

## CHAPTER 24

## MODEL COMPARISON

*“Entities are not to be multiplied without necessity”* - - - William of Ockham, *ca* 1330

We have seen in some detail how to conduct inferences – test hypotheses, estimate parameters, predict future observations – within the context of a preassigned model, representing some working hypothesis about the phenomenon being observed. But a scientist must be concerned also with a bigger problem; how to decide between different models when both seem able to account for the facts. Indeed, the progress of science requires comparison of different conceivable models; a false premise built into a model that is never questioned, cannot be removed by any amount of new data.

Stated very broadly, the problem is hardly new; some 650 years ago the Franciscan Monk William of Ockham perceived the logical error in the Mind Projection Fallacy.<sup>†</sup> This led him to teach that some religious issues might be settled by reason, but others only by faith. He removed the latter from his discourse, and concentrated on the areas where reason might be applied – just as Bayesians seek to do today when we discard orthodox mind-projecting mythology (such as assertions of limiting frequencies in experiments that have never been performed), and concentrate on the things that are meaningful in the real world. His propositions ‘amenable only to faith’ correspond roughly to what we should call non-Aristotelian propositions (or Aristotelian ones for which the available information is too meager to permit any inferences). His famous epigram quoted above, generally called “Ockham’s razor”, represents a good start on the principles of reasoning that he needed, and that we still need today. But it was also so subtle that only through modern Bayesian analysis has it been well understood.

Of course, from our present vantage point it is clear that this is really the same problem as that of compound hypothesis testing, considered already in Chapter 4. Here we need only generalize that treatment and work out further details, but some extra care is needed. As long as we work within a single model, normalization constants tend to cancel out and so need not be introduced at all. But when two different models appear in a single equation, the normalization constants do not cancel out, and it is imperative that all probabilities be correctly normalized.

### Formulation of the Problem

To see why this happens, recall first what Bayes’ theorem tells us about parameter estimation. A model  $M$  contains various parameters denoted collectively by  $\theta$ . Given data  $D$  and prior information  $I$ , and assuming the correctness of model  $M$ , to estimate the parameters we first apply Bayes’ theorem:

$$p(\theta|D, M, I) = p(\theta|M, I) \frac{p(D|\theta, M, I)}{p(D|M, I)} \quad (24-1)$$

in which the denominator serves as the normalizing constant:

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<sup>†</sup> Ockham’s position, stated in the language of his time, was that “Reality exists solely in individual things, and universals are merely abstract signs.” Translated into Twentieth Century language: the abstract creations of the mind are not realities in the external world. Unfortunately for him, some of the cherished ‘realities’ of contemporary orthodox theology were just the things to which he denied reality; so this got him into trouble with the Establishment. Evidently, Ockham was a forerunner of modern Bayesians, to whom all this sounds very familiar.

$$p(D|M, I) = \int p(D, \theta|M, I) d\theta = \int p(D|\theta, M, I) p(\theta|M, I) d\theta \quad (24-2)$$

which we see is the prior expectation of the likelihood  $L(\theta) = p(D|\theta, M, I)$ ; that is, its expectation over the prior probability distribution  $p(\theta|M, I)$  for the parameters.

Now we move up to a higher level problem; to judge, in the light of the prior information and data, which of a given set of different models  $\{M_1 \cdots M_r\}$  is most likely to be the correct one. Bayes' theorem gives the posterior probability for the  $j$ 'th model as

$$p(M_j|D, I) = p(M_j|I) \frac{p(D|M_j, I)}{p(D|I)}, \quad 1 \leq j \leq r. \quad (24-3)$$

But we may eliminate the denominator  $p(D|I)$  by calculating instead odds ratios as we did in Chap. 4. The posterior odds ratio for model  $M_j$  over  $M_k$  is

$$\frac{p(M_j|D, I)}{p(M_k|D, I)} = \frac{p(M_j|I)}{p(M_k|I)} \cdot \frac{p(D|M_j, I)}{p(D|M_k, I)} \quad (24-4)$$

and we see that the same probability  $p(D|M_j, I)$  that appears in the single-model parameter estimation problem (24-1) only as a normalizing constant, now appears as the fundamental quantity determining the status of model  $M_j$  relative to any other.<sup>†</sup> The exact measure of what the data have to tell us about this, is always the prior expectation of its likelihood function, over the prior probability  $p(\theta_j|M_j, I)$  for whatever parameters  $\theta_j$  may be in that model (they are generally different for different models). All probabilities must be correctly normalized here, otherwise we are violating our basic rules and the likelihood ratio in (24-4) is arbitrary nonsense even when it is not zero or infinite.

Intuitively, the model favored by the data is the one that assigns the highest probability to the observed data, and therefore “explains the data” best. This is just a repetition, at a higher level, of the likelihood principle for parameter estimation within a model.

But it is not yet clear how an Ockham principle can emerge from this. Indeed, the principle has never been stated in exact, well-defined terms. Later writers have tried, almost universally, to interpret it as saying that the criterion of choice is the ‘simplicity’ of the competing models, although it is not clear that Ockham himself used that term. Centuries of discussion by philosophers trying to make this interpretation brought no appreciable clarification of what is meant by ‘simplicity’.\* We think that concentration of attention exclusively on that undefined term has prevented understanding of the real point, which is merely that a model with unspecified parameters is a composite hypothesis, not a simple one. For this reason some interesting new features appear, arising from the internal structure of the parameter space.

