

CHAPTER 3a. INTRODUCTION TO NUMERICAL METHODS



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by

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Characteristics of Numerical Methods



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1. The solution procedure is iterative, with the accuracy of the estimated solution improving with each iteration.
2. The solution procedure provides only an approximation to true (exact), but unknown solution.
3. An initial estimate of the solution may be required.



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4. The solution procedure is conceptually simple, with algorithms representing the solution procedure that can be easily programmed on a digital computer.
5. The solution procedure may occasionally diverge from rather converge to the true solution.



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■ Example 1: Square Root

This example illustrates how to approach a solution for finding the square root of an arbitrary real number y using numerical methods.

$$f(y) = \sqrt{y}$$



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■ Example 1 (cont'd): Square Root

- The square root of any real number can be found using any computational aid such as a calculator or a spread sheet.
- On a calculator, you simply enter the number and then press $\sqrt{\quad}$ key.
- On a spread sheet, the function SQRT is used.



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■ Example 1 (cont'd): Square Root

- Strategy
 - Let's assume an initial value of x_0 for the square root.
 - Then x_0 will be in error by unknown amount Δx .
 - If we know Δx , then

$$x_0 + \Delta x = \sqrt{y}$$



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■ Example 1 (cont'd): Square Root

$$x_0 + \Delta x = \sqrt{y}$$

– If both sides of the above equation is squared, then

$$(x_0 + \Delta x)^2 = y$$

or

$$x_0^2 + 2x_0\Delta x + (\Delta x)^2 = y$$



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■ Example 1 (cont'd): Square Root

$$x_0^2 + 2x_0\Delta x + (\Delta x)^2 = y$$

(Note: An arrow points from the text below to the $(\Delta x)^2$ term, with a small ≈ 0 above it.)

– If we assume that $(\Delta x)^2$ is much smaller than Δx , then we have

$$\Delta x = \frac{y - x_0^2}{2x_0}$$



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■ Example 1 (cont'd): Square Root

- The value of Δx computed with the previous equation can be added to x_0 to get a revised estimate of x .
- Thus the new estimate x_1 of the true solution is given by

$$x_1 = x_0 + \Delta x$$



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■ Example 1 (cont'd): Square Root

- Generalizing the notation, we have

$$x_{i+1} = x_i + \Delta x \quad (1)$$

- where x_{i+1} and x_i are the estimates of x on trials i and $i + 1$, respectively, and

$$\Delta x = \frac{y - x_i^2}{2x_i} \quad (2)$$



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■ Example 1 (cont'd): Square Root

– To illustrate the numerical use of Eqs. 1 and 2:

- Assume $y = 150$
- We know that $12^2 = 144$
- So $x_0 = 12$, which is a reasonable estimate
- Therefore, the first iteration is given by Eq.2 as

$$\Delta x = \frac{y - x_0^2}{2x_0} = \frac{150 - (12)^2}{2(12)} = 0.25$$



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■ Example 1 (cont'd): Square Root

- and by Eq. 1 as

$$x_{i+1} = x_i + \Delta x$$

$$x_1 = x_0 + \Delta x = 12 + 0.25 = 12.25$$

- A second iteration can now be applied in Eqs. 2 and 1 to give, respectively

$$\Delta x = \frac{y - x_1^2}{2x_1} = \frac{150 - (12.25)^2}{2(12.25)} = -0.00255$$

$$x_{i+1} = x_i + \Delta x$$

$$x_2 = x_1 + \Delta x = 12.25 - 0.00255 = 12.24745$$



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■ Example 1 (cont'd): Square Root

- A third iteration, yields

$$\Delta x = \frac{y - x_2^2}{2x_2} = \frac{150 - (12.24745)^2}{2(12.24745)} = -1.28598 \times 10^{-6}$$

$$x_{i+1} = x_i + \Delta x$$

$$x_3 = x_2 + \Delta x = 12.24734 - 0.00000129 = 12.24744871$$

$$\text{True Value} = \sqrt{150} = 12.24744871$$

For 7 digits, the solution converges to true value in 3 iterations.



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■ Example 1 (cont'd): Square Root

$$\sqrt{y} = \sqrt{150}$$

| <i>i</i> | Δx | <i>x</i> | <i>y</i> | True Value | ABS error |
|----------|------------|------------|----------|------------|-------------|
| 0 | 0.25 | 12.0000000 | 150 | 12.2474487 | 0.247448714 |
| 1 | -0.003 | 12.2500000 | 150 | 12.2474487 | 0.002551286 |
| 2 | -3E-07 | 12.2474490 | 150 | 12.2474487 | 2.65676E-07 |
| 3 | -3E-15 | 12.2474487 | 150 | 12.2474487 | 3.55271E-15 |
| 4 | 0 | 12.2474487 | 150 | 12.2474487 | 0 |
| 5 | 0 | 12.2474487 | 150 | 12.2474487 | 0 |
| 6 | 0 | 12.2474487 | 150 | 12.2474487 | 0 |



