

Minimum Norm Construction

I 2.0

- Smallest, flattest models
- 2 data gravity problem
- Including a priori information through norms
- A generic flexible norm

Minimum Norm Construction : Accurate Data

Consider the geophysical experiment that yields data

$$d_j = (g_j, m) \quad j=1, N$$

Assume that the data are accurate.

Remarks: We recognize that there are infinitely many solutions. Our goal is to find one.

Some form of prior information must be supplied.

Our procedure is to incorporate this prior information into a model norm and then find the solution that has minimum norm.

We'll illustrate several types of prior information and the resulting models.

- (i) Smallest (l_2 -norm) solution (zero reference model)
- (ii) Smallest deviation (the roll of the reference model)
- (iii) Flattest models
- (iv) Weighted models.

Remark: All of the above components eventually will get combined into a generic model objective function that we will use.

We'll work on a simple example. 2-data gravity problem.

For the present we'll keep everything as analytic as possible. Working with functions and analytic data allows us to explore the fundamental problem of instability that arises.

①

Minimum Norm Construction : Inverse Problem #1

Consider a geophysical experiment in which the data are given by

$$d_j = (g_j, m) \quad j=1, N \quad (1)$$

These equations form a system of N constraints upon an unknown function m . We recognize that the solution is nonunique and therefore we construct a specific model that is of potential interest to us. Introducing a norm

$$\|m\| = (m, m)^{1/2} \quad (2)$$

we formulate the problem as finding an m that minimizes (2) subject to the constraints in (1).

The solution can be achieved in two ways:

- (i) using calculus of variations
- (ii) Projection theorem.

Calculus of Variations

To minimize a function subject to constraints we make a combined functional

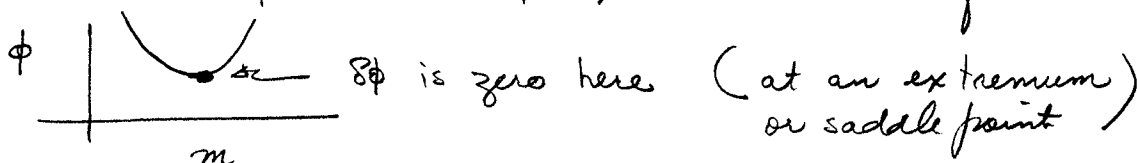
$$\phi(m) = \|m\|^2 + 2 \sum_j \alpha_j [d_j - (g_j, m)]$$

Comments: (1) Since $\|m\|$ is positive it doesn't matter whether we minimize $\|m\|$ or its square.

(2) The α_j 's are Lagrange multipliers. (Factor 2 is arbitrary)

$$\phi(m) = (m, m) + 2 \sum_j \alpha_j [d_j - (g_j, m)]$$

In a variational approach we introduce an arbitrary perturbation δm and observe the change in the functional ϕ . Then we look at $\delta\phi = \phi(m + \delta m) - \phi(m)$ and set it equal to zero.



(3)

The matrix Γ is positive definite and symmetric and therefore invertible. (details later)

$$\Gamma \bar{\alpha} = \bar{d}$$

$\Gamma : N \times N$ matrix

$$\Rightarrow \boxed{\bar{\alpha} = \Gamma^{-1} \bar{d}}$$

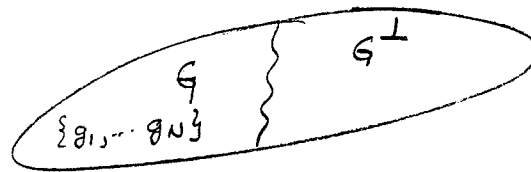
This solves for the coefficients. The minimum norm model is then obtained by

$$\boxed{m_0 = \sum x_j g_j}$$

Actually we have shown that $m = \sum x_j g_j$ is a stationary point. Technically we need to look at other derivatives to ensure that it is not a maximum or saddle point.

Method II: Using the Decomposition Theorem.

