Module 1 | Lesson 1 (Part 1)

The Squared Error Criterion and the Method of Least Squares

Module 1 | Least Squares

In this module

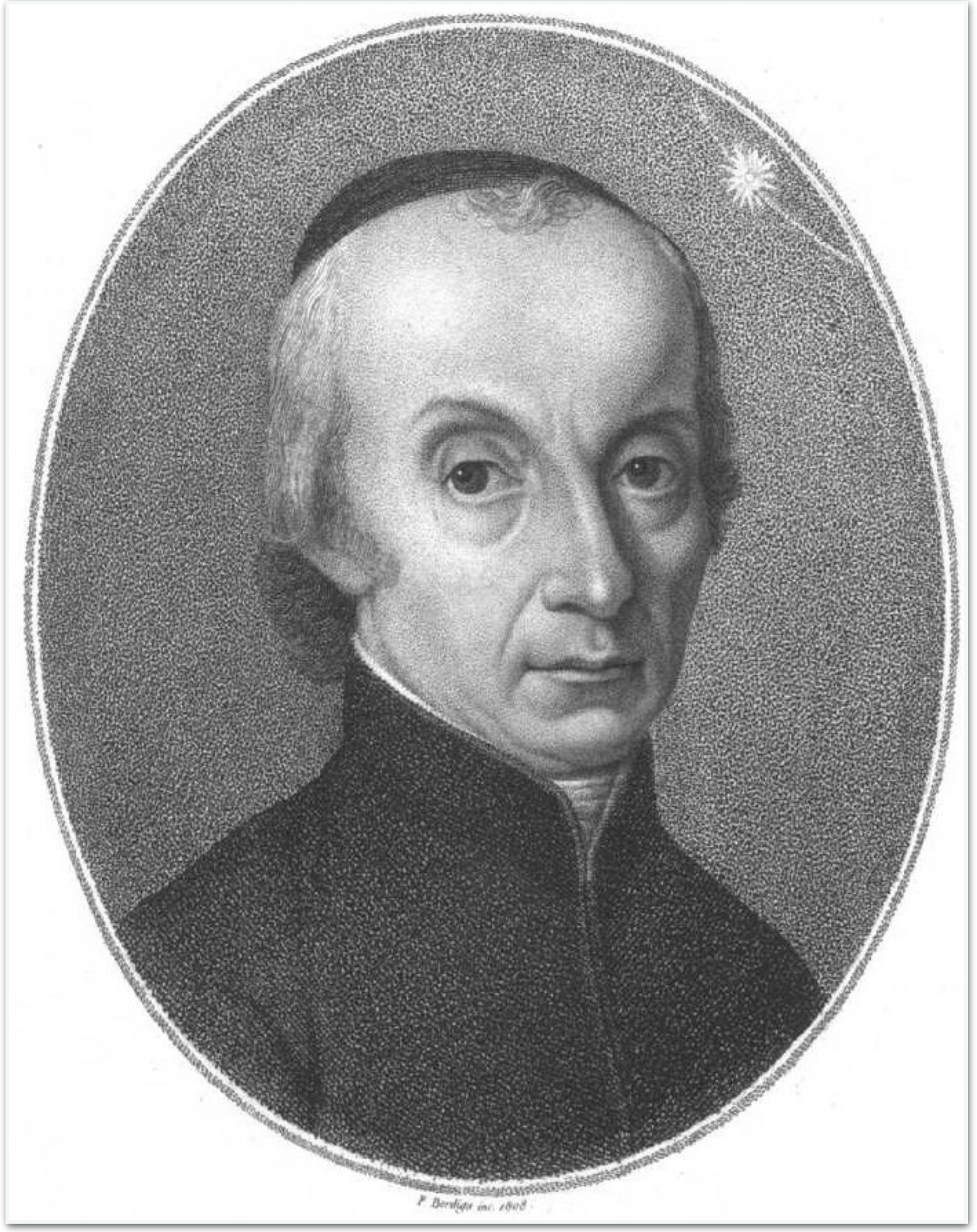
- The history of the method of *least squares*
- Ordinary and weighted least squares
- Recursive least squares
- Maximum likelihood and the method of least squares

