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

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.

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

facebook.com/acswebinars

@acswebinars

Search for “acswebinars” and connect!

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!
Have you discovered the missing element?


Find the many benefits of ACS membership!

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!


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

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 acswininars@acs.org
What is the Heroes of Chemistry Award?

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

ACS Professional Education Course with Stan and Steve!

Experimental Design for Productivity and Quality in Research & Development
- 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

http://bit.ly/acsProEd1

Process Capability: What It Is and How To Achieve It
- 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
- 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
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 $\mu$

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 $\mu$
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)

**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.
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 \( \mu \), and extending 1.96 standard deviations \( \sigma \) on either side of the true mean \( \mu \).

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.

Statistical Analysis: Gaussian Areas

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

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.
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.

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 $\mu$

the other interval does not include $\mu$
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 $\mu$, and approximately 5% of the intervals would not include $\mu$.

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 $\mu$ or not. All we need to know is $\sigma$.

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

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

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

or

CI for $\mu = x \pm z_{\alpha/2}\sigma$
**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 \( \mu \), and the expected 5 out of 100 confidence intervals do not include \( \mu \).

(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.)

---

**Challenge Question #2: Confidence Intervals**

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

A. less than 1.54

B. greater than 1.96
**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., $\sigma$ or $\mu$).

---

**Statistical Testing:** Testing For "Between"

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

The statistical question then becomes, "Is $\mu$ between $L$ and $U$?"

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

There is STATISTICAL STRENGTH in this statement.
Statistical Testing: Testing For "Between"

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

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

There is NO STATISTICAL STRENGTH in this statement.

Statistical Testing: Testing For "Between"

For this example, again we must answer, "No, we can't say with at least 95% confidence that $\mu$ 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 $\mu$ is outside the values.

But that isn't the question that was asked.
**Statistical Testing**: Testing For "Between"

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

1) We **can** say that $\mu$ is between L and U:
   
   $\mu > L$ and $\mu < U$

2) We **can't** say that $\mu$ is between L and U

The second outcome does not necessarily mean that $\mu$ is outside the specifications.

---

**Challenge Question #3**: An Uncertain World

A 95% confidence interval for the mean $\mu$ 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 $\mu$. 
**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 $\sigma$ is known, then

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

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

**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.
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?"

Hard Quiz #1: Sample Size (Answer)

Answer: The sample size can be found from the relationship

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

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

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

\[
n = 16
\]
**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!

---

**Improved Measurement:** Budgetary Considerations

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

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

0.05% toluene = \frac{0.05%}{\sqrt{n}}

$$
\sqrt{n} = \frac{0.05 \%}{0.05 \%} = 1
$$

$$
n = 1
$$

---

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

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)
ACS Professional Education Course with Stan and Steve!

Experimental Design for Productivity and Quality in Research & Development
- 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
- 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
- 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

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
“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 it is difficult to achieve good results all the time. This is just one of those successful stories.”

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


How has ACS Webinars® benefited you?

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

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

Search for “acswebinars” and connect!
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.


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.

Contact ACS Webinars ® at acswebinars@acs.org