



We will begin momentarily at 2pm ET



Slides available now! Recordings available as an exclusive ACS member benefit.

www.acs.org/acswebinars

Contact ACS Webinars[®] at acswebinars@acs.org

1



Benefits of ACS Membership



Chemical & Engineering News (C&EN)
The preeminent weekly news source.



NEW! Free Access to ACS Presentations on Demand[®]
ACS Member only access to over 1,000 presentation recordings from recent ACS meetings and select events.



NEW! ACS Career Navigator
Your source for leadership development, professional education, career services, and much more.

<http://bit.ly/benefitsACS>

2

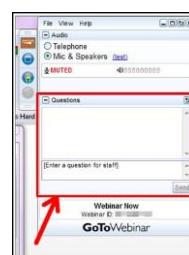


facebook.com/acswebinars
 @acswebinars
 youtube.com/acswebinars

Search for "acswebinars" and connect!

3

Have Questions?



Type them into questions box!

"Why am I muted?"

Don't worry. Everyone is muted except the presenter and host. Thank you and enjoy the show.

Contact ACS Webinars® at acswebinars@acs.org

4

Let's get Social...post, tweet, and link to ACS Webinars during today's broadcast!



facebook.com/acswebinars



[@acswebinars](https://twitter.com/acswebinars)



Search for "acswebinars" and connect!

5



Learn from the best and brightest minds in chemistry! Hundreds of webinars presented by subject matter experts in the chemical enterprise.

Recordings are available to current ACS members one week after the Live broadcast date. www.acs.org/acswebinars

Broadcasts of ACS Webinars® continue to be available to the general public LIVE every Thursday at 2pm ET!

www.acs.org/acswebinars

6



Have you discovered the missing element?



<http://bit.ly/benefitsACS>

Find the many benefits of ACS membership!

7

How has ACS Webinars® benefited you?



“This ACS Webinar showed me all the work and scientific knowledge that goes into the development of new drugs to treat malignancies that affect us all as humans. It gives me a better understanding on why is difficult to achieve good results all the time. This is just one of those successful stories.”

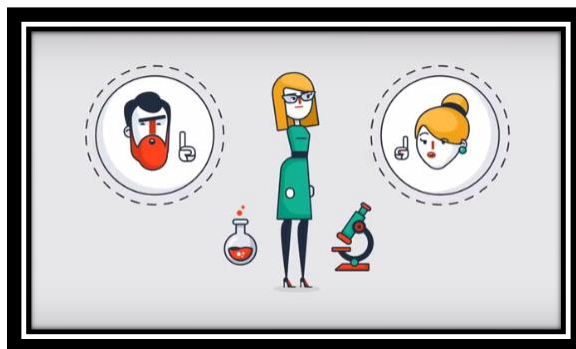
Fan of the Week

Francisco J. Ramirez
Chemist Supervisor - Organic Unit
Tucson Water Quality Laboratory
ACS member for 21 years strong!

<http://bit.ly/ACSvismodegib>

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org ⁸

An individual development planning tool for you!



- Know your career options
- Develop strategies to strengthen your skills
- Map a plan to achieve your career goals

ChemIDP.org

9

Upcoming ACS Webinars

www.acs.org/acswebinars



Thursday, September 14, 2017



How to Create Sustainable Product Design that Satisfies Production Demand and Eco-Awareness

Co-produced with ACS Green Chemistry Institute

Eric Beckman, Professor of Engineering, *University of Pittsburgh*

Joseph Fortunak, Professor of Chemistry, *Howard University*

Thursday, September 21, 2017



The Fantastic Phenols: Discover the Compounds That Give Wine its Allure

Co-produced with C&EN

Andrew Waterhouse, Professor of Enology, *UC Davis*

Bill Courtney, Grant Specialist, *Washington University*

Contact ACS Webinars[®] at acswebinars@acs.org

10

What is the Heroes of Chemistry Award?



“Their creative spirit, commitment to excellence, and technical talent are tangible evidence of the ACS Vision, ‘Improving people’s lives through the transforming power of chemistry.’”

ACS President Allison Campbell

Heroes of Chemistry is an annual award sponsored by the American Chemical Society that recognizes talented industrial chemical scientists whose work has led to the development of successful commercialized products ingrained with chemistry for the benefit of humankind.

