

Back to the pipette example

- Imagine that you are making dynamite
 - If you put less than 9.982 mL of a reagent, it will not explode
 - If you put more than 10.015 mL it will blow up in your face
- What is the probability for these events to occur?

Trial	Volume (ml)
1	9.991
2	10.005
3	9.983

$$\begin{aligned}\bar{V}_1 &= 9.993 \text{ mL} \\ S_1 &= 0.011 \text{ mL} \\ n_1 &= 3\end{aligned}$$

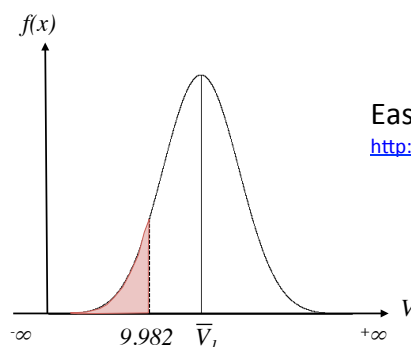
- Based on 3 measurements, we estimate that there is a 68% chance that we will deliver between $\bar{V}_1 - S_1 = 9.982 \text{ mL}$ and $\bar{V}_1 + S_1 = 10.004 \text{ mL}$ of reagent
- This does not tell me if the dynamite is bad or if a worker will be killed!

Bad dynamite

- We need to find:

$$P(V < 9.982 \text{ mL}) = \int_{-\infty}^{9.982} \frac{1}{S_1 \sqrt{2\pi}} e^{-\frac{(V - \bar{V}_1)^2}{2S_1^2}} dV$$

$$\begin{aligned}\bar{V}_1 &= 9.993 \text{ mL} \\ S_1 &= 0.011 \text{ mL} \\ n_1 &= 3\end{aligned}$$



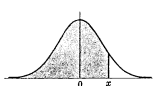
Easiest way is to use statistics tables:
<http://faculty.washington.edu/baneyx/436/Tables.pdf>

Approach

TABLE 47

AREAS UNDER THE STANDARD NORMAL CURVE
from $-\infty$ to z

$$\phi(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^z e^{-t^2/2} dt$$



NOTE: $\text{erf}(z) = 2\Phi(z\sqrt{2}) - 1$

2nd decimal

z	0	1	2	3	4	5	6	7	8	9
0.0	.5000	.5040	.5080	.5120	.5160	.5199	.5239	.5279	.5319	.5359
0.1	.5398	.5438	.5478	.5517	.5557	.5596	.5636	.5675	.5714	.5754
0.2	.5793	.5832	.5871	.5910	.5948	.5987	.6026	.6064	.6103	.6141
0.3	.6179	.6217	.6255	.6293	.6331	.6368	.6406	.6443	.6480	.6517
0.4	.6554	.6591	.6628	.6664	.6700	.6736	.6772	.6808	.6844	.6879
0.5	.6915	.6950	.6985	.7019	.7054	.7088	.7123	.7157	.7190	.7224
0.6	.7258	.7291	.7324	.7357	.7389	.7422	.7454	.7486	.7518	.7549
0.7	.7580	.7612	.7642	.7673	.7704	.7734	.7764	.7794	.7823	.7852
0.8	.7881	.7910	.7939	.7967	.7996	.8023	.8051	.8078	.8106	.8133
0.9	.8159	.8186	.8212	.8238	.8264	.8289	.8315	.8340	.8365	.8389
1.0	.8413	.8438	.8461	.8485	.8508	.8531	.8554	.8577	.8599	.8621
1.1	.8642	.8665	.8686	.8708	.8729	.8749	.8770	.8790	.8810	.8830
1.2	.8849	.8869	.8888	.8907	.8925	.8944	.8962	.8980	.8997	.9015
1.3	.9032	.9049	.9066	.9082	.9099	.9115	.9131	.9147	.9162	.9177
1.4	.9192	.9207	.9222	.9236	.9251	.9265	.9279	.9292	.9306	.9319
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1.6	.9452	.9463	.9474	.9484	.9495	.9505	.9515	.9525	.9535	.9545
1.7	.9554	.9564	.9573	.9582	.9591	.9599	.9608	.9616	.9625	.9633
1.8	.9641	.9649	.9656	.9664	.9671	.9678	.9686	.9693	.9699	.9706
1.9	.9713	.9719	.9726	.9732	.9738	.9744	.9750	.9756	.9761	.9767
2.0	.9772	.9778	.9783	.9788	.9793	.9798	.9803	.9808	.9812	.9817
2.1	.9821	.9826	.9830	.9834	.9838	.9842	.9846	.9850	.9854	.9857
2.2	.9861	.9864	.9868	.9871	.9875	.9878	.9881	.9884	.9887	.9890