The Squared Error Criterion and the Method of Least Squares

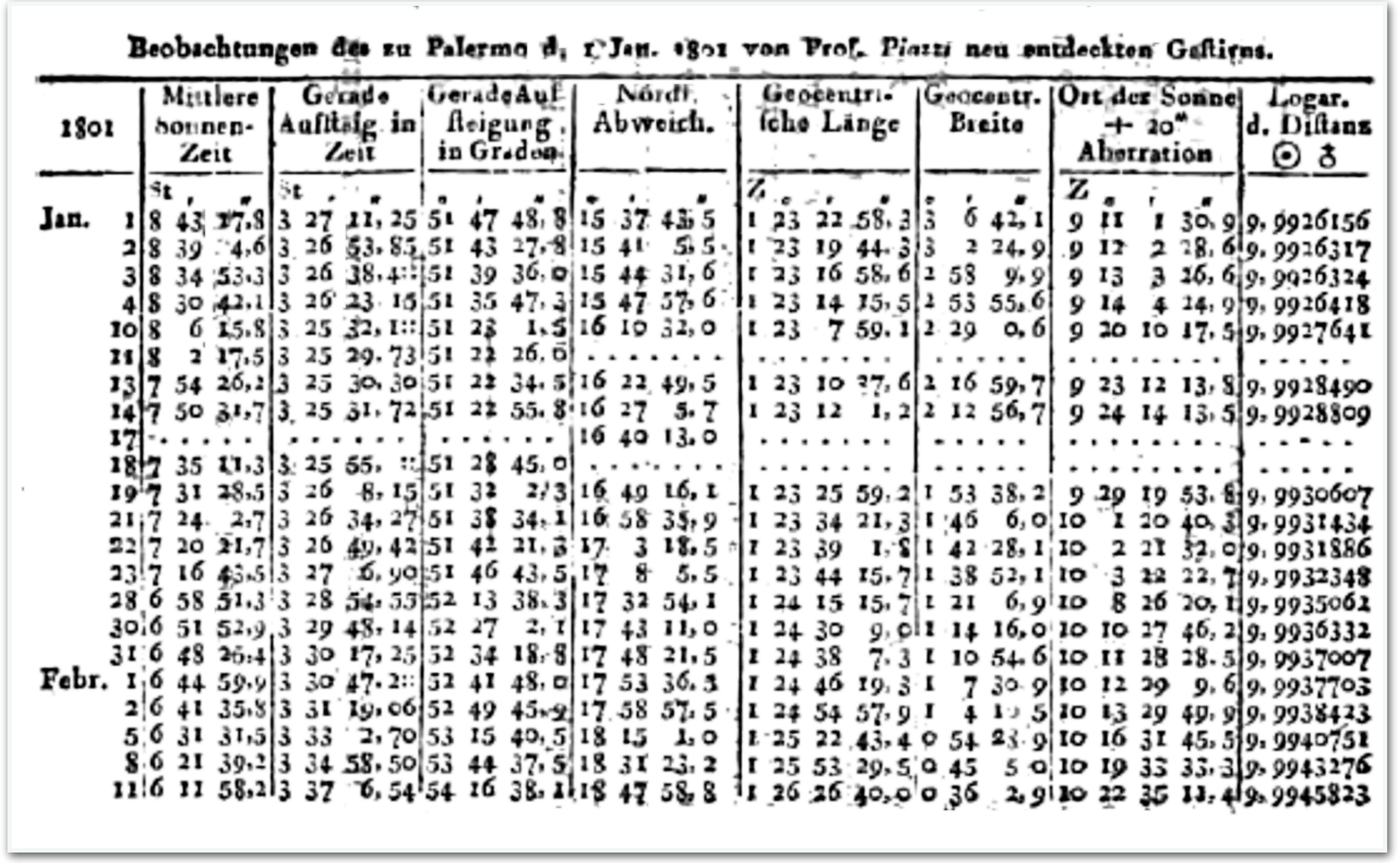
By the end of this video, you will be able to…

