Training Course on
Joint Inversions in Geophysics

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The linear case

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Objectives of this lecture

- Introduce useful concepts of parameter estimation
- Provide recipes to solve linear inverse problems
- Give simple examples

- Two useful books on the subject:
  - **Geophysical Data Analysis: Discrete Inverse Theory** (Revised Edition)
    William Menke (1989), Academic Press
  - **Parameter Estimation and Inverse Problems** (Second Edition)
    Richard C. Aster, Brian Borchers & Clifford H. Thurber (2013), Academic Press

Outline

- Introduction to discrete linear systems
- Vector norms
- Matrix norms
- Conditioning of a linear system
- Classification of linear inverse problems
- Solutions based on norm minimization
  - Overdetermined problems
  - Underdetermined problems
  - Mixed-determined problems
  - Damped least squares solutions
- Other a priori information
- Properties of generalized inverses: data and model resolution matrices
- Summary

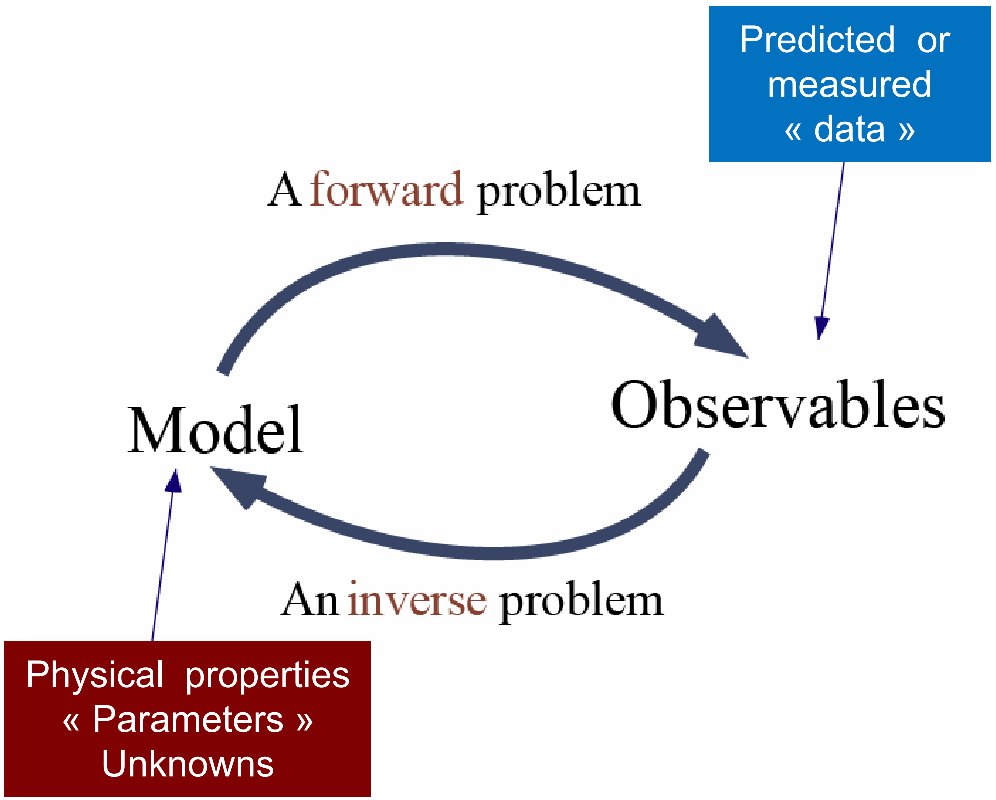
Mathematical representation and terminology

- We are interested in the relationships between physical (or chemical, economic, …) model parameters m and a set of data d.
- We assume a good knowledge of the laws governing the investigated phenomena (underlying physics), in the form of a function G such that

$$d = G(m)$$

- In the mathematical model $d = G(m)$, the forward modeling operator G can be defined as
  - a linear or nonlinear system of algebraic equations
  - the solution of an ODE or PDE
- **Forward problem**: find d given m
- **Inverse problem**: find m given d ←
- *Model identification problem*: find G knowing some values of d and m

Forward and inverse problems



Forward problem: **Model parameters ⇨ Forward modeling ⇨ Predicted data**

Inverse problem: **Observed data ⇨ Inverse modeling ⇨ Parameter estimation**

Continuous and discrete inverse problem (1)

- Quite often, our goal is to determine a finite number M of model parameters:
  - physical quantities, e.g. distributions of densities, temperatures, seismic velocities
  - coefficients entering functional relationships describing the mathematical model.
- In many cases also, we have a finite number N of data points.
- In such situations, the model parameters and data set can be expressed as vectors and we will write

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

  where $\mathbf{d}$ is a N-element vector, and $\mathbf{m}$, a M-element vector.
- In this case, finding $\mathbf{m}$ given $\mathbf{d}$ is a discrete inverse problem.
- In the other cases, when the model parameters and data are functions of continuous variables (time or space), we must solve a continuous inverse problem.

Continuous and discrete inverse problem (2)

$$d(x) = \int G(x,\xi)\, m(\xi)\, d\xi$$

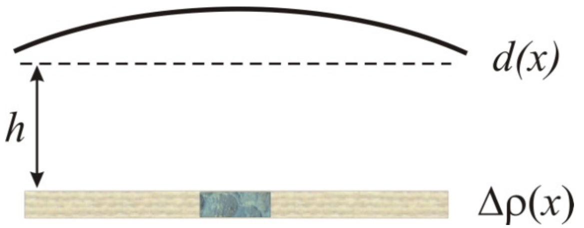
- In continuous inverse problems, and $G(x,\xi)$ is called the data kernel.
- When $G(x,\xi)$ can be written in the form $G(x-\xi)$, the integral representation above becomes a convolution integral and the inverse problem can be solved via a deconvolution.
- The theory of continuous inverse problems relies on functional analysis and is more abstract than the theory of discrete inverse problems.
- This is compensated for by gains in computation time since the computations can be partly carried out in symbolic form.
- Functional analysis also lends itself to a better physical interpretation of the operations needed to solve the inverse problem.
- Discrete inverse formulations are also applicable to properly sampled continuous problems, and therefore represent a vast domain of applications.

Example of convolution integral

- Example taken from Aster *et al.* (2013): Inversion of a vertical gravity anomaly $d(x)$, observed at some height h to estimate an unknown line mass density distribution relative to a background model $m(x) = \Delta\rho(x)$

$$d(x) = G\int_{-\infty}^{\infty} \frac{h}{\left[(\xi - x)^2 + h^2\right]^{3/2}} m(\xi)\, d\xi = \int_{-\infty}^{\infty} g(\xi - x)\, m(\xi)\, d\xi$$

where G is Newton's gravitational constant.



- Here, because the kernel is a smooth function, $d(x)$ will be a smoothed and scaled transformation of $m(x)$.
- The solution of the inverse problem $m(x)$ will be a roughened transformation of $d(x)$.
- Noise in the data can seriously affect the solution of the inverse problem.

Classification of inverse problems (1)

- We focus on discrete inverse problems: model parameters and data are represented by vectors

$$\mathbf{d} = \left(d_1\ d_2\ d_3 \cdots d_N\right)^T \text{ and } \mathbf{m} = \left(m_1\ m_2\ m_3 \cdots m_M\right)^T \text{respectively.}$$

- **Non-linear implicit equations**: series of L equations

$$\begin{cases} f_1(\mathbf{d},\mathbf{m}) = 0 \\ f_2(\mathbf{d},\mathbf{m}) = 0 \\ \vdots \\ f_L(\mathbf{d},\mathbf{m}) = 0 \end{cases} \quad \text{or, in matrix form,} \quad \boxed{\mathbf{f}(\mathbf{d},\mathbf{m}) = \mathbf{0}}$$

- **Linear implicit equations**

  Former matrix equation simplifies to:

$$\boxed{\mathbf{f}(\mathbf{d},\mathbf{m}) = \mathbf{0} = \mathbf{F}\left[\frac{\mathbf{d}}{\mathbf{m}}\right]}$$

  where $\mathbf{F}$ is a matrix of dimensions $L \times (M + N)$.

Classification of inverse problems (2)

- **Non-linear explicit equations**: when data and model parameters can be separated, $L = N$ equations can be written in matrix form

$$\mathbf{f}(\mathbf{d},\mathbf{m}) = \mathbf{0} = \mathbf{d} - \mathbf{g}(\mathbf{m})$$

  where $\mathbf{g}$ is a non-linear vector operator.

- **Linear explicit equations**: if $\mathbf{g}$ is a linear operator, the general equation writes

$$\mathbf{f}(\mathbf{d},\mathbf{m}) = \mathbf{0} = \mathbf{d} - \mathbf{G}\mathbf{m}$$

  where $\mathbf{G}$ is a $N \times M$ matrix. Matrix $\mathbf{F}$ defined above can then be partitioned in the form

$$\mathbf{F} = \left[\begin{array}{c|c} \mathbf{I} & \mathbf{0} \\ \hline \mathbf{0} & -\mathbf{G} \end{array}\right]$$

- In the following, we concentrate on the linear explicit equations $\mathbf{d} = \mathbf{G}\,\mathbf{m}$.

Discrete linear systems

- Simplest mathematical formulation. Uses linear algebra tools.
- Obey superposition and scaling laws:

$$\mathbf{G}(\mathbf{m}_1 + \mathbf{m}_2) = \mathbf{G}\mathbf{m}_1 + \mathbf{G}\mathbf{m}_2$$

$$\mathbf{G}(\alpha\mathbf{m}) = \alpha\,\mathbf{G}\mathbf{m}$$

- Broad range of applications: seemingly non-linear problems can be cast in a linear form (see next examples).
- Mathematical linearity is associated with physical linearity (straight rays, …)
- Can be used as local approximations for (weakly) non-linear problems

$$\mathbf{d} = \mathbf{g}(\mathbf{m}) \approx \mathbf{g}(\hat{\mathbf{m}}_n) + \nabla\mathbf{g}\left[\mathbf{m} - \hat{\mathbf{m}}_n\right] \quad \text{Taylor series expansion around } \hat{\mathbf{m}}_n$$

$$= \mathbf{g}(\hat{\mathbf{m}}_n) + \mathbf{G}_n \Delta\mathbf{m}_{n+1}\ ;\ n = 0, 1, 2, \ldots$$

where $\mathbf{G}_n = \nabla\mathbf{g}\big|_{\mathbf{m}=\hat{\mathbf{m}}_n}$; $\left(\mathbf{G}_n\right)_{ij} = \dfrac{\partial g_i}{\partial \hat{m}_j^{(n)}}$; $\Delta\mathbf{m}_{n+1} = \mathbf{m} - \hat{\mathbf{m}}_n$

$$\mathbf{d}' = \mathbf{d} - \mathbf{g}(\hat{\mathbf{m}}_n) = \mathbf{G}_n \Delta\mathbf{m}_{n+1} \quad \Rightarrow \text{Invert for } \Delta\mathbf{m}_{n+1} \text{ (starting from } \mathbf{m}_0)$$

Linear regression

- Problem of fitting a function to a data set. The function is defined by a series of parameters.
- When the problem can be solved as a linear inverse problem, it is referred to a linear regression.
- Example: ballistic trajectory

$$z(t) = m_1 + m_2 t - (1/2) m_3 t^2$$

Quadratic in time t, but linear with respect to m_i

$$\begin{bmatrix} 1 & t_1 & -1/2\, t_1^2 \\ 1 & t_2 & -1/2\, t_2^2 \\ 1 & t_3 & -1/2\, t_3^2 \\ \vdots & \vdots & \\ 1 & t_N & -1/2\, t_N^2 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_M \end{bmatrix}$$

(Space Archive)

Tomography

- Deals with path-integrated properties:
  - Travel times of acoustic, seismic, EM waves
  - Attenuation of waves, of X-rays, of muons
  - …
- In seismic traveltime tomography, the problem is non-linear if it is expressed in terms of wave velocities v.
- It is linearized by considering the wave slowness u.

