DL in Applied Mathematics

Lecture 15: Neural network augmented inverse problems for PDEs

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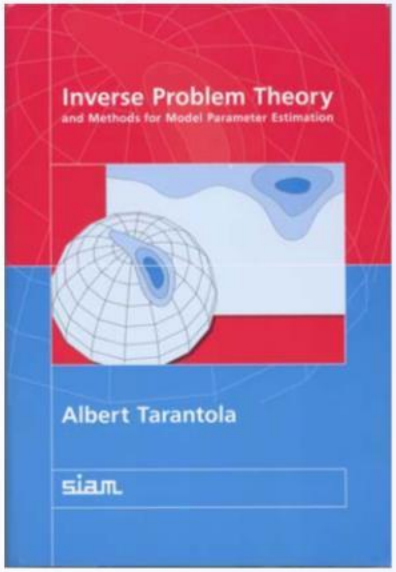
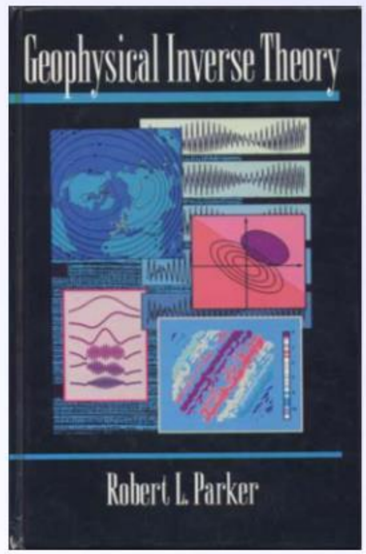
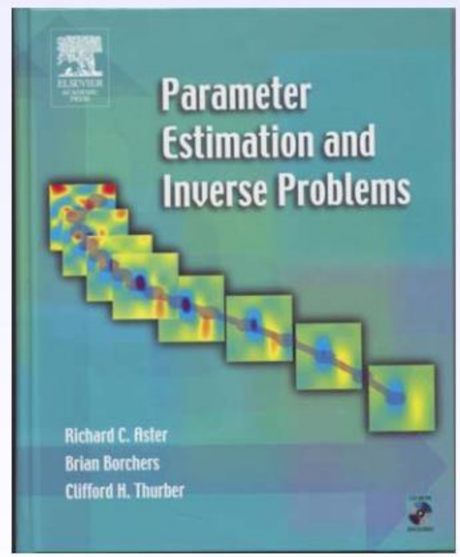
Course Contents

- Characterizing inverse problems
- Linear, discrete inverse problems
- Linearizing nonlinear problems
- Discrete ill-posed inverse problems
- Regularization
- Fully nonlinear inversion and parameter search
- Probabilistic inference

Books

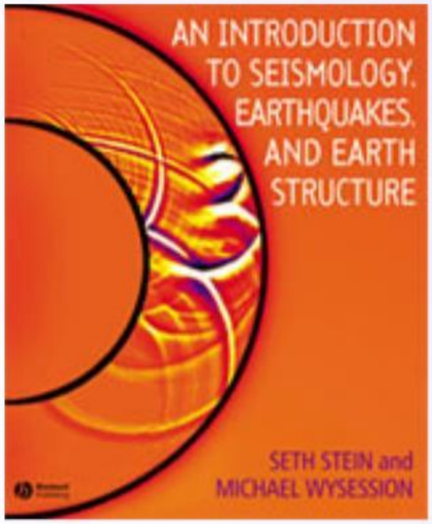




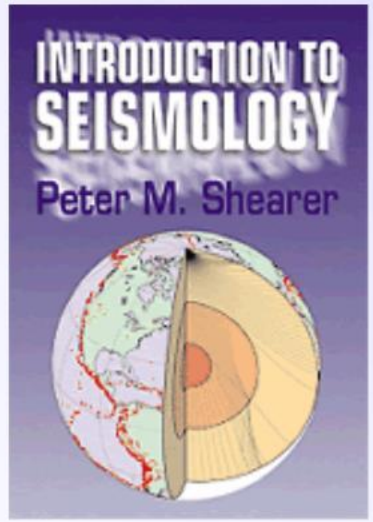


See also Menke '*Geophysical data analysis: discrete inverse theory*' (Academic Press, 1989)

Books

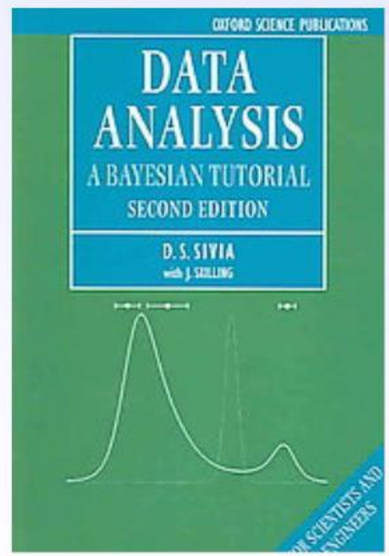


Chapter 7 on inverse problems



Introductory Chapter on inverse problems

Useful Bayesian tutorial
(First 5 chapters)



Reference works

Some papers:

- Understanding inverse theory
  Ann. Rev. Earth Planet. Sci., **5**, 35-64, Parker (1977).

- Interpretation of inaccurate, insufficient and inconsistent data
  Geophys. J. Roy. astr. Soc., **28**, 97-109, Jackson (1972).

- Monte Carlo sampling of solutions to inverse problems
  J. Geophys. Res., **100**, 12,431–12,447,
  Mosegaard and Tarantola, (1995)

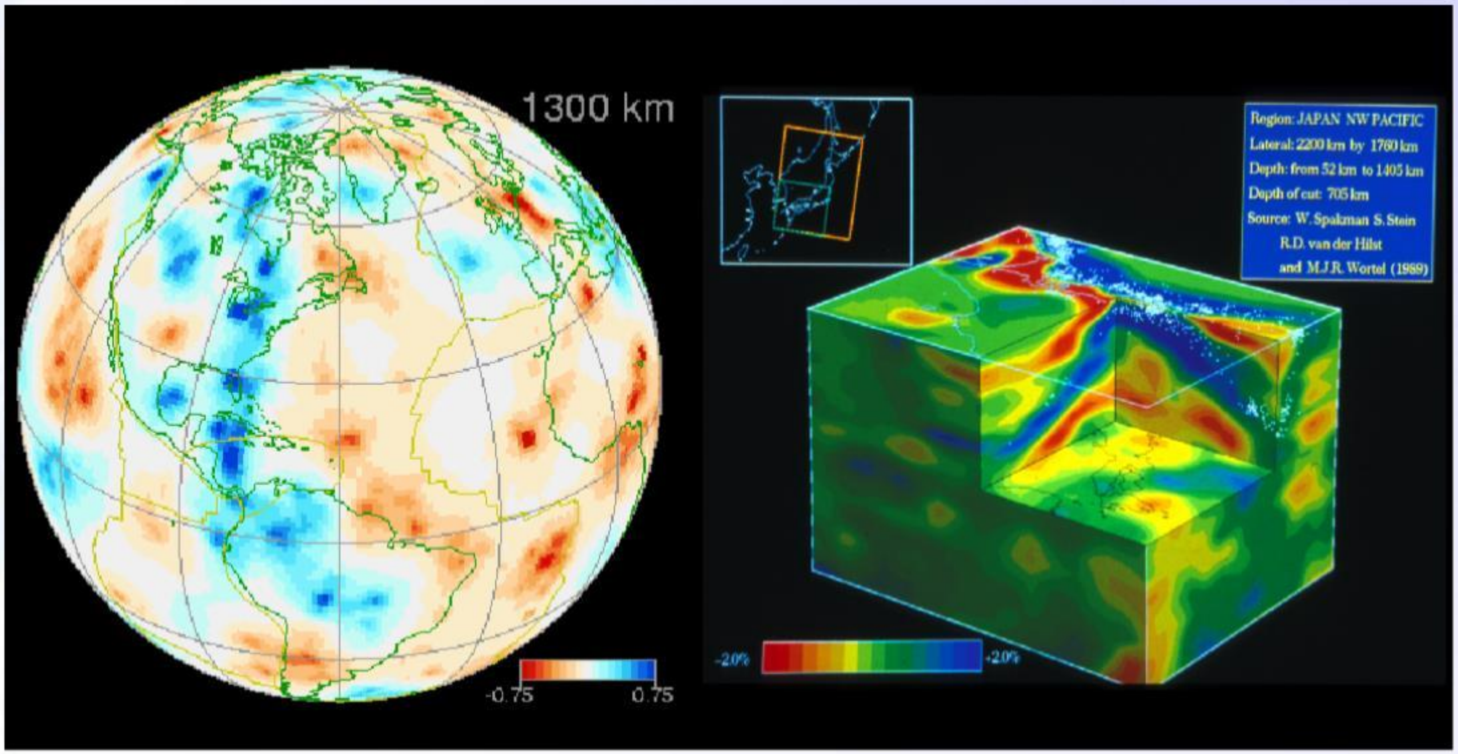
- *Monte Carlo methods in geophysical inverse problems,*
  Rev. of Geophys., 40, 3.1-3.29,
  Sambridge and Mosegaard (2002)