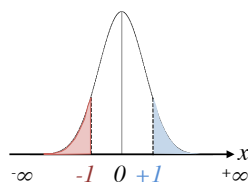
Need $P(V < 9.982 \text{ mL})$ knowing:

$$\bar{V}_1 = 9.993 \text{ mL}; S_1 = 0.008 \text{ mL}; n_1 = 3$$

Set:

$$x = \frac{(V - \bar{V}_1)}{S_1} = \frac{9.982 - 9.993}{0.011} = -1$$

This is not provided but the distribution is symmetrical:

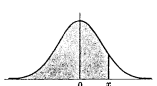


Approach

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from $-\infty$ to z

$$\phi(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^z e^{-t^2/2} dt$$

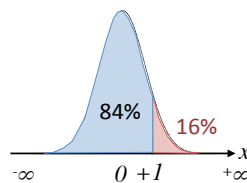


NOTE: $\text{erf}(z) = 2\Phi(z\sqrt{2}) - 1$

2nd decimal

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2.1	.9821	.9826	.9830	.9834	.9838	.9842	.9846	.9850	.9854	.9857
2.2	.9861	.9864	.9868	.9871	.9875	.9878	.9881	.9884	.9887	.9890

The area from $-\infty$ to $x = 1.00$ is 0.8413



We want what is left over, and $P_{\text{bad}} = 1 - 0.8413 = 0.1587 \approx 0.16$

- There is a 16% chance that the dynamite will be bad

Dangerous dynamite

- What about the probability for blowing up: $P(V > 10.015 \text{ mL})$

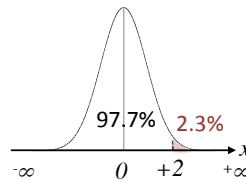
$$P(V > 10.015 \text{ mL}) = 1 - \int_{-\infty}^{10.015} \frac{1}{S_1 \sqrt{2\pi}} e^{-\frac{(V-\bar{V}_1)^2}{2S_1^2}} dV$$

$$x = \frac{(V - \bar{V}_1)}{S_1} = \frac{10.015 - 9.993}{0.011} = 2$$

TABLE 47	AREAS UNDER THE STANDARD NORMAL CURVE From $-\infty$ to x $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-t^2/2} dt$	
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NOTE: $\text{erf}(x) = 2\Phi(x\sqrt{2}) - 1$

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2.2	.9861	.9864	.9868	.9871	.9875	.9878	.9881	.9884	.9887	.9890



- There is a 2.3% chance of explosion

Dangerous dynamite

- For such an important outcome, do 9 replicates

$$\bar{V}_2 = 9.997 \text{ mL}$$

$$S_2 = 0.008 \text{ mL}$$

$$n_2 = 9$$

Bad or inactive: $P(V < 10.015 \text{ mL})$

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2.2	.9861	.9864	.9868	.9871	.9875	.9878	.9881	.9884	.9887	.9890

$$x = \frac{(V - \bar{V}_2)}{S_2} = \frac{10.015 - 9.997}{0.008} = 2.25$$

Area is 0.9878

$$P_{\text{blowup}} = 1 - 0.9878 = 1.23\%$$

Dangerous dynamite

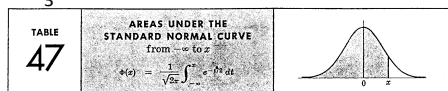
- What if you did 1000 replicates?