- Describe how the method of least squares was used in the discovery of Ceres
- Describe the least error criterion and how it's used in parameter estimation
- Derive the normal equations for least squares parameter estimation

Giuseppe Piazzi and Ceres



Giuseppe Piazzi



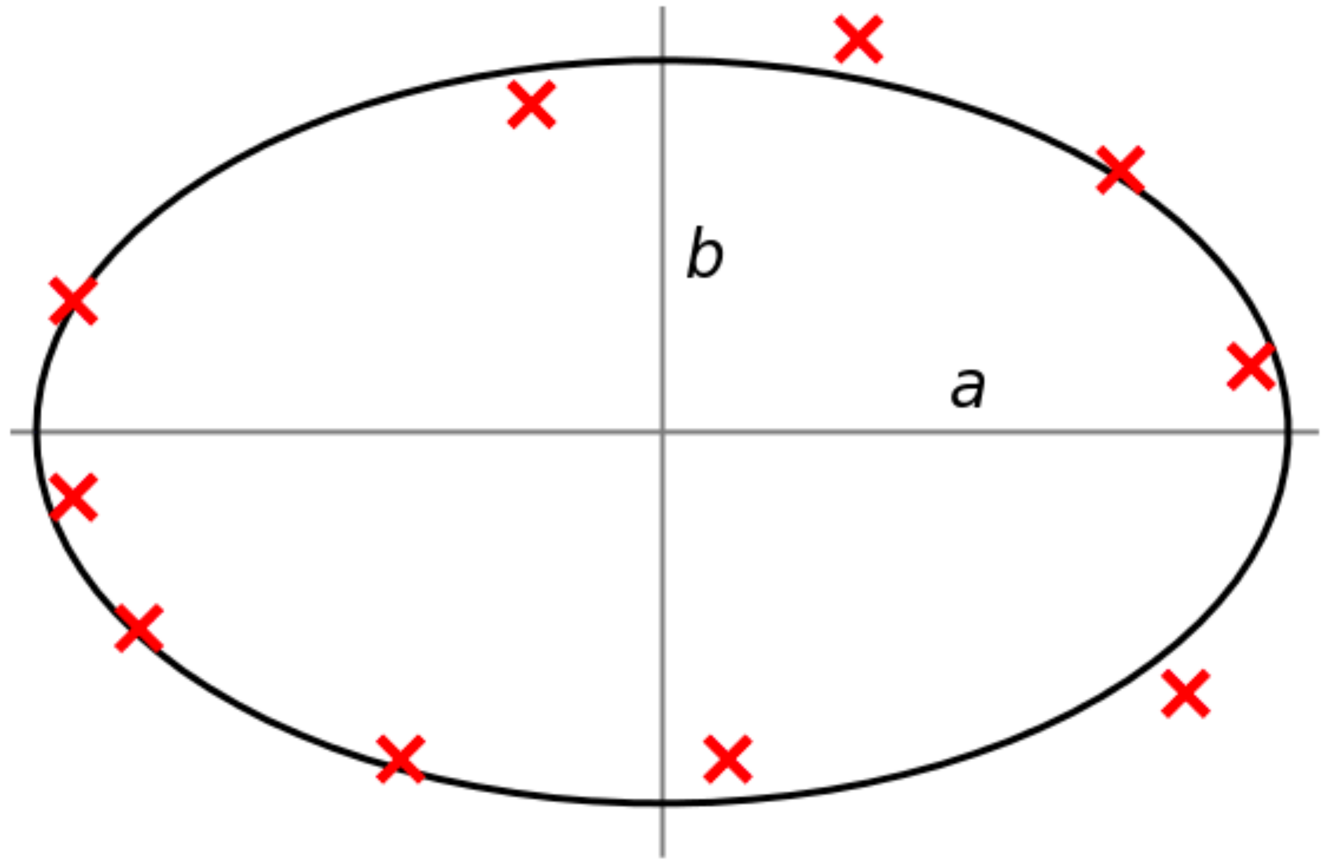
Beobachtungen des zu Palermo d. 1 Jan. 1801 von Prof. Piazzi neu entdeckten Gestirns.

