Softening a hard quadratic bound to a prior pdf — an example from geomagnetism

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Abstract. We discuss the problem of softening a hard quadratic bound to generate a personal prior probability distribution. The quadratic bound requires the model vector to live within a hyperspherical volume. Prior information suggests we may work in a finite-dimensional space, thus avoiding the known difficulties associated with infinite-dimensional spaces, and that values of the Euclidean 2-norm within the volume are uniformly distributed. The application is to the estimation of the magnetic field at the core-mantle boundary.

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INTRODUCTION

The Earth's magnetic field is generated in the liquid core of the earth, radius 3485km. The core is overlain by the silicate mantle, which we will take as a first approximation to be an insulator. The existence of the field is detected at the Earth's surface by direct measurement of its cartesian component values, and in the modern era, satellites can gather a dense global data set. What then can we infer about the morphology of the field at the core-mantle boundary, the boundary of the generation region? The problem is one of deconvolution with a known point-spread function (in the parlance of the astronomical community), albeit in a spherical geometry. This is the topic of this paper.

The magnetic field **B** is represented as the gradient of a potential V as a result of the insulating mantle approximation. Hence

$$\mathbf{B} = -\nabla V \tag{1}$$

and since **B** must be divergenceless by Maxwell's equations, we find that V satisfies Laplace's equation:

$$\nabla^2 V = 0 \tag{2}$$

In spherical coordinates (r, θ, ϕ) this is solved to give a general solution for V anywhere outside the core (radius c):

$$V = \sum_{l=1}^{\infty} \sum_{m=-l}^{l} c\beta_l^m(c) \left(\frac{c}{r}\right)^{l+1} Y_l^m(\theta, \phi) \tag{3}$$

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The $\beta_l^m(c)$ are often quoted in units of nanoTeslas (nT). In order to avoid complex coefficients, the spherical harmonics are defined here to be real with

$$Y_l^{|m|} = P_l^m(\cos\theta)\cos(m\phi); \quad Y_l^{-|m|} = P_l^m(\cos\theta)\sin(m\phi) \quad 0 \le m \le l \tag{4}$$

where P_l^m is a Legendre function. The normalisation is such that

$$\int_\Omega |Y_l^m|^2 \, d\Omega = \frac{4\pi}{2l+1} \tag{5}$$

where Ω is the sphere. The quantity that we wish to reconstruct on the core surface is B_r, the radial component of the magnetic field, which can be obtained easily from the potential:

$$B_r(\theta,\phi) = \sum_{l,m}(l+1)\beta_l^m(c)Y_l^m(\theta,\phi) \tag{6}$$

The data d_i are noisy observations of $\mathbf{B}$ related to the $\beta_l^m(c)$ via (1) and (3).

The need for prior information

Apart from a handful of problems in geophysics where the interesting parameters governing the system are finite in number (the problem of hypocentre location in seismology, and the determination of plate rotation poles in plate tectonics are the most readily accessible examples), most problems involve an Earth model which is a continuous function of the independent parameter (say time or position in one, two or three dimensions), and thus the Earth model is strictly infinite dimensional. The problem to hand is one such problem, where the quantity we seek is a continuous function of coordinates (θ,ϕ). Yet we only ever collect a finite data set consisting of D observations; since the work of Backus & Gilbert [7, 8] it has been known that such problems are fundamentally non-unique, and their solution requires the injection of prior information into the problem.

We shall see below that pertinent prior information does exist in this problem in the form of bounds on quadratic norms of the field, which take the form

$$\sum x_i^2 < 1 \tag{7}$$

where the x_i are parameters related linearly to the $\beta_l^m(c)$. The question we address here is how one might go about encoding information from (7) into a personal prior pdf which can be used in a Bayesian inference calculation to recover information about the $\beta_l^m(c)$.

PREVIOUS WORK

Much has been written about the problem of solving the linear inverse problem subject to a constraint of the form (7). Backus [3, 4, 5] comes to the conclusion that Bayesian inference is an unsafe way of proceeding when the prior information is really a hard quadratic bound and the dimensionality of the problem is really infinite, because the process of softening the bound to a personal pdf injects much more information than is contained in the bound, and some information that is contradictory to the bound. As a result, it is claimed that Bayesian calculations based on the softening of hard quadratic bounds are suspect. Backus [5] recommends the use of Neyman's method of confidence sets, Stark [14] suggests the use of minimax estimation, and Backus [6] advocates procrastination. As a consequence of these papers, geomagnetists have become paralysed, and no Bayesian calculations at all have been performed, when perhaps much could have been learned.

It seems to us that the apparatus of inductive inference is too valuable to give up lightly. We suggest that it might be of interest to make sensible Bayesian estimates in the case of the geomagnetic inverse problem, with which other calculations could be compared. We note that in the last 16 years since Backus' advocacy of confidence set inference, no actual data-based calculations have been made.

