#### Part 2

#### Inverse Problems for Geophysicists: Introduction to Linear Inverse Problems and Regularization Methods

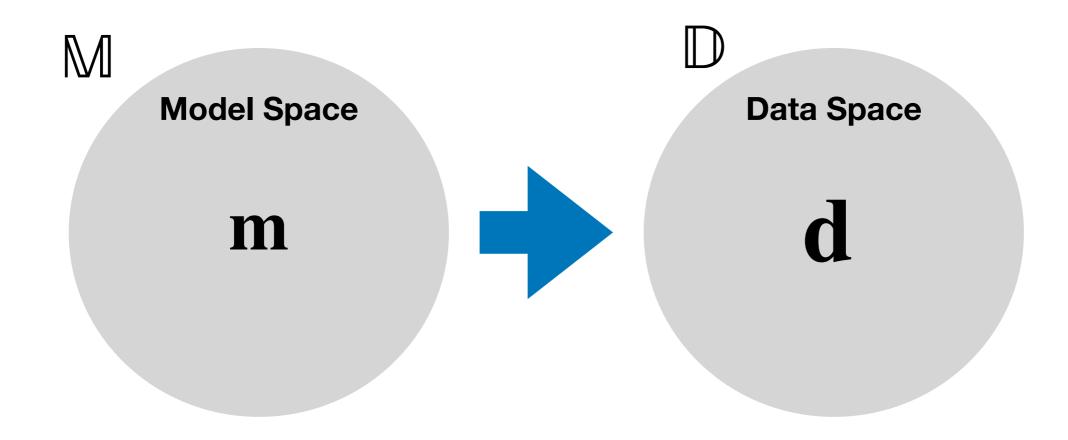
M D Sacchi UNLP Problemas Inversos

#### **Inverse Problems**

- An Inverse Problem is a mathematical problem where one attempts to estimate models that explain observations. We often name the observations d (data)
- Observations are generally measured on the surface of the earth and are discrete in time and space
- The subsurface is described by properties (density, velocity, reflectivity, resistivity, etc). These properties exist everywhere. We will refer to these properties as m(x,y,z) or m (model parameters)
- m(x,y,z) is the distribution of some property that can be discretized and represented via the vector m

#### Two spaces

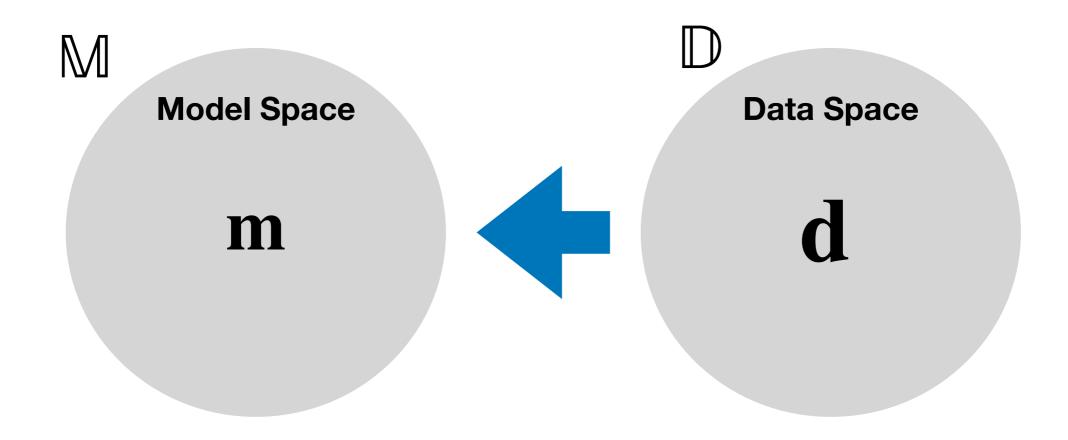
Forward Problem



$$F[\mathbf{m}] = \mathbf{d}$$

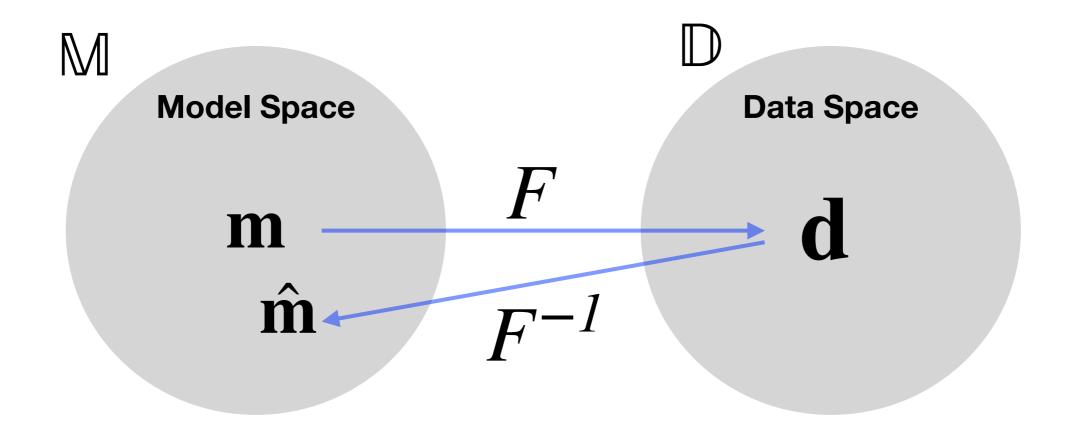
#### Two spaces

Inverse Problem



$$F^{-1}[\mathbf{d}] = \mathbf{m}$$

#### It is more complicated...



#### m: Solution

#### Geophysics and Inverse Problems

Data (What you can measure)	Model (What you would like to know)	Method
Gravity anomalies	Density	Potential Field Methods
Electrical potential	Resistivity	Potential Field Methods
Electrical and Magnetic Field	Electrical conductivity	EM/MT methods
Magnetic Fields	Susceptibility	Potential Field Methods
Seismic Waves	Velocities	Seismic Methods

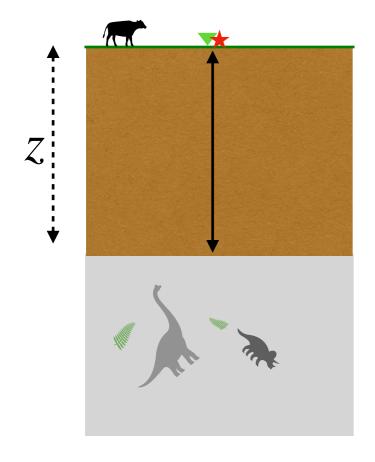
- Well-posed problem. A problem is said to be well-posed when
  - There is a solution
  - The solution is unique
  - The solution is stable
- If one of the above is not true, the problem is called an illposed problem
- Typical geophysical inverse problems are ill-posed problems (2 and 3 are not true)



Jacques Hadamard, 1865-1963

- There is a solution: YES
  - There is a solution otherwise we wouldn't be here
  - e.g. Rocks have density causing gravity anomalies

