Inverse Problems in Geophysics
Part 2: Matrix problems and Least Squares

2. MGPY+MGIN

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Recap

- Inversion: create model $\mathbf{m}$ that fits the data $\mathbf{d}$
- data vector along with measuring error
- model vector describes the subsurface
- number of data and model parameters important

Linear problems

$\mathbf{f}(\mathbf{m})$ is linear with respect to $\mathbf{m} \Rightarrow$ write as matrix-vector product

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

Examples

Gravimetry, Magnetics, Magnetic Resonance, VSP, straight-ray tomography, regression

Problem

$\mathbf{m} = \mathbf{G}^{-1}\mathbf{d}$? No, because is usually not invertible, not even quadratic.

Types of inverse problems

Important

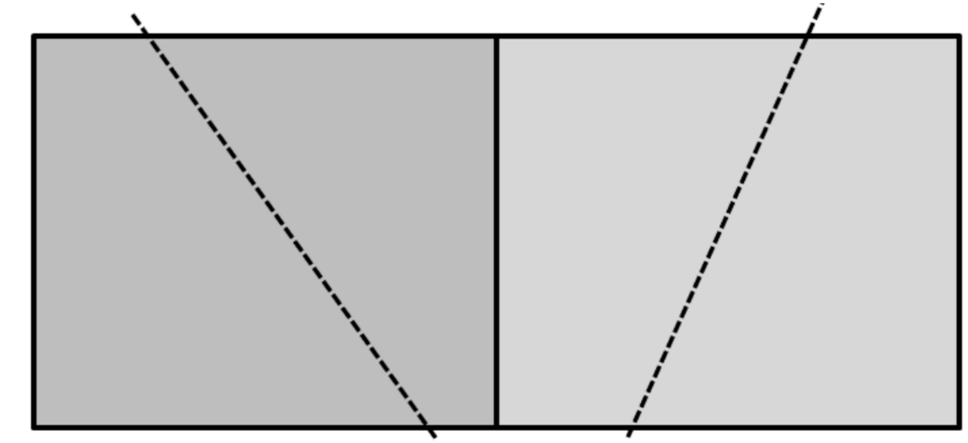
- every row stands for a measurement (data point)
- every column represents a model parameter

$$\mathbf{d} = \mathbf{G}\mathbf{m} + \mathbf{n} \Rightarrow \mathbf{G} \in \Re^{\mathbf{N} \times \mathbf{M}}$$

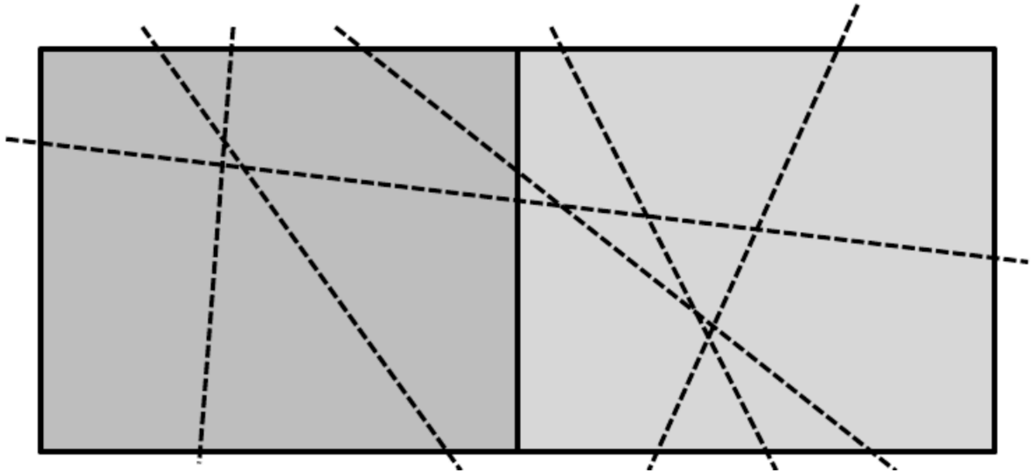
- N = M: even-determined
- N > M: over-determined problem (no existing solution)
- N < M: under-determined problem (no unique solution)
- mostly: (both over- and) under-determined model parts

Types of inverse problems (Menke, 2012)

