PART IV

Scientific data

DATA SHEET

DATA SHEET

Chi-squared distribution

Probability distribution sum of squares

$x_1, x_2, \ldots, x_\nu$ are independent, normally distributed variables with $E\{x_i\} = 0$ and $E\{x_i^2\} = 1$; ν = number of *degrees of freedom*; $\chi^2 = \sum_{i=1}^{\nu} x_i^2$. The probability density function of χ^2 is:

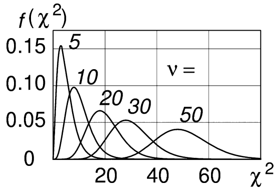
$$\boxed{f(\chi^2|\nu)\, d\chi^2 = [2^{\nu/2}\,\Gamma(\tfrac{\nu}{2})]^{-1}(\chi^2)^{\nu/2-1}\,\exp[-\chi^2/2]\, d\chi^2.}$$

Moments of $f(\chi^2|\nu)$:

mean	$\mu = E\{\chi^2\}$	$= \nu$
variance	$\sigma^2 = E\{(\chi^2 - \mu)^2\}$	$= 2\nu$
skewness	$\gamma_1 = E\{(\chi^2 - \mu)^3/\sigma^3\}$	$= 2\sqrt{(2/\nu)}$
excess	$\gamma_2 = E\{(\chi^2 - \mu)^4/\sigma^4 - 3\}$	$= 12/\nu$

Special cases

ν	$f(\chi^2\|\nu)$
1	$(2\pi)^{-1/2}\chi^{-1}\exp[-\chi^2/2]$
2	$\frac{1}{2}\exp[-\chi^2/2]$
3	$(2\pi)^{-1/2}\chi\exp[-\chi^2/2]$
∞	$(4\pi\nu)^{-1/2}\exp[-(\chi^2-\nu)^2/(4\nu)]$ normal with var $= 2\nu$



Relation to Poisson distribution (ν even)

$1 - F(\chi^2|\nu) =$
$= \sum_{j=0}^{c-1} e^{-m} m^j / j!$,
$c = \frac{1}{2}\nu$ $m = \frac{1}{2}\chi^2$).

Cumulative χ^2-distribution

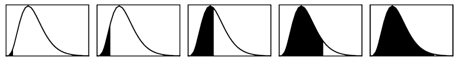
$F(\chi^2|\nu)$ = probability that sum of squares $< \chi^2$:

$$F(\chi^2|\nu) = \int_0^{\chi^2} f(S|\nu)\, dS.$$ *See table p. 2.*

Probability that χ^2 is exceeded is $1 - F(\chi^2)$.

Chi-squared distribution

Values of χ^2 for 1%, 10%, 50%, 90%, and 99%



$F = \nu$	0.01	0.10	0.50	0.90	0.99
1	0.000	0.016	0.455	2.706	6.635
2	0.020	0.211	1.386	4.605	9.210
3	0.115	0.584	2.366	6.251	11.35
4	0.297	1.064	3.357	7.779	13.28
5	0.554	1.610	4.351	9.236	15.09
6	0.872	2.204	5.348	10.65	16.81
7	1.239	2.833	6.346	12.02	18.48
8	1.646	3.490	7.344	13.36	20.09
9	2.088	4.168	8.343	14.68	21.67
10	2.558	4.865	9.342	15.99	23.21
11	3.053	5.578	10.34	17.28	24.73
12	3.571	6.304	11.34	18.55	26.22
13	4.107	7.042	12.34	19.81	27.69
14	4.660	7.790	13.34	21.06	29.14
15	5.229	8.547	14.34	22.31	30.58
20	8.260	12.44	19.34	28.41	37.57
25	11.52	16.47	24.34	34.38	44.31
30	14.95	20.60	29.34	40.26	50.89
40	22.16	29.05	39.34	51.81	63.69
50	29.71	37.69	49.34	63.17	76.15
60	37.49	46.46	59.34	74.40	88.38
70	45.44	55.33	69.33	85.53	100.4
80	53.54	64.28	79.33	96.58	112.3
90	61.75	73.29	89.33	107.6	124.1
100	70.07	82.36	99.33	118.5	135.8
∞	$\nu - a$	$\nu - b$	ν	$\nu + b$	$\nu + a$
	$a = 3.290\sqrt{\nu}$			$b = 1.812\sqrt{\nu}$	

F-distribution

F-distribution

Meaning of variable: F-ratio = ratio of mean squared deviations of two groups of samples.

$$F_{\nu_1,\nu_2} = \frac{\mathrm{MSD}_1}{\mathrm{MSD}_2} = \frac{\sum(\Delta y_{1i})^2/\nu_1}{\sum(\Delta y_{2i})^2/\nu_2}.$$

F-test: yields (cumulative) probability that both groups come from distributions with the same variance.

Probability density function:

$$f(F_{\nu_1,\nu_2}) = \frac{\Gamma\left(\frac{\nu_1+\nu_2}{2}\right)}{\Gamma\left(\frac{\nu_1}{2}\right)\Gamma\left(\frac{\nu_1}{2}\right)}\nu_1^{\nu_1/2}\nu_2^{\nu_2/2}F^{(\nu_1-2)/2}(\nu_2+\nu_1 F)^{-(\nu_1+\nu_2)/2}.$$

Cumulative distribution function:
$F(F_{\nu_1,\nu_2}) = \int_{-\infty}^{F} f(F')\,dF'$
$1 - F(F_{\nu_1,\nu_2}) = \int_{F}^{\infty} f(F')\,dF'$
mean: $m = \nu_2/(\nu_2-2), \quad \nu_2 > 2$
variance: $\sigma^2 = 2\nu_2^2(\nu_1+\nu_2-2)/[\nu_1(\nu_2-2)^2(\nu_2-4)], \quad \nu_2 > 4.$

Reflexive relation:
$F(F_{\nu_1,\nu_2}) = 1 - F(1/F_{\nu_2,\nu_1})$
e.g. $F_{10,5} = 4.74$ at the 95% level; then $F_{5,10} = 1/4.74 = 0.21$ at the 5% level.
Therefore tables can be restricted to F-ratios > 1.

Use in ANOVA (analysis of variance) in regression

Given: n data (x_i, y_i), $i = 1,\ldots,n$. Fit $f_i = ax_i + b$ by linear regression. The total sum of squared deviations SST can be divided into SSR (regression SSQ, explained by the model) and SSE (remaining error). ν = nr of degrees of freedom:
SST ($\nu = n-1$) = SSR ($\nu = 1$) + SSE ($\nu = n-2$)
$\mathrm{SST} = \sum(y_i - \langle y\rangle)^2$; $\mathrm{SSR} = \sum(f_i - \langle y\rangle)^2$; $\mathrm{SSE} = \sum(y_i - f_i)^2$
Perform F-test on $F_{1,n-2} = [\mathrm{SSR}/1]/[\mathrm{SSE}/(n-2)]$.

