Lecture 12

Equality and Inequality Constraints

Syllabus

Lecture 01 Describing Inverse Problems Probability and Measurement Error, Part 1 Lecture 02 Probability and Measurement Error, Part 2 Lecture 03 Lecture 04 The L₂ Norm and Simple Least Squares A Priori Information and Weighted Least Squared Lecture 05 **Resolution and Generalized Inverses** Lecture 06 Lecture 07 Backus-Gilbert Inverse and the Trade Off of Resolution and Variance Lecture 08 The Principle of Maximum Likelihood Lecture 09 **Inexact Theories** Lecture 10 Nonuniqueness and Localized Averages Vector Spaces and Singular Value Decomposition Lecture 11 Lecture 12 **Equality and Inequality Constraints** Lecture 13 L_1 , L_∞ Norm Problems and Linear Programming Lecture 14 Nonlinear Problems: Grid and Monte Carlo Searches Nonlinear Problems: Newton's Method Lecture 15 Lecture 16 Nonlinear Problems: Simulated Annealing and Bootstrap Confidence Intervals Lecture 17 **Factor Analysis** Varimax Factors, Empirical Orthogonal Functions Lecture 18 Lecture 19 Backus-Gilbert Theory for Continuous Problems; Radon's Problem Lecture 20 Linear Operators and Their Adjoints Lecture 21 Fréchet Derivatives Lecture 22 Exemplary Inverse Problems, incl. Filter Design Lecture 23 Exemplary Inverse Problems, incl. Earthquake Location Lecture 24 Exemplary Inverse Problems, incl. Vibrational Problems

Purpose of the Lecture

Review the Natural Solution and SVD

Apply SVD to other types of prior information and to equality constraints

Introduce Inequality Constraints and the Notion of Feasibility

Develop Solution Methods

Solve Exemplary Problems

Part 1

Review the Natural Solution and SVD

subspaces

model parameters \mathbf{m}_{p} can affect data \mathbf{m}_{0} cannot affect data

data \mathbf{d}_{p} can be fit by model \mathbf{d}_{0} cannot be fit by any model

natural solution

determine \mathbf{m}_{p} by solving \mathbf{d}_{p} - $\mathbf{G}\mathbf{m}_{p}$ =0

set $\mathbf{m}_0 = \mathbf{0}$

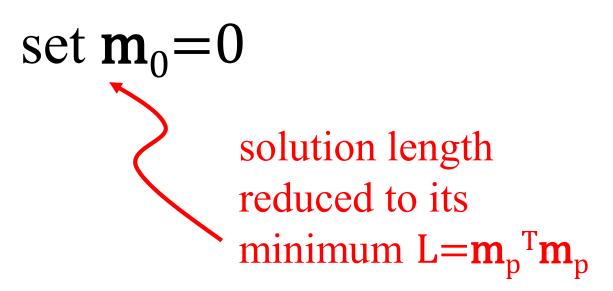
natural solution

determine \mathbf{m}_{p} by solving \mathbf{d}_{p} - $\mathbf{G}\mathbf{m}_{p}$ =0 set \mathbf{m}_{0} =0

error reduced to its minimum $E = \mathbf{e}_0^T \mathbf{e}_0$

natural solution

determine \mathbf{m}_{p} by solving \mathbf{d}_{p} - $\mathbf{G}\mathbf{m}_{p}$ =0



Singular Value Decomposition (SVD)

 $\mathbf{G} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\mathrm{T}}$

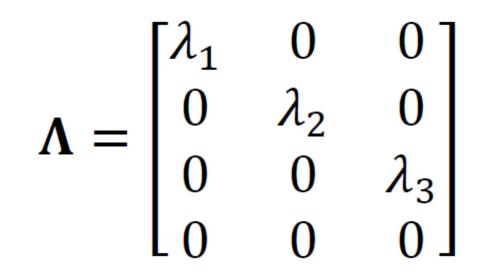
$N \times N$ matrix of eigenvectors $\mathbf{U} = \begin{bmatrix} \mathbf{u}^{(1)} & \mathbf{u}^{(2)} & \mathbf{u}^{(3)} & \cdots & \mathbf{u}^{N} \end{bmatrix}$

$M \times M \text{ matrix of eigenvectors}$ $\mathbf{V} = \begin{bmatrix} \mathbf{v}^{(1)} & \mathbf{v}^{(2)} & \mathbf{v}^{(3)} & \dots & \mathbf{v}^M \end{bmatrix}$ $\Lambda \text{ is an } N \times M \text{ diagonal matrix}$

