

# Weighted Averages

$$A: x = x_A \pm \sigma_A$$

$$B: x = x_B \pm \sigma_B$$

combining separate measurements: what is the best estimate for  $x$  ?

$$\text{Prob}_X(x_A) \propto \frac{1}{\sigma_A} e^{-(x_A - X)^2 / 2\sigma_A^2}$$

assume that measurements are governed by Gauss distribution with true value  $X$

$$\text{Prob}_X(x_B) \propto \frac{1}{\sigma_B} e^{-(x_B - X)^2 / 2\sigma_B^2}$$

probability that A finds  $x_A$

$$\text{Prob}_X(x_A, x_B) = \text{Prob}_X(x_A) \cdot \text{Prob}_X(x_B)$$

probability that A finds  $x_A$  and B finds  $x_B$

$$\propto \frac{1}{\sigma_A \sigma_B} e^{-\chi^2 / 2}$$

find maximum of probability

**principle of maximum likelihood**

the best estimate for  $X$  is that value for which  $\text{Prob}_X(x_A, x_B)$  is maximum

$$\chi^2 = \left( \frac{x_A - X}{\sigma_A} \right)^2 + \left( \frac{x_B - X}{\sigma_B} \right)^2$$

$$\frac{d\chi^2}{dX} = 0 \Rightarrow -2 \frac{x_A - X}{\sigma_A^2} - 2 \frac{x_B - X}{\sigma_B^2} = 0$$

chi squared – “sum of squares”

find minimum of  $\chi^2$

**method of least squares**

$$(\text{best estimate for } X) = \left( \frac{x_A}{\sigma_A^2} + \frac{x_B}{\sigma_B^2} \right) / \left( \frac{1}{\sigma_A^2} + \frac{1}{\sigma_B^2} \right)$$

$$= \frac{w_A x_A + w_B x_B}{w_A + w_B} = x_{\text{wav}}$$

weighted average

weights

$$w_A = \frac{1}{\sigma_A^2} \quad w_B = \frac{1}{\sigma_B^2}$$

# Weighted Averages

$x_1, x_2, \dots, x_N$  - measurements of a single quantity  $x$  with uncertainties  $\sigma_1, \sigma_2, \dots, \sigma_N$

$$x_1 \pm \sigma_1, x_2 \pm \sigma_2, \dots, x_N \pm \sigma_N$$

$$x_{wav} = \frac{\sum w_i x_i}{\sum w_i}$$

$$w_i = \frac{1}{\sigma_i^2}$$

$$\sigma_{wav} = \frac{1}{\sqrt{\sum w_i}}$$

← weighted average

← weights

← uncertainty in  $x_{wav}$   
can be calculated  
using error propagation

## Example Problem

Two students measure the radius of a planet and get final answers

$$R_A = 25,000 \pm 3,000 \text{ km and } R_B = 19,000 \pm 2,500 \text{ km.}$$

The best estimate of the true radius of a planet is the weighted average. Find the best estimate of the true radius of a planet and the error in that estimate.

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$$x_{\text{wav}} = \frac{w_A x_A + w_B x_B}{w_A + w_B} \quad w_A = \frac{1}{\sigma_A^2} \quad w_B = \frac{1}{\sigma_B^2} \quad \sigma_{\text{wav}} = \frac{1}{\sqrt{w_A + w_B}}$$

$$R_{\text{wav}} = \frac{\frac{R_A}{\sigma_A^2} + \frac{R_B}{\sigma_B^2}}{\frac{1}{\sigma_A^2} + \frac{1}{\sigma_B^2}} = \frac{\frac{25,000}{3,000^2} + \frac{19,000}{2,500^2}}{\frac{1}{3,000^2} + \frac{1}{2,500^2}} = 21,459 \text{ km} \rightarrow \underline{21,500 \text{ km}}$$

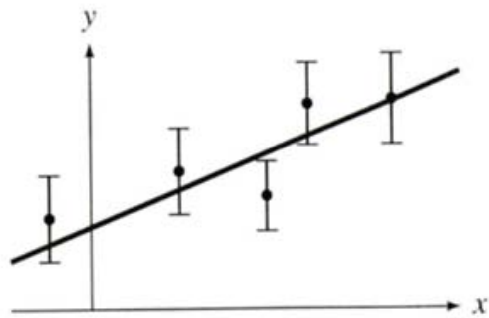
$$\sigma_{\text{wav}} = \frac{1}{\sqrt{\frac{1}{\sigma_A^2} + \frac{1}{\sigma_B^2}}} = \frac{1}{\sqrt{\frac{1}{3,000^2} + \frac{1}{2,500^2}}} = 1,921 \text{ km} \rightarrow \underline{1,900 \text{ km}}$$

