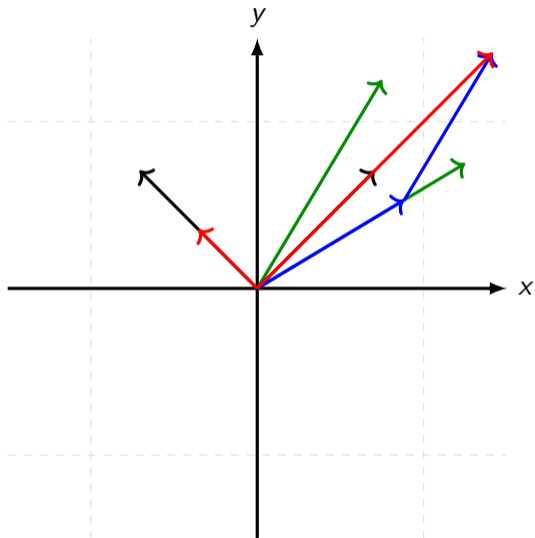
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CS551

26

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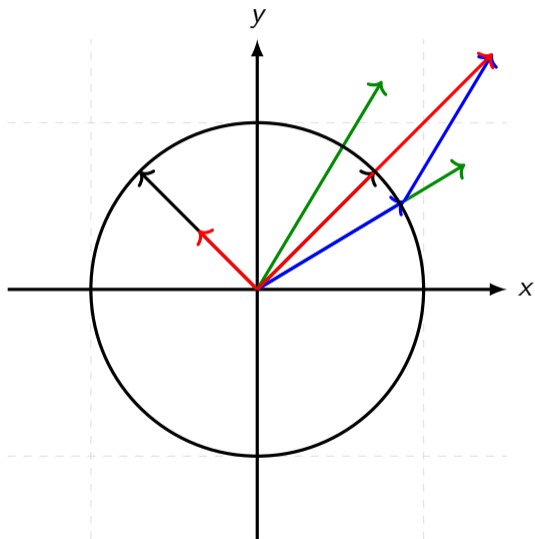
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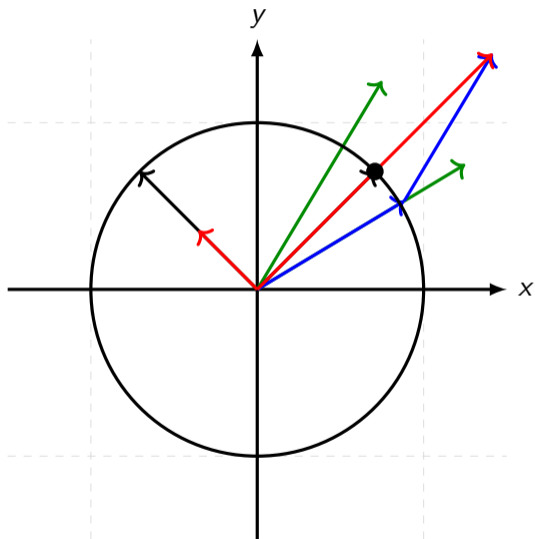
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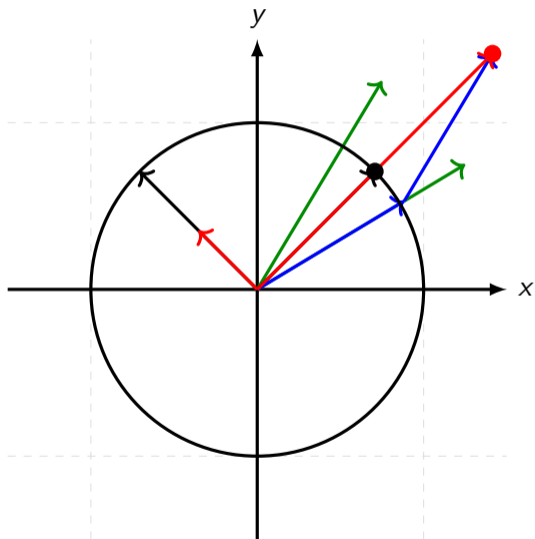
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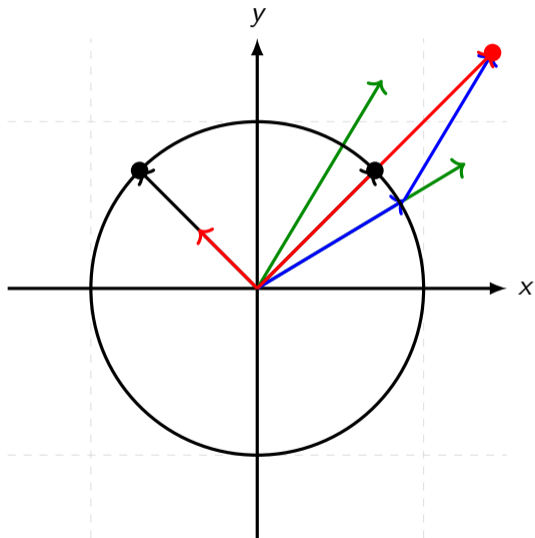
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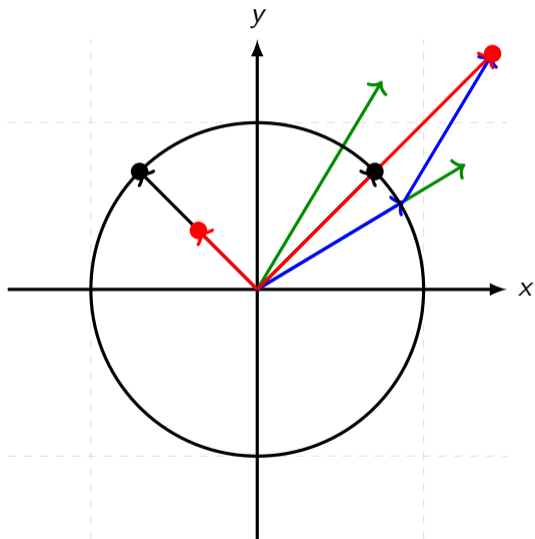Given $\|x\| = 1$, find Ax