Our model space can be divided into an activated and unactivated portion



$$m = m'' + m^\perp$$

$$\begin{aligned} m'' &\in G = \text{span}\{g_1, \dots, g_N\} \\ m^\perp &\in G^\perp \end{aligned}$$

Every element in G^\perp is perpendicular to every element in G . In particular:

$$(g_j, m^\perp) = 0 \quad j=1, N$$

Consider the data equations

$$\begin{aligned} d_j &= (g_j, m) \\ &= (g_j, m'' + m^\perp) = (g_j, m'') + \underbrace{(g_j, m^\perp)}_{=0} \end{aligned}$$

so

$$\boxed{d_j = (g_j, m'')}$$

(something that we knew before. The data are affected only by m'' .)

Now consider a minimum norm solution

$$\begin{aligned}
 \|m\|^2 &= \|m'' + m^\perp\|^2 \\
 &= (m'' + m^\perp, m'' + m^\perp) \\
 &= (m'', m'') + 2(m'', m^\perp) + (m^\perp, m^\perp) \\
 &= \|m''\|^2 + \|m^\perp\|^2
 \end{aligned}$$

Since m^\perp has no effect on the data we can include as much or as little of it as desired. From the point of view of minimizing $\|m\|^2$ we choose $m^\perp = 0$.

If $m^\perp = 0$ then the norm minimizing solution is $m_0 = m''$.
Thus

$$m_0 = \sum_{j=1}^N \alpha_j g_j$$

Substituting into the data equations yields, as before, a system of equations to be solved:

$$\Gamma \bar{\alpha} = \bar{d}$$

$$\Gamma_{ij} = (g_i, g_j)$$

Remark: We now have the algebra for our first inverse problem. Assuming that Γ^{-1} exists, and that we are not worried about computational efficiency, we can compute a minimum norm model that fits the data.

Remark: The algebra presented is completely general and is therefore valid for any Hilbert space. We consider two simple examples for illustration

(i) 2-data gravity problem

(ii) solution to an underdetermined system of equations.

2-Data Gravity Problem.

One of the simplest and yet informative problems in linear inverse theory is the two data gravity problem. The goal is to determine the density structure of a spherically symmetric body by measuring its mass and moment of inertia. The appropriate equations are

$$\begin{aligned} \frac{\bar{\rho}}{3} &= \int_0^1 r^2 \rho(r) dr \\ \frac{\bar{\rho} \gamma}{2} &= \int_0^1 r^4 \rho(r) dr \end{aligned} \quad (1)$$

where $\bar{\rho} = \frac{M_e}{\frac{4}{3}\pi a^3} = 5.5 \text{ Mg/m}^3$

'a' is radius of earth

$\gamma = \frac{C}{Ma^2} = .33078$

(C is moment of inertia about the spin axis)

In (1), the radius of the earth has been normalized to unity. So $r=0$ corresponds to the center of the earth, $r=1$ corresponds to the surface.

Remark: Remember, for a sphere if $\rho(r)$ is constant $\Rightarrow \gamma = 0.4$. For the earth $\gamma = .33078 < 0.4 \therefore$ The earth must be more dense toward the center.

Let

$$\begin{aligned} d_1 &= \frac{\bar{\rho}}{3} = 1.833 \text{ Mg/m}^3 \\ d_2 &= \frac{\bar{\rho} \gamma}{2} = .9095 \text{ Mg/m}^3 \end{aligned}$$

Then the two equations in (1) can be written as

$$\begin{aligned} d_j &= (g_j, m) \quad j=1,2 \\ \text{where } g_1 &= r^2, \quad g_2 = r^4 \end{aligned}$$