Remark: For regression with m parameters:
Perform F-test on $F_{m-1,n-m} = [\mathrm{SSR}/(m-1)]/[\mathrm{SSE}/(n-m)]$.

F-distribution

F-distribution, percentage points 95% and 99%

$F(F_{\nu_1,\nu_2}) = \mathbf{0.95}$

If $(\sum y_{1i}^2/\nu_1)/(\sum y_{2i}^2/\nu_2)$ exceeds the F-ratio F_{ν_1,ν_2} given in the table, the probability is $< 5\%$ that y and z are samples from distributions with equal variance.

ν_1 / ν_2	1	2	3	4	5	7	10	20	50	∞
2	18.5	19.0	19.2	19.3	19.3	19.4	19.4	19.5	19.5	19.5
3	10.1	9.55	9.28	9.12	9.01	8.89	8.79	8.66	8.58	8.53
4	7.71	6.94	6.59	6.39	6.26	6.09	5.96	5.80	5.70	5.63
5	6.61	5.79	5.41	5.19	5.05	4.88	4.74	4.56	4.44	4.36
7	5.59	4.74	4.35	4.12	3.97	3.79	3.64	3.44	3.32	3.23
10	4.96	4.10	3.71	3.48	3.33	3.14	2.98	2.77	2.64	2.54
20	4.35	3.49	3.10	2.87	2.71	2.51	2.35	2.12	1.97	1.84
50	4.03	3.18	2.79	2.56	2.40	2.20	2.03	1.78	1.60	1.44
∞	3.84	3.00	2.61	2.37	2.21	2.01	1.83	1.57	1.35	1.00

$F(F_{\nu_1,\nu_2}) = \mathbf{0.99}$

ν_1 / ν_2	1	2	3	4	5	7	10	20	50	∞
2	98.5	99.0	99.2	99.3	99.3	99.4	99.4	99.5	99.5	99.5
3	34.1	30.8	29.5	28.7	28.2	27.7	27.2	26.7	26.4	26.1
4	21,2	18.0	16.7	16.0	15.5	15.0	14.6	14.0	13.7	13.5
5	16.3	13.3	12.1	11.4	11.0	10.5	10.1	9.55	9.24	9.02
7	12.3	9.55	8.45	7.85	7.46	6.99	6.62	6.16	5.86	5.65
10	10.0	7.56	6.55	5.99	5.64	5.20	4.85	4.41	4.12	3.91
20	8.10	5.85	4.94	4.43	4.10	3.70	3.37	2.94	2.64	2.42
50	7.17	5.06	4.20	3.72	3.41	3.02	2.70	2.27	1.95	1.68
∞	6.63	4.61	3.78	3.32	3.02	2.64	2.32	1.88	1.53	1.00

Least-squares fitting

General least-squares fitting

Sum of weighted squared deviations

a. *Uncorrelated data*

Given n measured values y_i, $i=1,\dots n$, we seek m parameters $\hat{\theta}_k$, $k = 1\dots m$, $m < n$; such that:

$$\boxed{S = \sum_{i=1}^{n} w_i(y_i - f_i)^2 \text{ minimal}}$$

$f_i(\theta_1,\dots\theta_m)$ are functions of parameters. For the minimum: $S(\hat{\boldsymbol{\theta}}) = S_0$. Both y_i and f_i can be functions of one or more independent variables.

The *residuals* $\varepsilon_i = y_i - f_i$ are supposed to be samples from a random distribution with properties: $E[\varepsilon_i] = 0$; $E[\varepsilon_i\varepsilon_j] = \sigma_i^2\delta_{ij}$.

The *weight factors* w_i should be proportional to σ_i^{-2}.

If the variances σ_i of the deviations are known, a chi-squared test can be carried out on $\chi_0^2 = \min \sum_{i=1}^{n}[(y_i - f_i)/\sigma_i]^2$, for $\nu = n - m$ degrees of freedom.

b. *Correlated data*

$S = \sum_{i,j=1}^{n} w_{ij}(y_i - f_i)(y_j - f_j)$ minimal, with $\varepsilon_i = y_i - f_i$ samples from a random distribution with properties: $E[\varepsilon_i] = 0$; $E[\varepsilon_i\varepsilon_j] = \Sigma_{ij}$. $\boldsymbol{\Sigma}$ is the covariance matrix of the measured values. The matrix $\boldsymbol{W}$ of weight factors should be proportional to $\boldsymbol{\Sigma}^{-1}$.

Parameter covariances Likelihood of $\boldsymbol{\theta}$ is proportional to $\exp\left[-\frac{1}{2}\chi^2(\boldsymbol{\theta})\right]$. Since $E[\chi_0^2] = n - m$, $\chi^2(\boldsymbol{\theta})$ is estimated by scaling S:

$\hat{\chi}^2(\boldsymbol{\theta}) = (n-m)S(\boldsymbol{\theta})/S_0 = n - m + (\boldsymbol{\Delta\theta})^{\mathrm{T}}\boldsymbol{B}\boldsymbol{\Delta\theta}$, where $\boldsymbol{\Delta\theta} = \boldsymbol{\theta} - \hat{\boldsymbol{\theta}}$. The expectation of the parameter covariance matrix $\boldsymbol{C} = E[(\boldsymbol{\Delta\theta})(\boldsymbol{\Delta\theta})^{\mathrm{T}}]$ is given by:

$$\boxed{\boldsymbol{C} = \boldsymbol{B}^{-1}.}$$

$\sigma_k = \sqrt{C_{kk}}$; $\rho_{kl} = C_{kl}/(\sigma_k\sigma_l)$.