Email chemhero@acs.org or Visit www.acs.org/heroes

11

ACS Professional Education Course with Stan and Steve!



Experimental Design for Productivity and Quality in Research & Development

<http://bit.ly/acsProEd1>

- Basic concepts of experimental design
- Strengths and limitations of popular experimental design techniques
- Applicability of common designs
- Determining which experimental designs are appropriate or inappropriate for particular situations

Process Capability: What It Is and How To Achieve It

<http://bit.ly/acsProEd2>

- Why measurement variability is so important in process capability studies
- How to estimate measurement variability
- How to separate true process variability from apparent process variability to understand the true capability of a process
- Why setting specifications based on fitness for use is fundamental
- How to understand the two types of serious risk associated with setting specifications based on historical data

Statistical Analysis of Laboratory Data

<http://bit.ly/acsProEd3>

- How to apply statistical process control charts to measurement processes.
- How to correctly use outlier tests and when not to use them.
- How to know what statistical test to use when.
- How to recognize and reduce different types of errors.
- How to set in-house specifications.
- How to understand the influence of sample size on statistical significance and power.

<http://proed.acs.org/course-catalog/courses>

12

Statistical Analysis and Experimental Design



In this short webinar, you will learn to use:

1. Statistical analysis to create a 95% confidence interval for a true mean μ
2. Statistical testing to decide if you are probably between specifications
3. Experimental design to end up with a tighter, more useful confidence interval (sometimes expensive)
4. Improved measurement to end up with a tighter, more useful confidence interval (often cheaper)



“Chemistry in Numbers: How to Master the Statistical Analysis of Laboratory Data”
Session 8 of the 2017 Industry Science Series



Stanley Deming
President, Statistical Designs and
Professor Emeritus,
University of Houston



Stephen Morgan
Professor, Department of
Chemistry & Biochemistry,
University of South Carolina



Bryan Tweedy
Manager,
Office of Professional Education,
American Chemical Society

Slides available now! Recordings are an exclusive ACS member benefit.

www.acs.org/acswebinars

This ACS Webinar was co-produced by ACS Industry Member Programs,
C&EN, and ACS Committee on Corporation Associates

Statistical Analysis and Experimental Design

In this short webinar, you will learn to use:

1. Statistical analysis to create a 95% confidence interval for a true mean μ
2. Statistical testing to decide if you are probably between specifications
3. Experimental design to end up with a tighter, more useful confidence interval (sometimes expensive)
4. Improved measurement to end up with a tighter, more useful confidence interval (often cheaper)



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 15

Challenge Question #1: Gaussian Statistics

For a Gaussian distribution of data, how many standard deviations do you have to go on either side of the mean to include 95.00% of the data?

- A. 0.67
- B. 1.04
- C. 1.96
- D. 2.00
- E. 2.54
- F. None of the above.



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 16



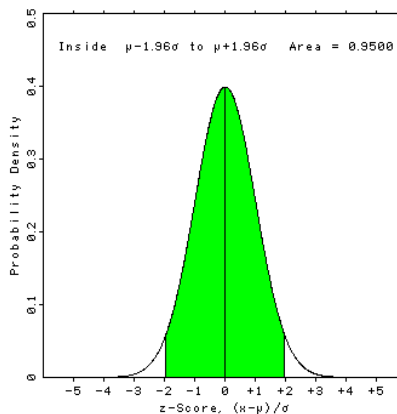
https://commons.wikimedia.org/wiki/File:Carl_Friedrich_Gauss.jpg

Statistical Analysis: Gaussian Areas and z values

When data are normally distributed, 95% of the values will lie inside the region centered at the true mean μ , and extending 1.96 standard deviations σ on either side of the true mean μ .

z values measure how many standard deviations you are away from the mean. If $z = 1.00$, you're 1.00 standard deviation above the mean. If $z = -1.96$, you're 1.96 standard deviations below the mean.

Thus, 95% of the values will lie between z values of -1.96 and +1.96.



