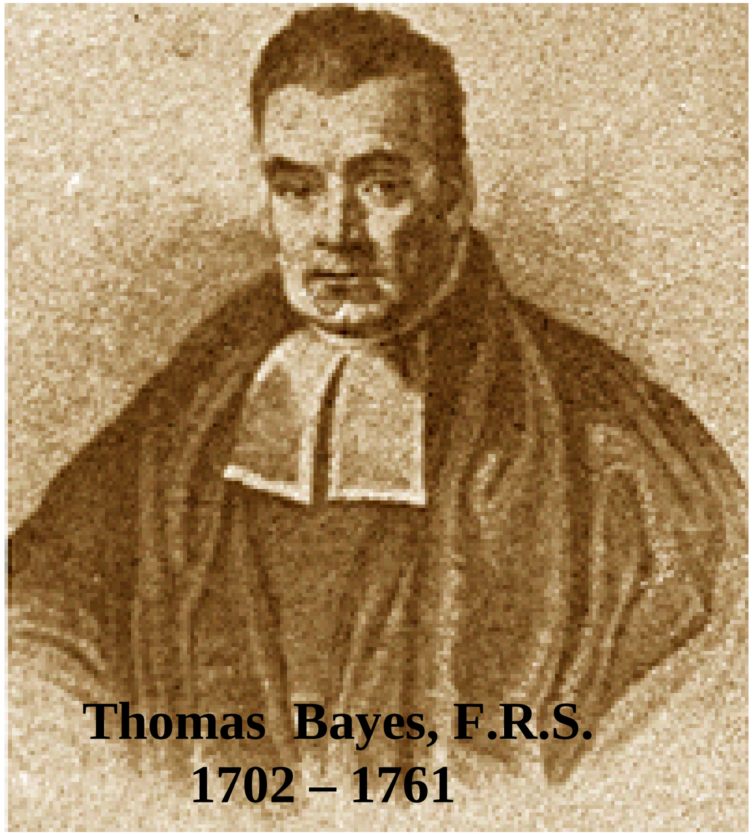


BEYOND LEAST SQUARES

V.Dose

Max Planck Institut
für Plasmaphysik

C. F. Gauss 1777 - 1855

1794 first use of quadratic distance measure

1798 probabilistic explanation

1821 quadratic measure ad hoc

first(?) mention of weights

1823 exact variances unknown

1826 data censoring unnecessary (?)

$$P(\boldsymbol{\theta}|\mathbf{D},\mathbf{M},I) = P(\mathbf{D}|\,\boldsymbol{\theta},\mathbf{M},I)\;P(\boldsymbol{\theta}|\mathbf{M},I)\;/\;P(\mathbf{D}|\mathbf{M},I)$$

$$\int P(x|I)\;P(y|x.I)\;dx = \int P(x,y|I)\;dx = P(y|I)$$

Sufficient statistic

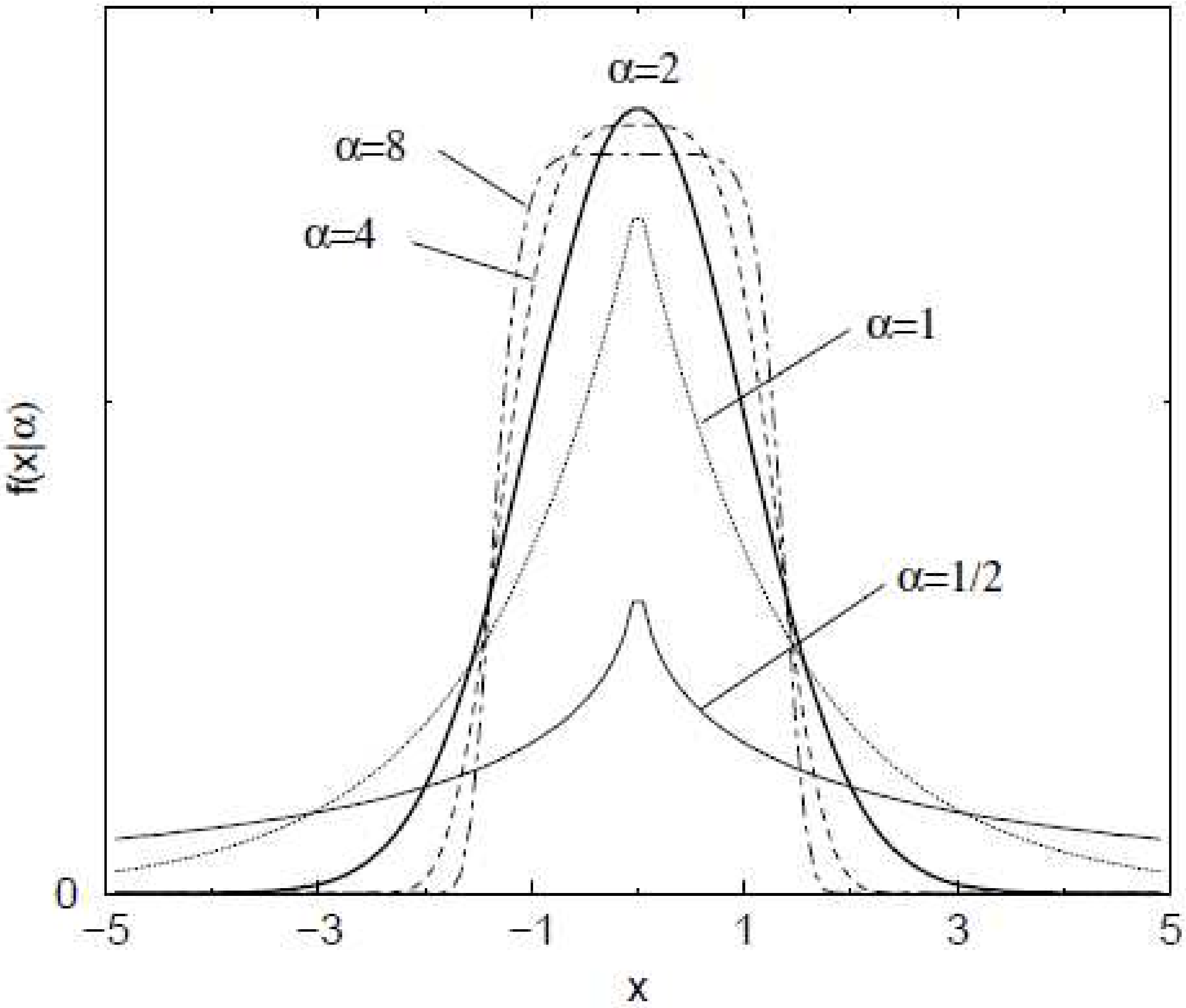
$$\hat{G} = u^2(\hat{G}) \sum_i d_i/\sigma_i^2 \quad , \quad u^2(\hat{G}) = 1/\sum_i 1/\sigma_i^2$$