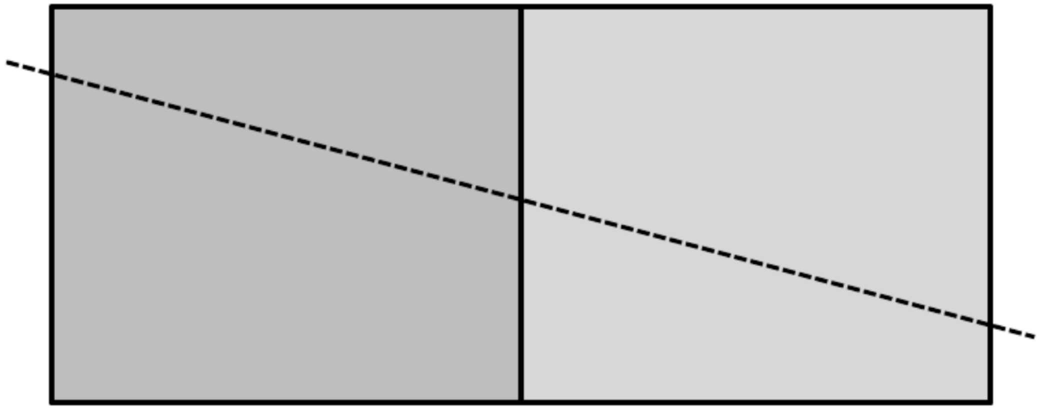
Even-determined



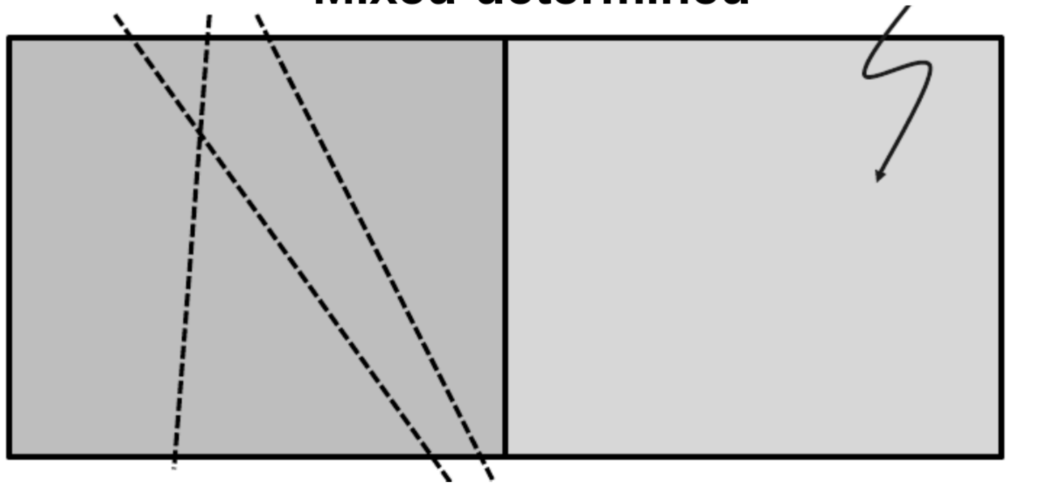
Over-determined



Under-determined



Mixed-determined

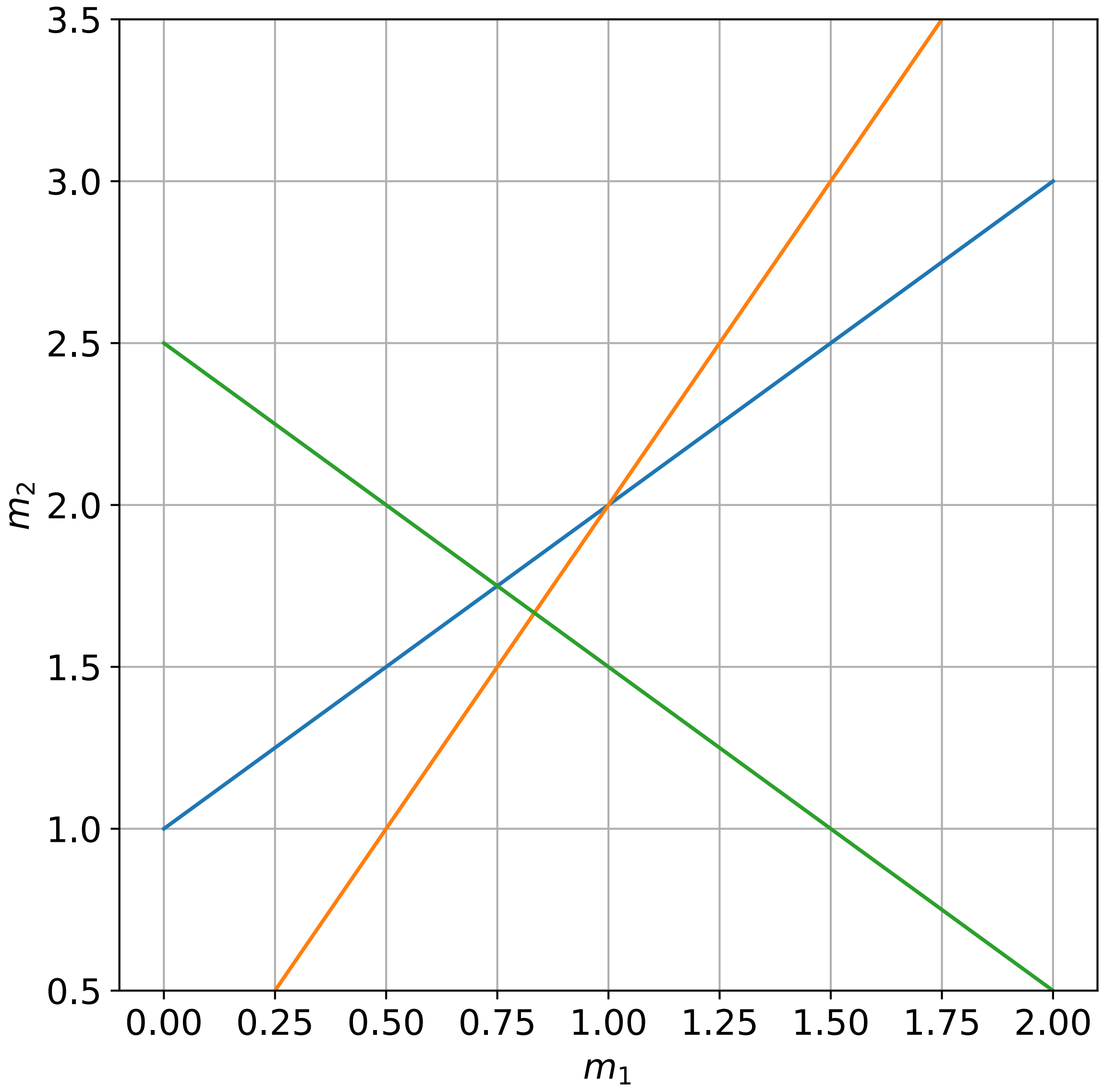


A simple matrix problem

$$m_1 - m_2 = -1$$
$$2m_1 - m_2 = 0$$
$$m_1 + m_2 = 2.5$$

$$\mathbf{G} = \begin{pmatrix} 1 & -1 \\ 2 & -1 \\ 1 & 1 \end{pmatrix}$$

