Bayesian Modeling, Inference, Prediction and Decision-Making

2c: Continuous Outcomes; Gaussian Modeling

David Draper

Department of Applied Mathematics and Statistics University of California, Santa Cruz

> draper@ams.ucsc.edu www.ams.ucsc.edu/~draper

> > eBay/Google

10 Fridays, 11 Jan-22 Mar 2013 (except 25 Jan)

Short course web page:

www.ams.ucsc.edu/~draper/eBay-Google-2013.html

© 2013 David Draper (all rights reserved)

Continuous Outcomes

For **continuous outcomes** there's an analogue of de Finetti's Theorem that's **equally central** to Bayesian model-building (e.g., Bernardo and Smith, 1994):

de Finetti's Theorem for Continuous Outcomes.

If Y_1, Y_2, \ldots is an infinitely exchangeable sequence of **real-valued** random quantities with probability measure p, there exists a probability measure Q over \mathcal{D} , the space of all distribution functions on R, such that the joint distribution function of Y_1, \ldots, Y_n has the form

$$p(y_1,\ldots,y_n) = \int_{\mathcal{D}} \prod_{i=1}^n F(y_i) \, dQ(F), \qquad (1)$$

where $Q(F) \stackrel{P}{=} \lim_{n \to \infty} p(F_n)$ and F_n is the **empirical** cumulative distribution function based on Y_1, \ldots, Y_n .

In other words, exchangeability of real-valued observables is **equivalent** to the hierarchical model

F	\sim	p(F)	(prior)	
$(Y_1,\ldots,Y_n F)$	$\stackrel{\mathrm{IID}}{\sim}$	F	(likelihood)	(2)

for some prior distribution p on the set \mathcal{D} of all possible distribution functions.

This prior makes the continuous form of de Finetti's Theorem **considerably harder to apply**: to take the elicitation task seriously is to try to specify a measure on a **function space** (*F* is in effect an **infinite-dimensional** parameter).

(NB This task is not unique to Bayesians—it's equivalent to asking "Where does the likelihood come from?" in frequentist analyses of observational data.)

Continuous Outcomes (continued)

What people often do in practice is to appeal to considerations that narrow down the field, such as an *a priori* judgment that the Y_i ought to be **symmetrically** distributed about a measure of center μ , and then try to use a fairly **rich parametric family** satisfying (e.g.) the symmetry restriction as a substitute for all of \mathcal{D} .

Strictly speaking you're not supposed to look at the Y_i while specifying your prior on \mathcal{D} — this can lead to a failure to fully assess and propagate **model uncertainty** — but not doing so can permit the data to surprise you in ways that would make you want to go back and revise your prior (an example of **Cromwell's Rule** in action).

As mentioned earlier, in this short course I'll suggest two potential ways out of this dilemma, based on **out-of-sample predictive validation** (the model-checking in the LOS data above was an example of this; also see topic 5) and **Bayesian nonparametrics/semi-parametrics** (which we will examine in topic 5).

<u>Case Study:</u> Measurement of physical constants. What used to be called the National Bureau of Standards (NBS) in Washington, DC, conducts extremely high precision measurement of physical constants, such as the actual weight of so-called **check-weights** that are supposed to serve as reference standards (like the official kg).

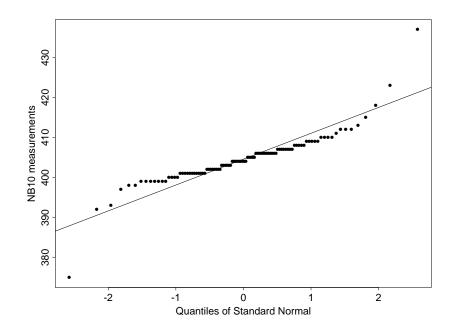
In 1962–63, for example, n = 100 weighings (listed below) of a block of metal called **NB10**, which was supposed to weigh exactly 10g, were made under conditions **as close to IID as possible** (Freedman et al., 1998).

Value	375	392	393	397	398	399	400	401
Frequency	1	1	1	1	2	7	4	12
Value	402	403	404	405	406	407	408	409
Frequency	8	6	9	5	12	8	5	5
Value	410	411	412	413	415	418	423	437

NB10 Modeling

Q: (a) How much does NB10 really weigh? (b) How certain are you given the data that the true weight of NB10 is less than (say) 405.25? And (c) How accurately can you predict the 101st measurement?

The graph below is a **normal qqplot** of the 100 measurements $y = (y_1, \ldots, y_n)$, which have a mean of $\overline{y} = 404.6$ (the units are **micrograms below 10g**) and an SD of s = 6.5.



Evidently it's plausible in answering these questions to assume **symmetry** of the "underlying distribution" *F* in de Finetti's Theorem.

One standard choice, for instance, is the **Gaussian**:

$$\begin{array}{ll} (\mu, \sigma^2) & \sim & p(\mu, \sigma^2) \\ (Y_i | \mu, \sigma^2) & \stackrel{\text{IID}}{\sim} & N(\mu, \sigma^2) \,. \end{array}$$
(3)

Here $N(\mu, \sigma^2)$ is the familiar **normal density**

$$p(y_i|\mu,\sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{y_i-\mu}{\sigma}\right)^2\right].$$
 (4)

Gaussian Modeling

Even though you can see from the previous graph that (3) is **not a good model** for the NB10 data, I'm going to fit it to the data for practice in working with the normal distribution from a Bayesian point of view (later we'll **improve** upon the Gaussian).

(3) is more **complicated** than the models in the AMI and LOS case studies because the parameter θ here is a **vector**: $\theta = (\mu, \sigma^2)$.

To warm up for this new complexity, let's first consider a **cut-down version of the model** in which we pretend that σ is known to be $\sigma_0 = 6.5$ (the sample SD).