<sup>†</sup> This logical structure is more general even than the Bayesian formalism; we shall see in Volume 2 that it persists in the pure maximum-entropy formalism, where in statistical mechanics the relative probability  $P_j/P_k$  of two different phases, such as liquid and solid, is the ratio of their partition functions  $Z_j/Z_k$ , which are the normalization constants for the sub-problems of prediction within one phase, although they are not expectations of any likelihoods. In Bayesian analysis, the data are indifferent between two models when their normalization constants become equal; in statistical mechanics the temperature of a phase transition is the one at which the two partition functions become equal. In chemical thermodynamics it is customary to state this as equality of the “free energies”  $F_j \simeq \log Z_j$ . This illustrates the basic unity of Bayesian and maximum-entropy reasoning, in spite of their superficial differences.

\* Indeed, for a time the notion of ‘simplicity’ was given up for dead, because of the seeming impossibility of defining it. The tedious details are recounted by Rosenkrantz (1977).

**Parameters Known in Advance:** To see this, suppose first that there is no such internal space; the parameters of a model are known exactly ( $\theta = \theta'$ ) in advance. This amounts to assigning a prior  $p(\theta_j|M_jI) = \delta(\theta_j - \theta'_j)$ , whereupon (24-2) reduces to

$$p(D|M_j, I) = p(D|\theta'_j, M_j, I) = L_j(\theta'_j) \quad (24-5)$$

just the likelihood of  $\theta'_j$  within the  $j$ 'th model. Evidently, this will be a maximum if  $\theta'_j$  happens to be equal to the maximum likelihood estimate  $\hat{\theta}_j$  for that model and the data. Then the posterior odds ratio (24-4) would reduce to

$$\frac{p(M_j|D, I)}{p(M_k|D, I)} = \frac{p(M_j|I)}{p(M_k|I)} \cdot \frac{(L_j)_{max}}{(L_k)_{max}} \quad (24-6)$$

This is the conventional Bayes' theorem result of Chapter 4. If the parameters were known to have, for each model, the most favorable values for the given data set, each model becomes in effect a simple hypothesis rather than a composite one [this is almost self-contradictory, for if the data were different one would have to suppose also different prior information about the parameters in order to retain (24-6)].

But this extreme case is also very unrealistic; usually, the parameters are unknown and in the problems 'amenable to reason' where useful inferences are possible, the data  $D$  will be more informative about the parameters within some model  $M_j$  than is the prior information; that is, as a function of  $\theta_j$  the likelihood function  $L_j(\theta_j) = p(D|\theta_j, M_j, I)$  will be more sharply peaked, at some point picked out by the data, than is the prior probability  $p(\theta_j|M_j, I)$ . Then in the exact integral (24-2) most of the contribution will come from a "high likelihood region"  $\Omega$  comprising a small neighborhood of that sharp peak. There is hardly any loss of generality in assuming this because, unless it is true, we would consider the data too meager to permit any useful new inferences and although the Bayesian procedure would still be valid in principle we would, like Ockham, 'remove the problem from our discourse' as being unproductive.

**Parameters Unknown:** Consider for the moment only the  $k$ 'th model and drop the index  $k$ . Let there be  $m$  parameters  $\theta \equiv \{\theta_1 \cdots \theta_m\}$  in the model and expand  $\log L(\theta)$  about the maximum likelihood point  $\hat{\theta} = \{\hat{\theta}_1 \cdots \hat{\theta}_m\}$ :

$$\log L(\theta_1 \cdots \theta_m) = \log L_{max} + \frac{1}{2} \sum_{i,j=1}^m \frac{\partial^2 \log L}{\partial \theta_i \partial \theta_j} (\theta_i - \hat{\theta}_i)(\theta_j - \hat{\theta}_j) + \cdots \quad (24-7)$$

Then near the peak a good approximation is a multivariate gaussian function:

$$L \simeq L_{max} \exp \left[ -\frac{1}{2} (\theta - \hat{\theta})' \Sigma^{-1} (\theta - \hat{\theta}) \right], \quad (24-8)$$

with the "inverse covariance matrix"

$$(\Sigma^{-1})_{i,j} \equiv - \left[ \frac{\partial^2 \log L}{\partial \theta_i \partial \theta_j} \right]_{\theta=\hat{\theta}} \quad (24-9)$$

Our supposition is that the prior density does not vary appreciably over the high likelihood region  $\Omega$ ; then if we were estimating the parameters  $\theta_j$ , in the approximation (24-8) we should be led to estimates of the form

$$(\theta_j)_{est} = \hat{\theta}_j \pm \sqrt{\Sigma_{jj}} \quad (24-10)$$

and the integral (24-2) is

$$p(D|M, I) \simeq L_{max} (2\pi)^{m/2} \sqrt{\det(\Sigma)} p(\hat{\theta}|M, I) \quad (24-11)$$

