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 perciesly 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:
$A(Q(PAQ)^gP)A = A$
So

$$Q(PAQ)^gP$$

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

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

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

1.10 General computation of A^+

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

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

2. Put the vectors
$u_1 = \frac{Av_1}{\sigma_1}, \ldots, u_r = \frac{Av_r}{\sigma_r}$
in the matrix $U = [u_1, \ldots, u_r]$
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 $\{(x_1, y_1), \ldots, (x_m, y_m)\} \in R^n \times R$. We are searching for

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

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

We introduce a **vector function**

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

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

2.2 Rate of convergence

Let us say that e_i is the i-th error of some method and α is a zero we are searching for. We can show that $|e_{i+1}| \le C \cdot \frac{1}{2}|e_i|^r$, where $C \in R > 0$ and $r \in N$. r is the rate of convergence of the method.

2.3 Case 1 for solving nonlinear equations ($p = m = 1$)

$g : R \rightarrow R$. We have to find a zero of the function g (let's call it α).

2.3.1 Tangent method

1. Select an initial approximation x_0.
2. Iterate $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, n = 0, 1, ...$ until it converges to α

Problem: the convergence of this method really needs a good initial approximation.
Theorem: The sequence x_i from the tangent method converges with the rate $r = 2$ if:

- $f'(\alpha) \neq 0$
- x_0 was close enough to α

2.3.2 Bisection

1. Start with x_0, x_1 such that $f(x_0)f(x_1) < 0$.
2. Compute $x_2 = \frac{x_0 + x_1}{2}$.
3. Choose $[x_0, x_2]$ if $f(x_0)f(x_2) < 0$, otherwise choose $[x_2, x_1]$.
4. Repeat.

Bisection always converges, but it is slow. Rate of convergence: We can show that $|e_{i+1}| \approx \frac{1}{2}|e_i|$. From here we can see that bisection has a linear rate of convergence.

2.3.3 Stopping criteria

Iterative method: $x_0, ..., x_n, x_n + 1$. How do we find n (how many steps of a method do we have to make)? This has to be true:

- $\frac{|x_{n+1} - x_n|}{|x_n|} <$ tolerance
- $|f(x_{n+1})| <$ tolerance

Tolerance is usually 10^{-10}.

2.4 Case 2 for solving nonlinear equations ($n = p > 1$)

$F : R^n \rightarrow R^n$. We have to find a zero of the function g (let's call it $\alpha \in R^n$). In this case we have a vector function of a vector variable.

$$F = \begin{bmatrix} F_1 \\ \vdots \\ F_n \end{bmatrix}, F_i : R^n \rightarrow R$$

2.4.1 Newton's method

$x^{(m+1)} = x^m - JF^{-1}(x^{(m)})F(x^{(m)})$ **(*)**

Where $x^m, x^{(m+1)} \in R^n$ are some approximations of α and JF is the Jacobi matrix of F:

$$JF(x^m) = \begin{bmatrix} gradF_1 \\ \vdots \\ gradF_n \end{bmatrix} = \begin{bmatrix} \frac{\partial F_1}{\partial x_1} \cdots \frac{\partial F_1}{\partial x_n} \\ \vdots \ddots \vdots \\ \frac{\partial F_n}{\partial x_1} \cdots \frac{\partial F_n}{\partial x_n} \end{bmatrix}$$

We multiply **(*)** by $JF(x^m)$ and solve this instead: $x^{(m+1)} = \Delta x^m + x^m$

2.4.2 Newton's or Tangent method

We construct a recursive sequence with: x_0 is an initial term

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

2.4.x Broyden's bethod It approximates $JF(x^{(m)})$ with some matrix B_bn where:

$$\text{slope} \approx f'(x_1)$$
$$\frac{f(x_2) - f(x_1)}{x_2 - x_1} \approx f(x_1)$$
$$f(x_2) - f(x_1) \approx f'(x)(x_2 - x_1)$$

Where $< f(x_2) - f(x_1) >$ is a vector, $< f(x_1) >$ is a $n \times n$ matrix B_n, and $< (x_2 - x_1) >$ a vector.

2.4.x Conclusion

1. Use Broyden's method first
2. If it doesn't converge, go and compute derivatives for Newtons method.
   (a) Do a few steps of gradient descent(GD)
   (b) Use the final approximate of GD as entry into Newton's method

3 Curves