This simpler model is then

$$\left\{\begin{array}{ccc} \mu & \sim & p(\mu) \\ IID & IID \\ (Y_i|\mu) & \sim & N(\mu, \sigma_0^2) \end{array}\right\}.$$
 (5)

The likelihood function in this model is

$$l(\mu|y) = \prod_{i=1}^{n} \frac{1}{\sigma_{0}\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma_{0}^{2}}(y_{i}-\mu)^{2}\right]$$

$$= c \exp\left[-\frac{1}{2\sigma_{0}^{2}}\sum_{i=1}^{n}(y_{i}-\mu)^{2}\right]$$

$$= c \exp\left[-\frac{1}{2\sigma_{0}^{2}}\left(\sum_{i=1}^{n}y_{i}^{2}-2\mu\sum_{i=1}^{n}y_{i}+n\mu^{2}\right)\right]$$

$$= c \exp\left[-\frac{1}{2\left(\frac{\sigma_{0}^{2}}{n}\right)}(\mu-\bar{y})^{2}\right].$$
(6)

Thus the likelihood function, when thought of as a **density** for μ , is a **normal distribution** with mean \overline{y} and SD $\frac{\sigma_0}{\sqrt{n}}$.

Gaussian Modeling (continued)

Notice that this SD is the same as the frequentist standard error for \overline{Y} based on an IID sample of size n from the $N(\mu, \sigma_0^2)$ distribution.

(6) also shows that the sample mean \bar{y} is a **sufficient statistic** for μ in model (5).

In finding the conjugate prior for μ , it would be nice if the **product of two normal distributions is another normal distribution**, because that would demonstrate that the conjugate prior is normal.

Suppose therefore, to see where it leads, that the **prior for** μ is (say) $p(\mu) = N(\mu_0, \sigma_{\mu}^2)$.

Then Bayes's Theorem would give

$$p(\mu|y) = c p(\mu) l(\mu|y)$$
(7)
= $c \exp\left[-\frac{1}{2\sigma_{\mu}^{2}}(\mu - \mu_{0})^{2}\right] \exp\left[-\frac{n}{2\sigma_{0}^{2}}(\mu - \bar{y})^{2}\right]$
= $c \exp\left\{-\frac{1}{2}\left[\frac{(\mu - \mu_{0})^{2}}{\sigma_{\mu}^{2}} + \frac{n(\mu - \bar{y})^{2}}{\sigma_{0}^{2}}\right]\right\},$

and we want this to be of the form

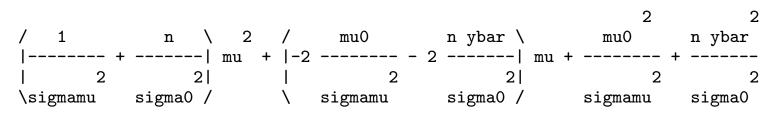
$$p(\mu|y) = c \exp\left\{-\frac{1}{2} \left[A(\mu - B)^2 + C\right]\right\}$$

= $c \exp\left\{-\frac{1}{2} \left[A\mu^2 - 2AB\mu + (AB^2 + C)\right]\right\}$ (8)

for some B, C, and A > 0.

Maple can help see if this works:

> collect((mu - mu0)^2 / sigmamu² +
 n * (mu - ybar)² / sigma0², mu);



6

Gaussian Modeling

Matching coefficients for A and B (we don't really care about C) gives

$$A = \frac{1}{\sigma_{\mu}^{2}} + \frac{n}{\sigma_{0}^{2}} \quad \text{and} \quad B = \frac{\frac{\mu_{0}}{\sigma_{\mu}^{2}} + \frac{ny}{\sigma_{0}^{2}}}{\frac{1}{\sigma_{\mu}^{2}} + \frac{n}{\sigma_{0}^{2}}}.$$
 (9)

Since A > 0 this demonstrates two things: (1) the **conjugate prior** for μ in model (5) is **normal**, and (2) the **conjugate updating rule** (when σ_0 is assumed known) is

$$\left\{ \begin{array}{c} \mu \sim N\left(\mu_{0}, \sigma_{\mu}^{2}\right) \\ \left(Y_{i}|\mu\right) \stackrel{\text{IID}}{\sim} N\left(\mu, \sigma_{0}^{2}\right), \\ i = 1, \dots, n \end{array} \right\} \rightarrow \left(\mu|y\right) = \left(\mu|\overline{y}\right) = N\left(\mu_{*}, \sigma_{*}^{2}\right), \quad (10)$$

where the posterior mean and variance are given by

$$\mu_* = B = \frac{\left(\frac{1}{\sigma_{\mu}^2}\right)\mu_0 + \left(\frac{n}{\sigma_0^2}\right)\bar{y}}{\frac{1}{\sigma_{\mu}^2} + \frac{n}{\sigma_0^2}} \quad \text{and} \quad \sigma_*^2 = A^{-1} = \frac{1}{\frac{1}{\sigma_{\mu}^2} + \frac{n}{\sigma_0^2}}.$$
 (11)

It becomes useful in understanding the meaning of these expressions to define the **precision** of a distribution, which is just the **reciprocal** of its variance: whereas the variance and SD scales measure **uncertainty**, the precision scale quantifies **information** about an unknown.

With this convention, (10) and (11) have a series of nice **intuitive interpretations**, as follows:

• The **prior**, considered as an **information source**, is Gaussian with mean μ_0 , variance σ_{μ}^2 , and **precision** $\frac{1}{\sigma_{\mu}^2}$, and when viewed as a data set consists of n_0 (to be determined below) observations;

• The likelihood, considered as an information source, is Gaussian with mean \bar{y} , variance $\frac{\sigma_0^2}{n}$, and precision $\frac{n}{\sigma_0^2}$, and when viewed as a data set consists of n observations;

Gaussian Modeling (continued)

• The **posterior**, considered as an **information source**, is Gaussian, and the posterior mean is a **weighted average** of the prior mean and data mean, with weights given by the **prior** and **data precisions**;

The posterior precision (the reciprocal of the posterior variance) is just the sum of the prior and data precisions (this is why Bayesians invented the idea of precision—on this scale information about μ in model (5) is additive); and

• Rewriting μ_* as

$$\mu_{*} = \frac{\left(\frac{1}{\sigma_{\mu}^{2}}\right)\mu_{0} + \left(\frac{n}{\sigma_{0}^{2}}\right)\bar{y}}{\frac{1}{\sigma_{\mu}^{2}} + \frac{n}{\sigma_{0}^{2}}} = \frac{\left(\frac{\sigma_{0}^{2}}{\sigma_{\mu}^{2}}\right)\mu_{0} + n\bar{y}}{\frac{\sigma_{0}^{2}}{\sigma_{\mu}^{2}} + n},$$
(12)

you can see that the **prior sample size** is

$$n_0 = \frac{\sigma_0^2}{\sigma_\mu^2} = \frac{1}{\left(\frac{\sigma_\mu}{\sigma_0}\right)^2},\tag{13}$$

which makes sense: the **bigger** σ_{μ} is in relation to σ_0 , the **less prior information** is being incorporated in the conjugate updating (10).