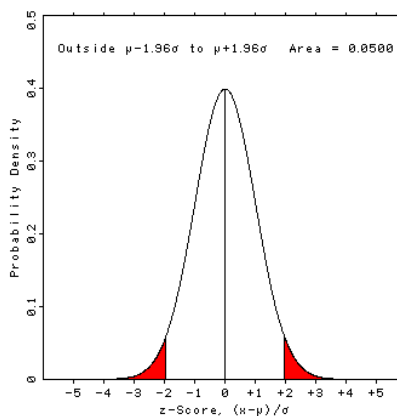
For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 17

Statistical Analysis: Gaussian Areas

When data are normally distributed, only 5% of the values will lie outside the region centered at the true mean μ and extending 1.96 standard deviations σ on either side of the true mean μ .

An equivalent way of saying this is that only 5% of the values will lie beyond z values of -1.96 and +1.96.

Half of the excluded area lies in the left tail; the other 2.5% of the area lies in the right tail.



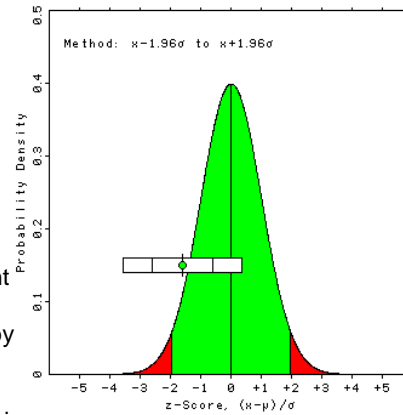
For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 18

Statistical Analysis: The Procedure Applied

Here is a procedure:

**For a given data point,
draw an interval extending
plus and minus 1.96 standard
deviations
from the data point**

Imagine that we select at random a data point from a distribution of data that is normally distributed. That data point might be shown by the single green dot in the figure at the right.



This procedure generates the interval shown in the figure.



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 19

Statistical Analysis: The Procedure Applied

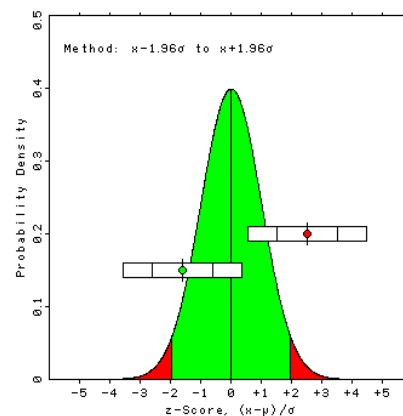
Imagine that we select at random a second data point from the same normal distribution.

That second data point and its interval might be shown by the upper red dot in the figure at the right.

In this example, the two intervals are different in an important way:

one interval includes μ

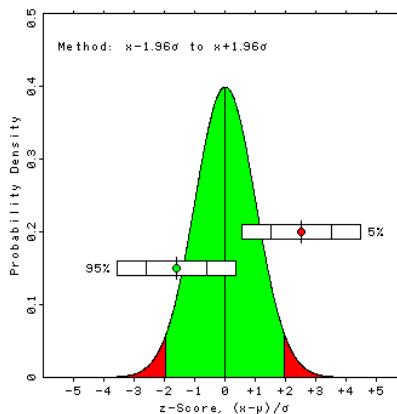
the other interval does not include μ



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 20

Statistical Analysis: The Procedure Applied

If we select at random a very large number of data points and apply the procedure to each of them, then we would expect that approximately 95% of the intervals would include μ , and approximately 5% of the intervals would not include μ .



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 21

Statistical Analysis: The Confidence Interval

These statements about the procedure apply to any data point taken from any Gaussian distribution, whether we know the value of the true mean μ or not. All we need to know is σ .

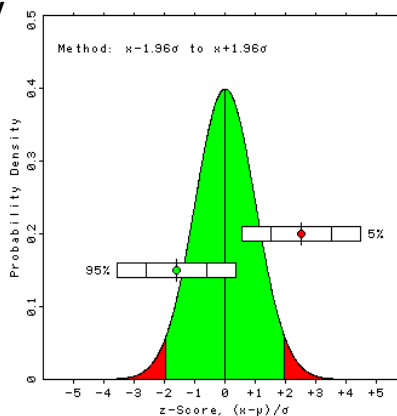
When we talk about confidence, we are expressing our confidence in the procedure.