$$m_2 = (d_i - G_{i1} \cdot m_1)/G_{i2}$$



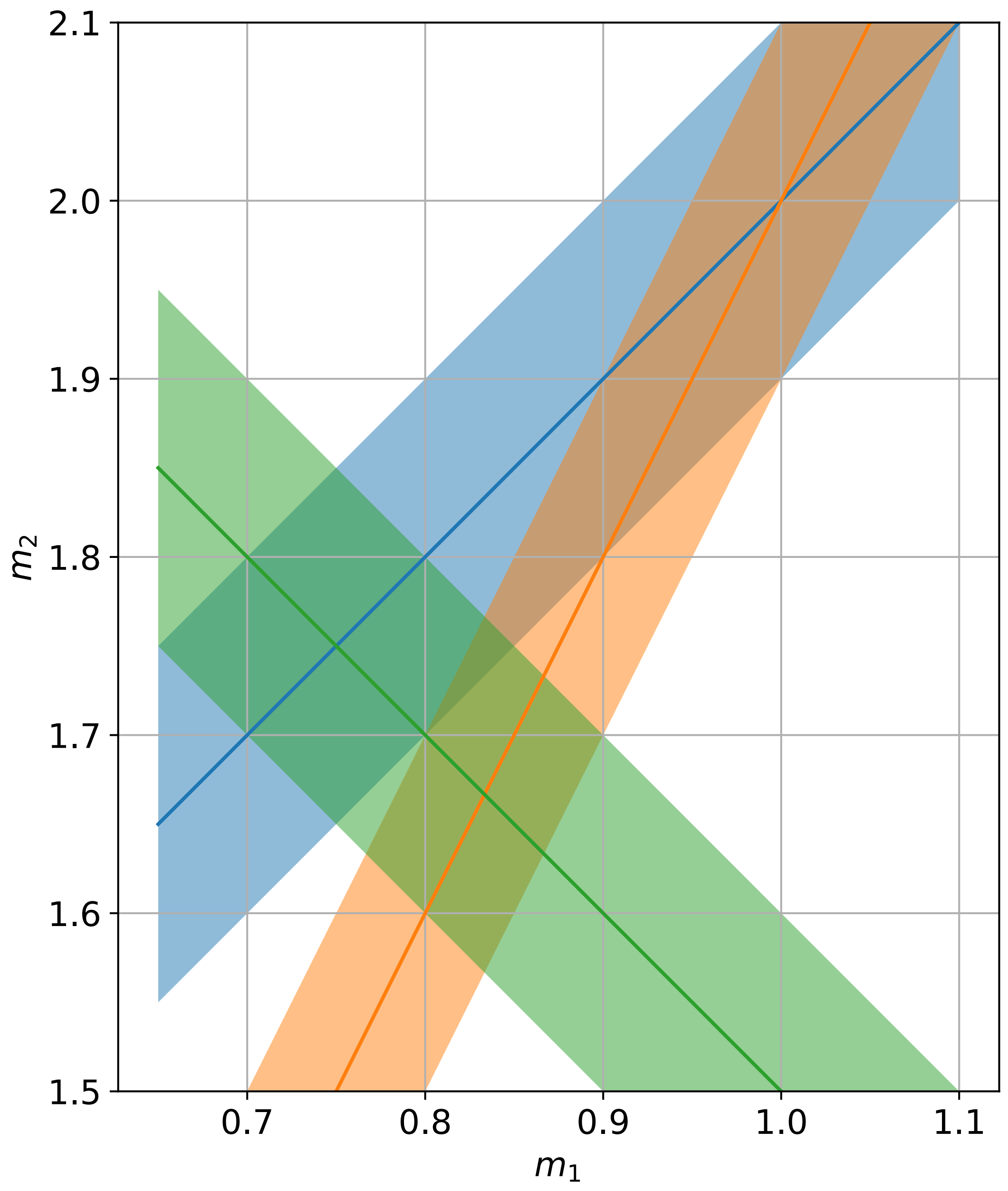
A simple matrix problem with errors

$$\mathbf{G} = \begin{pmatrix} 1 & -1 \\ 2 & -1 \\ 1 & 1 \end{pmatrix}$$

$$m_2 = (d_i - G_{i1} \cdot m_1)/G_{i2}$$

$$\delta m_2 = \delta d_i / G_{i2}$$

Data error of δd=0/0.05/0.1



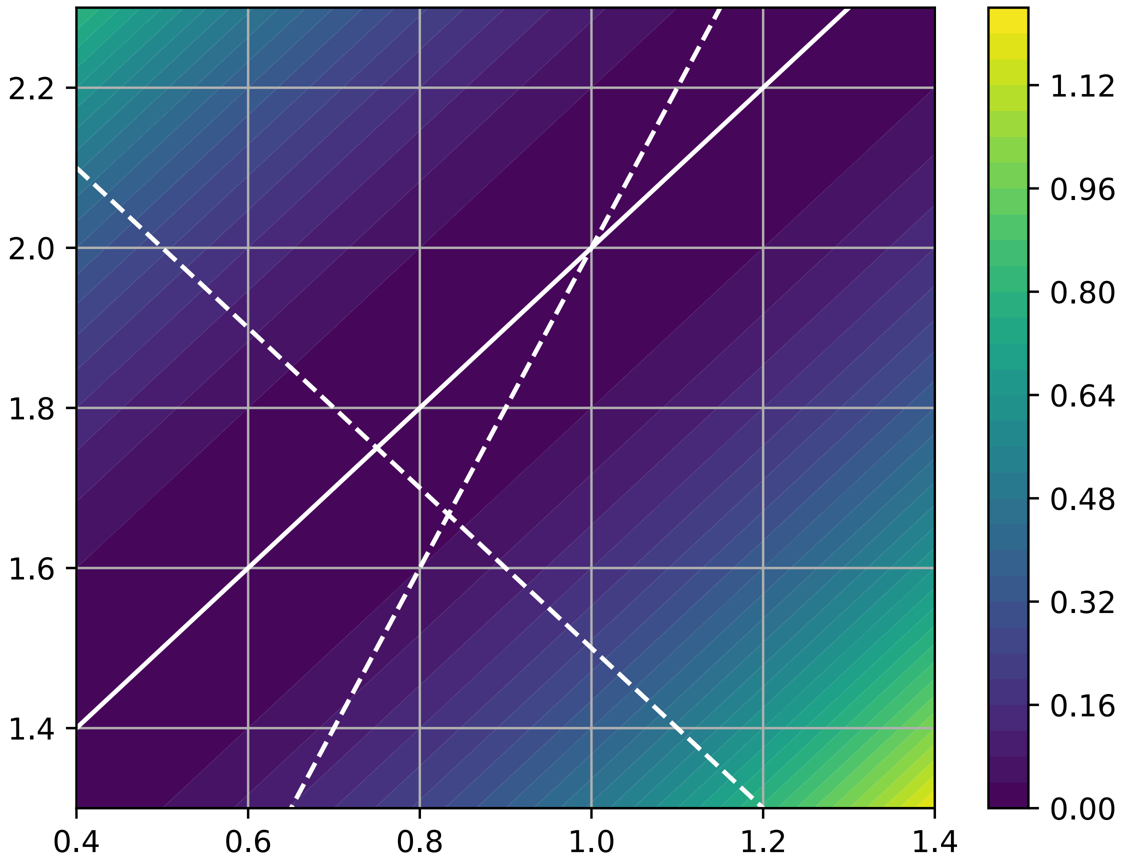