There are also several manuscripts on inverse problems available on the Internet. I can not vouch for any of them.
See http://www.ees.nmt.edu/Geop/Classes/GEOP529_book.html

Lecture 1: Introduction

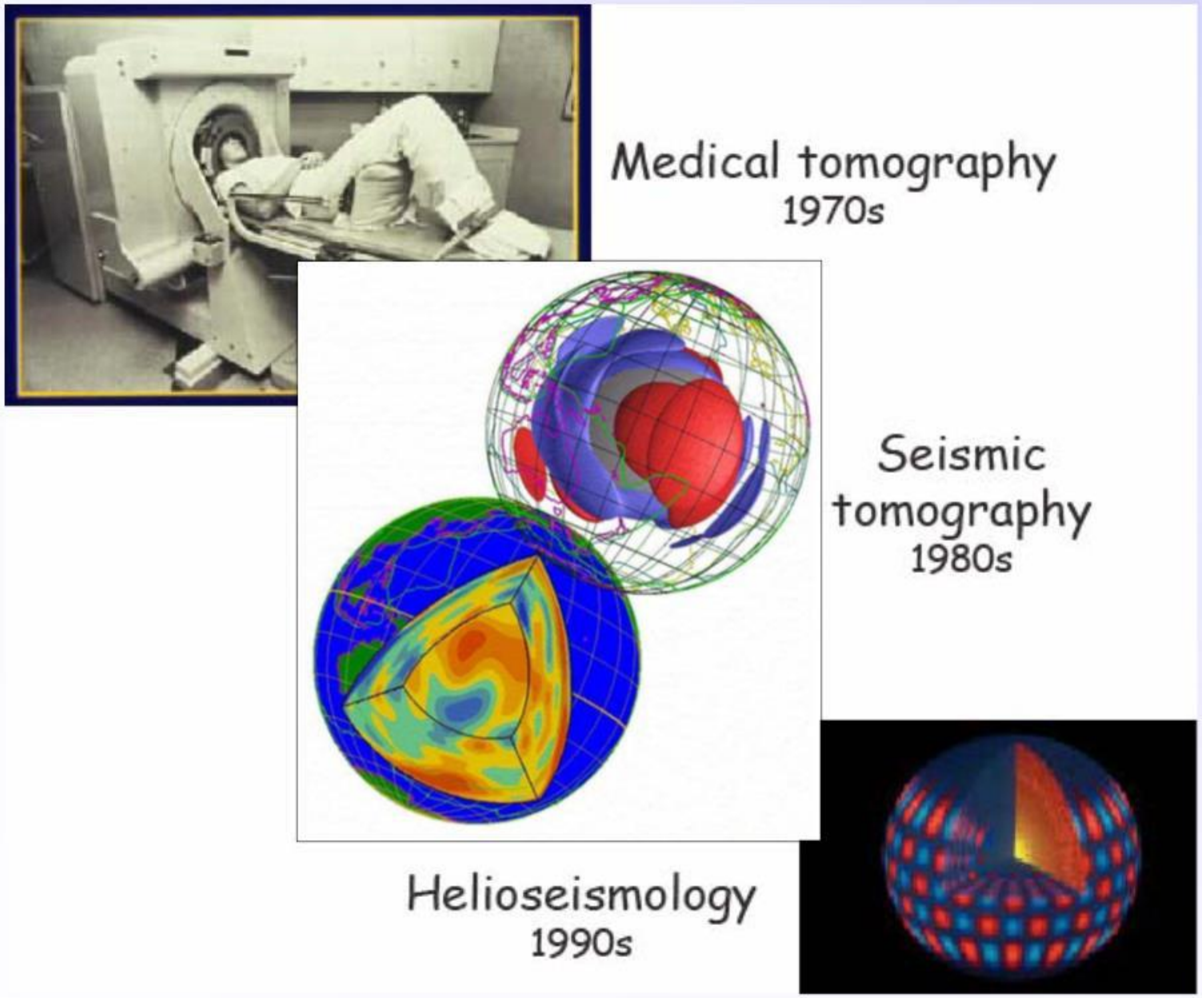
What are inverse problems and why do we care...

Geophysical inverse problems



Inferring seismic properties of the Earth's interior
from surface observations

Inverse problems are everywhere



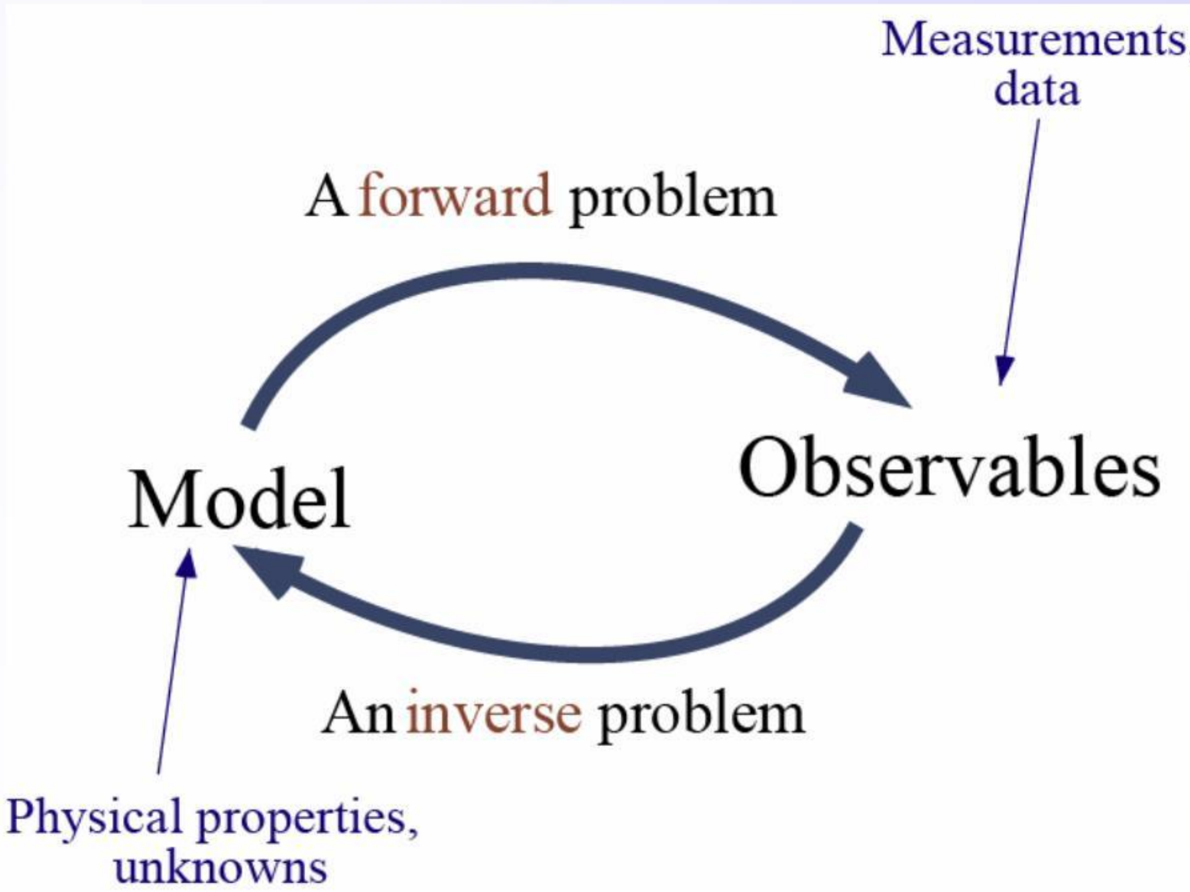
When data only indirectly constrain quantities of interest