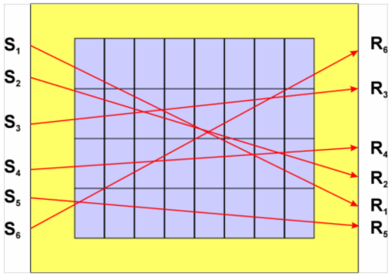
$$T = \int_s \frac{ds}{v(s)} = \int_s u(s)\, ds$$

- In case of slowness perturbations,

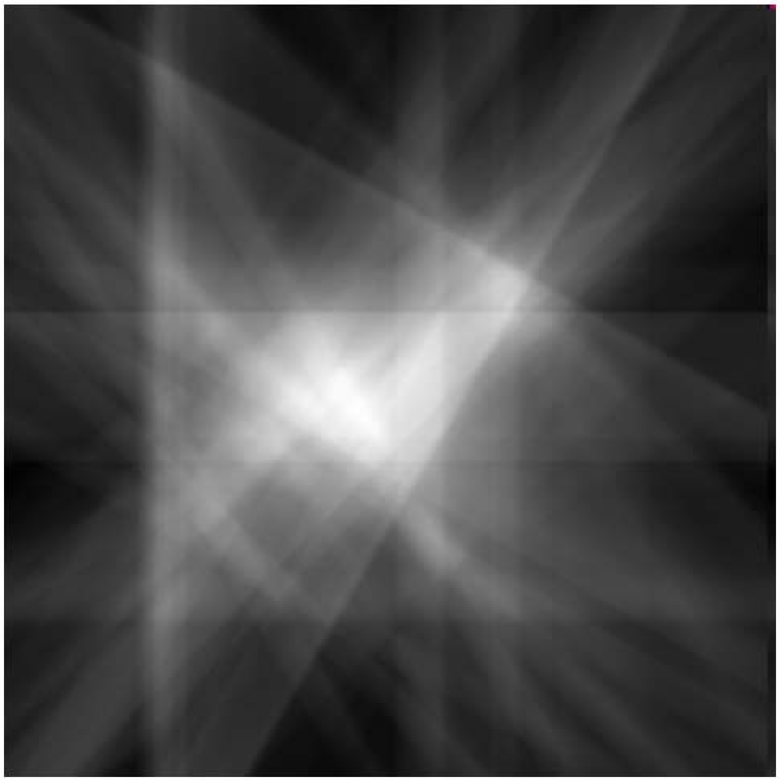
$$\Delta T = T_{obs} - T_{pred} = \int_s \Delta u(s)\, ds$$

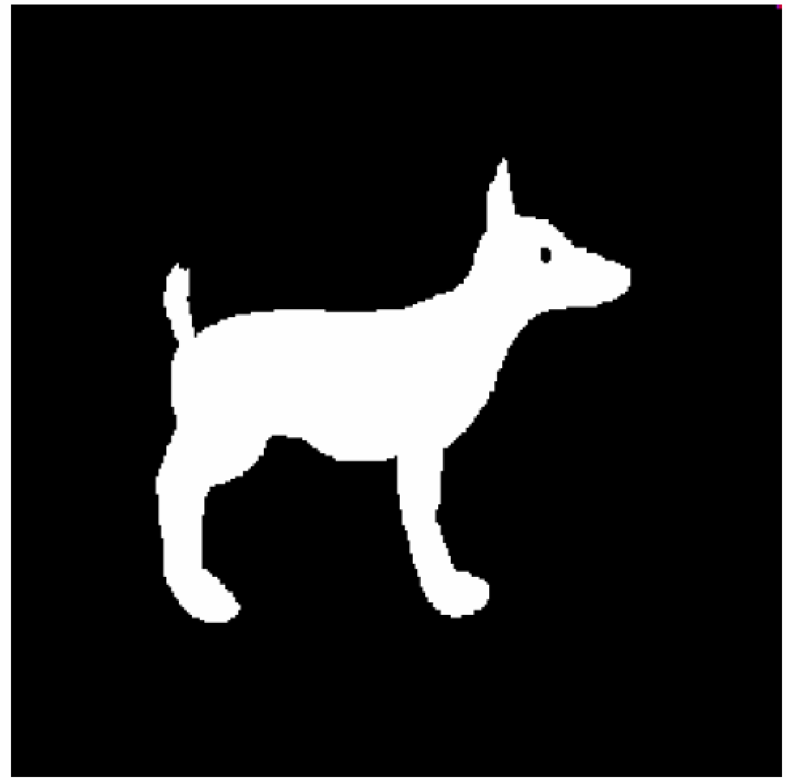
- If the medium is discretized into blocks

$$\Delta T_i = \sum_j l_{ij} \Delta u_j$$



Tomographic reconstruction via backprojection





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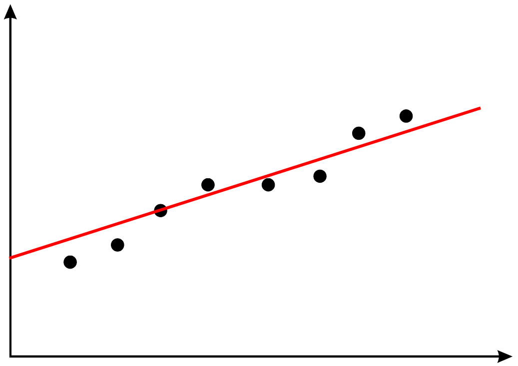
Vector norms (1)

- One way of solving the linear inverse problem is to measure the « length » of some vectors.
- This is related to the problem of minimizing a misfit function, which will be addressed later on in this course.
- For example, the linear regression problem is solved by the so-called least squares method in which one tries to minimize the overall error



$$E = \sum_{i=1}^{N} e_i^2 \quad \text{where} \quad e_i = d_i^{obs} - d_i^{pre} \; ; \mathbf{d}^{pre} = \mathbf{G}\mathbf{m}^{est}$$

$$E = \mathbf{e}^T \mathbf{e} \quad \text{(squared Euclidean length of vector } \mathbf{e}\text{).}$$

- The least squares method uses the L_2 (or Euclidean) norm which is defined, for a vector $\mathbf{v}$, by

$$\|\mathbf{v}\|_2 = \left(\sum_i |v_i|^2 \right)^{1/2} = (\mathbf{v}, \mathbf{v})^{1/2}$$

Vector norms (2)

- Other norms can be used such as

  the L_1 norm $\|\mathbf{v}\|_1 = \sum_i |v_i|$

  which is a particular case of the

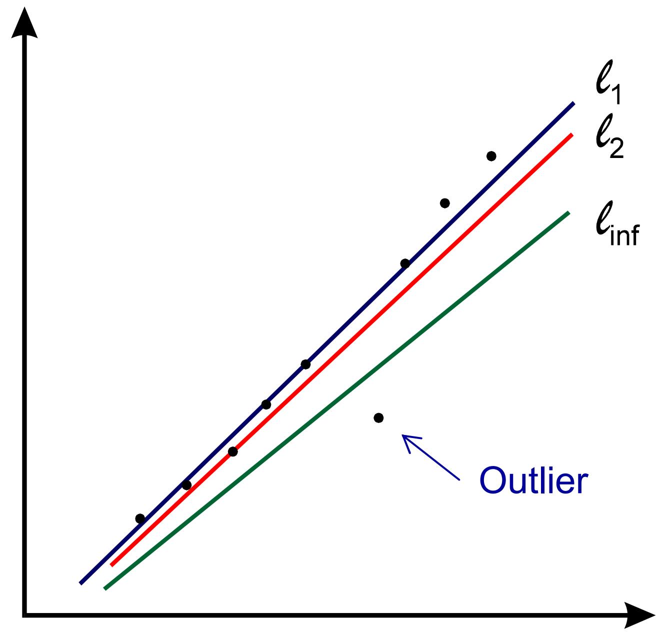
  L_p norm $$\|\mathbf{v}\|_p = \left(\sum_i |v_i|^p \right)^{1/p} \quad p \geq 1$$

- The higher norms give the largest element of vector $\mathbf{v}$ a larger weight.

- The limiting case $p \to \infty$ is the L_∞ norm

$$\|\mathbf{v}\|_\infty = \max_i |v_i|$$

which selects the vector element with the largest absolute value as the measure of length.



Vector norms (3)

- Why is the L_2 norm so frequently used? / Which norm should we use?

1. Computations are simpler with the L_2 norm than with the L_1 norm.
2. Depends on the importance one chooses to give to outliers, i.e., data that fall far from the mean trend:
   - If the data are very accurate with only a few outliers, we may want to be sensitive to these anomalous values. In this case, we would use a high-order norm.
   - On the contrary, if the data scatter widely around the trend, then the large prediction errors do not carry a special significance. In such cases, a low-order norm would be used because it gives a more balanced weight to errors of different size.
3. Similar arguments could be developed by considering a probabilistic approach of the inverse problem. Let us just point out that the L_2 norm implies that the data obey Gaussian statistics. Gaussians are rather short-tailed (limited support) distributions which imply very few scattered points.