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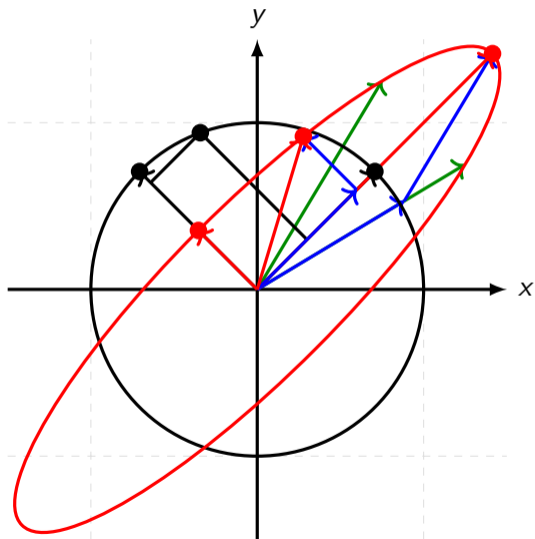
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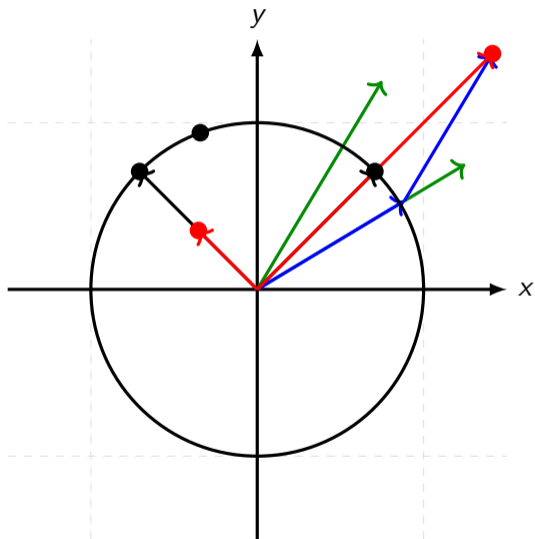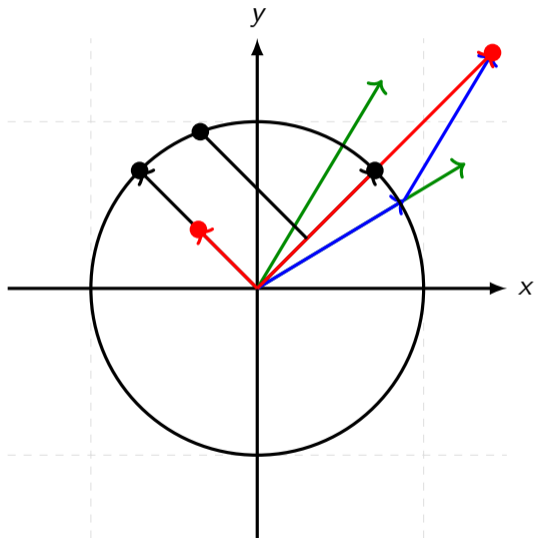Given $\|x\| = 1$, find Ax

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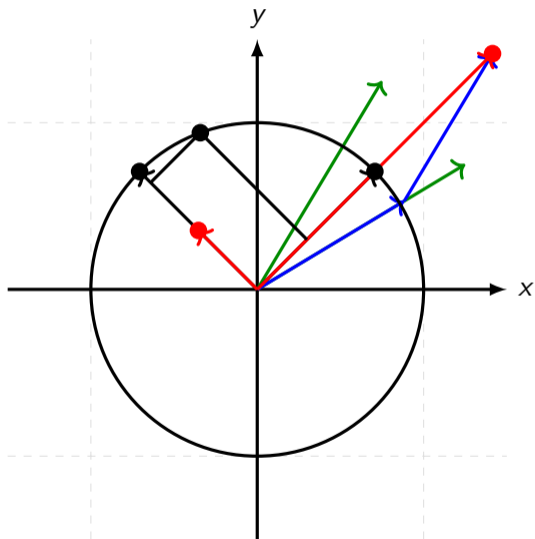$$A = \begin{bmatrix} 1.25 & 0.75 \\ 0.75 & 1.25 \end{bmatrix}$$

