Error & Uncertainty

Error

The error **is the** difference between a TRUE value, x, and a MEASURED value, x_i**:**

$$E = x - x_i$$

- **There is no error-free measurement.**
- **The significance of a measurement cannot be judged unless the associate error has been reliably estimated.**
- **Since the true value, x is generally unknown, then so is E.**

More on errors

- **Error is unknown. However, the** *likely errors* **can be ESTIMATED. They are called** *uncertainties***.**

$$\bar{x},$$

- **For multiple measurements, a** mean value **(also called** nominal **value),** **can be calculated. Hence, the error becomes:**

$$E = x - \bar{x}$$

- **Since x remains unknown, then E is still unknown.**

Uncertainty

The uncertainty, Δx, **is an** estimate of E as a possible range of errors.

$$\Delta x \approx E$$

- ***e.g.*, a velocity measurement can be reported as:**

$$V = 110\,m/s \pm 5\,m/s$$

uncertainty ($\pm 5\,m/s$)

- **The uncertainty may be expressed as physical units or as a %-age, *e.g.*,** $V = 110\,m/s \pm 4.5\%$

relative uncertainty ($\pm 4.5\%$)

Accuracy

The accuracy **is a** measure (or an estimate) of the maximum deviation of measured values, x_i, from the TRUE value, x:

$$\text{accuracy} = \text{estimate of } \max |x - x_i|$$

- **Again, since the TRUE value is unknown, neither is the maximum deviation. The accuracy is only an *estimate of the worst error*.**

- **Usually expressed as a percentage, *e.g*. "accurate to 5%"**
  - **Note this implies that 95% of the values are within the interval**

Example: pressure measurement

- **Given:** A measurement is claimed to be:

  P = 50 psi ± 5 psi.

- **Required:** What is the accuracy of the pressure probe used for making this measurement?

- **Answer:** The relative uncertainty $\Delta P / \bar{P}$ is about:

$$\frac{\Delta P}{\bar{P}} \approx \pm \frac{5}{50} \approx \pm 0.1 \approx \pm 10\%$$

The accuracy may be estimated to be (around) 10%.

Example

- Given: A pressure sensor is claimed to be accurate to 5%.

- Required: What will be the uncertainty (in psi) in the measurement of a pressure of 50 psi?

- Answer: The accuracy (≈ ± relative uncertainty) is 5%, so

$$\frac{\Delta P}{\overline{P}} \approx \pm 5\% \Rightarrow \Delta P \approx \pm 0.05 \times \overline{P} \approx \pm 0.05 \times 50 \approx \pm 2.5\,\text{psi}$$

The uncertainty in P in psi is ±2.5 psi, so the measurement should be reported as follows:

P = 50 psi ± 2.5 psi.

More on Accuracy

The question:

"Are the measured values accurate?"

can be reformulated as

"Are the measured values close to the true value?"

Or

"Are the measured values unbiased?"

Precision

The precision **is a** measure (or an estimate) of the reproducibility (i.e. repeatability) of repeated measurements. It is generally expressed as the deviation of a reading (measurement), x_i, from its mean value, $\bar{x}$:

$$precision = estimate\ of\ \max \left| x_i - \bar{x} \right|$$

- **The mean is not the same as the true value, unless the measurement is completely unbiased.**
- **Precision is a *characteristic of our measurement*.**
- **In this context: "accuracy" ≠ "precision"**

More on Precision

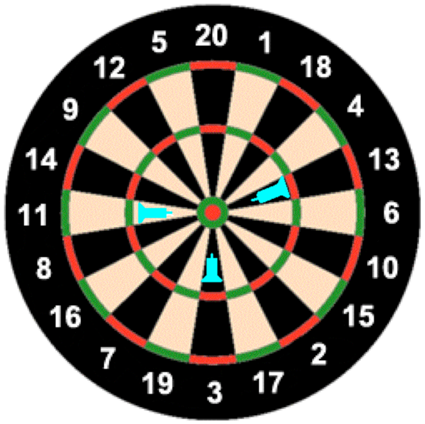
The question:

“Are the measured values precise?”

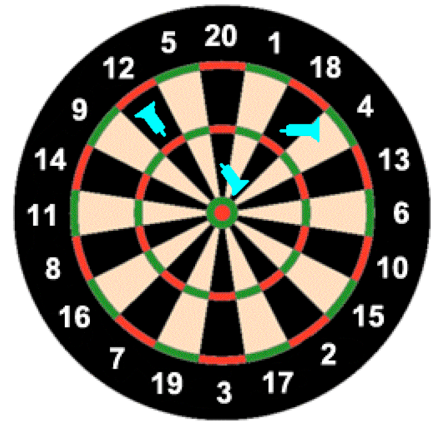
can be reformulated as

“Are the measured values close to each other?”