Least-squares fitting

Linear in the parameters

When f_i are linear functions of $\boldsymbol{\theta}$:
$f_i(\theta) = \sum_k A_{ik}\theta_k$; $\boldsymbol{f} = \boldsymbol{A}\,\boldsymbol{\theta}$ (general: $A_{ik} = \partial f_i/\partial\theta_k$)

$$\boxed{S = (\boldsymbol{y} - \boldsymbol{f})^{\mathrm{T}}\boldsymbol{W}(\boldsymbol{y} - \boldsymbol{f}) \text{ minimal}}$$

$$\boxed{\text{for } \hat{\boldsymbol{\theta}} = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{y},}$$

where $W_{ij} \propto \sigma_i^{-2}\delta_{ij}$ (uncorrelated data).
$S(\hat{\boldsymbol{\theta}}) = S_0$
Expectation of parameter covariance matrix $\boldsymbol{C} = E[(\boldsymbol{\Delta\theta})(\boldsymbol{\Delta\theta})^{\mathrm{T}}]$ is given by:

$$\boxed{\boldsymbol{C} = [S_0/(n-m)](\boldsymbol{A}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{A})^{-1}.}$$

Special case: linear function:
$f_i = f(x_i) = ax_i + b$ (a and b parameters):

$$\boxed{a = \langle(\Delta x)(\Delta y)\rangle/\langle(\Delta x)^2\rangle;\ b = \langle y\rangle - a\langle x\rangle.}$$

Here $\langle\ \rangle$ are *weighted* averages, such as:
$\langle\xi\rangle = (1/w)\sum_{i=1}^{n} w_i\,\xi_i;\ w = \sum_{i=1}^{n} w_i.$
$\Delta x = x - \langle x\rangle;\quad \Delta y = y - \langle y\rangle.$

Expectation of (co)variances of $\boldsymbol{a}$ and $\boldsymbol{b}$:
$E[(\Delta a)^2] = \sigma_a^2 = S_0/[n(n-2)\langle(\Delta x)^2\rangle]$
$E[(\Delta b)^2] = \sigma_b^2 = \langle x^2\rangle\sigma_a^2$
$E[\Delta a\Delta b] = -\langle x\rangle\sigma_a^2;\ \rho_{ab} = -\langle x\rangle\sigma_a/\sigma_b$
N.B.: a and b are uncorrelated if $\langle x\rangle = 0$.

Correlation coefficient *r* of *x* and *y*:

$$\boxed{r = \frac{\langle(\Delta x)(\Delta y)\rangle}{\sqrt{\langle(\Delta x)^2\rangle}\sqrt{\langle(\Delta y)^2\rangle}} = a\left(\frac{\langle(\Delta x)^2\rangle}{\langle(\Delta y)^2\rangle}\right)^{1/2}.}$$

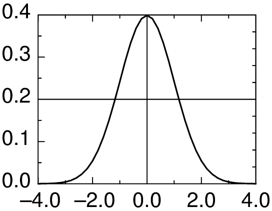
Normal distribution

One-dimensional Gauss function

Probability density function:

$$f(x)\,dx = (\sigma\sqrt{2\pi})^{-1}\ \exp[-(x-\mu)^2/(2\sigma^2)]\,dx$$

μ = *mean*,
σ^2 = *variance*,
σ = *standard deviation*.
Standard form:
$f(z) = (1/\sqrt{2\pi})\exp(-z^2/2)$,
$z = (x-\mu)/\sigma$.



Characteristic function: $\Phi(t) = \exp\left(-\frac{1}{2}\sigma^2 t^2\right)\exp(i\mu t)$.
Central moments $\mu_n = \int_{-\infty}^{\infty}(x-\mu)^n f(x)\,dx$,
$\mu_m = 0$ for m even, $\mu_{2n} = \sigma^{2n}\times 1\times 3\times 5\times(2n-1)$,
$\mu_2 = \sigma^2,\ \mu_4 = 3\sigma^4,\ \mu_6 = 15\sigma^6,\ \mu_8 = 105\sigma^8$.
skewness = 0, *excess* = 0.

Cumulative distribution function:
$F(x) = \int_{-\infty}^{x} f(x')\,dx' = \frac{1}{2}\{1+\mathrm{erf}\,(x/\sigma\sqrt{2})\}$,
$1-F(x) = F(-x) = \int_{x}^{\infty} f(x')\,dx' = \frac{1}{2}\,\mathrm{erfc}\,(x/\sigma\sqrt{2})$.

z	$f(z)$	$F(-z)$	z	$f(z)$	$F(-z)$
0.0	0.3989	0.5000	1.4	1.497e-01	8.076e-02
0.1	0.3970	0.4602	1.6	1.109e-01	5.480e-02
0.2	0.3910	0.4207	1.8	7.895e-02	3.593e-02
0.3	0.3814	0.3821	2.0	5.399e-02	2.275e-02
0.4	0.3683	0.3446	2.5	1.753e-02	6.210e-03
0.5	0.3521	0.3085	3.0	4.432e-03	1.350e-03
0.6	0.3332	0.2743	3.5	8.727e-04	2.326e-04
0.7	0.3123	0.2420	4.0	1.338e-04	3.167e-05
0.8	0.2897	0.2119	5.0	1.487e-06	2.866e-07
0.9	0.2661	0.1841	7.0	9.135e-12	1.280e-12
1.0	0.2420	0.1587	10	7.695e-23	7.620e-24
1.2	0.1942	0.1151	15	5.531e-50	3.671e-51

$$\text{large } z:\quad F(-z) = 1-F(z) \approx \frac{f(z)}{z}\left(1-\frac{1}{z^2+2}+\cdots\right)$$

Normal distribution

Multivariate Gauss functions

General *n*-dimensional form:

$$f(\mathbf{x})\,d\mathbf{x} = (2\pi)^{-n/2}\,(\det\mathbf{W})^{1/2}\exp\left[-\tfrac{1}{2}(\mathbf{x}-\mu)^{\mathrm{T}}\mathbf{W}(\mathbf{x}-\mu)\right]d\mathbf{x},$$

where $\mathbf{W}$ is the *weight matrix*. $\mathbf{W} = \mathbf{C}^{-1}$.
$\mathbf{C} \stackrel{\text{def}}{=} E[(\mathbf{x}-\mu)(\mathbf{x}-\mu)^{\mathrm{T}}]$ is the *covariance matrix*.

Bivariate normal distribution:

$$\mathbf{C} = \begin{pmatrix} \sigma_x^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_x\sigma_y & \sigma_y^2 \end{pmatrix}; \quad \rho \text{ is the } \textit{correlation coefficient}.$$

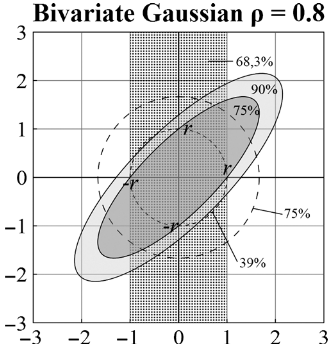
$$\mathbf{W} = \frac{1}{1-\rho^2}\begin{pmatrix} \sigma_x^{-2} & -\rho/(\sigma_x\sigma_y) \\ -\rho/(\sigma_x\sigma_y) & \sigma_y^{-2} \end{pmatrix}$$

$$f(x,y)\,dx\,dy = \frac{1}{2\pi\,\sigma_x\sigma_y\sqrt{1-\rho^2}}\exp\left[-\frac{z^2}{2(1-\rho^2)}\right]dx\,dy;$$

$$z^2 = \frac{(x-\mu_x)^2}{\sigma_x^2} - 2\frac{\rho(x-\mu_x)(y-\mu_y)}{\sigma_x\sigma_y} + \frac{(y-\mu_y)^2}{\sigma_y^2}.$$

Standard form:
$\mu_x = \mu_y = 0$; $\sigma_x = \sigma_y = 1$; $r^2 = x^2 - 2\rho xy + y^2$ is equation for ellipse at $+45°$ for $\rho > 0$ or $-45°$ for $\rho < 0$. Half major axis $a = r/\sqrt{1-|\rho|}$; half minor axis $b = r/\sqrt{(1+|\rho|}$. Cumulative probability integrated over ellipse: $1 - \exp\left[-\frac{1}{2}r^2/(1-\rho^2)\right]$.