1801	Mittlere Sonnen-Zeit	Gerade Aufstaig in Zeit	Gerade Aufsteigung in Graden	Nördl. Abweich.	Geocentrische Länge	Geocentr. Breite	Ort der Sonne + 20" Aberration	Logar. d. Distanz ☉ ♂
	St ' "	St ' "	° ' "	° ' "	Z ° ' "	° ' "	Z ° ' "	
Jan. 1	8 43 27,8	3 27 11,25	51 47 48,8	15 37 43,5	1 23 22 58,3	3 6 42,1	9 11 1 30,9	9,9926156
2	8 39 4,6	3 26 53,85	51 43 27,8	15 41 5,5	1 23 19 44,3	3 2 24,9	9 12 2 28,6	9,9926317
3	8 34 53,3	3 26 38,4::	51 39 36,0	15 44 31,6	1 23 16 58,6	2 58 9,9	9 13 3 26,6	9,9926324
4	8 30 42,1	3 26 23,15	51 35 47,3	15 47 57,6	1 23 14 15,5	2 53 55,6	9 14 4 24,9	9,9926418
10	8 6 15,8	3 25 32,1::	51 23 1,5	16 10 32,0	1 23 7 59,1	2 29 0,6	9 20 10 17,5	9,9927641
11	8 2 17,5	3 25 29,73	51 22 26,6	. . . .	. . . .	. . . . .	. . . .	. . . . .
13	7 54 26,2	3 25 30,30	51 22 34,5	16 22 49,5	1 23 10 27,6	2 16 59,7	9 23 12 13,8	9,9928490
14	7 50 31,7	3 25 31,72	51 22 55,8	16 27 5,7	1 23 12 1,2	2 12 56,7	9 24 14 13,5	9,9928809
17	. . . . . .	. . . .	. . . .	16 40 13,0	. . . .	. . . . .	. . . .	. . . . .
18	7 35 11,3	3 25 55,::	51 28 45,0	. . . .	. . . .	. . . . .	. . . .	. . . . .
19	7 31 28,5	3 26 8,15	51 32 2,3	16 49 16,1	1 23 25 59,2	1 53 38,2	9 29 19 53,8	9,9930607
21	7 24 2,7	3 26 34,27	51 38 34,1	16 58 35,9	1 23 34 21,3	1 46 6,0	10 1 20 40,3	9,9931434
22	7 20 21,7	3 26 49,42	51 42 21,3	17 3 18,5	1 23 39 1,8	1 42 28,1	10 2 21 32,0	9,9931886
23	7 16 43,5	3 27 6,90	51 46 43,5	17 8 5,5	1 23 44 15,7	1 38 52,1	10 3 22 22,7	9,9932348
28	6 58 51,3	3 28 54,55	52 13 38,3	17 32 54,1	1 24 15 15,7	1 21 6,9	10 8 26 20,1	9,9935062
30	6 51 52,9	3 29 48,14	52 27 2,1	17 43 11,0	1 24 30 9,0	1 14 16,0	10 10 27 46,2	9,9936332
31	6 48 26,4	3 30 17,25	52 34 18,8	17 48 21,5	1 24 38 7,3	1 10 54,6	10 11 28 28,5	9,9937007
Febr. 1	6 44 59,9	3 30 47,2::	52 41 48,0	17 53 36,3	1 24 46 19,3	1 7 30,9	10 12 29 9,6	9,9937703
2	6 41 35,8	3 31 19,06	52 49 45,9	17 58 57,5	1 24 54 57,9	1 4 1,5	10 13 29 49,9	9,9938423
5	6 31 31,5	3 33 2,70	53 15 40,5	18 15 1,0	1 25 22 43,4	0 54 23,9	10 16 31 45,5	9,9940751
8	6 21 39,2	3 34 58,50	53 44 37,5	18 31 23,2	1 25 53 29,5	0 45 5,0	10 19 33 33,3	9,9943276
11	6 11 58,2	3 37 6,54	54 16 38,1	18 47 58,8	1 26 26 40,0	0 36 2,9	10 22 35 11,4	9,9945823