Smallest Model Solution

The minimum norm model, when $\|g\| = (g, g)^{1/2}$ is given by

$$\rho(r) = \sum \alpha_j g_j = \alpha_1 r^2 + \alpha_2 r^4$$

where α 's are found by solving $\Pi \bar{\alpha} = \bar{d}$
 where $\Pi_{ij} = (g_i, g_j)$. Our inner product is

$$(g_i, g_j) = \int_0^1 g_i(r) g_j(r) dr$$

$$(g_1, g_1) = \int_0^1 r^4 dr = \frac{1}{5}$$

$$(g_1, g_2) = (g_2, g_1) = \frac{1}{7}$$

$$(g_2, g_2) = \frac{1}{9}$$

So

$$\Pi = \begin{pmatrix} \frac{1}{5} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{9} \end{pmatrix}$$

$$\Pi^{-1} = \frac{2205}{4} \begin{pmatrix} \frac{1}{9} & -\frac{1}{7} \\ -\frac{1}{7} & \frac{1}{5} \end{pmatrix}$$

$$\bar{\alpha} = \Pi^{-1} \bar{d} = \frac{2205}{4} \begin{pmatrix} \frac{1}{9} & -\frac{1}{7} \\ -\frac{1}{7} & \frac{1}{5} \end{pmatrix} \begin{pmatrix} 1.833 \\ .9095 \end{pmatrix} = \begin{pmatrix} 40.658 \\ -44.086 \end{pmatrix}$$

So

$$\boxed{\rho(r) = 40.658 r^2 - 44.086 r^4 \quad \frac{\text{Mg}}{\text{m}^3}}$$

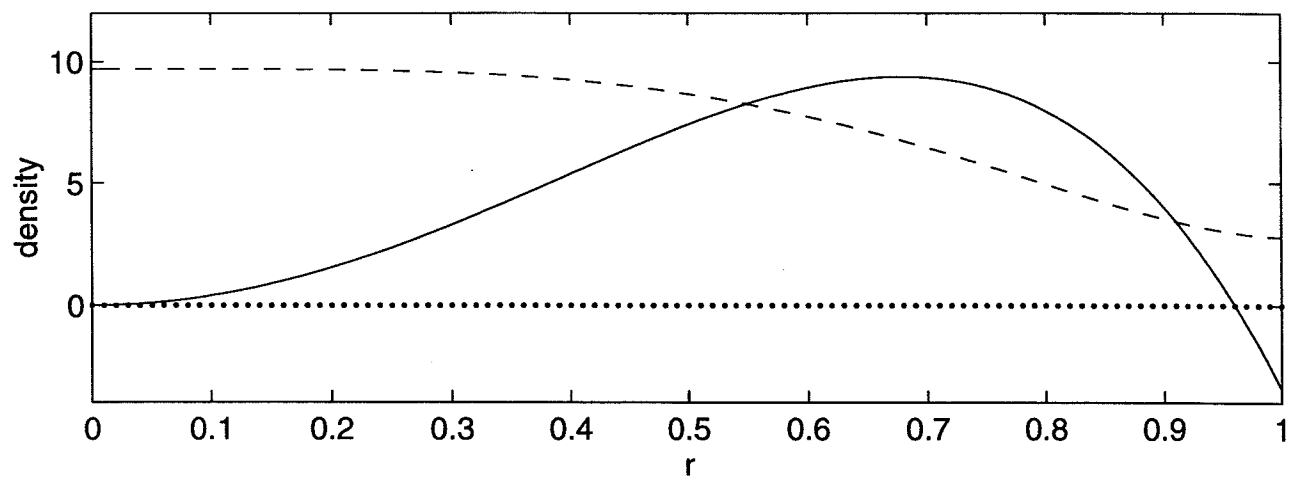
Remark: This density structure is plotted on the following graph.
 Places of interest are:

$r=0$ $\rho=0$ (center of the earth has zero density)