The objective function

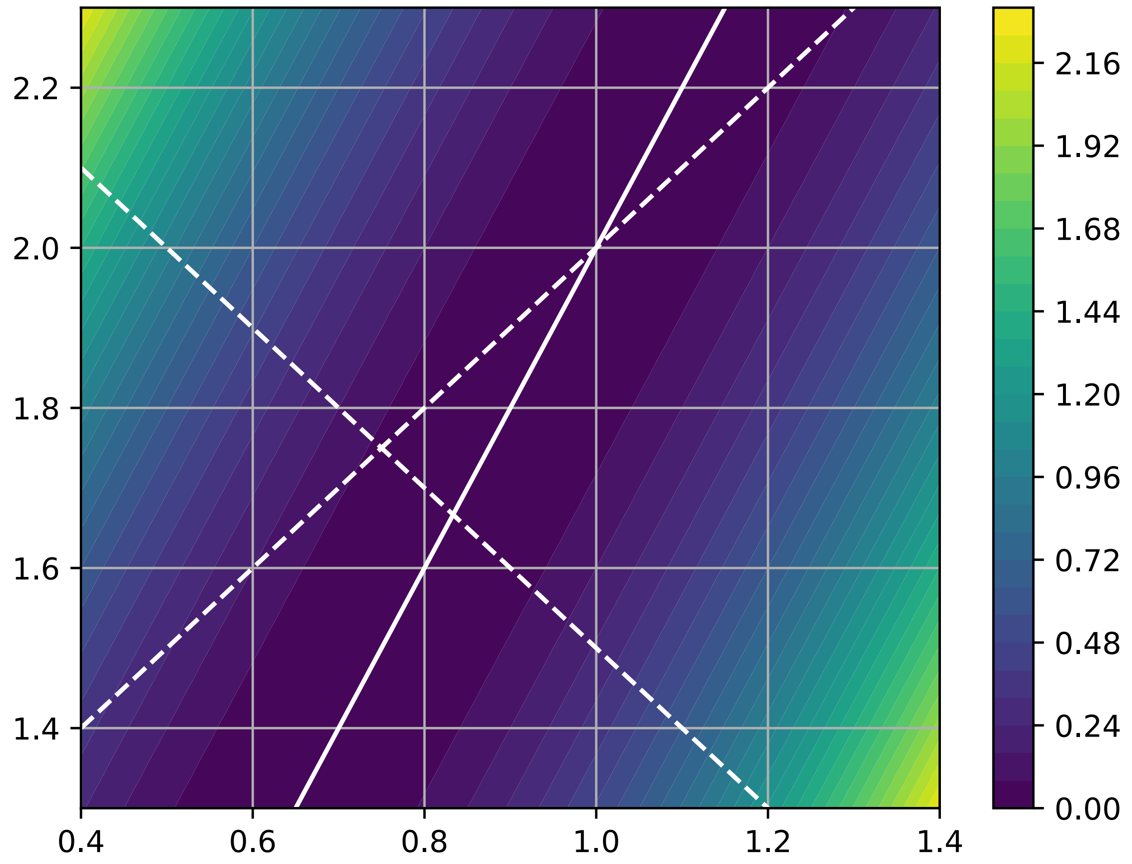
We minimize the L2-norm (summed squared distances) of the residual between data and model response:

$$\Phi = \|\mathbf{d} - \mathbf{Gm}\|_{\mathbf{2}}^{\mathbf{2}} = \sum_{\mathbf{1}}^{\mathbf{N}} (\mathbf{d_i} - \mathbf{g_i}(\mathbf{m}))^{\mathbf{2}} \rightarrow \min$$