Bivariate Gaussian ρ = 0.8



Marginal distr.: $f_x(x) = (\sigma_x\sqrt{2\pi})^{-1}\exp\left[-\frac{1}{2}((x-\mu_x)/\sigma_x)^2\right]$,
Conditional distribution:

$$f(x|y) = \frac{1}{\sigma_x\sqrt{2\pi(1-\rho^2)}}\exp\left[-\frac{\{x-\mu_x-\rho(\sigma_x/\sigma_y)(y-\mu_y)\}^2}{2\sigma_x^2(1-\rho^2)}\right].$$

Conditional expectation: $E[x|y] = \mu_x + \rho(\sigma_x/\sigma_y)(y-\mu_y)$.

Normal distribution

Probability that ≥1 ∈ *n* samples exceeds an interval

Probability that at least one out of n (independent, normally distributed) samples falls outside the interval $(\mu - d, \mu + d)$*:*

$$\Pr\{\geq 1; n, d\} = 1 - [1 - 2F(-d/\sigma)]^n \text{ (double-sided)}$$

$n \downarrow$	$d/\sigma \rightarrow$ 1.5	2	2.5	3	3.5	4
1	0.134	0.046	0.012	0.0027	4.7e-4	6.3e-5
2	0.249	0.089	0.025	0.0054	9.3e-4	1.3e-4
3	0.350	0.130	0.037	0.0081	0.0014	1.9e-4
4	0.437	0.170	0.049	0.0108	0.0019	2.5e-4
5	0.512	0.208	0.061	0.0134	0.0023	3.2e-4
6	0.577	0.244	0.072	0.0161	0.0028	3.8e-4
7	0.634	0.278	0.084	0.0187	0.0033	4.4e-4
8	0.683	0.311	0.095	0.0214	0.0037	5.1e-4
9	0.725	0.342	0.106	0.0240	0.0042	5.7e-4
10	0.762	0.372	0.117	0.0267	0.0046	6.3e-4
12	0.821	0.428	0.139	0.0319	0.0056	7.6e-4
15	0.884	0.503	0.171	0.0397	0.0070	9.5e-4
20	0.943	0.606	0.221	0.0526	0.0093	0.0013
25	0.972	0.688	0.268	0.0654	0.0116	0.0016
30	0.986	0.753	0.313	0.0779	0.0139	0.0019
40	0.997	0.845	0.393	0.102	0.0184	0.0025
50	0.999	0.903	0.465	0.126	0.0230	0.0032
70	1.000	0.962	0.583	0.172	0.0321	0.0044
100	1.000	0.991	0.713	0.237	0.0455	0.0063
150	1.000	0.999	0.847	0.333	0.0674	0.0095
200	1.000	1.000	0.918	0.418	0.0889	0.0126
300	1.000	1.000	0.976	0.556	0.130	0.0188
400	1.000	1.000	0.993	0.661	0.167	0.0250
500	1.000	1.000	0.998	0.741	0.208	0.0312

horizontal lines mark 5% level

DATA SHEET

Normal distribution

Probability that ≥1 ∈ *n* samples exceeds a value

Probability that at least one out of n (independent, normally distributed) samples is $>\mu + d$ *(or* $\ldots < \mu - d$*):*

$$\Pr\{\geq 1; n, d\} = 1 - [1 - F(-d/\sigma)]^n \text{ (single-sided)}$$

$n \downarrow$	$d/\sigma \rightarrow$ 1.5	2	2.5	3	3.5	4
1	0.067	0.023	0.0062	0.0014	2.3e-4	3.2e-5
2	0.129	0.045	0.012	0.0027	4.7e-4	6.3e-5
3	0.187	0.067	0.019	0.0040	6.9e-4	9.5e-5
4	0.242	0.088	0.025	0.0054	9.3e-4	1.3e-5
5	0.292	0.109	0.031	0.0067	0.0012	1.6e-4
6	0.340	0.129	0.037	0.0081	0.0014	1.9e-4
7	0.384	0.149	0.043	0.0094	0.0016	2.2e-4
8	0.425	0.168	0.049	0.011	0.0019	2.5e-4
9	0.463	0.187	0.055	0.012	0.0021	2.9e-4
10	0.499	0.206	0.060	0.013	0.0023	3.2e-4
12	0.564	0.241	0.072	0.016	0.0028	3.8e-4
15	0.646	0.292	0.089	0.020	0.0035	4.8e-4
20	0.749	0.369	0.117	0.027	0.0046	6.3e-4
25	0.823	0.438	0.144	0.033	0.0058	7.9e-4
30	0.874	0.499	0.170	0.038	0.0070	9.5e-4
40	0.937	0.602	0.221	0.053	0.0093	0.0013
50	0.968	0.684	0.268	0.065	0.012	0.0016
70	0.992	0.800	0.353	0.090	0.016	0.0022
100	0.999	0.900	0.464	0.126	0.023	0.0032
150	1.000	0.968	0.607	0.183	0.034	0.0047
200	1.000	0.990	0.712	0.237	0.045	0.0063
300	1.000	0.999	0.846	0.333	0.067	0.0095
400	1.000	1.000	0.917	0.417	0.089	0.0126
500	1.000	1.000	0.956	0.491	0.110	0.0157

horizontal lines mark 5% level

Physical constants

(*between parentheses: standard deviation*)