Let us interpret this result in terms of parameter space volumes. We may define the high likelihood region  $\Omega$  more explicitly by the conditions that:

- (1) It is as compact as possible; within  $\Omega$  the likelihood everywhere exceeds some nominal threshold value  $L_0$ . The volume of this region is then

$$V(\Omega) = \int_{L > L_0} d\theta_1 \cdots d\theta_m. \quad (24-12)$$

- (2) The integrated likelihood should be given by  $L_{max} V(\Omega)$ :

$$L_{max} V(\Omega) = \int L(\theta) d^m \theta = L_{max} (2\pi)^{m/2} \sqrt{\det \Sigma}. \quad (24-13)$$

Then a rectangular function equal to  $L_{max}$  on  $\Omega$ , zero elsewhere, is a crude approximation to the likelihood function and it has, in the present approximation, the same implications for model comparison as does the actual likelihood function. These conditions determine the effective high-likelihood volume of parameter space without any need to calculate the threshold  $L_0$ :

$$V(\Omega) = (2\pi)^{m/2} \sqrt{\det \Sigma} \quad (24-14)$$

Note that this is just the normalization constant for the above multivariate gaussian function;<sup>†</sup>

$$\int \exp \left[ -\frac{1}{2} (\theta - \hat{\theta})' \Sigma^{-1} (\theta - \hat{\theta}) \right] \cdot \frac{d\theta_1 \cdots d\theta_m}{V(\Omega)} = 1. \quad (24-15)$$

**Exercise (24.1).** Evaluate the threshold  $L_0$  and the dimensions  $(\theta - \hat{\theta})$  of the high-likelihood region  $\Omega$  by direct evaluation of the integral (24-12). Note that the matrix  $\Sigma$ , being real, symmetric, and positive definite, can be diagonalized:  $\Sigma = U \Lambda U^{-1}$ , where  $U$  is an  $(m \times m)$  real orthogonal matrix; that is, its transpose is  $U' = U^{-1}$  so  $\det(U) = \pm 1$ , and  $\Lambda_{ij} = \lambda_i \delta_{ij}$  is the diagonalized matrix. Now make the “spherical” change of variables from  $\{\theta_1 \cdots \theta_m\}$  to  $\{x_1 \cdots x_m\}$ , where

$$(\theta_k - \hat{\theta}_k) = \sum_{i=1}^m U_{ki} \sqrt{\lambda_i} x_i$$

and perform the integrations in the  $x$ -space. Show that, in  $x$ -space, the region  $\Omega$  is the interior of an  $m$ -dimensional sphere of radius  $R \simeq (m/e)^{1/2}$ ; and that the exact volume of such a sphere is  $\pi^{m/2} R^m / (m/2)!$ . As a check, in the cases  $m = (1, 2, 3)$  this reduces to  $(2R, \pi R^2, 4\pi R^3/3)$  respectively, as it should.

<sup>†</sup> Indeed, the maximum density for any continuous distribution  $p(x_1 \cdots x_n)$  is dimensionally the reciprocal of an  $n$ -dimensional volume, which can always be interpreted as the volume of a high-probability region.

The right-hand side of (24-11) becomes  $L_{max} V(\Omega) p(\hat{\theta}|M, I)$ . But since by hypothesis  $p(\theta|M, I)$  does not vary appreciably over  $\Omega$ , the quantity

$$W \equiv \frac{1}{L_{max}} \int L(\theta) p(\theta|MI) d^m \theta \simeq V(\Omega) p(\hat{\theta}|M, I) \quad (24-16)$$

is for all practical purposes just the *amount of prior probability* contained in the high likelihood region  $\Omega$ , and our fundamental model comparison rule now becomes

$$\frac{p(M_j|D, I)}{p(M_k|D, I)} = \frac{p(M_j|I)}{p(M_k|I)} \cdot \frac{(L_j)_{max}}{(L_k)_{max}} \cdot \frac{W_j}{W_k} \quad (24-17)$$

in which we see revealed, by comparison with (24-6), the Ockham factor ( $W_j/W_k$ ) arising from the internal parameter spaces of the models. In (24-17), the likelihood factor depends only on the data and the model, while the Ockham factor depends also on the prior information about its internal parameters. If two different models achieve the same likelihoods  $(L_j)_{max}$ , then in sampling theory terms they account for the data equally well, and one would think that we have no basis for choice between them. Yet Bayes' theorem tells us that there is another quality in the models; the prior information which may still give strong grounds for preference of one over the other. Indeed, the Ockham factor may be so strong that it reverses the likelihood judgment.

### But Where is the Idea of Simplicity?

The relation (24-17) has much meaning that unaided intuition could not (or at least, did not) see. If the data are highly informative compared to the prior information, then the relative merit of two models is determined by the product of two factors;

- (1) How high a likelihood can be attained on the parameter space of a model?
- (2) How much prior probability is concentrated in the high-likelihood region  $\Omega$  picked out by the data?

But neither of these seems concerned with the simplicity of the model (which seems for most of us to refer to the number of different assumptions that are made – for example, the number of different parameters that are introduced – in defining a model).