Thinking backwards

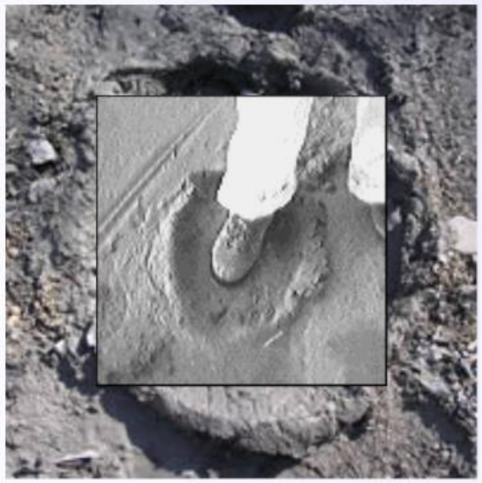
Most people, if you describe a train of events to them will tell you what the result will be. There are few people, however that if you told them a result, would be able to evolve from their own inner consciousness what the steps were that led to that result. This power is what I mean when I talk of reasoning backward.

Sherlock Holmes,
A Study in Scarlet,
Sir Arthur Conan Doyle (1887)

Reversing a forward problem



Inverse problems=quest for information



What is that ?

What can we tell about
Who/whatever made it ?

Collect data:

- Measure size, depth
  properties of the ground

Can we expect to reconstruct the
whatever made it from the evidence ?

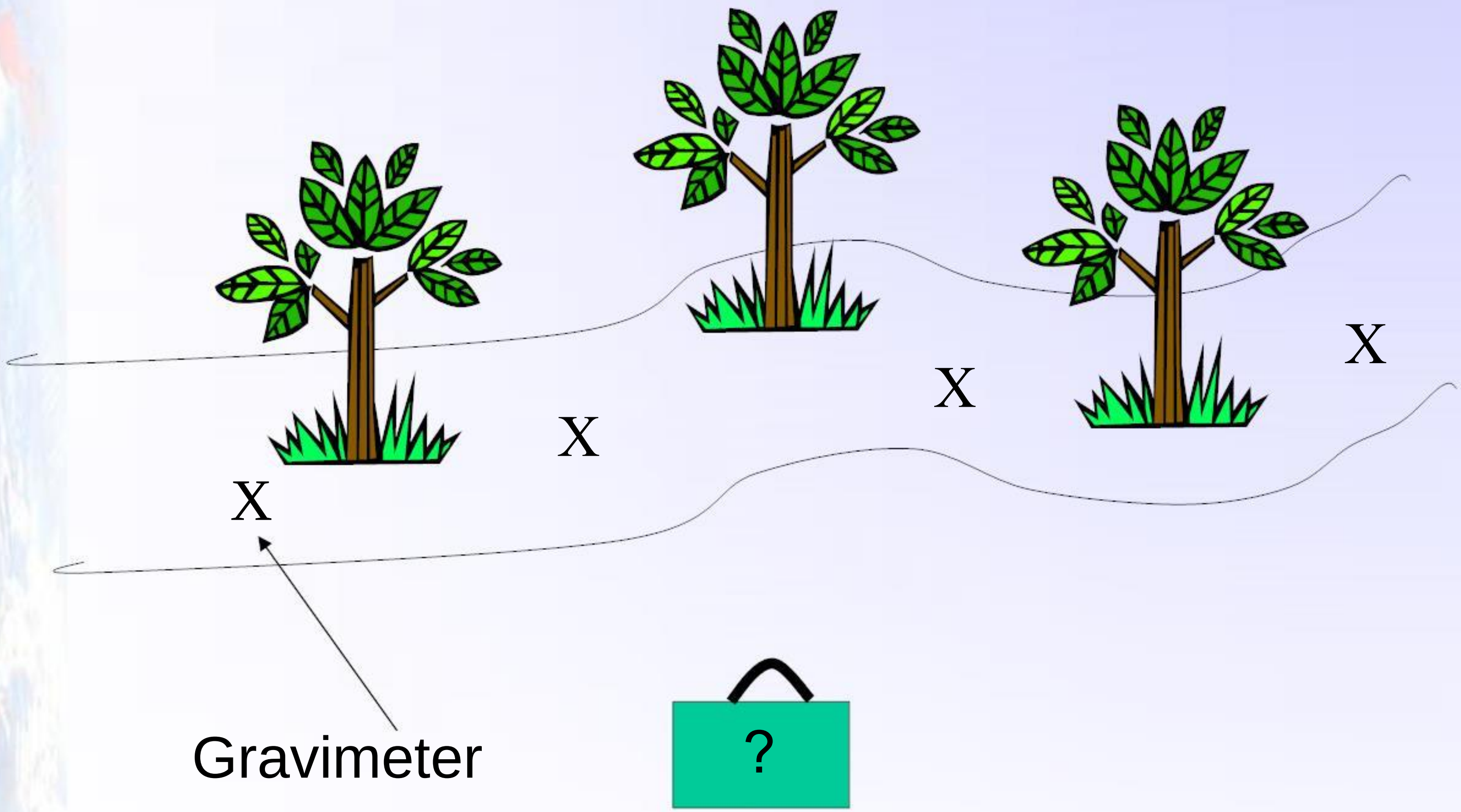
Use our prior knowledge:

- Who lives around here ?

Make guesses ?

Anatomy of an inverse problem

Hunting for gold at the beach with a gravimeter



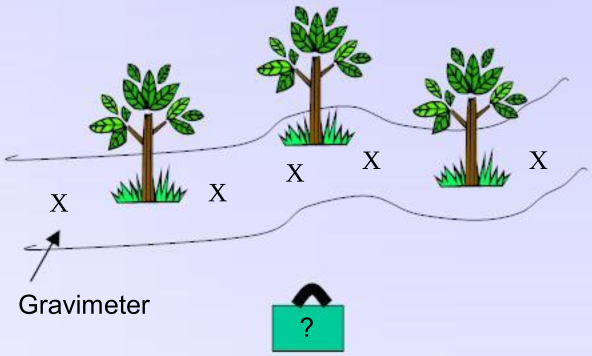
Courtesy Heiner Igel

Forward modelling example: Treasure Hunt

We have observed some values:

10, 23, 35, 45, 56 μ gals

How can we relate the observed gravity values to the subsurface properties?



We know how to do the *forward* problem:

$$\Phi(r) = \int \frac{G\rho(r')}{|r - r'|} dV'$$

This equation relates the (observed) gravitational potential to the subsurface density.

-> given a density model we can predict the gravity field at the surface!