velocity of light	$c = 299\,792\,458$ m/s (exact)
magnetic constant	$\mu_0 = 4\pi \times 10^{-7}$ N/A^2 (exact)
	$= 1.256\,637\,0614\ldots \times 10^{-6}$
electric constant	$\varepsilon_0 = 1/\mu_0 c^2$ (exact)
	$= 8.854\,187\,817\ldots \times 10^{-12}$ F/m
characteristic impedance	$Z_0 = \sqrt{\mu_0/\epsilon_0} = \mu_0 c$ (exact)
vacuum	$= 376.730\,313\,461\ldots\,\Omega$
Planck constant	$h = 6.626\,068\,96(33) \times 10^{-34}$ J s
Dirac constant $h/2\pi$	$\hbar = 1.054\,571\,628(53) \times 10^{-34}$ J s
gravitational constant	$G = 6.674\,28(67) \times 10^{-11}$ m^3 kg^{-1} s^{-2}
elementary charge	$e = 1.602\,176\,487(40) \times 10^{-19}$ C
mass electron	$m_e = 9.109\,382\,15(45) \times 10^{-31}$ kg
mass proton	$m_p = 1.672\,621\,637(83) \times 10^{-27}$ kg
	$= 1.007\,276\,466\,77(10)$ u
m_e/m_p	$= 5.446\,170\,2177(24) \times 10^{-4}$
atomic mass unit	$u = 1.660\,538\,782(83) \times 10^{-27}$ kg
Avogadro number	$N_A = 6.022\,141\,79(30) \times 10^{23}$ mol^{-1}
Boltzmann constant	$k = 1.380\,6504(24) \times 10^{-23}$ J/K
gas constant kN_A	$R = 8.314\,472(15)$ J mol^{-1} K^{-1}
molar volume	$V_m = 22.710\,98(40) \times 10^{-3}$ m^3/mol
ideal gas 273.15 K, 100 kPa	
Faraday eN_A	$F = 96\,485.3399(24)$ C/mol
Bohr radius	$a_0 = 5.291\,772\,0859(36) \times 10^{-11}$m
$a_0 = \hbar/(m_e c\alpha) = 10^7\,(\hbar/ce)^2/m_e$	
Bohr magneton	$\mu_B = 9.274\,009\,15(23) \times 10^{-24}$ J/T
$\mu_B = e\hbar/2m_e$	
nuclear magneton	$\mu_N = 5.050\,783\,24(13) \times 10^{-27}$ J/T
magnetic moment electron	$\mu_e = -9.284\,763\,77(23) \times 10^{-24}$ J/T
magnetic moment proton	$\mu_p = 1.410\,606\,662(37) \times 10^{-26}$ J/T
g-factor electron	$g_e = -2.002\,319\,304\,3622(15)$
g-factor proton	$g_p = 5.585\,694\,713(46)$
fine structure constant	$\alpha = 7.297\,352\,5376(50) \times 10^{-3}$
$\alpha^{-1} = 4\pi\varepsilon_0\hbar c/e^2$	$\alpha^{-1} = 137.035\,999\,679(94)$
proton gyromagnetic	$\gamma_p = 2.675\,222\,099(70) \times 10^8$ s^{-1}T^{-1}
ratio	$\gamma_p/2\pi = 42.577\,4821(11)$ MHz/T

Physical constants

conductance quantum $G_0 = 7.748\,091\,7004(53) \times 10^{-5}$ S
Josephson constant $K_J = 4.835\,978\,91(12) \times 10^{14}$ Hz/V
magnetic flux quantum $\Phi_0 = 2.067\,833\,667(52) \times 10^{-15}$ Wb
$G_0 = 2e^2/h;\ K_J = 2e/h;\ \Phi_0 = h/2e$
Stefan–Boltzmann constant $\sigma = 5.670\,400(40) \times 10^{-8}$
$\pi^2 k^4/(60\hbar^3 c^2);\ U = \sigma T^4$ (black body radiation) $\mathrm{W\,m^{-2}K^{-4}}$
Rydberg constant $R_\infty = 10\,973\,731{,}568\,527(73)\ \mathrm{m^{-1}}$
$\alpha^2 m_e c/2h$

masses of neutron (n), deuteron (d) and muon (μ)

n:	$1.674\,927\,211(84) \times 10^{-27}$ kg	$= 1.008\,664\,915\,97(43)$ u
d:	$3.343\,583\,20(17) \times 10^{-27}$ kg	$= 2.013\,553\,212\,724(78)$ u
μ:	$1.883\,531\,30(11) \times 10^{-28}$ kg	$= 0.113\,428\,9256(29)$ u

Relative standard deviations

g_e	7.4×10^{-13}	g_p	8.2×10^{-9}
R_∞	6.6×10^{-12}	$e,\ K_J,\ \Phi_0$	2.5×10^{-8}
m_d/u	3.9×10^{-11}	$h,\ N_A,\ u,\ m_e,$	
m_p/u	1.0×10^{-10}	$m_p,\ m_d,\ m_n$	5.0×10^{-8}
$m_e/u,\ m_n/u,$		$k,\ R,\ V_m$	1.7×10^{-6}
m_e/m_p	4.2×10^{-10}	σ (Stefan-B.)	7.0×10^{-6}
$\alpha,\ a_o,\ G_0$	6.8×10^{-10}	G	1.0×10^{-4}

Accuracies of derived quantities

If y_k is a product of powers of physical constants x_i:
$y_k = a_k \Pi_{i=1}^{N} x_i^{p_{ki}}$ (a_k is a constant), then

$$\epsilon_k^2 = \sum_{i=1}^{N} p_{ki}^2 \epsilon_i^2 + 2\sum_{j<i}^{N} p_{ki} p_{kj} r_{ij} \epsilon_i \epsilon_j,$$

where ϵ_k = relative standard deviation and r_{ij} = correlationcoefficient between i and j (For r: see website)

CODATA 2006 http://physics.nist.gov/cuu/constants/

Probability distributions

Continuous one-dimensional probability functions

x is a real variable from a *domain* $\mathcal{D}$; the *probability density function* (pdf) $p(x)$ is real; $p(x) \geq 0$. $p(x)\,dx$ is the probability of finding a sample X in the interval $(x, x + dx)$.
$p(x)$ is normalized: $\int_{\mathcal{D}} p(x)\,dx = 1$ (if $p(x)$ cannot be normalized, it is called an *improper* pdf).
The value of x for which $p(x)$ is a maximum, is called the *mode*.

The *expectation* or *expected value* of a function $g(x)$ over the pdf $p(x)$ is defined as the functional

$$E[g(x)] \stackrel{\text{def}}{=} \int_{\mathcal{D}} g(x)p(x)\,dx.$$

mean: $\mu = E[x]$.
variance: $\sigma^2 = E[(x - \mu)^2]$.
standard deviation (std) σ: root of the variance.
n-th moment: $\mu_n \stackrel{\text{def}}{=} E[x^n]$.
n-th central moment $\mu_n^c \stackrel{\text{def}}{=} E[(x - \mu)^n]$.
skewness: $E[(x - \mu)^3/\sigma^3]$.
kurtosis: $E[(x - \mu)^4/\sigma^4]$.
excess: *kurtosis*-3.

characteristic function $\Phi(t)$:

$$\Phi(t) \stackrel{\text{def}}{=} E[e^{itx}] = \int_{\infty}^{\infty} e^{itx}p(x)\,dx$$
$$= \sum_{n=0}^{\infty} \frac{(it)^n}{n!} E[x^n] = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \mu_n$$

$\Phi(t)$ generates the moments μ_n. The moments are also given by the *derivatives* of the characteristic function at $t = 0$:

$$\Phi^{(n)}(0) = \frac{d^n\Phi}{dt^n}|_{t=0} = i^n\mu_n.$$

Special case: $\mu_2 = \sigma^2 + \mu^2 = -(d^2\Phi(t)/dt^2)_{x=0}$.