Matrix norms (1)

- A vector-induced matrix norm is defined as

$$\|\mathbf{A}\| = \max_{\mathbf{v} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{v}\|}{\|\mathbf{v}\|} \qquad \text{or} \qquad \|\mathbf{A}\| = \max_{\|\mathbf{v}\| = 1} \|\mathbf{A}\mathbf{v}\|$$

- Therefore: $\|\mathbf{A}\mathbf{v}\| \leq \|\mathbf{A}\| \|\mathbf{v}\|$ and $\|\mathbf{I}\| = 1$
- The L_1 , L_2 and L_∞ norms thus correspond to

$$\|\mathbf{A}\|_1 = \max_{\mathbf{v} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{v}\|_1}{\|\mathbf{v}\|_1} = \boxed{\max_j \sum_i |a_{ij}| = \max_j \|\mathbf{c}_j\|_1}$$

where c_j is the j^{th} column of matrix $\mathbf{A}$

$$\|\mathbf{A}\|_2 = \max_{\mathbf{v} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{v}\|_2}{\|\mathbf{v}\|_2} = \boxed{\sqrt{\rho(\mathbf{A}^*\mathbf{A})} = \sqrt{\rho(\mathbf{A}\mathbf{A}^*)}} = \|\mathbf{A}^*\|_2$$

where $\rho(\mathbf{K})$ is the spectral radius of matrix $\mathbf{K}$; $\mathbf{A}^*$ is the adjoint of matrix $\mathbf{A}$

$$\|\mathbf{A}\|_\infty = \max_{\mathbf{v} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{v}\|_\infty}{\|\mathbf{v}\|_\infty} = \boxed{\max_i \sum_j |a_{ij}| = \max_i \|\mathbf{r}_i\|_1}$$

where r_i is the i^{th} row of matrix $\mathbf{A}$

Matrix norms (2)

- The L_1 norm of matrix $\mathbf{A}$ is the largest L_1 norm of the columns of the matrix.
- The L_∞ norm of matrix $\mathbf{A}$ is the largest L_∞ norm of the rows of the matrix.
- Both are easily calculated from the elements of matrix $\mathbf{A}$.
- The L_2 norm of matrix $\mathbf{A}$ requires more computations. Let us give a few practical reminders on matrix calculation.
  - Transpose $(\mathbf{A}^T)_{ij} = a_{ji}$
  - Adjoint $(\mathbf{A}^*)_{ij} = \overline{a}_{ji}$
  - Trace $\mathrm{tr}(\mathbf{A}) = \sum_{i=1}^{N} a_{ii}$
  - Eigenvalue / eigenvector problem $\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{x}$
  - Characteristic polynomial $\det(\mathbf{A} - \lambda\,\mathbf{I}_N) = 0$
  - Spectral radius $\rho(\mathbf{A}) = \max_{1 \le i \le N} \left\{ \left| \lambda_i(\mathbf{A}) \right| \right\}$
  - Singular values $\mu_i(\mathbf{A}) = \sqrt{\lambda_i(\mathbf{A}^T\mathbf{A})} = \sqrt{\lambda_i(\mathbf{A}\mathbf{A}^T)}$

For square matrices

Matrix norms (3)

- The L_2 norm of matrix $\mathbf{A}$ is the largest square root of the eigenvalue of matrix $\mathbf{AA}^*$ or matrix $\mathbf{A}^*\mathbf{A}$.
- It is the largest singular value of matrix $\mathbf{A}$.
- If matrix $\mathbf{A}$ is hermitian (or self-adjoint) $\mathbf{A} = \mathbf{A}^*$, or symmetric $\mathbf{A} = \mathbf{A}^T$, its L_2 norm is the spectral radius of matrix $\mathbf{A}$:

$$\|\mathbf{A}\|_2 = \rho(\mathbf{A}).$$

For any norm, $\|\mathbf{A}\| \geq \rho(\mathbf{A})$

- The Frobenius norm is not vector-induced but can easily be computed

$$\|\mathbf{A}\|_F = \left(\sum_{i=1}^{N} \sum_{j=1}^{M} |a_{ij}|^2 \right)^{1/2}$$

or

$$\|\mathbf{A}\|_F = \left\{ \mathrm{tr}\left(\mathbf{A}^* \mathbf{A} \right) \right\}^{1/2}$$

- It is an effective way to compute the L_2 norm of a matrix since

$$\|\mathbf{A}\|_2 \leq \|\mathbf{A}\|_F \leq \sqrt{N}\, \|\mathbf{A}\|_2$$

for a $N \times N$ matrix.

Conditioning of a linear system (1)

- Let's consider the linear system $\mathbf{Au} = \mathbf{b}$ (taken from Ciarlet, 1994)

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix} \quad \text{whose solution is} \quad \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix},$$

and the perturbed system

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} u_1 + \delta u_1 \\ u_2 + \delta u_2 \\ u_3 + \delta u_3 \\ u_4 + \delta u_4 \end{pmatrix} = \begin{pmatrix} 32.1 \\ 22.9 \\ 33.1 \\ 30.9 \end{pmatrix} \quad \text{whose solution is} \quad \begin{pmatrix} 9.2 \\ -12.6 \\ 4.5 \\ -1.1 \end{pmatrix}.$$

- A very weak relative perturbation of the RHS $\|\Delta \mathbf{b}\| / \|\mathbf{b}\| = 0.2/60 \approx 0.0033$
  induces an important relative error of the solution $\|\Delta \mathbf{u}\| / \|\mathbf{u}\| = 16.4/2 = 8.2$
  that is, an amplification of the relative errors of $8.2 / 0.003 = 2461$.

Conditioning of a linear system (2)

- Let's also consider a perturbed system in which we slightly modify the elements of matrix $\mathbf{A}$:

$$\begin{pmatrix} 10 & 7 & 8.1 & 7.2 \\ 7.08 & 5.04 & 6 & 5 \\ 8 & 5.98 & 9.89 & 9 \\ 6.99 & 4.99 & 9 & 9.98 \end{pmatrix} \begin{pmatrix} u_1 + \Delta u_1 \\ u_2 + \Delta u_2 \\ u_3 + \Delta u_3 \\ u_4 + \Delta u_4 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix} \quad \text{whose solution is} \quad \begin{pmatrix} -80.33 \\ 136 \\ -34.10 \\ 21.97 \end{pmatrix}.$$

- These error amplifications may be surprising in this example, considering the good aspect of the original matrix $\mathbf{A}$ which is symmetric and full, its determinant is equal to 1, and its inverse

$$\mathbf{A}^{-1} = \begin{pmatrix} 25 & -41 & 10 & -6 \\ -41 & 68 & -17 & 10 \\ 10 & -17 & 5 & -3 \\ -6 & 10 & -3 & 2 \end{pmatrix}$$

doesn't show anything special.

Conditioning of a linear system (3)

- These behaviors can be analyzed by considering the norms of matrices $\mathbf{A}$ and $\mathbf{A}^{-1}$.

- In the first case, we compare the solutions $\mathbf{u}$ and $\boldsymbol{\delta}\mathbf{u}$ of the systems

$$\begin{cases} \mathbf{A}\,\mathbf{u} = \mathbf{b} \\ \mathbf{A}(\mathbf{u} + \delta\,\mathbf{u}) = \mathbf{b} + \delta\,\mathbf{b} \end{cases} \quad \Rightarrow \quad \mathbf{A}\,\delta\,\mathbf{u} = \delta\,\mathbf{b}$$

- For any vector norm and its induced matrix norm, we infer from

$$\begin{cases} \mathbf{b} = \mathbf{A}\mathbf{u} \\ \delta\mathbf{u} = \mathbf{A}^{-1}\delta\mathbf{b} \end{cases} \quad \text{that} \quad \begin{cases} \|\mathbf{b}\| \le \|\mathbf{A}\|\,\|\mathbf{u}\| \quad \Rightarrow \quad \|\mathbf{u}\| \ge \dfrac{\|\mathbf{b}\|}{\|\mathbf{A}\|} \\ \|\delta\,\mathbf{u}\| \le \left\|\mathbf{A}^{-1}\right\|\,\|\delta\,\mathbf{b}\| \end{cases}$$

- The relative error on the result is therefore bounded by the quantity

$$\frac{\|\delta\,\mathbf{u}\|}{\|\mathbf{u}\|} \le \left\{ \|\mathbf{A}\|\,\left\|\mathbf{A}^{-1}\right\| \right\} \frac{\|\delta\,\mathbf{b}\|}{\|\mathbf{b}\|}$$

Conditioning of a linear system (4)

- In the second case, we compare the solutions $\mathbf{u}$ and $\mathbf{\Delta u}$ of the systems

$$\begin{cases} \mathbf{A}\,\mathbf{u} = \mathbf{b} \\ (\mathbf{A} + \Delta\,\mathbf{A})(\mathbf{u} + \Delta\,\mathbf{u}) = \mathbf{b} \end{cases} \Rightarrow \quad \mathbf{A}\,\Delta\,\mathbf{u} = -\Delta\,\mathbf{A}(\mathbf{u} + \Delta\,\mathbf{u})$$

- We infer from the last equality that

$$\|\Delta\mathbf{u}\| \leq \|\mathbf{A}^{-1}\|\,\|\Delta\mathbf{A}\|\,\|\mathbf{u} + \Delta\mathbf{u}\| \quad \text{that is,} \quad \frac{\|\Delta\,\mathbf{u}\|}{\|\mathbf{u} + \Delta\,\mathbf{u}\|} \leq \left\{\|\mathbf{A}\|\,\|\mathbf{A}^{-1}\|\right\}\frac{\|\Delta\,\mathbf{A}\|}{\|\mathbf{A}\|}$$

- For small perturbations $\mathbf{\Delta A}$, $\dfrac{\|\Delta\,\mathbf{u}\|}{\|\mathbf{u} + \Delta\,\mathbf{u}\|}$ is a good approximation of $\dfrac{\|\Delta\,\mathbf{u}\|}{\|\mathbf{u}\|}$

  and therefore, $$\frac{\|\Delta\,\mathbf{u}\|}{\|\mathbf{u}\|} \leq \left\{\|\mathbf{A}\|\,\|\mathbf{A}^{-1}\|\right\}\frac{\|\Delta\,\mathbf{A}\|}{\|\mathbf{A}\|}$$

- In both cases, the relative error on the result is bounded by the relative error of the modified quantities multiplied by which is the condition number of matrix $\mathbf{A}$.

$$\boxed{\operatorname{cond}(\mathbf{A}) = \|\mathbf{A}\|\,\|\mathbf{A}^{-1}\|}$$

Conditioning of a linear system (5)

- The condition number measures the sensitivity of the solution $\mathbf{u}$ of system $\mathbf{Au} = \mathbf{b}$ with respect to variations in data $\mathbf{b}$ or in elements of matrix $\mathbf{A}$.
- A linear system is well-conditioned if its condition number is small; it is ill-conditioned if its condition number is large.
- Properties

$$\text{cond}(\mathbf{A}) \geq 1 \qquad \text{(since } \mathbf{A}\mathbf{A}^{-1} = \mathbf{I},\ 1 = \|\mathbf{I}\| \leq \|\mathbf{A}\|\,\|\mathbf{A}^{-1}\|\text{)}$$

$$\text{cond}(\mathbf{A}) = \text{cond}(\mathbf{A}^{-1})$$

$$\text{cond}(\alpha\,\mathbf{A}) = \text{cond}(\mathbf{A})$$

$$\text{cond}_2(\mathbf{A}) = \frac{\max_i \mu_i(\mathbf{A})}{\min_i \mu_i(\mathbf{A})}$$

where $\mu_i(\mathbf{A})$ denote the non-zero **singular values** of matrix $\mathbf{A}$

$$\text{cond}_2(\mathbf{A}) = \frac{\max_i |\lambda_i(\mathbf{A})|}{\min_i |\lambda_i(\mathbf{A})|}$$

where $\lambda_i(\mathbf{A})$ denote the non-zero **eigenvalues** of matrix $\mathbf{A}$ if $\mathbf{A}$ is a normal matrix $(\mathbf{A}\,\mathbf{A}^* = \mathbf{A}^*\mathbf{A})$

$$\text{cond}_2(\mathbf{A}) = 1$$

if $\mathbf{A}$ is a unitary matrix $(\mathbf{A}\,\mathbf{A}^* = \mathbf{A}^*\mathbf{A} = \mathbf{I})$

Conditioning of a linear system (6)

- Finally, $\mathrm{cond}_2(\mathrm{A})$ is invariant by unitary transformation. $\mathbf{U}\mathbf{U}^* = \mathbf{U}^*\mathbf{U} = \mathbf{I}$

  then $\mathrm{cond}_2(\mathbf{A}) = \mathrm{cond}_2(\mathbf{UA}) = \mathrm{cond}_2(\mathbf{AU}) = \mathrm{cond}_2(\mathbf{U}^*\mathbf{AU})$.