- The solution is unique: Generally NO
- For instance, Depth-Velocity ambiguity:  $t = \frac{2z}{v}$
- Assume two-way traveltime for a vertical incidence plane wave

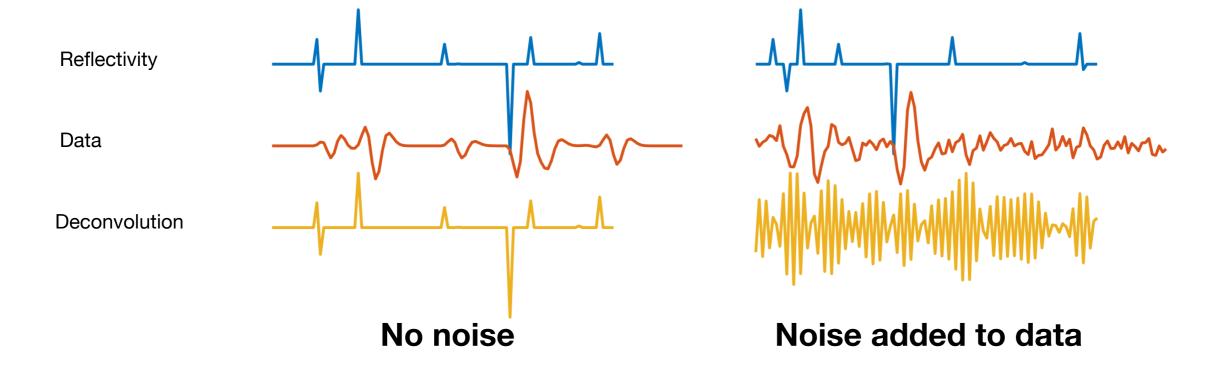


$$t = \frac{2 \times 1000m}{2000m/s} = \frac{2 \times 1500m}{3000m/s}$$

Sol 1	Sol 2
1000m	1500m
2000m/s	3000m/s

Clearly, there is an infinite number of solutions

- The solution is stable: Not true
  - A small perturbation in the data causes a large perturbation in the solution
  - e.g. Deconvolution



- The solution is stable: Not true
  - A small perturbation can cause a large perturbation in the solution
  - Assume perfect data and an invertible operator

$$d = F(m) \to \hat{m} = F^{-1}(d)$$

Assume perturbed data (inaccurate data)

$$\hat{m} + \delta m = F^{-1}(d+n)$$

- The solution is stable: Not true
  - Solution for perturbed data

$$\hat{m} + \delta m = F^{-1}(d+n)$$

The solution is not stable. The latter means

$$if |n| = small, |\delta m| = large$$

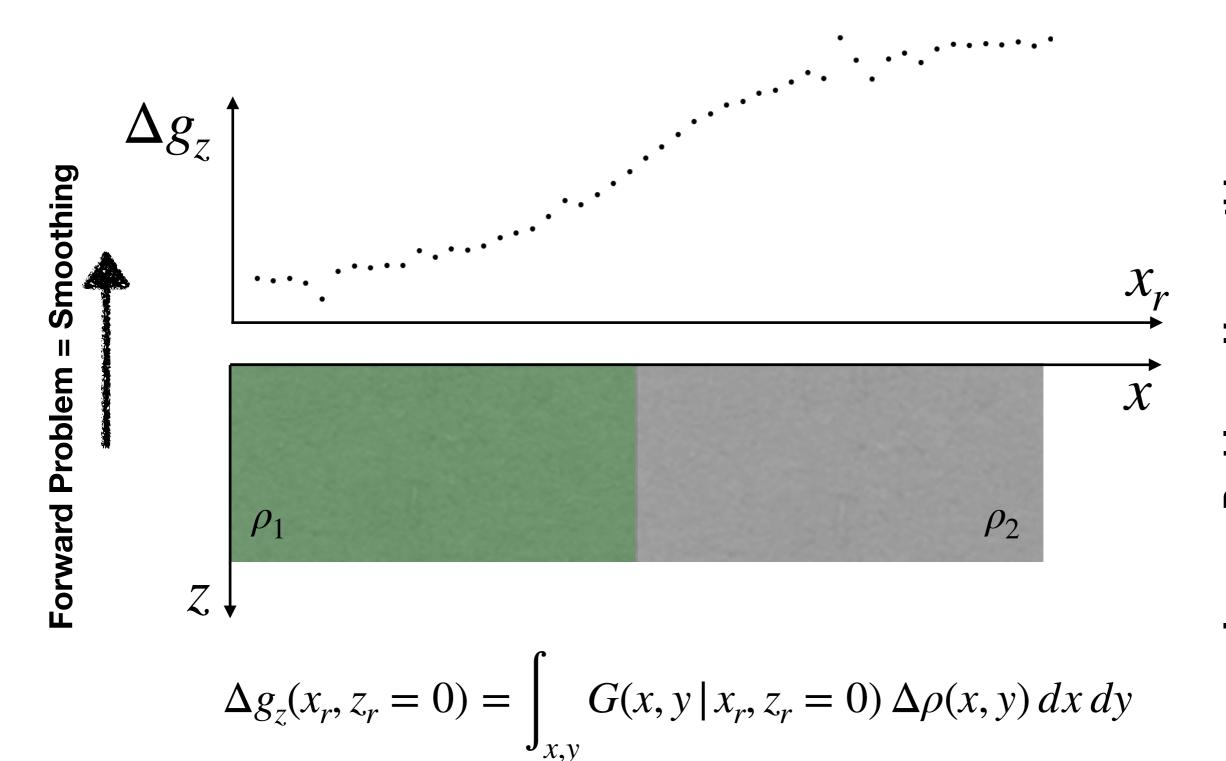
 This is the main problem we face in geophysical inversion and often in data processing. You can think that somewhere one is trying to divide by small numbers and hence, whatever you are doing to your data leads to "noise amplification".

# Why geophysical problems are ill-posed?

- Not enough data (insufficient spatial data or insufficient bandwidth)
- Presence of noise also leads to unstable solutions
- A central characteristic of the forward problem:
  - The Forward Problem smoothes the unknown subsurface properties. Seismic waves, gravity anomalies, electrical potential, etc are nice smooth functions of space and time. Subsurface properties, on the other hand, might or might not be smooth!
- The next slide illustrates the aforementioned concept