Of the useful bounds that can be applied to the geomagnetic inverse problem, we list two in order of certainty. The first quadratic bound [3] is that the energy contained in the magnetic field must be less than the rest mass of the Earth. In terms of the Schmidt quasi-normalised Gauss coefficients at the core-mantle boundary $\beta_l^m(c)$, this leads to

$$\sum_{l,m} \frac{(l+1)}{(2l+1)} |\beta_l^m(c)|^2 < \Gamma_e \tag{8}$$

where $\Gamma_e = 1 \times 10^{24} \mathrm{nT}^2$. The second, the so-called "heat flux bound", states that the amount of dissipation in the core associated with the magnetic field must be less than the heat flow out of the Earth's surface. This leads to [13, 11, 3]

$$\sum_{l,m} \frac{(l+1)(2l+1)(2l+3)}{l} |\beta_l^m(c)|^2 < \Gamma_h \tag{9}$$

where $\Gamma_h = 3 \times 10^{17} \mathrm{nT}^2$; this quantity arises from converting the observed heat flow out of the Earth Q into geomagnetic units by

$$\Gamma_h = \frac{Q\sigma\mu_0^2}{4\pi c} \tag{10}$$

and using values for the conductivity σ of the core ($3 \times 10^5 \mathrm{Sm}^{-1}$) and the permeability of free space μ_0.

In treating these bounds it is much more convenient to put them into the form of (7). We do this by a simple redefinition of the model in terms of new parameters x_l^m. In the case of the heat flux bound we write

$$x_l^m = \sqrt{\frac{(l+1)(2l+1)(2l+3)}{\Gamma_h l}} \beta_l^m(c) \tag{11}$$

There is a concomitant amendment to the form of the forward problem to account for this. We will normally use a single subscript i to index the x_l^m, where $l^2 \leq i \leq l(l+2)$ indexes all the coefficients with degree l and $(2l+1)$ different orders m.

More on the heat flux bound

We need more background on the physics on which the heat flux bound is based. Let Φ_{true} be the true dissipation in the core. Then a lower bound Φ on Φ_{true} can be written in terms of suitably normalised coefficients x_i at the CMB with suitable weights w_i as we have seen:

$$\sum_i w_i x_i^2 = \Phi < \Phi_{\text{true}} \tag{12}$$

The usual argument made is that $\Phi_{\text{true}} < Q$, where Q is the observed heat flow through the Earth's surface, and therefore the quadratic form on the left of (12) must be less than Q.

But let us examine the inequality in more detail. The left hand side depends only on the poloidal coefficients of the magnetic field, and quite possibly the toroidal magnetic field may generate anything from 1–100 times more Ohmic dissipation than the poloidal field, so quite probably $\Phi << \Phi_{\text{true}}$. We can say more. The heat flowing out of the core is probably much less than Q, since much of Q is accounted for by radioactivity in the mantle. If $Q \sim 44$TW, the observed global heat loss from the Earth, then the heat flowing out of the core Q_{core} might be only 6-12 TW. It is theoretically possible for the dissipation to exceed the heat flowing out of the core [1, 12] because of the so-called thermodynamic efficiency; we have the inequality

$$\Phi_{\text{true}} \leq (T_{\max}/T_{\min} - 1) Q_{\text{core}} \tag{13}$$

for maximum and minimum temperatures in the core $T_{\max}$ and $T_{\min}$ respectively. Mineral physics suggests that $T_{\max}/T_{\min} \sim 1.2$ perhaps in the core, thus it seems likely that the dynamo is quite inefficient, and so Φ_{true} might only be 1/5 of the heat flow out of the core-mantle boundary. Conversely, when very large temperature differences are extant, and the dynamo returns its heat to the hottest part of the core for re-use, it is clearly possible to have an efficiency greater than one.

We can see how these inequalities add up to lead to the possibility that Φ might be only perhaps a thousandth of Q, and yet it is feasible that only the strict inequality $\Phi < Q$ may be pertinent (if we ignore efficiencies greater than 1 as being geophysically indefensible). Some authors even admit that $\Phi < Q$ might be strictly in error, since a heat pulse of dissipation in the core in the distant past might not yet be seen in the heat flow at the Earth surface. Discounting this possibility, it seems to us that we need a way of encoding all this imprecision into a prior probability distribution for $\{x_i\}$ that says that virtually the whole range of $0 \leq \Phi \leq Q$ should be possible (there seems to be no lower bound on Φ, because prior to receiving the data, we know nothing about the size of the magnetic field $\mathbf{B}$ and the dissipation scales with this).