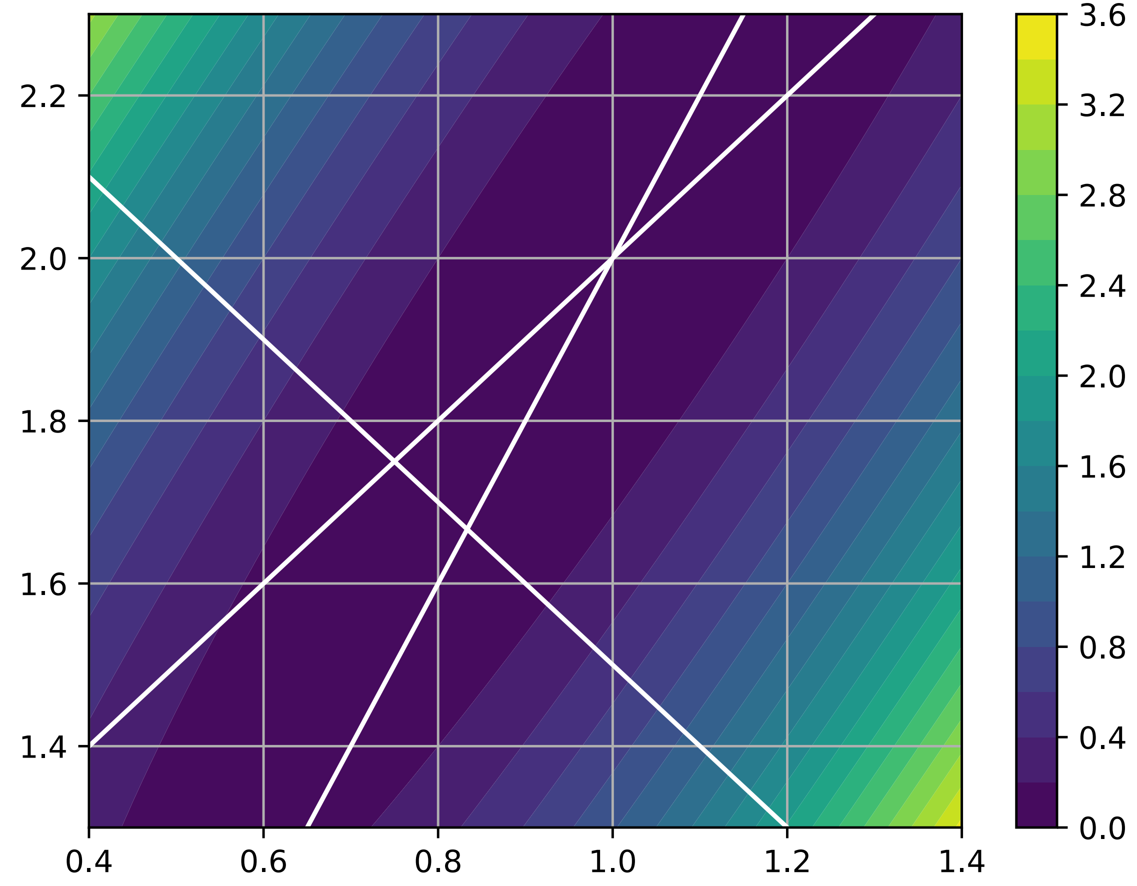
Let’s compute the objective function for a range of values for m_1 and m_2 (grid search).

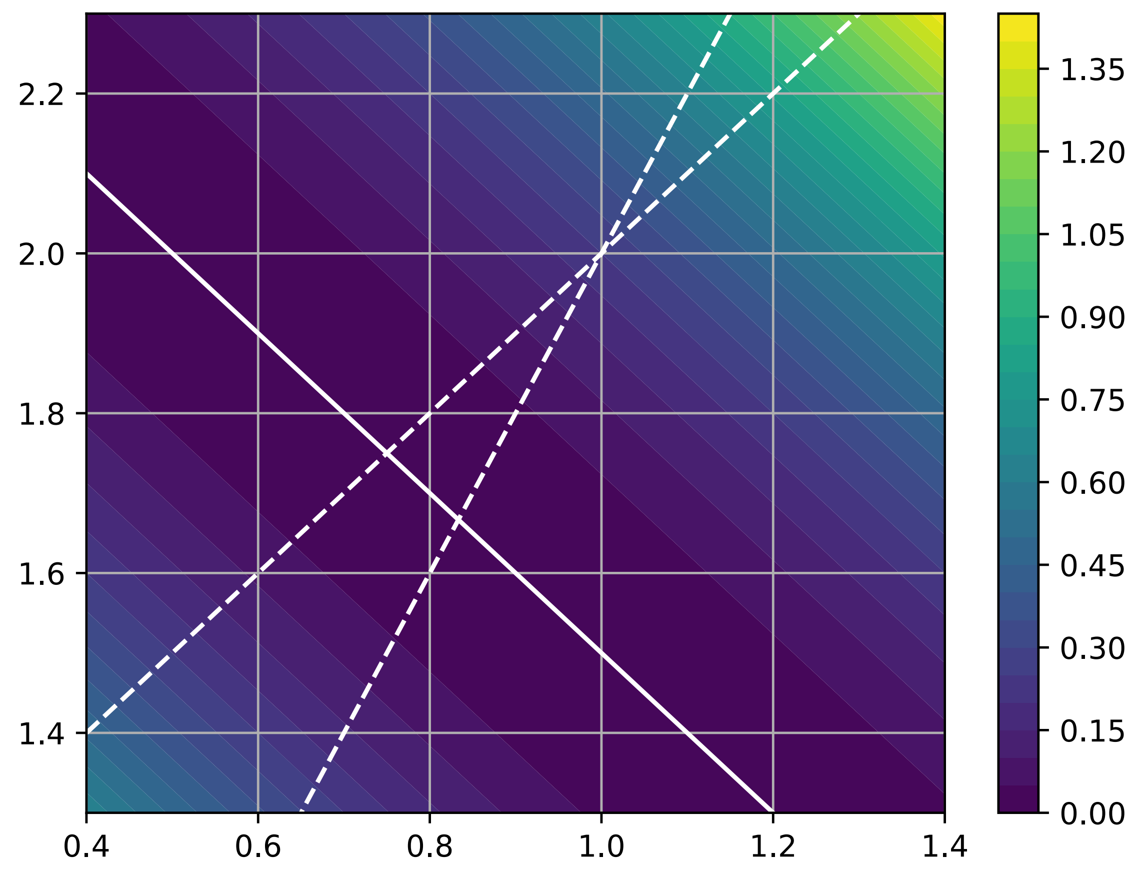
Distance function for the first two data