singular value decomposition

 $\mathbf{G} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\mathrm{T}}$

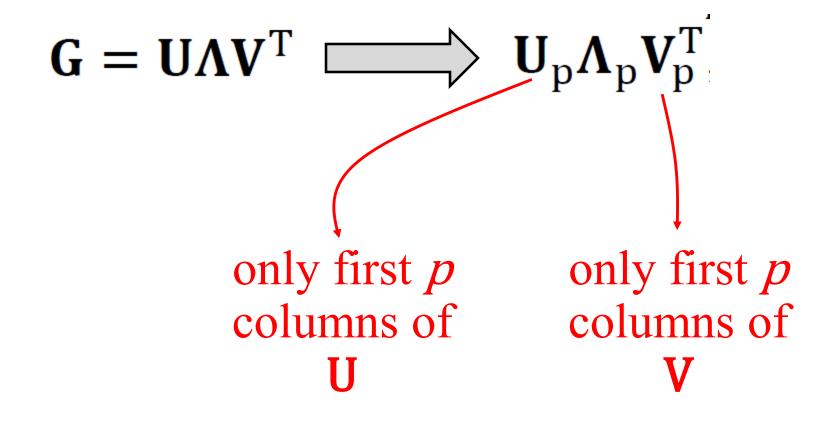
$\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{I}$ and $\mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}$



suppose only $p \lambda$'s are non-zero

$\boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda}_{\mathrm{p}} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix}$

suppose only $p \lambda$'s are non-zero



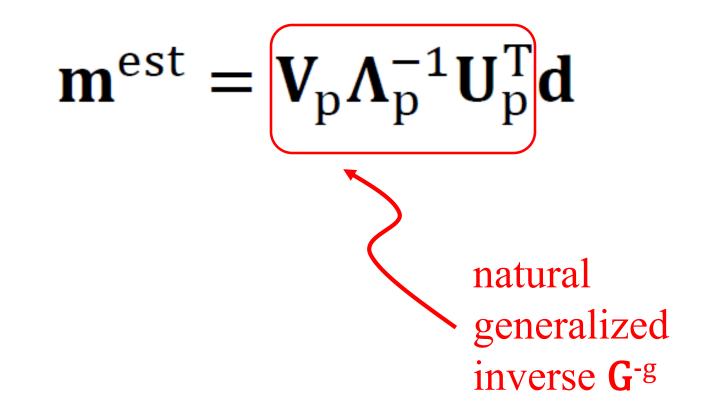
$\mathbf{U}_{p}^{T}\mathbf{U}_{p}=\mathbf{I} \text{ and } \mathbf{V}_{p}^{T}\mathbf{V}_{p}=\mathbf{I}$ since vectors mutually pependicular and of unit length

$\mathbf{U}_{p}\mathbf{U}_{p}^{T} \neq \mathbf{I}$ and $\mathbf{V}_{p}\mathbf{V}_{p}^{T} \neq \mathbf{I}$ since vectors do not span entire space

The Natural Solution

$\mathbf{m}^{\text{est}} = \mathbf{V}_{\text{p}} \mathbf{\Lambda}_{\text{p}}^{-1} \mathbf{U}_{\text{p}}^{\text{T}} \mathbf{d}$

The Natural Solution



resolution and covariance

$$\mathbf{R} = \mathbf{G}^{-g}\mathbf{G} = \{\mathbf{V}_{p}\boldsymbol{\Lambda}_{p}^{-1}\mathbf{U}_{p}^{T}\}\{\mathbf{U}_{p}\boldsymbol{\Lambda}_{p}\mathbf{V}_{p}^{T}\} = \mathbf{V}_{p}\mathbf{V}_{p}^{T}$$
$$\mathbf{N} = \mathbf{G}\mathbf{G}^{-g} = \{\mathbf{U}_{p}\boldsymbol{\Lambda}_{p}\mathbf{V}_{p}^{T}\}\{\mathbf{V}_{p}\boldsymbol{\Lambda}_{p}^{-1}\mathbf{U}_{p}^{T}\} = \mathbf{U}_{p}\mathbf{U}_{p}^{T}$$

$$= \sigma_d^2 \{ \mathbf{V}_p \mathbf{\Lambda}_p^{-1} \mathbf{U}_p^T \} \{ \mathbf{V}_p \mathbf{\Lambda}_p^{-1} \mathbf{U}_p^T \}^T = \sigma_d^2 \mathbf{V}_p \mathbf{\Lambda}_p^{-2} \mathbf{V}_p^T$$

Part 2

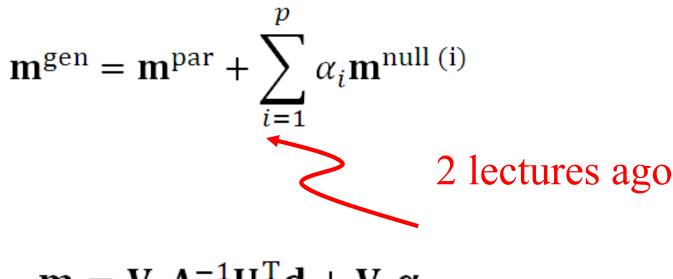
Application of SVD to other types of prior information and to equality constraints

general solution to linear inverse problem

$$\mathbf{m}^{\text{gen}} = \mathbf{m}^{\text{par}} + \sum_{i=1}^{p} \alpha_i \mathbf{m}^{\text{null (i)}}$$