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Given $\|x\| = 1$, find Ax

Eigen decomposition (contd)

- **Every real symmetric matrix can be decomposed into an expression using only real valued eigen value and eigen vector**

$$A = Q \Lambda Q^T$$

  - Q **is orthogonal matrix correspond of eigen vector of** A
  - Λ **- Diagonal matrix**
    - $\Lambda_{i,i}$ is associated with eigen vector in column *i* of Q ie. $Q_{:i}$
  - **As** Q **is orthogonal,** A **is scaling space by** λ_i **in** v^i
- **Real symmetric matrix is guaranteed to have eigen decomposition but not unique**
  - **Two or more eigen vector can have same eigen value**
  - **Sort the entries of** Λ **in descending order**

- **Matrix is said to be singular if any one of the eigen value is 0**
- **Eigen decomposition can be used for optimization for the expression** $f(\mathsf{x}) = \mathsf{x}^T A\mathsf{x}$ **subject to** $\|\mathsf{x}\|_2 = 1$

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  - **Whenever x is equal to an eigen vector of A, f takes on the value of corresponding eigen value**

Eigen decomposition (contd)

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- **Matrices with**
  - **All positive eigen value — Positive definite** ($x^T A x > 0$)
  - **All positive or 0 eigen value — Positive semidefinite** ($x^T A x \geq 0$)
  - **All negative eigen value — Negative definite** ($x^T A x < 0$)

Eigenvalue decomposition

- Any $n \times n$ symmetric matrix M can be decomposed into the sum of its n eigenvector products
- Let (λ_i, U_i) be the eigen pairs $i = 1, \ldots, n$ and assume $\lambda_i \geq \lambda_{i+1}$
- Each eigenvector U_i is an $n \times 1$ matrix, multiplying it by its transpose yields an $n \times n$ matrix, product $U_i U_i^T$ same dimension as M
- Linear combination of these matrices weighted by its corresponding eigenvalue gives the original matrix $M = \sum_{i=1}^{n} \lambda_i U_i U_i^T$
  - It holds for symmetric matrices
  - Can be applied on covariance matrix
- Using only the vector associated with the largest eigenvalues, a good approximation of the matrix can be made

- **Covariance of Lincoln & $M - U_1 U_1^T$**

image source: Data Science Design Manual
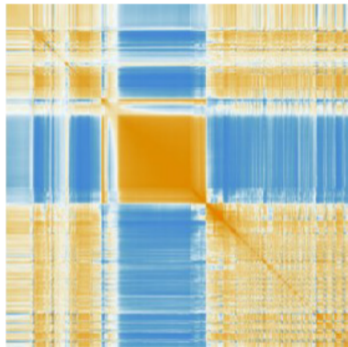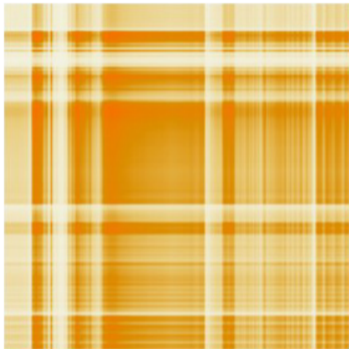
Error plot

- **Reconstructing the Lincoln memorial from the one, five, fifty eigenvectors**

image source: Data Science Design Manual
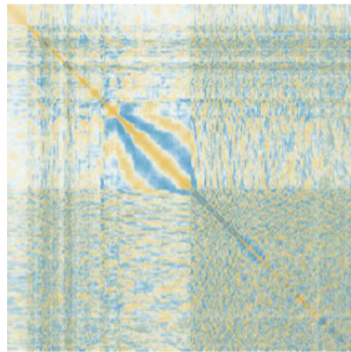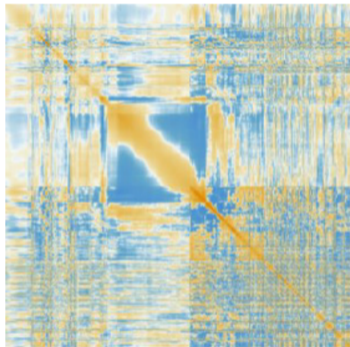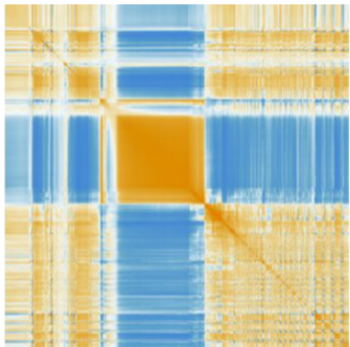
Singular Value Decomposition

- **Every real matrix has a singular value decomposition but the same is not true for eigen value decomposition**
- **EVD —** $A = V\mathbf{diag}(\boldsymbol{\lambda})V^{-1}$
- **SVD —** $A = UDV^T$
  - $A = m \times n$, $U = m \times m$, $D = m \times n$, $V = n \times n$
  - U, V **are orthogonal**
  - D **- diagonal matrix not necessary square**
    - **Diagonal elements of** D **are known as singular value of** A
    - U **is left singular vector**
    - V **is right singular vector**