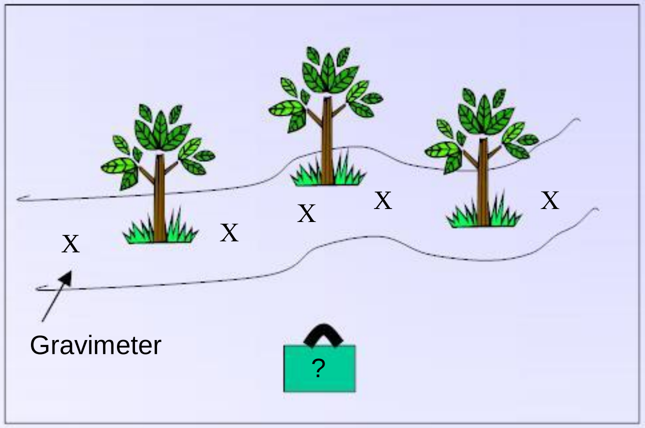
Treasure Hunt: Trial and error

What else do we know?

Density sand: 2.2 g/cm^3
Density gold: 19.3 g/cm^3

Do we know these values *exactly*?

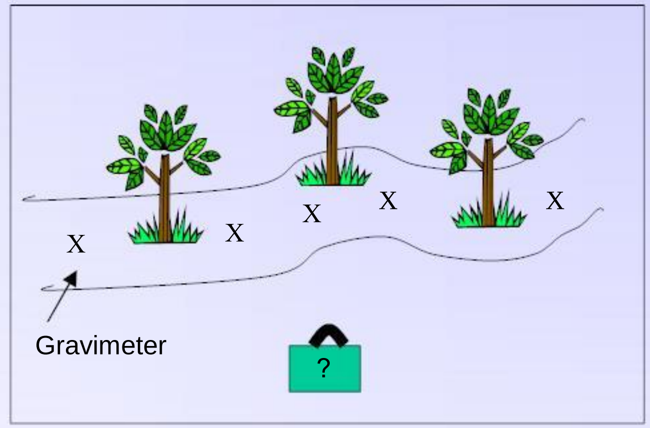
Where is the box with gold?



One approach is trial and (t)error forward modelling

Use the *forward* solution to calculate many models for a rectangular box situated somewhere in the ground and compare the *theoretical* (*synthetic*) data to the observations.

Treasure Hunt: model space

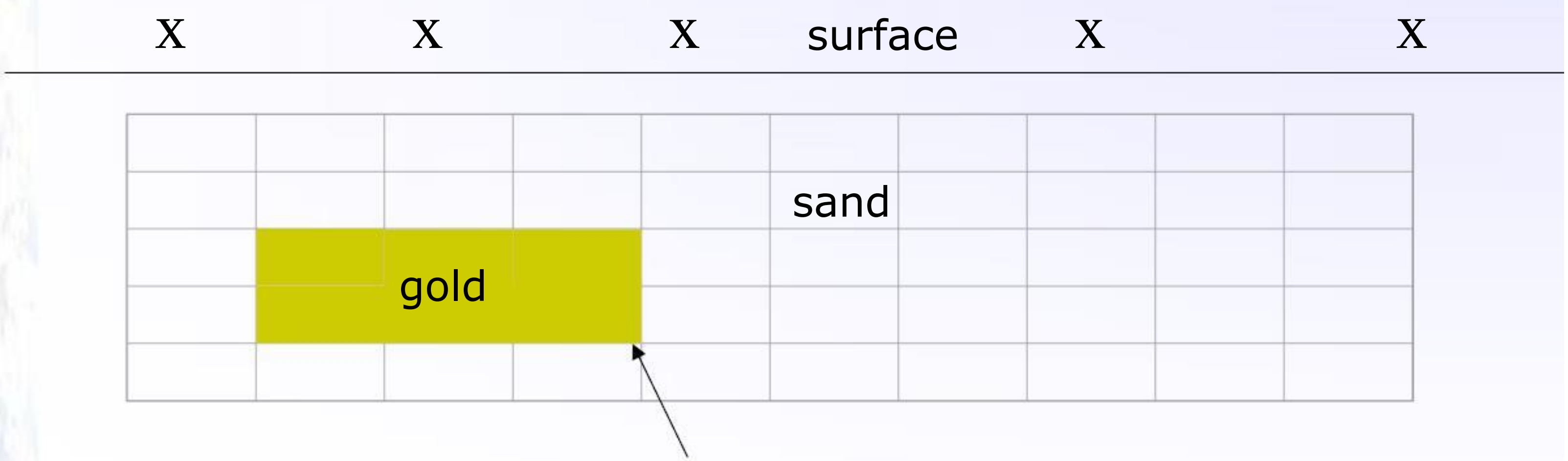


But ...

... we have to define *plausible* models for the beach. We have to somehow describe the model geometrically.

We introduce simplifying approximations

- divide the subsurface into rectangles with variable density
- Let us assume a flat surface



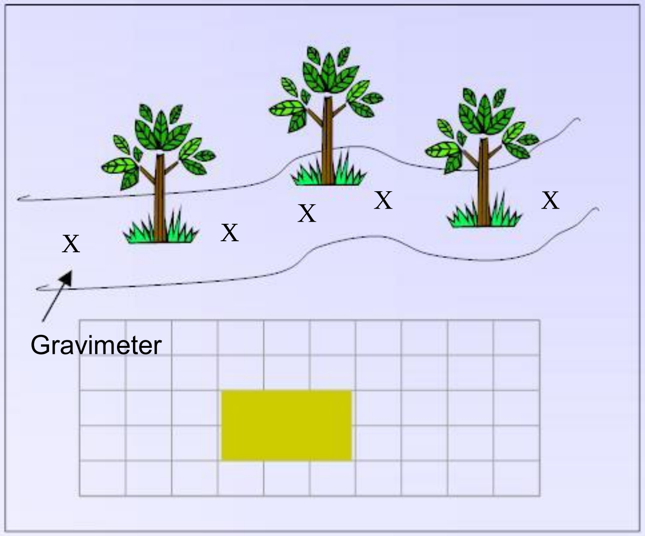
Treasure Hunt: Non-uniqueness

Could we compute all possible models and compare the synthetic data with the observations?

- at every rectangle two possibilities (sand or gold)
- $2^{50} \sim 10^{15}$ possible models

(Age of universe $\sim 10^{17}$ s)

Too many models!



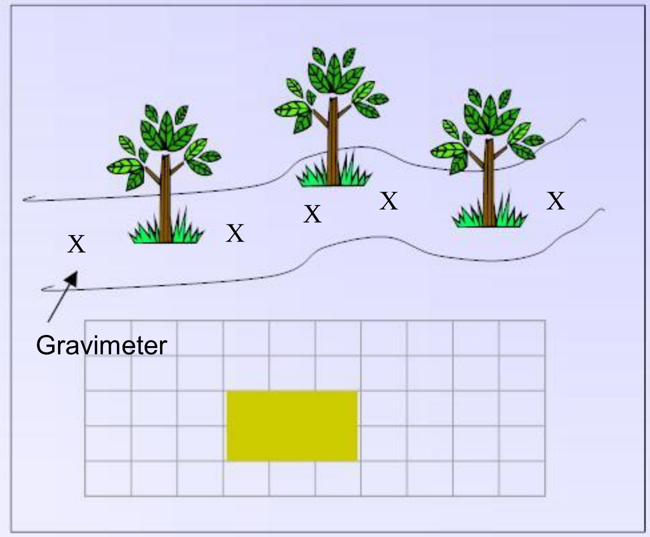
- We have 10^{15} possible models but only 5 observations!
- It is likely that two or more models will fit the data (maybe exactly)

Non-uniqueness is likely

Treasure hunt: a priori information

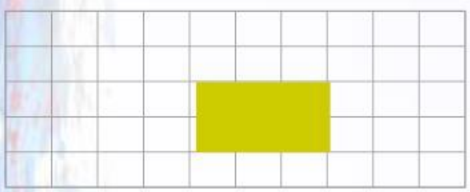
Is there anything we know about the treasure?

How large is the box?
Is it still intact?
Has it possibly disintegrated?
What was the shape of the box?