- Numerical analysis of the previous example

  The eigenvalues of symmetric matrix

  $$\mathbf{A} = \begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix}$$

  are equal to its singular values

  $$\lambda_1 = 30.2887 \quad > \quad \lambda_2 = 3.858 \quad > \quad \lambda_3 = 0.8431 \quad > \quad \lambda_4 = 0.01015$$

  Using L_2 norm, $\mathrm{cond}_2(\mathbf{A}) = \dfrac{\lambda_1}{\lambda_4} = 2984.108$; $\dfrac{\|\boldsymbol{\delta}\mathbf{u}\|_2}{\|\mathbf{u}\|_2} = \dfrac{16.397}{2}$; $\dfrac{\|\boldsymbol{\delta}\mathbf{b}\|_2}{\|\mathbf{b}\|_2} = \dfrac{0.2}{60.025}$

  so that condition $\dfrac{\|\boldsymbol{\delta}\mathbf{u}\|_2}{\|\mathbf{u}\|_2} \le \mathrm{cond}_2(\mathbf{A}) \dfrac{\|\boldsymbol{\delta}\mathbf{b}\|_2}{\|\mathbf{b}\|_2}$ becomes $8.199 < 9.942$.

Conditioning of a linear system (7)

- The Frobenius norm is useful to evaluate the L_2 norm of a matrix without knowing its singular values.
- Here, for symmetric matrix $\mathbf{A}$,

$$\begin{aligned} \|\mathbf{A}\|_2 &= \rho(\mathbf{A}) &&= \lambda_1 &&= 30.2887 &&< 30.5450 &&= \|\mathbf{A}\|_F \\ \|\mathbf{A}^{-1}\|_2 &= \rho(\mathbf{A}^{-1}) &&= \frac{1}{\lambda_4} &&= 98.5222 &&< 98.5292 &&= \|\mathbf{A}^{-1}\|_F \end{aligned}$$

- Therefore, $\mathrm{cond}_2(\mathbf{A}) = \|\mathbf{A}\|_2 \, \|\mathbf{A}^{-1}\|_2 = 2984 \quad < \quad 3009 = \|\mathbf{A}\|_F \, \|\mathbf{A}^{-1}\|_F = \mathrm{cond}_F(\mathbf{A})$

  which verifies property $\|\mathbf{A}\|_2 \le \|\mathbf{A}\|_F \le \sqrt{N}\,\|\mathbf{A}\|_2$ seen previously

- We also verify that $\dfrac{\|\Delta\mathbf{u}\|}{\|\mathbf{u}+\Delta\mathbf{u}\|} \le \mathrm{cond}(\mathbf{A}) \dfrac{\|\Delta\mathbf{A}\|}{\|\mathbf{A}\|}$

$\dfrac{\|\Delta\mathbf{u}\|_F}{\|\mathbf{u}+\Delta\mathbf{u}\|_F} = \dfrac{162{,}825}{163{,}079}$; $\dfrac{\|\Delta\mathbf{A}\|_F}{\|\mathbf{A}\|_F} = \dfrac{0{,}266645}{30{,}5450}$ leading to $0{,}998 < 26{,}267$.

Classification of linear inverse problems (1)

- When solving the linear inverse problem $\mathbf{d} = \mathbf{G}\mathbf{m}$, several cases must be distinguished according to the quantity of information contained in the equation $\mathbf{d} = \mathbf{G}\mathbf{m}$.

- This information depends on number N of data and number M of model parameters, but it also depends on the structure of matrix $\mathbf{G}$ which can be sparse or full.

- If $\boldsymbol{N} > \boldsymbol{M}$, there are more data than unknowns, i.e., too much information to exactly solve the inverse problem.

  This corresponds to an **overdetermined problem**.

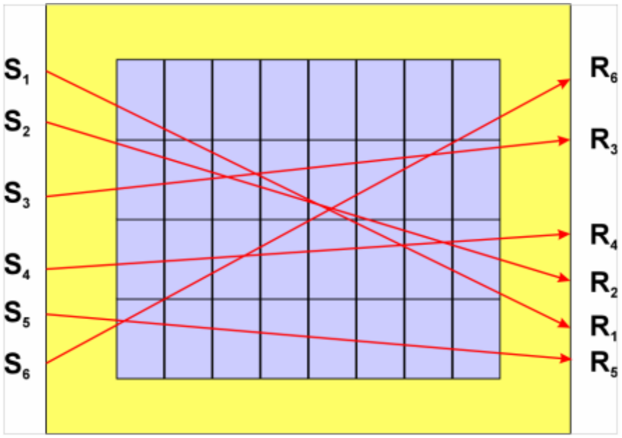
  Curve (or surface) fitting procedures are typical overdetermined problems.

- If $\boldsymbol{N} < \boldsymbol{M}$, there are more unknowns than data:we do not have enough information to determine all model parameters.

  This corresponds to an **underdetermined problem**.

Classification of linear inverse problems (2)

- In reality, we often must deal with **mixed-determined problems**, which are partly overdetermined and partly undertermined.
  This can happen even if $N > M$.
- This situation is typical of tomographic experiments when the medium is divided into blocks: some blocks are crossed by many rays whereas others are not crossed by any rays.
- Each of the situations described above must be solved in an appropriate manner.
- The solution for mixed-determined problems applies to all situations but is not necessarily optimal.



Solutions based on norm minimization

- Minimization of the prediction error in overdetermined problems.
- Minimization of the norm of the estimated solution in underdetermined problems.
- Combination of the two approaches in mixed-determined problems.

Overdetermined problems (1)

- Consider the prediction error $\mathbf{e} = \mathbf{d} - \hat{\mathbf{d}}$ between observations $\mathbf{d}$ and data $\hat{\mathbf{d}} = \mathbf{G}\hat{\mathbf{m}}$ predicted from the model $\hat{\mathbf{m}}$ we seek to find.
- Minimization of $E = \mathbf{e}^T\mathbf{e} = (\mathbf{d} - \mathbf{G}\hat{\mathbf{m}})^T(\mathbf{d} - \mathbf{G}\hat{\mathbf{m}})$ by canceling the derivatives $\partial E / \partial \hat{m}_q$ with respect to parameter $\hat{m}_q$
- Explicitly,

$$E = \sum_{i=1}^{N} \left\{ \left[d_i - \sum_{j=1}^{M} G_{ij}\hat{m}_j \right] \left[d_i - \sum_{j=1}^{M} G_{ij}\hat{m}_j \right] \right\}$$

$$\frac{\partial E}{\partial \hat{m}_q} = \sum_{i=1}^{N} \left\{ -G_{iq} \left[d_i - \sum_{j=1}^{M} G_{ij}\hat{m}_j \right] + \left[d_i - \sum_{j=1}^{M} G_{ij}\hat{m}_j \right] (-G_{iq}) \right\} = -2 \sum_{i=1}^{N} \left\{ G_{iq} d_i - G_{iq} \sum_{j=1}^{M} G_{ij}\hat{m}_j \right\}$$

$$\frac{\partial E}{\partial \hat{m}_q} = 0 \quad \Rightarrow \quad \sum_{i=1}^{N} G_{iq} d_i - \sum_{j=1}^{M} \left\{ \left[\sum_{i=1}^{N} G_{iq} G_{ij} \right] \hat{m}_j \right\} = 0$$

Overdetermined problems (2)

- The last equation can be written in matrix form as

$$\mathbf{G}^T\mathbf{d} - \mathbf{G}^T\mathbf{G}\hat{\mathbf{m}} = \mathbf{0}, \text{ where}$$

$$\mathbf{G}^T\mathbf{G} = \begin{bmatrix} G_{11} & G_{21} & \cdots & \cdots & G_{N1} \\ G_{12} & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ G_{1M} & \cdots & \cdots & \cdots & G_{NM} \end{bmatrix} \begin{bmatrix} G_{11} & G_{12} & \cdots & G_{1M} \\ G_{21} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ G_{N1} & \cdots & \cdots & G_{NM} \end{bmatrix}$$

is a $M \times M$ square matrix.

- If inverse $\left[\mathbf{G}^T\mathbf{G}\right]^{-1}$ exists, then the estimated model is given by the least squares solution

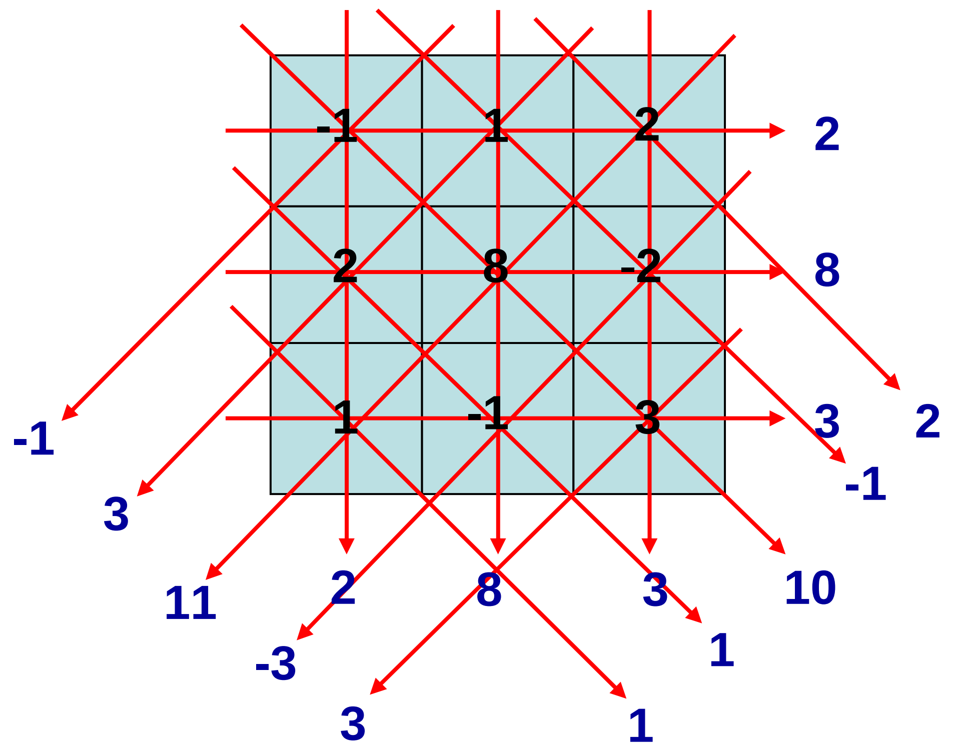
$$\hat{\mathbf{m}} = \left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{G}^T\mathbf{d}$$