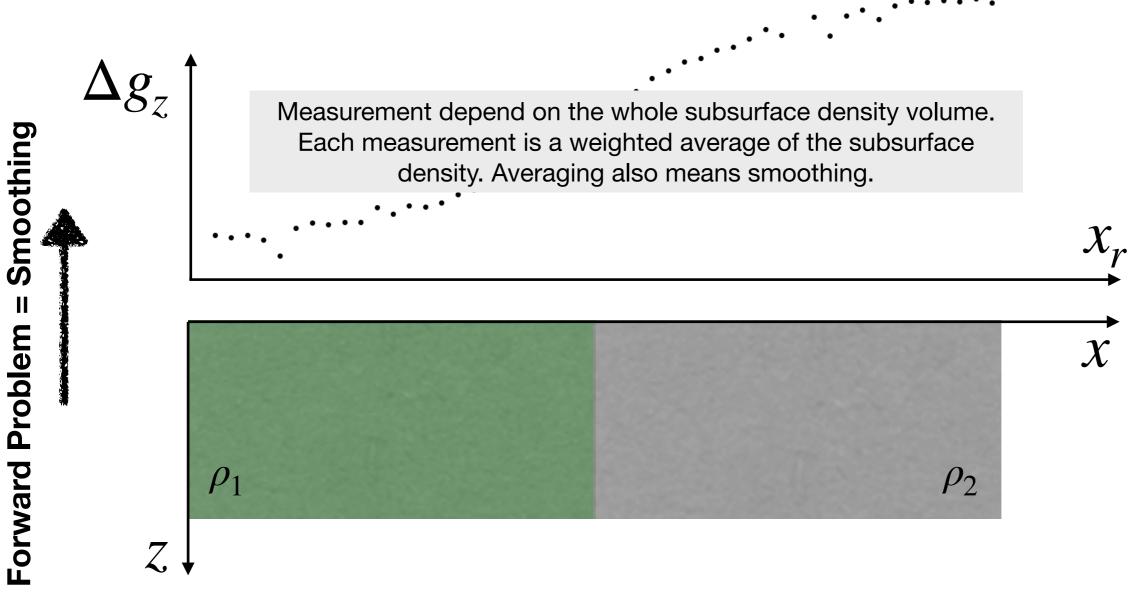
# Inverse Problem = Unsmoothing

#### Example: Inversion of gravity anomalies



# Inverse Problem = Unsmoothing

#### Example: Inversion of gravity anomalies



$$\Delta g_z(x_r, z_r = 0) = \int_{x,y} G(x, y | x_r, z_r = 0) \, \Delta \rho(x, y) \, dx \, dy$$

### Key points

- Previous example shows an interesting feature of the Forward Problem:
  - Observations (data) are a weighted average of density. The averaging kernel smoothes the density anomaly (The physics, in this case given by Newton's gravitational attraction, is the cause of this behaviour)
  - Inverse Problem: Recovering the density from the data entails the opposite of smoothing (un-smoothing); an unstable operation
  - Smoothing = is a low pass operation = Stable
  - Un-smoothing = is a high pass operation = Unstable
  - Solving an inverse problem in many cases entails controlling instability

### Key points

 Subsurface properties (such as density anomalies) are a function of space (that exists everywhere). The observed gravity anomalies are given by a finite number of observations

$$d(\mathbf{r}_j) = \int G(\mathbf{x} \mid \mathbf{r}_j) m(\mathbf{x}) d\mathbf{x} \qquad j = 1...N$$

 So inversion, theoretically, attempt to go from a finite number of observations to a function

$$\mathbf{d} \in \mathbb{R}^N, m(\mathbf{x}) \in \mathbb{R}^\infty$$

There is a natural underdeterminacy in an inverse problem

#### Linear inverse problems

- Many inverse problems in seismology entail solving integral equations. Others entail
  solving PDEs. We will start with simple problems that can be written as integral
  equations that after discretization lead to discrete system of equations.
  - Integral equations
  - Linear discrete system of equations
  - Regularization methods
  - Connection to exploration seismology:
    - Deconvolution
    - AVO inversion
    - Linearized seismic imaging (Forward and Adjoint Operators)
      - Migration & Least-Squares migration

#### Linear inverse problems

Fredholm integral equation of 1st kind

$$d(r_j) = \int_X G(r_j, x) m(x) dx \qquad j = 1...N$$

We can discretize the model

$$x_k = x_0 + (k-1)\Delta x$$
  $k = 1...M$ 

$$d(r_j) = \sum_{k=1}^{M} G(r_j, x_k) m(x_k) \Delta x$$
  $j = 1...N$ 

Which leads to a system of equations

$$\mathbf{d} = \mathbf{Lm}, \quad \mathbf{d} \in \mathbb{R}^N, \quad \mathbf{m} \in \mathbb{R}^M$$

#### Examples

$$d(r_j) = \int_X G(r_j, x) m(x) dx \qquad j = 1...N$$

$$s(t_i) = \int w(t_i - \tau) \, r(\tau) \, d\tau$$

Convolution

$$T(r_j) = \int_0^{r_j} s(l) \, dl$$

**Travel-time tomography** 

$$d(\omega, s_i, r_j) = \int_x \int_z B(\omega, x, y \mid s_i, r_j) m(x, z) dx dz$$
 Born imaging

#### TWO IMPORTANT MATRICES (OPERATORS)

Two special operations (or operators?)

Forward :  $\mathbf{d} = \mathbf{L}\mathbf{m}$ Transpose or adjoint :  $\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{d}$ 

- L is a linear operator (Forward modelling operator).
- Why are them special?
  - Iterative solvers for large inverse problems only need to evaluate  $\mathbf{L}[\ \cdot\ ]$  and  $\mathbf{L}^T[\ \cdot\ ]$  We pretend these are Matrices but in reality these are linear operators (codes)
  - I usually interpret operators as matrices. In reality, operators are codes that apply an operation *on the flight* (implicit form)
  - We will see these operators everywhere today

When L is a real matrix

$$\mathbf{L}' = \mathbf{L}^T$$

• When L is a complex matrix

$$\mathbf{L}' = \mathbf{L}^H$$

Two special operations (or operators)

Forward : 
$$\mathbf{d} = \mathbf{L}\mathbf{m}$$
 (1)  
Transpose or adjoint :  $\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{d}$  (2)

• Replace (1) into (2)

$$\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{L} \mathbf{m}$$

- Questions:
  - Is the adjoint model a good representation of the true model?
  - Can I remove the distortion?

**See:** Migration vs. Least-squares Migration: Least-squares migration of incomplete reflection data. Nemeth et al. GEOPHYSICS (1999), 64(1)

Two special operations (or operators)

Forward : 
$$d = Lm$$
 (1)

Conjugate transpose or adjoint :  $\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{d}$  (2)

(2) into (1) 
$$\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{L} \mathbf{m}$$

m is a distorted version of m

Forward : d = Lm

Conjugate transpose or adjoint :  $\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{d}$ 

$$\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{L} \mathbf{m}$$

$$\tilde{\mathbf{m}} \approx \mathbf{m} \ if \ \mathbf{L}^T \mathbf{L} \approx \mathbf{I}$$

The adjoint, in some instances, is good enough to estimate m. An example is RTM which can be considered the adjoint of Born modelling

Forward : d = Lm

Conjugate transpose or adjoint :  $\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{d}$ 

$$\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{L} \mathbf{m}$$

$$\mathbf{L}^T \mathbf{L} \approx \operatorname{diag}(\mathbf{L}^T \mathbf{L}) = \mathbf{D}, \qquad \hat{\mathbf{m}} = \mathbf{D}^{-1} \tilde{\mathbf{m}}$$

This is an inexpensive way of partially correcting the adjoint to make it look closer to the desired solution

**Example: Averaging** 

$$d = \begin{bmatrix} 1/3 & 1/3 & 1/3 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} = \mathbf{Lm} \quad \text{Averaging operator}$$

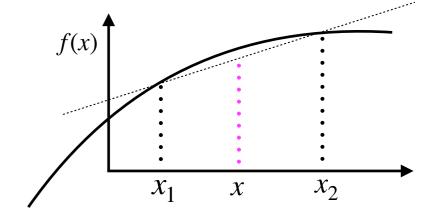
$$ilde{\mathbf{m}}=egin{bmatrix} \tilde{m}_1 \\ \tilde{m}_2 \\ \tilde{m}_3 \end{bmatrix} = egin{bmatrix} d/3 \\ d/3 \end{bmatrix} = \mathbf{L}^T d$$
 Adjoint of the averaging operator

Question: Can you recover m from  $\tilde{\mathbf{m}} = \mathbf{L}^T \mathbf{L} \mathbf{m}$ ?