$$\underline{R_{\text{wav}} = 21,500 \pm 1,900 \text{ km}}$$

# Least-Squares Fitting

consider two variables  $x$  and  $y$  that are connected by a linear relation

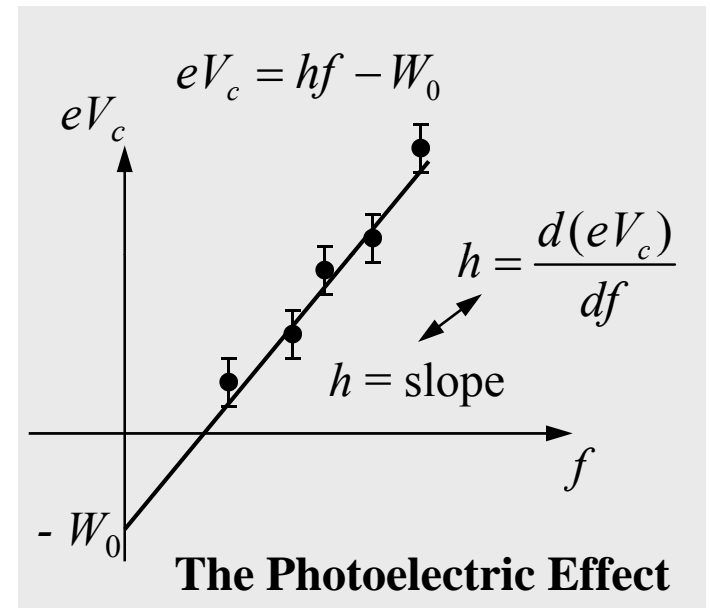
$$y = A + Bx$$



graphical method of finding the best straight line to fit a series of experimental points

$$\begin{array}{l} x_1, x_2, \dots, x_N \\ y_1, y_2, \dots, y_N \end{array} \longrightarrow \text{find } A \text{ and } B$$

analytical method of finding the best straight line to fit a series of experimental points is called **linear regression** or **the least-squares fit for a line**



# Calculation of the Constants A and B

(true value for  $y_i$ ) =  $A + Bx_i$

$\text{Prob}_{A,B}(y_1) \propto \frac{1}{\sigma_y} e^{-(y_1 - A - Bx_1)^2 / 2\sigma_y^2}$  ← probability of obtaining the observed value of  $y_1$

$\text{Prob}_{A,B}(y_1, \dots, y_N) = \text{Prob}_{A,B}(y_1) \cdots \text{Prob}_{A,B}(y_N)$  ← probability of obtaining the set  $y_1, \dots, y_N$

$\propto \frac{1}{\sigma_y^N} e^{-\chi^2/2}$  ← find maximum of probability

$\chi^2 = \sum_{i=1}^N \frac{(y_i - A - Bx_i)^2}{\sigma_y^2}$  ← chi squared – “sum of squares”

← find minimum of  $\chi^2$

least squares fitting

$$\left| \frac{\partial \chi^2}{\partial A} = \frac{-2}{\sigma_y^2} \sum_{i=1}^N (y_i - A - Bx_i) = 0 \right.$$

$$\left| \frac{\partial \chi^2}{\partial B} = \frac{-2}{\sigma_y^2} \sum_{i=1}^N x_i (y_i - A - Bx_i) = 0 \right.$$