Tomographic reconstruction of a 3 × 3 model (1)

3 × 3 model

$$\mathbf{M} = \begin{bmatrix} -1 & 1 & 2 \\ 2 & 8 & -2 \\ 1 & -1 & 3 \end{bmatrix}$$

16-ray scan of the model



Note: it is assumed that all ray segments have unit length

Tomographic reconstruction of a 3 × 3 model (2)

Cell numbering adopted

1	2	3
4	5	6
7	8	9

$$\mathbf{m} = \begin{bmatrix} -1 \\ 1 \\ 2 \\ 2 \\ 8 \\ -2 \\ 1 \\ -1 \\ 3 \end{bmatrix}$$

$$\mathbf{G} = \begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\
1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}$$

3 horizontal rays (from top to bottom)

3 vertical rays (from left to right)

5 oblique rays "NW - SE"
(from upper right corner to lower left corner)

5 oblique rays "NE - SW"
(from upper left corner to lower right corner)

$$\mathbf{d} = \begin{bmatrix} 2 \\ 8 \\ 3 \\ 2 \\ 8 \\ 3 \\ 2 \\ -1 \\ 10 \\ 1 \\ 1 \\ -1 \\ 3 \\ 11 \\ -3 \\ 3 \end{bmatrix}$$

Data vector **d**

Matrix of raypaths (other expressions are also possible)

Tomographic reconstruction of a 3 × 3 model (3)

True model

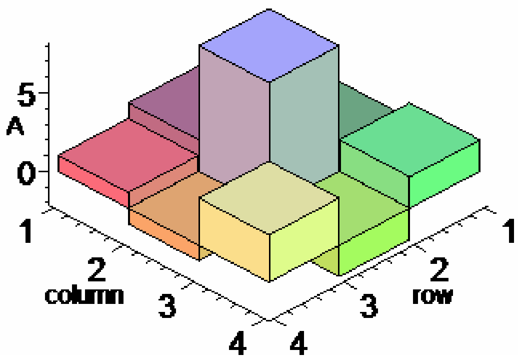
$$\mathbf{m}$$

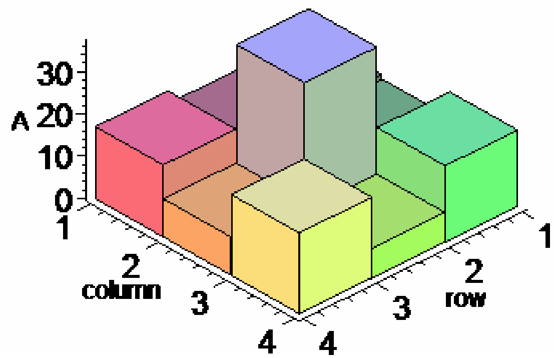
Back-projection

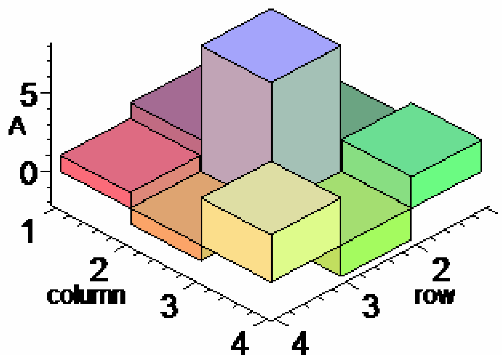
$$\hat{\mathbf{m}} = \mathbf{G}^T \mathbf{d}$$

Filtered back-projection

$$\tilde{\mathbf{m}} = \left[\mathbf{G}^T \mathbf{G}\right]^{-1} \mathbf{G}^T \mathbf{d} = \left[\mathbf{G}^T \mathbf{G}\right]^{-1} \hat{\mathbf{m}}$$







$$\mathbf{M} = \begin{bmatrix} -1 & 1 & 2 \\ 2 & 8 & -2 \\ 1 & -1 & 3 \end{bmatrix}$$

$$\hat{\mathbf{M}} = \begin{bmatrix} 13 & 12 & 18 \\ 14 & 37 & 7 \\ 17 & 9 & 19 \end{bmatrix}$$

$$\tilde{\mathbf{M}} = \begin{bmatrix} -1 & 1 & 2 \\ 2 & 8 & -2 \\ 1 & -1 & 3 \end{bmatrix}$$

(Maple computations and graphics)

Underdetermined problems (1)

- When the number of unknowns, M, exceeds the number of data, N, the problem admits an infinity of solutions.
- To obtain a solution, one has to provide some a priori information (e.g., physical constraints) to reduce the number of solutions.
- We can also find a solution minimizing the norm of the model while imposing at the same time a zero prediction error.

$$\begin{cases} L = \hat{\mathbf{m}}^T \hat{\mathbf{m}} = \sum_{j=1}^{M} \hat{m}_j^2 \quad \text{Minimum} \\ \mathbf{e} = \mathbf{d} - \mathbf{G}\hat{\mathbf{m}} = \mathbf{0} \end{cases}$$

- This problem can be solved with Lagrange multipliers which we first illustrate with the minimization of a function of two variables $E(x,y)$ subject to a constraint $\varphi(x,y) = 0$ defined implicitly.
- Minimize $dE + \lambda d\phi = \left(\frac{\partial E}{\partial x} + \lambda \frac{\partial \phi}{\partial x}\right) dx + \left(\frac{\partial E}{\partial y} + \lambda \frac{\partial \phi}{\partial y}\right) dy = 0$ λ: Lagrange multiplier

Underdetermined problems (2)

- Since dx and dy are not independent, we have to consider the 3 equations

$$\left(\frac{\partial E}{\partial x} + \lambda \frac{\partial \phi}{\partial x}\right) = 0 \quad ; \quad \left(\frac{\partial E}{\partial y} + \lambda \frac{\partial \phi}{\partial y}\right) = 0 \quad ; \quad \phi(x,y) = 0$$

  that will allow us to determine the 3 unknowns: the values of x and y at the minimum of function E, and λ (not needed).

- When we have M unknowns in a vector $\hat{\mathbf{m}}$ and N constraints $\phi(\hat{\mathbf{m}})$, we introduce a Lagrange multiplier for each constraint.
  We then have to solve $M+N$ simultaneous equations for $M+N$ unknowns.

- In our underdetermined problem, we minimize the function

$$\psi(\hat{\mathbf{m}}) = L + \sum_{i=1}^{N} \lambda_i e_i = \sum_{j=1}^{M} \hat{m}_j^2 + \sum_{i=1}^{N} \left\{ \lambda_i \left[d_i - \sum_{j=1}^{M} G_{ij} \hat{m}_j \right] \right\}$$

  with respect to variables $\hat{m}_q,\ q = 1, \dots M$

Underdetermined problems (3)

- The differenciation gives

$$\frac{\partial \psi}{\partial \hat{m}_q} = 2\sum_{j=1}^{M} \frac{\partial \hat{m}_j}{\partial \hat{m}_q}\hat{m}_j - \sum_{i=1}^{N}\lambda_i \sum_{j=1}^{M} G_{ij}\frac{\partial \hat{m}_j}{\partial \hat{m}_q} = 2\hat{m}_q - \sum_{i=1}^{N}\lambda_i G_{iq} = 0$$

or, in matrix form, $2\hat{\mathbf{m}} - \mathbf{G}^T\boldsymbol{\lambda} = \mathbf{0}$,

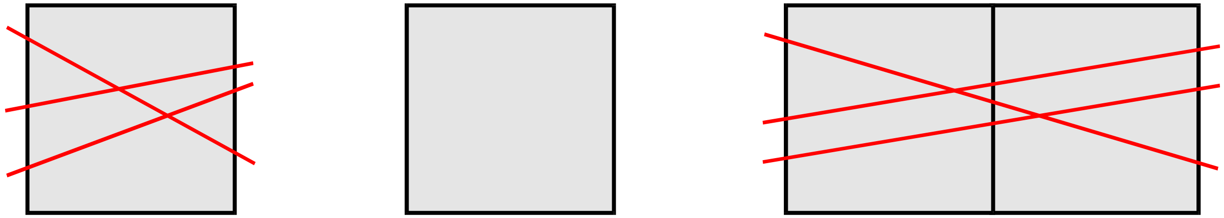
an equation that must be solved with the constraint $\mathbf{e} = \mathbf{d} - \mathbf{G}\hat{\mathbf{m}} = \mathbf{0}$

which implies $\mathbf{d} = \mathbf{G}\hat{\mathbf{m}} = \mathbf{G}\mathbf{G}^T\frac{\boldsymbol{\lambda}}{2}$

- $\mathbf{G}\mathbf{G}^T$ is a $N \times N$ square matrix. If it is invertible, then $\boldsymbol{\lambda} = 2\left[\mathbf{G}\mathbf{G}^T\right]^{-1}\mathbf{d}$
and by using the first matrix equation, we obtain the « minimum length » solution

$$\boxed{\hat{\mathbf{m}} = \mathbf{G}^T\left[\mathbf{G}\mathbf{G}^T\right]^{-1}\mathbf{d}}$$

Mixed-determined problems (1)



- Example taken from Menke (1984).
- We can only determine the average properties of the two cells in case c).

$$\begin{cases} G_{11}m_1 + G_{12}m_2 = d_1 \\ G_{21}m_1 + G_{22}m_2 = d_2 \\ G_{31}m_1 + G_{32}m_2 = d_3 \end{cases} \quad \text{By introducing} \quad \begin{cases} m_1' = \dfrac{m_1 + m_2}{2} \\ m_2' = \dfrac{m_1 - m_2}{2} \end{cases} \quad \text{then} \quad \begin{cases} m_1 = m_1' + m_2' \\ m_2 = m_1' - m_2' \end{cases}$$

$$\begin{cases} \left(G_{11} + G_{12}\right) m_1' = d_1 \\ \left(G_{21} + G_{22}\right) m_1' = d_2 \\ \left(G_{31} + G_{32}\right) m_1' = d_3 \end{cases} \quad \text{since} \quad G_{11} = G_{12} \; ; G_{21} = G_{22} \; ; G_{31} = G_{32}$$

Mixed-determined problems (2)

- This shows that parameter m'_1 is overdetermined whereas parameter m'_2 is underdetermined. This suggests a partitioning of the equations into overdetermined and underdetermined parts by forming linear combinations of the initial parameters.

$$\left[\begin{array}{c|c} \mathbf{G}'_{over} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{G}'_{under} \end{array}\right] \left[\begin{array}{c} \mathbf{m}'_{over} \\ \hline \mathbf{m}'_{under} \end{array}\right] = \left[\begin{array}{c} \mathbf{d}'_{over} \\ \hline \mathbf{d}'_{under} \end{array}\right]$$

- The new problem $\mathbf{d'}=\mathbf{G'm'}$ can be solved by using the least squares solution for the overdetermined part and the minimum length solution for the underdetermined part, i.e., we minimize the data prediction error and introduce only minimal a priori information.