To understand this, let us ask: “How do we all decide these things intuitively?” Having observed some facts, what is the real criterion that leads us to prefer one explanation of them over another? Suppose that two explanations, *A* and *B*, could account for some proven historical facts equally well. But *A* makes four assumptions, each of which seemed to us already highly plausible; while *B* makes only two assumptions, but they seem strained, far-fetched, and unlikely to be true. Every historian finds himself in situations like this; and he does not hesitate to opt for explanation *A*, although *B* is intuitively simpler. Thus our intuition asks, fundamentally, not how *simple* the hypotheses are; but rather how *plausible* they are.

But there is a loose connection between simplicity and plausibility, because the more complicated a set of possible hypotheses, the larger the manifold of conceivable alternatives, and so the smaller must be the prior probability of any particular hypothesis in the set.

Now we see why ‘simplicity’ could never be given a satisfactory definition (that is, a definition that accounted in a satisfactory way for these inferences); it was a poorly chosen word, directing one’s attention away from the essential component of the inference. But from Centuries of unquestioned acceptance, the idea of ‘simplicity’ became implanted with such an unshakable mindset that several workers, even after applying Bayes’ theorem where the contrary fact stares you in the face, continued doggedly to try to interpret the Bayesian analysis in terms of simplicity!<sup>†</sup>

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<sup>†</sup> Indeed, one author, for whom Ockham’s razor was *by definition* concerned with simplicity, rejected Bayesian analysis because of its failure to exhibit that error.

Generations of philosophers opined vaguely that ‘simple hypotheses are more plausible’ without giving any logical reason why this should be so. We suggest that this should be turned around: we should say rather that ‘more plausible hypotheses tend to be simpler’. An hypothesis that we consider simpler is one that has fewer equally plausible alternatives.

None of this could be comprehended at all within the confines of orthodox statistical theory, whose ideology did not allow the concept of a probability for a model or for a fixed but unknown parameter. Orthodoxy tried to compare models entirely in terms of their different sampling distributions, which took no note of *either* the simplicity of the model or the prior information! But it was unable to do even this, because then all the parameters within a model became ‘nuisance parameters’ and that same ideology denied one any way to deal with them.\* Thus orthodox statistics was a total failure on this problem, and this held up progress for most of the 20<sup>th</sup> Century.

It is remarkable that, although the point at issue is trivial mathematically, generations of mathematically competent people failed to see it because of that conceptual mindset. But once the point is seen, it seems intuitively obvious and one cannot comprehend how anyone could ever have imagined that ‘simplicity’ alone was the criterion for judging models. This just reminds us again that the human brain is an imperfect reasoning device; although it is fairly good at drawing reasonable conclusions, it often fails to give a convincing rationale for those conclusions. For this we really do need the help of probability theory as logic.

Of course, Bayes’ theorem does recognize simplicity as one component of the inference. But by what mechanism does this happen? Although Bayes’ theorem always gives us the correct answer to whatever question we ask of it, it often does this in such a slick, efficient way that we are left bewildered and not quite understanding how it happened. The present problem is a good example of this, so let us try to understand the situation better intuitively.

Denote by  $M_n$  a model for which  $\theta = \{\theta_1, \dots, \theta_n\}$  is  $n$ -dimensional, ranging over a parameter space  $S_n$ . Now introduce a new model  $M_{n+1}$  by adding a new parameter  $\theta_{n+1}$  and going to a new parameter space  $S_{n+1}$ , in such a way that  $\theta_{n+1} = 0$  represents the old model  $M_n$ . We shall presently give an explicit calculation with this scenario, but first let us think about it in general terms.

On the subspace  $S_n$  the likelihood is unchanged by this change of model;  $p(D|\theta, M_{n+1}, I) = p(D|\theta, M_n, I)$ ,  $\theta \in S_n$ . But the prior probability  $p(\theta|M_{n+1}, I)$  must now be spread over a larger parameter space than before and will, in general, assign a lower probability to a neighborhood  $\Omega$  of a point in  $S_n$  than did the old model.

For a reasonably informative experiment, we expect that the likelihood will be rather strongly concentrated in small subregions  $\Omega_n \in S_n$  and  $\Omega_{n+1} \in S_{n+1}$ . Therefore, if with  $M_{n+1}$  the maximum likelihood point occurs at or near  $\theta_{n+1} = 0$ ,  $\Omega_{n+1}$  will be assigned less prior probability than is  $\Omega_n$  with model  $M_n$ , and we have  $p(D|M_n, I) > p(D|M_{n+1}, I)$ ; the likelihood ratio generated by the data will favor  $M_n$  over  $M_{n+1}$ . This is the Ockham phenomenon.

Thus, if the old model is already flexible enough to account well for the data, then as a general rule Bayes’ theorem will, like Ockham, tell us to prefer the old model. It is intuitively simpler if by ‘simpler’ we mean a model that occupies a smaller volume of parameter space, and thus *restricts us to a smaller range of possible sampling distributions*. Generally, the inequality will go the other way only if the maximum likelihood point is far from  $\theta_{n+1} = 0$  (*i.e.* a significance test would indicate a need for the new parameter), because then the likelihood will be so much smaller on  $\Omega_n$  than on  $\Omega_{n+1}$  that it more than compensates for the lower prior probability of the latter; as noted, Ockham would not disagree.