Piazzi's 24 observations

Karl Friedrich Gauss

Karl Friedrich Gauss
'Princeps mathematicorum'

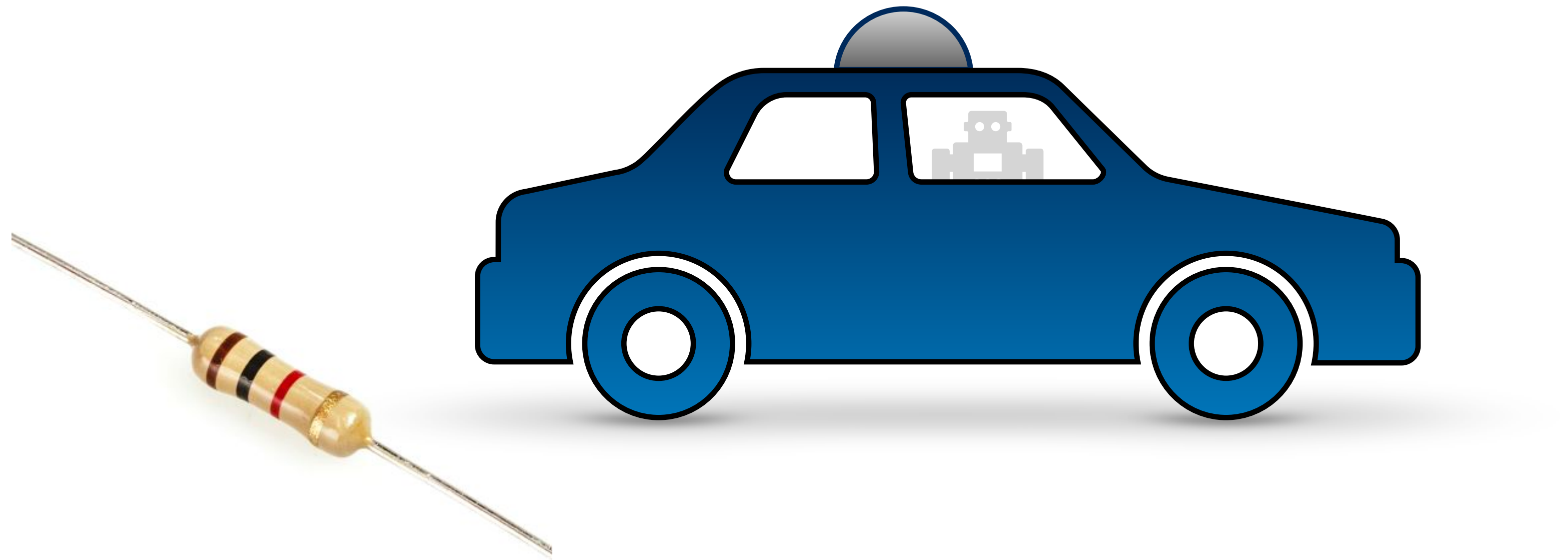


*Gauss used the **method of least squares** to determine the orbital parameters of Ceres.*

Least Squares

*The **most probable value** of the unknown quantities will be that in which the **sum of the squares** of the differences between the actually observed and the computed values multiplied by numbers that measure the degree of precision is a **minimum**.*

- Karl Friedrich Gauss



Resistor in the drive-system of a car

Multimeter

Estimating Resistance

Measurement	Resistance (Ohms)
1	1068
2	988
3	1002
4	996

R?

Estimating Resistance

Measurement	Resistance (Ohms)
1	1068
2	988
3	1002
4	996

Let x be the resistance. Assume it is a **constant**, but **unknown**.

We make measurements, y, of the resistance.