Bayesian inference with multivariate θ . Returning now to model (3) with σ^2 unknown, (as mentioned above) this model has a (k = 2)-dimensional **parameter vector** $\theta = (\mu, \sigma^2)$.

When k > 1 you can still use Bayes' Theorem directly to obtain the **joint posterior distribution**,

$$p(\theta|y) = p(\mu, \sigma^2|y) = c p(\theta) l(\theta|y)$$

= $c p(\mu, \sigma^2) l(\mu, \sigma^2|y),$ (14)

<u>Multivariate</u> Unknown θ

where $y = (y_1, \ldots, y_n)$, although making this calculation directly requires a k-dimensional **integration** to evaluate the normalizing constant c; for example, in this case

$$c = [p(y)]^{-1} = \left(\iint p(\mu, \sigma^2, y) \, d\mu \, d\sigma^2 \right)^{-1}$$
$$= \left(\iint p(\mu, \sigma^2) \, l(\mu, \sigma^2 | y) \, d\mu \, d\sigma^2 \right)^{-1}. \tag{15}$$

Usually, however, you'll be more interested in the marginal posterior distributions, in this case $p(\mu|y)$ and $p(\sigma^2|y)$.

Obtaining these requires k integrations, each of dimension (k-1), a process that people refer to as marginalization or integrating out the nuisance parameters — for example,

$$p(\mu|y) = \int_0^\infty p(\mu, \sigma^2|y) \, d\sigma^2 \,. \tag{16}$$

Predictive distributions also involve a k-dimensional integration: for example, with $y = (y_1, \ldots, y_n)$,

$$p(y_{n+1}|y) = \iint p(y_{n+1}, \mu, \sigma^2|y) d\mu d\sigma^2 \qquad (17)$$
$$= \iint p(y_{n+1}|\mu, \sigma^2) p(\mu, \sigma^2|y) d\mu d\sigma^2.$$

And, finally, if you're interested in a **function of the parameters**, you also have some more hard integrations ahead of you.

For instance, suppose you wanted the posterior distribution for the **coefficient of variation** $\lambda = g_1(\mu, \sigma^2) = \frac{\sqrt{\sigma^2}}{\mu}$ in model (3).

<u>Multivariate</u> Unknown θ

Then one fairly direct way to get this posterior (e.g., Bernardo and Smith, 1994) is to (a) introduce a **second function** of the parameters, say $\eta = g_2(\mu, \sigma^2)$, such that the mapping $f = (g_1, g_2)$ from (μ, σ^2) to (λ, η) is **invertible**; (b) compute the joint posterior for (λ, η) through the usual **change-of-variables formula**

$$p(\lambda,\eta|y) = p_{\mu,\sigma^2} \big[f^{-1}(\lambda,\eta)|y \big] |J_{f^{-1}}(\lambda,\eta)|, \qquad (18)$$

where $p_{\mu,\sigma^2}(\cdot,\cdot|y)$ is the joint posterior for μ and σ^2 and $|J_{f^{-1}}|$ is the **determinant** of the **Jacobian** of the inverse transformation; and (c) **marginalize** in λ by integrating out η in $p(\lambda,\eta|y)$, in a manner analogous to (16).

Here, for instance, $\eta = g_2(\mu, \sigma^2) = \mu$ would create an invertible f, with **inverse** defined by $(\mu = \eta, \sigma^2 = \lambda^2 \eta^2)$; the **Jacobian determinant** comes out $2\lambda\eta^2$ and (18) becomes $p(\lambda, \eta|y) = 2\lambda\eta^2 p_{\mu,\sigma^2}(\eta, \lambda^2\eta^2|y)$.

This process involves **two integrations**, one (of dimension k) to get the normalizing constant that defines (18) and one (of dimension (k-1)) to get rid of η .

You can see that when k is a lot bigger than 2, all these integrals may create **severe computational problems** this has been the **big stumbling block** for applied Bayesian work for a long time.

More than 200 years ago Laplace (1774) — perhaps the second Bayesian in history (after Bayes himself) — developed, as one avenue of solution to this problem, what people now call Laplace approximations to high-dimensional integrals of the type arising in Bayesian calculations (see, e.g., Tierney and Kadane, 1986).

Starting in the next case study after this one, we'll use another, computationally intensive, **simulation-based** approach: **Markov chain Monte Carlo** (MCMC).

Gaussian Modeling

Back to model (3). The conjugate prior for $\theta = (\mu, \sigma^2)$ in this model (e.g., Gelman et al., 2003) turns out to be most simply described **hierarchically**:

$$\sigma^{2} \sim \operatorname{SI-}\chi^{2}(\nu_{0}, \sigma_{0}^{2})$$
$$(\mu|\sigma^{2}) \sim N\left(\mu_{0}, \frac{\sigma^{2}}{\kappa_{0}}\right).$$
(19)

Here saying that $\sigma^2 \sim \text{SI-}\chi^2(\nu_0, \sigma_0^2)$, where SI stands for **scaled inverse**, amounts to saying that the precision $\tau = \frac{1}{\sigma^2}$ follows a **scaled** χ^2 distribution with parameters ν_0 and σ_0^2 .

The scaling is chosen so that σ_0^2 can be interpreted as a **prior estimate** of σ^2 , with ν_0 the **prior sample size** of this estimate (i.e., **think of a prior data set with** ν_0 **observations and sample SD** σ_0).