- For this, we write equation $\mathbf{d}=\mathbf{Gm}$ in the form $\mathbf{d}_r+\mathbf{d}_0=\mathbf{G}(\mathbf{m}_r+\mathbf{m}_0)$, where $\mathbf{m}_0$ and $\mathbf{d}_0$ belong to the model nul space and data nul space, respectively: $\mathbf{Gm}_0=\mathbf{0}$ and $\mathbf{d}_0^T\mathbf{Gm}=0$.

Mixed-determined problems (3)

- With this decomposition, prediction error E and norm of solution L write:

$$E = [\mathbf{d} - \mathbf{Gm}]^T [\mathbf{d} - \mathbf{Gm}]$$

$$= [\mathbf{d}_r - \mathbf{Gm}_r]^T [\mathbf{d}_r - \mathbf{Gm}_r] + \mathbf{d}_0^T \mathbf{d}_0 \quad \text{as} \quad \mathbf{Gm}_0 = \mathbf{0} \ \text{ and } \ \mathbf{d}_0^T \mathbf{d}_r = \mathbf{d}_r^T \mathbf{d}_0 = 0$$

$$L = \mathbf{m}^T \mathbf{m} \ = \ \mathbf{m}_r^T \mathbf{m}_r + \mathbf{m}_0^T \mathbf{m}_0 \quad \text{since} \quad \mathbf{m}_r^T \mathbf{m}_0 = \mathbf{m}_0^T \mathbf{m}_r = 0$$

- Returning to the fact that we want to minimize the data prediction error and introduce only minimal a priori information, we therefore impose

$$E_r = [\mathbf{d}_r - \mathbf{Gm}_r]^T [\mathbf{d}_r - \mathbf{Gm}_r] = 0 \qquad \text{(Error on } \mathbf{d}_0 \text{ cannot be reduced)}$$

and we may choose $\mathbf{m}_0 = \mathbf{0}$ to limit a priori information.

- The vector subspaces $\mathbf{m}_r, \mathbf{m}_0, \mathbf{d}_r$ and $\mathbf{d}_0$ belong to can be identified by a SVD of matrix $\mathbf{G}$ which writes $\boxed{\mathbf{G} = \mathbf{U}_r \Sigma_r \mathbf{V}_r^T}$
- $\mathbf{U}_r, \Sigma_r$ and $\mathbf{V}_r$ are matrices of dimensions $N \times r$, $r \times r$, and $M \times r$, respectively.

Mixed-determined problems (4)

- Σ_r is a diagonal matrix containing the r non-zero singular values of matrix $\mathbf{G}$.
- $\mathbf{U}_r$ contains the eigenvectors associated with the non-zero eigenvalues of matrix $\mathbf{GG}^{\mathrm{T}}$.
- $\mathbf{V}_r$ contains the eigenvectors associated with the non-zero eigenvalues of matrix $\mathbf{G}^{\mathrm{T}}\mathbf{G}$.
- We introduce $\mathbf{U}_0$ and $\mathbf{V}_0$ as the contributions of zero singular values of $\mathbf{G}$.
- With these definitions, $\mathbf{m}_r$, $\mathbf{m}_0$, $\mathbf{d}_r$ and $\mathbf{d}_0$ belong to the subspaces spanned by $\mathbf{V}_r$, $\mathbf{V}_0$, $\mathbf{U}_r$ and $\mathbf{U}_0$.
- Notes on the nul spaces $\mathbf{U}_0$ and $\mathbf{V}_0$:
  - It is easy to verify that $\mathbf{U}_0^T\mathbf{Gm} = \mathbf{U}_0^T\mathbf{U}_r\Sigma_r\mathbf{V}_r^T\mathbf{m} = \mathbf{0}$ because $\mathbf{U}_0 \perp \mathbf{U}_r$.
    This implies that the data cannot entirely be described by operator G
  - $\mathbf{V}_0$ is responsible for the non-uniqueness of the solutions because

$$\forall\ \mathbf{m}_0 \in \mathbf{V}0,\ \ \mathbf{G}(\mathbf{m}_1 + \mathbf{m}_0) = \mathbf{Gm}_1 \quad \text{since} \quad \mathbf{Gm}_0 = \mathbf{0}$$

Mixed-determined problems (5)

- By analogy with square matrices $\mathbf{G}$, for which the inverse operator is $\mathbf{G}^{-1}$, since we have $\mathbf{G} = \mathbf{U}_r \Sigma_r \mathbf{V}_r^T$, we define for our mixed-determined problem $\mathbf{d} = \mathbf{Gm}$ a « generalized » inverse

$$\mathbf{G}^{-g} = \mathbf{V}_r \Sigma_r^{-1} \mathbf{U}_r^T$$

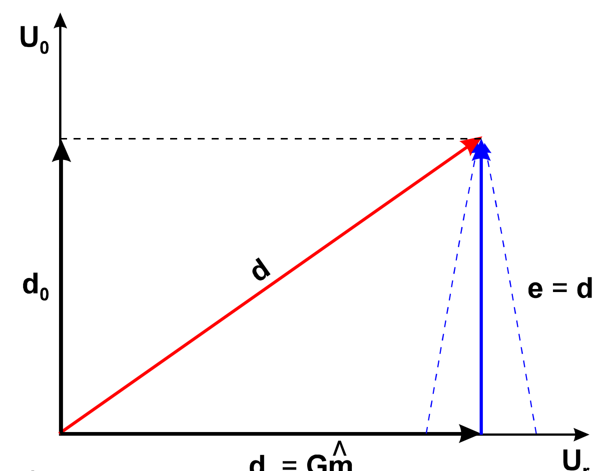
  so that

$$\hat{\mathbf{m}} = \mathbf{G}^{-g}\mathbf{d} = \mathbf{V}_r \Sigma_r^{-1} \mathbf{U}_r^T \mathbf{d}$$

- We can easily verify that this solution
  - Has no component in the model nul space $\mathbf{V}_0$: $\mathbf{V}_0^T \hat{\mathbf{m}} = \mathbf{V}_0^T \mathbf{V}_r \Sigma_r^{-1} \mathbf{U}_r^T \mathbf{d} = 0$ as $\mathbf{V}_0 \perp \mathbf{V}_r$
  - Error $\mathbf{e}$ has no components in $\mathbf{U}_r$ subspace

Since $\mathbf{U}_r^T \mathbf{U}_r = \mathbf{I}_r$ and $\mathbf{V}_r^T \mathbf{V}_r = \mathbf{I}_r$

$$\begin{aligned} \mathbf{U}_r^T \mathbf{e} &= \mathbf{U}_r^T [\mathbf{d} - \mathbf{G}\hat{\mathbf{m}}] \\ &= \mathbf{U}_r^T [\mathbf{d} - \mathbf{U}_r \Sigma_r \mathbf{V}_r^T \mathbf{V}_r \Sigma_r^{-1} \mathbf{U}_r^T \mathbf{d}] \\ &= \mathbf{U}_r^T [\mathbf{d} - \mathbf{U}_r \mathbf{U}_r^T \mathbf{d}] = \mathbf{U}_r^T \mathbf{d} - \mathbf{U}_r^T \mathbf{d} = \mathbf{0} \end{aligned}$$



Mixed-determined problems (6)

- In addition to being the natural solution for mixed-determined problems, the generalized inverse $\mathbf{G}^{-g}$ can be used in all situations described previously: over-, under-, and exactly-determined problems.
- It contains all solutions derived before:
  - When $\mathbf{U}_0$ and $\mathbf{V}_0$ are of zero dimension, $r = N = M$, $\mathbf{G}^{-g} = \mathbf{G}^{-1}$ (exact determination)
  - When $\mathbf{U}_0$ has zero dimension and $\mathbf{V}_0$ has non-zero dimension (overdetermination),

$$\hat{\mathbf{m}} = \left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{G}^T\mathbf{d} = \mathbf{V}_r\boldsymbol{\Sigma}_r^{-2}\mathbf{V}_r^T\mathbf{V}_r\boldsymbol{\Sigma}_r\mathbf{U}_r^T\mathbf{d} = \mathbf{V}_r\boldsymbol{\Sigma}_r^{-1}\mathbf{U}_r^T\mathbf{d} = \mathbf{G}^{-g}\mathbf{d}$$

  - When $\mathbf{U}_0$ has non-zero dimension and $\mathbf{V}_0$ has zero dimension (underdetermination),

$$\mathbf{G}^T\left[\mathbf{G}\mathbf{G}^T\right]^{-1} = \left[\mathbf{V}_r\Sigma_r\mathbf{U}_r^T\right]\left\{\left[\mathbf{U}_r\Sigma_r\mathbf{V}_r^T\right]\left[\mathbf{V}_r\Sigma_r\mathbf{U}_r^T\right]\right\}^{-1} = \left[\mathbf{V}_r\Sigma_r\mathbf{U}_r^T\right]\left\{\mathbf{U}_r\Sigma_r^{-2}\mathbf{U}_r^T\right\}$$

$$= \mathbf{V}_r\Sigma_r^{-1}\mathbf{U}_r^T = \mathbf{G}^{-g}$$

Weak underdetermination

- In case of weak underdetermination, rather than partitioning vectors $\mathbf{m}$ and $\mathbf{d}$, we can minimize a combination of the data prediction error E and length of the solution L, i.e., we minimize a function

$$\psi(\hat{\mathbf{m}}) = E + \varepsilon^2 L = \mathbf{e}^T \mathbf{e} + \varepsilon^2 \hat{\mathbf{m}}^T \hat{\mathbf{m}}$$

  with respect to elements $\hat{m}_q$ of model $\hat{\mathbf{m}}$ we seek to find.

- Factor ε determines the importance of length L relative to error E in the minimization of function $\psi(\hat{\mathbf{m}})$.

- By solving this minimization problem explicitly, we end up with the damped least squares solution

$$\hat{\mathbf{m}} = \left[\mathbf{G}^T \mathbf{G} + \varepsilon^2 \mathbf{I}\right]^{-1} \mathbf{G}^T \mathbf{d}$$

- The additional term $\varepsilon^2\mathbf{I}$ regularizes matrix $\mathbf{G}^T\mathbf{G}$ and stabilizes its inverse, at the expense of the model resolution.

Other a priori information (1)

- The criterion that was adopted (minimization of $L = \mathbf{m}^T \mathbf{m}$) is not always suitable. It can be generalized in several ways.
- For instance, we can introduce an a priori information on the model and consider minimizing

$$L = \left(\mathbf{m} - \mathbf{m}_{priori}\right)^T \left(\mathbf{m} - \mathbf{m}_{priori}\right)$$

- In other cases, we will be looking for smooth solutions by introducing weighting factors in the form of a $M \times M$ matrix $\mathbf{W}_{\mathrm{m}}$:

$$L = \mathbf{m}^T \mathbf{W}_m \mathbf{m}.$$

- We may estimate the roughness of discrete model parameters via

$$\Delta = \mathbf{Dm} = \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & \ddots & \ddots \\ & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ \vdots \\ m_M \end{pmatrix}$$

Other a priori information (2)

- Matrix $\mathbf{D}$ is an approximate differenciation operator. Minimizing the roughness of vector $\mathbf{m}$ amounts to minimize

$$L = \Delta^T \Delta = (\mathbf{Dm})^T (\mathbf{Dm}) = \mathbf{m}^T \left(\mathbf{D}^T \mathbf{D}\right)\mathbf{m} = \mathbf{m}^T \mathbf{W}_m \mathbf{m}$$

- The off-diagonal terms of matrix $\mathbf{W}_\mathrm{m}$ represent the interdependence of the model parameters. Matrix $\mathbf{W}_\mathrm{m}$ can be designed to impose some relationship between the model parameters.