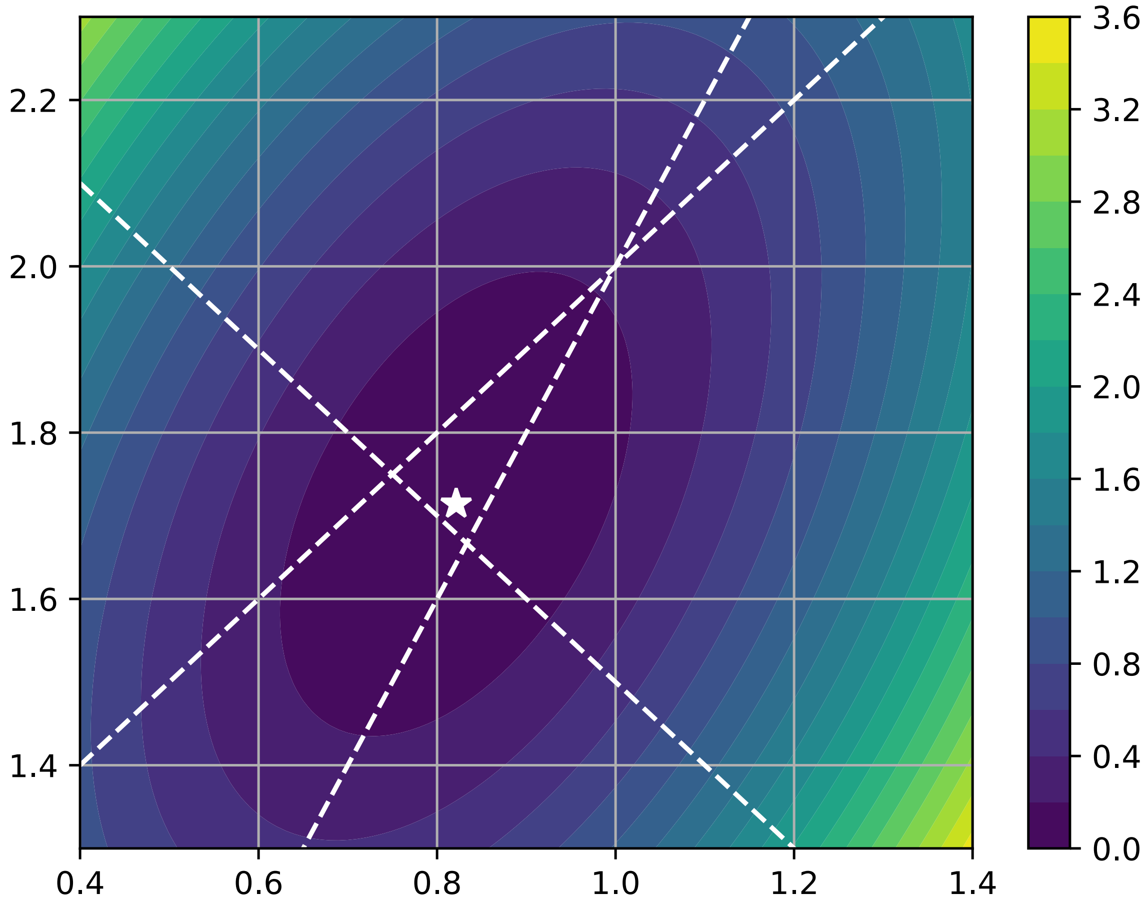


Distance function of 1st + 2nd and 3rd





Total objective function



- Add all three squared distances.
- ellipsoidal minimum shape
- The minimum pixel (grid spacing of 0.1) lies at (0.82, 1.71).

How can we determine the absolute minimum value?

The method of least squares

Derivation

$$\Phi = \|\mathbf{d} - \mathbf{Gm}\|_2^2 = (\mathbf{d} - \mathbf{Gm})^T(\mathbf{d} - \mathbf{Gm})$$

$$\nabla_m = \left(\frac{\partial}{\partial m_1}, \frac{\partial}{\partial m_2}, \ldots, \frac{\partial}{\partial m_M}\right)^T$$

$$\nabla_m \Phi = \nabla_m (\mathbf{Gm} - \mathbf{d})^T (\mathbf{Gm} - \mathbf{d}) = 0$$

$$\nabla_m \Phi = \nabla_m (\mathbf{m}^T \mathbf{G}^T - \mathbf{d}^T)(\mathbf{Gm} - \mathbf{d}) = 0$$

$$\nabla_m \Phi = \nabla_m \mathbf{m}^T \mathbf{G}^T (\mathbf{Gm} - \mathbf{d}) = 0$$

Derivation (cont.)

$$\nabla_m \Phi = \nabla_m \mathbf{m}^T \mathbf{G}^T (\mathbf{G}\mathbf{m} - \mathbf{d}) = 0$$

$$\nabla_m \Phi = \mathbf{G}^T (\mathbf{G}\mathbf{m} - \mathbf{d}) = \mathbf{G}^T \mathbf{G}\mathbf{m} - \mathbf{G}^T \mathbf{d} = 0$$

$$\Rightarrow \qquad \mathbf{m} = (\mathbf{G}^T \mathbf{G})^{-1} \mathbf{G}^T \mathbf{d} = \mathbf{G}^\dagger \mathbf{d}$$