$$\mathbf{m} = \mathbf{V}_{\mathrm{p}} \mathbf{\Lambda}_{\mathrm{p}}^{-1} \mathbf{U}_{\mathrm{p}}^{\mathrm{T}} \mathbf{d} + \mathbf{V}_{\mathrm{0}} \boldsymbol{\alpha}$$

general minimum-error solution



 $\mathbf{m} = \mathbf{V}_{\mathrm{p}} \mathbf{\Lambda}_{\mathrm{p}}^{-1} \mathbf{U}_{\mathrm{p}}^{\mathrm{T}} \mathbf{d} + \mathbf{V}_{\mathrm{0}} \boldsymbol{\alpha}$

general minimum-error solution

$$\mathbf{m}^{\text{gen}} = \mathbf{m}^{\text{par}} + \sum_{i=1}^{p} \alpha_i \mathbf{m}^{\text{null (i)}}$$

$$\mathbf{m} = \mathbf{V}_{p} \mathbf{\Lambda}_{p}^{-1} \mathbf{U}_{p}^{T} \mathbf{d} + \mathbf{V}_{0} \boldsymbol{\alpha}$$
plus amount
plus amount
 $\boldsymbol{\alpha}$ of null
vectors

you can adjust α to match whatever a priori information you want

$$\mathbf{m} = \mathbf{V}_{\mathrm{p}} \mathbf{\Lambda}_{\mathrm{p}}^{-1} \mathbf{U}_{\mathrm{p}}^{\mathrm{T}} \mathbf{d} + \mathbf{V}_{\mathrm{0}} \boldsymbol{\alpha}$$

for example $\mathbf{m} = < \mathbf{m} >$ by minimizing $L = ||\mathbf{m} - < \mathbf{m} > ||_2$ w.r.t. α

you can adjust α to match whatever a priori information you want

$$\mathbf{m} = \mathbf{V}_{\mathrm{p}} \mathbf{\Lambda}_{\mathrm{p}}^{-1} \mathbf{U}_{\mathrm{p}}^{\mathrm{T}} \mathbf{d} + \mathbf{V}_{\mathrm{0}} \mathbf{\alpha}$$

for example m = < m >by minimizing $L = ||m - < m > ||_2$ w.r.t. α

get $\alpha = V_0^T < m >$ so $m = V_p \Lambda_p^{-1} U_p^T d + V_0^T V_0^T < m >$

equality constraints

minimize *E* with constraint **Hm=h**

Step 1 find part of solution constrained by Hm=h

SVD of H (not G)

 $H = V_{p} \Lambda_{p} U_{p}^{T}$ SO $m = V_{p} \Lambda_{p}^{-1} U_{p}^{T} h + V_{0} \alpha$

Step 2 convert Gm=dinto and equation for α

$\mathbf{GV_p \Lambda_p^{-1} U_p^T h + GV_0 \alpha = d}$ and rearrange

 $[\mathbf{G}\mathbf{V}_0]\boldsymbol{\alpha} = [\mathbf{d} - \mathbf{G}\mathbf{V}_{\mathbf{p}}\boldsymbol{\Lambda}_{\mathbf{p}}^{-1}\mathbf{U}_{\mathbf{p}}^{\mathsf{T}}\mathbf{h}]$ $\mathbf{G}'\boldsymbol{\alpha} = \mathbf{d}'$

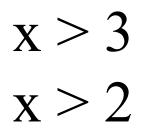
Step 3 solve $G'\alpha = d'$ for α using least squares

Step 4 reconstruct **m** from α $\mathbf{m} = \mathbf{V}_{\mathbf{p}} \Lambda_{\mathbf{p}}^{-1} \mathbf{U}_{\mathbf{p}}^{\mathrm{T}} \mathbf{h} + \mathbf{V}_{0} \alpha$

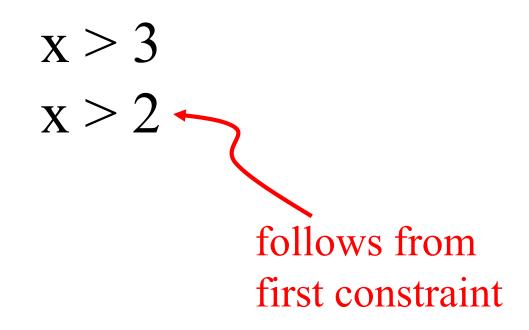
Part 3

Inequality Constraints and the Notion of Feasibility

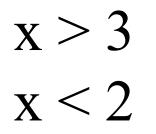
Not all inequality constraints provide new information



