

# EECS 545: Machine Learning

## Linear Algebra Review

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Portions of this presentation adapted from  
EECS 545 Winter 2010, Stanford CS229 Lecture Notes, CMU 10-701,  
Delaware CISC 489/689 review slides.

# Outline

- Basic Concepts and Notation
- Matrix Multiplication
- Operations and Properties
- Matrix Calculus

# Outline

- **Basic Concepts and Notation**
- Matrix Multiplication
- Operations and Properties
- Matrix Calculus

# Basic Concepts

- Why linear algebra?
  - Compact representation
  - Efficient representation
  - Tools like Matlab
  - Help appreciate Machine Learning

- Can represent:

$$4x_1 - 5x_2 = -13$$

$$-2x_1 - 3x_2 = 9$$

As:

$$Ax = b$$

Where:

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

- Generalizes well to many machine learning contexts

# Basic Notation

- $x \in \mathfrak{R}^n$  is a vector with  $n$  entries.

- $x_i$  is the  $i^{th}$  entry of  $x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$

# Basic Notation

- $A \in \mathfrak{R}^{m \times n}$  is a matrix with  $m$  rows and  $n$  columns.
- $a_{ij}$  or  $A_{ij}$  is the entry in the  $i^{th}$  row and  $j^{th}$  column of  $A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$
- $a_j$  is the  $j^{th}$  column of  $A$
- $a_i^T$  is the  $i^{th}$  row of  $A$

# Transpose

- The transpose of a matrix  $A \in \mathfrak{R}^{m \times n}$  is the matrix  $A^T \in \mathfrak{R}^{n \times m}$ , where:

$$(A^T)_{ij} = A_{ji}$$

- Properties of transposes

$$- (A^T)^T = A$$

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

$$- (A + B)^T = A^T + B^T$$

$$\begin{pmatrix} a \\ b \end{pmatrix}^T = (a \quad b)$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

- A matrix where  $A = A^T$  is said to be *symmetric*.
- A matrix where  $A = -A^T$  is said to be *anti-symmetric*.

# Outline

- Basic Concepts and Notation
- **Matrix Multiplication**
- Operations and Properties
- Matrix Calculus



# Vector-Vector Multiplication

- Inner product (dot product)

$$x^T y \in \mathbb{R} = [x_1 \quad x_2 \quad \cdots \quad x_n] \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^n x_i y_i$$

- Outer product

$$xy^T \in \mathbb{R}^{m \times n} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} [y_1 \quad y_2 \quad \cdots \quad y_n] = \begin{bmatrix} x_1 y_1 & x_1 y_2 & \cdots & x_1 y_n \\ x_2 y_1 & x_2 y_2 & \cdots & x_2 y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_m y_1 & x_m y_2 & \cdots & x_m y_n \end{bmatrix}$$

- Useful for compactly representing a matrix where all rows are a multiples of each other

# Matrix-Vector Multiplication

- The product of a matrix  $A \in \mathbb{R}^{m \times n}$  and a vector  $x \in \mathbb{R}^n$  is a vector  $y \in \mathbb{R}^m$ , where

$$y = Ax = \begin{bmatrix} \leftarrow & a_1^T & \rightarrow \\ \leftarrow & a_2^T & \rightarrow \\ & \vdots & \\ \leftarrow & a_m^T & \rightarrow \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_1^T x \\ a_2^T x \\ \vdots \\ a_m^T x \end{bmatrix}$$

or

$$y_i = \sum_{k=1}^n a_{ik} x_k$$

# Matrix-Matrix Multiplication

- The product of a matrix  $A \in \mathfrak{R}^{m \times n}$  and a matrix in  $B \in \mathfrak{R}^{n \times p}$  is a matrix  $C \in \mathfrak{R}^{m \times p}$ , where

$$C = AB = \begin{bmatrix} \leftarrow & a_1^T & \rightarrow \\ \leftarrow & a_2^T & \rightarrow \\ & \vdots & \\ \leftarrow & a_m^T & \rightarrow \end{bmatrix} \begin{bmatrix} \uparrow & \uparrow & & \uparrow \\ b_1 & b_2 & \cdots & b_p \\ & \downarrow & & \downarrow \end{bmatrix} = \begin{bmatrix} a_1^T b_1 & a_1^T b_2 & \cdots & a_1^T b_p \\ a_2^T b_1 & a_2^T b_2 & \cdots & a_2^T b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^T b_1 & a_m^T b_2 & \cdots & a_m^T b_p \end{bmatrix}$$

or

$$c_{ij} = \sum_{k=1}^n a_{ik} b_{kj}$$

- Notice, vector-vector and matrix-vector are special cases of matrix-matrix multiplication