- **Trace operator**

  - $Tr(\mathsf{A}) = \sum_i A_{i,i}$

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  - $Tr(A) = \sum_i A_{i,i}$
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Trace operator & Determinant

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- **Determinant of** A **is denoted as** $\det(\mathrm{A})$
  - **Defined only for square matrix**
  - **Product of all eigen value of the matrix**

- **Let** $y = Ax$ **then** $\dfrac{\partial y}{\partial z} = A\dfrac{\partial x}{\partial z}$

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Matrix calculus

- **Let** $y = Ax$ **then** $\dfrac{\partial y}{\partial z} = A\dfrac{\partial x}{\partial z}$

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Principal Component Analysis

- **We have m points $\left\{ x^1, x^2, \ldots, x^m \right\}$ in $\mathbb{R}^n$**

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Principal Component Analysis

- **We have m points $\{x^1, x^2, \ldots, x^m\}$ in $\mathbb{R}^n$**
- **Representing these points using a lossy compression**
  - **For each point choose a lower dimension ie. $x^i \in \mathbb{R}^n \to c^i \in \mathbb{R}^l$**
  - **Target is to find out f such that $f(x) = c$ and a decode function g such that $x \approx g(f(x))$**
- **Let $g(c) = Dc$ where $D \in \mathbb{R}^{n \times l}$**
  - **PCA constraints the column of D to be orthogonal**
    - D **is not orthogonal matrix**
    - **For unique solution columns of D have unit norm**
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- **Generate optimal code point c^* for each x**
  - **Minimize distance between x and $g(c^*)$**
  - **We use L^2 norm ie. $c^* = arg_c \min \|x - g(c)\|_2$**
  - **We can switch to squared L^2 norm $c^* = arg_c \min \|x - g(c)\|_2^2$**

- **We need to minimize**

$$(x - g(c))^T (x - g(c))$$

- **We need to minimize**

$$(x - g(c))^T (x - g(c))$$
$$\Rightarrow \ x^T x - x^T g(c) - g(c)^T x + g(c)^T g(c)$$

- **We need to minimize**

$$(x - g(c))^T(x - g(c))$$
$$\Rightarrow \quad x^Tx - x^Tg(c) - g(c)^Tx + g(c)^Tg(c)$$
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Principal Component Analysis (contd.)

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- **Therefore we have,**

$$c^* \quad = \quad arg_c \min(x^Tx - 2x^Tg(c) + g(c)^Tg(c))$$

Principal Component Analysis (contd.)

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$$\Rightarrow \quad x^T x - x^T g(c) - g(c)^T x + g(c)^T g(c)$$
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- **Therefore we have,**

$$c^* \quad = \quad arg_c \min(x^T x - 2x^T g(c) + g(c)^T g(c))$$
$$\Rightarrow \quad arg_c \min(-2x^T Dc + c^T D^T Dc)$$

- **We need to minimize**

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- **Therefore we have,**

$$
\begin{aligned}
c^* \;&=\; arg_c \min(x^T x - 2x^T g(c) + g(c)^T g(c)) \\
&\Rightarrow\; arg_c \min(-2x^T Dc + c^T D^T Dc) \\
&\Rightarrow\; arg_c \min(-2x^T Dc + c^T c)
\end{aligned}
$$

- **We need to minimize**

$$(x - g(c))^T(x - g(c))$$
$$\Rightarrow \quad x^Tx - x^Tg(c) - g(c)^Tx + g(c)^Tg(c)$$
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- **Therefore we have,**

$$c^* \quad = \quad arg_c \min(x^Tx - 2x^Tg(c) + g(c)^Tg(c))$$
$$\Rightarrow \quad arg_c \min(-2x^TDc + c^TD^TDc)$$
$$\Rightarrow \quad arg_c \min(-2x^TDc + c^Tc)$$

- **Optimization problem can be solved by differentiating**

$$\nabla_c(-2x^TDc + c^Tc) \quad = \quad 0$$

Principal Component Analysis (contd.)

- **We need to minimize**

$$(x - g(c))^T (x - g(c))$$
$$\Rightarrow \; x^T x - x^T g(c) - g(c)^T x + g(c)^T g(c)$$
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$$

- **Optimization problem can be solved by differentiating**

$$
\begin{aligned}
\nabla_c (-2x^T Dc + c^T c) \; &= \; 0 \\
-2D^T x + 2c \; &= \; 0
\end{aligned}
$$

Principal Component Analysis (contd.)

- **We need to minimize**

$$(x - g(c))^T (x - g(c))$$
$$\Rightarrow x^T x - x^T g(c) - g(c)^T x + g(c)^T g(c)$$
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- **Therefore we have,**

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&\Rightarrow arg_c \min(-2x^T Dc + c^T D^T Dc) \\
&\Rightarrow arg_c \min(-2x^T Dc + c^T c)
\end{aligned}
$$

- **Optimization problem can be solved by differentiating**

$$
\begin{aligned}
\nabla_c(-2x^T Dc + c^T c) &= 0 \\
-2D^T x + 2c &= 0 \\
c &= D^T x
\end{aligned}
$$

- **Optimal encoding can be done using matrix-vector multiplication** $f(x) = D^T x$

Principal Component Analysis (contd.)