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■ Example 2: Root of a Polynomial

This example illustrates how to approach a solution for finding one root of a polynomial using numerical methods.

$$x^3 - 3x^2 - 6x + 8 = 0$$



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■ Example 2 (cont'd): Root of a Polynomial

– Strategy

- Dividing both sides of the equation by x , yields

$$x^2 - 3x - 6 + \frac{8}{x} = 0$$

- Solving for x using the x^2 term, gives

$$x = \sqrt{3x + 6 - \frac{8}{x}} \quad (3)$$



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■ Example 2 (cont'd): Root of a Polynomial

– Eq. 3 can be solved iteratively as follows:

$$x_{i+1} = \sqrt{3x_i + 6 - \frac{8}{x_i}} \quad (4)$$

– If an initial value of 2 ($x_0 = 2$) is assumed for x , then

$$x_1 = \sqrt{3x_0 + 6 - \frac{8}{x_0}} = \sqrt{3(2) + 6 - \frac{8}{2}} = 2.828427$$



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■ Example 2 (cont'd): Root of a Polynomial

– Now $x_1 = 2.828427$

– A second iteration will yield

$$x_2 = \sqrt{3x_1 + 6 - \frac{8}{x_1}} = \sqrt{3(2.828427) + 6 - \frac{8}{2.828427}} = 3.414213$$

– A third iteration results in

$$x_3 = \sqrt{3x_2 + 6 - \frac{8}{x_2}} = \sqrt{3(3.414213) + 6 - \frac{8}{3.414213}} = 3.728202$$



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■ Example 2 (cont'd): Root of a Polynomial

- The results of 20 iteration are shown Table 1 of the next viewgraph.
- It is evident from the table that the solution converges to the true value of 4 after the the 20th iteration.



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■ Example 2 (cont'd): Root of a Polynomial

Table 1

| <i>i</i> | x_i | True Value | Abs Error | <i>i</i> | x_i | True Value | Abs Error |
|----------|----------|------------|-------------|----------|----------|------------|-------------|
| 0 | 2 | 4 | 2 | 10 | 3.999127 | 4 | 0.000872759 |
| 1 | 2.828427 | 4 | 1.171572875 | 11 | 3.999618 | 4 | 0.000381862 |
| 2 | 3.414214 | 4 | 0.585786438 | 12 | 3.999833 | 4 | 0.000167071 |
| 3 | 3.728203 | 4 | 0.271797358 | 13 | 3.999927 | 4 | 7.30945E-05 |
| 4 | 3.877989 | 4 | 0.122010596 | 14 | 3.999968 | 4 | 3.1979E-05 |
| 5 | 3.946016 | 4 | 0.053983839 | 15 | 3.999986 | 4 | 1.39909E-05 |
| 6 | 3.976265 | 4 | 0.023734503 | 16 | 3.999994 | 4 | 6.12101E-06 |
| 7 | 3.989594 | 4 | 0.010406236 | 17 | 3.999997 | 4 | 2.67794E-06 |
| 8 | 3.995443 | 4 | 0.00455702 | 18 | 3.999999 | 4 | 1.1716E-06 |
| 9 | 3.998005 | 4 | 0.001994519 | 19 | 3.999999 | 4 | 5.12576E-07 |
| | | | | 20 | 4 | 4 | 0 |



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- In view of Examples 1 and 2, we conclude that
 - The solution procedure is iterative, with the accuracy of the estimated solution improving with each iteration.
 - The solution procedure provides only an approximation to true (exact), but unknown solution



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- An initial estimate of the solution may be required.
- The solution procedure is conceptually simple, with algorithms representing the solution procedure that can be easily programmed on a digital computer.



Accuracy, Precision, and Bias

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■ Bias

An estimate of a parameter θ made from sample statistic is said to be an unbiased estimate if the expected value of the sample quantity $\hat{\theta}$ is θ ; that is

$$E(\hat{\theta}) = \theta$$

The bias is defined as

$$[E(\hat{\theta}) - \theta]$$



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■ Bias

– Definition:

Bias is a systematic deviation of values from the true value



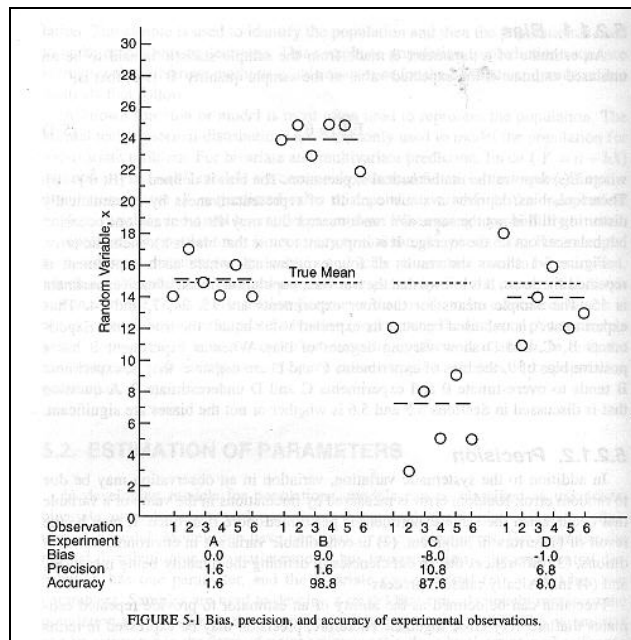
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■ Bias

- Consider four experiments where each experiment is repeated six times.
- The following table shows the results of the four experiments:

| | True (Population) | Exp. A | Exp. B | Exp. C | Exp D |
|------|-------------------|--------|--------|--------|-------|
| Mean | 15 | 15 | 24 | 7 | 14 |





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■ Bias

- Experiment A is unbiased because its expected value (mean) equals the true mean.
- Experiments B, C, and D show varying degrees of bias.
- Experiment B has a positive bias of 9, whereas the bias of C and D are negative.
- Experiment B tends to overestimate θ , while C and D tend to underestimate θ .



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■ Precision

– Definition:

Precision is defined as the ability of an estimator to give repeated estimates that are very close to each other.



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■ Precision

- Precision can be expressed in terms of the variance of the estimator.

| | Precision |
|---------------------------------|--------------------|
| $\text{Var}(\theta) \uparrow$ | Lack of precision |
| $\text{Var}(\theta) \downarrow$ | High precision |
| $\text{Var}(\theta) = 0$ | Absolute precision |



Accuracy, Precision, and Bias

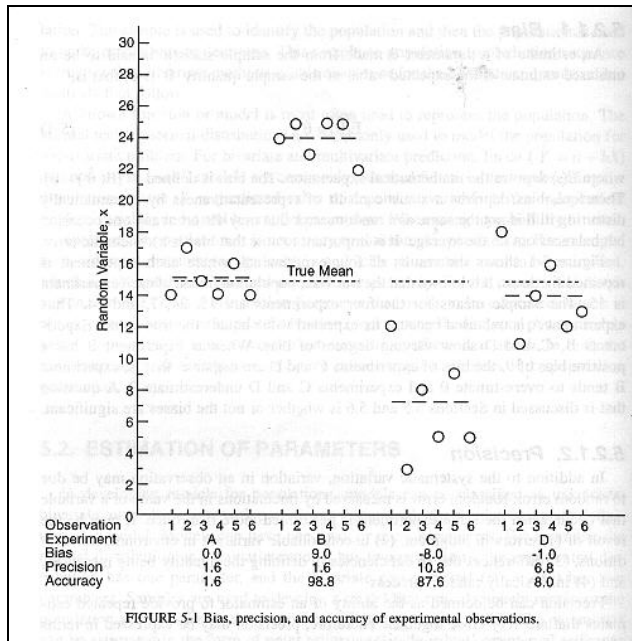
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■ Precision

- Consider four experiments where each experiment is repeated six times.
- The following table shows the results of the four experiments:

| | Exp. A | Exp. B | Exp. C | Exp D |
|-----|--------|--------|--------|-------|
| Var | 1.6 | 1.6 | 10.6 | 6.8 |

Note: Variance is about the sample mean for each experiment



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■ Precision

- Experiment A and B show considerably more precision (i.e., they have lower variances).
- Experiment C has the largest variation, therefore, it is the least precise.
- Experiments A and B have the same level of variation, however, A is unbiased, whereas B is highly biased.



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■ Accuracy

– Definition:

Accuracy is defined as the closeness or nearness of the measurements to the true or actual value of the quantity being measured.



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■ Accuracy

– Bias and Precision are considered elements of Accuracy.

$$\text{Bias} + \text{Precision} \Rightarrow \text{Accuracy}$$

– Inaccuracy can result from either a bias or a lack of precision.



