

# *Introduction to Statistical Machine Learning*

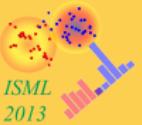
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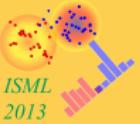
Canberra  
February – June 2013

(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")



## *Outlines*

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## Part III

# *Linear Algebra*

*Basic Concepts*

*Linear Transformations*

*Trace*

*Inner Product*

*Projection*

*Rank, Determinant, Trace*

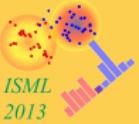
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# Intuition

## Geometry

- Points and Lines
- Vector addition and scaling
- Humans have experience with 3 dimensions (less with 1, 2 though)

Generalisation to  $N$  dimensions (possibly  $N \rightarrow \infty$ )

- Line  $\rightarrow$  vector space  $\mathbb{V}$
- Point  $\rightarrow$  vector  $x \in \mathbb{V}$
- Example :  $X \in \mathbb{R}^{n \times m}$
- Space of matrices  $\mathbb{R}^{n \times m}$  and the space of vectors  $\mathbb{R}^{n \cdot m}$  are isomorphic

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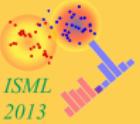
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# Vector Space $\mathcal{V}$ , underlying Field $\mathcal{F}$

Given vectors  $\mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathcal{V}$  and scalars  $\alpha, \beta \in \mathcal{F}$ , the following holds:

- Associativity of addition :  $\mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w}$  .
- Commutativity of addition :  $\mathbf{v} + \mathbf{w} = \mathbf{w} + \mathbf{v}$  .
- Identity element of addition :  $\exists \mathbf{0}$  such that  $\mathbf{v} + \mathbf{0} = \mathbf{v}, \forall \mathbf{v} \in \mathcal{V}$ .
- Inverse of addition : For all  $\mathbf{v} \in \mathcal{V}, \exists \mathbf{w} \in \mathcal{V}$ , such that  $\mathbf{v} + \mathbf{w} = \mathbf{0}$ . The additive inverse is denoted  $-\mathbf{v}$ .
- Distributivity of scalar multiplication with respect to vector addition :  $\alpha(\mathbf{v} + \mathbf{w}) = \alpha\mathbf{v} + \alpha\mathbf{w}$  .
- Distributivity of scalar multiplication with respect to field addition :  $(\alpha + \beta)\mathbf{v} = \alpha\mathbf{v} + \beta\mathbf{v}$  .
- Compatibility of scalar multiplication with field multiplication :  $\alpha(\beta\mathbf{v}) = (\alpha\beta)\mathbf{v}$  .
- Identity element of scalar multiplication :  $1\mathbf{v} = \mathbf{v}$ , where 1 is the identity in  $\mathcal{F}$  .

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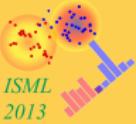
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# Matrix-Vector Multiplication

```
1  for i in xrange(m):  
    R[i] = 0.0;  
    for j in xrange(n):  
        R[i] = R[i] + A[i,j] * V[j]
```

Listing 1: Code for elementwise matrix multiplication.

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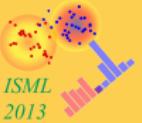
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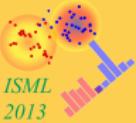
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# Matrix-Vector Multiplication

```
1  for i in xrange(m):
    R[i] = 0.0;
    for j in xrange(n):
        R[i] = R[i] + A[i,j] * V[j]
```

Listing 2: Code for elementwise matrix multiplication.