Since χ^2 is a special case of the Gamma distribution, SI- χ^2 must be a special case of the **inverse Gamma** family — its **density** (see Gelman et al. (2003), Appendix A) is

$$\sigma^{2} \sim \text{SI-}\chi^{2}(\nu_{0},\sigma_{0}^{2}) \leftrightarrow$$

$$p(\sigma^{2}) = \frac{\left(\frac{1}{2}\nu_{0}\right)^{\frac{1}{2}\nu_{0}}}{\Gamma\left(\frac{1}{2}\nu_{0}\right)} \left(\sigma_{0}^{2}\right)^{\frac{1}{2}\nu_{0}} \left(\sigma^{2}\right)^{-\left(1+\frac{1}{2}\nu_{0}\right)} \exp\left(\frac{-\nu_{0}\sigma_{0}^{2}}{2\sigma^{2}}\right).$$
(20)

As may be verified with Maple, this distribution has **mean** (provided that $\nu_0 > 2$) and **variance** (provided that $\nu_0 > 4$) given by

$$E(\sigma^2) = \frac{\nu_0}{\nu_0 - 2} \sigma_0^2 \quad \text{and} \quad V(\sigma^2) = \frac{2\nu_0^2}{(\nu_0 - 2)^2(\nu_0 - 4)} \sigma_0^4.$$
(21)

Gaussian Modeling (continued)

The parameters μ_0 and κ_0 in the second level of the prior model (19), $(\mu | \sigma^2) \sim N\left(\mu_0, \frac{\sigma^2}{\kappa_0}\right)$, have **simple parallel interpretations** to those of σ_0^2 and ν_0 : μ_0 is the **prior estimate** of μ , and κ_0 is the **prior effective sample size** of this estimate.

The likelihood function in model (3), with both μ and σ^2 unknown, is

$$l(\mu, \sigma^{2}|y) = c \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^{2}}} \exp\left[-\frac{1}{2\sigma^{2}}(y_{i}-\mu)^{2}\right]$$

$$= c (\sigma^{2})^{-\frac{1}{2}n} \exp\left[-\frac{1}{2\sigma^{2}}\sum_{i=1}^{n}(y_{i}-\mu)^{2}\right]$$

$$= c (\sigma^{2})^{-\frac{1}{2}n} \exp\left[-\frac{1}{2\sigma^{2}}\left(\sum_{i=1}^{n}y_{i}^{2}-2\mu\sum_{i=1}^{n}y_{i}+n\mu^{2}\right)\right].$$

(22)

The expression in brackets in the last line of (22) is

$$\begin{bmatrix} \cdot \end{bmatrix} = -\frac{1}{2\sigma^2} \left[\sum_{i=1}^n y_i^2 + n(\mu - \bar{y})^2 - n\bar{y}^2 \right]$$
(23)
$$= -\frac{1}{2\sigma^2} \left[n(\mu - \bar{y})^2 + (n - 1)s^2 \right],$$

where $s^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2$ is the sample variance. Thus

$$l(\mu, \sigma^2 | y) = c \, (\sigma^2)^{-\frac{1}{2}n} \exp\left\{-\frac{1}{2\sigma^2} \left[n(\mu - \bar{y})^2 + (n - 1)s^2\right]\right\},\,$$

and it's clear that the **vector** (\bar{y}, s^2) is **sufficient** for $\theta = (\mu, \sigma^2)$ in this model, i.e., $l(\mu, \sigma^2|y) = l(\mu, \sigma^2|\bar{y}, s^2)$.

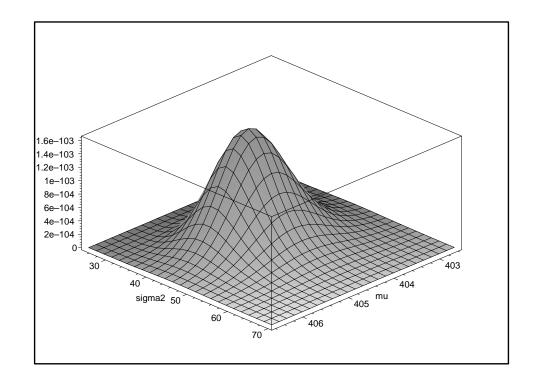
Gaussian Analysis

Maple can be used to make **3D** and **contour plots** of this likelihood function with the NB10 data:

- > l := (mu, sigma2, ybar, s2, n) -> sigma2^(n / 2) *
 exp((n * (mu ybar)^2 + (n 1) * s2) / (2 * sigma2));
- 1 := (mu, sigma2, ybar, s2, n) ->

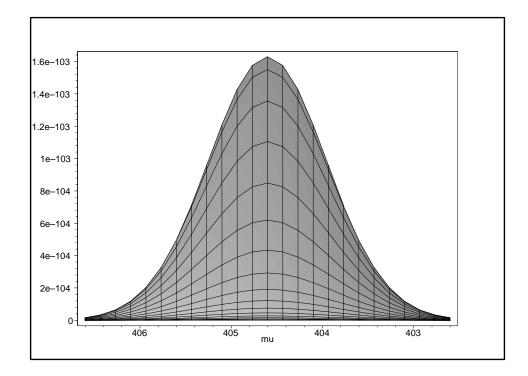
2 (- 1/2 n) n (mu - ybar) + (n - 1) s2 sigma2 exp(- 1/2 ------) sigma2

- > plotsetup(x11);
- > plot3d(l(mu, sigma2, 404.6, 42.25, 100), mu = 402.6 .. 406.6, sigma2 = 25 .. 70);

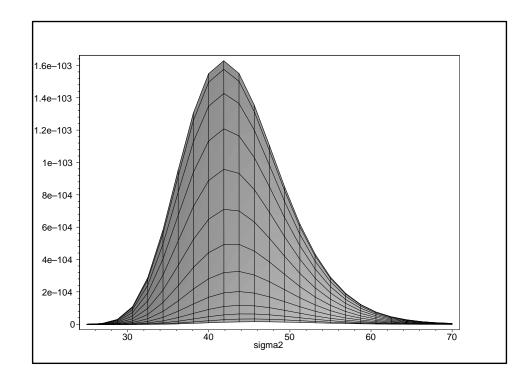


You can use the mouse to **rotate** 3D plots and get **other useful views** of them:

Gaussian Analysis

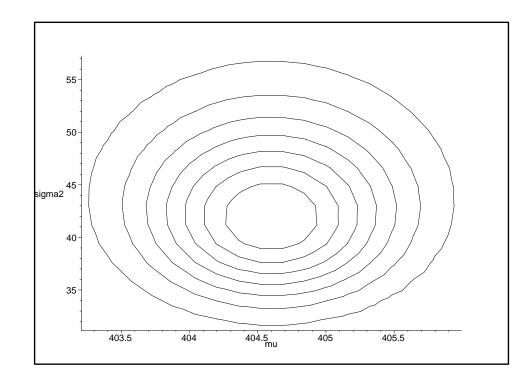


The **projection** or **shadow plot** of μ looks a lot like a **normal** (or maybe a *t*) distribution.