**Example: Linear Interpolator (this is used a lot!!)** 

$$f(x) = af(x_1) + bf(x_2)$$

**Linear Interpolator (LI)** 



$$f(x) = \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \end{bmatrix}$$

$$\begin{bmatrix} \tilde{f}(x_1) \\ \tilde{f}(x_2) \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} f(x)$$

$$\tilde{f}(x_1) = af(x)$$

$$\tilde{f}(x_2) = bf(x)$$

**Adjoint of LI** 

Forward: 2 samples make 1, Adjoint: 1 sample makes 2

## DISCRETE LINEAR INVERSE PROBLEMS IN EXPLICIT FORM (WITH MATRICES)

#### Discrete Linear Inverse Problems

$$\mathbf{d} = \mathbf{Lm}, \quad \mathbf{L} \in \mathscr{R}^{N \times M}$$

- A) N>M: More observations than data = Overdetermined problem
- B) N<M: Less observations than data = Underdetermined problem</li>
- Let's consider Problem B)
  - Underdetermined Problem with Accurate Data
  - Underdetermined Problem with Noisy (inaccurate) Data

#### Discrete Linear Inverse Problems

(1) Accurate data 
$$d = Lm$$

(2) Inaccurate data 
$$d = Lm + e \rightarrow d \approx Lm$$

Consider discrete data and discrete vector of model parameters

## Discrete Linear Inverse Problem with Accurate Data

$$d = Lm$$

$$\mathbf{d} \in R^N$$
,  $\mathbf{m} \in R^M$ 

We assume an under-determined problem  $\,M>N\,$ 

- We have more unknowns than observations.
- Hence, we have an infinite number of solutions.
- One needs to pick one. Which one?

## Discrete Linear Inverse Problem with Accurate Data: Minimum Norm Solution

 Among all possible solution select the one with minimum Euclidian norm. In other words,

Minimize 
$$\|\mathbf{m}\|_2^2$$

Subject to 
$$d = Lm$$

 The latter is solved using the Method of Lagrange Multipliers. We minimized an augmented cost function

$$J = \|\mathbf{m}\|_2^2 + \mathbf{b}^T (\mathbf{Lm} - \mathbf{d})$$

•  $\mathbf{b} \in \mathbb{R}^N$  is the vector of Lagrange Multipliers, one multiplier per observation

## Discrete Linear Inverse Problem with Accurate Data: Minimum Norm Solution

 To solve the problem we need to minimize the cost respect to m and b

$$J = \|\mathbf{m}\|_2^2 + \mathbf{b}^T (\mathbf{Lm} - \mathbf{d})$$

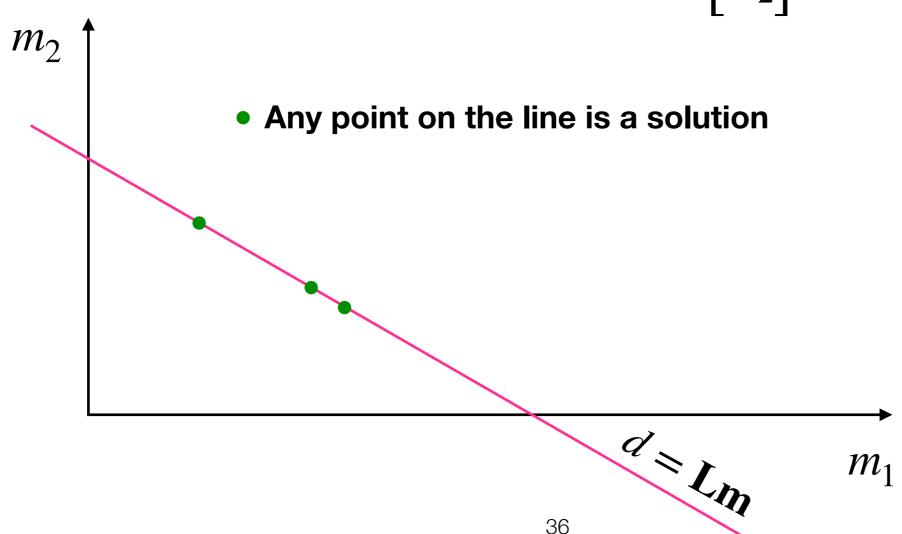
 Which leads to the so called minimum norm solution (I will do it in the whiteboard)

$$\mathbf{m}_{mn} = \mathbf{L}^T (\mathbf{L} \mathbf{L}^T)^{-1} \mathbf{d}$$

## Discrete Linear Inverse Problem with Accurate Data: Minimum Norm Solution

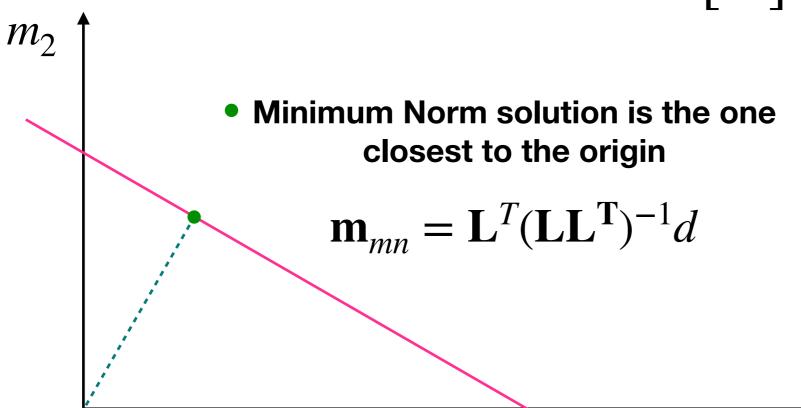
• N=1, M=2 (2 unknowns and 1 equation)

$$d = \mathbf{Lm} = \begin{bmatrix} L_{11} & L_{12} \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix}$$



• N=1, M=2 (2 unknowns and 1 equation)

$$d = \mathbf{Lm} = \begin{bmatrix} L_{11} & L_{12} \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix}$$