$$d_i \longrightarrow d_i + \gamma(d_i - \hat{G})$$ invariance!

generalised Gauss :

$$p(d|G,\sigma,\alpha) = \frac{1}{2\sigma\sqrt{2}\Gamma(1+1/\alpha)} \exp\left\{-\left|\frac{d-G}{\sigma\sqrt{2}}\right|^{\alpha}\right\}$$

generalised Gauss



alpha marginalisation

$$p(\vec{d}|G,\vec{\sigma},\alpha) = \frac{1}{\{\Gamma(1+1/\alpha)\}^N} \cdot \prod_i \frac{1}{2\sigma_i\sqrt{2}} \exp\left\{-\left|\frac{d_i - G}{\sigma_i\sqrt{2}}\right|^\alpha\right\}$$

$$p(\vec{d}|G,\vec{\sigma}) = \int_0^\infty \mathrm{d}\alpha \; p(\alpha) p(\vec{d}|G,\vec{\sigma},\alpha)$$

Zellner's maximum data information prior

$$-H(p) = \int p(\mathbf{d},\alpha) \log p(\mathbf{d},\alpha)\, d\mathbf{d}\, d\alpha \,,$$

$$p(\mathbf{d},\alpha) = p(\alpha)\, p(\mathbf{d}|\alpha)$$

$$-H(p) = \int I(\alpha)\, p(\alpha)\, d\alpha + \int p(\alpha) \log p(\alpha)\, d\alpha$$

$$I(\alpha) = \int p(\mathbf{d}|\alpha) \log p(\mathbf{d}|\alpha)\, d\mathbf{d}$$

Zellner's maximum data information prior ctd

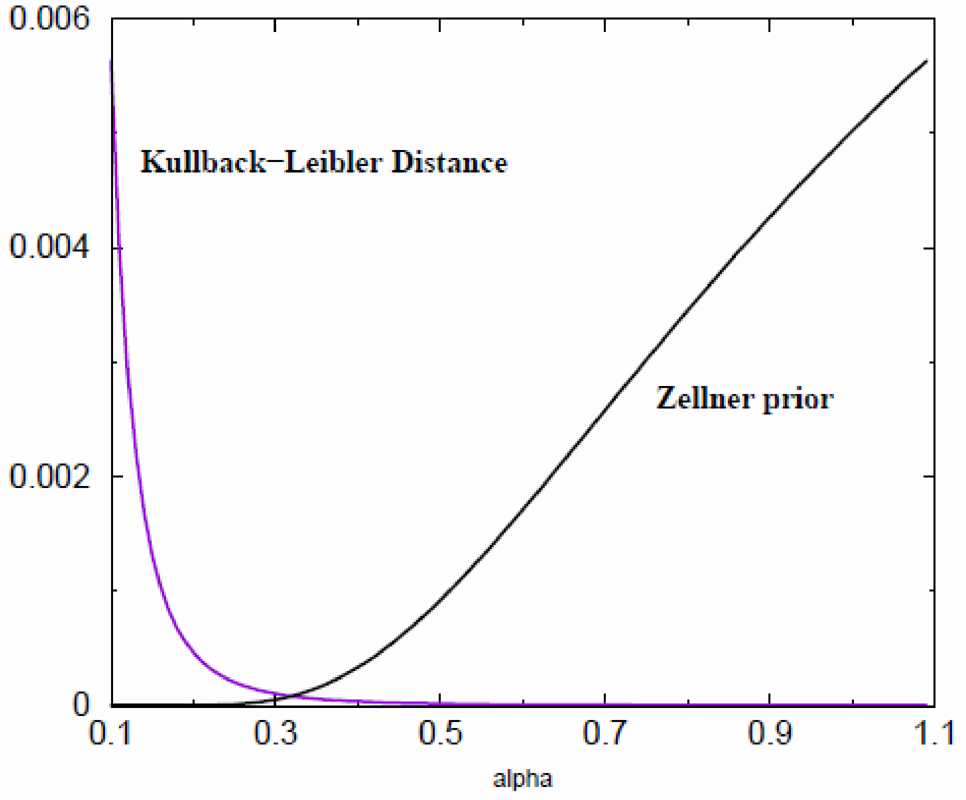
$$I(\alpha) = \int p(\mathbf{d}|\alpha) \log p(\mathbf{d}|\alpha) \, d\mathbf{d}$$

$$\Phi(p) = -\int p(\alpha) \log p(\alpha) \, d\alpha + \int I(\alpha) \, p(\alpha) \, d\alpha$$