Not all inequality constraints provide new information



Some inequality constraints are incompatible



Some inequality constraints are incompatible

x > 3x < 2 both bigger than 3 and smaller than 2

every row of the inequality constraint

$Hm \ge h$

divides the space of **m** into two parts

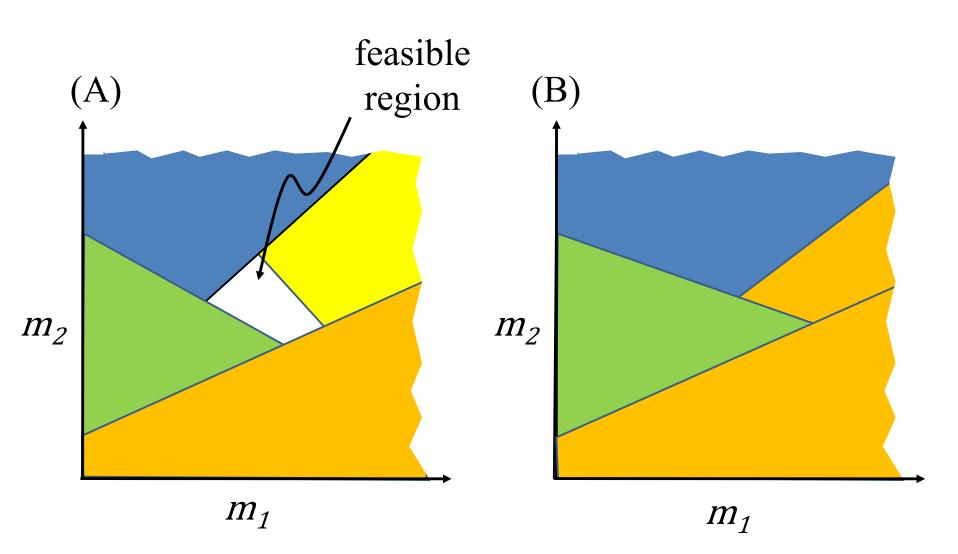
one where a solution is *feasible* one where it is *infeasible*

the boundary is a planar surface

when all the constraints are considered together they either create a feasible volume or they don't

if they do, then the solution must be in that volume

if they don't, then no solution exists



now consider the problem of minimizing the error Esubject to inequality constraints $\mathbf{Hm} \ge \mathbf{h}$

if the global minimum is inside the feasible region

then

the inequality constraints have no effect on the solution

but if the global minimum is outside the feasible region

then

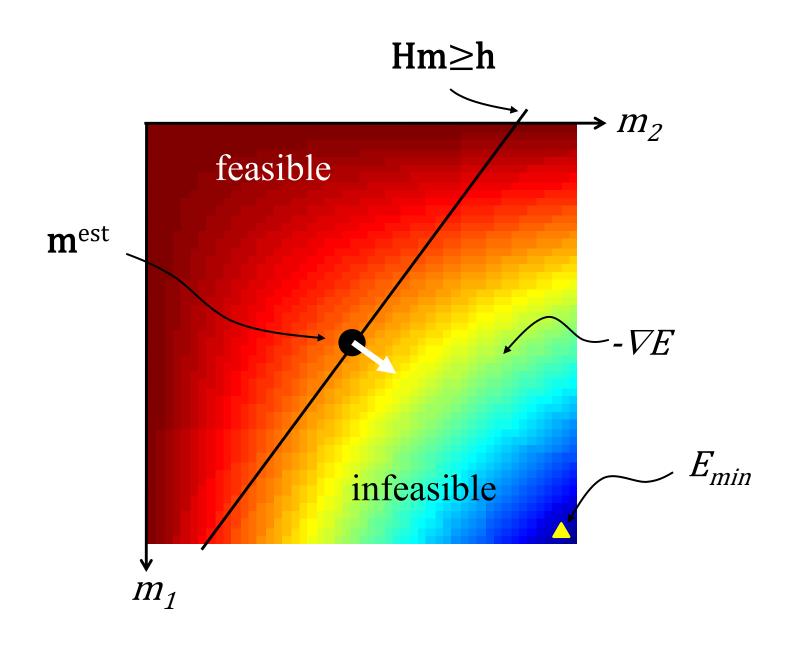
the solution is on the surface of the feasible volume

but if the global minimum is outside the feasible region

then

the solution is on the surface of the feasible volume

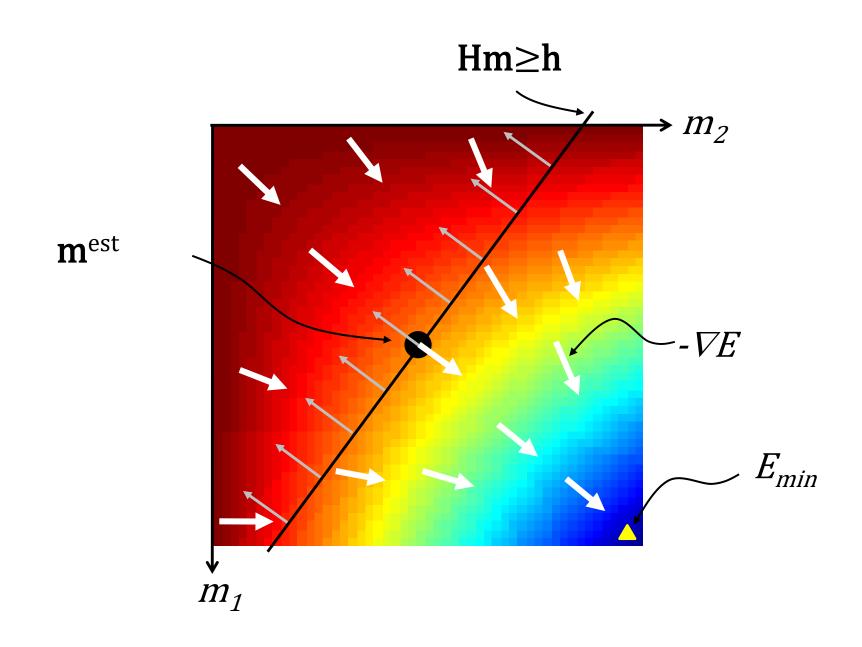
the point on the surface where E is the smallest