Probability distributions

(one-dimensional functions – continued)
Cumulative distribution function (cdf) $P(x)$:

$$P(x) \stackrel{\text{def}}{=} \int_a^x p(x')\,dx',$$

where a is the lower limit of the domain of x (usually $-\infty$). $P(x)$ is a monotonously non-decreasing function of x, starting at 0 and ending at 1. The value of x for which $P(x) = 0.5$ is the *median*; when $P(x) = 0.25, x$ is the *first quartile*; when $P(x) = 0.75, x$ is the *third quartile*; when $P(x) = 0.01n, x$ is the n-th *percentile*.
Survival function (sf): $S(x) = 1 - P(x)$.

Continuous two-dimensional probability functions

Joint pdf: $p(x, y)\,dx\,dy$ is the probability for a sample pair (X, Y) to find the value X in the interval $(x, x + dx)$ *and* the value Y in the interval $(y, y + dy)$. $p(x, y) \geq 0$; $\int p(x, y)\,dx\,dy = 1$.
Conditional pdf: $p(x|y)\,dx$ (*p of x given y*) is the probability for a sample pair (X, Y) that a sample X occurs in the interval $(x, x + dx)$ *while* Y has the value y.
Marginal pdf: $p_x(x) = \int p(x, y)\,dy$ is the probability for a sample pair (X, Y) that a sample X occurs in the interval $(x, x + dx)$ *irrespective* of the value of Y.

$p(x|y) = p(x, y)/p_y(y)$,
$p(x, y) = p_x(x)\,p(y|x) = p_y(y)\,p(x|y)$,
$p(x|y) = p_x(x)$ if x and y are independent,
$p(x, y) = p_x(x)\,p_y(y)$ if x and y are independent.

Expectation of $g(x, y)$: $E[g(x, y)] = \int dx \int dy\, g(x, y)\, p(x, y)$.
Mean of x: μ_x is the expectation $E[x] = \int dx \int dy\, x\, p(x, y) =$
$= \int x\, p_x(x)\, dx$.
Variance of x: $\sigma_x^2 = C_{xx} = E[(x - \mu_x)^2]$.
Covariance of x and y: $C_{xy} = E[(x - \mu_x)(y - \mu_y)] =$
$= \int dx \int dy (x - \mu_x)(y - \mu_y) p(x, y)$.
Correlation coefficient between x and y: $\rho_{xy} = C_{xy}/(\sigma_x \sigma_y)$.
$\mathbf{C} = E[\mathbf{x}\mathbf{x}^{\mathrm{T}}]$ is the *correlation matrix* ($\mathbf{x}$ is the column vector of deviations from the mean).

Student's t-distribution

Student's t-distribution

Let X be a normally distributed variable with expectation 0 and variance σ^2 and Y^2/σ^2 an independent chi-squared distributed variable with ν degrees of freedom. Then $t = \frac{X\sqrt{\nu}}{Y}$ is distributed according to a Student's t-distribution $f(t|\nu)$ with ν degrees of freedom, independent of σ:

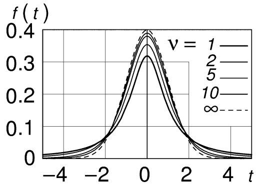
$$f(t|\nu)\,dt = \frac{1}{\sqrt{\nu\pi}}\,\frac{\Gamma[(\nu+1)/2]}{\Gamma(\nu/2)}\left(1+\frac{t^2}{\nu}\right)^{-(\nu+1)/2} dt.$$

Application: accuracy of the mean

Let $x_1, \ldots, x_n$ be n independent samples from a normal distribution with unknown expectation μ and unknown variance σ^2; let $\langle x\rangle = \frac{1}{n}\sum_{i=1}^{n} x_i$; $S = \sum_{i=1}^{n}(x_i - \langle x\rangle)^2$ and $\hat{\sigma} = \sqrt{S/(n-1)}$, then $t = [(\langle x\rangle - \mu)\sqrt{n}]/\hat{\sigma}$ is distributed according to a Student's t-distribution with $\nu = n-1$ degrees of freedom. The best estimate for σ is $\hat{\sigma}$. If σ is known, then $\langle x\rangle$ is distributed normally with mean μ and variance σ^2/n. In the latter case $\chi^2 = S/\sigma^2$ satisfies a chi-squared distribution with $\nu = n-1$ degrees of freedom.

Properties and moments

f is symmetric: $f(-t) = f(t)$; mean = 0
variance $\sigma^2 = \nu/(\nu-2)$ $(\nu > 2)$; 'skewness' $\gamma_1 = 0$
"excess" $\gamma_2 = E\{t^4\}/\sigma^4 - 3 = 6/(\nu-4)$
$\lim_{\nu\to\infty} f(t|\nu) = (1/\sqrt{2\pi})\exp(-t^2/2)$



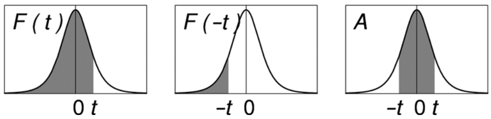
Cumulative distribution

$F(t|\nu) = \int_{-\infty}^{t} f(t'|\nu)\,dt'$
$F(-t|\nu) = 1 - F(t|\nu)$

see table p. 2

Student's t-distribution

Values of *t* at 75%, 90%, 95%, 99%, and 99.5%



A = acceptance level for two-sided interval $(-t, t)$

$F(t) =$	0.75	0.90	0.95	0.99	0.995
$F(-t) =$	0.25	0.10	0.05	0.01	0.005
$A(\%)$	50	80	90	98	99
$\nu = 1$	1.000	3.078	6.314	31.821	63.657
2	0.816	1.886	2.920	6.965	9.925
3	0.765	1.638	2.353	4.541	5.841
4	0.741	1.533	2.132	3.747	4.604
5	0.727	1.467	2.015	3.365	4.032
6	0.718	1.440	1.943	3.143	3.707
7	0.711	1.415	1.895	2.998	3.499
8	0.706	1.397	1.860	2.896	3.355
9	0.703	1.383	1.833	2.821	3.250
10	0.700	1.372	1.812	2.764	1.169
11	0.697	1.363	1.796	2.718	3.106
12	0.695	1.356	1.782	2.681	3.055
13	0.694	1.350	1.771	2.650	3.012
14	0.692	1.345	1.761	2.624	2.977
15	0.691	1.341	1.753	2.602	2.947
20	0.687	1.325	1.725	2.528	2.845
25	0.684	1.316	1.708	2.485	2.787
30	0.683	1.310	1.697	2.457	2.750
40	0.681	1.303	1.684	2.423	2.704
50	0.679	1.299	1.676	2.403	2.678
60	0.697	1.296	1.671	2.390	2.660
70	0.678	1.294	1.667	2.381	2.648
80	0.678	1.292	1.664	2.374	2.639
100	0.677	1.290	1.660	2.364	2.626
∞	0.674	1.282	1.645	2.326	2.576