The two-sided or two-tailed confidence interval (CI) for μ can be expressed as

$$(x - z_{w/2}\sigma) \leq \mu \leq (x + z_{w/2}\sigma)$$

or

$$\text{CI for } \mu = x \pm z_{w/2}\sigma$$



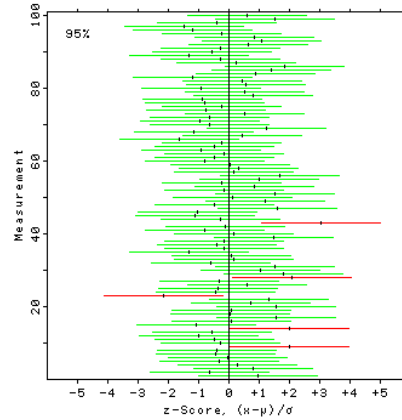
For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 22

Statistical Analysis: 95% Confidence Intervals

The figure at the right shows the results of drawing at random 100 data points from a z distribution and applying the 95% confidence interval procedure.

As shown in the figure, the expected 95 out of 100 confidence intervals include μ , and the expected 5 out of 100 confidence intervals do not include μ .

(It is rare that a relatively small sample of 100 data points will give the exact expectation values. Figures in this module will show the exact expectation values. In real life, this won't always happen.)



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 23

Challenge Question #2: Confidence Intervals

If you want more than 95% of your confidence intervals to include the true mean μ , then the z multiplier used to generate the confidence interval must be:

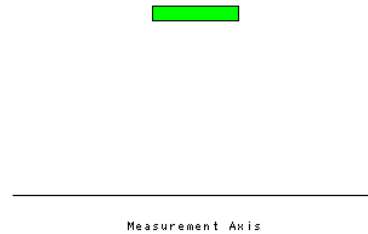
- A. less than 1.54
- B. greater than 1.96



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 24

Statistical Testing: Confidence Interval Details

In the figure at the right, the horizontal axis is a measurement axis. The vertical dimension has no meaning. The rectangular box represents a two-sided confidence interval for a population parameter (e.g., σ or μ).



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 25

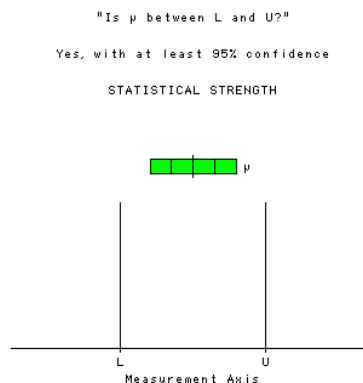
Statistical Testing: Testing For "Between"

Sometimes we want to know if a true mean μ is between two specified values — a lower specification L, and an upper specification U.

The statistical question then becomes, "Is μ between L and U?"

In this example, because the confidence interval for μ is both greater than L and less than U, we can state with at least 95% confidence that μ is probably between the values.

There is STATISTICAL STRENGTH in this statement.



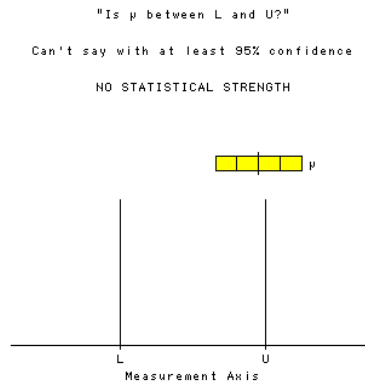
For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 26

Statistical Testing: Testing For "Between"

In this example, the confidence interval for μ includes the upper specification U. The true mean μ might be below U, or it might be above U. If we ask the question, "Is the true mean μ between the values L and U?" then we must answer, "No, we can't say with at least 95% confidence that μ is between L and U."

In this case, we can't say much more.

There is NO STATISTICAL STRENGTH in this statement.