furthermore

the feasible-pointing normal to the surface must be parallel to ∇E

else you could slide the point along the surface to reduce the error *E*

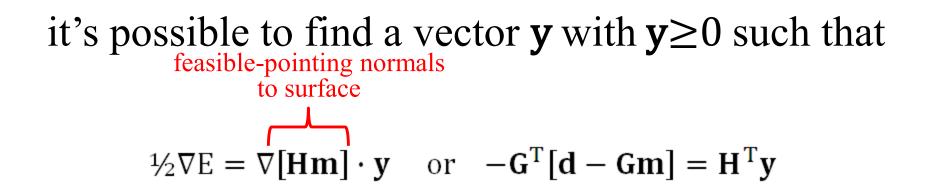


Kuhn – Tucker theorem

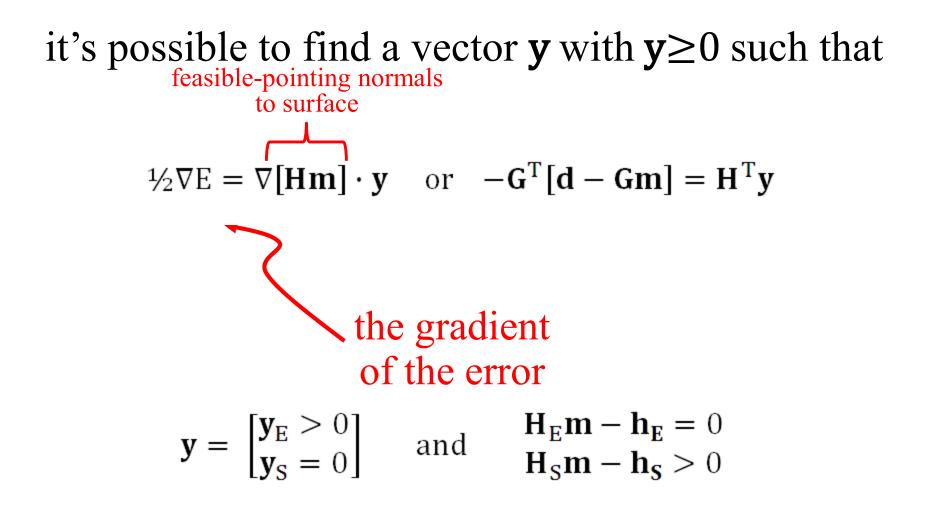
it's possible to find a vector **y** with $y_i \ge 0$ such that

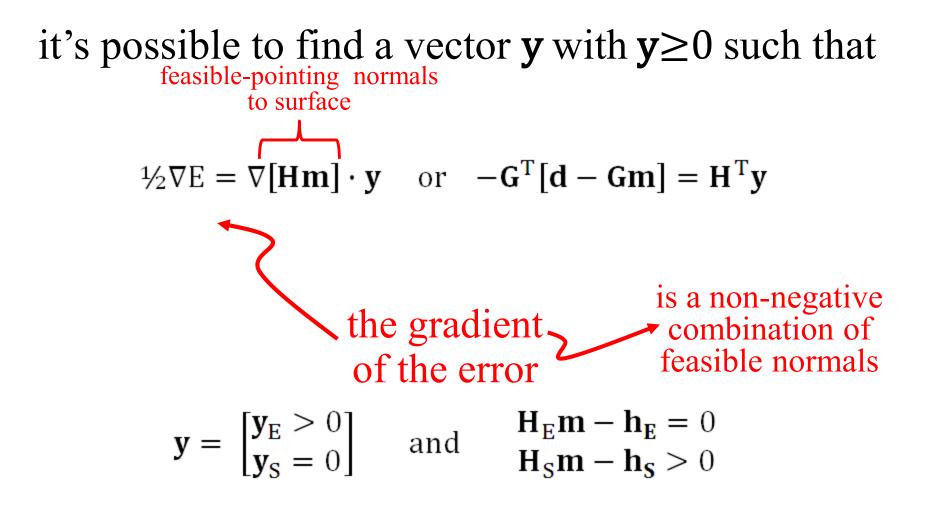
 $\frac{1}{2}\nabla \mathbf{E} = \nabla [\mathbf{H}\mathbf{m}] \cdot \mathbf{y}$ or $-\mathbf{G}^{\mathrm{T}}[\mathbf{d} - \mathbf{G}\mathbf{m}] = \mathbf{H}^{\mathrm{T}}\mathbf{y}$