$$p(\alpha) = \exp(I(\alpha)) / Z$$

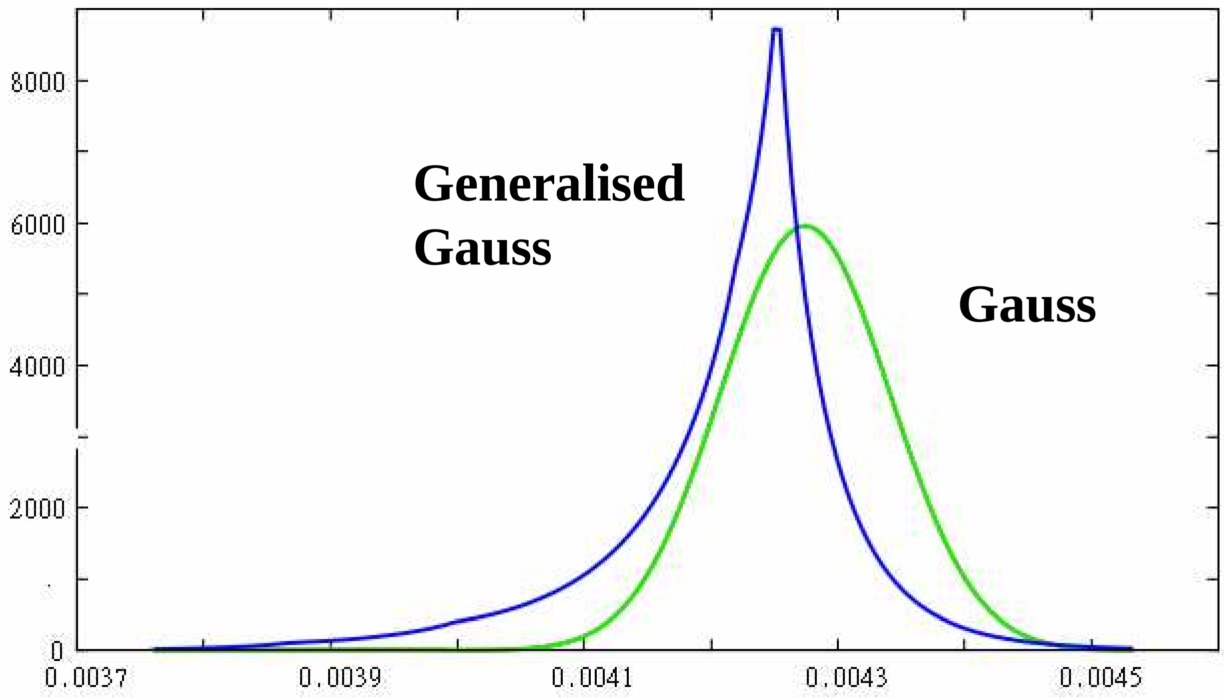
$$p(\alpha) = \frac{\exp\{-1/\alpha\}}{\Gamma(1+1/\alpha)} \frac{1}{Z(\alpha_0)} \quad , \quad 0 \leq \alpha \leq \alpha_0$$

Zellner prior and K/L-distance



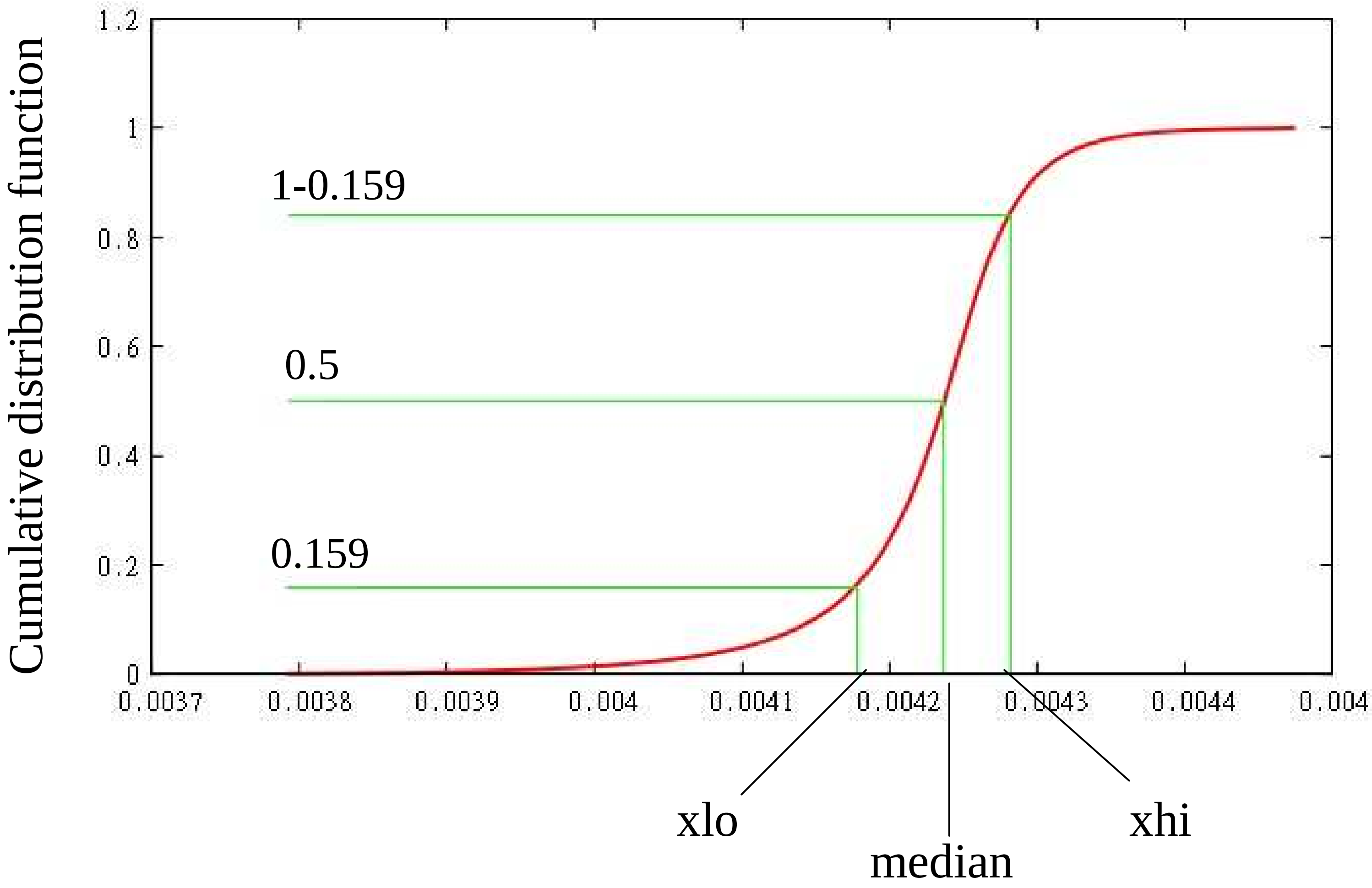
$$K/L(\alpha) = \int dx\, f(x|\alpha+\varepsilon) \log f(x|\alpha),\ \varepsilon=0.001$$