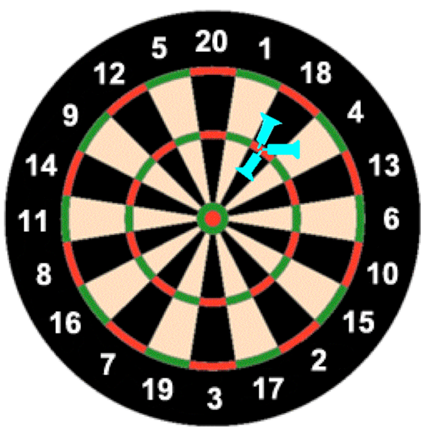
Accurate but NOT precise



Neither accurate nor precise



Precise but NOT accurate



Both accurate and precise

Types of errors

A systematic error is one that happens consistently – a bias or constant difference between the measurement and the true value

- **Human components of measurement systems are often responsible for systematic errors, *e.g*., systematic errors are common in reading of a pressure indicated by an inclined manometer.**
- In theory, these can be anticipated **and/or** measured **and then** corrected, **even** after the fact.
- **A** random error **is just that** – random and uncontrollable!

How to reduce systematic errors?

Calibration: **Check the measuring instrument against a known standard.**

→ ***involves comparison with either*:**

a) ***A primary standard*** (given by the “National Institute of standards and technology” – NIST – *ex* “National Bureau of Standards)

b) ***A secondary standard*** (with higher accuracy that instrument)

c) ***A known input source***.

How to reduce random errors?

- **There is NO random error free measurements.**
- **Hence, the random errors CANNOT be eliminated.**
- **However, the easiest ways to reduce random errors is to <u>take more measurements</u> because:**

ON AVERAGE, random errors
tend to cancel out

Uncertainty in multi-sample measurements

Multi-Sample Measurements

Multi-sample **measurements are significant number of data collected from enough experiments so that the reliability of the results can be assured by statistics.**

- ***In other words*, a significant number of measurements of the same quantity (for fixed system variables) under varying test conditions (*i.e.* different samples and/or different instruments) so that the uncertainties can be reduced by the number of observations.**

Arithmetic Mean and SD

If each reading is x_i and there are n readings, then the arithmetic mean value is given by:

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}$$

The standard deviation is given by:

$$\sigma = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n-1}}$$

Due to random errors data is dispersed in a Gaussian or Normal Distribution.

The Gaussian or Normal Distribution

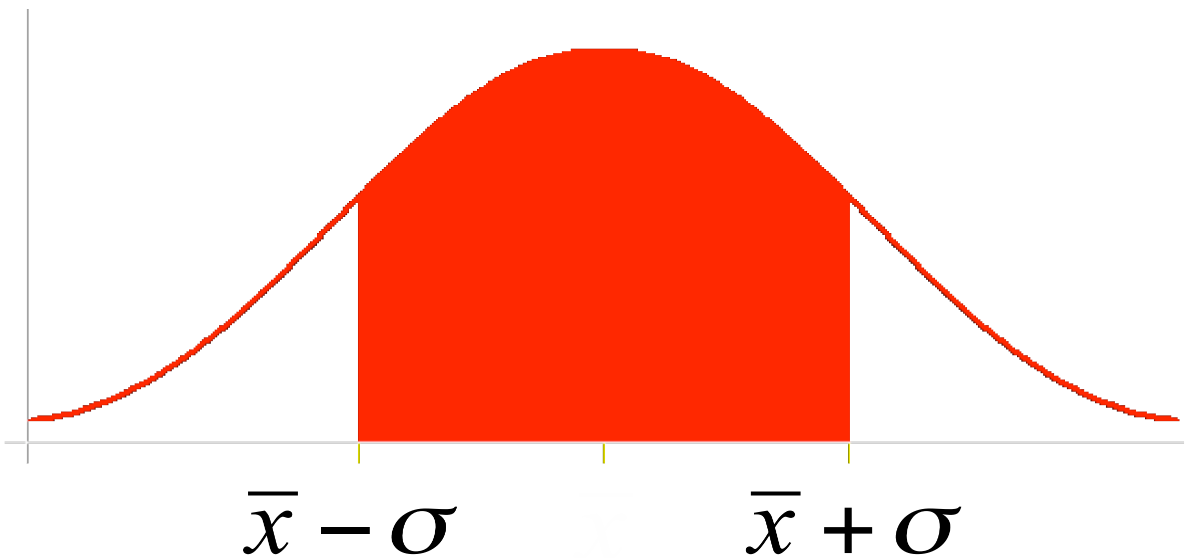
- This is the distribution followed by random errors.
- It is often referred to as the "bell" curve as it looks like the outline of a bell.
- The peak of the distribution occurs at the mean of the random variable, and the standard deviation is a common measure for how "fat" this bell curve is.
- The mean and the standard deviation are all the information that is necessary to completely describe any normally-distributed random variable.