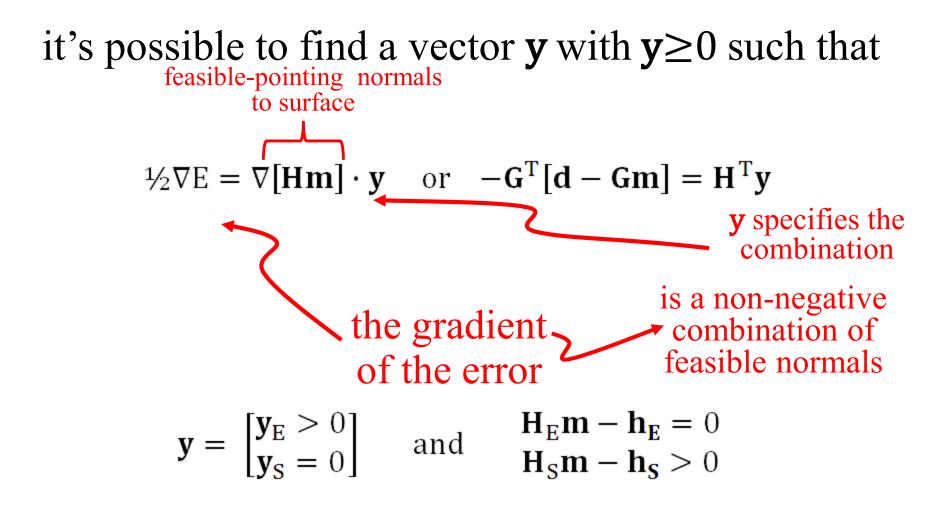
$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_{\mathrm{E}} > 0 \\ \mathbf{y}_{\mathrm{S}} = 0 \end{bmatrix} \quad \text{and} \quad \begin{array}{l} \mathbf{H}_{\mathrm{E}}\mathbf{m} - \mathbf{h}_{\mathrm{E}} = 0 \\ \mathbf{H}_{\mathrm{S}}\mathbf{m} - \mathbf{h}_{\mathrm{S}} > 0 \end{array}$$



$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_{\mathrm{E}} > 0 \\ \mathbf{y}_{\mathrm{S}} = 0 \end{bmatrix} \quad \text{and} \quad \begin{array}{l} \mathbf{H}_{\mathrm{E}}\mathbf{m} - \mathbf{h}_{\mathrm{E}} = 0 \\ \mathbf{H}_{\mathrm{S}}\mathbf{m} - \mathbf{h}_{\mathrm{S}} > 0 \end{array}$$







$$\frac{1}{2}\nabla \mathbf{E} = \nabla [\mathbf{H}\mathbf{m}] \cdot \mathbf{y} \quad \text{or} \quad \mathbf{G}^{\mathrm{T}}[\mathbf{d} - \mathbf{G}\mathbf{m}] = -\mathbf{H}^{\mathrm{T}}\mathbf{y}$$

$$\int \mathbf{for \ linear \ case \ with \ \mathbf{Gm} = \mathbf{d}}$$

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_{\mathrm{E}} > 0 \\ \mathbf{y}_{\mathrm{S}} = 0 \end{bmatrix} \quad \text{and} \quad \begin{array}{l} \mathbf{H}_{\mathrm{E}}\mathbf{m} - \mathbf{h}_{\mathrm{E}} = 0 \\ \mathbf{H}_{\mathrm{S}}\mathbf{m} - \mathbf{h}_{\mathrm{S}} > 0 \end{array}$$

 $\frac{1}{2}\nabla E = \nabla [Hm] \cdot y$ or $G^{T}[d - Gm] = -H^{T}y$

some coefficients
$$y_i$$

are positive
 $\mathbf{y} = \begin{bmatrix} \mathbf{y}_E > 0 \\ \mathbf{y}_S = 0 \end{bmatrix}$ and $\mathbf{H}_E \mathbf{m} - \mathbf{h}_E = 0$
 $\mathbf{H}_S \mathbf{m} - \mathbf{h}_S > 0$

$$\frac{1}{2}\nabla \mathbf{E} = \nabla [\mathbf{H}\mathbf{m}] \cdot \mathbf{y}$$
 or $\mathbf{G}^{\mathrm{T}}[\mathbf{d} - \mathbf{G}\mathbf{m}] = -\mathbf{H}^{\mathrm{T}}\mathbf{y}$

some coefficients
$$y_i$$
 the solution is on the
are positive y_i corresponding constraint
surface
 $\mathbf{y} = \begin{bmatrix} \mathbf{y}_E > 0 \\ \mathbf{y}_S = 0 \end{bmatrix}$ and $\begin{aligned} \mathbf{H}_E \mathbf{m} - \mathbf{h}_E = 0 \\ \mathbf{H}_S \mathbf{m} - \mathbf{h}_S > 0 \end{aligned}$