Gauss and generalized Gauss



$\Delta G = G - G_0$

asymmetric posterior (cdf)



Newtonian constant of gravitation

	point est.	uncertainty
least squares	6.674274	(+67, -67)
Gauss generalised	6.674200	(+71, -103)
CODATA 06	6.67428	(+670, -670)

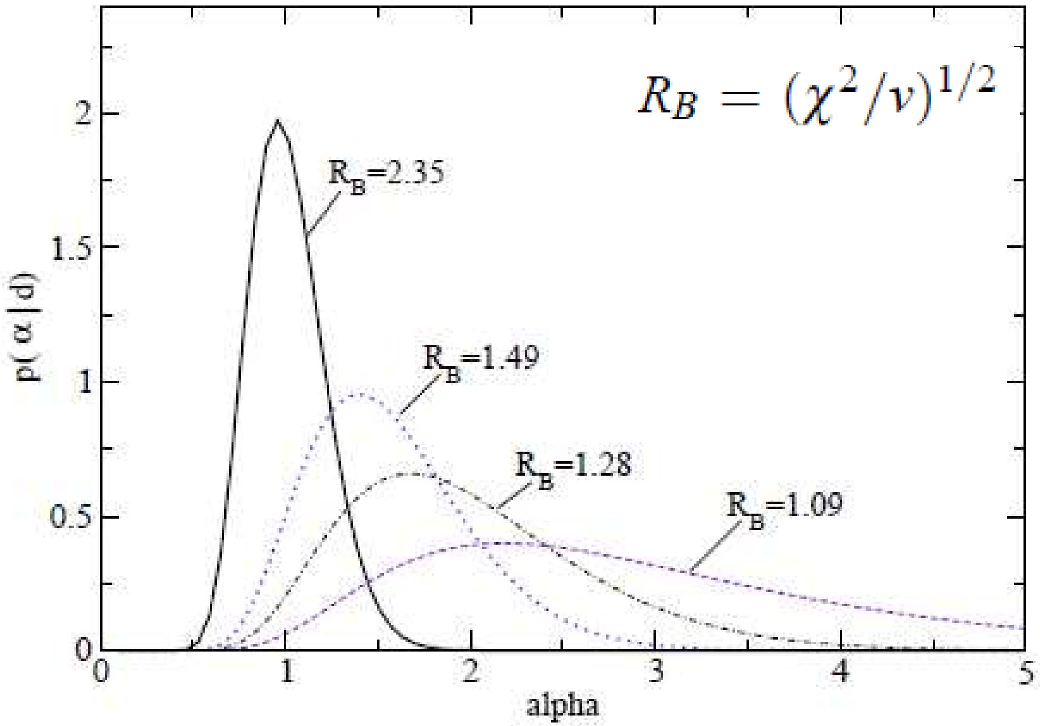
Units of 10^{11} kg^{-1} s^{-2} m^3

posterior alpha distribution

$$p(\mathbf{d}|\alpha,\boldsymbol{\sigma}) = \int dG \; p(G) \; p(\mathbf{d}|G, \alpha,\boldsymbol{\sigma})$$

$$p(\alpha|\mathbf{d},\boldsymbol{\sigma}) = p(\alpha) \; p(\mathbf{d}|\alpha,\boldsymbol{\sigma}) \; / p(\mathbf{d}| \; \boldsymbol{\sigma})$$

alpha distributions, real data



uncertainties:

generate $r_i(0,1]$, scale by $\lambda = \frac{1}{u^2(\hat{G})\sum_i r_i}$ $\tilde{\sigma}_i = 1/\sqrt{\lambda r_i}$