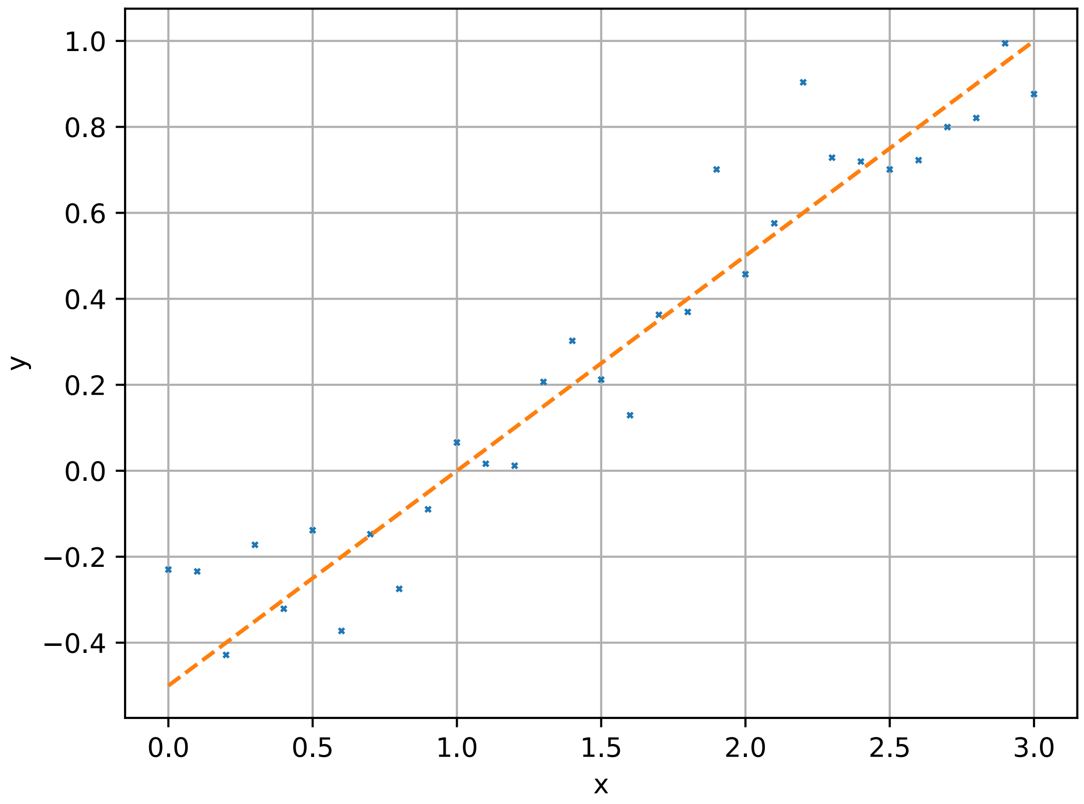
$$\text{mit} \quad \mathbf{G}^\dagger = (\mathbf{G}^T \mathbf{G})^{-1} \mathbf{G}^T$$

(generalized inverse or Pseudo-inverse, in Matlab/Julia `G\d`)

The solution $\mathbf{m}_{LS} = \mathbf{G}^\dagger \mathbf{d}$ is the least-squares solution

Application to the matrix problem

Linear regression



- x - measuring positions
- y - measurements (data)
- $\mathbf{y} = a \cdot \mathbf{x} + b + \mathbf{n}$
- model: slope & intersection
  $\mathbf{m} = (a, b)^T$
- How is $\mathbf{G}$ looking like?
  $\mathbf{Gm} = a \cdot \mathbf{x} + b$

Resolution analysis

Model resolution

$$\mathbf{d} = \mathbf{G}\mathbf{m}^{\text{true}} + \mathbf{n}$$

Matrix inversion with inverse operator $\mathbf{G}\dagger$:

$$\mathbf{m}^{\text{est}} = \mathbf{G}^{\dagger}\mathbf{d} = \mathbf{G}^{\dagger}\mathbf{G}\mathbf{m}^{\text{true}} + \mathbf{G}^{\dagger}\mathbf{n} = \mathbf{R}^{M}\mathbf{m}^{\text{true}} + \mathbf{G}^{\dagger}\mathbf{n}$$

with the model resolution matrix $\mathbf{R}^{M} = \mathbf{G}^{\dagger}\mathbf{G}$

$\Rightarrow$ How is the true model ($\mathbf{m}^{\text{true}}$) reflected in the estimated ($\mathbf{m}^{\text{est}}$)?

Data resolution

$$\mathbf{m}^{\text{est}} = \mathbf{G}^{\dagger}\mathbf{d}^{\text{obs}}$$

How are the data explained by the model?

$$\mathbf{d}^{\text{est}} = \mathbf{G}\mathbf{m}^{\text{est}} = \mathbf{G}\mathbf{G}^{\dagger}\mathbf{d}^{\text{obs}} = \mathbf{R}^{D}\mathbf{d}^{\text{obs}}$$

with the data resolution (information density) matrix:

$$\mathbf{R}^{D} = \mathbf{G}\mathbf{G}^{\dagger}$$

Diagonal of R^{D}: information content of individual data

Overdetermined problems

$$\mathbf{G}^{\dagger} = (\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T$$

$$\Rightarrow \mathbf{R}^M = (\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T\mathbf{G} = \mathbf{I}$$

perfect model resolution

$$\mathbf{G}^{\dagger} = (\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T \quad \Rightarrow \quad \mathbf{R}^D = \mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T$$

Wrap-up overdetermined problems ($N > M$)