• N=1, M=2 (2 unknowns and 1 equation)

$$d = \mathbf{Lm} = \begin{bmatrix} L_{11} & L_{12} \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix}$$

- $m_2$  (Q) What is the big deal about the minimum norm solution?
  - (A) It avoids solutions where  $m_1 \to \pm \infty$  ,  $m_2 \to \pm \infty$  It is a conservative solution that guarantees stability

**Problem** 

$$d = Lm$$

**Minimum norm solution** 

$$\mathbf{m}_{mn} = \mathbf{L}^T (\mathbf{L} \mathbf{L}^T)^{-1} \mathbf{d}$$

We can replace the data back into the solution  $\mathbf{m}_{mn} = \mathbf{L}^T (\mathbf{L} \mathbf{L}^T)^{-1} \mathbf{L} \mathbf{m}$ 

**Model resolution matrix is not identity** 

$$\mathbf{m}_{mn} = \mathbf{R}_{m}\mathbf{m}$$

$$\mathbf{R}_m = \mathbf{L}^T (\mathbf{L} \mathbf{L}^T)^{-1} \mathbf{L} \neq \mathbf{I}$$

So, unless the "true solution" is the minimum norm solution, we cannot recover the "true solution"...

**Problem** 

$$d = Lm$$

**Minimum norm solution** 

$$\mathbf{m}_{mn} = \mathbf{L}^T (\mathbf{L} \mathbf{L}^T)^{-1} \mathbf{d}$$

**Predicted data** 

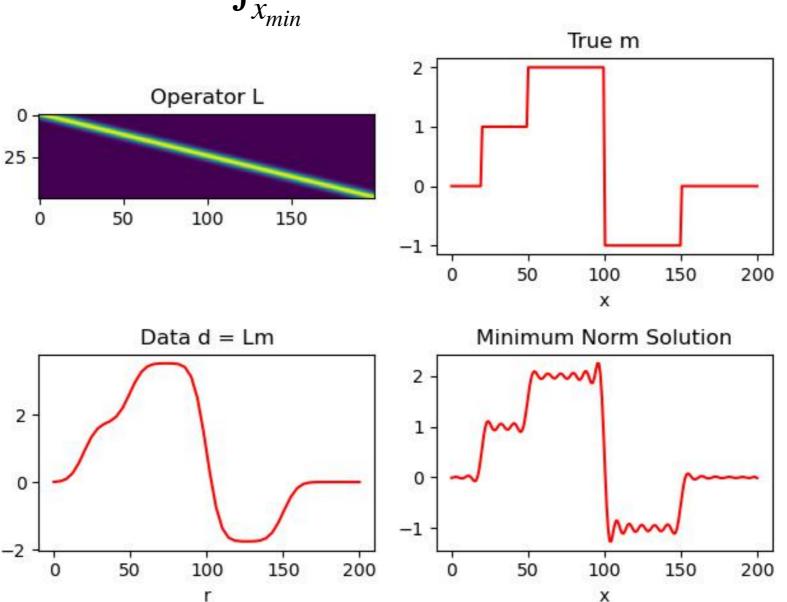
$$\mathbf{d}^{pred} = \mathbf{L}\mathbf{m}_{mn} = \mathbf{L}\mathbf{L}^{T}(\mathbf{L}\mathbf{L}^{T})^{-1}\mathbf{d}$$

**Data resolution matrix** is the identity

$$\mathbf{d}^{pred} = \mathbf{R}_d \mathbf{d} = \mathbf{d}$$
$$\mathbf{R}_d = \mathbf{L} \mathbf{L}^T (\mathbf{L} \mathbf{L}^T)^{-1} = \mathbf{I}$$

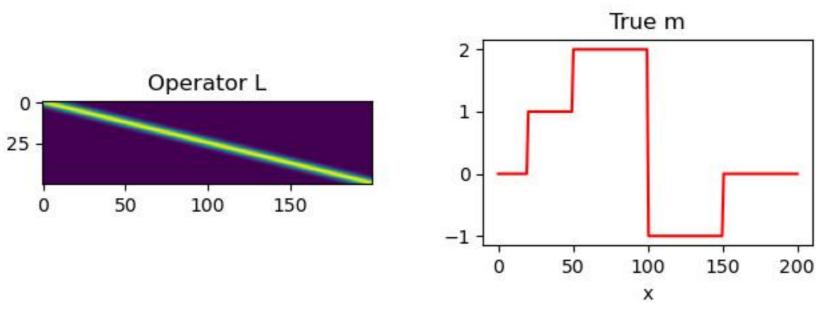
It is obvious that I can recover the data exactly because the data was used as an exact constraint when we constructed the minimum norm solution.

• Example 
$$d(r_j) = \int_{x_{min}}^{x_{max}} Ae^{-\alpha(r_j - x)^2} m(x) dx$$

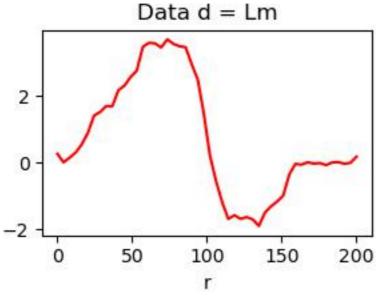


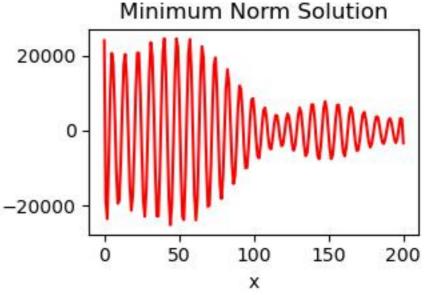
demo\_1.ipynb

• Example 
$$d(r_j) = \int_{x}^{x_{max}} Ae^{-\alpha(r_j - x)^2} m(x) dx + \sigma n(r_j)$$



demo\_2.ipynb





This is not working because I am fitting the data "exactly" and the data now contains noise!

 Among all possible solution select the one with minimum Weighted Euclidian norm. In other words,

Minimize 
$$\|\mathbf{Wm}\|_2^2$$
  
Subject to  $\mathbf{d} = \mathbf{Lm}$ 

 The latter is solved using the Method of Lagrange Multipliers. We minimized an augmented cost function

$$J = \|\mathbf{W}\mathbf{m}\|_{2}^{2} + \mathbf{b}^{T}(\mathbf{L}\mathbf{m} - \mathbf{d})$$

•  $\mathbf{b} \in \mathbb{R}^N$  is the vector of Lagrange Multipliers, one multiplier per observation

 To solve the problem we need to minimize the cost respect to m and b

$$J = \|\mathbf{W}\mathbf{m}\|_{2}^{2} + \mathbf{b}^{T}(\mathbf{L}\mathbf{m} - \mathbf{d})$$

 Which leads to the so called weighted minimum norm solution (I will do it in the whiteboard)

$$\mathbf{Q} = (\mathbf{W}^T \mathbf{W})^{-1}$$
$$\mathbf{m}_{wmn} = \mathbf{Q} \mathbf{L}^T (\mathbf{L} \mathbf{Q} \mathbf{L}^T)^{-1} \mathbf{d}$$