Units

Definitions SI basic units

SI: *Système International d'Unités*

Source http://physics.nist.gov/cuu/Units

length: **meter** (m) length of the path traveled by light in vacuum during 1/299 792 458 second (1983).

mass: **kilogram** (kg) mass of the international prototype of the kilogram (1901).

time: **second** (s) duration of 9 192 631 770 periods of the transition between two hyperfine levels of the ground state of the cesium-133 atom (1967).

current: **ampere** (A) current in two infinitely long and thin straight parallel conductors, placed 1 meter apart in vacuum, that exert a force on each other of 2×10^{-7} newton per meter length (1948).

thermodynamic temperature: **kelvin** (K) fraction 1/273.16 of the thermodynamic temperature of the triple point of water (1967).

amount of substance: **mol** (mol) amount of substance which contains as many elementary entities as there are atoms in 0.012 kg of carbon 12. The entities (atoms, molecules, ions, electrons, etc.) must be specified (1971).

luminous intensity: **candela** (cd) radiant intensity of a source that emits monochromatic radiation of frequency 540×10^{12} Hz in a given direction, with intensity of 1/683 W/sr (watt per steradian) (1979).

10^{-1}	deci	d	10^{-2}	centi	c	10^{-3}	milli	m
10^{-6}	micro	μ	10^{-9}	nano	n	10^{-12}	pico	p
10^{-15}	femto	f	10^{-18}	atto	a	10^{-21}	zepto	z
10^{-24}	yocto	y						
10^{1}	deca	da	10^{2}	hecto	h	10^{3}	kilo	k
10^{6}	mega	M	10^{9}	giga	G	10^{12}	Tera	T
10^{15}	peta	P	10^{18}	exa	E	10^{21}	zetta	Z
10^{24}	yotta	Y						

DATA SHEET

Units

Derived SI units

plane angle (circle: 2π)	$\alpha, \ldots$	**radian**	rad
solid angle (sphere: 4π)	ω, Ω	**steradian**	sr
area	A, S		m^2
volume	V		m^3
frequency	ν	**hertz**	$\mathrm{Hz} = \mathrm{s}^{-1}$
linear momentum	p		$\mathrm{kg\,m\,s}^{-1}$
angular momentum	L, J		$\mathrm{kg\,m}^2\mathrm{s}^{-1}$
specific mass	ρ		$\mathrm{kg/m}^3$
moment of inertia	I		$\mathrm{kg\,m}^2$
force	F	**newton**	$\mathrm{N} = \mathrm{kg\,m\,s}^{-2}$
torque	M		$\mathrm{N\,m}$
pressure	p, P	**pascal**	$\mathrm{Pa} = \mathrm{N/m}^2$
viscosity	η		$\mathrm{N\,s\,m}^{-2} = \mathrm{kg\,m}^{-1}\mathrm{s}^{-1}$
energy	E, w	**joule**	$\mathrm{J} = \mathrm{N\,m} = \mathrm{kg\,m}^2\mathrm{s}^{-2}$
power	P	**watt**	$\mathrm{W} = \mathrm{J/s}$
charge	q, Q	**coulomb**	$\mathrm{C} = \mathrm{A\,s}$
electric potential	V, Φ	**volt**	$\mathrm{V} = \mathrm{J/C}$
electric field	E		$\mathrm{V/m}$
dielectric displacement	D		$\mathrm{C/m}^2$
capacity	C	**farad**	$\mathrm{F} = \mathrm{C/V}$
resistance	R	**ohm**	$\Omega = \mathrm{V/A}$
specific resistance	ρ		$\Omega\,\mathrm{m}$
conductance	G	**siemens**	$\mathrm{S} = \Omega^{-1}$
specific conductance	σ, κ		$\mathrm{S/m}$
inductance	L	**henry**	$\mathrm{H} = \mathrm{Wb/A}$
magnetic flux	Φ	**weber**	$\mathrm{Wb} = \mathrm{V\,s}$
magnetic field	H		$\mathrm{A/m}$
magnetic flux density	B	**tesla**	$\mathrm{T} = \mathrm{Wb/m}^2$
luminous flux	Φ	**lumen**	$\mathrm{lm} = \mathrm{cd.sr}$
illuminance	I	**lux**	$\mathrm{lx} = \mathrm{lm/m}^2$
activity (radionuclide)	A	**becquerel**	$\mathrm{Bq} = \mathrm{s}^{-1}$
absorbed dosis	D	**gray**	$\mathrm{Gy} = \mathrm{J/kg}$
dose equivalent	H	**sievert**	$\mathrm{Sv} = \mathrm{J/kg}$

Units

Non-SI units (incl. British, US) (see also **atomic units** on p. 5)

length: **fermi** (fm) = 10^{-15} m; **Ångstrom** (Å) = 10^{-10} m; **mil** (mil) = 0.001 in; **inch** (in) = 2.54 cm (exact); **foot** (ft) = 12 in = 0.304 8 m; **yard** (yd) = 3 ft = 0.914 4 m; **fathom** = 6 ft = 1.828 8 m; **cable** = 720 ft = 185.2 m; **(statute) mile** = 1760 yd = 1609.34 m; **nautical mile** (nm) = 1852 m; **astronomical unit** (AU) = $1.495\,978\,70 \times 10^{11}$ m; **light year** (Ly) = 9.4605×10^{15} m; **parsec** (pc) = 3.086×10^{16} m.

area: **barn** (b) = 10^{-28} m^2 = 100 fm^2; **are** (a) = 100 m^2; **hectare** (ha) = 10^4 m^2; **acre** = 4840 sq. yd = 4046.87 m^2; **sq. mile** = 640 acres = 2.59 km^2.

volume: **Br. fluid ounce** fl oz) = 28.41 cm^3; **US fl. oz** = 29.572 9 cm^3; **US liq. pint** = 16 US fl. oz = 473.2 cm^3; **Br. pint** (pt) = 20 Br. fl. oz = 568.2 cm^3; **US liq. quart** = 2 US liq. pt = 946.3 cm^3; **liter** (l) = 1 dm^3; **Br. quart** (qt) = 2 Br. pt = 1.136 dm^3; **US gallon** = 4 US liq. qt = 231 in^3 = 3.785 4 dm^3; **(Br.) imperial gallon** (gal) = 4 Br. qt = 4.546 dm^3; **bushel** = 8 imp. gal; **barrel** = 42 US gal.; **ton** = 1 m^3; **register ton** = 100 ft^3 = 2.83 m^3.