$$\left| \sum y_i - AN - B \sum x_i = 0 \right.$$

$$\left| \sum x_i y_i - A \sum x_i - B \sum x_i^2 = 0 \right.$$



$$A = \frac{\sum x^2 \sum y - \sum x \sum xy}{\Delta}$$

$$B = \frac{N \sum xy - \sum x \sum y}{\Delta}$$

$$\Delta = N \sum x^2 - (\sum x)^2$$

# Uncertainties in $y$ , $A$ , and $B$

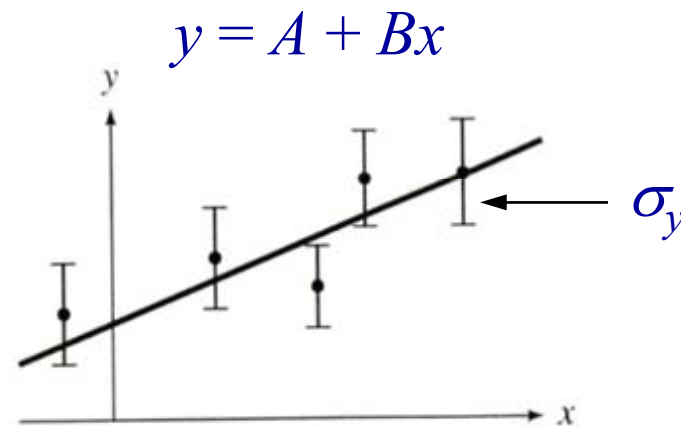
$$\sigma_y = \sqrt{\frac{1}{N-2} \sum_{i=1}^N (y_i - A - Bx_i)^2}$$

$$\sigma_A = \sigma_y \sqrt{\frac{\sum x^2}{\Delta}}$$

$$\sigma_B = \sigma_y \sqrt{\frac{N}{\Delta}}$$

uncertainty in the measurement of  $y$

uncertainties in the constants  $A$  and  $B$   
given by error propagation in terms  
of uncertainties in  $y_1, \dots, y_N$



# Example of Calculation of the Constants $A$ and $B$

$$T = A + B P$$

if volume of an ideal gas is kept constant,  
its temperature is a linear function of its pressure

$i$	$P_i$	$T_i$
1	65	-20
2	75	17
3	85	42
4	95	94
5	105	127

absolute zero of temperature  $A = ?$

$$\sum P = 425$$

$$\sum P^2 = 37,125$$

$$\sum T = 260$$

$$\sum PT = 25,810$$

$$\Delta = N \sum P^2 - (\sum P)^2 = 5,000$$

$$A = \frac{\sum P^2 \sum T - \sum P \sum PT}{\Delta} = -263.35$$

$$B = \frac{N \sum PT - \sum P \sum T}{\Delta} = 3.71$$

$$\sigma_T = \sqrt{\frac{1}{N-2} \sum (T_i - A - B P_i)^2} = 6.7$$

$$\sigma_A = \sigma_T \sqrt{\frac{\sum P^2}{\Delta}} = 18$$

$$A = -263.35 \pm 18^\circ \text{C}$$

$$\underline{A = -263 \pm 18^\circ \text{C}}$$

$$A = \frac{\sum x^2 \sum y - \sum x \sum xy}{\Delta}$$

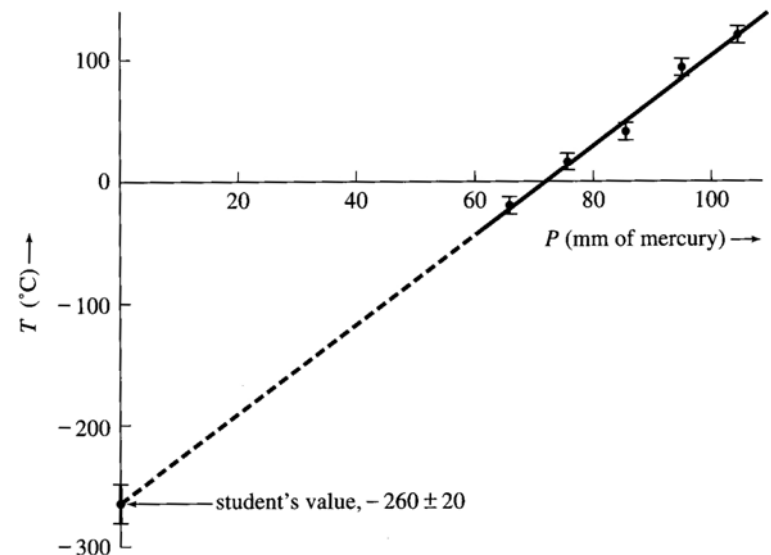
$$B = \frac{N \sum xy - \sum x \sum y}{\Delta}$$

$$\Delta = N \sum x^2 - (\sum x)^2$$

$$\sigma_y = \sqrt{\frac{1}{N-2} \sum_{i=1}^N (y_i - A - B x_i)^2}$$

$$\sigma_A = \sigma_y \sqrt{\frac{\sum x^2}{\Delta}}$$

absolute zero of  
temperature =  $-273.15^\circ \text{C}$



# Covariance

$$x = \bar{x} \pm \delta x \rightarrow q(x, y) = \bar{q} \pm \delta q$$

$$y = \bar{y} \pm \delta y$$

find  $\bar{q}$  and  $\delta q$

$N$  pairs of data  $(x_1, y_1), \dots, (x_N, y_N)$

$$x_1, \dots, x_N \rightarrow \bar{x} \text{ and } \sigma_x$$

$$y_1, \dots, y_N \rightarrow \bar{y} \text{ and } \sigma_y$$

$$q_i = q(x_i, y_i)$$

$$q_1, \dots, q_N \rightarrow \bar{q} \text{ and } \sigma_q$$

$$\rightarrow q_i \approx q(\bar{x}, \bar{y}) + \frac{\partial q}{\partial x} (x_i - \bar{x}) + \frac{\partial q}{\partial y} (y_i - \bar{y})$$