## Linear Inverse Problems with inaccurate data

Including noise into the problem

```
\mathbf{d} = \mathbf{Lm} + \mathbf{e}
\mathbf{d} : N \times 1 \qquad \mathbf{m} : M \times 1 \qquad \mathbf{L} : N \times M
```

- e represents "nice" Gaussian additive noise
- Given the vector of observed data d, one wishes to estimate the vector of model parameters m

## Linear Inverse Problems with inaccurate data: Regularized least-squares solution

Cost function for least-squares problems

$$J = \|\mathbf{e}\|_2^2 = \|\mathbf{d} - \mathbf{Lm}\|_2^2$$

The principle is simple, find  $\mathbf{m}$  that minimize the sum of the squares of the errors

$$\nabla J = 0 \to (\mathbf{L}^T \mathbf{L}) \mathbf{m} = \mathbf{L}^T \mathbf{d}$$

To compute the solution we now have to invert a matrix. Assume the matrix is invertible then

$$\mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L})^{-1} \mathbf{L}^T \mathbf{d} \qquad M < < N$$

Careful here: This is valid for overdetermined problems where the matrix to invert is full rank

## Linear Inverse Problems with inaccurate data: Regularized least-squares solution

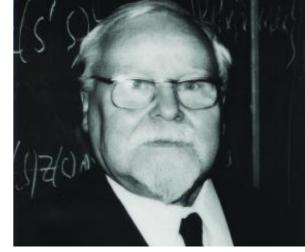
The latter is a naive solution because inverse problems are ill-posed and regularization is needed and, in general, they are not well-posed over-determined problems. In other words, one cannot safely compute:  $(\mathbf{L}^T \mathbf{L})^{-1}$ 

- Either is non invertible
- Or the Matrix has a large condition number (It will amplify noise)
- Condition Number  $\kappa = \frac{\lambda_{max}(\mathbf{L}^T\mathbf{L})}{\lambda_{min}(\mathbf{L}^T\mathbf{L})}$

Matrix computations
GH Golub, CF Van Loan, 2013 (4th edition)

### Regularization (a solution to ill-conditioning)

- Main idea of regularization methods:
  - Take an ill-posed problem and turn into a well-posed problem by introducing constraints that lead to a stable solution. The solution often depends on a trade-off parameter. Therefore, regularization methods create a family of solutions with different properties (e.g. smoothness). One can modify the solution by changing the tradeoff parameter
  - Often called Tikhonov regularization



A. N. Tikhonov (1906-1993)

Replace cost function to minimize

$$J = \|\mathbf{d} - \mathbf{Lm}\|_2^2$$
 — Cost with no regularization term

by

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{Wm}\|_{2}^{2}$$

- μ Is the infamous trade-off parameter or regularization parameter. Why infamous?
- W is a matrix/operator of weights

Evaluate the solution, as usual, by minimizing a cost function

$$\mathbf{m}_{sol} = \underset{\mathbf{m}}{\operatorname{argmin}} J$$

$$= \underset{\mathbf{m}}{\operatorname{argmin}} \{ \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{W}\mathbf{m}\|_{2}^{2} \}$$

Taking derivatives and equating them to zero

$$\nabla J = 0 \rightarrow \mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{R})^{-1} \mathbf{L}^T \mathbf{d}$$
$$\mathbf{R} = \mathbf{W}^T \mathbf{W}$$

Anatomy of the cost function

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{Wm}\|_{2}^{2}$$

$$Error Norm Model Norm$$

$$J = \underbrace{\|\mathbf{e}\|_{2}^{2}}_{Error\ Norm} + \mu \quad \underbrace{\|\mathbf{u}\|_{2}^{2}}_{Model\ Norm}$$

• To minimize J is equivalent to simultaneously minimize  ${\bf e}$  and  ${\bf u}$ 

• To minimize J is equivalent to simultaneously minimize  ${\bf e}$  and  ${\bf u}$ 

$${f e}={f d}-{f Lm}pprox {f 0}$$
 Minimize the residuals  ${f u}={f Wm}pprox {f 0}$  Minimize the bad features of  ${f m}$ 

- W is a high-pass operator therefore it penalizes roughness. The vector u represents amplified bad features of m
- Examples of W are first and second order derivatives

## Regularization with first order derivative smoothing

$$\mathbf{W} = \mathbf{D}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

$$\frac{\partial f(x)}{\partial x} \leftrightarrow ikF(k)$$

The derivative operator is high pass because it amplifies high frequencies

## Regularization with second order derivative smoothing

$$\mathbf{W} = \mathbf{D}_2 = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix}$$

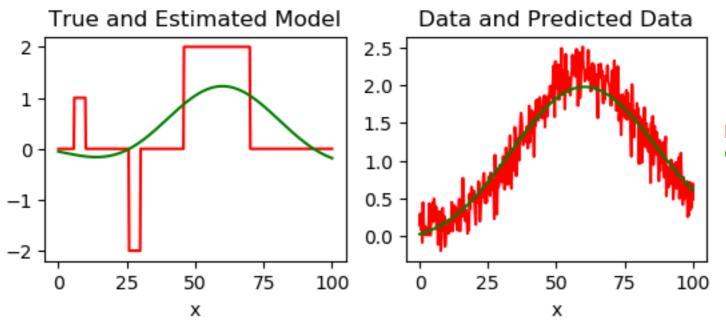
$$\frac{\partial^2 f(x)}{\partial x^2} \leftrightarrow -k^2 F(k)$$
 Second Derivative is also a high-pass operator

### Damped LS solution is when W=I

$$\mathbf{m}_{sol} = \underset{\mathbf{m}}{\operatorname{argmin}} J$$

$$= \underset{\mathbf{m}}{\operatorname{argmin}} \{ \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{m}\|_{2}^{2} \}$$

$$\frac{\partial J}{\partial \mathbf{m}} = 0 \to \mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{I})^{-1} \mathbf{L}^T \mathbf{d}$$