But intuition does not tell us at all, quantitatively, how great this discrepancy in likelihoods must be in order to bring us to the point of indifference between the models. Furthermore, having

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\* This and other criticisms of orthodox hypothesis testing theory were made long ago by Pratt (1961).

seen this mechanism, it is easy to invent cases (for example, if the introduction of the new parameter is accompanied by a redistribution of prior probability on the old subspace  $S_n$ ) in which Bayes' theorem may contradict Ockham because it is taking account further circumstances undreamt of in Ockham's philosophy. So we need specific calculations to make these things quantitative.

### An Example: Linear Response Models

Now we give a simple analysis that illustrates the above conclusions and allows us to calculate definite numerical values for the likelihood and Ockham factors. We have a data set  $D \equiv \{(x_1, y_1) \cdots (x_n, y_n)\}$  consisting of measured values of  $(x, y)$  in  $n$  pairs of observations. We may think of  $x$  as the 'cause' and  $y$  as the 'effect' although this is not required. For the general relations below the 'independent variables'  $x_i$  need not be uniformly spaced or even monotonic increasing in the index  $i$ . From these data and any prior information we have, we are to decide between two conceivable models for the process generating the data. For model  $M_1$  the responses are, but for irregular measurement errors  $e_i$ , linear in the cause:

$$M_1 : \quad y_i = \alpha x_i + e_i, \quad 1 \leq i \leq n \quad (24-18)$$

while for model  $M_2$  there is also a quadratic term:

$$M_2 : \quad y_i = \alpha x_i + \beta x_i^2 + e_i, \quad (24-19)$$

which represents, if  $\beta$  is negative, an incipient saturation or stabilizing effect (if  $\beta$  is positive, an incipient instability). We may think, for concreteness, of  $x_i$  as the dose of some medicine given to the  $i$ 'th patient,  $y_i$  as the resulting increase in blood pressure. Then we are trying to decide whether the response to this medicine is linear or quadratic in the dosage. But this mathematical model applies equally well to many different scenarios.<sup>†</sup> Whichever model is correct, the errors of measurement of  $y_i$  are supposed to be the same, and we assign a joint sampling distribution to them:

$$p(e_1 \cdots e_n | I) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp \left\{ -\frac{e_i^2}{2\sigma^2} \right\} = \left( \frac{w}{2\pi} \right)^{n/2} \exp \left\{ -\frac{w}{2} \sum_i e_i^2 \right\} \quad (24-20)$$

where  $w \equiv 1/\sigma^2$  is the 'weight' parameter, more convenient in calculations than  $\sigma^2$ .

**Digression: The Old Sermon Still Another Time:** Again, we belabor the meaning of this, as discussed in Chapter 7. In orthodox statistics, a sampling distribution is always referred to as if it represented an 'objectively real' fact, the frequency distribution of the errors. But we doubt whether anybody has ever seen a real problem in which one had prior knowledge of any such frequency distribution, or indeed prior knowledge that any limiting frequency distribution exists.

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<sup>†</sup> For example,  $x_i$  might be the amount of ozone in the air in the  $i$ 'th year,  $y_i$  the average temperature in January of that year. Or,  $x_i$  may be the amount of some food additive ingested by the  $i$ 'th Canadian rat,  $y_i$  the binary decision whether that rat did or did not develop cancer. Or,  $x_i$  may be the amount of acid rain falling on Northern Germany in the  $i$ 'th year,  $y_i$  the number of pine trees that died in that year; and so on. In other words, we are now in the realm of what were called 'linear response models' in the Preface, and the results of these calculations have a direct bearing on many currently controversial health and environmental issues. Of course, many real problems will require more sophisticated models than we are considering now; but having seen this simple calculation it will be clear how to generalize it in many different ways.

How could one ever acquire information about the long-run results of an experiment that has never been performed? That is part of the Mind-Projecting Mythology that we discard.

We recognize, then, that assigning this sampling distribution is only a means of describing our own *prior state of knowledge* about the measurement errors. The parameter  $\sigma$  indicates the general magnitude of the errors that we expect; The prior information  $I$  might, for example, be the variability observed in past examples of such data; or in a physics experiment it might not be the result of any observations, but rather obtained from the principles of statistical mechanics, indicating the level of Nyquist noise for the known temperature of the apparatus.

In particular, the absence of correlations in (24-20) is not an assertion that no correlations exist in the real data; it is only a recognition that we have no knowledge of such correlations, and therefore to suppose correlations of either sign is as likely to hurt as to help the quality of our inferences. Thus in one sense, by being noncommittal about it, we are only being honest and frankly acknowledging our ignorance. But in another sense, we are taking the safest, most conservative course; using a sampling distribution which will yield reasonable results whether or not correlations actually exist. But if we knew of any such correlations, we would be able to make still better inferences (although not much better) by use of a sampling distribution which contains them.

The reason for this is that correlations in a sampling distribution tell the robot that some regions of the vector sample space are more likely than others even though they have the same error magnitudes; then some details of the data that it would have to dismiss as probably noise, can be recognized as providing further evidence about systematic effects in the model.