$$\bar{V}_3 = 10.001 \text{ mL}$$

$$S_3 = 0.009 \text{ mL}$$

$$n_3 = 1000$$

Bad or inactive: $P(V < 10.015 \text{ mL})$



NOTE: $\text{erf}(z) = 2\Phi(z\sqrt{2}) - 1$

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$$x = \frac{(V - \bar{V}_2)}{S_2} = \frac{10.015 - 10.001}{0.009} = 1.56$$

Area is 0.9406

$$P_{\text{blowup}} = 1 - 0.9406 = 6\%$$

- The more replicates you do, the more confident you are that \bar{X} and S are good estimates of μ and σ

Confidence testing

- I would like to report how confident I am in my data
 - Example: "I am 95% confident that the measured volume of 9.993 mL is within $\pm \lambda$ of the *population* mean"
 - This is very different from: "There is a 68% chance that a measured volume will fall between $\bar{V} \pm S$ "
- λ is the *confidence interval* and it also depends on n

$$\lambda = \frac{t \cdot S}{\sqrt{n}}$$

S: sample standard deviation
n: number of measurements
t: obtained from statistics table

<http://faculty.washington.edu/baneyx/436/Tables.pdf>

Critical values of t

Table 1 CRITICAL VALUES OF t^a

DF ^b	P					
	50	20	10	5	1	0.1
1	1.00	3.08	6.31	12.7	63.7	637.0
2	0.816	1.89	2.92	4.30	9.92	31.6
3	0.765	1.64	2.35	3.18	5.84	12.9
4	0.741	1.53	2.13	2.78	4.60	8.61
5	0.727	1.48	2.01	2.57	4.03	6.86
6	0.718	1.44	1.94	2.45	3.71	5.96
7	0.711	1.42	1.89	2.36	3.50	5.40
8	0.706	1.40	1.86	2.31	3.36	5.04
9	0.703	1.38	1.83	2.26	3.25	4.78
10	0.700	1.37	1.81	2.23	3.17	4.59
15	0.691	1.34	1.75	2.13	2.95	4.07
20	0.687	1.32	1.72	2.09	2.85	3.85
30	0.683	1.31	1.70	2.04	2.75	3.65
∞	0.674	1.28	1.64	1.96	2.58	3.29

^a The P values are the probabilities (in %) that the absolute value of t will exceed the tabular entry if there is no real difference between the means being tested.

^b DF is the number of degrees of freedom.

- Degrees of freedom: $DF = n - 1$
- To determine a 95% confidence interval, use $P=5$; For a 99% confidence interval, use $P=1$, etc.

Example

$$\bar{V}_1 = 9.993 \text{ mL}$$

$$S_1 = 0.011 \text{ mL}$$

$$n_1 = 3$$

$$DF = 3 - 1 = 2 \Rightarrow t = 4.3$$

$$\lambda = \frac{t \cdot S}{\sqrt{n}} = \frac{4.3 \times 0.011}{\sqrt{3}} = 0.0273$$

I am 95% confident that the volume of the pipette is in the range: $V = 9.993 \pm 0.028$ mL based on 3 measurements

$$V = 9.993 \pm 0.028 \text{ mL (95% confidence, } n=3)$$

DF ^b	P					
	50	20	10	5	1	0.1
1	1.00	3.08	6.31	12.7	63.7	637.0
2	0.816	1.89	2.92	4.30	9.92	31.6
3	0.765	1.64	2.35	3.18	5.84	12.9
4	0.741	1.53	2.13	2.78	4.60	8.61
5	0.727	1.48	2.01	2.57	4.03	6.86
6	0.718	1.44	1.94	2.45	3.71	5.96
7	0.711	1.42	1.89	2.36	3.50	5.40
8	0.706	1.40	1.86	2.31	3.36	5.04
9	0.703	1.38	1.83	2.26	3.25	4.78
10	0.700	1.37	1.81	2.23	3.17	4.59
15	0.691	1.34	1.75	2.13	2.95	4.07
20	0.687	1.32	1.72	2.09	2.85	3.85
30	0.683	1.31	1.70	2.04	2.75	3.65
∞	0.674	1.28	1.64	1.96	2.58	3.29