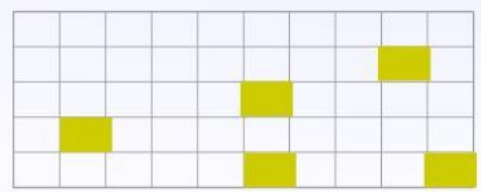
This is called *a priori* (or prior) information.
It will allow us to define plausible, possible, and unlikely models:

plausible



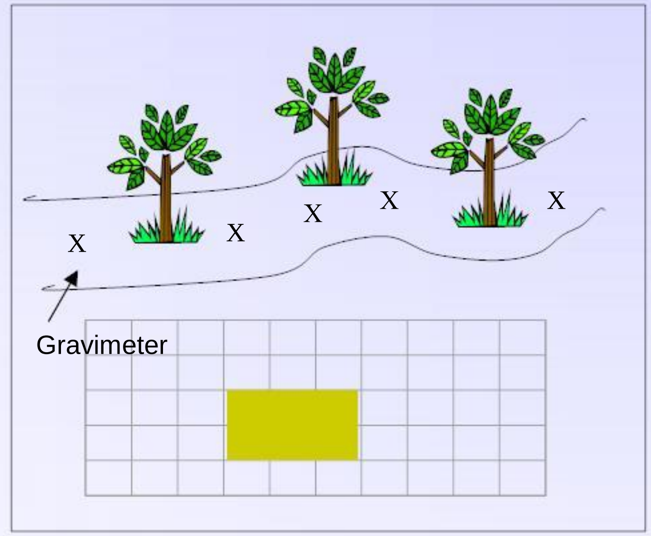
possible

unlikely



Treasure hunt: data uncertainties

Things to consider in formulating the inverse problem

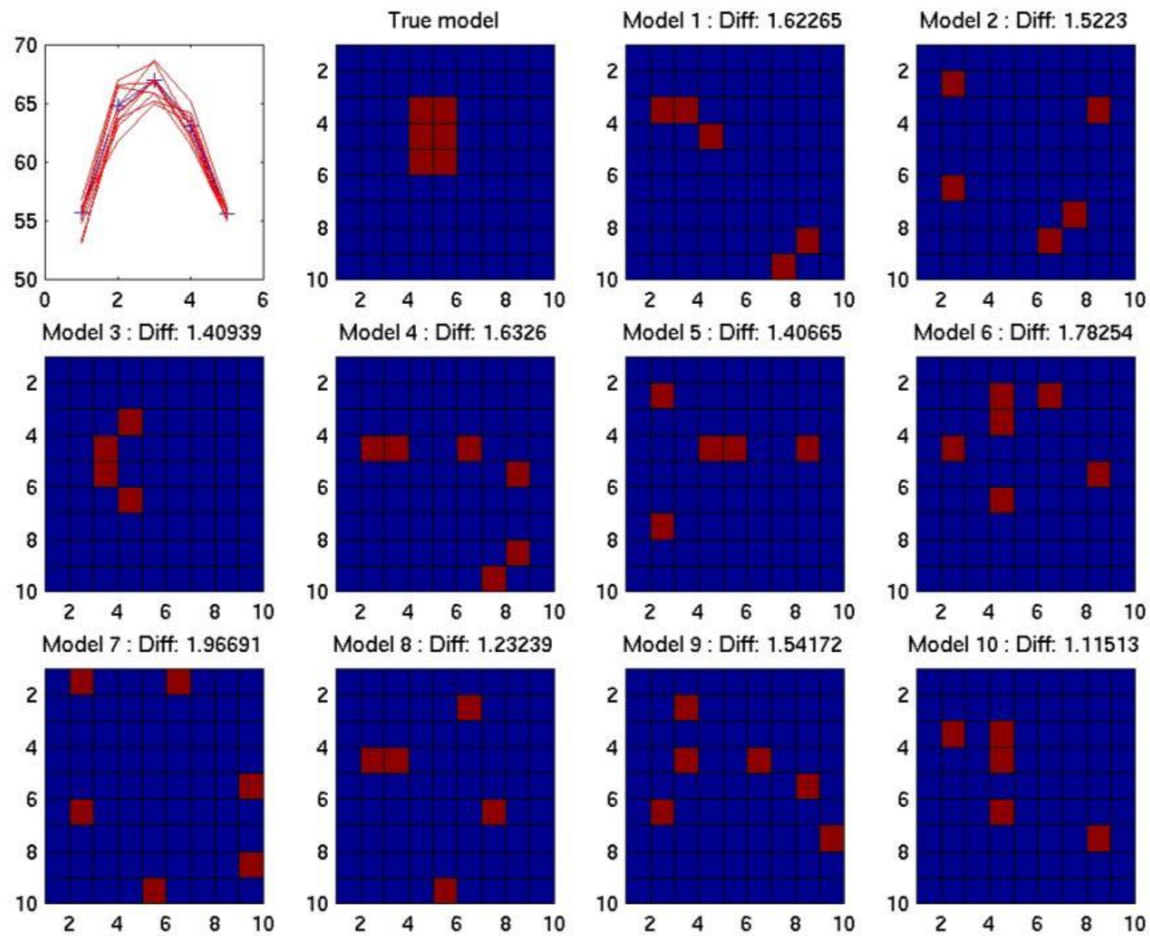


- Do we have errors in the data ?
  - Did the instruments work correctly ?
  - Do we have to correct for anything?
    (e.g. topography, tides, ...)
- Are we using the right theory ?
  - Is a 2-D approximation adequate ?
  - Are there other materials present other than gold and sand ?
  - Are there adjacent masses which could influence observations ?

Answering these questions often requires introducing more simplifying assumptions and guesses.
All inferences are dependent on these assumptions. (GIGO)