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 27

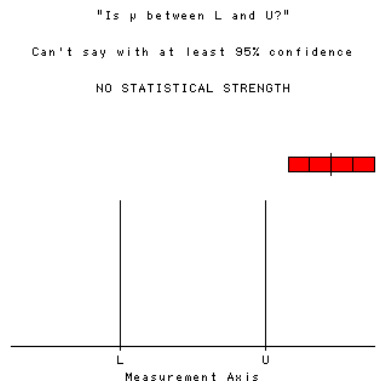
Statistical Testing: Testing For "Between"

For this example, again we must answer, "No, we can't say with at least 95% confidence that μ is between L and U."

There is NO STATISTICAL STRENGTH — for the question that was asked.

With this result we could say more. We can say something about the opposite of the sense of the question. We can be at least 95% confident that μ is outside the values.

But that isn't the question that was asked.



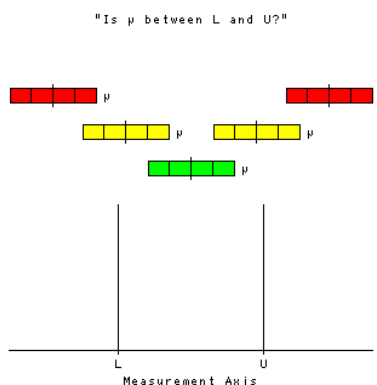
For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 28

Statistical Testing: Testing For "Between"

To summarize: it is appropriate to use a two-sided confidence interval to see if μ is between L and U at some level of confidence. There are two possible outcomes:

- 1) We **can** say that μ is between L and U:
 $\mu > L$ and $\mu < U$
- 2) We **can't** say that μ is between L and U

The second outcome does not necessarily mean that μ is outside the specifications.

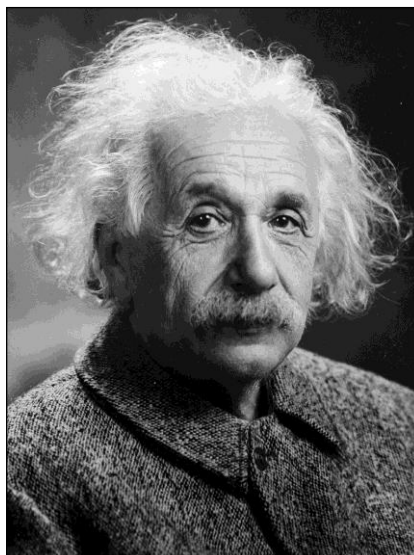


For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 29

Challenge Question #3: An Uncertain World

A 95% confidence interval for the mean μ is calculated based on a set of eight replicate measurements. Which of the following statements is not true?

- A. 95% of all future measurements will be within this interval.
- B. The mean of the eight replicate measurements is inside the confidence interval.
- C. The confidence interval might not contain μ .



https://commons.wikimedia.org/wiki/Category:Albert_Einstein#/media/File:Albert_Einstein_Head.jpg

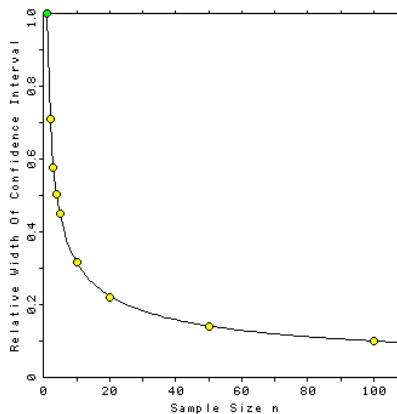
For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 30

Experimental Design: Mathematical Description

The width of the confidence interval depends on the number of measurements that go into determining the mean. If the true standard deviation σ is known, then

$$\text{CI for } \mu = \bar{x} \pm z_{\alpha/2} \sigma_{\bar{x}} = \bar{x} \pm \frac{z_{\alpha/2} \sigma}{\sqrt{n}}$$

The width of the confidence interval decreases by a factor of $1/\sqrt{n}$.



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 31

Experimental Design: Sample Size

A simple question that researchers frequently ask statisticians is,

"How big should my sample size be?"

And the researchers expect a simple answer ("Four!").

But statisticians always reply that there is no simple answer — it depends.

It depends on how small the desired standard deviation of the mean must be, and it depends on how large the standard deviation of the raw data is. And now you can figure out how big your sample size should be — you don't have to ask a statistician.