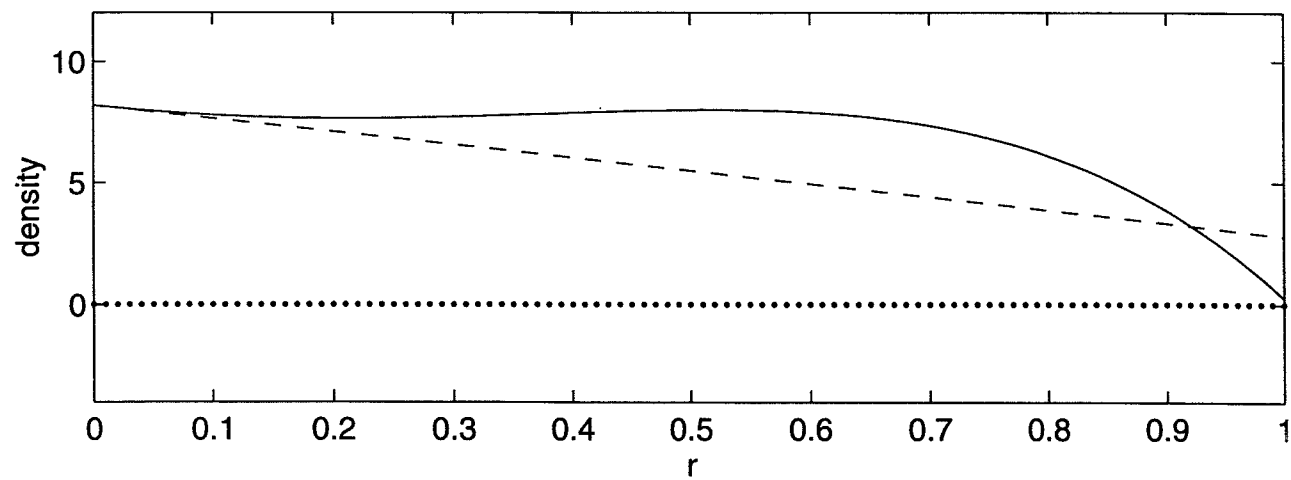
$r=1$ $\rho = -3.428 \text{ Mg/m}^3$ (surface of the earth has negative density)

*: We have constructed a mathematical solution to the problem but not a geophysical solution. For this example, the smallest model was not the best norm to be minimized.

Smallest and flattest models



Smallest deviatoric model



Smallest deviatoric model.

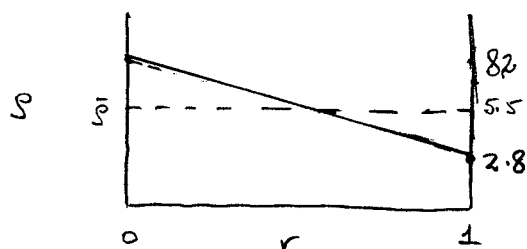
Remark: The density structure produced by minimizing $\|g\|^2$ was unacceptable on physical grounds. Does this mean that a smallest model formulation is not appropriate for the 2-data gravity problem?

Remark: In minimizing $\int_0^1 \rho(r)^2 dr$ we have attempted to find a model that is close to zero everywhere. But really, this is not a result that is consistent even with elementary geophysics. Let's examine what we know.

(1) average density for the earth is $\bar{\rho} = 5.5 \text{ Mg/m}^3$

(2) surface rocks (if we think of the "surface" as being a planetary surface and think of the average properties of the top 100 km) the a reasonable estimate for the density at the surface is $\rho_s \sim 2.8 \text{ Mg/m}^3$. If the average value is 5.5 Mg/m^3 then we would estimate that the density at the center of the earth is greater than 5.5 Mg/m^3 . This of course is entirely in accordance with our ideas of compaction and compression of rocks as we descend into the earth.

So, a guess for the earth density



Choose $\rho_0(r) = 8.2 - 5.4r \quad \frac{\text{Mg}}{\text{m}^3}$

So $\rho_0(r)$ is a "guess" at what the density structure might be even if it isn't a particularly brilliant guess.

Remark: If $\rho_0(r)$ is our current best estimate for the density then we would like our density structure which fits the two data to be close to $\rho_0(r)$. That is we want to minimize

$$\phi = \|\rho - \rho_0\| \quad \text{subject to data constraints.}$$

(8)

but $p(r) = p_0(r) + \delta p(r)$. Minimizing $\|p - p_0\|$ is the same as minimizing $\|\delta p\|$. Write the data equations in terms of δp

$$\begin{aligned} d_j &= (g_j, p) = (g_j, p_0 + \delta p) \\ &= (g_j, p_0) + (g_j, \delta p) \end{aligned}$$

but p_0 is known so (g_j, p_0) can be evaluated and taken to the other side.

$$d_j - (g_j, p_0) = (g_j, \delta p)$$

Introducing new data we have

$$\begin{aligned} f_j &= (g_j, \delta p) \\ f_j &= d_j - (g_j, p_0) \end{aligned}$$

But this is same type of equation that we had before. The only change is that

- (i) new data
- (ii) "model" is now δp .