More on Probability Distribution Functions

The probability for a reading to fall in the range $\pm \infty$ of the mean is 100 %.

- If you integrate under the curve of the normal distribution from negative to positive infinity, the area is 1.0. (*i.e.* 100 %)

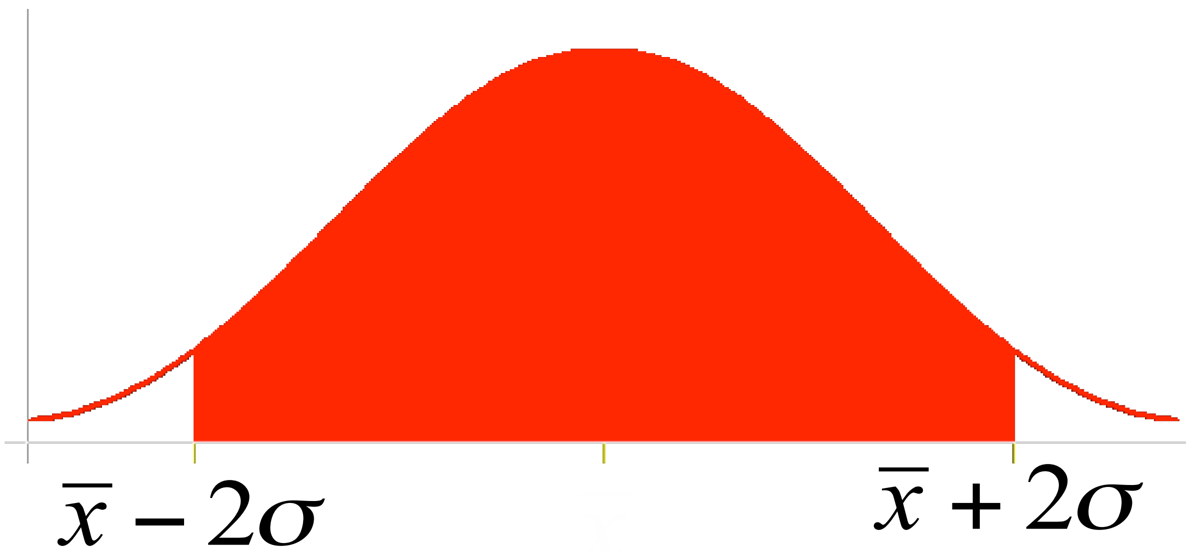
More on Probability Distribution Functions



The probability for a reading to fall in the range ± _ of the mean is about 68 %.

- Integrating over a range within ± _ from the mean value, the resulting value is 0.6826.