Accuracy, Precision, and Bias

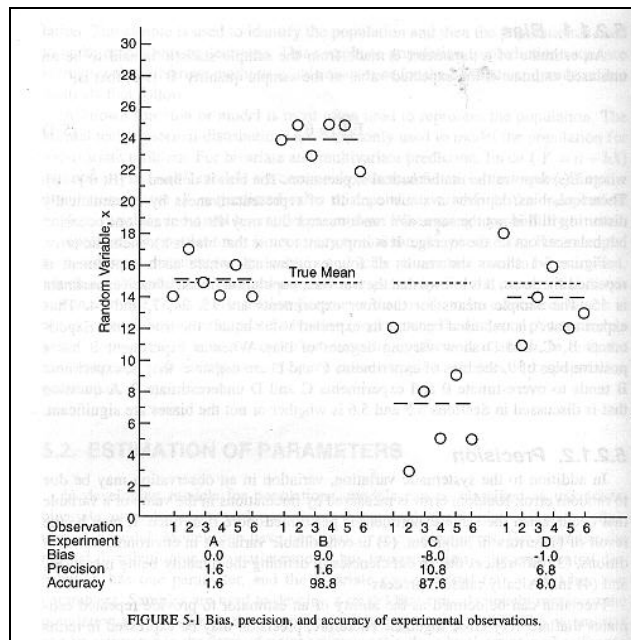
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■ Accuracy

- Consider four experiments where each experiment is repeated six times.
- The following table shows the results of the four experiments:

| | Exp. A | Exp. B | Exp. C | Exp D |
|-----|--------|--------|--------|-------|
| Var | 1.6 | 98.8 | 87.6 | 8.0 |

Note: Variance is about the true mean of the population (i.e., 15)





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■ Bias, Precision, and Accuracy

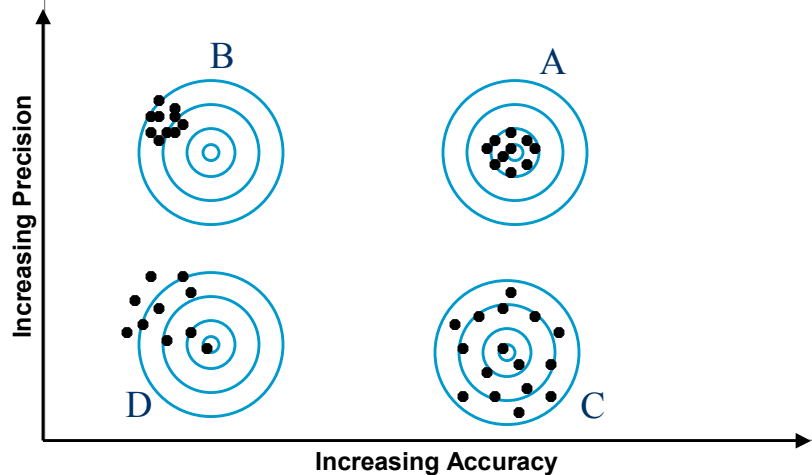
- Consider the four dartboards of the following figure.
- Assuming that these shooting at the targets were aiming at the center, the person shooting at target A was successful.



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Bias, Precision, and Accuracy

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■ Bias, Precision, and Accuracy

- The holes in target B are similarly clustered as in target B, but they show large deviation from the center.
- The holes in target C are very different in character from the holes in either target A or B.
- They are not near the center, and they are not near each other.



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■ Bias, Precision, and Accuracy

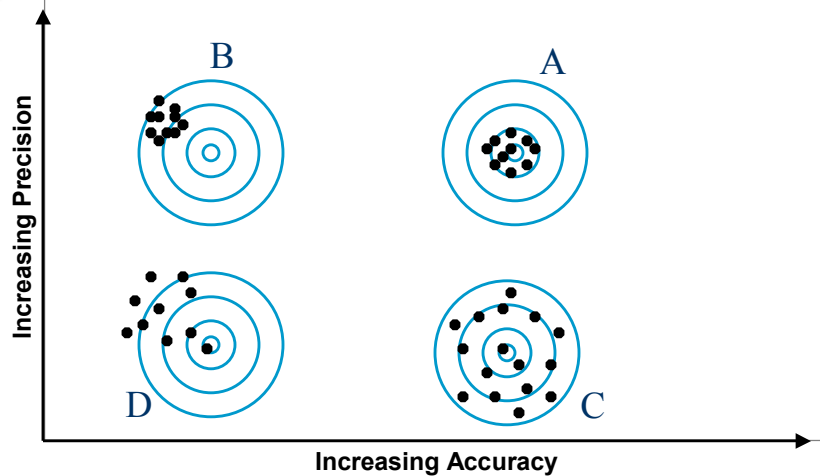
- The holes in target A and B show a measure of precision, therefore, the shooters were precise.
- The shooters of targets C and D were imprecise since the holes show a lot of scatter.
- The holes in targets B and D are consistently to the left, that is, there is a systematic distortion of the hole with respect to the center of the target.



Accuracy, Precision, and Bias

Bias, Precision, and Accuracy

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■ Bias, Precision, and Accuracy

- The holes in targets B and D show a systematic deviation to the left.
- Targets A and C are considered to *unbiased* because there is no systematic deviation.
- In the figure, accuracy increases as precision increases, therefore, the shooter of target A is the most accurate.

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