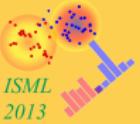
$$\begin{array}{c} A \qquad \qquad \qquad V \qquad \qquad \qquad R \\[10pt]
 \left[ \begin{array}{cccc} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{array} \right] \left[ \begin{array}{c} v_1 \\ v_2 \\ \dots \\ v_n \end{array} \right] = \left[ \begin{array}{c} a_{11}v_1 + a_{12}v_2 + \dots + a_{1n}v_n \\ a_{21}v_1 + a_{22}v_2 + \dots + a_{2n}v_n \\ \dots \\ a_{m1}v_1 + a_{m2}v_2 + \dots + a_{mn}v_n \end{array} \right] \end{array}$$



$$\begin{matrix} A & V & = & R \\ 
 \left[ \begin{matrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{matrix} \right] \left[ \begin{matrix} v_1 \\ v_2 \\ \dots \\ v_n \end{matrix} \right] & = & \left[ \begin{matrix} a_{11}v_1 + a_{12}v_2 + \dots + a_{1n}v_n \\ a_{21}v_1 + a_{22}v_2 + \dots + a_{2n}v_n \\ \dots \\ a_{m1}v_1 + a_{m2}v_2 + \dots + a_{mn}v_n \end{matrix} \right]
 \end{matrix}$$

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# Matrix-Vector Multiplication



$$A \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = R$$
$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} a_{11}v_1 + a_{12}v_2 + \cdots + a_{1n}v_n \\ a_{21}v_1 + a_{22}v_2 + \cdots + a_{2n}v_n \\ \cdots \\ a_{m1}v_1 + a_{m2}v_2 + \cdots + a_{mn}v_n \end{bmatrix}$$