# Properties of Matrix Multiplication

- Matrix multiplication is associative:

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

- Matrix multiplication is distributive:

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

- Matrix multiplication is **not** necessarily commutative:

$$AB \neq BA$$

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# The Identity Matrix

- Identity is the matrix  $I \in \mathbb{R}^{n \times n}$ , where:

$$I = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

Or

$$I_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

- And has the property:

$$AI = A = IA$$

- Special case of the more general diagonal matrix  $D$ , where

$$D_{ij} = \begin{cases} d_i & i = j \\ 0 & i \neq j \end{cases}$$

# Other Special matrices

$$\begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \quad \text{diagonal} \quad \begin{pmatrix} a & b & c \\ 0 & d & e \\ 0 & 0 & f \end{pmatrix} \quad \text{upper-triangular}$$

$$\begin{pmatrix} a & b & 0 & 0 \\ c & d & e & 0 \\ 0 & f & g & h \\ 0 & 0 & i & j \end{pmatrix} \quad \text{tri-diagonal} \quad \begin{pmatrix} a & 0 & 0 \\ b & c & 0 \\ d & e & f \end{pmatrix} \quad \text{lower-triangular}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{I (identity matrix)}$$

# The Inverse

- The inverse,  $A^{-1}$ , of a square matrix  $A \in \mathfrak{R}^{n \times n}$  is the unique matrix such that

$$A^{-1}A = I = AA^{-1}$$

- A matrix  $A$  is ***invertible*** or ***non-singular*** if  $A^{-1}$  exists, and ***non-invertible*** or ***singular*** otherwise.

$$\forall A, B \in \mathfrak{R}^{n \times n}$$

- $(A^{-1})^{-1} = A$
  - $(AB)^{-1} = B^{-1}A^{-1}$
  - $(A^{-1})^T = (A^T)^{-1}$
- If  $Ax = b$ , then  $x = A^{-1}b$ .



# The Matrix Trace

- The trace of a square matrix  $A \in \mathfrak{R}^{n \times n}$  is the sum of its diagonal elements:

$$\text{tr}A = \text{tr}(A) = \sum_{i=1}^n A_{ii}$$

- Properties:

$$- \text{tr}(A) = \text{tr}(A^T)$$

$$- \text{tr}(A + B) = \text{tr}(A) + \text{tr}(B) \quad (A, B \in \mathfrak{R}^{n \times n})$$

$$- \text{tr}(tA) = t \cdot \text{tr}(A)$$

$$- \text{tr}(AB) = \text{tr}(BA) \quad (A \in \mathfrak{R}^{n \times m}, B \in \mathfrak{R}^{m \times n})$$

# Linear independence

- A set of vectors is **linearly independent** if none of them can be written as a linear combination of the others.
- Vectors  $v_1, \dots, v_k$  are linearly independent if  $c_1 v_1 + \dots + c_k v_k = 0$  implies  $c_1 = \dots = c_k = 0$

$$\begin{pmatrix} | & | & | \\ v_1 & v_2 & v_3 \\ | & | & | \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

e.g.  $\begin{pmatrix} 1 & 0 \\ 2 & 3 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$

$(u,v)=(0,0)$ , i.e. the columns are linearly independent.

$$x_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \quad x_2 = \begin{bmatrix} 4 \\ 1 \\ 5 \end{bmatrix} \quad x_3 = \begin{bmatrix} 2 \\ -3 \\ -1 \end{bmatrix} \quad x_3 = -2x_1 + x_2$$