$$\bar{q} = \frac{1}{N} \sum_{i=1}^N q_i$$

$$= \frac{1}{N} \sum_{i=1}^N \left[ q(\bar{x}, \bar{y}) + \frac{\partial q}{\partial x} (x_i - \bar{x}) + \frac{\partial q}{\partial y} (y_i - \bar{y}) \right]$$

$$\sum (x_i - \bar{x}) = 0 \Rightarrow \underline{\bar{q} = q(\bar{x}, \bar{y})}$$

$$\sigma_q^2 = \frac{1}{N} \sum (q_i - \bar{q})^2$$

$$= \frac{1}{N} \sum \left[ \frac{\partial q}{\partial x} (x_i - \bar{x}) + \frac{\partial q}{\partial y} (y_i - \bar{y}) \right]^2$$

$$= \left( \frac{\partial q}{\partial x} \right)^2 \frac{1}{N} \sum (x_i - \bar{x})^2 + \left( \frac{\partial q}{\partial y} \right)^2 \frac{1}{N} \sum (y_i - \bar{y})^2$$

$$+ 2 \frac{\partial q}{\partial x} \frac{\partial q}{\partial y} \frac{1}{N} \sum (x_i - \bar{x})(y_i - \bar{y})$$

$\sigma_q$  for arbitrary  $\sigma_x$  and  $\sigma_y$

$\sigma_x$  and  $\sigma_y$  can be correlated  $\longrightarrow$

covariance  $\sigma_{xy}$   $\longrightarrow$

$$\sigma_q^2 = \left( \frac{\partial q}{\partial x} \right)^2 \sigma_x^2 + \left( \frac{\partial q}{\partial y} \right)^2 \sigma_y^2 + 2 \frac{\partial q}{\partial x} \frac{\partial q}{\partial y} \sigma_{xy}$$

$$\sigma_{xy} = \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})$$

when  $\sigma_x$  and  $\sigma_y$  are independent  $\sigma_{xy} = 0 \longrightarrow$

$$\sigma_q^2 = \left( \frac{\partial q}{\partial x} \right)^2 \sigma_x^2 + \left( \frac{\partial q}{\partial y} \right)^2 \sigma_y^2$$



# Coefficient of Linear Correlation

$N$  pairs of values  $(x_1, y_1), \dots, (x_N, y_N)$

$$y = A + Bx$$



do  $N$  pairs of  $(x_i, y_i)$  satisfy a linear relation ?

$$r = \frac{\sigma_{xy}}{\sigma_x \cdot \sigma_y}$$

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$



linear correlation coefficient  
or correlation coefficient

$$-1 \leq r \leq 1$$

Suppose  $(x_i, y_i)$  all lie exactly  
on the line  $y = A + Bx$

$$y_i = A + Bx_i$$

$$\bar{y} = A + B\bar{x}$$

$$y_i - \bar{y} = B(x_i - \bar{x})$$

$$r = \frac{B \sum (x_i - \bar{x})^2}{\sqrt{\sum (x_i - \bar{x})^2 \cdot B^2 \sum (x_i - \bar{x})^2}} = \frac{B}{|B|} = \pm 1$$

Suppose, there is no relationship  
between  $x$  and  $y$

$$\sum (x_i - \bar{x})(y_i - \bar{y}) \rightarrow 0$$

$$r = 0$$

if  $r$  is close to  $\pm 1$

when  $x$  and  $y$  are linearly correlated

if  $r$  is close to 0

when there is no relationship between  $x$  and  $y$   
 $x$  and  $y$  are uncorrelated