- **Optimal encoding can be done using matrix-vector multiplication** $f(x) = D^T x$
- **PCA reconstruction** $r(x) = g(f(x)) = DD^T x$

Principal Component Analysis (contd.)

- Optimal encoding can be done using matrix-vector multiplication $f(\mathrm{x}) = \mathrm{D}^T\mathrm{x}$
- PCA reconstruction $r(\mathrm{x}) = g(f(\mathrm{x})) = \mathrm{DD}^T\mathrm{x}$
- D can be determined by minimizing distance between inputs and reconstruction ie.

$$\mathrm{D}^* = \arg_\mathrm{D} \min \sqrt{\sum_{i,j} \left(x_j^{(i)} - r(x^{(i)})_j\right)^2} \text{ subject to } \mathrm{D}^T\mathrm{D} = \mathrm{I}_l$$

Principal Component Analysis (contd.)

- **Optimal encoding can be done using matrix-vector multiplication** $f(\mathbf{x}) = \mathbf{D}^T \mathbf{x}$
- **PCA reconstruction** $r(\mathbf{x}) = g(f(\mathbf{x})) = \mathbf{D}\mathbf{D}^T \mathbf{x}$
- $\mathbf{D}$ **can be determined by minimizing distance between inputs and reconstruction ie.**

$$\mathbf{D}^* = \arg_{\mathbf{D}} \min \sqrt{\sum_{i,j} \left(x_j^{(i)} - r(x^{(i)})_j \right)^2} \text{ subject to } \mathbf{D}^T\mathbf{D} = \mathbf{I}_l$$

- **To derive** $\mathbf{D}^*$**, we start by considering** $l = 1$
  - $\mathbf{D}$ **becomes** $\mathbf{d}$

- **Simplifying based on the assumptions**

$$d^* = \arg_d \min \sum_i \|x^{(i)} - dd^T x^{(i)}\|_2^2 \text{ subject to } \|d\|_2 = 1$$

Principal Component Analysis (contd.)

- **Simplifying based on the assumptions**

$$d^* = \arg_d \min \sum_i \|x^{(i)} - dd^T x^{(i)}\|_2^2 \text{ subject to } \|d\|_2 = 1$$

- $d^T x^{(i)}$ **is scalar, hence** $dd^T x^{(i)} = d^T x^{(i)} d = x^{(i)T} dd$

- **We get,** $d^* = \arg_d \min \sum_i \|x^{(i)} - x^{(i)T} dd\|_2^2 \text{ subject to } \|d\|_2 = 1$

Principal Component Analysis (contd.)

- **Simplifying based on the assumptions**

$$d^* = \arg_d \min \sum_i \|x^{(i)} - dd^T x^{(i)}\|_2^2 \text{ subject to } \|d\|_2 = 1$$

  - $d^T x^{(i)}$ **is scalar, hence** $dd^T x^{(i)} = d^T x^{(i)} d = x^{(i)T} dd$

- **We get,** $d^* = \arg_d \min \sum_i \|x^{(i)} - x^{(i)T} dd\|_2^2$ **subject to** $\|d\|_2 = 1$

- **Rewriting in terms of single design matrix**

$$d^* = \arg_d \min \|X - Xdd^T\|_2^2 \text{ subject to } \|d\|_2 = 1$$

Principal Component Analysis (contd.)

- **Simplifying based on the assumptions**

$$d^* = \arg_d \min \sum_i \|x^{(i)} - dd^Tx^{(i)}\|_2^2 \text{ subject to } \|d\|_2 = 1$$

- $d^Tx^{(i)}$ **is scalar, hence** $dd^Tx^{(i)} = d^Tx^{(i)}d = x^{(i)T}dd$

- **We get,** $d^* = \arg_d \min \sum_i \|x^{(i)} - x^{(i)T}dd\|_2^2 \text{ subject to } \|d\|_2 = 1$

- **Rewriting in terms of single design matrix**

$$d^* = \arg_d \min \|X - Xdd^T\|_2^2 \text{ subject to } \|d\|_2 = 1$$

- **Now we have,** $\arg_d \min \|X - Xdd^T\|_F^2 \text{ subject to } \|d^Td\| = 1$

- **Simplifying,**

$$\arg_{\mathbf{d}} \min \|\mathsf{X} - \mathsf{X}\mathbf{d}\mathbf{d}^{T}\|_{F}^{2}$$

- **Simplifying,**

$$\arg_{\mathbf{d}} \min \|\mathsf{X} - \mathsf{X}\mathbf{d}\mathbf{d}^T\|_F^2$$
$$= \arg_{\mathbf{d}} \min Tr\left((\mathsf{X} - \mathsf{X}\mathbf{d}\mathbf{d}^T)^T(\mathsf{X} - \mathsf{X}\mathbf{d}\mathbf{d}^T)\right)$$