- By combining the a priori information $\mathbf{m}_\mathrm{priori}$ and weighting matrix $\mathbf{W}_\mathrm{m}$,

$$L = \left[\mathbf{m} - \mathbf{m}_{priori}\right]^T \mathbf{W}_m \left[\mathbf{m} - \mathbf{m}_{priori}\right]$$

- We can similarly define a $N \times N$ weighting matrix $\mathbf{W}_\mathrm{d}$ for the data to favor the « good » data at the expense of the noisy data and define a generalized prediction error

$$E = \mathbf{e}^T \mathbf{W}_d \mathbf{e}$$

$\mathbf{W}_\mathrm{d}$ is a diagonal matrix when there is no coupling between the data.

Other a priori information (3)

- We thus obtain new solutions of the discrete linear inverse problem, which generalize the expressions obtained so far.
- **Overdetermined problems**

  Minimization of $E = \mathbf{e}^T \mathbf{W}_d \mathbf{e}$ leads to the weighted least squares solution

$$\hat{\mathbf{m}} = \left[\mathbf{G}^T \mathbf{W}_d \mathbf{G}\right]^{-1} \mathbf{G}^T \mathbf{W}_d \mathbf{d}$$

- **Purely underdetermined problems**

  Minimization of $L = \left[\mathbf{m} - \mathbf{m}_{priori}\right]^T \mathbf{W}_m \left[\mathbf{m} - \mathbf{m}_{priori}\right]$ with constaint $E = 0$

  leads to the weighted minimal length solution

$$\hat{\mathbf{m}} = \mathbf{m}_{priori} + \mathbf{W}_m \mathbf{G}^T \left[\mathbf{G}\mathbf{W}_m \mathbf{G}^T\right]^{-1} \left[\mathbf{d} - \mathbf{G}\mathbf{m}_{priori}\right]$$

Other a priori information (4)

- **Weakly underdetermined problems**

Minimization of quantity $\psi(\hat{\mathbf{m}}) = E + \varepsilon^2 L = \mathbf{e}^T \mathbf{W}_d \mathbf{e} + \varepsilon^2 \left[\hat{\mathbf{m}} - \mathbf{m}_{priori}\right]^T \mathbf{W}_m \left[\hat{\mathbf{m}} - \mathbf{m}_{priori}\right]$

leads to the damped and weighted least squares solution which can be written

$$\hat{\mathbf{m}} = \mathbf{m}_{priori} + \left[\mathbf{G}^T \mathbf{W}_d \mathbf{G} + \varepsilon^2 \mathbf{W}_m\right]^{-1} \mathbf{G}^T \mathbf{W}_d \left[\mathbf{d} - \mathbf{G}\mathbf{m}_{priori}\right]$$

$$\hat{\mathbf{m}} = \mathbf{m}_{priori} + \mathbf{W}_m^{-1} \mathbf{G}^T \left[\mathbf{G}\mathbf{W}_m^{-1}\mathbf{G}^T + \varepsilon^2 \mathbf{W}_d^{-1}\right]^{-1} \left[\mathbf{d} - \mathbf{G}\mathbf{m}_{priori}\right]$$

- **Linear equality constraints**: yet another class of a priori information

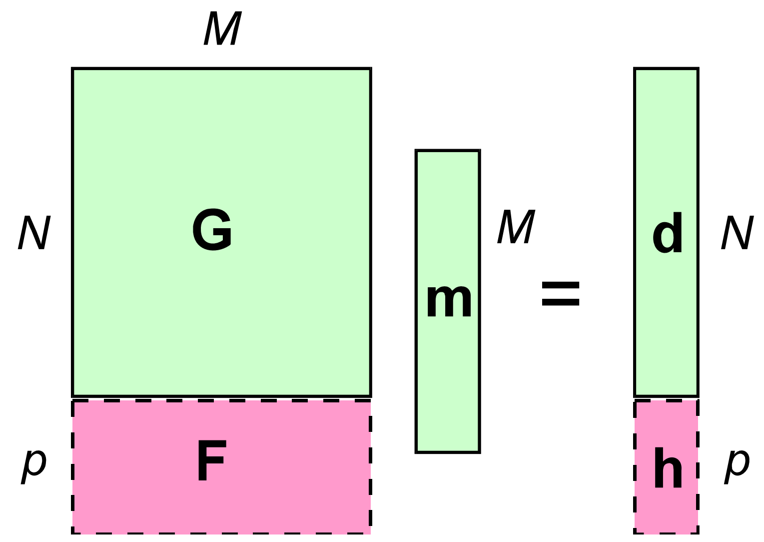
Linear combinations of model parameters can be expressed as $\mathbf{h} = \mathbf{F}\mathbf{m}$.

For example, if the average of the model parameters is equal to a constant μ, then

$$\mathbf{F}\mathbf{m} = \frac{1}{M}\begin{bmatrix}1 & 1 & 1 \ldots 1\end{bmatrix}\begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_M \end{bmatrix} = [\mu] = \mathbf{h}$$

Other a priori information (5)

- Other example: in a curve fitting procedure, impose that the curve passes through a specified point.
- One way to account for linear equality constraints is to combine the p equations $\mathbf{h} = \mathbf{Fm}$ with the N equations $\mathbf{d} = \mathbf{Gm}$ and to put strong weights on equations $\mathbf{h} = \mathbf{Fm}$.
- This will impose a prediction error which is very small for the equations $\mathbf{h} = \mathbf{Fm}$ at the expense of the prediction error of equations $\mathbf{d} = \mathbf{Gm}$ which can be important.



Other a priori information (6)

- Another solution to this problem is to minimize the prediction error $E = \mathbf{e}^{\mathrm{T}}\mathbf{e}$ with the p constraints $\mathbf{Fm} - \mathbf{h} = \mathbf{0}$ by using the Lagrange multipliers technique once more.
- We minimize the function

$$\psi(\hat{\mathbf{m}}) = \sum_{i=1}^{N}\left\{\sum_{j=1}^{M} G_{ij}\hat{m}_j - d_i\right\}^2 + 2\sum_{i=1}^{p}\left\{\lambda_i\left[\sum_{j=1}^{M} F_{ij}\hat{m}_j - h_i\right]\right\} \quad \textit{wrt} \text{ variables } \hat{m}_q,\ q = 1,\ldots M$$

- In matrix form:

$$\left[\begin{array}{c|c} \mathbf{G}^T\mathbf{G} & \mathbf{F}^T \\ \hline \mathbf{F} & \mathbf{0} \end{array}\right]\left[\begin{array}{c} \hat{\mathbf{m}} \\ \hline \lambda \end{array}\right] = \left[\begin{array}{c} \mathbf{G}^T\mathbf{d} \\ \hline \mathbf{h} \end{array}\right]$$

- Finally, the solution of the overdetermined problem $\mathbf{d} = \mathbf{Gm}$ with linear constraints $\mathbf{h} = \mathbf{Fm}$ is

$$\hat{\mathbf{m}} = \underbrace{\left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{G}^T\mathbf{d}}_{\text{sol. without constraint}} - \left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{F}^T\left\{\mathbf{F}\left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{F}^T\right\}^{-1}\left\{\mathbf{F}\left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{G}^T\mathbf{d} - \mathbf{h}\right\}$$

Properties of generalized inverses (1)

- We have obtained model parameters estimates in various situations that we can write $\mathbf{m}^{est} = \mathbf{G}^{-g}\mathbf{d}^{obs} + \mathbf{v}$
- The inverse operator $\mathbf{G}^{-g}$ is not a matrix inverse in the classical sense (except in the exactly determined problem where $\mathbf{G}^{-g} = \mathbf{G}^{-1}$). The matrix products $\mathbf{G}\mathbf{G}^{-g}$ and $\mathbf{G}^{-g}\mathbf{G}$ are generally not identity matrices.
- Data predicted from the estimated models are obtained via

$$\mathbf{d}^{pre} = \mathbf{G}\mathbf{m}^{est} = \mathbf{G}\left[\mathbf{G}^{-g}\mathbf{d}^{obs}\right] = \left[\mathbf{G}\mathbf{G}^{-g}\right]\mathbf{d}^{obs} = \mathbf{N}\,\mathbf{d}^{obs}$$

- The $N \times N$ square matrix $\mathbf{N} = \mathbf{G}\mathbf{G}^{-g}$ is the data resolution matrix, which should ideally be the $\mathbf{I}_N$ identity matrix. In this case, the data prediction error would be zero.
- The importance of off-diagonal terms can be evaluated by defining

$$\mu(\mathbf{N}) = \left\|\mathbf{N} - \mathbf{I}_N\right\|_F^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\left[n_{ij} - \delta_{ij}\right]^2$$

Properties of generalized inverses (2)

- Similarly, we may wonder how close the estimated model $\mathbf{m}^{\mathrm{est}}$ is from the true model $\mathbf{m}^{\mathrm{true}}$ which is such that $\mathbf{G}\mathbf{m}^{\mathrm{true}} = \mathbf{d}^{\mathrm{obs}}$.
- Therefore, $\mathbf{m}^{est} = \mathbf{G}^{-g}\mathbf{d}^{obs} = \mathbf{G}^{-g}\left[\mathbf{G}\mathbf{m}^{true}\right] = \left[\mathbf{G}^{-g}\mathbf{G}\right]\mathbf{m}^{true} = \mathbf{R}\,\mathbf{m}^{true}$
- The $M \times M$ square matrix $\boxed{\mathbf{R} = \mathbf{G}^{-g}\mathbf{G}}$ is the model resolution matrix, which should ideally be the $\mathbf{I}_M$ identity matrix to uniquely determine each model parameter.
- The importance of off-diagonal terms can be evaluated by defining

$$\mu(\mathbf{R}) = \left\|\mathbf{R} - \mathbf{I}_M\right\|_F^2 = \sum_{i=1}^{M}\sum_{j=1}^{M}\left[r_{ij} - \delta_{ij}\right]^2$$

- The unit covariance matrix characterizes the degree of error amplification that occurs in the mapping from data to model parameters. If the data are all uncorrelated and have equal variance σ^2, the unit covariance matrix is given by

$$\mathbf{\Gamma} = \sigma^{-2}\mathbf{G}^{-g}\mathbf{C}_d\mathbf{G}^{-g^T} \boxed{= \mathbf{G}^{-g}\mathbf{G}^{-g^T}}$$

Summary (1)

Resolution of linear systems $\mathbf{d} = \mathbf{Gm}$ for N data and M unknowns using the L_2 norm