The minimum norm solution, minimizing $\|\delta p\|$ is completely appropriate.

I: Compute the new data.

$$(g_1, p_0) = \int_0^1 r^2 (8.2 - 5.4r) dr = \frac{8.2}{3} - \frac{5.4}{4} = 1.383$$

$$(g_2, p_0) = \int_0^1 r^4 (8.2 - 5.4r) dr = \frac{8.2}{5} - \frac{5.4}{6} = .740$$

$$\text{so } f_1 = d_1 - (g_1, p_0) = 1.833 - 1.383 = .45$$

$$f_2 = d_2 - (g_2, p_0) = .9095 - .740 = .1695$$

$$\vec{f} = (.45, .1695)^T \quad \text{are new data.}$$

The smallest norm solution $\delta p = \alpha_1 r^2 + \alpha_2 r^4$

(9)

$$\vec{\alpha} = \vec{P}^{-1} \vec{f} = \frac{2205}{4} \begin{pmatrix} \frac{1}{9} & -\frac{1}{7} \\ -\frac{1}{7} & \frac{1}{5} \end{pmatrix} \begin{pmatrix} .533 \\ .203 \end{pmatrix} = \begin{pmatrix} 16.66 \\ -19.59 \end{pmatrix}$$

so $\delta r = 16.66 r^2 - 19.59 r^4$

and

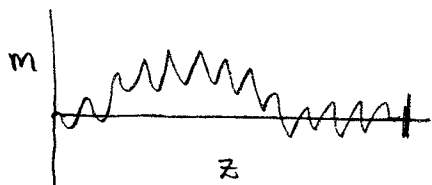
$$\rho(r) = 8.2 - 5.4r + 16.66 r^2 - 19.59 r^4 \quad \frac{\text{Mg}}{\text{m}^3}$$

How does this look?

$$\left. \begin{aligned} \rho(0) &= 8.2 \text{ Mg/m}^3 \\ \rho(1) &= 0.262 \text{ Mg/m}^3 \end{aligned} \right\} \text{ See handout.}$$

So we still don't have a good geophysical answer but we're getting close. This is certainly a better result than we had previously. If we had made an estimate with $\rho_0(0)$ to be larger, we would have done better with respect to the surface density.

Remark: The above cases are a bit pessimistic to be generalized. Usually smallest, or smallest deviatoric, models can be constructed which look reasonably geophysical. A characteristic of these models however is that they tend to have fluctuations.



← typical result of trying to construct a model which is as close to zero everywhere (subject to data constraints).

This may be undesirable. Is there a way around this. Can a solution be formulated which doesn't suffer from these oscillations.

Remark: Consider integral equations of the form

$$d_j = \int_a^b g_j(x) m(x) dx = (g_j, m) \quad j=1, N$$

Integrate these equations by parts. Let

$$h_j(x) = \int_a^x g_j(u) du \quad \left| (h_j(x) = g_j^{(-1)}(x) \text{ in Parker's notation} \right.$$

be the indefinite integrals of the kernel functions. we obtain

$$\begin{aligned} d_j &= h_j(x) m(x) \Big|_a^b - \int_a^b h_j(x) m'(x) dx \\ &= h_j(b) m(b) - \underbrace{h_j(a) m(a)}_{=0} - \int_a^b h_j(x) m'(x) dx \end{aligned}$$

Suppose that $m(b)$ is known. Then

$$\boxed{h_j(b) m(b) - d_j = \int_a^b h_j(x) m'(x) dx} \quad (1)$$

So we have a new system of equations

$$\boxed{f_j = (h_j, m')} \quad j=1, N \quad (2)$$

where $f_j = h_j(b) m(b) - d_j$ are new data
 $h_j(x)$: are new kernels
 $m'(x)$: new "model".