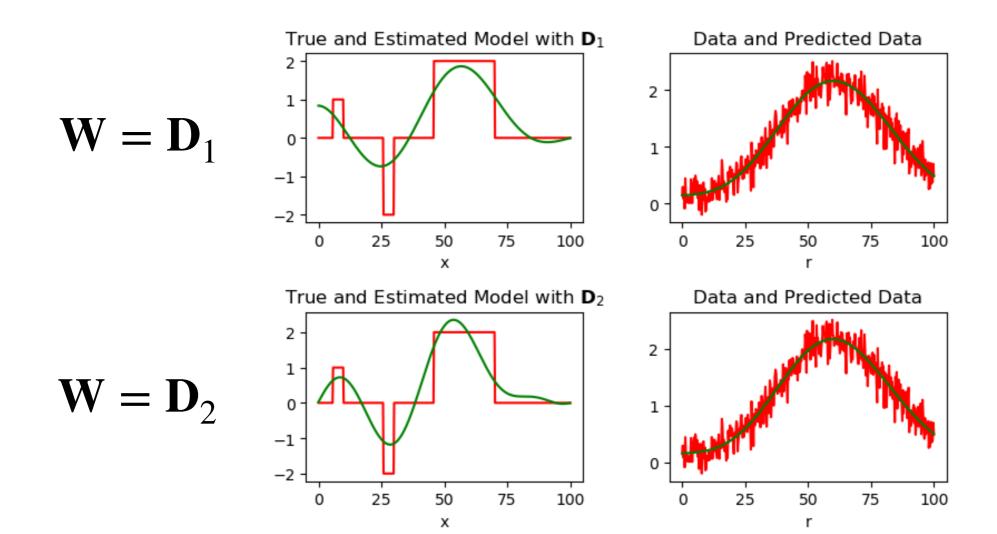


Red: True Model | Observed data
Green: Estimated Model | Predicted data

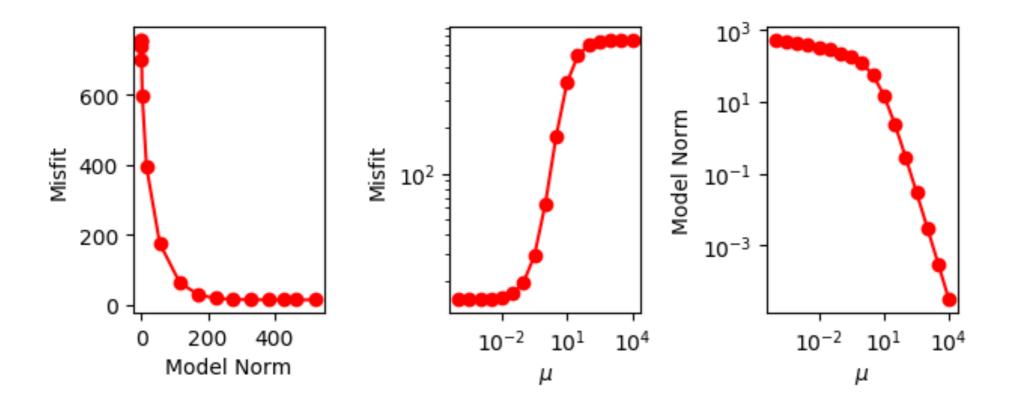
### **Example: Solution with smoothing**

$$\mathbf{m}_{sol} = \underset{\mathbf{m}}{\operatorname{argmin}} \{ \|\mathbf{d} - \mathbf{L}\mathbf{m}\|_{2}^{2} + \mu \|\mathbf{W}\mathbf{m}\|_{2}^{2} \}$$

$$\frac{\partial J}{\partial \mathbf{m}} = 0 \rightarrow \mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{W}^T \mathbf{W})^{-1} \mathbf{L}^T \mathbf{d}$$



## Trade-off curves (for Damped least-squares)



#### Underdetermined Problem with inaccurate data

#### **Minimum Norm Solution**

$$J = Misfit + \mu Model Norm$$

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{m}\|_{2}^{2}$$

Make residuals small = Find a model that fits the data

Make model parameters small = Stable solution that does not blow up

 $\mu$  : Trade-off parameter of the inverse problem

So we solve the problem

$$d = Lm + n$$

by minimizing the cost  $J = \|\mathbf{d} - \mathbf{L}\mathbf{m}\|_2^2 + \mu \|\mathbf{m}\|_2^2$ 

- We already discussed how one can compute derivatives of the scalar function J with respect to a vector.
- Condition for minimum

$$\frac{dJ}{d\mathbf{m}} = 0 \to (\mathbf{L}^T \mathbf{L} + \mu \mathbf{I}) \,\mathbf{m} = \mathbf{L}^T \mathbf{d}$$

Cost 
$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{m}\|_{2}^{2}$$

- Solution  $\mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{I})^{-1} \mathbf{L}^T \mathbf{d}$
- Predicted data  $\mathbf{d}_{pred} = \mathbf{L}\mathbf{m}_{sol} = \mathbf{L}(\mathbf{L}^T\mathbf{L} + \mu\mathbf{I})^{-1}\mathbf{L}^T\mathbf{d}$
- Predicted residuals  $\mathbf{r} = \mathbf{d}_{pred} \mathbf{d}$
- You can also show the following important identity:

$$\mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{I})^{-1} \mathbf{L}^T \mathbf{d} = \mathbf{L}^T (\mathbf{L} \mathbf{L}^T + \mu \mathbf{I})^{-1} \mathbf{d}$$

$$\mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{I})^{-1} \mathbf{L}^T \mathbf{d} = \mathbf{L}^T (\mathbf{L} \mathbf{L}^T + \mu \mathbf{I})^{-1} \mathbf{d}$$
1 2

1 looks like the least-squares solution for overdetermined problems, so it is often called the regularized least-squares solution. Also called damped least-squares, ridge regression solution, least-squares solution with zero-order quadratic regularization, Tikhonov solution, etc.

2 looks like the minimum norm solution for exact data but now there is an additional constant diagonal term.

The method we described is also called Tikhonov regularization, so the solution given by either 1) or 2) is also the Tikhonov solution.

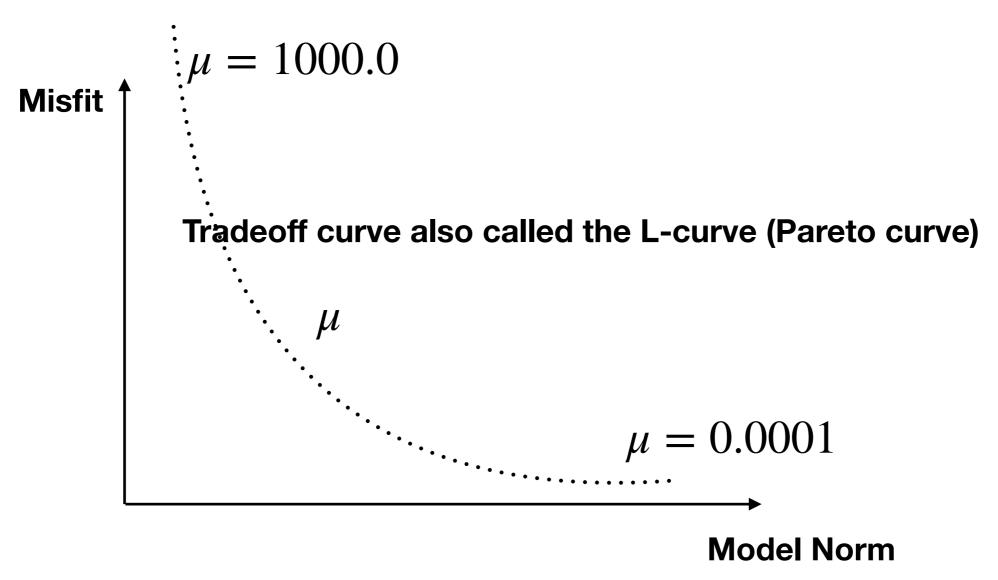
$$\mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{I})^{-1} \mathbf{L}^T \mathbf{d} = \mathbf{L}^T (\mathbf{L} \mathbf{L}^T + \mu \mathbf{I})^{-1} \mathbf{d}$$

Where does the name <u>damped least-squares solution</u> come from? As one increases  $\mu$ , more damping is introduced. In other words, the solution becomes smaller and less oscillatory!