We model our measurements as corrupted by noise v.

$$\boxed{y = x + v}$$

Estimating Resistance

Measurement	Resistance (Ohms)
1	1068
2	988
3	1002
4	996

Measurement Model

'Actual' resistance *Measurement noise*

$$y_1 = x + v_1$$

$$y_2 = x + v_2$$

$$y_3 = x + v_3$$

$$y_4 = x + v_4$$

Estimating Resistance

#	Resistance (Ohms)
1	1068
2	988
3	1002
4	996

Measurement Model

$$y_1 = x + v_1$$

$$y_2 = x + v_2$$

$$y_3 = x + v_3$$

$$y_4 = x + v_4$$

Squared Error

$$e_1^2 = (y_1 - x)^2$$

$$e_2^2 = (y_2 - x)^2$$

$$e_3^2 = (y_3 - x)^2$$

$$e_4^2 = (y_4 - x)^2$$

The squared error *criterion*:

$$\hat{x}_{\mathrm{LS}} = \operatorname{argmin}_x \left(e_1^2 + e_2^2 + e_3^2 + e_4^2\right) = \mathscr{L}_{\mathrm{LS}}(x)$$

squared error cost func.
or loss func.

The 'best' estimate of resistance is the one that minimizes the sum of squared errors

Minimizing the Squared Error Criterion

$$\boxed{\hat{x}_{\mathrm{LS}} = \mathrm{argmin}_{\,x} \left(e_1^2 + e_2^2 + e_3^2 + e_4^2\right) = \mathscr{L}_{\mathrm{LS}}(x)}$$

Let's re-write our criterion using vectors:

This matrix is called the 'Jacobian'

$$\mathbf{e} = \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix} = \mathbf{y} - \mathbf{H}x$$

$$= \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} x$$

Minimizing the Squared Error Criterion

$$\boxed{\hat{x}_{\text{LS}} = \text{argmin}_{\,x} \left(e_1^2 + e_2^2 + e_3^2 + e_4^2\right) = \mathscr{L}_{\text{LS}}(x)}$$

Now, we can express our criterion as follows,

$$\begin{aligned}
\mathscr{L}_{\text{LS}}(x) = e_1^2 + e_2^2 + e_3^2 + e_4^2 &= \mathbf{e}^T\mathbf{e} \\
&= (\mathbf{y} - \mathbf{H}x)^T(\mathbf{y} - \mathbf{H}x) \\
&= \mathbf{y}^T\mathbf{y} - x^T\mathbf{H}^T\mathbf{y} - \mathbf{y}^T\mathbf{H}x + x^T\mathbf{H}^T\mathbf{H}x
\end{aligned}$$

Minimizing the Squared Error Criterion

$$\boxed{\mathscr{L}(x) = \mathbf{e}^T\mathbf{e} = \mathbf{y}^T\mathbf{y} - x^T\mathbf{H}^T\mathbf{y} - \mathbf{y}^T\mathbf{H}x + x^T\mathbf{H}^T\mathbf{H}x}$$

To minimize this, we can compute the partial derivative with respect to our parameter, set to 0, and solve for an extremum:

$$\left.\frac{\partial \mathscr{L}}{\partial x}\right|_{x=\hat{x}} = -\mathbf{y}^T\mathbf{H} - \mathbf{y}^T\mathbf{H} + 2\hat{x}^T\mathbf{H}^T\mathbf{H} = 0$$

$$-2\mathbf{y}^T\mathbf{H} + 2\hat{x}^T\mathbf{H}^T\mathbf{H} = 0$$

Re-arranging, we arrive at:

$$\hat{x}_{\text{LS}} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$$

x-hat minimizes our squared error criterion!

Minimizing the Squared Error Criterion

Careful! We will only be able to solve for $\hat{x}$ if $(\mathbf{H}^T\mathbf{H})^{-1}$ exists.