# Rank of a Matrix

- $\text{rank}(A)$  (the rank of a  $m$ -by- $n$  matrix  $A$ ) is

The maximal number of linearly independent columns

=The maximal number of linearly independent rows

=The dimension of  $\text{col}(A)$

=The dimension of  $\text{row}(A)$

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 2 & 1 \\ 4 & 2 \end{pmatrix}$$

- If  $A$  is  $n$  by  $m$ , then

–  $\text{rank}(A) \leq \min(m, n)$

– If  $n = \text{rank}(A)$ , then  $A$  has full row rank

– If  $m = \text{rank}(A)$ , then  $A$  has full column rank

# Linear Independence and Matrix Rank

- A set of vectors  $\{x_1, x_2, \dots, x_n\}$  is **linearly independent** if no vector can be written as a linear combination ( $x_n = \sum_{i=1}^{n-1} \alpha_i x_i$ ) of the remaining vectors, and **linearly dependent** otherwise.
- The **rank** of a matrix is the largest number of linearly independent rows.
  - $\text{rank}(A) \leq \min(m, n)$  (full rank if =)  $\forall A \in \mathbb{R}^{m \times n}$
  - $\text{rank}(A) = \text{rank}(A^T)$   $\forall A \in \mathbb{R}^{m \times n}$
  - $\text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B)$   $\forall A, B \in \mathbb{R}^{m \times n}$
  - $\text{rank}(AB) \leq \min(\text{rank}(A), \text{rank}(B))$   $\forall A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times p}$

# Orthogonal and Normal Matrices

- Two vectors are *orthogonal* if  $x^T y = 0$
- A vector is said to be *normalized* if  $\|x\|_2 = 1$
- A square matrix  $U \in \mathbb{R}^{n \times n}$  is orthogonal if all columns are normalized and orthogonal to each other

$$U^T U = I = U U^T$$

or

$$U^{-1} = U^T$$

# Quadratic Forms

- Given a square matrix  $A \in \mathfrak{R}^{n \times n}$  and a vector  $x \in \mathfrak{R}^n$ , the scalar value  $x^T A x$  is called a quadratic form. Written explicitly, we see that

$$x^T A x = \sum_{i=1}^n x_i (A x)_i = \sum_{i=1}^n x_i \left( \sum_{j=1}^n A_{ij} x_j \right) = \sum_{i=1}^n \sum_{j=1}^n A_{ij} x_i x_j$$

$$x^T A x = (x^T A x)^T = x^T A^T x = x^T \left( \frac{1}{2} A + \frac{1}{2} A^T \right) x,$$

# Positive Semidefinite Matrices

- A symmetric matrix  $A \in S^n$  is **positive definite** (PD), usually denoted  $A \succ 0$  (or just  $A > 0$ ), if for all non-zero vectors  $x \in R^n$ ,  $x^T A x > 0$ .
- A symmetric matrix  $A \in S^n$  is **positive semidefinite** (PSD), denoted  $A \succeq 0$ , if for all vectors  $x \in R^n$ ,  $x^T A x \geq 0$ .
- A symmetric matrix  $A \in S^n$  is **negative definite** (ND), denoted  $A \prec 0$ , if for all non-zero vectors  $x \in R^n$ ,  $x^T A x < 0$ .
- A symmetric matrix  $A \in S^n$  is **negative semidefinite** (NSD), denoted  $A \preceq 0$ , if for all non-zero vectors  $x \in R^n$ ,  $x^T A x \leq 0$ .
- Finally, a symmetric matrix  $A \in S^n$  is **indefinite**, if it is neither positive semidefinite nor negative semidefinite.