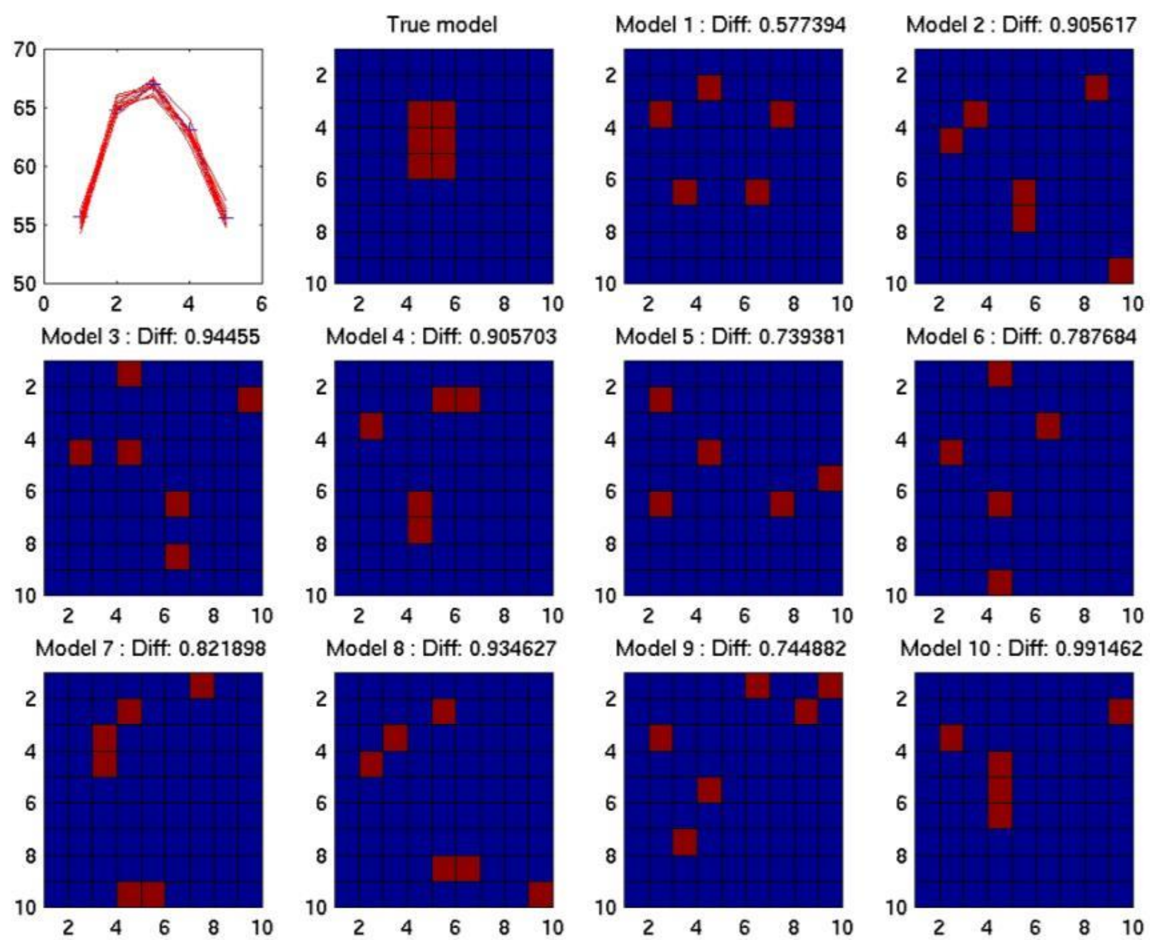
Treasure Hunt: solutions

Models with less than 2% error.



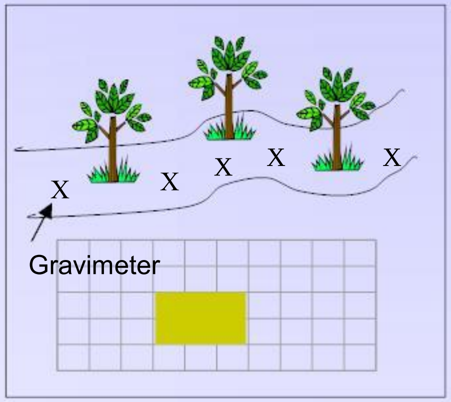
Treasure Hunt: solutions

Models with less than 1% error.



What we have learned from one example

Inverse problems = inference about physical systems from data



- Data usually contain errors (data uncertainties)
- Physical theories require approximations
- Infinitely many models will fit the data (non-uniqueness)
- Our physical theory may be inaccurate (theoretical uncertainties)
- Our forward problem may be highly nonlinear
- We always have a finite amount of data

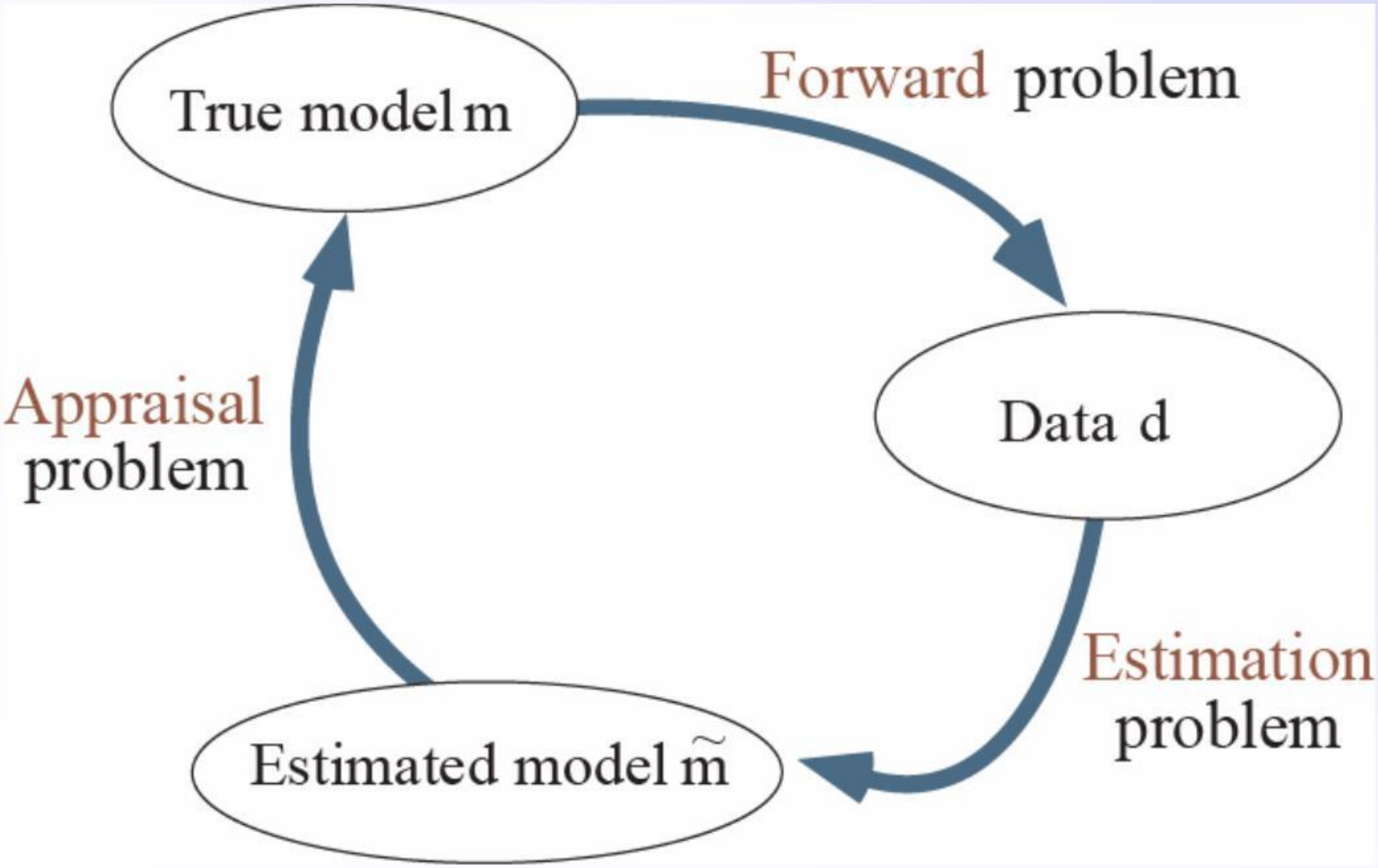
Detailed questions are:

How accurate are our data?

How well can we solve the forward problem?

What independent information do we have on the model space (a priori information) ?

Estimation and Appraisal



Let’s be a bit more formal…

What is a model ?

A simplified way of representing physical reality:

- A seismic model of the Lithosphere might consist of a set of layers with P-wavespeed of rocks as a constant in each layer. This is an approximation. The real Earth is more complex.

- A model of density structure that explains a local gravity anomaly might consist of a spherical body of density $\rho + \Delta\rho$ and radius *R,* embedded in a uniform half-space.

- A model may consist of:
  - A finite set of unknowns representing parameters to be solved for,

$$\boldsymbol{m} = \left[m_1, m_2, \ldots, m_j, \ldots, m_M\right]$$

    e.g. the intercept and gradient in linear regression.

  - A continuous function,

$$m(\mathbf{x})$$

    e.g. the seismic velocity as a function of depth.