And the shadow plot of σ^2 looks a lot like a **Gamma** (or maybe an **inverse Gamma**) distribution.

Gaussian Analysis



The **contour plot** shows that μ and σ^2 are **uncorrelated** in the likelihood distribution, and the **skewness** of the marginal distribution of σ^2 is also evident.

Posterior analysis. Having adopted the **conjugate prior** (19), what I'd like next is simple expressions for the **marginal posterior distributions** $p(\mu|y)$ and $p(\sigma^2|y)$ and for **predictive distributions** like $p(y_{n+1}|y)$.

Fortunately, in model (3) all of the integrations (such as (16) and (17)) may be done analytically (see, e.g., Bernardo and Smith 1994), yielding the following results:

$$(\sigma^{2}|y,\mathcal{G}) \sim \operatorname{SI-}\chi^{2}(\nu_{n},\sigma_{n}^{2}),$$

$$(\mu|y,\mathcal{G}) \sim t_{\nu_{n}}\left(\mu_{n},\frac{\sigma_{n}^{2}}{\kappa_{n}}\right), \text{ and} \qquad (24)$$

$$(y_{n+1}|y,\mathcal{G}) \sim t_{\nu_{n}}\left(\mu_{n},\frac{\kappa_{n}+1}{\kappa_{n}}\sigma_{n}^{2}\right).$$

NB10 Gaussian Analysis

In the above expressions

$$\nu_{n} = \nu_{0} + n,
\sigma_{n}^{2} = \frac{1}{\nu_{n}} \left[\nu_{0} \sigma_{0}^{2} + (n-1)s^{2} + \frac{\kappa_{0}n}{\kappa_{0} + n} (\bar{y} - \mu_{0})^{2} \right], \quad (25)
\mu_{n} = \frac{\kappa_{0}}{\kappa_{0} + n} \mu_{0} + \frac{n}{\kappa_{0} + n} \bar{y}, \quad \text{and}
\kappa_{n} = \kappa_{0} + n,$$

 \bar{y} and s^2 are the usual **sample mean** and **variance** of y, and \mathcal{G} denotes the assumption of the **Gaussian model**.

Here $t_{\nu}(\mu, \sigma^2)$ is a **scaled** version of the usual t_{ν} distribution, i.e., $W \sim t_{\nu}(\mu, \sigma^2) \iff \frac{W-\mu}{\sigma} \sim t_{\nu}$.

The scaled t distribution (see, e.g., Gelman et al. (2003) Appendix A) has **density**

$$\eta \sim t_{\nu}(\mu, \sigma^2) \leftrightarrow p(\eta) = \frac{\Gamma\left[\frac{1}{2}(\nu+1)\right]}{\Gamma\left(\frac{1}{2}\nu\right)\sqrt{\nu\pi\sigma^2}} \left[1 + \frac{1}{\nu\sigma^2}(\eta-\mu)^2\right]^{-\frac{1}{2}(\nu+1)}.$$
(26)

This distribution has **mean** μ (as long as $\nu > 1$) and **variance** $\frac{\nu}{\nu-2}\sigma^2$ (as long as $\nu > 2$).

Notice that, as with all previous conjugate examples, the posterior mean is again a **weighted average** of the prior mean and data mean, with weights determined by the **prior sample size** and the **data sample size**:

$$\mu_n = \frac{\kappa_0}{\kappa_0 + n} \mu_0 + \frac{n}{\kappa_0 + n} \bar{y}.$$
(27)

NB10 Gaussian Analysis (continued)

NB10 Gaussian Analysis. Question (a): I don't know anything about what NB10 is supposed to weigh (down to the nearest microgram) or about the accuracy of the NBS's measurement process, so I want to use a **diffuse prior** for μ and σ^2 .

Considering the meaning of the **hyperparameters**, to provide little prior information I want to choose both ν_0 and κ_0 close to 0.

Making them exactly 0 would produce an **improper** prior distribution (which doesn't integrate to 1), but choosing positive values as close to 0 as you like yields a **proper and highly diffuse prior**.

You can see from (24, 25) that the result is then

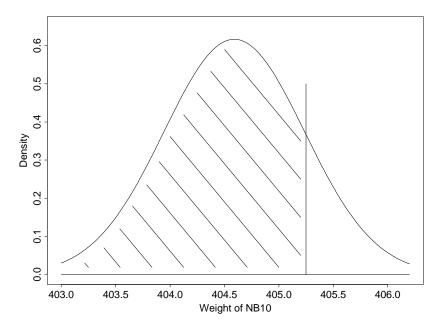
$$(\mu|y,\mathcal{G}) \sim t_n \left[\bar{y}, \frac{(n-1)s^2}{n^2} \right] \doteq N\left(\bar{y}, \frac{s^2}{n} \right),$$
 (28)

i.e., with diffuse prior information (as with the Bernoulli model in the AMI case study) the 95% central Bayesian interval **virtually coincides** with the usual frequentist 95% confidence interval

$$\bar{y} \pm t_{n-1}^{.975} \frac{s}{\sqrt{n}} = 404.6 \pm (1.98)(0.647) = (403.3, 405.9).$$

Thus both {frequentists who assume G} and {Bayesians who assume G with a diffuse prior} conclude that **NB10 weighs about** 404.6µg **below 10g, give or take about** 0.65µg.

<u>Question (b)</u>. If interest focuses on whether NB10 weighs **less than some value** like 405.25, when reasoning in a Bayesian way you can answer this question directly: the posterior distribution for μ is shown below, and $P_B(\mu < 405.25|y, \mathcal{G}, \text{diffuse prior}) \doteq .85$, i.e., your **betting odds** in favor of the proposition that $\mu < 405.25$ are about 5.5 to 1.