**Back to the Problem:** The sampling distribution for model  $M_1$  is then

$$M_1 : \quad p(D|\alpha M_1) = \left(\frac{w}{2\pi}\right)^{n/2} \exp \left\{ -\frac{w}{2} \sum_{i=1}^n (y_i - \alpha x_i)^2 \right\} \quad (24-21)$$

The sum is

$$\Sigma = \sum_i (y_i^2 - 2\alpha y_i x_i + \alpha^2 x_i^2) = n(\overline{y^2} - 2\alpha \overline{xy} + \alpha^2 \overline{x^2}) \quad (24-22)$$

where the bars denote, as before, averages over the data. The maximum likelihood estimate (MLE) of  $\alpha$  is then found from  $\partial \Sigma / \partial \alpha = n(-2\overline{xy} + 2\alpha \overline{x^2}) = 0$ , or,

$$\alpha = \hat{\alpha} \equiv \frac{\overline{xy}}{\overline{x^2}} \quad (24-23)$$

which in this case is also called the ‘ordinary least squares’ (OLS) estimate. The likelihood (24-21) for model  $M_1$  is then

$$L(\alpha, M_1) = \left(\frac{w}{2\pi}\right)^{n/2} \exp \left\{ -\frac{nw}{2} [\overline{y^2} - \hat{\alpha}^2 \overline{x^2} + \overline{x^2}(\alpha - \hat{\alpha})^2] \right\} \quad (24-24)$$

and we note in passing that, if we were using this to estimate  $\alpha$  from the data, our result would be

$$(\alpha)_{est} = \hat{\alpha} \pm \frac{1}{\sqrt{nw\overline{x^2}}} \quad (24-25)$$

Now, using (24-23), the ‘global’ sampling distribution for model  $M_1$  in (24-3) contains two factors:

$$p(D|M_1 I) = \int p(D|\alpha M_1) p(\alpha|M_1 I) d\alpha = L_{max}(M_1) \cdot W \quad (24-26)$$



where

$$L_{max}(M_1) = \left(\frac{w}{2\pi}\right)^{n/2} \exp \left\{ -\frac{nw}{2} (\overline{y^2} - \hat{\alpha}^2 \overline{x^2}) \right\} = \left(\frac{w}{2\pi}\right)^{n/2} \exp \left\{ \frac{nw}{2} \frac{\overline{xy^2} - \overline{x^2 y^2}}{\overline{x^2}} \right\} \quad (24-27)$$

$$W_1 = \int \exp \left\{ -\frac{nw}{2} \overline{x^2} (\alpha - \hat{\alpha})^2 \right\} p(\alpha|M_1 I) d\alpha. \quad (24-28)$$

Now we are obliged to use a normalized prior for  $\alpha$ ; almost always it will be known that  $|\alpha|$  cannot be enormously large (else there would be such a catastrophe that we would not be concerned with this problem); but we would seldom have any more specific prior information about it. We can indicate this by assigning a prior density

$$p(\alpha|M_1 I) = \frac{1}{\sqrt{2\pi}\delta^2} \exp \left\{ -\frac{\alpha^2}{2\delta^2} \right\} \quad (24-29)$$

which says that we do not know whether  $\alpha$  is positive or negative, but it is highly unlikely that  $|\alpha|$  is much greater than  $\delta$ . As we saw in Chapter 6, when we are estimating parameters within a single given model and have such vague prior information about them, the exact analytical form of the prior makes no difference in the conclusions. That is, the effect of different reasonable priors first appears in our conclusions in perhaps the tenth decimal place; but since we are calculating those final conclusions only to three or four decimal places, the effect of different priors is not just negligibly small; it is strictly nil. All priors that are essentially equal to a constant  $C = p(\hat{\alpha}|M, I)$  over the region  $\Omega$  of high likelihood, lead to the same conclusions; even the value of the constant  $C$  cancels out. But when we are comparing different models,  $C$  does not cancel out; it expresses the prior range (in this case,  $C \simeq 1/2\delta$ ) of values that  $\alpha$  might have. Then we are free to choose a Gaussian analytical form which makes it easy to do the integrations. Indeed, this choice can be justified also as representing the actual state of knowledge that we have in real problems. Then the likely error  $\sigma$  of our measurements is so much smaller than  $\delta$  that over the high likelihood region  $\Omega$ , the prior density for  $\alpha$  is essentially constant and equal to  $(2\delta)^{-1}$ . Had we chosen a rectangular prior with width  $2\delta$ , it would have led to just the same result.