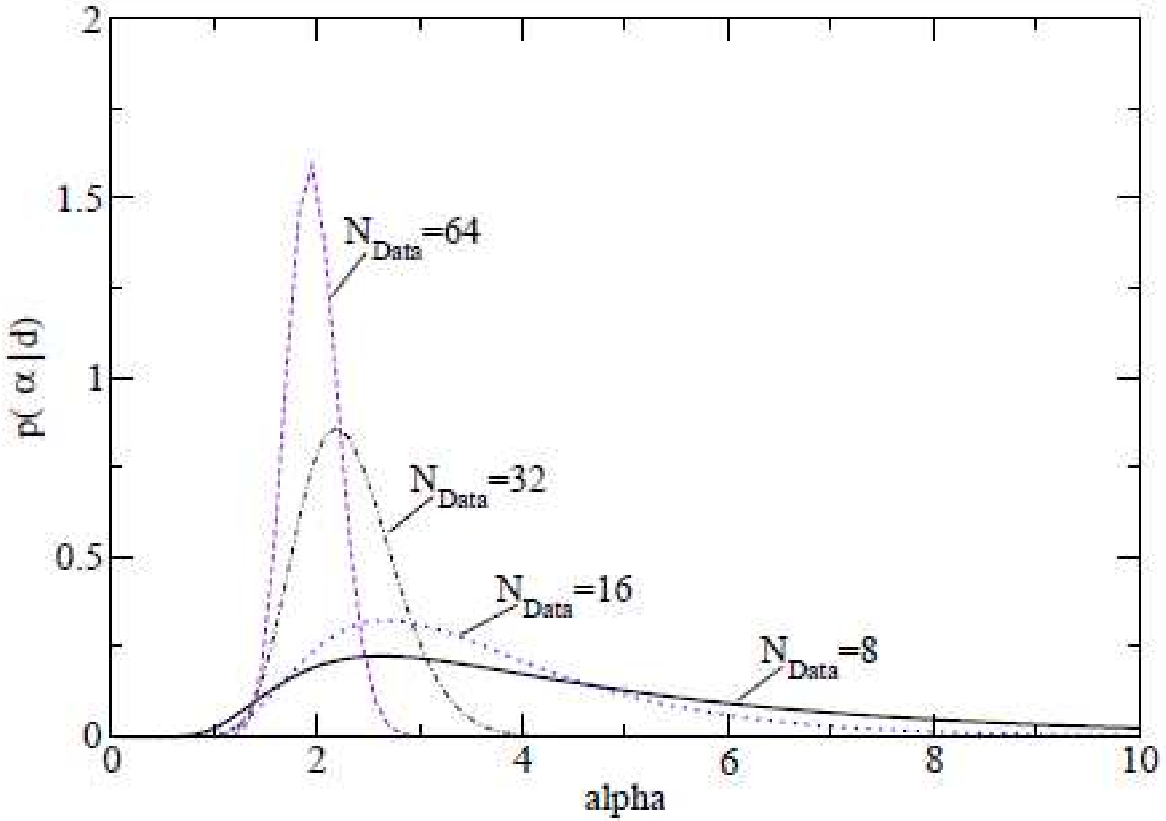
data:

generate $\mathrm{rnd}_G(\hat{G}, u^2(\hat{G}))$

adjust scatter $d_i \to d_i + \gamma(d_i - \hat{G})$

impose $R_\gamma = 1$, $R_\gamma = R_0(1+\gamma)$

alpha distributions, surrogate data



Gauss 1823:

„….the variances of the measurement σ_i^2 *are practically never exactly known………"*

Precision of errors unknown

$$p(\sigma_i|s_i,\omega_i) = \delta\left(\sigma_i - \frac{s_i}{\omega_i}\right)$$

$\langle\omega_i\rangle = 1$ for all i ⟶ $p(\vec{\omega}) = \exp\left\{-\sum_i \omega_i\right\}$

$$p(\vec{d}|G,\vec{s}) = \int d\vec{\omega}\, p(\vec{\omega}) \int d\vec{\sigma} \prod_i \delta\left(\sigma_i - \frac{s_i}{\omega_i}\right) p(d_i|G,\sigma_i)$$

$$x_i = (d_i - G)/s_i\sqrt{2}$$

$$p(\vec{d}|G,\vec{s}) = \prod_i \frac{1}{s_i\sqrt{2\pi}} \int_0^\infty d\omega_i\, \omega_i \exp\left\{-\omega_i - \omega_i^2 x_i^2\right\}$$