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 32

Hard Quiz #1: Sample Size

Problem: The percentage of toluene in 1000 chemical samples of gasoline is to be estimated by making multiple gas chromatographic measurements for each gasoline sample and using the statistical sample mean as an estimate of the toluene percentage. Previous experience has indicated that individual measurements produce a confidence interval that is 0.2% toluene wide.

How many measurements (n) must be taken to make the confidence interval less than or equal to 0.05% toluene?

"How big should my sample size be?"



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 33

Hard Quiz #1: Sample Size (Answer)

Answer: The sample size can be found from the relationship

$$\text{width for } n = (\text{width for } n = 1) / \sqrt{n}$$

$$0.05 \% \text{ toluene} = 0.2 \% \text{ toluene} / \sqrt{n}$$

$$\sqrt{n} = 0.2 \% \text{ toluene} / 0.05 \% \text{ toluene} = 4$$

$$n = 16$$



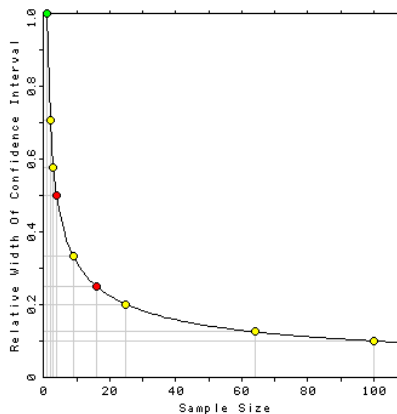
For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 34

Experimental Design: Budgetary Considerations

The $1/\sqrt{n}$ effect is like a "statistical sledgehammer" — it is a brute-force way of making the confidence interval of the mean as small as desired, simply by making n sufficiently large.

In the previous problem, there were 1000 gasoline samples to be analyzed, each involving 16 measurements, for a total of 16,000 gas chromatographic determinations. That can be expensive!

Is there a less expensive way to reduce the standard deviation of the mean? Yes!



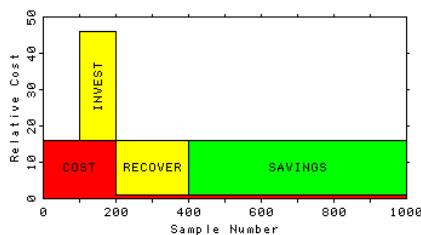
For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 35

Improved Measurement: Budgetary Considerations

Instead of using the current measurement method with its inherent σ of 0.2% toluene, acquire a better measurement method with an inherent σ of 0.05% toluene. Then

$$\begin{aligned} \text{width for } n &= (\text{width for } n = 1) / \sqrt{n} \\ 0.05 \% \text{ toluene} &= 0.05 \% \text{ toluene} / \sqrt{n} \\ \sqrt{n} &= 0.05 \% / 0.05 \% = 1 \\ n &= 1 \end{aligned}$$

**Do not try to do with statistics
what you can do cheaper
with improved measurement**



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 36

Statistical Analysis and Experimental Design

In this short webinar, you have learned to use:

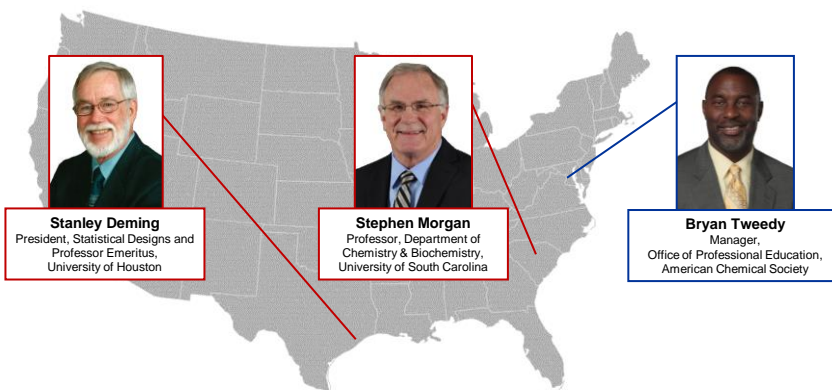
1. Statistical analysis to create a 95% confidence interval for a true mean μ
2. Statistical testing to decide if you are probably between specifications
3. Experimental design to end up with a tighter, more useful confidence interval (sometimes expensive)
4. Improved measurement to end up with a tighter, more useful confidence interval (often cheaper)