 $\frac{1}{2}\nabla E = \nabla [Hm] \cdot y$ or $G^{T}[d - Gm] = -H^{T}y$

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_{\mathrm{E}} > 0 \\ \mathbf{y}_{\mathrm{S}} = 0 \end{bmatrix} \text{ and } \begin{array}{l} \mathbf{H}_{\mathrm{E}}\mathbf{m} - \mathbf{h}_{\mathrm{E}} = 0 \\ \mathbf{H}_{\mathrm{S}}\mathbf{m} - \mathbf{h}_{\mathrm{S}} > 0 \end{array}$$
some coefficients \mathbf{y}_{i}
are zero

 $\frac{1}{2}\nabla E = \nabla [Hm] \cdot y$ or $G^{T}[d - Gm] = -H^{T}y$

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_{\mathrm{E}} > 0 \\ \mathbf{y}_{\mathrm{S}} = 0 \end{bmatrix} \text{ and } \begin{array}{c} \mathbf{H}_{\mathrm{E}}\mathbf{m} - \mathbf{h}_{\mathrm{E}} = 0 \\ \mathbf{H}_{\mathrm{S}}\mathbf{m} - \mathbf{h}_{\mathrm{S}} > 0 \\ \text{some coefficients } y_{i} \\ \text{are zero} \end{array}$$
 the solution is on the feasible side of the corresponding constraint surface

Part 4

Solution Methods

simplest case

minimize E subject to $m_i > 0$ (H=I and h=0)

iterative algorithm with two nested loops

Start with an initial guess for **m**

The particular initial guess m=0 is feasible

It has all its elements in $\mathbf{m}_{\rm E}$ constraints satisfied in the equality sense

Any model parameter m_i in \mathbf{m}_E that has associated with it a negative gradient $[\nabla E]_i$ can be changed both to decrease the error and to remain feasible.

If there is no such model parameter in $\mathbf{m}_{\rm E}$, the Kuhn – Tucker theorem indicates that this \mathbf{m} is the solution to the problem.

If some model parameter m_i in \mathbf{m}_E has a corresponding negative gradient, then the solution can be changed to decrease the prediction error.

- To change the solution, we select the model parameter corresponding to the most negative gradient and move it to the set \mathbf{m}_{S} .
- All the model parameters in \mathbf{m}_{S} are now recomputed by solving the system $\mathbf{G}_{S}\mathbf{m'}_{S}=\mathbf{d}_{S}$ in the least squares sense. The subscript S on the matrix indicates that only the columns multiplying the model parameters in \mathbf{m}_{S} have been included in the calculation.
- All the $\mathbf{m}_{\rm E}$'s are still zero. If the new model parameters are all feasible, then we set $\mathbf{m} = \mathbf{m}'$ and return to Step 2.

- If some of the elements of $\mathbf{m'}_{S}$ are infeasible, however, we cannot use this vector as a new guess for the solution.
- So, we compute the change in the solution and add as much of this vector as possible to the solution \mathbf{m}_{S} without causing the solution to become infeasible.
- We therefore replace $\mathbf{m}_{\rm S}$ with the new guess $\mathbf{m}_{\rm S} + \alpha \, \delta \mathbf{m}$, where is the largest choice that can be made without some $\mathbf{m}_{\rm S}$ becoming infeasible. At least one of the $m_{\rm Si}$'s has its constraint satisfied in the equality sense and must be moved back to $\mathbf{m}_{\rm E}$. The process then returns to Step 3.

In MatLab

mest = lsqnonneg(G,dobs);



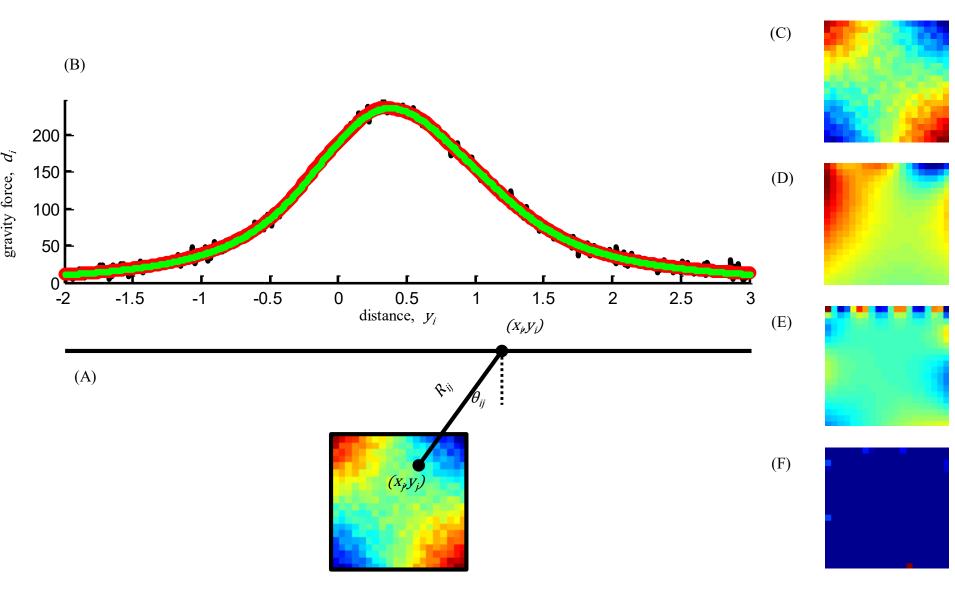
gravitational field depends upon density