error marginalisation ctd

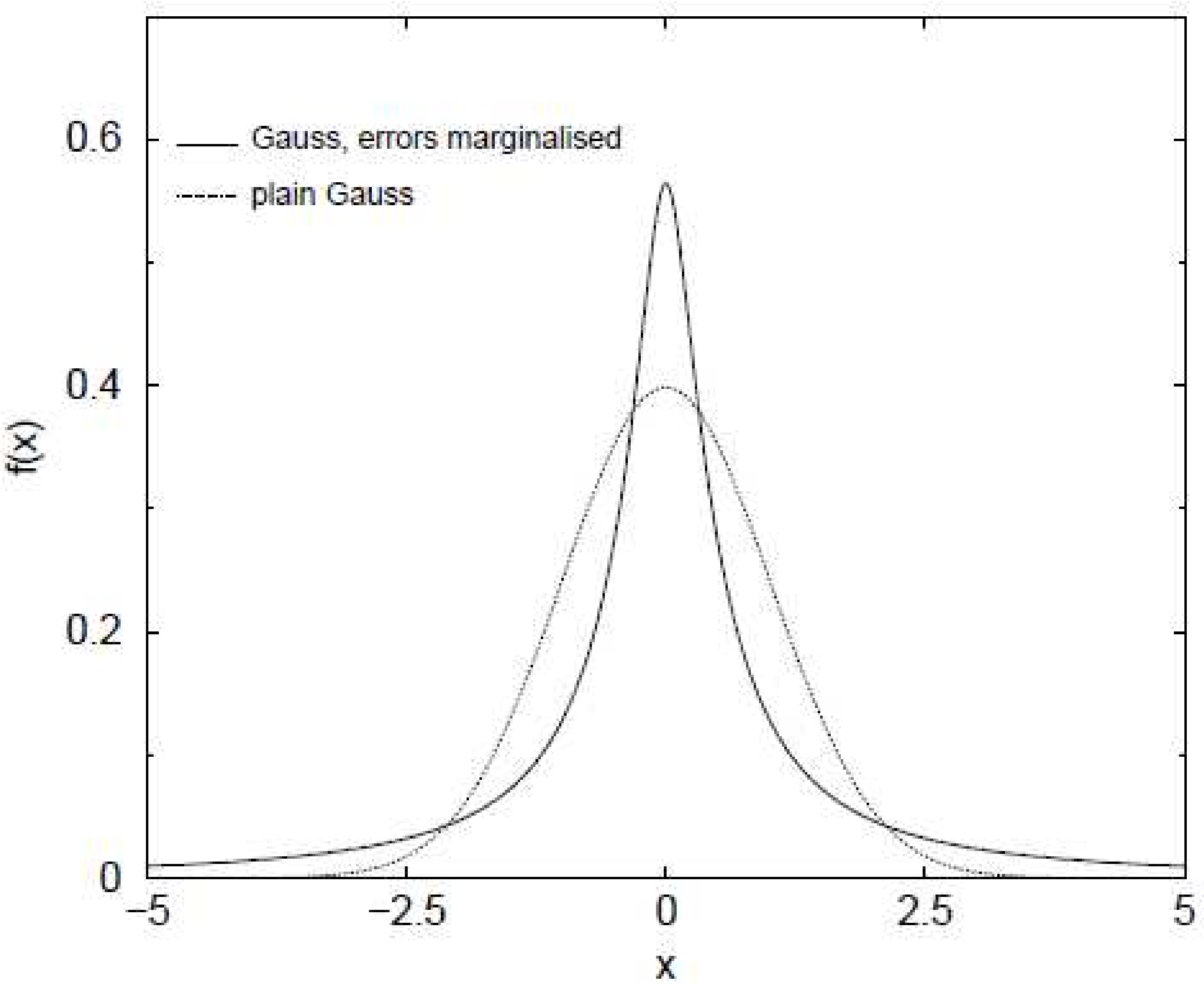
$$x_i = (d_i - G)/s_i\sqrt{2}$$

$$p(\vec{d}|G,\vec{s}) = \prod_i \frac{1}{s_i\sqrt{2\pi}} \frac{1}{2x_i^2}\left[1 - \frac{\sqrt{\pi}}{2x_i} e^{\frac{1}{4x_i^2}} \operatorname{erfc}\left\{\frac{1}{2x_i}\right\}\right]$$

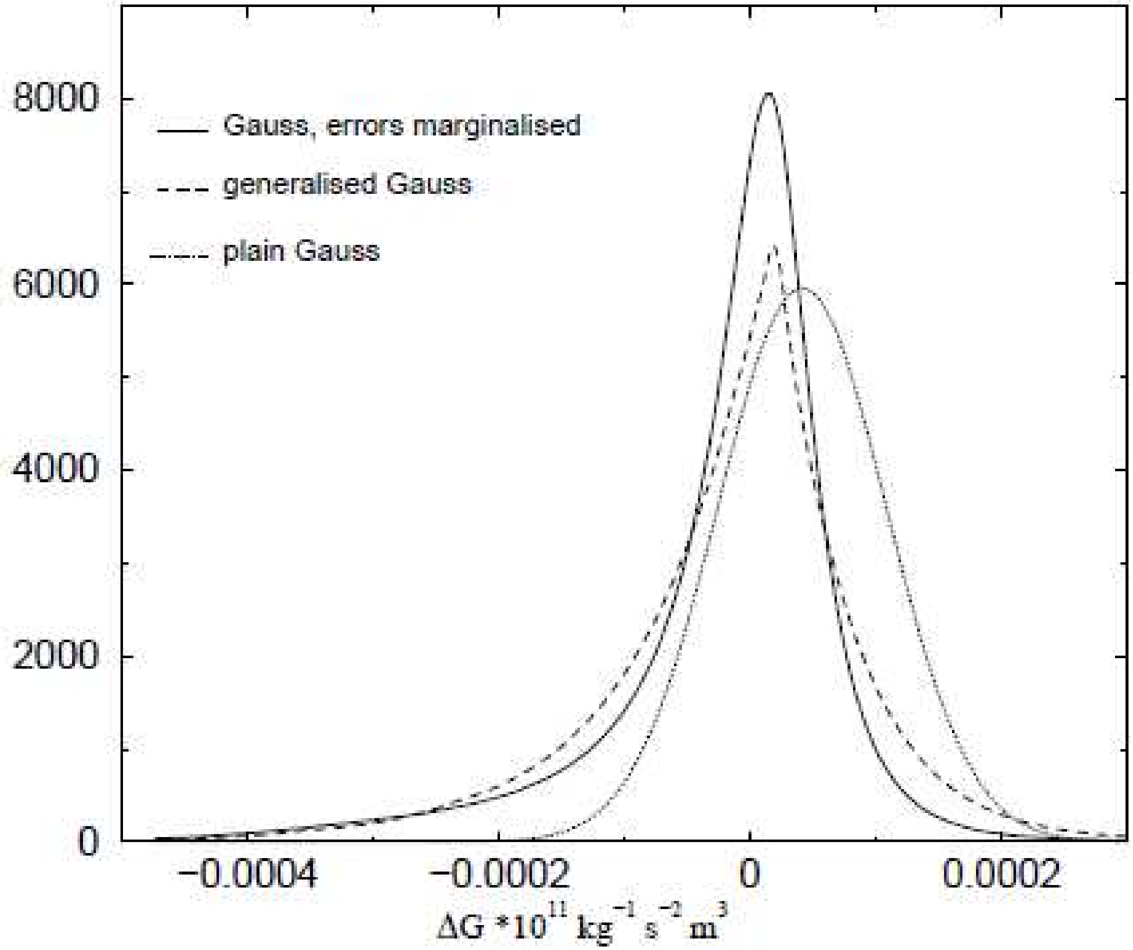
$$z = 1/2x \qquad \operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$$

$$\sqrt{\pi} \cdot z \cdot e^{z^2} \operatorname{erfc}\{z\} \sim 1 - \frac{1}{2z^2} + \frac{1 \cdot 3}{(2z^2)^2} - \frac{1 \cdot 3 \cdot 5}{(2z^2)^3} + \ldots$$