For participants in ACS Webinar 7 September 2017. DO NOT COPY Copyright © 2017 by Stanley N. Deming and Stephen L. Morgan. All rights reserved. Slide 37



“Chemistry in Numbers: How to Master the Statistical Analysis of Laboratory Data”
Session 8 of the 2017 Industry Science Series



Slides available now! Recordings are an exclusive ACS member benefit.

www.acs.org/acswebinars

This ACS Webinar was co-produced by ACS Industry Member Programs,
C&EN, and ACS Committee on Corporation Associates

38

ACS Professional Education Course with Stan and Steve!



Experimental Design for Productivity and Quality in Research & Development

<http://bit.ly/acsProEd1>

- Basic concepts of experimental design
- Strengths and limitations of popular experimental design techniques
- Applicability of common designs
- Determining which experimental designs are appropriate or inappropriate for particular situations

Process Capability: What It Is and How To Achieve It

<http://bit.ly/acsProEd2>

- Why measurement variability is so important in process capability studies
- How to estimate measurement variability
- How to separate true process variability from apparent process variability to understand the true capability of a process
- Why setting specifications based on fitness for use is fundamental
- How to understand the two types of serious risk associated with setting specifications based on historical data

Statistical Analysis of Laboratory Data

<http://bit.ly/acsProEd3>

- How to apply statistical process control charts to measurement processes.
- How to correctly use outlier tests and when not to use them.
- How to know what statistical test to use when.
- How to recognize and reduce different types of errors.
- How to set in-house specifications.
- How to understand the influence of sample size on statistical significance and power.

<http://proed.acs.org/course-catalog/courses>

39

Upcoming ACS Webinars www.acs.org/acswebinars



Thursday, September 14, 2017



How to Create Sustainable Product Design that Satisfies Production Demand and Eco-Awareness

Co-produced with ACS Green Chemistry Institute

Eric Beckman, Professor of Engineering, *University of Pittsburgh*

Joseph Fortunak, Professor of Chemistry, *Howard University*

Thursday, September 21, 2017



The Fantastic Phenols: Discover the Compounds That Give Wine its Allure

Co-produced with C&EN

Andrew Waterhouse, Professor of Enology, *UC Davis*

Bill Courtney, Grant Specialist, *Washington University*

Contact ACS Webinars[®] at acswebinars@acs.org

40

How has ACS Webinars® benefited you?



“This ACS Webinar showed me all the work and scientific knowledge that goes into the development of new drugs to treat malignancies that affect us all as humans. It gives me a better understanding on why is difficult to achieve good results all the time. This is just one of those successful stories.”

Fan of the Week

Francisco J. Ramirez
Chemist Supervisor - Organic Unit
Tucson Water Quality Laboratory
ACS member for 21 years strong!

FREE WEBINAR | AUGUST 3 AT 2PM ET
DISCOVERING VISMODEGIB
IN THE FIGHT AGAINST SKIN CANCER
WITH DAN SUTHERLIN
Contentmark

<http://bit.ly/ACSvismodegib>

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org ⁴¹



facebook.com/acswebinars
@acswebinars
youtube.com/acswebinars

Stay connected...
Email us!
acswebinars@acs.org

ACS Webinars®
CLICK • WATCH • LEARN • DISCUSS
www.acs.org/acswebinars

Search for “acswebinars” and connect!

42



Benefits of ACS Membership



Chemical & Engineering News (C&EN)

The preeminent weekly news source.



NEW! Free Access to ACS Presentations on Demand®

ACS Member only access to over 1,000 presentation recordings from recent ACS meetings and select events.



NEW! ACS Career Navigator

Your source for leadership development, professional education, career services, and much more.

<http://bit.ly/benefitsACS>

43



ACS Webinars® does not endorse any products or services. The views expressed in this presentation are those of the presenter and do not necessarily reflect the views or policies of the American Chemical Society.



Mike

Russell

Erik

Kaye

John

Contact ACS Webinars® at acswebinars@acs.org

44