Example

$$\bar{V}_2 = 9.997 \text{ mL} \quad DF = 9 - 1 = 8 \quad \Rightarrow \quad t = 2.31$$

$$S_2 = 0.008 \text{ mL}$$

$$n_2 = 9$$

$$\lambda = \frac{t \cdot S}{\sqrt{n}} = \frac{2.31 \times 0.008}{\sqrt{9}} = 0.006$$

I am 95% confident that the volume of the pipette is in the range: $V = 9.997 \pm 0.006$ mL based on 9 measurements

$$V = 9.997 \pm 0.006 \text{ mL (95% confidence, } n=9)$$

DF ^b	P					
	50	20	10	5	1	0.1
1	1.00	3.08	6.31	12.7	63.7	637.0
2	0.816	1.89	2.92	4.30	9.92	31.6
3	0.765	1.64	2.35	3.18	5.84	12.9
4	0.741	1.53	2.13	2.78	4.60	8.61
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∞	0.674	1.28	1.64	1.96	2.58	3.29

Example

$$\bar{V}_3 = 10.001 \text{ mL} \quad DF = \infty \quad \Rightarrow \quad t = 1.96$$

$$S_3 = 0.009 \text{ mL}$$

$$n_3 = 1000$$

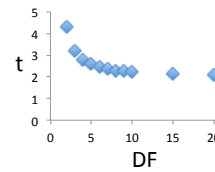
$$\lambda = \frac{t \cdot S}{\sqrt{n}} = \frac{1.96 \times 0.009}{\sqrt{1000}} = 0.00055 \approx 0.001$$

$$V = 10.001 \pm 0.001 \text{ mL (95% confidence, } n=1000)$$

DF ^b	P					
	50	20	10	5	1	0.1
1	1.00	3.08	6.31	12.7	63.7	637.0
2	0.816	1.89	2.92	4.30	9.92	31.6
3	0.765	1.64	2.35	3.18	5.84	12.9
4	0.741	1.53	2.13	2.78	4.60	8.61
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∞	0.674	1.28	1.64	1.96	2.58	3.29

Notes

- Effect of replicates on t attenuates above 6 to 8
- This remains an measure of precision (closeness to true population mean), not of accuracy



DF ^a	P					
	50	20	10	5	1	0.1
1	1.00	3.08	6.31	12.7	63.7	637.0
2	0.816	1.89	2.92	4.30	9.92	31.6
3	0.765	1.64	2.35	3.18	5.84	12.9
4	0.741	1.53	2.13	2.78	4.60	8.61
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∞	0.674	1.28	1.64	1.96	2.58	3.29

Estimating error

- In some cases, I will need to estimate error
 - Make it large enough so that it is safe
 - Do not make it too large so that it detracts from value
- Approach:
 - Account for instrument characteristics (fluctuations, least significant digit...)
 - Account for quality of calibration
 - Rely on familiarity with technique
- Example: timing falling sphere
 - Best: multiple repeats
 - If not: estimated on/off delay (0.1 s) + parallax (0.1-0.2s)

$$\lambda \approx 0.3 \text{ s (95\% conf., est.)}$$

Estimating error

- In some cases, I will need to estimate error
 - Make it large enough so that it is safe
 - Do not make it too large so that it detracts from value
- Approach:
 - Account for instrument characteristics (fluctuations, least significant digit...)
 - Account for quality of calibration
 - Rely on familiarity with technique
- Example: using a digital meter
 - Best: multiple repeats
 - If not: do you trust calibration, how much fluctuation is there and between what values, what is the least significant digit?
 - So for a stable reading of 6.2 mA, a reasonable estimate might

$$\lambda \approx 0.1 \text{ mA (95\% conf., est.)}$$

I am 95% confident that the meter would register a different value if the current varied by 0.1 mA

Significance testing

Is a measured value accurate (e.g., does it differ significantly from an accepted literature value or a calculated theoretical value)?

or

Do two experimental studies differ from one other because of real difference in technique or random events?