Gauss & marginalised Gauss



posterior distributions of G

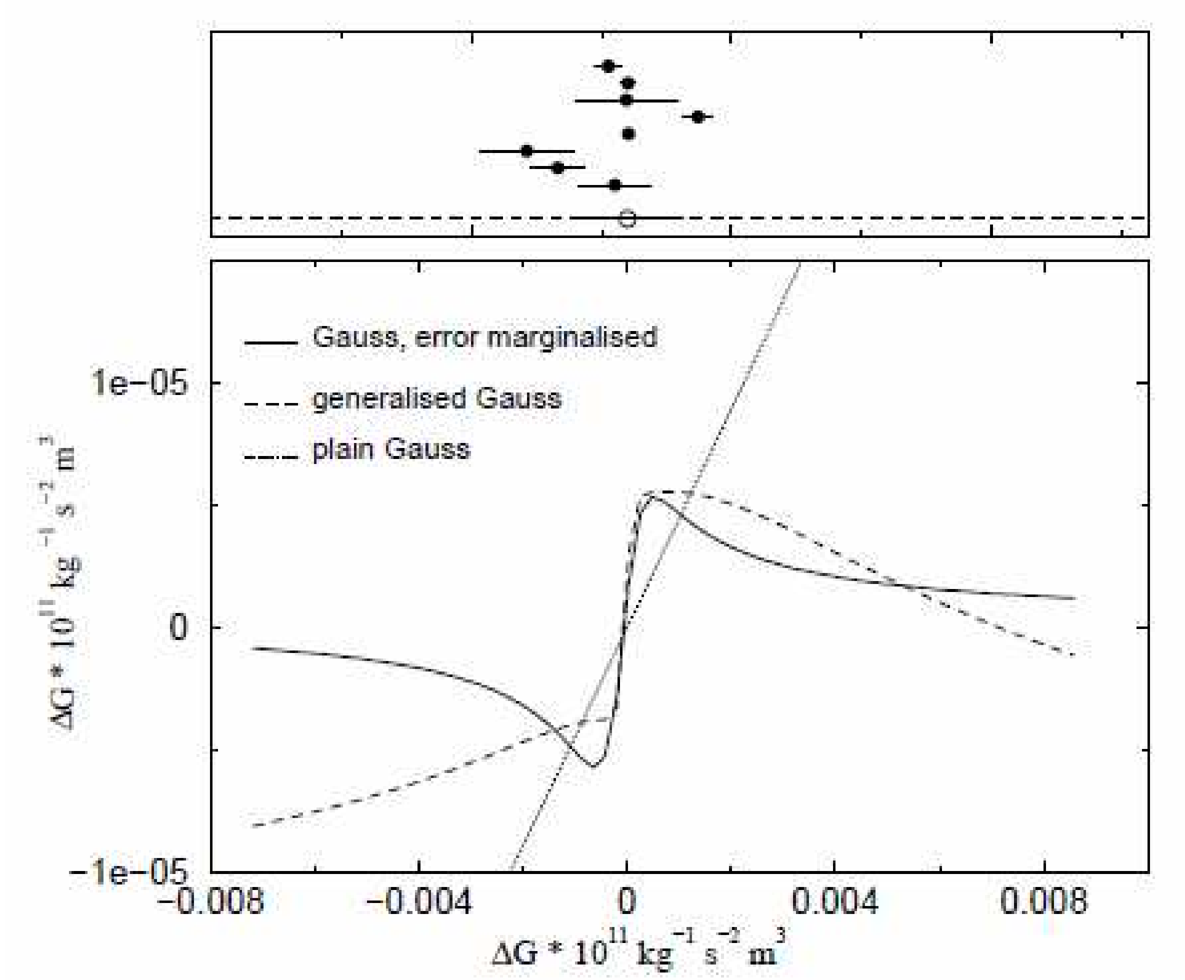


Newtonian constant of gravitation

	point est.	uncertainty
least squares	6.674274	(+67, -67)
Gauss generalised	6.674200	(+71, -103)
Gauss marginalised	6.674233	(+49, -88)
CODATA 06	6.67428	(+670, -670) !!

Units of 10^{11} kg^{-1} s^{-2} m^{3}

robustness in G-estimation



electron charge e and Planck's constant h

CODATA 2006: $e_0 = 1.602\ 176\ 487 \cdot 10^{-19}$ C , $h_0 = 6.626\ 068\ 96 \cdot 10^{-34}$ Js

