LEAST SQUARES AND FITTING

Why? Because in real life measurements come with errors, and "noise". Many times the given data "overdetermine" the problem (see example below) making a solution nonexistent.

Simple Example: Solve
\[ x_1 + x_2 = 2 \]
\[ x_1 - x_2 = 1 \]
\[ x_1 + x_2 = 3 \]

What do you see? Anything you do not like? This is what data from real life look like. We still need to solve this never the less! The system in this example is called inconsistent. i.e. \# of equations > \# of unknowns

Instead we find a solution which comes as "close" as possible to solving this system.

If we let "close" = in terms of Euclidean distance then method has a name: LEAST SQUARES

\[ \text{Least squares produces the line with the smallest } \]
\[ R^2 = \text{Squared Error} = d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2 \]

How? Note that
\[ d_1^2 = (y_1 - (a + bx_1))^2 \]
\[ d_2^2 = (y_2 - (a + bx_2))^2 \]
\[ d_3^2 = (y_3 - (a + bx_3))^2 \]
\[ d_4^2 = (y_4 - (a + bx_4))^2 \]
\[ d_5^2 = (y_5 - (a + bx_5))^2 \]
\[ d_6^2 = (y_6 - (a + bx_6))^2 \]

\[ \text{So } R^2 = \sum_{i=1}^{n} (y_i - (a + bx_i))^2 \]
So \( R^2 = \sum_{i=1}^{n} [y_i - (a+bx_i)]^2 \) \\
We wish to find \( a \) and \( b \) which will make this a min. 
We know from analysis how to minimize a function in two variables. 
1) Take the derivatives \( = 0 \) 
2) Solve for variables ... 
So lets define \( f(a,b) = \sum_{i=1}^{n} [y_i - (a+bx_i)]^2 \) and 
\[
\begin{align*}
\frac{\partial f}{\partial a} &= 0 = -2 \sum_{i=1}^{n} [y_i - (a+bx_i)] \\
\frac{\partial f}{\partial b} &= 0 = -2 \sum_{i=1}^{n} x_i [y_i - (a+bx_i)] \\
\end{align*}
\]
and solve.

This leads to the equations 
\[
\begin{align*}
& a \sum x_i + b \sum x_i^2 = \sum y_i \\
& a \sum x_i^2 + b \sum x_i = \sum x_i y_i \\
\end{align*}
\]
or in matrix form
\[
\begin{bmatrix}
\sum x_i & \sum x_i^2 \\
\sum x_i & \sum x_i^2 \\
\end{bmatrix}
\begin{bmatrix}
\alpha \\
\beta \\
\end{bmatrix}
=
\begin{bmatrix}
\sum y_i \\
\sum x_i y_i \\
\end{bmatrix}
\]

Solution
\[
\begin{align*}
\alpha &= \frac{\sum x_i^2 \sum x_i y_i - \sum x_i \sum x_i y_i}{\sum x_i^2 - n \bar{x}^2} \\
b &= \frac{\sum x_i y_i - n \bar{x} \bar{y}}{\sum x_i^2 - n \bar{x}^2}
\end{align*}
\]
Alternatively: Given the system \( Ax = B \) 
Normal equations (for least squares) 
First multiply with \( A^T \) 
\( A^T A x = A^T B \) \( \leftarrow \) this makes the system consistent.

Example: \( A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \), \( B = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \)

\( A^T A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix} \), \( A^T B = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \)
The normal equations are

\[
\begin{bmatrix}
3 & 1 \\
1 & 3
\end{bmatrix}
\begin{bmatrix}
x_1^y \\
x_2^y
\end{bmatrix} =
\begin{bmatrix}
6 \\
4
\end{bmatrix}
\]

Solution (any way you like) is

\[
\begin{bmatrix}
x_1^y \\
x_2^y
\end{bmatrix} =
\begin{bmatrix}
7/4 \\
3/4
\end{bmatrix}
\]

What is \( R^2 = ? \)

\[
(B - Ax)^2 = \left( \begin{bmatrix}
3 \\
1 \\
2.5
\end{bmatrix} - \begin{bmatrix}
.5 \\
.5 \\
.5
\end{bmatrix} \right)^2 = \frac{1}{4} + 0 + \frac{1}{4} = \frac{1}{2}
\]

Use matlab to see the results.

the least squares fit is the line \( y = \frac{7}{4} + \frac{3}{4} t \)

\[\text{Find the line that best fits the data points (1,2), (-1,1) and (1,3).}\]

\[\text{The model is} \quad y = a + bt \]

\[\text{So} \quad \begin{bmatrix}
2 \\
1 \\
3
\end{bmatrix} = \begin{bmatrix}
a \\
b
\end{bmatrix} = \begin{bmatrix}
1 & 1 \\
1 & -1 \\
1 & 1
\end{bmatrix} \begin{bmatrix}
a \\
b
\end{bmatrix} \]

or \( B = A \cdot x \)

We solved this by linear least squares method

by multiplying with \( A^T \) on both sides.

\[A^TA \cdot x = A^TB\]

\[
\begin{bmatrix}
3 & 1 \\
1 & 3
\end{bmatrix}
\begin{bmatrix}
a \\
b
\end{bmatrix} =
\begin{bmatrix}
6 \\
4
\end{bmatrix}
\]

with solution \( a = \frac{7}{4} \)

\( b = \frac{3}{4} \)

and residual \( r = B - Ax = \begin{bmatrix}
-5/4 \\
7/4
\end{bmatrix} \)

and \( r^2 = \frac{1}{4} + 0 + \frac{1}{4} = \frac{1}{2} \)

Applications in data compression.

Can we do better with the least squares method?

How about a non-linear function?

\[\text{Example: Fit the data (-1,1), (0,0), (1,0), (2,-2) with} \]
\[\text{a function} \quad y = \text{c}_1 + \text{c}_2 t + \text{c}_3 t^2 \]

\[\text{Applying the data to this function gives} \]

\[
\begin{align*}
\text{c}_1 + \text{c}_2 t + \text{c}_3 t^2 &= y \\
\text{c}_1 + \text{c}_2 (-1) + \text{c}_3 \cdot 1 &= 1 \\
\text{c}_1 + \text{c}_2 \cdot 0 + \text{c}_3 \cdot 0 &= 0
\end{align*}
\]
\begin{align*}
&c_1 + c_2 \cdot 1 + c_3 \cdot 1 = 0 \\
&c_1 + c_2 \cdot 2 + c_3 \cdot 4 = -2 \\
&\begin{pmatrix}
1 & -1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 1 \\
1 & 2 & 4
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2 \\
c_3
\end{pmatrix}
= \begin{pmatrix}
1 \\
0 \\
0 \\
-2
\end{pmatrix} \\
\mathbf{A^T A} \cdot \mathbf{c} = \mathbf{A^T B} \\
\begin{pmatrix}
4 & 2 & 6 \\
2 & 6 & 8 \\
6 & 8 & 18
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2 \\
c_3
\end{pmatrix}
= \begin{pmatrix}
-1 \\
-5 \\
-9
\end{pmatrix}
\text{Solving this gives} \\
c_1 = 0.45 \\
c_2 = -0.65 \\
c_3 = -0.25
\end{align*}

Therefore \( y = 0.45 - 0.65t - 0.25t^2 \)

Here \( R^2 = 0.15^2 + (-0.45)^2 + (0.45)^2 + (-0.15)^2 = 0.95 \)