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# Matrix Calculus

- First derivative: The Gradient
- Second derivative: The Hessian

# The Gradient

- Suppose that  $f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$  is a function that takes as input a matrix  $A$  of size  $m \times n$  and returns a real value (scalar). Then the gradient of  $f$  (with respect to  $A \in \mathbb{R}^{m \times n}$ ) is the matrix of partial derivatives, defined as:

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

$$(\nabla_A f(A))_{ij} = \frac{\partial f(A)}{\partial A_{ij}}.$$

# The Gradient

Note that the size of  $\nabla_A f(A)$  is always the same as the size of  $A$ . So if, in particular,  $A$  is just a vector  $x \in \mathbb{R}^n$ ,

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

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

# Gradient of Linear Functions

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

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

$$\nabla_x b^T x = b$$

# The Hessian

Suppose that  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is a function that takes a vector in  $\mathbb{R}^n$  and returns a real number. Then the **Hessian** matrix with respect to  $x$ , written  $\nabla_x^2 f(x)$  or simply as  $H$  is the  $n \times n$  matrix of partial derivatives,

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

# The Hessian

In other words,  $\nabla_x^2 f(x) \in \mathbb{R}^{n \times n}$ , with

$$(\nabla_x^2 f(x))_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}.$$

Note that the Hessian is always symmetric, since

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} = \frac{\partial^2 f(x)}{\partial x_j \partial x_i}.$$

Similar to the gradient, the Hessian is defined only when  $f(x)$  is real-valued.

# Hessians of Quadratic Functions

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

$$\nabla_x^2 x^T A x = 2A$$

# Gradients and Hessians of Quadratic and Linear Functions (Recap)

- $\nabla_x b^T x = b$
- $\nabla_x x^T A x = 2Ax$  (if  $A$  symmetric)
- $\nabla_x^2 x^T A x = 2A$  (if  $A$  symmetric)



# Linear Regression

- Main idea:
  - Compute gradient and set gradient to 0.  
(condition for optimal solution)
  - Solve the equation in a closed form

- Objective function:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \left( \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}^{(n)}) - y^{(n)} \right)^2$$

- We will derive the gradient from matrix calculus

# Linear Regression

- The design matrix is an NxM matrix, applying
  - the M basis functions (columns)
  - to N data points (rows)

$$\Phi = \begin{pmatrix} \phi_0(\mathbf{x}^{(1)}) & \phi_1(\mathbf{x}^{(1)}) & \dots & \phi_{M-1}(\mathbf{x}^{(1)}) \\ \phi_0(\mathbf{x}^{(2)}) & \phi_1(\mathbf{x}^{(2)}) & \dots & \phi_{M-1}(\mathbf{x}^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}^{(N)}) & \phi_1(\mathbf{x}^{(N)}) & \dots & \phi_{M-1}(\mathbf{x}^{(N)}) \end{pmatrix}$$

$$\Phi \mathbf{w} \approx \mathbf{y}$$

$$\Phi = \begin{pmatrix} \phi_0(\mathbf{x}^{(1)}) & \phi_1(\mathbf{x}^{(1)}) & \dots & \phi_{M-1}(\mathbf{x}^{(1)}) \\ \phi_0(\mathbf{x}^{(2)}) & \phi_1(\mathbf{x}^{(2)}) & \dots & \phi_{M-1}(\mathbf{x}^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}^{(N)}) & \phi_1(\mathbf{x}^{(N)}) & \dots & \phi_{M-1}(\mathbf{x}^{(N)}) \end{pmatrix}$$

$$\begin{aligned} E(\mathbf{w}) &= \frac{1}{2} \sum_{n=1}^N \left( \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}^{(n)}) - y^{(n)} \right)^2 \\ &= \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^T \phi(\mathbf{x}^{(n)}) - y^{(n)})^2 \\ &= \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^T \phi(\mathbf{x}^{(n)}))^2 - \sum_{n=1}^N y^{(n)} \mathbf{w}^T \phi(\mathbf{x}^{(n)}) + \frac{1}{2} \sum_{n=1}^N y^{(n)2} \end{aligned}$$

$$\Phi = \begin{pmatrix} \phi_0(\mathbf{x}^{(1)}) & \phi_1(\mathbf{x}^{(1)}) & \dots & \phi_{M-1}(\mathbf{x}^{(1)}) \\ \phi_0(\mathbf{x}^{(2)}) & \phi_1(\mathbf{x}^{(2)}) & \dots & \phi_{M-1}(\mathbf{x}^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}^{(N)}) & \phi_1(\mathbf{x}^{(N)}) & \dots & \phi_{M-1}(\mathbf{x}^{(N)}) \end{pmatrix}$$