With the prior (24-29) we can do the integration (24-28) exactly, with the result

$$W_1 = \frac{1}{\sqrt{1 + nw\overline{x^2}\delta^2}} \exp \left\{ -\frac{nw\overline{x^2}\hat{\alpha}^2}{2(1 + nw\overline{x^2}\delta^2)} \right\} \quad (24-30)$$

But this can be simplified greatly. In the first place, we see from (24-25) that the accuracy with which the experiment can measure  $\alpha$  is  $\sigma/\sqrt{n\overline{x^2}}$ , and  $\delta$  is surely at least 100 times this, so

$$nw\overline{x^2}\delta^2 = n\overline{x^2}\frac{\delta^2}{\sigma^2} = \left( \frac{\text{prior range for } \alpha}{\text{accuracy of the measurement of } \alpha} \right)^2 \quad (24-31)$$

and this is typically very large numerically, of the order of  $10^4$  or greater. Therefore (24-30) may be written

$$W_1 = \frac{1}{\sqrt{nw\overline{x^2}\delta^2}} \exp \left\{ -\frac{\hat{\alpha}^2}{2\delta^2} \right\} \quad (24-32)$$

But now  $\delta$  is surely also at least 100 times greater than  $\hat{\alpha}$ ; so  $\hat{\alpha}^1/2\delta^2$  is less than  $10^{-4}$ ; and the Ockham factor reduces, to all the accuracy we could use, simply to

$$W_1 = \frac{\text{accuracy of } \alpha \text{ measurement}}{\text{prior range for } \alpha} \quad (24-33)$$

\*\*\*\*\* MORE HERE!! \*\*\*\*\*

## COMMENTS

Religious scholars who failed to heed the teachings of William of Ockham about issues amenable to reason and issues amenable only to faith, were doomed to a lifetime of generating nonsense. Let us note some of the forms this nonsense has taken.

### Final Causes

It seems that any discussion of scientific inference must deal, sooner or later, with the issue of belief or disbelief in final causes. Expressed views range all the way from Jacques Monod's forbidding us even to mention purpose in the Universe, to the religious fundamentalist who insists that it is evil not to believe in such a purpose.<sup>†</sup> We are astonished by the emotional, dogmatic intensity with which opposite views are proclaimed, by persons who do not have a shred of supporting factual evidence for their views.

But almost everyone who has discussed this has supposed that by a 'final cause' one means some supernatural force that suspends Natural Law and takes over control of molecular events (that is, alters molecular positions and/or velocities in a way inconsistent with the equations of motion) in order to ensure that some desired final condition is attained. In our view, almost all past discussions have been flawed by failure to recognize that operation of a final cause does not imply controlling molecular details.

When the author of a textbook says: "My purpose in writing this book was to ...", he is disclosing that there was a true "final cause" governing many activities of writer, pen, paper, secretary, word processor, typesetter, printer, extending usually over several years. When a chemist imposes conditions on his system which forces it to have a certain volume and temperature, he is just as truly the wielder of a final cause dictating the final thermodynamic state that he wished it to have. A bricklayer and a cook are likewise engaged in the art of making final causes. But – and this is the point usually missed – these final causes are *macroscopic*; they do not determine any particular "molecular" details. In all cases, had the fine details been different in any one of billions of ways, the final cause could have been satisfied just as well.

The final cause may then be said to possess an entropy, indicating the number of microscopic ways in which its purpose could have been realized; and the larger that entropy, the greater is the probability that it will be realized. Thus the Principle of Maximum Entropy applies also here.

In other words, while the idea of a microscopic final cause runs counter to all the instincts of a scientist, a macroscopic final cause is a perfectly familiar and real phenomenon, which we all invoke daily. We can hardly deny the existence of purpose in the Universe when virtually everything we do is done with some definite purpose in mind. Indeed, anybody who fails to pursue some definite long-run purpose in the conduct of his life, is dismissed as an idler by his colleagues. Obviously, this is just a familiar fact with no religious connotations; every scientist believes in macroscopic final causes without thereby believing in supernatural contravention of the laws of physics. The

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<sup>†</sup> For some, reasoning itself is evil: as one TV evangelist put it, "*Reasoning is a sure sign that one is not trusting God.*"

wielder of the final cause is not suspending physical law; he is merely choosing the Hamiltonian with which the molecules of a system interact, whatever their precise microstate.

But while all this has no religious connotations, neither does it have any anti-religious ones. Turning to the Universe as a whole, nothing compels us to suppose – or forbids us to suppose – that some kind of conscious and purposive God is the ultimate controlling force; even one in charge of all molecular details. But on what grounds does one suppose that He is concerned with human welfare, much less that He created the solar system specifically for our benefit? \* Indeed, how do we know that the opposite is not true? Perhaps God regards all life as an accidental cancerous growth that can be tolerated for the moment, but which must be wiped out if it starts interfering with His real design. How could anyone disprove that hypothesis? In a similar way, we tolerate the existence of insect life out in the forest – as long as it stays there and does not interfere with our purposes. But when the bugs creep into our gardens, houses, and granaries, we wipe them out.

### **Darwinian Evolution vs. Creationism**

These considerations seem always to invoke another issue, for reasons that we do not understand except that it is suggested by the book of Genesis in the Bible (although the issue itself makes no reference to any particular religion). For some, belief in detailed final causes for everything is tied to the dogma that every form of life must have been created by God for some specific purpose, and this becomes a premise from which to attack the idea of Darwinian evolution.

Our problem with this is that we are unable to see any functional difference between Darwinian evolution and Creationism; in what way would the observable facts be any different? Since the extinction of species and appearance of new species is not a mere ‘theory’ but an unquestioned fact (there are no dinosaurs or dodos running about today, and there is no evidence that humans or horses existed in the time of the dinosaurs and plenty of evidence that they did not), one who believes in an omnipotent God as the controlling force behind it all must, it seems to us, also believe that whatever may be the facts, those must have been His intention; otherwise He could not be omnipotent.