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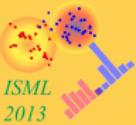
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```
R = A[:,0] * V[0];
for j in xrange(1, n):
    R += A[:, j] * V[j];
```

Listing 4: Code for columnwise matrix multiplication.



- Denote the  $n$  columns of  $A$  by  $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$
- Each  $\mathbf{a}_i$  is now a (column) vector

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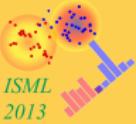
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$$A \quad V = R$$
$$\begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \dots & \mathbf{a}_n \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1 v_1 + \mathbf{a}_2 v_2 + \dots + \mathbf{a}_n v_n \end{bmatrix}$$



- Given  $R = AV$ ,

$$R = \left[ \mathbf{a}_1 v_1 + \mathbf{a}_2 v_2 + \cdots + \mathbf{a}_n v_n \right]$$

- What is  $R^T$  ?

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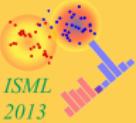
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# Transpose of R

- Given  $R = AV$ ,

$$R = \begin{bmatrix} \mathbf{a}_1 v_1 + \mathbf{a}_2 v_2 + \cdots + \mathbf{a}_n v_n \end{bmatrix}$$

- What is  $R^T$  ?

- 

$$R^T = [v_1 \mathbf{a}_1^T + v_2 \mathbf{a}_2^T + \cdots + v_n \mathbf{a}_n^T]$$

- NOT equal to  $A^T V^T$  ! (In fact,  $A^T V^T$  is not even defined.)

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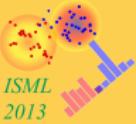
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- Reverse order rule :  $(AV)^T = V^T A^T$

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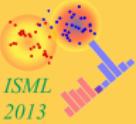
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- Reverse order rule :  $(AV)^T = V^T A^T$

$$\begin{matrix} V^T & A^T & R^T \end{matrix}$$
$$\begin{bmatrix} v_1 & v_2 \dots v_n \end{bmatrix} \begin{bmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \dots \\ \mathbf{a}_n^T \end{bmatrix} = [v_1 \mathbf{a}_1^T + v_2 \mathbf{a}_2^T + \dots + v_n \mathbf{a}_n^T]$$

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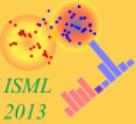
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- The trace of a square matrix  $A$  is the sum of all diagonal elements of  $A$ .

$$\text{tr}\{A\} = \sum_{k=1}^n A_{kk}$$

- Example

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

$$\text{tr}\{A\} = 1 + 5 + 9 = 15$$

- The trace does not exist for a non-square matrix.

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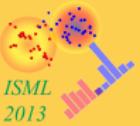
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# vec( $x$ ) operator

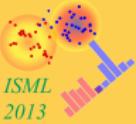
- Define  $\text{vec}(X)$  as the vector which results from stacking all columns of a matrix  $A$  on top of each other.
- Example

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

$$\text{vec}(A) = \begin{bmatrix} 1 \\ 4 \\ 7 \\ 2 \\ 5 \\ 8 \\ 3 \\ 6 \\ 9 \end{bmatrix}$$

- Given two matrices  $\mathbf{X}, \mathbf{Y} \in \mathbb{R}^{n \times p}$ , the trace of the product  $\mathbf{X}^T \mathbf{Y}$  can be written as

$$\text{tr}\{\mathbf{X}^T \mathbf{Y}\} = \text{vec}(\mathbf{X})^T \text{vec}(\mathbf{Y})$$



- Mapping from two vectors  $x, y \in \mathbb{V}$  to a field of scalars  $\mathbb{F}$   
(  $\mathbb{F} = \mathbb{R}$  or  $\mathbb{F} = \mathbb{C}$  ):

$$\langle \cdot, \cdot \rangle : \mathbb{V} \times \mathbb{V} \rightarrow \mathbb{F}$$

- Conjugate Symmetry :

$$\langle x, y \rangle = \overline{\langle y, x \rangle}$$

- Linearity :

$$\langle ax, y \rangle = a \langle x, y \rangle, \text{ and } \langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle$$