Josephson constant $K_J = 2e/h = 2(e_0+\Delta e)/(h_0+\Delta h)$

$$\approx 2(e_0/h_0)(1+ \Delta e/e_0 - \Delta h/h_0)$$

v.Klitzing constant $R_K = h/e^2 = (h_0+\Delta h)/(e_0+\Delta e)^2$

$$\approx (h_0/e_0^2)(1+2\ \Delta e/e_0\ )$$

Product $K_J^2 R_K = 4/h = 4/(h_0+ \Delta h) \approx (4/h_0)(1- \Delta h/h_0)$

Likelihood

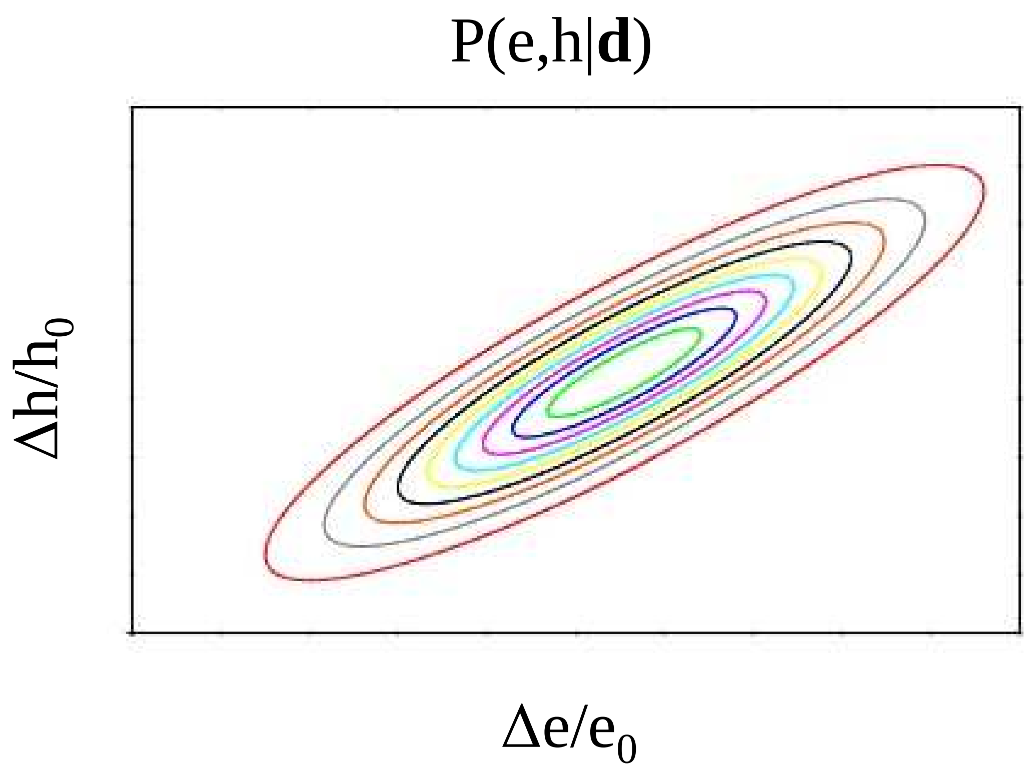
$$L_1(e,h) = \mathrm{p}(\mathrm{d\_R_K}|\mathrm{e,h})$$

$$L_2(e,h) = \mathrm{p}(\mathrm{d\_K_J}|\mathrm{e,h})$$

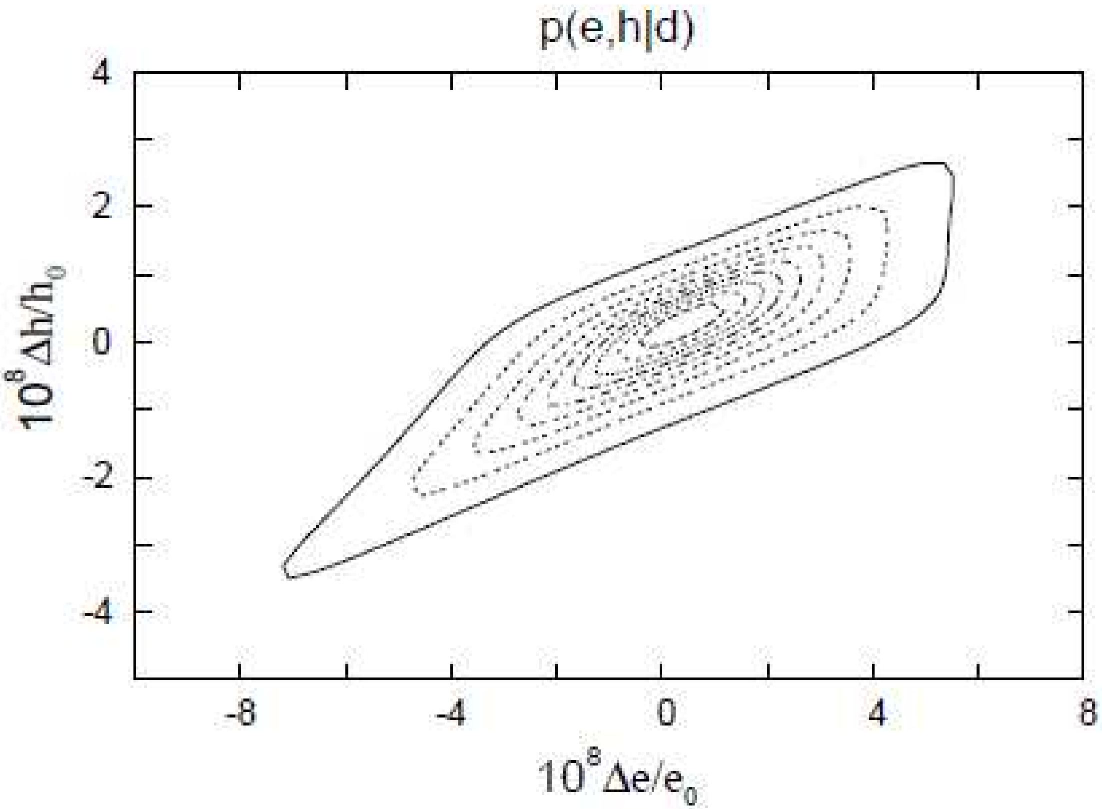
$$L_3(e,h) = \mathrm{p}(\mathrm{d\_K_J{}^2R_K}|\mathrm{e,h})$$

$$L(e,h) = L_1(e,h) * L_2(e,h) * L_3(e,h)$$

2-D Gaussian posterior



e/h posterior



Bayesian result : $P(e,h|D)$

Marginals : $P(e|D) = \int P(e,h|D)\, dh$

$P(h|D) = \int P(e,h|D)\, de$

Summaries : mean & variance

median & tails

results on e and h

TABLE 3. Estimates of e and h using traditional least squares and marginalised Gauss (16). CODATA-06 adjustments are shown for comparison.

	$e \cdot 10^{19}$ / C
least squares	1.602 176 459 (+30, -30)
marg. Gauss	1.602 176 454 (+27, -33)
CODATA-06	1.602 176 487 (+40, -40)
	$h \cdot 10^{34}$ / Js
least squares	6.626 068 88 (+22,-22)
marg. Gauss	6.626 068 86 (+16,-25)
CODATA-06	6.626 068 96 (+33,-33)

THE END

Thank you for your attention,
the talk is open for discussion