- **Simplifying,**

$$
\begin{aligned}
&\arg_{\mathbf{d}} \min \|X - Xdd^T\|_F^2 \\
=\ &\arg_{\mathbf{d}} \min Tr\left((X - Xdd^T)^T(X - Xdd^T)\right) \\
=\ &\arg_{\mathbf{d}} \min Tr(X^TX - X^TXdd^T - dd^TX^TX + dd^TX^TXdd^T)
\end{aligned}
$$

- **Simplifying,**

$$\arg_{\mathbf{d}} \min \|X - Xdd^T\|_F^2$$
$$= \arg_{\mathbf{d}} \min Tr\left((X - Xdd^T)^T(X - Xdd^T)\right)$$
$$= \arg_{\mathbf{d}} \min Tr(X^TX - X^TXdd^T - dd^TX^TX + dd^TX^TXdd^T)$$
$$= \arg_{\mathbf{d}} \min -2\, Tr(X^TXdd^T) + Tr(X^TXdd^Tdd^T)$$

Principal Component Analysis (contd.)

- **Simplifying,**

$$\arg_d \min \|X - Xdd^T\|_F^2$$
$$= \arg_d \min Tr\left((X - Xdd^T)^T(X - Xdd^T)\right)$$
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$$= \arg_d \min - Tr(X^TXdd^T)$$

- **Simplifying,**

$$\arg_{\mathsf{d}} \min \|\mathsf{X} - \mathsf{X}\mathsf{d}\mathsf{d}^T\|_F^2$$
$$= \arg_{\mathsf{d}} \min Tr\left((\mathsf{X} - \mathsf{X}\mathsf{d}\mathsf{d}^T)^T(\mathsf{X} - \mathsf{X}\mathsf{d}\mathsf{d}^T)\right)$$
$$= \arg_{\mathsf{d}} \min Tr(\mathsf{X}^T\mathsf{X} - \mathsf{X}^T\mathsf{X}\mathsf{d}\mathsf{d}^T - \mathsf{d}\mathsf{d}^T\mathsf{X}^T\mathsf{X} + \mathsf{d}\mathsf{d}^T\mathsf{X}^T\mathsf{X}\mathsf{d}\mathsf{d}^T)$$
$$= \arg_{\mathsf{d}} \min -2\, Tr(\mathsf{X}^T\mathsf{X}\mathsf{d}\mathsf{d}^T) + Tr(\mathsf{X}^T\mathsf{X}\mathsf{d}\mathsf{d}^T\mathsf{d}\mathsf{d}^T)$$
$$= \arg_{\mathsf{d}} \min -Tr(\mathsf{X}^T\mathsf{X}\mathsf{d}\mathsf{d}^T)$$
$$= \arg_{\mathsf{d}} \min -Tr(\mathsf{d}^T\mathsf{X}^T\mathsf{X}\mathsf{d})$$

CS551

39

Principal Component Analysis (contd.)

- **Simplifying,**

$$\arg_{\mathbf{d}} \min \|\mathbf{X} - \mathbf{X}\mathbf{d}\mathbf{d}^T\|_F^2$$
$$= \arg_{\mathbf{d}} \min Tr\left((\mathbf{X} - \mathbf{X}\mathbf{d}\mathbf{d}^T)^T(\mathbf{X} - \mathbf{X}\mathbf{d}\mathbf{d}^T)\right)$$
$$= \arg_{\mathbf{d}} \min Tr(\mathbf{X}^T\mathbf{X} - \mathbf{X}^T\mathbf{X}\mathbf{d}\mathbf{d}^T - \mathbf{d}\mathbf{d}^T\mathbf{X}^T\mathbf{X} + \mathbf{d}\mathbf{d}^T\mathbf{X}^T\mathbf{X}\mathbf{d}\mathbf{d}^T)$$
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$$= \arg_{\mathbf{d}} \min - Tr(\mathbf{X}^T\mathbf{X}\mathbf{d}\mathbf{d}^T)$$
$$= \arg_{\mathbf{d}} \min - Tr(\mathbf{d}^T\mathbf{X}^T\mathbf{X}\mathbf{d})$$