$$\begin{aligned} E(\mathbf{w}) &= \frac{1}{2} \sum_{n=1}^N \left( \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}^{(n)}) - y^{(n)} \right)^2 \\ &= \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^T \phi(\mathbf{x}^{(n)}) - y^{(n)})^2 \\ &= \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^T \phi(\mathbf{x}^{(n)}))^2 - \sum_{n=1}^N y^{(n)} \mathbf{w}^T \phi(\mathbf{x}^{(n)}) + \frac{1}{2} \sum_{n=1}^N y^{(n)2} \\ &= \frac{1}{2} \mathbf{w}^T \Phi^T \Phi \mathbf{w} - \mathbf{w}^T \Phi^T \mathbf{y} + \frac{1}{2} \mathbf{y}^T \mathbf{y} \end{aligned}$$

# Linear Regression

- Objective function:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \left( \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}^{(n)}) - y^{(n)} \right)^2$$

# Linear Regression

- Objective function:

$$\begin{aligned} E(\mathbf{w}) &= \frac{1}{2} \sum_{n=1}^N \left( \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}^{(n)}) - y^{(n)} \right)^2 \\ &= \frac{1}{2} \sum_{n=1}^N \left( \mathbf{w}^T \phi(\mathbf{x}^{(n)}) - y^{(n)} \right)^2 \end{aligned}$$

# Linear Regression

- Objective function:

$$\begin{aligned} E(\mathbf{w}) &= \frac{1}{2} \sum_{n=1}^N \left( \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}^{(n)}) - y^{(n)} \right)^2 \\ &= \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^T \phi(\mathbf{x}^{(n)}) - y^{(n)})^2 \\ &= \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^T \phi(\mathbf{x}^{(n)}))^2 - \sum_{n=1}^N y^{(n)} \mathbf{w}^T \phi(\mathbf{x}^{(n)}) + \frac{1}{2} \sum_{n=1}^N y^{(n)2} \end{aligned}$$

# Linear Regression

- Objective function:

$$\begin{aligned} E(\mathbf{w}) &= \frac{1}{2} \sum_{n=1}^N \left( \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}^{(n)}) - y^{(n)} \right)^2 \\ &= \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^T \phi(\mathbf{x}^{(n)}) - y^{(n)})^2 \\ &= \frac{1}{2} \sum_{n=1}^N (\mathbf{w}^T \phi(\mathbf{x}^{(n)}))^2 - \sum_{n=1}^N y^{(n)} \mathbf{w}^T \phi(\mathbf{x}^{(n)}) + \frac{1}{2} \sum_{n=1}^N y^{(n)2} \\ &= \frac{1}{2} \mathbf{w}^T \Phi^T \Phi \mathbf{w} - \mathbf{w}^T \Phi^T \mathbf{y} + \frac{1}{2} \mathbf{y}^T \mathbf{y} \end{aligned}$$

- Trick: vectorization (by defining data matrix)



# Linear Regression

- Compute gradient and set to zero

$$\begin{aligned}\nabla_{\mathbf{w}} E(\mathbf{w}) &= \nabla_{\mathbf{w}} \left( \frac{1}{2} \mathbf{w}^T \Phi^T \Phi \mathbf{w} - \mathbf{w}^T \Phi^T \mathbf{y} + \frac{1}{2} \mathbf{y}^T \mathbf{y} \right) \\ &= \Phi^T \Phi \mathbf{w} - \Phi^T \mathbf{y} \\ &= 0\end{aligned}$$

- Solve the resulting equation (normal equation)

$$\Phi^T \Phi \mathbf{w} = \Phi^T \mathbf{y}$$

$$\mathbf{w}_{ML} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y}$$

This is the *Moore-Penrose pseudo-inverse*:  $\Phi^\dagger = (\Phi^T \Phi)^{-1} \Phi^T$

applied to:  $\Phi \mathbf{w} \approx \mathbf{y}$