When reasoning in a frequentist way $P_F(\mu < 405.25)$ is **undefined**; about the best you can do is to test $H_0: \mu < 405.25$, for which the *p*-value would (approximately) be $p = P_{F,\mu=405.25}(\bar{y} > 405.59) = 1 - .85 = .15$, i.e., **insufficient evidence to reject** H_0 at the usual significance levels (note the **connection** between the *p*-value and the posterior probability, which arises in this example because the null hypothesis is **one-sided**).

NB The significance test tries to answer a **different question**: in Bayesian language it looks at $P(\bar{y}|\mu)$ instead of $P(\mu|\bar{y})$.

Many people find the latter quantity more interpretable.

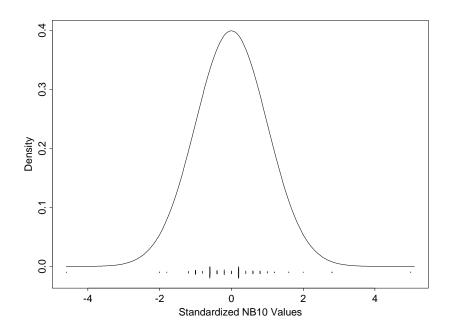
Question (c). We saw earlier that in this model

$$(y_{n+1}|y,\mathcal{G}) \sim t_{\nu_n} \left[\mu_n, \frac{\kappa_n + 1}{\kappa_n} \sigma_n^2 \right],$$
 (29)

and for *n* large and ν_0 and κ_0 close to 0 this is $(y_{n+1}|y,\mathcal{G}) \stackrel{\cdot}{\sim} N(\bar{y},s^2)$, i.e., a **95% posterior predictive** interval for y_{n+1} is (392,418).

Model Expansion

A standardized version of this predictive distribution is plotted below, with the standardized NB10 data values superimposed.



It's evident from this plot (and also from the normal qqplot given earlier) that the Gaussian model provides a **poor fit** for these data: the three most extreme points in the data set in standard units are -4.6, 2.8, and 5.0.

With the **symmetric heavy tails** indicated in these plots, in fact, the empirical CDF looks quite a bit like that of a *t* distribution with a rather small number of **degrees of freedom**.

This suggests revising the previous model by **expanding** it: **embedding** the Gaussian in the *t* family and adding a parameter *k* for **tail-weight**.

Unfortunately there's no standard closed-form conjugate choice for the prior on k.

A more **flexible** approach to computing is evidently needed — this is where **Markov chain Monte Carlo** methods (our next main topic) come in.

The Exponential Family

It was noticed a long time ago that many of the standard sampling distributions that you're likely to want to use in constructing likelihood functions have the **same general** form, which is referred to as the **exponential family**:

Definition (e.g., Bernardo and Smith, 1994): Given data y_1 (a sample of size 1) and a parameter vector $\theta = (\theta_1, \dots, \theta_k)$, the (marginal) sampling distribution $p(y_1|\theta)$ belongs to the *k*-dimensional exponential family if it can be expressed in the form

$$p(y_1|\theta) = c f_1(y_1) g_1(\theta) \exp\left[\sum_{j=1}^k \phi_j(\theta) h_j(y_1)\right]$$
(30)

for $y_1 \in \mathcal{Y}$ and 0 otherwise; if \mathcal{Y} does not depend on θ the family is called **regular**.

 $(\phi_1(\theta), \dots, \phi_k(\theta))$ in (30) is referred to as the **natural parameterization** of the exponential family.

In this case the **joint distribution** $p(y|\theta)$ of a **sample** $y = (y_1, \ldots, y_n)$ of size n which is conditionally IID from (30) (which also defines, as usual, the **likelihood function** $l(\theta|y)$) will be

$$p(y|\theta) = l(\theta|y) = \prod_{i=1}^{n} p(y_i|\theta)$$
(31)
$$= c \left[\prod_{i=1}^{n} f_1(y_i)\right] [g_1(\theta)]^n \exp\left[\sum_{j=1}^{k} \phi_j(\theta) \sum_{i=1}^{n} h_j(y_i)\right].$$

This leads to **another way** to define the exponential family: in (30) take $f(y) = \prod_{i=1}^{n} f_1(y_i)$ and $g(\theta) = [g_1(\theta)]^n$ to yield

<u>Definition</u>: Given data $y = (y_1, \ldots, y_n)$ (a conditionally IID sample of size n) and a parameter vector $\theta = (\theta_1, \ldots, \theta_k)$, the (joint) sampling distribution $p(y|\theta)$ belongs to the

k-dimensional exponential family if it can be expressed in the form

$$p(y|\theta) = c f(y) g(\theta) \exp\left[\sum_{j=1}^{k} \phi_j(\theta) \sum_{i=1}^{n} h_j(y_i)\right].$$
 (32)

Either way you can see that $\{\sum_{i=1}^{n} h_1(y_i), \dots, \sum_{i=1}^{n} h_k(y_i)\}$ is a set of **sufficient** statistics for θ under this sampling model, because the likelihood $l(\theta|y)$ depends on y only through the values of $\{h_1, \dots, h_k\}$.

I bring up the exponential family in part because, if the likelihood $l(\theta|y)$ is of the form (32), then in searching for a **conjugate** prior $p(\theta)$ — that is, a prior of the same functional form as the likelihood — you can see directly what will work:

$$p(\theta) = c g(\theta)^{\tau_0} \exp\left[\sum_{j=1}^k \phi_j(\theta) \tau_j\right], \qquad (33)$$

for some $\tau = (\tau_0, \dots, \tau_k).$

With this choice the **posterior** for θ will be

$$p(\theta|y) = c g(\theta)^{1+\tau_0} \exp\left\{\sum_{j=1}^k \phi_j(\theta) \left[\tau_j + \sum_{i=1}^n h_j(y)\right]\right\},$$
(34)

which is indeed of the same form (in θ) as (33).