- Positive-definiteness :

$$\langle x, x \rangle \geq 0, \text{ and } \langle x, x \rangle = 0 \text{ for } x = 0 \text{ only.}$$

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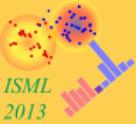
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# Canonical Inner Products

- Inner product for real numbers  $x, y \in \mathbb{R}$ :

$$\langle x, y \rangle = xy$$

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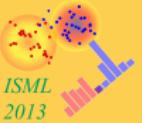
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# Canonical Inner Products

- Inner product for real numbers  $x, y \in \mathbb{R}$ :

$$\langle x, y \rangle = xy$$

- Dot product between two vectors:

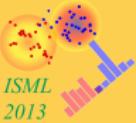
Given  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y} \equiv \sum_{k=1}^n x_k y_k = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n$$

- Canonical inner product for matrices :

Given  $\mathbf{X}, \mathbf{Y} \in \mathbb{R}^{n \times p}$

$$\begin{aligned} \langle \mathbf{X}, \mathbf{Y} \rangle &= \text{tr} \{ \mathbf{X}^T \mathbf{Y} \} = \sum_{k=1}^p (\mathbf{X}^T \mathbf{Y})_{kk} = \sum_{k=1}^p \sum_{l=1}^n (\mathbf{X}^T)_{kl} (\mathbf{Y})_{lk} \\ &= \sum_{k=1}^p \sum_{l=1}^n \mathbf{X}_{lk} \mathbf{Y}_{lk} \end{aligned}$$



# Calculations with Matrices

- Denote  $(i, j)^{\text{th}}$  element of matrix  $\mathbf{X}$  by  $\mathbf{X}_{ij}$
- Transpose :  $(\mathbf{X}^T)_{ij} = \mathbf{X}_{ji}$
- Product :  $(\mathbf{XY})_{ij} = \sum_{k=1}^m \mathbf{X}_{ik} \mathbf{Y}_{kj}$
- Proof of the linearity of the canonical matrix inner product :

$$\langle \mathbf{X} + \mathbf{Y}, \mathbf{Z} \rangle = \text{tr} \left\{ (\mathbf{X} + \mathbf{Y})^T \mathbf{Z} \right\} = \sum_{k=1}^p ((\mathbf{X} + \mathbf{Y})^T \mathbf{Z})_{kk}$$

$$= \sum_{k=1}^p \sum_{l=1}^n ((\mathbf{X} + \mathbf{Y})^T)_{kl} \mathbf{Z}_{lk} = \sum_{k=1}^p \sum_{l=1}^n (\mathbf{X}_{lk} + \mathbf{Y}_{lk}) \mathbf{Z}_{lk}$$

$$= \sum_{k=1}^p \sum_{l=1}^n \mathbf{X}_{lk} \mathbf{Z}_{lk} + \mathbf{Y}_{lk} \mathbf{Z}_{lk}$$

$$= \sum_{k=1}^p \sum_{l=1}^n (\mathbf{X}^T)_{kl} \mathbf{Z}_{lk} + (\mathbf{Y}^T)_{kl} \mathbf{Z}_{lk}$$

$$= \sum_{k=1}^p (\mathbf{X}^T \mathbf{Z})_{kk} + (\mathbf{Y}^T \mathbf{Z})_{kk}$$

$$= \text{tr} \left\{ \mathbf{X}^T \mathbf{Z} \right\} + \text{tr} \left\{ \mathbf{Y}^T \mathbf{Z} \right\} = \langle \mathbf{X}, \mathbf{Z} \rangle + \langle \mathbf{Y}, \mathbf{Z} \rangle$$

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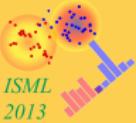
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# Projection

- In linear algebra and functional analysis, a **projection** is a linear transformation  $P$  from a vector space  $\mathbb{V}$  to itself such that

$$P^2 = P$$

Projection transformation can only have effective influence for one time, because after first time projection, we can not move it anymore by further applying that transformation.



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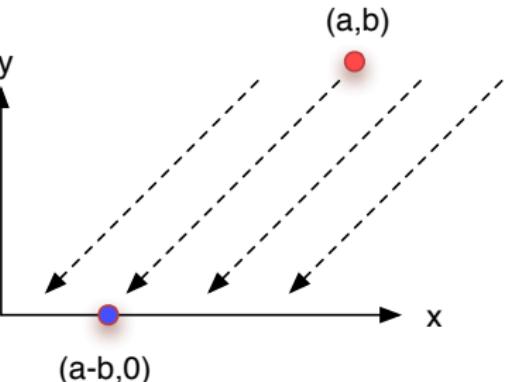
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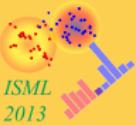
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- In linear algebra and functional analysis, a projection is a linear transformation  $P$  from a vector space  $\mathbb{V}$  to itself such that

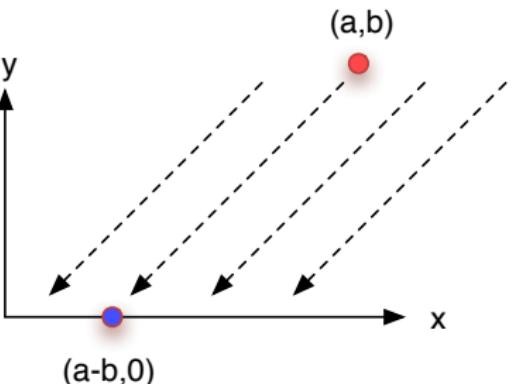
$$P^2 = P$$





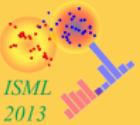
- In linear algebra and functional analysis, a projection is a linear transformation  $P$  from a vector space  $\mathbb{V}$  to itself such that