But these equations are precisely the same as those we solved previously for a minimum norm model. (minimize $\phi = (m', m)$)
The solution is therefore

$$m'(x) = \sum_{j=1}^N \beta_j \cdot h_j(x) \quad (3)$$

where

$$\Pi \vec{\beta} = \vec{f} \quad \text{and} \quad \Pi_{ij} = (h_i, h_j)$$

Once $m'(x)$ is found, we can integrate to obtain $m(x)$.

$$m(x) = \int_x^x m'(u) du + C \quad (4)$$

The constant is evaluated by requiring that the known boundary condition at $x=b$ is satisfied. ($m(b)$ was presumed to be known in order evaluate the new data f_j)

* (Note $m(x) = \int_x^x \sum_{j=1}^N \beta_j h_j(u) du = \sum_{j=1}^N \beta_j g^{(-2)}(x) + C$) : So the model is made doubly smoothed ker

Remark: The above procedure required that a value of the model be supplied at the right hand endpoint. Suppose however that $m(a)$ was known rather than $m(b)$. Is there a way to alter the formulation?

Fundamental Theorem of Calculus.

$$m(b) - m(a) = \int_a^b m'(x) dx$$

So we could alter (1) by substituting for $m(b)$ to get

$$h_j(b) m(b) - d_j = \int_a^b h_j(x) m'(x) dx$$

$$h_j(b) \left\{ m(a) + \int_a^b m'(x) dx \right\} - d_j = \int_a^b h_j(x) m'(x) dx$$

$$h_j(b) m(a) - d_j = \int_a^b (h_j(x) - h_j(b)) m'(x) dx$$

so

$$\tilde{f}_j = d_j - h_j(b) m(a) = \int_a^b [h_j(b) - h_j(x)] m'(x) dx$$

Remark: This process of integration by parts may be continued indefinitely so long as values of the function and its derivative are known at a boundary.

eg: with the next integration by parts we obtain equations of the form

$$p_j' = (r_j, m'')$$

$$r_j = g_j^{(-2)} \quad (\text{double indefinite integral})$$

The smallest norm model minimizing $\phi = (m'', m'')$ is called the "smoothest" model (at least by me!)

Flattest model for the 2-data gravity problem.

The information we had about the surface rocks was that $g(1) = 2.8 \frac{Mg}{m^3}$. Use a flattest model formulation that requires knowledge of the model at its right hand endpoint.

$$h_j(1)g(1) - d_j = \int_0^1 h_j(r)g'(r)dr$$

$$h_1(r) = \int_0^r u^2 du = \frac{r^3}{3}$$

$$h_2(r) = \int_0^r u^4 du = \frac{r^5}{5}$$

$$h_1(1) = \frac{1}{3}$$

$$h_2(1) = \frac{1}{5}$$

$$g(1) = 2.8 \frac{Mg}{m^3}$$

$$\bar{g} = 5.5 Mg/m^3$$

$$f_1 = h_1(1)g(1) - d_1 = \frac{g(1)}{3} - \frac{\bar{g}}{3} = \frac{1}{3}(g(1) - \bar{g})$$

$$f_2 = h_2(1)g(1) - d_2 = \frac{g(1)}{5} - \frac{\bar{g}}{2} = \frac{1}{5}\left(g(1) - \frac{5}{2}\bar{g}\right)$$

$$\frac{1}{3}(g(1) - \bar{g}) = \int_0^1 \frac{r^3}{3} g'(r) dr$$

$$\frac{1}{5}\left(g(1) - \frac{5}{2}\bar{g}\right) = \int_0^1 \frac{r^5}{5} g'(r) dr$$

We obtain

$$-2.7 = \int_0^1 r^3 \rho'(r) dr$$

$$-1.7482 = \int_0^1 r^5 \rho'(r) dr$$

$$\bar{\Gamma} = \begin{pmatrix} \frac{1}{7} & \frac{1}{9} \\ \frac{1}{9} & \frac{1}{11} \end{pmatrix} \quad \bar{\Gamma}^{-1} = 1559.25 \begin{pmatrix} \frac{1}{11} & -\frac{1}{9} \\ -\frac{1}{9} & \frac{1}{7} \end{pmatrix}$$

$$\vec{\beta} = \bar{\Gamma}^{-1} \bar{f} = -1559.25 \begin{pmatrix} \frac{1}{11} & -\frac{1}{9} \\ -\frac{1}{9} & \frac{1}{7} \end{pmatrix} \begin{pmatrix} -2.7 \\ -1.7482 \end{pmatrix} = \begin{pmatrix} -79.849 \\ 78.363 \end{pmatrix}$$