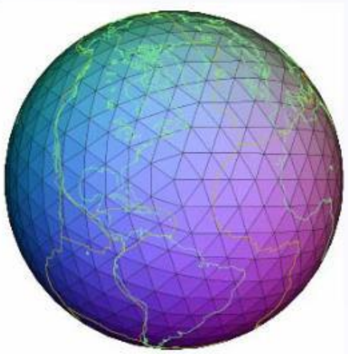
Discretizing a continuous model

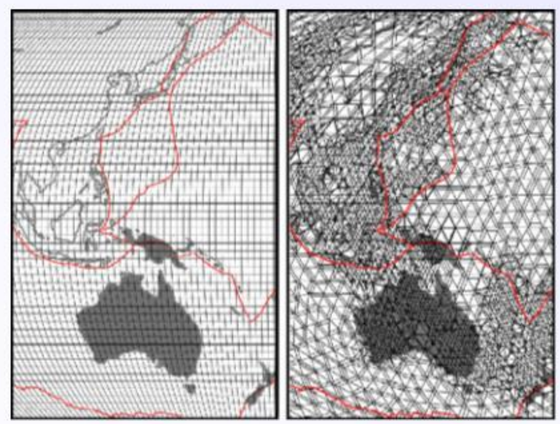
Often continuous functions are discretized to produce a finite set of unknowns. This requires use of *Basis functions*

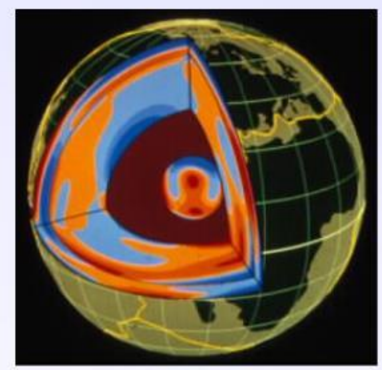
$$m(\mathbf{x}) = \sum_{j=1}^{M} m_j \phi_j(\mathbf{x})$$

m_j become the unknowns $(j = 1, \ldots, M)$

$\phi_j(\mathbf{x})$ are the *chosen* basis functions





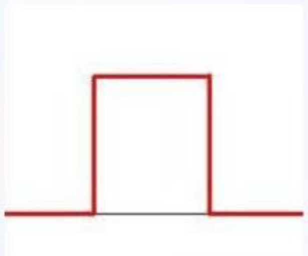


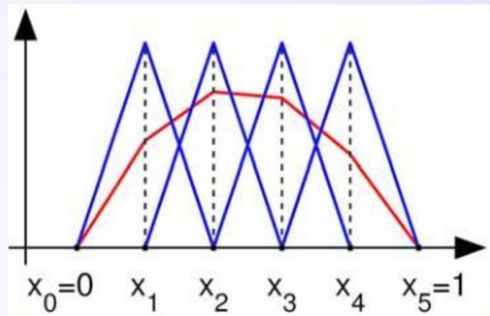
All inferences we can make about the continuous function will be influenced by the choice of basis functions. They must suit the physics of the forward problem. They bound the resolution of any model one gets out.

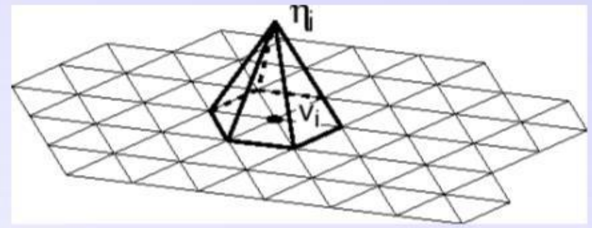
Discretizing a continuous model

Example of *Basis functions*

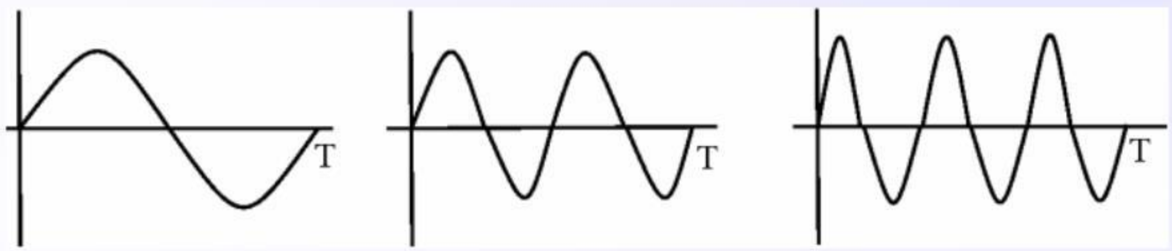
Local support

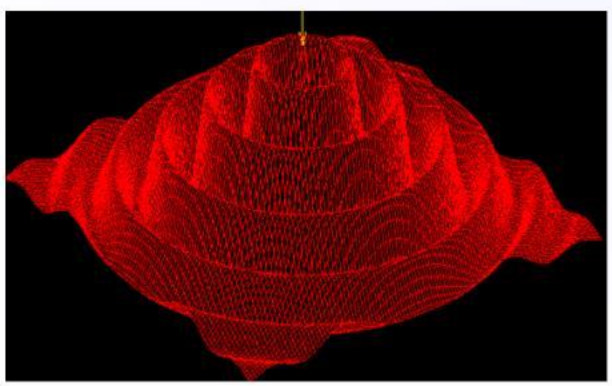


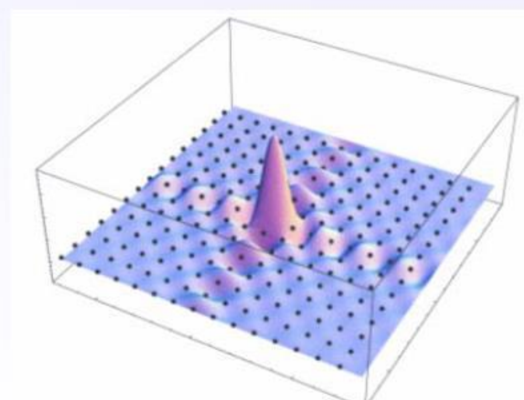




Global support







Forward and inverse problems

- Given a model **m** the *forward problem* is to predict the data that it would produce **d**

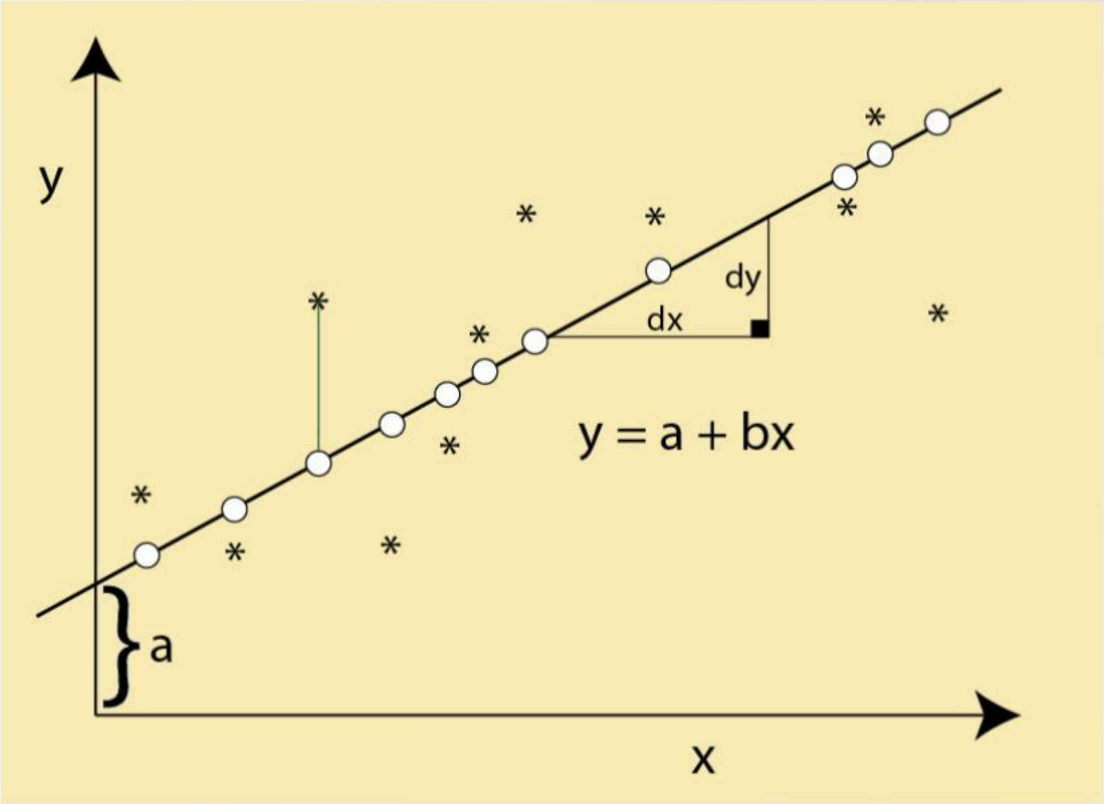
$$\boldsymbol{d} = g(\boldsymbol{m})$$

- Given data **d** the *inverse problem* is to find the model **m** that produced it.