If we have m measurements, and n unknown parameters, then:

$$\mathbf{H} \in \mathbb{R}^{m \times n} \qquad \mathbf{H}^T\mathbf{H} \in \mathbb{R}^{n \times n}$$

This means that $(\mathbf{H}^T\mathbf{H})^{-1}$ exists only if there are at least as many measurements as there are unknown parameters:

$$m \geq n$$

Minimizing the Squared Error Criterion

Returning to our problem, we see that:

#	Resistance (Ohms)
1	1068
2	988
3	1002
4	996

$$\mathbf{y} = \begin{bmatrix} 1068 \\ 988 \\ 1002 \\ 996 \end{bmatrix} \qquad \mathbf{H} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\hat{x}_{\mathrm{LS}} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$$

$$= \left([1 1 1 1] \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \right)^{-1} [1 1 1 1] \begin{bmatrix} 1068 \\ 988 \\ 1002 \\ 996 \end{bmatrix} = \frac{1}{4}(1068 + 988 + 1002 + 996) = 1013.5 \quad \text{Ohms}$$

The least squares solution is just the mean of our measurements!

Method of Least Squares | Assumptions

- Our measurement model, $y = x + v$, is **linear.**
- Measurements are **equally weighted.**
  (we do not suspect that some have more noise than others).

Summary | The Method of Least Squares

- Pioneered by Gauss to determine the orbit of the planetoid *Ceres*
- Least squares finds the parameters which minimize the *Least Squares Criterion*
- Ordinary least squares assumes that measurements are weighted equally, measurement model is linear

Module 1 | Lesson 1 (Part 2)

Weighted Least Squares

Weighted Least Squares

By the end of this video, you will be able to…

- Derive the weighted least squares criterion given varying measurement noise variance
- Compare weighted least squares to ordinary least squares

Method of *Weighted* Least Squares

- Suppose we take measurements with multiple multimeters, some of which are better than others

vs.

Method of *Weighted* Least Squares

Consider the general linear measurement model for m measurements and n unknowns:

$$\begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} = \mathbf{H} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} v_1 \\ \vdots \\ v_m \end{bmatrix}$$

$$\mathbf{y} = \mathbf{H}\mathbf{x} + \mathbf{v}$$

In regular least squares, we implicitly assumed that each noise term was of equal variance:

$$\mathbb{E}[v_i^2] = \sigma^2 \quad (i = 1, \ldots, m) \qquad\qquad \mathbf{R} = \mathbb{E}[\mathbf{v}\mathbf{v}^T] = \begin{bmatrix} \sigma^2 & & 0 \\ & \ddots & \\ 0 & & \sigma^2 \end{bmatrix}$$

Method of *Weighted* Least Squares

If we assume each noise term is independent, but of different variance,

$$\mathbb{E}[v_i^2] = \sigma_i^2, \quad (i = 1, \ldots, m) \qquad \mathbf{R} = \mathbb{E}[\mathbf{v}\mathbf{v}^T] = \begin{bmatrix} \sigma_1^2 & & 0 \\ & \ddots & \\ 0 & & \sigma_m^2 \end{bmatrix}$$

Then we can define a *weighted* least squares criterion as:

$$\begin{aligned} \mathscr{L}_{\mathrm{WLS}}(\mathbf{x}) &= \mathbf{e}^T\mathbf{R}^{-1}\mathbf{e} \\ &= \frac{e_1^2}{\sigma_1^2} + \frac{e_2^2}{\sigma_2^2} + \ldots + \frac{e_m^2}{\sigma_m^2} \end{aligned}$$

where

$$\begin{bmatrix} e_1 \\ \vdots \\ e_m \end{bmatrix} = \mathbf{e} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} - \mathbf{H} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

The higher the expected noise, the lower the weight we place on the measurement.

Re-deriving regular least squares

What happens if all of our variances are the same?

$$\begin{aligned}\mathscr{L}_{\mathrm{WLS}}(\mathbf{x}) &= \frac{e_1^2}{\sigma^2} + \frac{e_2^2}{\sigma^2} + \ldots + \frac{e_m^2}{\sigma^2} \\ &= \frac{1}{\sigma^2}(e_1^2 + \ldots + e_m^2)\end{aligned}$$