As a first example, with $s = \sum_{i=1}^{n} y_i$, the **Bernoulli/binomial** likelihood (equation (6) in part 2) can be written

$$l(\theta|y) = \theta^{s}(1-\theta)^{n-s}$$

= $(1-\theta)^{n} \left(\frac{\theta}{1-\theta}\right)^{s}$ (35)
= $(1-\theta)^{n} \exp\left[s \log\left(\frac{\theta}{1-\theta}\right)\right],$

which shows (a) that this sampling distribution is a member of the **exponential family** with k = 1, $g(\theta) = (1 - \theta)^n$, the natural parameterization $\phi_1(\theta) = \log\left(\frac{\theta}{1-\theta}\right)$ (<u>NB</u> the basis of **logistic regression**), and $h_1(y_i) = y_i$, and (b) that $\sum_{i=1}^n h_1(y_i) = s$ is sufficient for θ .

Then (33) says that the **conjugate prior** for the Bernoulli/binomial likelihood is

$$p(\theta) = c (1-\theta)^{n\tau_0} \exp\left[\tau_1 \log\left(\frac{\theta}{1-\theta}\right)\right]$$
$$= c \theta^{\alpha-1} (1-\theta)^{\beta-1} = \text{Beta}(\alpha,\beta)$$
(36)

for some α and β , as we've already seen is **true**.

As an example of a **non-regular** exponential family, suppose that a reasonable model for the data is to take the observed values $(y_i|\theta)$ to be conditionally IID from the **uniform** distribution

 $U(0,\theta)$ on the interval $(0,\theta)$ for unknown θ :

$$p(y_1|\theta) = \left\{ \begin{array}{ll} \frac{1}{\theta} & \text{for } 0 < y_1 < \theta \\ 0 & \text{otherwise} \end{array} \right\} = \frac{1}{\theta} I(0,\theta), \quad (37)$$

where I(A) = 1 if A is true and 0 otherwise.

 θ in this model is called a **range-restriction** parameter; such parameters are fundamentally different from **location** and **scale** parameters (like the mean μ and variance σ^2 in the $N(\mu, \sigma^2)$ model, respectively) or **shape** parameters (like the degrees of freedom ν in the t_{ν} model).

(37) is an **example of (30)** with $c = 1, f_1(y) = 1, g_1(\theta) = \frac{1}{\theta}, h_1(y) = 0$, and $\phi_1(\theta) =$ anything you want (e.g., 1), but only when the set $\mathcal{Y} = (0, \theta)$ is taken to depend on θ .

(**Truncated** distributions with **unknown truncation point** also lead to non-regular exponential families.)

It turns out that inference in non-regular exponential families is **similar** in some respects to the story when the exponential family is regular, but there are some **important differences** too (e.g., with a conditionally IID sample of size *n* from (37), $V(\theta|y) = O(n^{-2})$ (!) instead of the more familiar $O(n^{-1})$).

For an example with p > 1, take $\theta = (\mu, \sigma^2)$ with the **Gaussian likelihood**:

$$l(\theta|y) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma^{2}}(y_{i}-\mu)^{2}\right] \quad (38)$$
$$= \sigma^{-n}(2\pi)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^{2}}\left(\sum_{i=1}^{n}y_{i}^{2}-2\mu\sum_{i=1}^{n}y_{i}+n\mu^{2}\right)\right].$$

This is of the form (32) with k = 2, $c = (2\pi)^{-\frac{n}{2}}$, f(y) = 1, $g(\theta) = \sigma^{-n} \exp\left(-\frac{n\mu^2}{2\sigma^2}\right)$, $\phi_1(\theta) = -\frac{1}{2\sigma^2}$, $\phi_2(\theta) = \frac{\mu}{\sigma^2}$, $h_1(y_i) = y_i^2$, and $h_2(y_i) = y_i$, which shows that $[h_1(y) = \sum_{i=1}^n y_i^2, h_2(y) = \sum_{i=1}^n y_i] \text{ or equivalently}$ $(\bar{y}, s^2) \text{ is sufficient for } \theta.$

Some **unpleasant algebra** then demonstrates that an application of (33) leads to (19) as the **conjugate prior** for the Gaussian likelihood when both μ and σ^2 are unknown.

In Dispraise of Hypothesis Testing

Setup: Controlled experiment of new versus old treatment, with n (human) subjects randomized, $\frac{n}{2}$ to old, $\frac{n}{2}$ to new, n (fairly) large.

 θ = the mean difference (new – old), on the most important outcome of interest (scaled, without loss of generality, so that large values are better than small), in the population \mathcal{P} of subjects judged exchangeable with those in the trial.

(This is like imagining that the *n* trial subjects were randomly sampled from \mathcal{P} [of course this is typically not how subjects are actually enlisted in the trial] and then randomized to new or old, which gives θ a causal interpretation as the mean improvement per person caused by receiving the new treatment instead of the old.)

As we've noted earlier, two frequentist schools of inference about θ developed in the twentieth century:

• The Fisherian approach, which has two parts:

(a) **Point** and **interval estimates** of θ based on the **likelihood function**; and

(b) Summarization of the evidence against a null hypothesis like H_0 : $\theta = 0$ via *P*-values (the chance, if the null is true, of getting data as extreme as, or more extreme than, what you got).

Hypothesis Testing (continued)

• The Neyman-Pearson approach, which also has two parts:

(c) **Testing** $H_0: \theta = 0$ against $H_1: \theta \neq 0$ by developing rules (as a function of *n*) that **reject** H_0 with a pre-specified **Type I error probability** α (the chance of **incorrectly rejecting** H_0), and then (having first specified α) choosing *n* so that the **Type II error probability** β (the chance of **incorrectly failing to reject** H_0) is no more than some **pre-specified threshold** when θ actually is some **pre-specified positive value** θ_1 (this is equivalent to choosing *n* so that the **power** $(1 - \beta)$ of the test is not less than a pre-specified threshold when $\theta = \theta_1$); and

(d) Constructing a **confidence interval** for θ with some pre-specified **confidence level** $100(1 - \gamma)$ %.

In practice a **combined frequentist approach** has somehow evolved in which randomized trials are often **designed** from the **Neyman-Pearson** point of view (c) but then **summarized** with **Fisherian** P-values (b) as **measures of** evidence against H_0 .