A possible prior probability density

Obviously (12) is invariant under interchange of labels on parameters, and defines the interior of a hypersphere. We aim to convert this into an isotropic probability density function (pdf) which encapsulates the information contained therein, as well as the previous discussion which shows that the quadratic form could equally likely live anywhere in the hypersphere. Backus [2, 4] has treated the problem of constructing isotropic pdfs corresponding to (12) in the case where $N = \infty$. He shows that in this case it is impossible to construct a prior pdf that encapsulates (12) without injecting extra information into the problem not contained in (12). Thus the problem of "softening" the hard prior bound into a pdf appears to be intractable.

It seems to us that we know more about the length scales over which dissipation occurs. It is much more likely that the spectrum of the dissipation has non-zero contributions up to a certain wavenumber, after which it decays rapidly, than it is that the converse be true. One thing we know is that turbulence plays a role in the core. In order to have dynamo action at all, the magnetic Reynolds number R_m must be larger than a critical value, of order 10-100. But since the magnetic Prandtl number P_m of most liquid metals is small (10^{-6} being typical), this means that the hydromagnetic Reynolds number (which is R_m/P_m) must be very large indeed. Braginsky & Meytlis [10] (see also Braginsky & Roberts [9]) estimate that the shortest length scale of the anisotropic turbulence to be perhaps 1km. This would have associated magnetic fields with wavenumbers $l \sim 40,000$, and hence a parameter space dimension $N \sim 10^9$. We will take this as a likely value, but we can always study the dependency of the solution to the exact dimension of the parameter space, and equally to the exact value of Γ_h used. It is worth noting that this $N \gg D$ for all practical data sets.

Let us define some terminology. Let $p(\mathbf{x})$ be the pdf for $\mathbf{x} = \{x_i\}$. In our development below we use n to define the dimension of the space; we are interested in all spaces with dimension $1 \leq n \leq N$. The inequality (12) defines the interior of a hypersphere, so it makes sense to work in terms of radius $r_n : 1 \leq n \leq N$ where $r_n^2 = \sum_1^n x_i^2$. It is known [4] that we need to avoid independent pdfs for each x_i, since the Central Limit Theorem leads to unavoidable concentration of $E\{r_n^2\}$.

We require $p(r_n)$ where clearly

$$p(r_n) = 0 \quad r_n > 1 \tag{14}$$

The pdf must be normalised so that

$$\int_\Theta p(r_n)\, d^n x = 1 \tag{15}$$

over the hypersphere $\Theta : r_n < 1$. We perform the integral (15) in spherical coordinates. Let S_n be the surface area of a unit sphere in n-dimensional space (note that this notation is not universal — some would call a sphere in 3-d space the "two-sphere"). Then we can write (15) in the form

$$\int S_n r^{n-1} p(r)\, dr = 1 \tag{16}$$

with

$$S_n = \frac{2\pi^{n/2}}{\Gamma(n/2)} \tag{17}$$

(e.g. Zwillinger 1996, p315).

Let us step back to the discussion of what we really know about Φ: we discovered that really all values are likely up to Q. In our non-dimensional variables, we would like all values of "energy" $E = r_n^2$ to be equally likely. We assume then

$$p(E) = 1 \quad 0 \leq E \leq 1 \tag{18}$$

and zero otherwise. What then is the corresponding pdf of $\mathbf{x}$? It follows that

$$p(r) = p(E)dE/dr = 2r \tag{19}$$

In order to conserve probability mass this generates the multidimensional probability distribution p($\mathbf{x}$) which satisfies

$$2r\delta r = p(\mathbf{x})\delta^n \mathbf{x} = p(\mathbf{x}) S_n r^{n-1} \delta r \tag{20}$$

and hence

$$p(\mathbf{x}) = \frac{2}{S_n r^{n-2}} \tag{21}$$

In particular, $< r_n^2 >$ (the expected value of r_n^2) and its standard deviation are

$$< r_n^2 >= 1/2 \tag{22}$$

and

$$\sigma(r_n^2) = \sqrt{\frac{1}{12}} \sim 0.28 \tag{23}$$

regardless of the dimension n. It is the correlation inherent in (21) that evades the otherwise inevitable concentration of the Central Limit Theorem.

To show that (21) is isotropic in all spaces below n, we need to consider the joint pdf in one space lower by marginalising over one of the variables, say x_n. If $p(r_{n-1}^2)$ is the marginal of p in $n-1$ dimensional space, we have

$$p(r_{n-1}^2) = 2\int_0^{\sqrt{1-r_{n-1}^2}} p(r_{n-1}^2 + z^2)\, dz \tag{24}$$

which is clearly a function of only r_{n-1}^2, showing that it too is isotropic.

