1 Linear Models

1.1 Types of errors

Errors come from: impercise data, mistakes in the model, computational percision,.. We know two types of errors:

- **Absolute** error = approximate value - correct value

$$\Delta x = \overline{x} - x$$

- **Relative** error = $\dfrac{\text{absolute err}}{\text{correct value}}$

$$\delta x = \frac{\Delta x}{x}$$

1.2 Mathematical model is **linear**, when the function F is a linear function of the parameters:

$$F(x, a_1, \ldots, a_p) = a_1\phi_1(x) + \cdots + a_p\phi_p(x)$$

where $\phi_1, \ldots, \phi_p$ are functions of a specific type.

1.3 Least squares method Given points

$$\{(x_1, y_1), \ldots, (x_m, y_m)\}, x_i \in R^n, y_i \in R$$

the task is to find a function $F(x, a_1, \ldots, a_p)$ that is good fit for the data. The values of the parameters $a_1, \ldots, a_p$ should be chosen so that the equations

$$y_i = F(x, a_1, \ldots, a_p), i = 1, \ldots, m$$

are satisified or, it this is not possible, that the error is as small as possible.
We use **Least squares method** to determine that the sum od squared errors is as small as possible.

$$\sum_{i=1}^{m}(F(x_i, a_1, \ldots, a_p) - y_i)^2$$

1.4 Systems of linear equations

A system of linear equations in the matrix form is given by $A\vec{x} = \vec{b}$, where:

- A is the matrix of coefficients of order $m \times n$ where m is the number of equations and n is the number of unknowns,
- $\vec{x}$ is the vector of unknowns and
- $\vec{b}$ is the right side vector

$$\begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & \ldots & \phi_p(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \ldots & \phi_p(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_n) & \phi_2(x_n) & \ldots & \phi_p(x_n) \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_p \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{bmatrix}$$

1.5 Existance of solutions in linear equations

Let A = $[\vec{a_1}, \ldots, \vec{a_n}]$, where $\vec{a_i}$ are vector representing the columns of A. For any vector

$$\vec{x} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{bmatrix}$$

the produdct $A\vec{x}$ is a linear combination $A\vec{x} = \sum_i x_i a_i$. The system is **solvable** iff the vector $\vec{b}$ can be expressed as a linear combination of the columns of A, that is it is in the column space of A, $\vec{b} \in C(A)$.
By adding $\vec{b}$ to the columns of A we obtain the extended matrix of the system:

$$[A|\vec{b}] = [\vec{a_1}, \ldots, \vec{a_n}|b]$$

The system $A\vec{x} = \vec{b}$ is solvable iff the rank of A equals the rank of the extended matrix $[A|\vec{b}]$, i.e.:

$$rankA = rank[A|\vec{b}] =: r$$

The solution is unique if the rank of the two matrices equals num of unknowns (r = n).

1.6 Properties of **squared matrices**
Let $A \in R^{n \times n}$ be a square matrix. The following conditions are equivalent and characterize when a matrix A is **invertible** or **nonsingular**:

- The matrix A has an inverse
- rank A = n
- $\det(A) \neq 0$
- The null space $N(A) = \{\vec{x} : A\vec{x} = 0$ is trivial
- All eigenvalues of A are nonzero
- For each $\vec{b}$ the system of equations $A\vec{x} = \vec{b}$ has percisely one solution

1.7 Generalized inverse of a matrix $A \in R^{n \times m}$ is a matrix $G \in R^{m \times n}$ such that

$$AGA = A$$

Let G be a generalized inverse of A. Multiplying $AGA = A$ with A^{-1} from the left and the right side we obtain:
LHS: $A^{-1}GAA^{-1} = IGI = G$
RHS: $A^{-1}AA^{-1} = IA^{-1} = A^{-1}$
where I is the identity matrix. The equality LHS=RHS implies that $G = A^{-1}$.
Every matrix $A \in R^{n \times m}$ **has** a generalized inverse. When computing a generalized inverse we come across two cases:

1. rank A = rank A_{11} where

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

And $A_{11} \in R^{r \times r}, A_{12} \in R^{r \times (m-r)}, A_{21} \in R^{(n-r) \times r}, A_{22} \in R^{(n-r) \times (m-r)}$. We claim that

$$G = \begin{bmatrix} A_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix}$$

where 0s denote zero matrices of appropriate sizes, is the generalized inverse of A.

2. The upper left $r \times r$ submatrix of A is **not** invertible.
One way to hanlde this case is to use permutation matrices P and Q, such that

$$PAQ = \begin{bmatrix} \tilde{A_{11}} & \tilde{A_{12}} \\ \tilde{A_{21}} & \tilde{A_{22}} \end{bmatrix},$$

$\tilde{A_{11}} \in R^{r \times r}$ and rank $\tilde{A_{11}} = r$. By case 1 generalized inverse of PAQ equals to

$$(PAQ)^g = \begin{bmatrix} \tilde{A_{11}}^{-1} & 0 \\ 0 & 0 \end{bmatrix}$$

Thus $(PAQ)(PAQ)^g(PAQ) = PAQ$ holds, Multiplying from the left by P^{-1} and from the right by Q^{-1} we get:
$A(Q(PAQ)^g P)A = A$
So

$$Q(PAQ)^g P$$

is a **generalized** inverse of A.