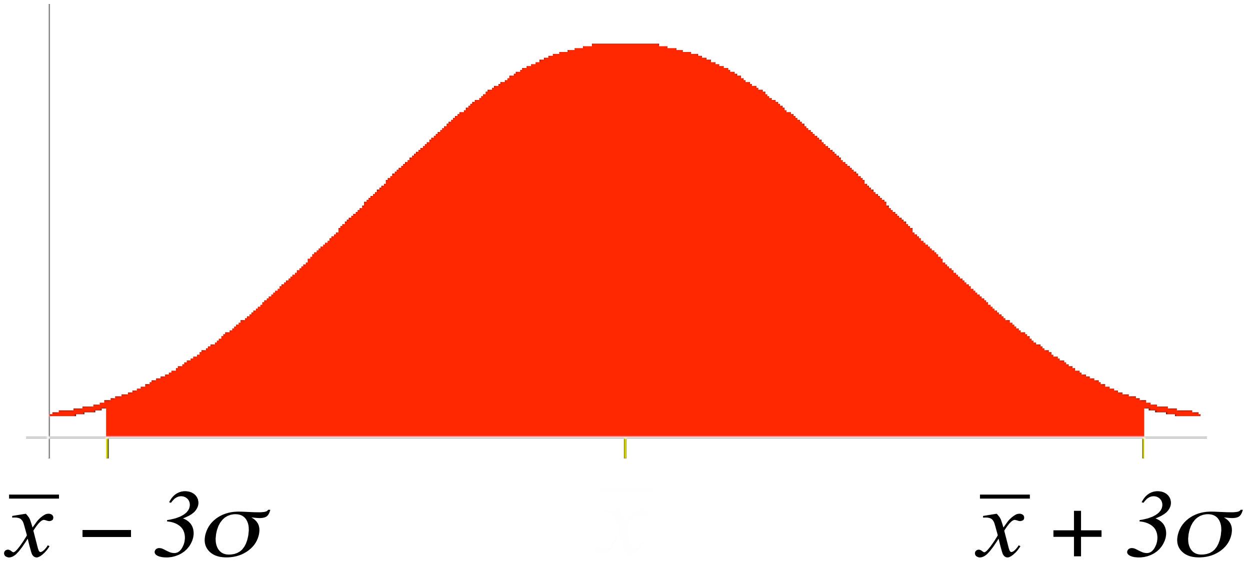
More on Probability Distribution Functions



- Integrating over a range within ± 2_ from the mean value, the resulting value is 0.954.

The probability for a reading to fall in the range ± 2_ of the mean is about 95 %.

More on Probability Distribution Functions



- Integrating over a range within ± 3_ from the mean value, the resulting value is 0.997.

The probability for a reading to fall in the range ± 3_ of the mean is almost 100 %.

Probability for Gaussian Distribution
(this is tabulated in any statistics book)

Probability	± value of the mean
50%	0.6754 _
68.3%	_
86.6%	1.5 _
95.4%	2_
99.7%	3_

The Lognormal distribution

- Most environmental exposure data has a lognormal distribution
- The same formulas and statistical methods that apply to a normal distribution can be used if we use the logarithum of the sample data
- For summary data, conversion formulas also may be used

$$\bar{x}_l = \ln(GM) \quad S_l = \ln(GSD)$$

$$\bar{x}_l = mean\ of\ \ln(data)$$

$$S_l = std.dev.\ of\ \ln(data)$$

Estimating Uncertainty

- Often we represent the uncertainty as a 95% confidence interval. *In other words,* if I state the uncertainty to be Δx with 95% conficence, I am suggesting that I am 95% sure that any reading x_i will be within the range $\pm \Delta x$ of the mean.

- The probability of a sample chosen at random of being within the range ± 2_ of the mean is about 95%.

95% Uncertainty ≈ twice the standard deviation

Δx ≈ 2_

Propagation of errors
RMS error: (Est of Std Dev or CV)

- **Addition or Subtraction: z = x + y or z = x – y**

$$\Delta z = \sqrt{(\Delta x)^2 + (\Delta y)^2 + \ldots}$$

- **Multiplication or Division: z = x y or z = x/y**

$$\frac{\Delta z}{z} = \sqrt{\left(\frac{\Delta x}{x}\right)^2 + \left(\frac{\Delta y}{y}\right)^2 + \ldots}$$

- **Products of powers:**

$z = x^m y^n$

$$\frac{\Delta z}{z} = \sqrt{\left(\frac{m\,\Delta x}{x}\right)^2 + \left(\frac{n\,\Delta y}{y}\right)^2 + \cdots}$$

Propagation of errors
Max error

- Addition or Subtraction: z = x + y or z = x – y

$$\Delta z = |\Delta x| + |\Delta y| + \ldots$$

- Multiplication or Division: z = x y or z = x/y

$$\frac{\Delta z}{z} = \frac{\Delta x}{x} + \frac{\Delta y}{y} + \ldots$$

- Products of powers:

$z = x^m y^n$

$$\frac{\Delta z}{z} = |m|\frac{\Delta x}{x} + |n|\frac{\Delta y}{y} + \ldots$$

Example

- Say we collected 50 well water samples containing Xylene, with an average value X, of 40 ± 16 ppb (95% CI).
- What does that mean?
- The ± 16 ppb would represent a 95% confidence interval.
- That is, if you randomly select many samples of water from this well you should find that 95% of the samples meet the stated limit of 40 ± 16 ppb.
- This does not mean that you couldn’t get a sample that has a xylene value of 16 ppb, it just means that it is very unlikely.