# Quantitative Significance of $r$

Student $i$	1	2	3	4	5	6	7	8	9	10
Homework $x_i$	90	60	45	100	15	23	52	30	71	88
Exam $y_i$	90	71	65	100	45	60	75	85	100	80

calculate correlation coefficient

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

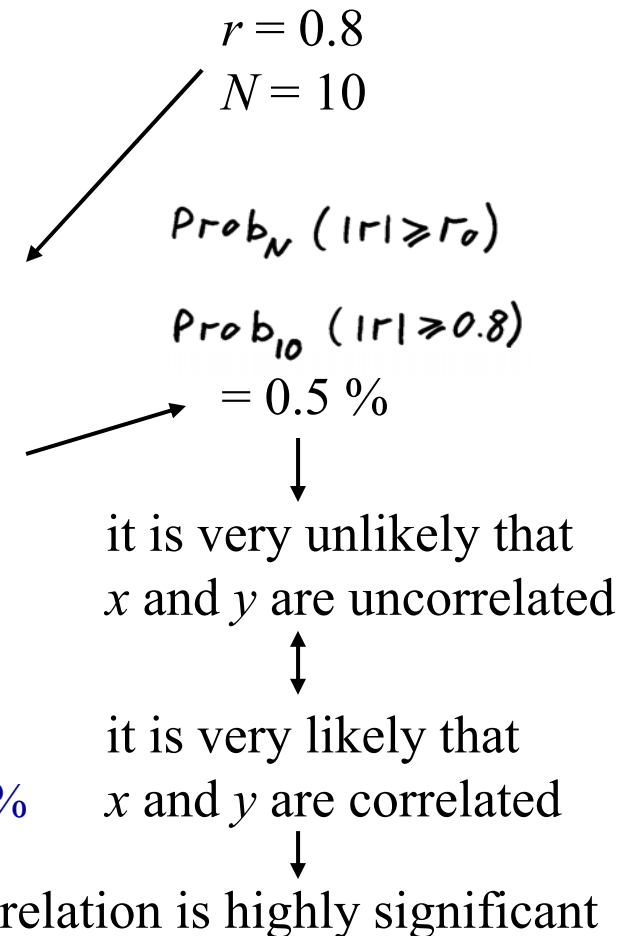
probability that  $N$  measurements of two uncorrelated variables  $x$  and  $y$  would produce  $r \geq r_0$   $\longrightarrow$  **Table C**

**Table 9.4.** The probability  $Prob_N(|r| \geq r_0)$  that  $N$  measurements of two uncorrelated variables  $x$  and  $y$  would produce a correlation coefficient with  $|r| \geq r_0$ . Values given are percentage probabilities, and blanks indicate values less than 0.05%.

$N$	$r_0$										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
3	100	94	87	81	74	67	59	51	41	29	0
6	100	85	70	56	43	31	21	12	6	1	0
10	100	78	58	40	25	14	7	2	0.5	0	0
20	100	67	40	20	8	2	0.5	0.1		0	0
50	100	49	16	3	0.4					0	0

correlation is “significant” if  $Prob_N(|r| \geq r_0)$  is less than 5 %

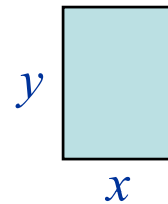
correlation is “highly significant” if  $Prob_N(|r| \geq r_0)$  is less than 1 %



Example:

Calculate the covariance and the correlation coefficient  $r$  for the following six pairs of measurements of two sides  $x$  and  $y$  of a rectangle. Would you say these data show a significant linear correlation coefficient? Highly significant?

	A	B	C	D	E	F	
$x =$	71	72	73	75	76	77	mm
$y =$	95	96	96	98	98	99	mm



$$\bar{x} = 74$$

$$\bar{y} = 97$$

covariance  $\sigma_{xy} = \frac{1}{N} \sum (x_i - \bar{x})(y_i - \bar{y}) = \frac{1}{6} ((-3) \times (-2) + \dots + 3 \times 2) = \underline{3}$

correlation coefficient  $r = \frac{\sigma_{xy}}{\sigma_x \sigma_y} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}} = \underline{0.98}$

**Table C**  $Prob_6(|r| \geq 0.98) \approx 0.2\%$  therefore, the correlation is both significant and highly significant



# Chi Squared Test for a Distribution

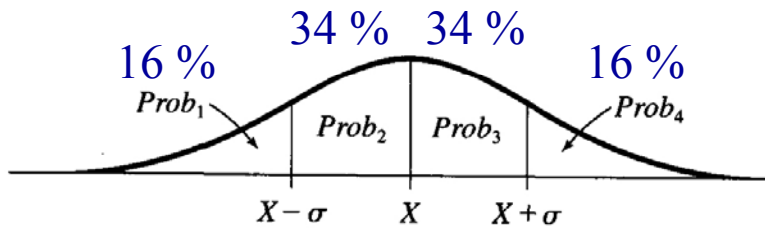
40 measured values of  $x$  (in cm)