- **Optimization problem can be solved by eigen decomposition**

Principal Component Analysis (contd.)
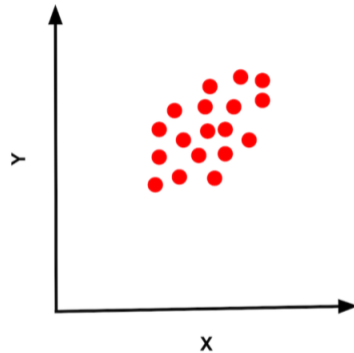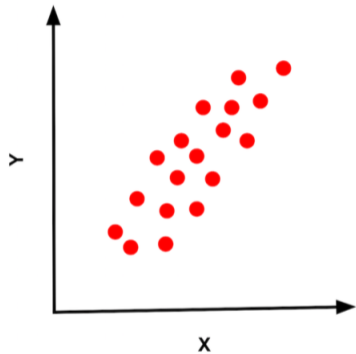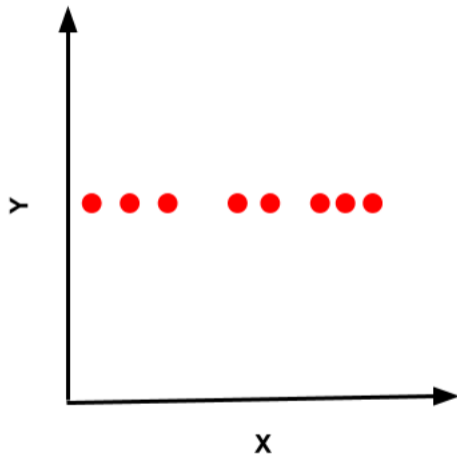
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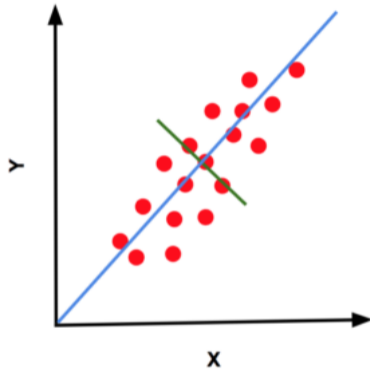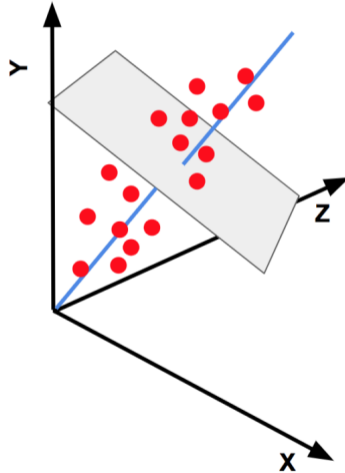
Principal Component Analysis (contd.)

- **Assemble data matrix** $A = \begin{bmatrix} x_1 & x_2 & \ldots & x_n \\ y_1 & y_2 & \ldots & y_n \\ z_1 & z_2 & \ldots & z_n \end{bmatrix}$

- **Calculate mean** $\mu_x = \dfrac{1}{n} \sum_i x_i$, $\mu_y = \dfrac{1}{n} \sum_i y_i$, $\mu_z = \dfrac{1}{n} \sum_i z_i$

- **Subtract mean from data matrix**

$$M = \begin{bmatrix} x_1 - \mu_x & x_2 - \mu_x & \ldots & x_n - \mu_x \\ y_1 - \mu_y & y_2 - \mu_y & \ldots & y_n - \mu_y \\ z_1 - \mu_z & z_2 - \mu_z & \ldots & z_n - \mu_z \end{bmatrix}$$

- **Calculate covariance matrix** $C = MM^T$

- **Find eigen vector and value of** C

Overview of Probability

Probability

- **Mathematical framework for representing uncertain statements**
- **Possible source of uncertainty**
  - **Inherent stochasticity**
  - **Incomplete observability**
  - **Incomplete model**
- **Two broad categories**
  - **Frequentist**
    - **Getting a card**
  - **Bayesian**
    - **Chance of having flu**

Random Variable

- **Variable that can take different values randomly**
- **Example**
  - X **is random variable that can take value** x_1 **or** x_2

Probability Distribution

- How likely a random variable is to take on each of its possible states

Probability Distribution

- **How likely a random variable is to take on each of its possible states**
- **Probability Mass Function**
  - **Discrete**
  - **Maps state to probability of taking that state**

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- **Joint probability distribution**
  - $P(X = x, Y = y)$ — **probability of X taking value x and Y taking value y**

Probability Distribution

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  - **Discrete**
  - **Maps state to probability of taking that state**
- **Joint probability distribution**
  - $P(X = x, Y = y)$ **— probability of** X **taking value** x **and** Y **taking value** y
- **Probability function** P **on** X
  - **The domain of** P **is set of all possible state of** X
  - $\forall x \in X \quad 0 \le P(x) \le 1$
  - $\displaystyle\sum_{x \in X} P(x) = 1$
- **Example**
  - **Uniform distribution with** k **different states** $1/k$

Probability Density Function

- **Continuous variable (*p*)**

Probability Density Function

- **Continuous variable (p)**
  - **The domain of p is set of all possible state of X**
  - $\forall x \in X \quad p(x) \geq 0$
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Probability Density Function

- **Continuous variable (p)**
  - **The domain of p is set of all possible state of X**
  - $\forall x \in X \quad p(x) \geq 0$
  - $\displaystyle \int_{x \in X} p(x)\,dx = 1$
- **Example**
  - **Uniform distribution in $[a, b]$ is represented as $X \sim U(a, b)$**

Marginal Probability

- **Probability distribution over the subset**
- **Let X, Y be random variables and $P(x, y)$ is known**
  - $P(x) = \displaystyle\sum_{y \in Y} P(x, y)$
  - $p(x) = \displaystyle\int_{y \in Y} p(x, y)\, dy$