$$P^2 = P$$



$$A \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a - b \\ 0 \end{bmatrix} \quad A = \begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix}$$

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# Orthogonal Projection

- Orthogonality : need an **inner product**  $\langle x, y \rangle$
- Choose two arbitrary vectors  $x$  and  $y$ . Then  $Px$  and  $y - Py$  are orthogonal.

$$0 = \langle Px, y - Py \rangle = (Px)^T(y - Py) = x^T(P - P^T P)y$$

## • Orthogonal Projection

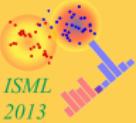
$$P^2 = P \quad P = P^T$$

- Example : Given some unit vector  $u \in \mathbb{R}^n$  characterising a line through the origin in  $\mathbb{R}^n$
- project an arbitrary vector  $x \in \mathbb{R}^n$  onto this line by

$$P = uu^T$$

- Proof :  $P = P^T$ , and

$$P^2x = (uu^T)(uu^T)x = uu^Tx = Px$$



# Orthogonal Projection

- Given a matrix  $\mathbf{A} \in \mathbb{R}^{n \times p}$  and a vector  $\mathbf{x}$ . What is the closest point  $\tilde{\mathbf{x}}$  to  $\mathbf{x}$  in the column space of  $\mathbf{A}$  ?
- Orthogonal Projection into the column space of  $\mathbf{A}$

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

- Projection matrix

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

- Proof

$$P^2 = \mathbf{A}(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{A}(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T = \mathbf{A}(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T = P$$

- Orthogonal projection ?

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

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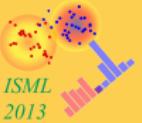
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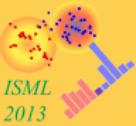
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$$a_1 \mathbf{v}_1 + a_2 \mathbf{v}_2 + \cdots + a_k \mathbf{v}_k = \mathbf{0} \equiv \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

has only the trivial solution

$$a_1 = a_2 = a_k = 0$$



- The **column rank** of a matrix  $A$  is the maximal number of linearly independent columns of  $A$ .
- The **row rank** of a matrix  $A$  is the maximal number of linearly independent rows of  $A$ .
- For every matrix  $A$ , the row rank and column rank are equal, called **the rank** of  $A$ .

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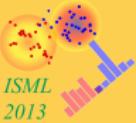
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Let  $S_n$  be the set of all permutation of the numbers  $\{1, \dots, n\}$ .  
The determinant of the square matrix  $A$  is then given by

$$\det \{A\} = \sum_{\sigma \in S_n} \text{sgn}(\sigma) \prod_{i=1}^n A_{i,\sigma(i)}$$

where  $\text{sgn}$  is the signature of the permutation (+1 if the permutation is even, -1 if the permutation is odd).

- $\det \{AB\} = \det \{A\} \det \{B\}$  for  $A, B$  square matrices.
- $\det \{A^{-1}\} = \det \{A\}^{-1}$ .
- $\det \{A^T\} = \det \{A\}$ .

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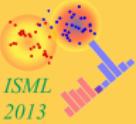
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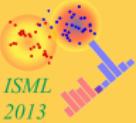
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# Matrix Inverse

- Identity Matrix  $I$
- $I = AA^{-1} = A^{-1}A$
- The matrix inverse  $A^{-1}$  does only exist for square matrices which are NOT singular.
- Singular matrix
  - at least one eigenvalue is zero,
  - determinant  $|A| = 0$ .
- Inversion 'reverses the order' (like transposition)

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

(Only then is  $(AB)(AB)^{-1} = (AB)B^{-1}A^{-1} = AA^{-1} = I$ .)