- objective function Φ as squared data misfit
- weighting of individual data (unitless, more flexible & objective)
- broad minimum of the objective function
- grid search to plot $\phi \Rightarrow$ only nice for M=2
- least squares method yields
- resolution matrices for model (perfect) and data (distributed)

Appendix

The generalized inverse

The matrix

$$\mathbf{G}^{\dagger} = (\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T$$

is called pseudo-inverse (Moore-Penrose inverse)

The solution $\mathbf{m}_{LS} = \mathbf{G}^{\dagger}\mathbf{d}$ is the least-squares solution

Error weighting

Unweighted residual norm (root-mean square RMS)

$$\|\mathbf{d} - \mathbf{f}(\mathbf{m})\| = \sqrt{1/N \sum (d_i - f_i(\mathbf{m}))^2}$$

Weighting by individual error ϵ_i (chi-square value):

$$\chi^2 = \frac{1}{N} \sum \left(\frac{d_i - f_i(\mathbf{m})}{\epsilon_i} \right)^2 \to \min$$

In case of exact error estimates: $\chi^2 = 1$

Error weighting

replace d_i by $\hat{d}_i = d_i/\epsilon_i$ leads to

$$\mathbf{m} = (\hat{\mathbf{G}}^T\hat{\mathbf{G}})^{-1}\hat{\mathbf{G}}^T\hat{\mathbf{d}}$$

with $\hat{\mathbf{G}} = \mathrm{diag}(1/\epsilon_i) \cdot \mathbf{G}$

Derivation (1)

$$\Phi = \|\mathbf{d} - \mathbf{Gm}\|_2^2 = (\mathbf{d} - \mathbf{Gm})^T(\mathbf{d} - \mathbf{Gm})$$

$$\Phi = (\mathbf{Gm} - \mathbf{d})^T(\mathbf{Gm} - \mathbf{d})$$

$$\frac{\partial \Phi}{\partial m} = \frac{\partial}{\partial m}(\mathbf{Gm} - \mathbf{d})^T(\mathbf{Gm} - \mathbf{d}) + (\mathbf{Gm} - \mathbf{d})^T \frac{\partial}{\partial m}(\mathbf{Gm} - \mathbf{d}) =$$

$$\mathbf{G}^T\mathbf{Gm} - \mathbf{G}^T\mathbf{d} + \mathbf{G}^T\mathbf{Gm} - \mathbf{G}^T\mathbf{d} = 0$$

$$\mathbf{G}^T\mathbf{Gm} = \mathbf{G}^T\mathbf{d} \quad \Rightarrow \quad \mathbf{m} = \mathbf{G}^\dagger\mathbf{d} \quad \mathrm{mit} \quad \mathbf{G}^\dagger = (\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T$$

Derivation (2)

$$\Phi = (\mathbf{d} - \mathbf{Gm})^T(\mathbf{d} - \mathbf{Gm}) = \sum_i \Bigg[(d_i - \sum_j G_{ij} m_j)(d_i - \sum_k G_{ij} m$$

$$\Phi = \sum_i \Bigg[d_i d_i - d_i \sum_k G_{ik} m_k - d_i \sum_j G_{ij} m_j + \sum_j G_{ij} m_j \sum_k G_{ik} m$$

$$\Phi = \sum_i d_i d_i - 2 \sum_j m_j \sum d_i Gij + \sum_i \sum_j \sum_k m_j G_{ij} G_{ik} m_j m_k$$

$$\Phi = \sum_i d_i d_i - 2\sum_j m_j \sum_i d_i Gij + \sum_j \sum_k m_j m_k \sum_i G_{ij} G_{ik}$$

$$\partial\Phi = \partial m_q = \sum_i \sum_k (\delta_{iq} m_k + m_j \delta_{ik}) \sum G_{ij} G_{ik} - 2\sum_j \delta_{iq} \sum G_{ij} d$$

$$0 = 2\sum_k \sum_i G_{iq} G_{ik} - 2\sum_i G_{iq} d_i = \mathbf{2G}^T\mathbf{G} - \mathbf{2G}^T\mathbf{d}$$

Derivation by change $t\delta\mathbf{m}$

$$\Phi(t) = (\mathbf{d} - \mathbf{G}(\mathbf{m} + t\delta\mathbf{m}))^T(\mathbf{d} - \mathbf{G}(\mathbf{m} + t\delta\mathbf{m}))$$

$$\Phi(t) = (\mathbf{m} + t\delta\mathbf{m})^T\mathbf{G}^T\mathbf{G}(\mathbf{m} + t\delta\mathbf{m}) - 2(\mathbf{m} + t\delta\mathbf{m})\mathbf{G}^T\mathbf{d} + \mathbf{d}^T\mathbf{d}$$

$$\Phi(t) = t^2(\delta\mathbf{m}\mathbf{G}^T\mathbf{G}\delta\mathbf{m}) + 2t(\delta\mathbf{m}\mathbf{G}^T\mathbf{G}\mathbf{m} - \delta\mathbf{m}^T\mathbf{G}^T\mathbf{d}) + (\mathbf{m}^T\mathbf{G}^T\mathbf{G}$$

$\Phi(t)$ has a minimum at $t = 0$, therefore $\partial\Phi/\partial t$ must be 0

$$\partial\Phi(t=0)/\partial t = 2(\delta\mathbf{m}^T\mathbf{G}^T\mathbf{G}\mathbf{m} - \delta\mathbf{m}^T\mathbf{G}\mathbf{d}) = 2\delta\mathbf{m}^T(\mathbf{G}^T\mathbf{G}\mathbf{m} - \mathbf{G}^T$$

As this holds for every $\delta\mathbf{m}$, we obtain $\mathbf{G}^T\mathbf{G}\mathbf{m} = \mathbf{G}^T\mathbf{d}$