Example (cont'd)

- If we assume that variations in the water samples follow a normal distribution and the xylene concentration, X, is within the range 40 ± 16 ppb (95%CI).

  What is the standard deviation, _?

- Uncertainty ≈ 95% of confidence interval ≈ 2_

$$\Rightarrow \pm 16\,ppb \approx \pm 2\sigma \Rightarrow \boxed{\sigma \approx 8\,ppb}$$

Example (cont'd)

- If you assume that average = 40 ± 16 ppb (95%CI).

  Estimate the probability of findings a sample from this population Xylene concentration ≤ to 16 ppb.

$$E \leq 16\ ppb \quad \Rightarrow \quad E \in]-\infty, \bar{E} - 3\sigma]$$

Since _ = 8 ppb, a value of 16 ppb is: (40-16)/8 = 3 _ from the average value of 40

- Recall that a ±3 _ interval contains 99.7 % of values;
- Therefore:

$$\mathrm{P}(E < 16\,ppb) = \frac{100 - 99.7}{2} = 0.15\%$$

Data Quality Control and Control Charts

Outliers

- Consider an experiment in which we measure the weight of ten individual “identical” blank filter samples:
- The scale readings (in grams) are:

  2.41, 2.42, 2.43, 2.43, 2.44, 2.44, 2.45, 2.46, 2.47 and 4.85

- The 4.85 g reading seems too high and likely represents an error in your measurement, but *what if the readings were 2.50 or 2.51 g ?*
- At what point can you flag or toss out suspect readings?

Outliers: Chauvenet's Criterion

- Of a group of *n* readings, a reading may be rejected if the probability of obtaining that particular reading is less than *1/2n*. The probability distribution used is the normal distribution.
- It is applied *once* to the complete data set, and readings meeting the criterion are eliminated.
- The mean and standard deviation may then be recalculated using the reduced data set.

Chauvenet's criterion

- The values x_i which are outside of the range

$$\overline{x} \pm C\sigma$$

are declared outliers (errors) and can be excluded for the analysis.

- Excluding outliers can be controversial; proceed with caution!

Number of sample	C
5	1.65
10	1.96
15	2.13
25	2.33
50	2.57
100	2.81

Methodology for discarding outlier:

1. After running an experiment, sort the outcomes from lowest to highest value.

   The suspect outliers will then be at the top and/or the bottom of your list

2. Calculate the mean value and the standard deviation.

3. Using Chauvenet's criterion, discard outliers.

4. Recalculate the mean value and the standard deviation of smaller sample and STOP. (Do not repeat!)

Data Quality Control – example

1. The readings (in grams) were: 2.41, 2.42, 2.43, 2.43, 2.44, 2.44, 2.45, 2.46, 2.47 and 4.85
2. Calculate $\overline{m} = 2.68\,g \quad and \quad \sigma = 0.76\,g$
3. Apply Chauvenet's criterion (for n=10, C=1.96): Any values, m_i, outside the range:

$$\overline{m} - C\sigma \leq m_i \leq \overline{m} + C\sigma \;\Rightarrow\; 1.19\,g \leq m_i \leq 4.17\,g$$

   is an outliers and should be discarded.

4. Clearly the 4.85 value is an outlier. No other points are.

Control Charts

- Control charts (Shewhart charts) are a useful graphical tool for performing quality control analysis developed in the 1920s by Dr. Walter A. Shewhart of the Bell Telephone Labs.
- Control charts show a graphical display of a quality characteristic that's measured from a sample versus the sample number (or time).
- Control charts contain:
  - a center line that represents the average value of the measured quality characteristic (the in-control state);
  - Two other horizontal lines, called the upper control limit (UCL) and the lower control limit (LCL) (the out of control state);
- The control limits are chosen so that if the process is in statistical control, nearly all of the sample points will fall between them. Typically this is 3*Std. Dev. of the measured quantity. As long as the points plot within the control limits, the process is assumed to be in control, and no action is necessary.