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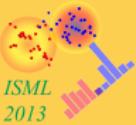
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# Matrix Inverse and Transpose

- $(A^{-1})^T$  ?

# Matrix Inverse and Transpose



- $(A^{-1})^T$  ?
- need to assume that  $(A^{-1})$  exists
- rule :  $(A^{-1})^T = (A^T)^{-1}$

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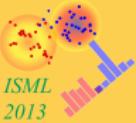
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$$(A^{-1} + B^T C^{-1} B)^{-1} B^T C^{-1} = A B^T (B A B^T + C)^{-1}$$

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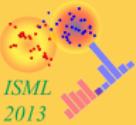
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$$(A^{-1} + B^T C^{-1} B)^{-1} B^T C^{-1} = A B^T (B A B^T + C)^{-1}$$

- How to analyse and prove such an equation?
- $A^{-1}$  must exist, therefore  $A$  must be square, say  $A \in \mathbb{R}^{n \times n}$ .
- Same for  $C^{-1}$ , so let's assume  $C \in \mathbb{R}^{m \times m}$ .
- Therefore,  $B \in \mathbb{R}^{m \times n}$ .

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$$(A^{-1} + B^T C^{-1} B)^{-1} B^T C^{-1} = AB^T (BAB^T + C)^{-1}$$

- Multiply by  $(BAB^T + C)$

$$(A^{-1} + B^T C^{-1} B)^{-1} B^T C^{-1} (BAB^T + C) = AB^T$$

- Simplify the left-hand side

$$\begin{aligned}& (A^{-1} + B^T C^{-1} B)^{-1} [B^T C^{-1} B (AB^T) + B^T] \\&= (A^{-1} + B^T C^{-1} B)^{-1} [B^T C^{-1} B + A^{-1}] AB^T \\&= AB^T\end{aligned}$$

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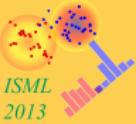
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$$(A + BD^{-1}C)^{-1} = A^{-1} - A^{-1}B(D + CA^{-1}B)^{-1}CA^{-1}$$

- Useful if  $A$  is diagonal and easy to invert, and  $B$  is very tall (many rows, but only a few columns) and  $C$  is very wide (few rows, many columns).

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# Manipulating Matrix Equations



- Don't multiply by a matrix which does not have full rank.  
**Why?** In the general case, you will loose solutions.
- Don't multiply by nonsquare matrices.
- Don't assume a matrix inverse exists because a matrix is square. The matrix might be singular and you are making the same mistake as if deducing  $a = b$  from  $a 0 = b 0$ .

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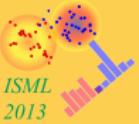
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# Eigenvectors

- Every square matrix  $A \in \mathbb{R}^{n \times n}$  has an Eigenvector decomposition

$$Ax = \lambda x$$

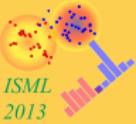
where  $x \in \mathbb{R}^n$  and  $\lambda \in \mathbb{C}$ .

- Example:

$$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} x = \lambda x$$

$$\lambda = \{-i, i\}$$

$$x = \left\{ \begin{bmatrix} i \\ 1 \end{bmatrix}, \begin{bmatrix} -i \\ 1 \end{bmatrix} \right\}$$



- How many eigenvalue/eigenvector pairs?
- 

$$Ax = \lambda x$$

is equivalent to

$$(A - \lambda I)x = 0$$

- Has only non-trivial solution for  $\det\{A - \lambda I\} = 0$
- polynom of  $n$ th order; at most  $n$  distinct solutions

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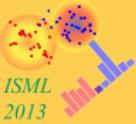
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- How can we enforce **real eigenvalues**?
- Let's look at matrices with complex entries  $A \in \mathbb{C}^{n \times n}$ .
- **Transposition is replaced by Hermitian adjoint**, e.g.

$$\begin{bmatrix} 1 + i2 & 3 + i4 \\ 5 + i6 & 7 + i8 \end{bmatrix}^H = \begin{bmatrix} 1 - i2 & 5 - i6 \\ 3 - i4 & 7 - i8 \end{bmatrix}$$

- Denote the complex conjugate of a complex number  $\lambda$  by  $\bar{\lambda}$ .