Algorithm for computing A^g:

1. Find any nonsingular submatrix B in A of order $r \times r$,

2. in A substitute
   - elements of submatrix B for corresponding elements of $(B^{-1})^T$,
   - all other elements with 0

3. the transpose of the obtained matrix is generalized inverse G

solutions:
Let $A \in R^{n \times m}$ and $\vec{b} \in R^m$. If the system $A\vec{x} = \vec{b}$ is solvable (that is, $\vec{b} \in$ C(A)) and G is a generalized inverse of A, then $\vec{x} = G\vec{b}$ is a solution of the system. Moreover, all solutions of system are exactly vectors of the form

$$x_z = G\vec{b} + (GA - I)z$$

1.8 The Moore-Penrose generalized inverse
The MP inverse of $A \in R^{n \times m}$ is any matrix $A^+ \in R^{n \times m}$ satisfying the following four conditions:

1. A^+ is a generalized inverse of A: $AA^+A = A$

2. A is a generalized inverse of A^+ : $A^+AA^+ = A^+$

3. The square matrix $AA^+ \in R^{n \times n}$ is symetric: $(AA^+)^T = AA^+$

4. The square matrix $A^+A \in R^{m \times m}$ is symmetric: $(A^+A)^T = A^+A$

Properties:

- If A is a square invertible matrix, then it $A^+ = A^{-1}$

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

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

Construction of the MP inverse (4 cases):

1. $A^T A \in R^{m \times m}$ is an invertible matrix $(m \le n)$

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

2. AA^T is an invertible matrix $(n \le m)$

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

3. $\Sigma \in R^{n \times m}$ is diagonal matrix of the form

$$\Sigma = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{bmatrix}$$

Then the MP inverse is:

$$\Sigma = \begin{bmatrix} \sigma_1^+ & & \\ & \ddots & \\ & & \sigma_n^+ \end{bmatrix}$$

where $\sigma_i^+ = \begin{cases} \frac{1}{\sigma_i} & \sigma_i \neq 0 \\ 0 & \sigma_i = 0 \end{cases}$

4. a general matrix A (using SVD)

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

1.9 SVD computation

1. Compute the eigenvalues and an orthonormal basis consistiong of eigenvectors of the symetric matrix $A^T A$ or AA^T (depending on which of them is of smaller size)

2. the singular values of the matrix $A \in R^{n \times m}$ are equal to $\sigma_i = \sqrt{\lambda_i}$

3. the left singular vectors are the corresponding orthonormal eigenvectors of AA^T

4. the right singular vectors are the corresponding orthonormal eigenvectors of $A^T A$

5. If u (resp. v) is a left (resp. right) singular vector corresponding to the singular value σ_i, then $v = Au$ (resp. $u = A^T v$) is a right (resp left) singular vector corresponding to the same singular value

6. the remaining columns of U (resp. V) consist of an orthonormal basis of the kernel (i.e., the eigenspace of $\lambda = 0$) of AA^T (resp. $A^T A$)

1.10 General computation of A^+

1. For $A^T A$ compute its **nonzero** eigenvalues $\lambda_1 \ge \cdots \ge \lambda_r > 0$, and the corresponding orthonormal eigenvectors $v_1, \dots, v_r$, and form the matrices:

$$S = diag(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_r}) \in R^{r \times r}$$
$$V = [v_1 \dots v_r] \in R^{m \times r}$$

2. Put the vectors
$u_1 = \dfrac{Av_1}{\sigma_1}, \dots, u_r = \dfrac{Av_r}{\sigma_r}$
in the matrix $U = [u_1, \dots, u_r]$

3. Then $A^+ = V\Sigma^+ U^T$

1.11 Undetermined systems
Let $A \in R^{n \times m}$, where $m > n$. A system of equiations that has more variables than constraints. Typically such system has infinitely many solutions, but it may happen that it has no solutions $\rightarrow$ such system is undetermined.

1. An undetermined system of linear equations $Ax = b$ is solvable iff $AA^+b = b$.

2. If there are infinitely many solutions, the solution A^+b is the one with the smallest norm, i.e

$$||A^+b|| = min\{||x|| : Ax = b\}$$

Moreover, it is the unique solution of smallest norm.

1.12 Overdetermined systems
Let $A \in R^{n \times m}$, where $n > m$. A system of equations that has more constraints than variables. Typically such system has no soluitons, but it may happen that it migh have one or even infinitely many solutions.

2 Nonlinear Models

2.1 Definition
Given is a sample of data points $(x_1, y_1), \dots, (x_m, y_m) \in R^n \times R$. We are searching for

$$F : R^n \times R^p \rightarrow R,$$
$$F(x_i, a_i, \dots, a_p) = y_i,$$
$$i = 1, \dots, m$$

which can be nonlinear in parameters $a_i, \dots, a_p$.
Examples: exponential decay/growth, Gaussian model, logistic model,...

We introduce a vector function

$$G : R^p \rightarrow R^m, G = (g_1, \dots, g_m)$$
$$g_1(a_1, \dots, a_p) = F(x_1, a_1, \dots a_p) - y_1$$
$$\dots$$
$$g_m(a_1, \dots, a_p) = F(x_m, a_1, \dots a_p) - y_m$$

Solving $F(x_i, a_i, \dots, a_p) = y_i$, is equicalent to solving $G(a_1, \dots, a_p) = (0, \dots, 0)$. Newton's method will solve the latter system.