731	772	771	681	722	688	653	757	733	742
739	780	709	676	760	748	672	687	766	645
678	748	689	810	805	778	764	753	709	675
698	770	754	830	725	710	738	638	787	712

are these measurements governed by a Gauss distribution ?

$$\bar{x} = \frac{\sum x_i}{N} = 730.1 \text{ cm}$$

$$\sigma = \sqrt{\frac{\sum (x_i - \bar{x})^2}{N-1}} = 46.8 \text{ cm}$$



$$\frac{O_k - E_k}{\sqrt{E_k}} = \frac{\text{deviation}}{\text{expected size of its fluctuation}} \sim 1 ?$$

$$\chi^2 = \sum_{k=1}^n \frac{(O_k - E_k)^2}{E_k}$$

chi squared

Bin number $k$	Observed number $O_k$	Expected number $E_k = N \text{Prob}_k$	Difference $O_k - E_k$
1	8	6.4	1.6
2	10	13.6	-3.6
3	16	13.6	2.4
4	6	6.4	-0.4

$\chi^2 \lesssim n$  observed and expected distributions agree about as well as expected

$\chi^2 \gg n$  significant disagreement between observed and expected distributions

$O_k$  – observed number  
 $E_k$  – expected number  
 $\sqrt{E_k}$  – fluctuations of  $E_k$

$$\begin{aligned} \chi^2 &= \sum_{k=1}^4 \frac{(O_k - E_k)^2}{E_k} \\ &= \frac{(1.6)^2}{6.4} + \frac{(-3.6)^2}{13.6} + \frac{(2.4)^2}{13.6} + \frac{(-0.4)^2}{6.4} \\ &= 1.80 < n \end{aligned}$$

no reason to doubt that the measurements were governed by a Gauss distribution

# Degrees of Freedom and Reduced Chi Squared

a better procedure is to compare  $\chi^2$  not with the number of bins  $n$  but instead with the number of degree of freedom  $d$

$n$  is the number of bins

$c$  is the number of parameters that had to be calculated from the data to compute the expected numbers  $E_k$

$c$  is called the number of constrains

$d$  is the number of degrees of freedom

$$\underline{d = n - c}$$

test for a GAUSS distribution  $G_{\mu, \sigma}(x) \rightarrow c = 3$   $\begin{matrix} \swarrow N \\ \leftarrow \mu \\ \swarrow \sigma \end{matrix}$

(expected average value of  $\chi^2$ ) =  $d = n - c$

$\tilde{\chi}^2 = \chi^2 / d$  reduced chi squared

(expected average value of  $\tilde{\chi}^2$ ) = 1

# Probabilities of Chi Squared

quantitative measure of agreement between observed data and their expected distribution

$$(\text{expected average value of } \chi^2) = d = n - c$$

$$\tilde{\chi}^2 = \chi^2 / d$$

$$(\text{expected average value of } \tilde{\chi}^2) = 1$$

$$\chi^2 = 1.80$$

$$d = 4 - 3 = 1$$

$$\tilde{\chi}^2 = 1.80$$

$$\text{Prob}(\tilde{\chi}^2 \geq 1.80) \approx 18\% \quad \leftarrow \text{Table D}$$

d	$\tilde{\chi}_0^2$												
	0	0.25	0.5	0.75	1.0	1.25	1.5	1.75	2	3	4	5	6
1	100	62	48	39	32	26	22	19 X	16	8	5	3	1
2	100	78	61	47	37	29	22	17	14	5	2	0.7	0.2
3	100	86	68	52	39	29	21	15	11	3	0.7	0.2	—
5	100	94	78	59	42	28	19	12	8	1	0.1	—	—
10	100	99	89	68	44	25	13	6	3	0.1	—	—	—
15	100	100	94	73	45	23	10	4	1	—	—	—	—

probability of obtaining a value of  $\tilde{\chi}^2$  greater or equal to  $\tilde{\chi}_0^2$ , assuming the measurements are governed by the expected distribution

disagreement is “significant” if  $\text{Prob}_N(\tilde{\chi}^2 \geq \tilde{\chi}_0^2)$  is less than 5 %

disagreement is “highly significant” if  $\text{Prob}_N(\tilde{\chi}^2 \geq \tilde{\chi}_0^2)$  is less than 1 %

reject the expected distribution