These marginals can be continued all the way down to $p(x_1)$, the marginal for one variable. It is simpler to note that any point at a fixed value of x in the n-sphere is actually in an $(n-1)$-sphere of radius $\sqrt{1-x^2}$. We find

$$p(x_1) = \frac{S_{n-1}}{S_n} \int_0^{\sqrt{1-x_1^2}} \frac{2r^{n-2}}{(r^2 + x_1^2)^{(n-2)/2}}\, dr \tag{25}$$

This can be evaluated in terms of Hypergeometric functions ${}_2F_1$ [15], but the answer is not terribly illuminating:

$$p(x) = \frac{S_{n-1}}{S_n} \left(\frac{x^{2-n} \left(1-x^2\right)^{\frac{n-1}{2}} \Gamma(\frac{n}{2})\, {}_2F_1(\frac{n-2}{2}, \frac{n-1}{2}, \frac{n+1}{2}, 1-x^{-2})}{(n-1)\sqrt{\pi}\,\Gamma(\frac{n}{2}-\frac{1}{2})} \right) \tag{26}$$

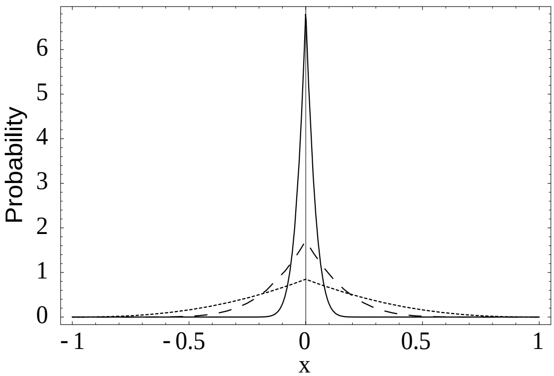

FIGURE 1. Marginalised pdfs $p_1(x)$ for $N = 300$ (solid), $N = 20$ (dashed) and $N = 6$ (dotted).

Integration of (25) by parts shows that the marginal is in fact non-singular everywhere, despite the apparent singularity of (21). The marginals integrate to unity regardless of the dimension of the space, as they must. Figure 1 shows the marginalised pdf $p(x)$ for three examples of $n = N$ which are much lower than the hypothesized $N \sim 10^9$. As the chosen value of N increases the pdf is increasingly concentrated at the origin.

It is perhaps interesting to note that our assignment is the same as that which maximises the entropy of the distribution subject to the constraints. Since there are no moment constraints, the flat distribution is the maximum entropy choice.

The subspace for computation is less than the dimension of the space

Although the dimension of the space N is large, the dimension of the space in which computations need to be performed can be considerably smaller, because the magnetic fields associated with the highest degree spherical harmonics are attenuated so much by the distance from the core surface to the Earth's surface. As a result, the is a maximum degree L beyond which nothing can be learned about the core field from noisy data at the Earth's surface. This exemplifies the ill-posedness of the inverse problem. Our knowledge of the spherical harmonics beyond L must remain as the prior knowledge we have about them.

Backus [3] uses Schwartz' inequality to show that the net effect of all magnetic fields at the core surface with $l > 31$ cannot produce a magnetic field of rms value in excess of 1nT at the Earth's surface if they obey the heat flux bound. At the time, 1nT was much less than the observational errors associated with satellite data. At the present time, it is expected to be able to collect satellite data with sub-nanoTesla errors, so one might want to find the degree beyond which fields of, say, 1% of 1nT are produced.

It is straightforward to see how L is calculated. Without loss of generality, we restrict attention to axisymmetric fields. Clearly, any field obeying (9) will have a $g_l^0(c)$ for which

$$(l+1)(2l+1)(2l+3)l^{-1}(\beta_l^0)^2 < \Gamma_h \tag{27}$$

At the north pole on the Earth's surface (radius $r = a$) this generates a radial field B_r of strength

$$B_r(0,0) = (l+1)\left(\frac{c}{a}\right)^{l+2} Y_l^0(0,0)\beta_l^0(c) \tag{28}$$

which we require to be less than ε, the largest acceptable error. Using (27) in (28) and the fact that with Schmidt quasi-normalisation, $Y_l^0(0,0) = 1$, we find

$$\left(\frac{c}{a}\right)^{l+2} \sqrt{\frac{\Gamma_h l(l+1)}{(2l+1)(2l+3)}} < \varepsilon \tag{29}$$

If $\varepsilon = .01$nT, an $l = 38$ field exceeds the bound, and if $\varepsilon = .1$nT, an $l = 34$ field exceeds the bound; hence, the appropriate truncation levels are $L = 37$ and $L = 33$ respectively.

Discussion

We now have our prior for the vector **x**. The pdf of interest is, of course, the posterior p(**x**|**d**). The likelihood for the data is usually assumed to be Gaussian, and then it is certainly possible to compute the maximum of the *a posteriori* distribution by methods of optimization; however, it is important to characterise fully the acceptable ranges of parameters given by the posterior. Sampling the posterior and the calculation of the relevant integrals appears to be most easily accomplished by numerical sampling schemes, the results of which will be forthcoming.

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