Control Charts - 2

- There are many types of charts for sequential QC data;
  - Control charts for individual samples or X charts
  - Control charts for sample means or $\overline{X}$ charts
  - A control chart for variability, using the sample range (R charts) or standard deviation (Sigma charts)
- All charts have the same general form:

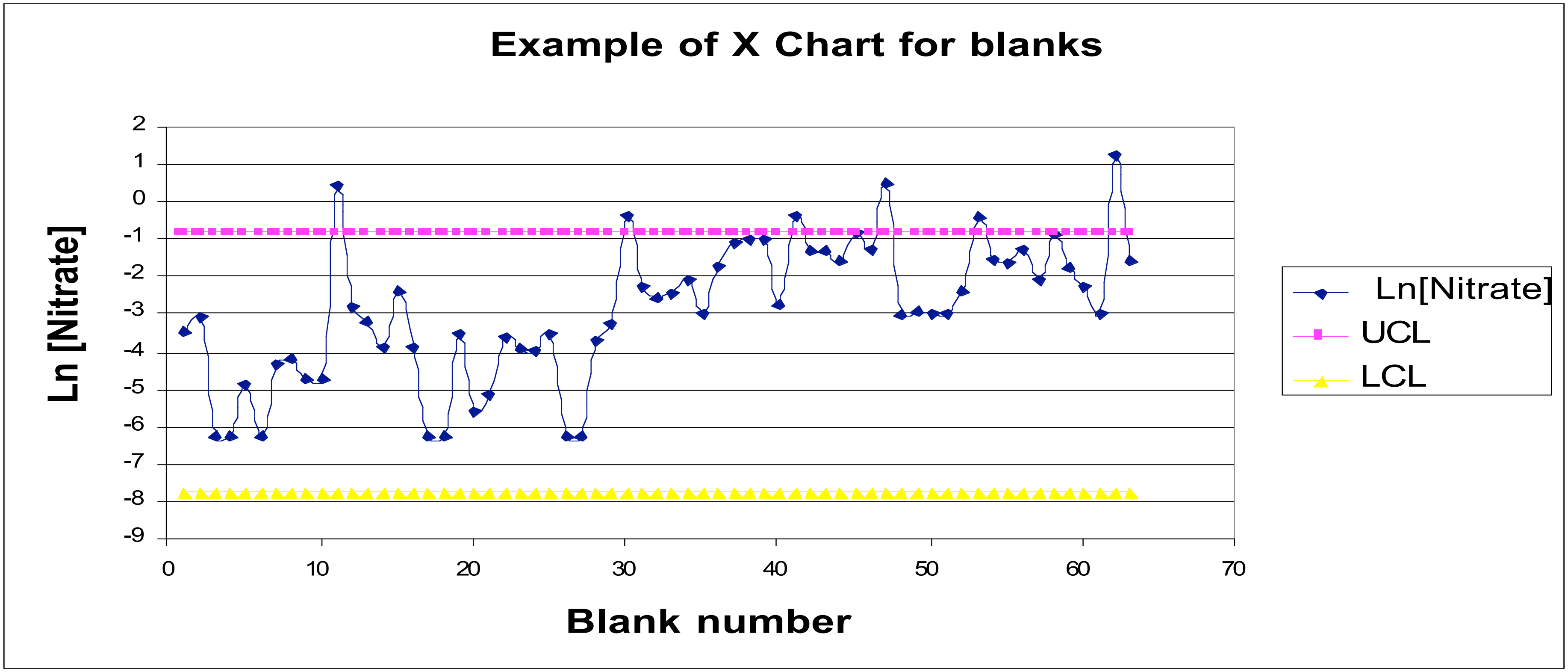
$$\overline{X} = sample\ mean$$

$$UCL = \overline{X}_n + A \cdot S_n$$

$$LCL = \overline{X}_n - A \cdot S_n$$

- Where S_n is the measure of variability under normal conditions

Xi Control Chart



Moving Range Chart of individual data (Xi)

A *moving range average* is calculated by taking pairs of data (x1,x2), (x2,x3), (x3,x4),..., (xn-1,xn), taking the sum of the absolute value of the differences between them and dividing by the number of pairs (one less than the number of pieces of data). This is shown mathematically as:

$$MRBAR = \frac{1}{n-1}\sum_{i=1}^{n-1}\left|x_{i+1} - x_i\right|$$

Xi Chart- continued

An estimate of the process standard deviation is given by:

$$\hat{\sigma} = \frac{MRBAR}{1.128}$$

The three sigma control limits become:

$$UCL = XBAR + 2.66 * MRBAR$$

$$LCL = XBAR - 2.66 * MRBAR$$

Plot the centerline XBAR, LCL, UCL, and the process X(i)

- Note XBAR=mean of data

Data Analysis: Outline

1. Examine the data for consistency:
   - Points that do not appear proper should be flagged / eliminated.
   - Check the entire experimental procedure if there are too many “inconsistent data”.
2. Plot or check standards for consistency.
3. Perform a statistical analysis of data where appropriate (& validate assumptions).
4. Estimate the uncertainties in the results.