via the inverse square law

example

gravitational force depends upon density observations model parameters

via the inverse square law theory



more complicated case

minimize $||\mathbf{m}||_2$ subject to $\mathbf{Hm} \ge \mathbf{h}$

this problem is solved by transformation to the previous problem

solve by non-negative least squares $\mathbf{G'm'} = \mathbf{d'} = \begin{bmatrix} \mathbf{H}^T \\ \mathbf{h}^T \end{bmatrix} \mathbf{m'} = \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}$

then compute m_i as

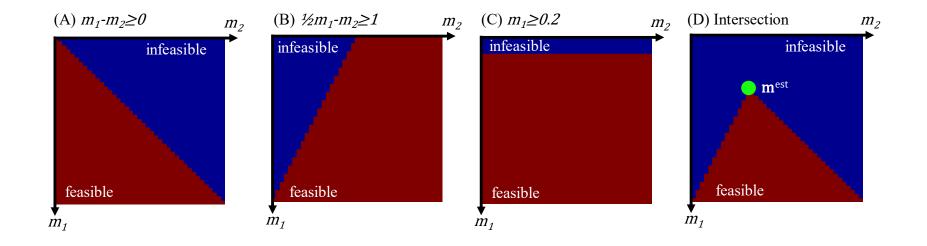
$$-e'_{i}/e'_{M+1}$$

with e'=d'-G'm'

In MatLab

$$Gp = [H, h]';$$

- dp = [zeros(1, length(H(1, :))), 1]';
- mp = lsqnonneg(Gp,dp);
- ep = dp Gp*mp;
- m = -ep(1:end-1)/ep(end);

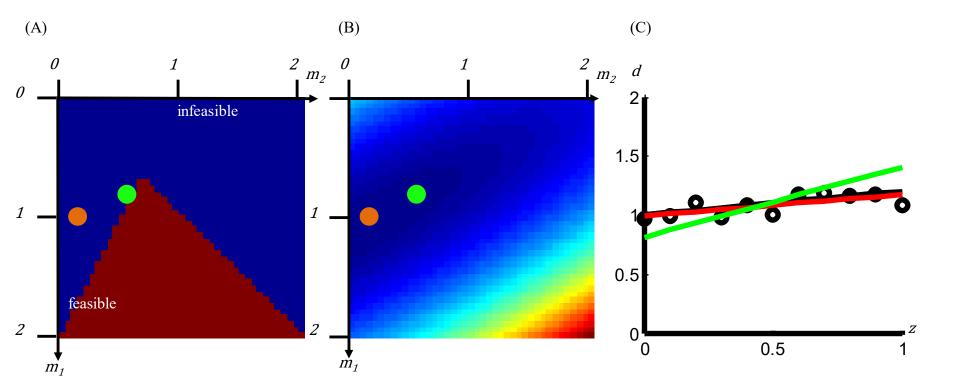


yet more complicated case

minimize $||\mathbf{d}-\mathbf{Gm}||_2$ subject to $\mathbf{Hm} \ge \mathbf{h}$

this problem is solved by transformation to the previous problem

minimize ||m'|| subject to H'm'≥h' where $\left\{-HV_{\mathbf{p}}\Lambda_{\mathbf{p}}^{-1}\right\}m' \geq \left\{h - HV_{\mathbf{p}}\Lambda_{\mathbf{p}}^{-1}U_{\mathbf{p}}^{\mathrm{T}}d\right\} \quad \mathrm{or} \quad H'm' \geq h'$ and $\mathbf{T}_{\mathrm{p}} \mathbf{m} = \mathbf{V}_{\mathrm{p}} \mathbf{\Lambda}_{\mathrm{p}}^{-1} |\mathbf{d}_{\mathrm{p}} - \mathbf{m}'| = |\mathbf{V}_{\mathrm{p}} \mathbf{\Lambda}_{\mathrm{p}}^{-1} |\mathbf{U}_{\mathrm{p}}^{\mathrm{T}} \mathbf{d} - \mathbf{m}'|$



In MatLab

```
[Up, Lp, Vp] = svd(G,0);
lambda = diag(Lp);
rlambda = 1./lambda;
Lpi = diag(rlambda);
```

```
% transformation 1
Hp = -H*Vp*Lpi;
hp = h + Hp*Up'*dobs;
```

```
% transformation 2
Gp = [Hp, hp]';
dp = [zeros(1,length(Hp(1,:))), 1]';
mpp = lsqnonneg(Gp,dp);
ep = dp - Gp*mpp;
mp = -ep(1:end-1)/ep(end);
```

```
% take mp back to m
mest = Vp*Lpi*(Up'*dobs-mp);
dpre = G*mest;
```