So $\rho'(r) = \beta_1 r^3 + \beta_2 r^5$

$$\Rightarrow \rho(r) = \frac{\beta_1 r^4}{4} + \frac{\beta_2 r^6}{6} + C$$

$$\boxed{\rho(r) = C - 19.962 r^4 + 13.06 r^6}$$

Adjust the constant of integration C to make a surface density $\rho(1) = 2.8 \Rightarrow C = 9.702$.

$$\therefore \boxed{\rho(r) = 9.702 - 19.962 r^4 + 13.06 r^6}$$

This curve monotonically decreases from the core to the surface.

$$\rho(0) = 9.7 \text{ Mg/m}^3$$

Remark: This is definitely a geophysically acceptable density distribution.

Summary: a-data gravity problem

- (1) We can rigorously generate models that fit the data
- (2) Depending upon what objective function is minimized we get models with different character.
 - some intuitively simple mathematical norms (eg $\|m\|^2$) don't produce physically appealing models
 - others, like minimizing $\|m'\|^2$ or $\|m - m_{ref}\|^2$ produce more reasonable models.

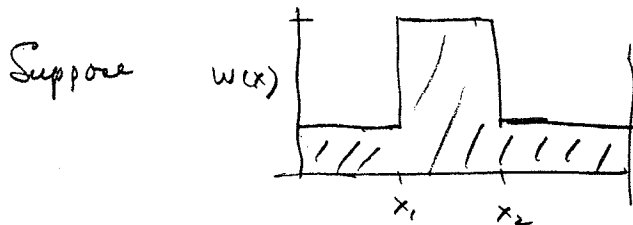
Clearly the approach we are establishing is to first "design" the right kind of objective f^m for the problem. That is, the model that minimizes $\phi_m(m)$ should have the "right character" and be consistent with any a-priori information we have about the model.

We already have some components for building up a general objective f^m but we need one more.

Weighted model objective f^m

$$\text{let } \phi_m = \int_a^b w(x) m^2(x) dx \quad \text{or} \quad \int_a^b w(x) (m(x) - m_{ref}(x))^2 dx$$

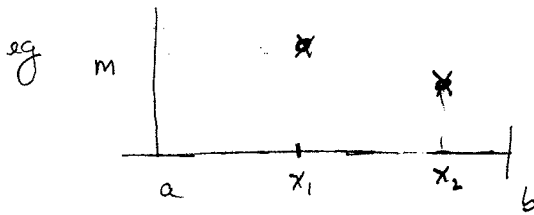
where $w(x) > 0$ $w \in [a, b]$



This weighting discriminates against $m_c(x)$ (constructed model) to have energy in this region.

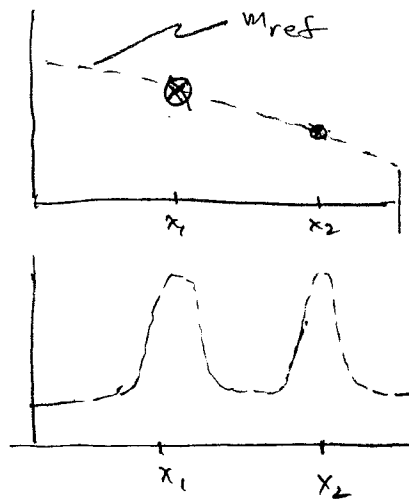
Potential uses of the weighting f^m

- (1) Construct a model which includes local knowledge obtained from previous investigations



Estimates of $m(x)$ are obtained at x_1, x_2

We want the constructed model to be close to these values at these locations.