From a **Bayesian** point of view this approach **perversely emphasizes the worst** of both the Fisherian and Neyman-Pearson schools, by failing to focus on the **most scientifically relevant summary** of any given trial: an (interval) **estimate** of θ on the scale of the most **important outcome variable** (recall de Finetti's Bayesian emphasis on **predicting** data values on the scales on which they're measured).

Hypothesis Testing (continued)

A good rule of thumb: don't wander off onto the probability scale (as *P*-values do) when you can stay on the data scale (as interval estimates do), because it's harder to think about whether probabilities are important scientifically ("Is P = 0.03 small enough?") than it is to think about whether changes on the main outcome scale of interest are real-world relevant ("Would it positively affect eBay's bottom line if the change to the web experience we're now studying increased the percentage of visits to the eBay web page that end in a sale from 10% to 12%?").

Standard example: I've run my experiment and the *P*-value comes out **0.02**, which is **"small enough to publish"**; but can I tell from this whether the difference I've found is **real-world meaningful**?

In a **two-tailed** test of H_0 : $\theta = 0$ against H_1 : $\theta \neq 0$ I can work backwards from P = 0.02 to figure out that the value of the standard **test statistic**

$$z = \frac{\overline{\mathsf{new}} - \overline{\mathsf{old}}}{\widehat{SE}(\overline{\mathsf{new}} - \overline{\mathsf{old}})}$$
(39)

that gave rise to P = 0.02 was ± 2.3 (taking *n* to be **large**), but

(1) I can't even tell from the *P*-value whether the new treatment was **better or worse than the old**,

(2) the thing I really want to know to judge the **practical significance** of this finding is the **numerator** of (39),

(3) the thing I really want to know to judge the **statistical significance** of this finding is the **denominator** of (39), and

(4) the *P*-value has **thrown away crucial information** by (in effect) specifying only the **ratio** of (2) and (3) rather than their **separate**, and **separately important**, values.

Hypothesis Testing (continued)

If I have to work out the **numerator** and **denominator** of (39) **separately** to pin down both the **practical** and **statistical** significance of my result, both of which are **key scientific summaries**, then **what's the point** of calculating the *P*-value at all?

Why not **dispense with it altogether** and go directly to the (e.g., 95%) interval estimate

$$(\overline{\text{new}} - \overline{\text{old}}) \pm 2\widehat{SE}(\overline{\text{new}} - \overline{\text{old}})?$$
 (40)

(This is a large-*n* approximation to the Bayesian solution to the inference problem when prior information is diffuse.)

For me the above argument **demolishes the use of** *P*-values in inference (although in part 5 I'll make better use of them in **diagnostic checking** of a **statistical model**, which is another task altogether).

The Fisherian point and interval estimates (a) and the Neyman-Pearson confidence intervals (d) are much more in keeping with the scientifically compelling idea of staying on the data scale, but they have the following two drawbacks in relation to the Bayesian approach:

- They fail to incorporate relevant prior information about θ when it's available, and
- They don't necessarily work very well (i.e., they don't necessarily live up to their advertised frequentist properties) when the likelihood function is heavily skewed and/or when n is small.

References

Bernardo JM, Smith AFM (1994). Bayesian Theory. New York: Wiley.

- Craig PS, Goldstein M, Seheult AH, Smith JA (1997). Constructing partial prior specifications for models of complex physical systems. *The Statistician*, **46**, forthcoming.
- Draper D (1995). Inference and hierarchical modeling in the social sciences (with discussion). *Journal of Educational and Behavioral Statistics*, **20**, 115–147, 233–239.
- Draper D, Hodges JS, Mallows CL, Pregibon D (1993). Exchangeability and data analysis (with discussion). *Journal of the Royal Statistical Society, Series A*, **156**, 9–37.
- de Finetti B (1930). Funzione caratteristica di un fenomeno aleatorio. *Mem. Acad. Naz. Lincei*, **4**, 86–133.
- de Finetti B (1964). Foresight: its logical laws, its subjective sources. In *Studies in Subjective Probability*, HE Kyburg, Jr., and HE Smokler, eds., New York: Wiley (1980), 93–158.

de Finetti B (1974/5). Theory of Probability, 1–2. New York: Wiley.

- Fisher RA (1922). On the mathematical foundations of theoretical statistics. *Philosophical Transactions of the Royal Society of London A*, **222**, 309–368.
- Fisher RA (1956). *Statistical Methods and Scientific Inference*. London: Oliver and Boyd.
- Freedman D, Pisani R, Purves R, Adhikari A (1998). *Statistics*, third edition. New York: Norton.
- Gelman A, Carlin JB, Stern HS, Rubin DB (2003). *Bayesian Data Analysis*, second edition. London: Chapman & Hall.
- Hacking I (1975). *The Emergence of Probability*. Cambridge: Cambridge University Press.
- Johnson NL, Kotz S (1970). *Distributions in statistics: Continuous univariate distributions*, **1**. New York: Wiley.
- Kadane JB, Dickey JM, Winkler RL, Smith WS, Peters SC (1980). Interactive elicitation of opinion for a normal linear model. *Journal of the American Statistical Association*, **75**, 845–854.

References (continued)

- Kadane JB, Wolfson LJ (1997). Experiences in elicitation. *The Statistician*, **46**, forthcoming.
- Kahn K, Rubenstein L, Draper D, Kosecoff J, Rogers W, Keeler E, Brook R (1990). The effects of the DRG-based Prospective Payment System on quality of care for hospitalized Medicare patients: An introduction to the series. *Journal of the American Medical Association*, **264**, 1953–1955 (with editorial comment, 1995–1997).
- Laplace PS (1774). Mémoire sur la probabilité des causes par les évenements. *Mémoires de l'Academie des Sciences de Paris*, **6**, 621–656. English translation in 1986 as "Memoir on the probability of the causes of events," with an introduction by SM Stigler, *Statistical Science*, **1**, 359–378.
- O'Hagan A (1997). Eliciting expert beliefs in substantial practical applications. *The Statistician*, **46**, forthcoming.
- Samaniego FJ, Reneau DM (1994). Toward a reconciliation of the Bayesian and frequentist approaches to point estimation. *Journal of the American Statistical Association*, **89**, 947–957.
- Tierney L, Kadane JB (1986). Accurate approximations for posterior moments and marginal densities. *Journal of the American Statistical Association*, **81**, 82–86.