So when Darwin points out that there is a simple mechanism (natural selection) that can bring about automatically the changes that we observe, in what way does this contradict the hypothesis of an omnipotent God? Since that mechanism obviously exists, a believer in such a God must also believe that He created that mechanism for the purpose of carrying out His plan. Indeed, a God who failed to make use of such an obvious labor-saving device would seem rather stupid. Far from attacking Darwin, creationists ought to thank him profusely for showing them how to make their position so much more rational. We see this as much like the phenomenon noted in our opening paragraph: a false premise that is irremovable because it is built into a model that is never questioned.

Whatever the facts of biology – or physics, or chemistry, or geology, or astronomy – one is always free to postulate that behind it all is a purposive God; and this hypothesis cannot be confirmed or refuted by observation because it is consistent with all facts whatever they may be. So everyone is free to believe what he wishes about this, and whatever new knowledge we may acquire in the future will never require him to change this opinion. But this is hardly a new discovery; a famous exchange about it is reported to have occurred in 18<sup>th</sup> Century France:

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\* Some such hypothesis seems to have been considered obvious by nearly everyone except Spinoza up to the time of Newton; indeed, Newton himself thought that if the solar system were to drift gradually into a configuration incompatible with human life, it would be necessary for God to intervene and nudge the planets back on their proper courses to save us. This seems hopelessly arrogant to us today, as Einstein once noted in reply to a question from a news reporter. Much of the current discussion merely elaborates views that Einstein expressed many years ago.

**Act I:** Laplace sends Napoleon a just completed volume of his *Mécanique Céleste*. Although Napoleon is incapable of comprehending a word of it, when next they meet he has to say something about it in acknowledgment.

Napoleon: “How is it that, although you say so much about the Universe, you say nothing about its Creator?”

Laplace: “No, Sire, I had no need of that hypothesis.”

**Act II:** Napoleon reports this conversation to Lagrange, who will never pass up an opportunity to get in a holier-than-thou dig at the atheist Laplace:

Lagrange: “Ah, but it is such a good hypothesis: it explains so many things!”

**Act III:** Napoleon reports Lagrange’s comment back to Laplace, who has learned to expect such posturing and is ready for it:

Laplace: “Indeed, Sire, Monsieur Lagrange has, with his usual sagacity, put his finger on the precise difficulty with the hypothesis: it explains everything, but predicts nothing.”

In other words, the hypothesis of a God is, as Laplace saw, logically disconnected from the subject matter of science. That is the reason why scientists – Lagrange just as much as Laplace – have no way of using the hypothesis in the conduct of science; and why science in turn can offer no evidence for or against the hypothesis. We need not take such extreme positions as either Monod or the religious fundamentalists; it is sufficient if we recognize that, because of their logical independence, we cannot use their relation to advance either science or religion – or to disprove either. Curiously, nearly everyone who raises such issues does so in the belief that by denigrating science he is somehow advancing religion; hardly anyone, except perhaps Richard Dawkins (1987), imagines that by denigrating religion one is advancing science.

After all this, I shall surely be accused of cowardice if I fail to reveal my own personal views. Of course, I do not believe in any theological system as actual fact, because for a scientist supernatural explanations do not explain anything and there is no factual evidence for them in historical records or archæology. But I recognize that, as a human institution, religion has filled a need, brought comfort to many, and that over the Centuries human behavior has undoubtedly been better than it would have been without religion. So I do not advocate abandoning religion; only that religion should now become more rational by abandoning claims of miracles, which only discredit it in the minds of educated persons today. It would be greatly in their own interest to accept and use the truths of science.<sup>†</sup>

For me, somewhat the same purpose is served instead by classical music. Thus, while I do not participate in any religious activities, I will spend hours at the piano striving for exactly the right phrasing of a short passage in a Beethoven sonata; and feel great satisfaction when I finally succeed. But whatever ‘reality’ can be attributed to either religious or musical feelings is just what we ourselves choose to attribute to them; it is in the eye of the beholder.

This discussion has taken us rather far afield, so we conclude it by listing where interested readers may find a great deal about what modern scholarship has to say about the basis of Christianity and the Bible as historical fact. The Old Testament is analyzed in vast detail by Robert H. Pfeiffer (1948). F. C. Conybeare (1958) gives what we should call a rational analysis – indeed,

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<sup>†</sup> Although I was raised as a Methodist Christian, I now recognize that the Jewish religion comes closer to this goal than does Christianity, because it lays more emphasis on ethical teachings, and less on some arbitrary system of theology tied to miracles.

the only one known to us – of the origins of the New Testament, as a beautiful example of complex plausible reasoning leading to virtually certain conclusions. Also, there is a peculiar difficulty about the existence of a town called Nazareth in these early times, discussed by W. B. Smith (1905). However, the field has erupted into controversy again in recent years, with many different conclusions asserted for many different motives, by persons who simply ignore the facts of science. For an account of this, see L. T. Johnson (1996).