- If $N > M$: *Overdetermined problem*
  - Minimization of prediction error $E = [\mathbf{d} - \mathbf{Gm}]^T [\mathbf{d} - \mathbf{Gm}]$
  - Least squares solution $\hat{\mathbf{m}} = \left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{G}^T\mathbf{d}$
  - Data resolution matrix $\mathbf{N} = \mathbf{G}\left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{G}^T$
  - Model resolution matrix $\mathbf{R} = \mathbf{I}_M$
  - Unit covariance matrix $\mathbf{\Gamma} = \left[\mathbf{G}^T\mathbf{G}\right]^{-1}$
- If $N < M$: *Underdetermined problem*
  - Minimization of norm of solution $L = \mathbf{m}^T\mathbf{m}$ with constraint $E = 0$
  - Minimum length solution $\hat{\mathbf{m}} = \mathbf{G}^T\left[\mathbf{G}\mathbf{G}^T\right]^{-1}\mathbf{d}$
  - Data resolution matrix $\mathbf{N} = \mathbf{I}_N$
  - Model resolution matrix $\mathbf{R} = \mathbf{G}^T\left[\mathbf{G}\mathbf{G}^T\right]^{-1}\mathbf{G}$
  - Unit covariance matrix $\mathbf{\Gamma} = \mathbf{G}^T\left[\mathbf{G}\mathbf{G}^T\right]^{-2}\mathbf{G}$

Summary (2)

Resolution of linear systems $\mathbf{d} = \mathbf{Gm}$ for N data and M unknowns using the L_2 norm

- For any given N, M: *Mixed-determined problem*
  - Singular value decompostion $\mathbf{G} = \mathbf{U}_r \boldsymbol{\Sigma}_r \mathbf{V}_r^T$
  - Generalized inverse solution $\hat{\mathbf{m}} = \mathbf{V}_r \boldsymbol{\Sigma}_r \mathbf{U}_r^T \mathbf{d}$
  - Data resolution matrix $\mathbf{N} = \mathbf{U}_r \mathbf{U}_r^T$
  - Model resolution matrix $\mathbf{R} = \mathbf{V}_r \mathbf{V}_r^T$
  - Unit covariance matrix $\boldsymbol{\Gamma} = \mathbf{V}_r \boldsymbol{\Sigma}_r^{-2} \mathbf{V}_r^T$
- *Damped least squares solutions*

$$\hat{\mathbf{m}} = \left[\mathbf{G}^T\mathbf{G} + \varepsilon^2 \mathbf{I}_M\right]^{-1} \mathbf{G}^T \mathbf{d}$$

$$\hat{\mathbf{m}} = \mathbf{G}^T\left[\mathbf{G}\mathbf{G}^T + \varepsilon^2 \mathbf{I}_N\right]^{-1} \mathbf{d}$$

Exercise: medium described by 4 cells

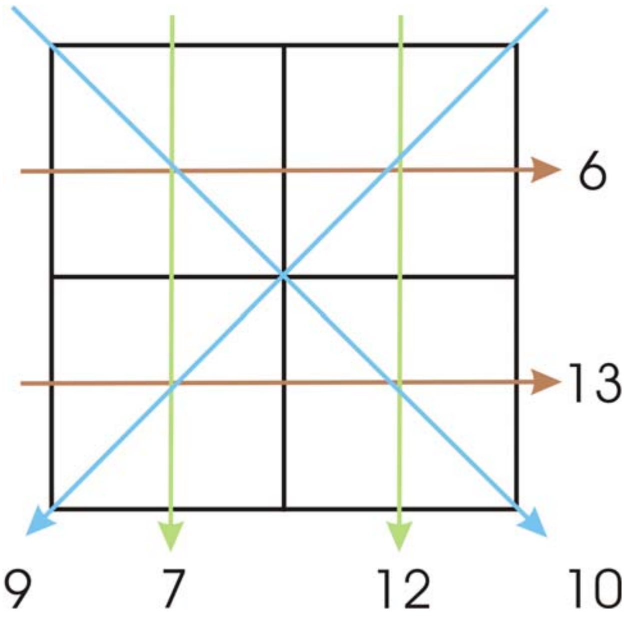
- Compute solutions with

$$\hat{\mathbf{m}}_1 = \left[\mathbf{G}^T\mathbf{G}\right]^{-1}\mathbf{G}^T\mathbf{d}$$

$$\hat{\mathbf{m}}_3 = \mathbf{G}^T\left[\mathbf{G}\mathbf{G}^T + \varepsilon^2\mathbf{I}_N\right]^{-1}\mathbf{d} \quad ; \quad \varepsilon = 0.01, 0.1, 1$$

$$\hat{\mathbf{m}}_3 = \left[\mathbf{G}^T\mathbf{G} + \varepsilon^2\mathbf{I}_M\right]^{-1}\mathbf{G}^T\mathbf{d} \quad ; \quad \varepsilon = 0.01, 0.1, 1$$

$$\hat{\mathbf{m}}_4 = \mathbf{V}_r\,{}_r\mathbf{U}_r^T\mathbf{d}$$



- In all these cases, compute

  the solution length $L = \hat{\mathbf{m}}^T\hat{\mathbf{m}}$

  the data prediction error $E = \mathbf{e}^T\mathbf{e} = \left(\mathbf{d} - \mathbf{G}\hat{\mathbf{m}}\right)^T\left(\mathbf{d} - \mathbf{G}\hat{\mathbf{m}}\right)$

Exercise: medium described by 4 cells

- Use your preferred computation tool to do the matrix operations:
  - Matlab, Octave
  - Maple, Mathematica
  - LibreOffice, Gnumeric, Excel (MMULT, MINVERSE, TRANSPOSE, …)(*)
  - Python, R
  - Fortran, C

  (*) Norms can be tricky to compute

Exercise: medium described by 4 cells

- Main results:

$$\hat{m}_1 = [2 \quad 4 \quad 5 \quad 8] \quad ; \quad E_1 = 0 \quad ; \quad L_1 = 109$$

$$\hat{m}_2 = [2.000090 \quad 3.999990 \quad 4.999940 \quad 7.999790]$$

$$E_2 = .1479000000\text{e-}6 \quad ; \quad L_2 = 108.9963201 \quad [\varepsilon = 0.01]$$

$$\hat{m}_2 = [2.00577777 \quad 3.99582753 \quad 4.99085241 \quad 7.97592705]$$

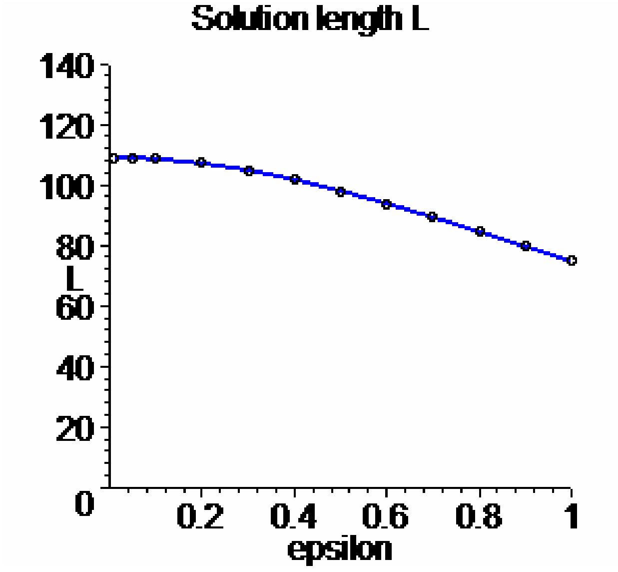
$$E_2 = .2427478313\text{e-}2 \quad ; \quad L_2 = 108.5138021 \quad [\varepsilon = 0.1]$$

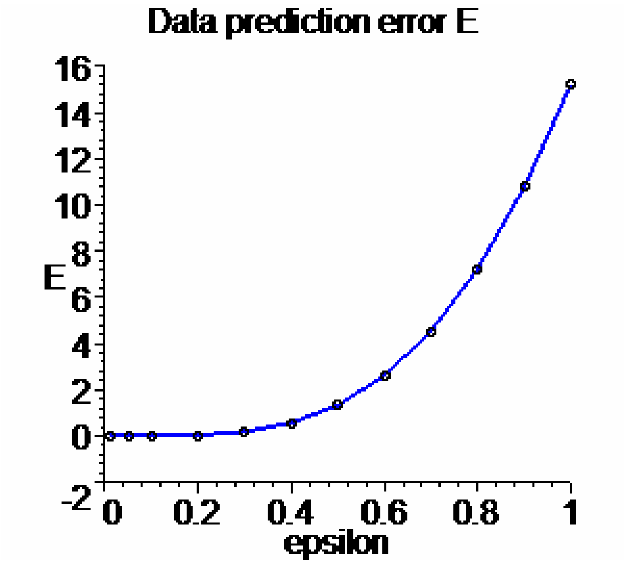
$$\hat{m}_3 = [2.005778095 \quad 3.995827847 \quad 4.990852723 \quad 7.975927349]$$

$$E_3 = .2427360908\text{e-}2 \quad ; \quad L_3 = 108.5138140 \quad [\varepsilon = 0.1]$$

Exercise: medium described by 4 cells

- Main results (*continued*):





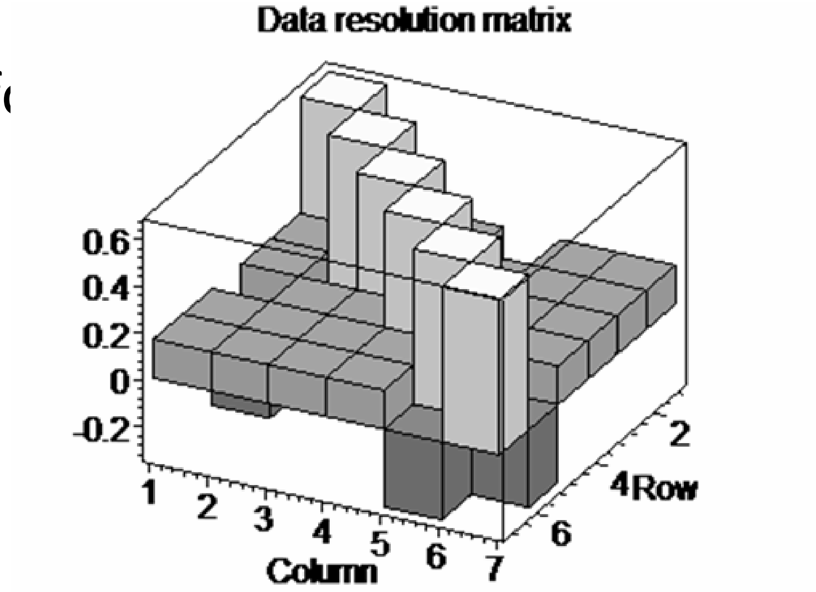
Solid line: damped overdetermined solution
Symbols: damped underdetermined solution

Exercise: medium described by 4 cells

- Main results (*continued*):

  6×6 **data resolution matrix** f[ ]
  the least squares solution (1)

  Data predicted from the estimated model do not entirely explain the data (they are slightly smoothed)



  4×4 **model resolution matrix** for the least squares solution is

  $\mathbf{I}_4$ identity matrix

Exercise: medium described by 4 cells

- Main results (*continued*):

  When ε increases (> 0.6), we degrade both the data and model resolutions (smoothing)

  Trade-off between resolution and variance