Terminology can be a problem. Applied mathematicians often call the equation above a *mathematical model* and **m** as its parameters, while other scientists call *G* the *forward operator* and **m** the model.

Consider the example of linear regression...

Linear Regression



What is the forward problem ?

What is the inverse problem ?

Characterizing inverse Problems

They come in all shapes and sizes…

Types of inverse problem

Can you think of examples in each category ?

- Nonlinear and discrete

$$d = g(m)$$

m and **d** are vectors of finite length and G is a function

- Linear and discrete

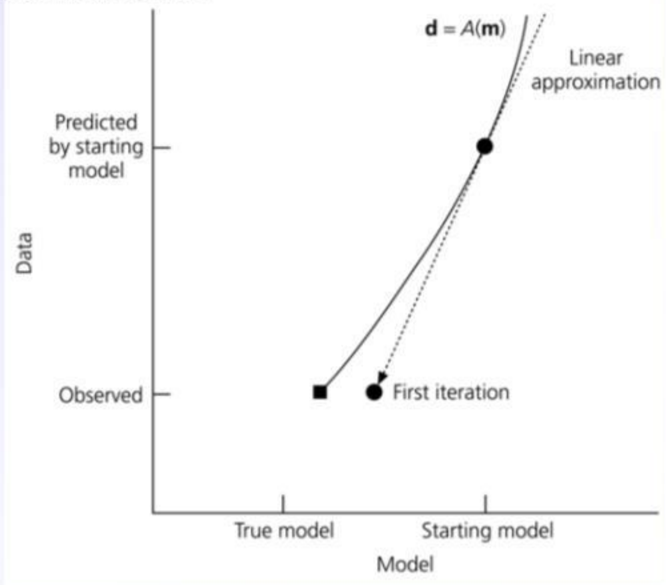
$$d = Gm$$

m is a vector of M unknowns
d is a vector of N data
and G is an M x N matrix.

- Linearized

$$\delta d = G\delta m$$

Figure 7.2-2: Illustration of the the effect of linearizing about an inverse problem starting model.



Perturbations in model parameters from a reference model related linearly to differences between observations and predictions from the reference model.

Types of inverse problem

- Linear and continuous

$$\int_a^b g(s,x)m(x)dx = d(s)$$

$G(x)$ is called an operator and $g(s,x)$ is a kernel.

Fredholm integral equation of the first kind
(these are typically ill-posed)

Can you think of examples in each category ?

- Non-Linear and continuous

$$\int_a^b g(s,x,m(x))dx = d(s)$$

$g(s,x,m(x))$ is a nonlinear function of the unknown

function $m(x)$

Linear functions

- A linear function or operator obey the following rules

Superposition $$G(m_1 + m_2) = G(m_1) + G(m_2)$$

Scaling $$G(\lambda m) = \lambda G(m)$$

Are the following linear or nonlinear inverse problems

1. We want to predict rock density ρ in the Earth at a given radius r from its center from the known mass M and moment of inertia I of the Earth. We use the following relation:

$$d_i = \int_0^a g_i(r)\rho(r)dr$$

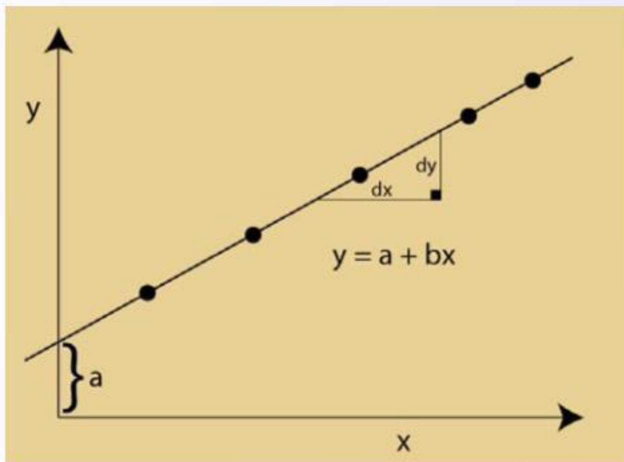
where d_1 = M and d_2 = I and $g_i(r)$ are the corresponding Frechet kernels: $g_1(r) = 4 \text{ pi } r^2$ and $g_2(r) = 8/3\, \pi\, r^4$.

2. We want to determine v(**r**) of the medium from measuring ttravel time, t for many wave paths.

$$t_i = \int_{R_i} \frac{1}{V(r)} ds$$

Formulating inverse problems

Regression



$$\mathbf{d} = G\mathbf{m}$$

$$\mathbf{d} = [y_1, y_2, \ldots, y_N]^T$$

$$\mathbf{m} = [a, b]^T$$

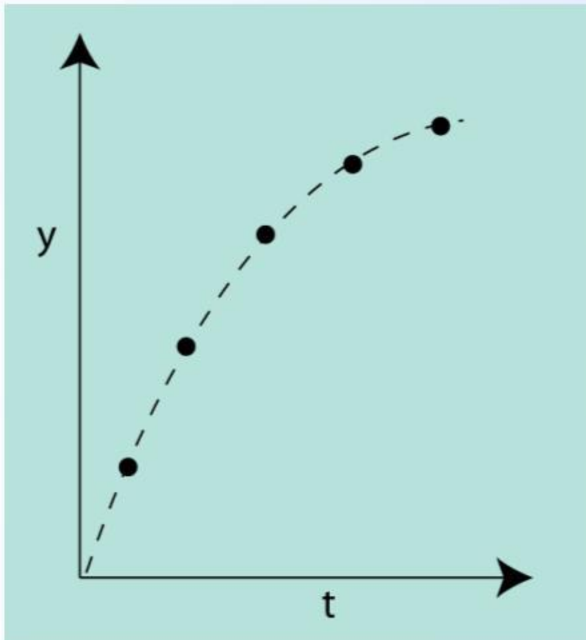
$$G = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{pmatrix}$$

Discrete or continuous ?
Linear or nonlinear ? Why ?
What are the data ?
What are the model parameters ?
Unique or non-unique solution ?

$$y = a + bx$$

Formulating inverse problems

Ballistic trajectory



$$d = Gm$$

$$d = [y_1, y_2, \ldots, y_N]^T$$

$$m = [m_1, m_2, m_3]^T$$

$$G = \begin{pmatrix} 1 & t_1 & -1/2t_1^2 \\ 1 & t_2 & -1/2t_2^2 \\ \vdots & \vdots & \vdots \\ 1 & t_M & -1/2t_M^2 \end{pmatrix}$$

Discrete or continuous ?
Linear or nonlinear ? Why ?
What are the data ?
What are the model parameters ?
Unique or non-unique solution ?

$$y = m_1 + m_2 t - \frac{1}{2} m_3 t^2$$

Recap: Characterising inverse problems

- Inverse problems can be continuous or discrete
- Continuous problems are often discretized by choosing a set of basis functions and projecting the continuous function on them.
- The forward problem is to take a model and predict observables that are compared to actual data. Contains the Physics of the problem. This often involves a mathematical model which is an approximation to the real physics.
- The inverse problem is to take the data and constrain the model in some way.
- We may want to build a model or we may wish to ask a less precise question of the data !

Three classical questions
(from Backus and Gilbert, 1968)

The problem with constructing a solution

- The existence problem

  Does any model fit the data ?

- The uniqueness problem

  Is there a unique model that fits the data ?

- The stability problem

  Can small changes in the data produce large changes in the solution ?

  (Ill-posedness)

Backus and Gilbert (1970)
Uniqueness in the inversion of inaccurate gross earth data.
*Phil. Trans. Royal Soc. A, **266**, 123-192, 1970.*