Significance testing

- Different ways to test significance
 - Is the measured $S_x^2 \approx \sigma_x^2$? (χ^2 test)
 - Is the measured $S_1^2 \approx S_2^2$? (F test)
 - Is the measured $\bar{X} \approx \mu$? (t test)
 - Is the measured $\bar{X}_1 \approx \bar{X}_2$? (t test)
- The t test provides an answer to both our questions

Comparing your results to accepted value

- Calculate t value using:

$$t = \frac{|\bar{X} - \mu|}{\frac{S}{\sqrt{n}}}$$

- Pipette example:

$$\begin{array}{l} \bar{V}_1 = 9.997 \text{ mL} \\ S_1 = 0.008 \text{ mL} \\ n = 9 \end{array} \quad t = \frac{|9.994 - 10|}{\frac{0.008}{\sqrt{9}}} = 2.25 \quad \text{DF} = n-1 = 8$$

- Look at the table

Comparing your results to accepted value

DF = 8 and t= 2.25

DF ^b	P					
	50	20	10	5	1	0.1
1	1.00	3.08	6.31	12.7	63.7	637.0
2	0.816	1.89	2.92	4.30	9.92	31.6
3	0.765	1.64	2.35	3.18	5.84	12.9
4	0.741	1.53	2.13	2.78	4.60	8.61
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15	0.691	1.34	1.75	2.13	2.95	4.07
20	0.687	1.32	1.72	2.09	2.85	3.85
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∞	0.674	1.28	1.64	1.96	2.58	3.29

- By interpolation $P = 5.67\%$
- Based on a t test there is a $\approx 6\%$ chance that the deviation from the “true” value is due to random fluctuation
- There is a $\approx 94\%$ chance that the deviation from the “true” value is due to systematic error

Comparing your results to someone else's

- Calculate t value using data from distributions 1 and 2 and:

$$t = \frac{|\bar{X}_1 - \bar{X}_2|}{\left(\frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2}{n_1 + n_2 - 2} \right)^{\frac{1}{2}}} \left(\frac{n_1 n_2}{n_1 + n_2} \right)^{\frac{1}{2}}$$

Denominator: pooled variance (S if $S_1=S_2=S$)
 n_1+n_2-2 : total number of degree of freedoms

- Obtain P value from the table to get contribution of random errors

Comparing your results to someone else's

- Example: drain pipettes by touching walls or not

<i>Touching</i>	<i>Not touching</i>
$\bar{V}_1 = 9.994 \text{ mL}$	$\bar{V}_2 = 9.983 \text{ mL}$
$S_1 = 0.008 \text{ mL}$	$S_2 = 0.008 \text{ mL}$
$n_1 = 6$	$n_2 = 8$

$$t = \frac{|9.994 - 9.983|}{\left(\frac{5 \times 0.008^2 + 7 \times 0.008^2}{6 + 8 - 2} \right)^{\frac{1}{2}}} \left(\frac{6 \times 8}{6 + 8} \right)^{\frac{1}{2}} = 2.55$$

- With $DF = n_1 + n_2 - 2 = 12$, we get a 2 to 3% chance that the difference is random.
- Thus, there is a 97-98% chance that the difference in data sets is due to systematic error. Here, a difference in technique.

Expectations for Experiment 1

- Measure of precision in your data by calculation of 95% confidence interval

$$\lambda = \frac{t \cdot S}{\sqrt{n}} \quad \text{for} \quad P = 5$$

$$X = \bar{X} \pm \lambda_x \quad (95\% \text{ confidence, } n = \alpha)$$

I am 95% confident that if I were to do this measurement an infinity of times, the mean would fall into the range $\pm \lambda_x$.

- Measure of accuracy of your data by comparing to an accepted or literature value

$$t = \frac{|\bar{X} - \mu|}{S / \sqrt{n}}$$

How likely is it that the mean that I would find after an infinity of measurements would equal the accepted value