Since our variance is constant, it will not affect our final estimate! *This results in the same estimate as regular least squares:*

$$\sigma_1^2 = \sigma_2^2 = \ldots \sigma_m^2 = \sigma^2 \rightarrow \quad \hat{\mathbf{x}}_{\mathrm{WLS}} = \hat{\mathbf{x}}_{\mathrm{LS}} = \operatorname{argmin}_{\mathbf{x}} \mathscr{L}_{\mathrm{LS}}(\mathbf{x}) = \operatorname{argmin}_{\mathbf{x}} \mathscr{L}_{\mathrm{WLS}}(\mathbf{x})$$

Minimizing the *Weighted* Least Squares Criterion

Expanding our new criterion,

$$\begin{aligned}\mathscr{L}_{\text{WLS}}(\mathbf{x}) &= \mathbf{e}^T\mathbf{R}^{-1}\mathbf{e} \\ &= (\mathbf{y} - \mathbf{H}\mathbf{x})^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}\mathbf{x})\end{aligned}$$

We can minimize it as before, but accounting for the new weighting term:

$$\hat{\mathbf{x}} = \text{argmin}_{\,\mathbf{x}}\, \mathscr{L}(\mathbf{x}) \longrightarrow \left.\frac{\partial \mathscr{L}}{\partial \mathbf{x}}\right|_{\mathbf{x}=\hat{\mathbf{x}}} = \mathbf{0} = -\mathbf{y}^T\mathbf{R}^{-1}\mathbf{H} + \hat{\mathbf{x}}^T\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$$

$$\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\hat{\mathbf{x}}_{\text{WLS}} = \mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}$$

The weighted normal equations!

Method of *Weighted* Least Squares

The weighted normal equations

$$\boxed{\hat{\mathbf{x}} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}}$$

Let's adapt our example:

	Resistance Measurements (Ohms)	
#	Multimeter A ($\sigma = 20$ Ohms)	Multimeter B ($\sigma = 2$ Ohms)
1	1068	
2	988	
3		1002
4		996

Method of *Weighted* Least Squares

Once we define the relevant quantities, we plug-and-chug to get:

$$\mathbf{H} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 1068 \\ 988 \\ 1002 \\ 996 \end{bmatrix} \qquad \mathbf{R} = \begin{bmatrix} \sigma_1^2 & & & \\ & \sigma_2^2 & & \\ & & \sigma_3^2 & \\ & & & \sigma_4^2 \end{bmatrix} = \begin{bmatrix} 400 & & & \\ & 400 & & \\ & & 4 & \\ & & & 4 \end{bmatrix}$$

$$\begin{aligned}
\hat{x}_{\mathrm{WLS}} &= (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{y} \\
&= \left([1111] \begin{bmatrix} 400 & & & \\ & 400 & & \\ & & 4 & \\ & & & 4 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \right)^{-1} [1111] \begin{bmatrix} 400 & & & \\ & 400 & & \\ & & 4 & \\ & & & 4 \end{bmatrix}^{-1} \begin{bmatrix} 1068 \\ 988 \\ 1002 \\ 996 \end{bmatrix} \\
&= \frac{1}{1/400 + 1/400 + 1/4 + 1/4} \left(\frac{1068}{400} + \frac{988}{400} + \frac{1002}{4} + \frac{996}{4} \right) \\
&= 999.3 \text{ Ohms}
\end{aligned}$$

Ordinary versus Weighted Least Squares

	Least Squares	Weighted Least Squares
Loss / Criterion	$\mathscr{L}_{\text{LS}}(\mathbf{x}) = \mathbf{e}^T\mathbf{e}$	$\mathscr{L}_{\text{WLS}}(\mathbf{x}) = \mathbf{e}^T\mathbf{R}^{-1}\mathbf{e}$
Solution	$\hat{\mathbf{x}}_{\text{LS}} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$	$\hat{\mathbf{x}}_{\text{WLS}} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{y}$
Limitations	$m \geq n$	$m \geq n$ $\sigma_i^2 > 0$

Accurate noise modelling is crucial to utilize various sensors effectively!

Summary | Weighted Least Squares

- Measurements can come from sensors that have different noisy characteristics
- Weighted least squares lets us weight each measurement according to noise *variance*