Construct m_{ref}

at x_1, x_2 the weight $w(x)$ is large $\Rightarrow m_c(x)$ will tend to be close to $m_{ref}(x_1), m_{ref}(x_2)$

But away from those locations our confidence in m_{ref} is diminished

so we are not distressed if our reconstructed model differs substantially.

Remark: As we shall see, there are other ways to include this type of information, but the above scenario is valid.

- (2) Specific appraisal analysis

Suppose



Question: is this feature really there (?). Or is it in the right location (maybe it should be shallower or deeper)

Design an objective f^m to discriminate against the feature or put it in a different location.

(3) General exploration of model space.

Generic Model Objective Function

If we combine all of the previous ideas we obtain one (of many) useful forms for a model objective J^m . It's one that we will use here

$$J_m = \alpha_s \int w_s(x) (m - m_{ref})^2 dx + \alpha_x \int w_x \left(\frac{d(m - m_{ref})}{dx} \right)^2 dx$$

α_s, α_x : positive constants

$w_s(x)$: weighting J^m for the smallest model component

$w_x(x)$: weighting J^m for the derivative

m_{ref} : reference model (often leave it out of the second term)

Remark: This form of objective J^m is chosen because of its simplicity and yet great functionality. By varying a relatively few constants or functions, one can generate quite different kinds of models, put in a priori information and explore model space.

Remark: We will later add even more flexibility to the problem by
(i) replacing the l_2 -norms with more general l_p norms

So, we should be all ready to solve our inverse problem.
 Let's consider a simple, but typical example (One related to the NMR experiment and also, more generally, a Laplace Transform)
 (This example is one that you'll do for an assignment so I don't want to do everything for you here, but we do need to illustrate the effects of instability or ill-posedness).

Problem: Given data $d_j = (g_j, m)$

$$\boxed{g_j(x) = e^{-jx}} \quad \begin{matrix} x \in [0, 1] \\ j = 0, 20 \end{matrix}$$

Generate true data using a model

$$\boxed{m(x) = 1 - \frac{1}{2} \cos 2\pi x}$$

Compute the smallest model $(\phi_m = (m, m))$ that reproduces the data.

Solution is $m_c(x) = \sum \alpha_j g_j(x)$

$$\Gamma \alpha = d$$

$$\Gamma_{ij} = (g_i, g_j)$$

Do everything in double precision arithmetic. Data and inner product matrix is generated from analytic expressions. (You'll derive them in your homework)

Examples: (1) Data, true & recovered model. (few data, lots of data)
 (2) Perturbed data

Summary: (numerical test examples)

We have found a way to overcome the fundamental problem of non-uniqueness (namely to generate a model with certain characteristics) but there is a further problem of numerical instability.

The inverse problem is ill-posed because of this instability.

Basically, for our calculation, we had

$$\Gamma a = d$$

Γ is symmetric and positive definite (s. long as the kernels are linearly independent), so

$$\Gamma = R \Lambda R^T$$

Γ is $N \times N$

where $R = \begin{pmatrix} | & & | \\ r_1 & \dots & r_N \\ | & & | \end{pmatrix}$ is an orthonormal matrix

$$\Lambda = \text{diag}(\lambda_1, \dots, \lambda_N)$$

$\lambda_1 > \lambda_2 > \dots > \lambda_N$ are the eigenvalues of $\Gamma \vec{r}_i = \lambda_i \vec{r}_i$

So

$$R \Lambda R^T a = d$$

$$R^T a = \Lambda^{-1} R^T d$$

$$a = R \Lambda^{-1} R^T d$$

$$\left(a = \sum_{i=1}^N \frac{(r_i^T d)}{\lambda_i} \vec{r}_i \right)$$

$$m(x) = \sum_{i=1}^N d_i g_i(x)$$

So the numerical difficulties stem from the small eigenvalues of the inner product matrix. Effectively Γ is almost singular

$$\det \Gamma = \prod_{i=1}^N \lambda_i \lambda_2 \dots \lambda_N \sim 0$$

Note that difficulties will arise because of numerical imprecision as the number of data grow! There will also be problem if the data vector d is incorrect.