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# Real Eigenvalues

- How can we enforce real eigenvalues?
- Let's assume  $A \in \mathbb{C}^{n \times n}$ , Hermitian ( $A^H = A$ ).
- Calculate

$$x^H A x = \lambda x^H x$$

for an eigenvector  $x \in \mathbb{C}^n$  of  $A$ .

- Another possibility to calculate  $x^H A x$

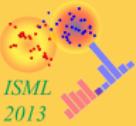
$$\begin{aligned} x^H A x &= x^H A^H x && (A \text{ is Hermitian}) \\ &= (x^H A x)^H && (\text{reverse order}) \\ &= (\lambda x^H x)^H && (\text{eigenvalue}) \\ &= \bar{\lambda} x^H x \end{aligned}$$

- and therefore

$$\lambda = \bar{\lambda} \quad (\lambda \text{ is real}).$$

- If  $A$  is Hermitian, then all eigenvalues are real.
- Special case: If  $A$  has only real entries and is symmetric, then all eigenvalues are real.

# Singular Value Decomposition



Every matrix  $A \in \mathbb{R}^{n \times p}$  can be decomposed into a product of three matrices

$$A = U\Sigma V^T$$

where  $U \in \mathbb{R}^{n \times n}$  and  $V \in \mathbb{R}^{p \times p}$  are orthogonal matrices ( $U^T U = I$  and  $V^T V = I$ ), and  $\Sigma \in \mathbb{R}^{n \times p}$  has nonnegative numbers on the diagonal.

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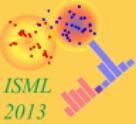
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# How to calculate a gradient?

- Given a vector space  $\mathcal{V}$ , and a function  $f : \mathcal{V} \rightarrow \mathbb{R}$ .
- Example:  $X \in \mathbb{R}^{n \times p}$ , arbitrary  $C \in \mathbb{R}^{n \times n}$ ,

$$f(X) = \text{tr} \{ X^T C X \}.$$

- How to calculate the gradient of  $f$  ?

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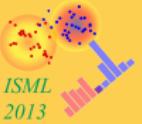
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# How to calculate a gradient?

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- Example:  $X \in \mathbb{R}^{n \times p}$ , arbitrary  $C \in \mathbb{R}^{n \times n}$ ,

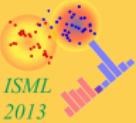
$$f(X) = \text{tr} \{ X^T C X \}.$$

- How to calculate the gradient of  $f$  ?
- Ill-defined question. There is no gradient in a vector space.
- Only a Directional Derivative at point  $X \in \mathcal{V}$  in direction  $\xi \in \mathcal{V}$ .

$$\mathcal{D}f(X)(\xi) = \lim_{h \rightarrow 0} \frac{f(X + h\xi) - f(X)}{h}$$

- For the example  $f(X) = \text{tr} \{ X^T C X \}$

$$\begin{aligned}\mathcal{D}f(X)(\xi) &= \lim_{h \rightarrow 0} \frac{\text{tr} \{ (X + h\xi)^T C (X + h\xi) \} - \text{tr} \{ X^T C X \}}{h} \\ &= \text{tr} \{ \xi^T C X + X^T C \xi \} = \text{tr} \{ X^T (C^T + C) \xi \}\end{aligned}$$



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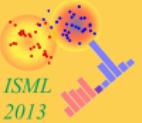
# How to calculate a gradient?

- Given a vector space  $\mathcal{V}$ , and a function  $f : \mathcal{V} \rightarrow \mathbb{R}$ .
  - How to calculate the gradient of  $f$  ?
- ① Calculate the Directional Derivative
- ② Define an inner product  $\langle A, B \rangle$  on the vector space
- ③ The gradient is now defined as

$$\mathcal{D}f(X)(\xi) = \langle \text{grad } f, \xi \rangle$$

- For the example  $f(X) = \text{tr}\{X^T C X\}$
- Define the inner product  $\langle A, B \rangle = \text{tr}\{A^T B\}$  .
- Write the Directional Derivative as an inner product with  $\xi$

$$\begin{aligned}\mathcal{D}f(X)(\xi) &= \text{tr}\{X^T (C^T + C)\xi\} \\ &= \langle (C + C^T)X, \xi \rangle = \langle \text{grad } f, \xi \rangle\end{aligned}$$



- Gilbert Strang, "Introduction to Linear Algebra", Wellesley Cambridge, 2009.
- David C. Lay, "Linear Algebra and Its Applications", Addison Wesley, 2005.

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