Conditional Probability

- **Probability of some event given that some other event has happened**

$$P(Y = y | X = x) = \frac{P(Y = y, X = x)}{P(X = x)}$$

Conditional Probability

- **Probability of some event given that some other event has happened**

$$P(Y = y | X = x) = \frac{P(Y = y, X = x)}{P(X = x)}$$

- **Chain rule:** $P(x_1 x_2 \ldots x_n) = P(x_1) \prod_{i=2}^{n} P(x_i | x_1 \ldots x_{i-1})$
  - $P(a, b, c) = P(a | b, c) P(b | c) P(c)$

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- **Independence of random variable**

Conditional Probability

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  - $P(a, b, c) = P(a | b, c) P(b | c) P(c)$
- **Independence of random variable**
  - $\forall x \in X, y \in Y \quad p(X = x, Y = y) = p(X = x) p(Y = y)$
  - **Conditional independence**
    - $p(x, y | z) = p(x | z) p(y | z)$

Expectation

- **Expected value of some function with respect to probability distribution** $P(x)$

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Expectation

- **Expected value of some function with respect to probability distribution $P(x)$**

  - $\mathbb{E}_{X \sim P}[f(x)] = \sum_x P(x)f(x)$

  - $\mathbb{E}_{X \sim p}[f(x)] = \int_x P(x)f(x)\,dx$

  - $\mathbb{E}_X[\alpha f(x) + \beta g(x)] = \alpha \mathbb{E}_X[f(x)] + \beta \mathbb{E}_X[g(x)]$

- **How much the values of a given function vary as we sample different values of x from its probability distribution**

Variance & Covariance

- **How much the values of a given function vary as we sample different values of x from its probability distribution**
  - **Var**$(f(x)) = \mathbb{E}[(f(x) - \mathbb{E}[f(x)])^2]$

Variance & Covariance

- How much the values of a given function vary as we sample different values of x from its probability distribution
  - $\text{Var}(f(x)) = \mathbb{E}[(f(x) - \mathbb{E}[f(x)])^2]$
- How much two values are linearly related

Variance & Covariance

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  - **Var**$(f(x)) = \mathbb{E}[(f(x) - \mathbb{E}[f(x)])^2]$
- How much two values are linearly related
  - $Cov(f(x), g(y)) = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])(g(y) - \mathbb{E}[g(y)])\right]$

Variance & Covariance

- How much the values of a given function vary as we sample different values of x from its probability distribution
  - **Var**$(f(x)) = \mathbb{E}[(f(x) - \mathbb{E}[f(x)])^2]$
- How much two values are linearly related
  - $Cov(f(x), g(y)) = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])(g(y) - \mathbb{E}[g(y)])\right]$
    - It can be positive or negative

- **Suppose $P(y|x)$ and $P(x)$ known and need to find out $P(x|y)$**

$$P(x|y) = \frac{P(x)P(y|x)}{P(y)}$$

Bayes' rule

- **Suppose $P(y|x)$ and $P(x)$ known and need to find out $P(x|y)$**

$$P(x|y) = \frac{P(x)P(y|x)}{P(y)}$$

- **Now $P(y)$ can be found out from**

$$P(y) = \sum_x P(y|x)P(x)$$

Problems

- Suppose that we have two bags each containing black and white balls. One bag contains three times as many white balls as blacks. The other bag contains three times as many black balls as white. Suppose we choose one of these bags at random. For this bag we select five balls at random, replacing each ball after it has been selected. The result is that we find 4 white balls and one black. What is the probability that we were using the bag with mainly white balls?

- Given the following statistics, what is the probability that a person has cancer if he has a positive pathological result?
  - One percent of people over 50 have this cancer.
  - Ninety percent of people who have this cancer test positive on pathological report.
 - Eight percent of people will have false positives.

Information theory

- **Quantifying how much information is present in a signal**
  - **The sun rises in the east. — uninformative**
  - **There was a solar eclipse this morning. — informative**
- **Therefore, we would like to quantify**
  - **Likely event should have low information content**
    - **Events guaranteed to happen should have no information**
  - **Less likely event should have higher information content**
  - **Independent event should have additive information**
- **Information of an event $X = x$ be $I(x) = -\log P(x)$**
  - **Natural logarithm, with base e**
  - **Unit of $I(x)$ is *nat***

Gaussian distribution

- **Also, known as Normal Distribution**

$$\mathcal{N}(x; \mu, \sigma^2) = \sqrt{\frac{1}{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right)$$
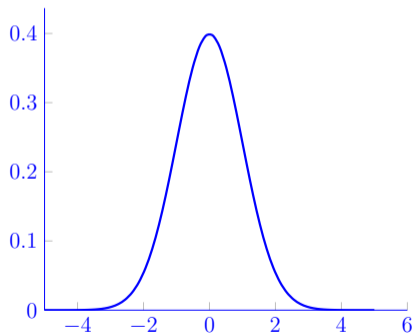
Multivariate normal distribution

- **Defined as**

$$\mathcal{N}(\mathsf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sqrt{\frac{1}{(2\pi)^n \mathbf{det}(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\mathsf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathsf{x} - \boldsymbol{\mu})\right)$$

- $\boldsymbol{\mu}$ — mean of the distribution
- $\boldsymbol{\Sigma}$ — Covariance matrix of the distribution

References

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CS551

59