mass: **u** (unified atomic mass unit) = $1.660\,538\,782(83) \times 10^{-27}$ kg; **grain avdp** (gr) = 64.79891 mg (exact); **(Br.) drachme** = **(US) dram** = 60 gr = 3.887 934 6 g; **ounce avdp** (oz) = 28.349 527 g (exact); **troy ounce (apothecary ounce)** = 480 gr = 31.103 4768 g; **pound avoirdupois** (lb) = 16 oz = 7000 grain = 0.453 592 37 kg (exact); **(Br.) stone** = 14 lbs = 6.35 kg; **ton** = 1000 kg.

time: **minute** (min) = 60 s; **hour** (h) = 3600 s.

temperature: t **degree Celsius** (°C) = $t + 273.15$ K; f **degree Fahrenheit** (°F) = $(f - 32) \times 5/9$ °C.

velocity: **knot** = nautical mile/h = 0.514 44 m/s.

force: **dyne** (dyn) = 10^{-5} N; **poundforce** (lbf) = 4.448 22 N; **kilogramforce** (kgf) = 9.806 65 N (exact).

Units

(non SI units, *continued*)

pressure: **mm Hg** (torr) = 101 325/760 Pa (exact) = 133.322 Pa; **pound per sq. inch** (psi) = 6 894.76 Pa; **technical atmosphere** (at) = kgf/cm^2 = 98 066.5 Pa (exact); **bar** (bar) = 10^5 Pa; **normal atmosphere** (atm) = 101 325 Pa (exact).

energy: **hartree** (E_h) = 4.359 743 94(22) $\times 10^{-18}$ J; **erg** (erg) = 10^{-7} J; **thermochemical calorie** (cal_{th}) = 4.184 J; **15° calorie** (cal_{15}) = 4.1855 J; **Int. Table calorie** (cal_{IT}) = 4.1868 J; **Br. thermal unit** (Btu) = 1055.87 J; **kilowatt hour** (kWh) = 3.6 MJ; **ton coal equiv.** (tse) = 29.3 GJ; **ton oil equiv.** (toe) = 45.4 GJ; m^3 **natural gas** (average, 0 °C, 1 atm) = 39.4 MJ.

power: **horsepower** (metric, PS) = 75 kgf m/s = 735.5 W; **horsepower** (mechanical, hp) = 550 lbf ft/s = 745.7 W.

viscosity: **poise** (p) = g cm^{-1}s^{-1} = 0.1 kg m^{-1}s^{-1}; *kinematic viscosity:* **stokes** (St) = 10^{-4} m^2/s

(radio)activity, dose: **curie** (Ci) = 3.7×10^{10} Bq; **röntgen** (R) = 2.58×10^{-4} C/kg; **rad** (rad, rd) = 0.01 Gy; **rem** (rem) = 0.01 Sv.

light: **stilb** (sb) = cd/cm^2; **phot** (ph) = cd cm^{-2}sr^{-1}.

electrostatic units (esu): c.g.s. unit of charge (g$^{1/2}$cm$^{3/2}$s^{-1}), such that $4\pi\varepsilon_0 = 1$ (dimensionless): *charge:* 10^{-9}/ 2.997 924 58 C; *current:* 10^{-9}/2.99... A; *dipole moment:* 10^{-11}/2.99... C m; **debye** (D) = 10^{-18} esu = 10^{-29}/2.99... C; *el. pot.:* 299.7... V; *el. field:* 2.99... × 10^4 V/m.

electromagnetic units (emu): c.g.s. unit of current (g$^{1/2}$cm$^{1/2}$s^{-1}), such that $\mu_0/4\pi = 1$ (dimensionless): *current:* **abampere** (abamp) = 10 A; *magn. field:* **oerstedt** (Oe) = $(1/4\pi)$ abamp/cm = $10^3/4\pi$ A/m; *magn. flux density ("induction"):* **gauss** (G) = 10^{-4} T; *magn. flux:* **maxwell** (Mx) = 10^{-8} Wb.

Units

Atomic units (a.u.)

The basic a.u. are the Bohr radius a_0, the electron mass m_e, Dirac's constant $\hbar$ and the elementary charge e: $m_e = 1$ a.u., $\hbar = 1$ a.u., $c = 1/\alpha$ a.u., $e = 1$ a.u., $4\pi\varepsilon_0 = 1$ a.u.

mass	m_e	$= 9.109\,382\,15(45)\times 10^{-31}$ kg
length	a_0	$= 5.291\,772\,0859(36)\times 10^{-11}$ m
charge	e	$= 1.602\,176\,487(40)\times 10^{-19}$ C
time	$a_0/(\alpha c)$	$= 2.418\,884\,326\,505(16)\times 10^{-17}$ s
		$= (4\pi R_\infty c)^{-1}$
velocity	αc	$= 2.187\,691\,2541(15)\times 10^{6}$ m/s
energy	$\hbar^2/(m_e a_0^2)$	$= e^2/(4\pi\varepsilon_0 a_0) = \alpha^2 mc^2$
		$= 2R_\infty hc =$
(**hartree**)	E_h	$= 4.359\,743\,94(22)\times 10^{-18}$ J
		$= 2\,625.312\,93(13)$ kJ/mol
		$= 627.464\,850(32)$ kcal/mol
		$= 27.211\,383\,86(68)$ eV

Molecular units

This is a consistent system of units for 'molecular' quantities, useful for molecular modeling and simulation. Coulomb forces have an *electric factor* coefficient $f = 1/(4\pi\varepsilon_0)$: $F = fq_1q_2/r^2$ (see table). The unit for f is kJ mol^{-1} nm e^{-2}.

mass	u	$= 1.660\,538\,86(28)\times 10^{-27}$ kg
length	nm	$= 10^{-9}$ m
time	ps	$= 10^{-12}$ s
velocity	nm/ps	$= 1000$ m/s
energy	kJ/mol	$= 1.660\,538\,86\times 10^{-21}$ J
force	kJ mol^{-1} nm^{-1}	$= 1.660\,538\,86\times 10^{-12}$ N
pressure	kJ mol^{-1} nm^{-3}	$= 1.660\,538\,86\times 10^{5}$
		$= 16.605\,3886$ bar
charge	e	$= 1.602\,176\,53(14)\times 10^{-19}$ C
electric factor	f	$= 138.935\,4574(14)$