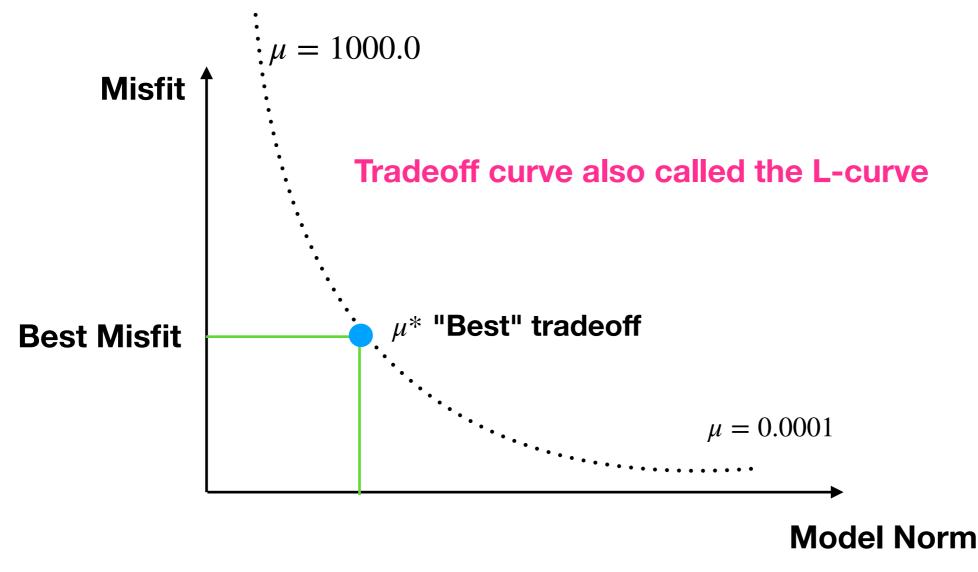
The tradeoff parameter  $\mu$  is sometimes also call the damping parameter.

The tradeoff parameter must be provided and it defines a family of solutions. I should have written  $\mathbf{m}_{sol}(\mu)$  to indicate the dependency of the solution on the tradeoff parameter.

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{m}\|_{2}^{2} = \mathbf{Misfit} + \mu \, \mathbf{Model \, Norm}$$



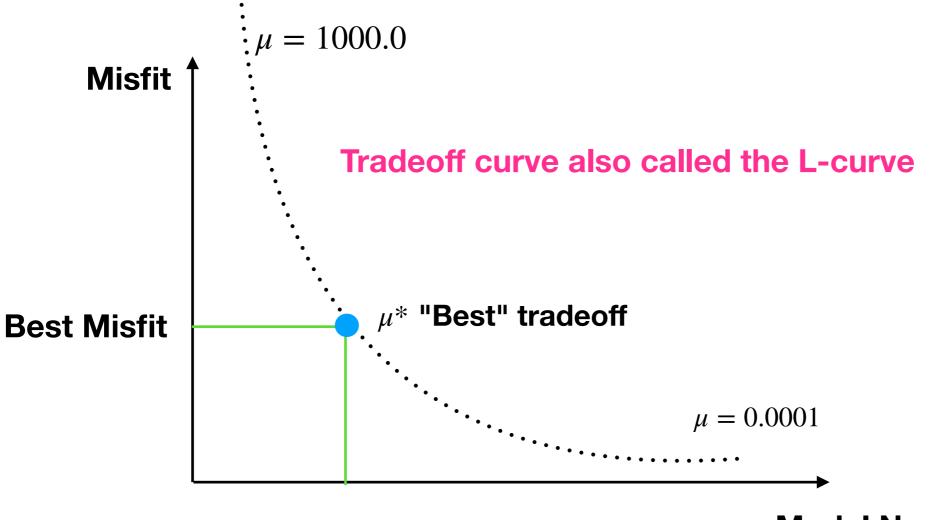
$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{m}\|_{2}^{2} = \mathbf{Misfit} + \mu \, \mathbf{Model \, Norm}$$



Recall original problem: d = Lm + n.

Assume you know the variance of the noise:  $\sigma^2$ 

Best misfit = 
$$\|\mathbf{d} - \mathbf{Lm}_{sol}(\mu^*)\|_2^2 = N \times \sigma^2$$

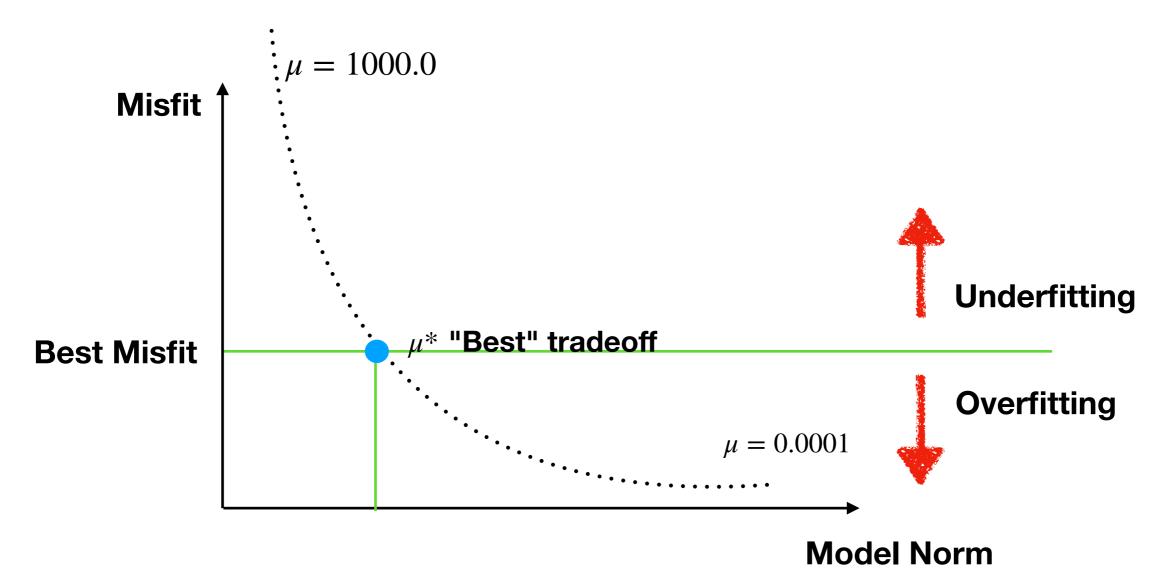


**Model Norm** 

Recall original problem: d = Lm + n.

Assume you know the variance of the noise:  $\sigma^2$ 

Best misfit = 
$$\|\mathbf{d} - \mathbf{Lm}_{sol}(\mu^*)\|_2^2 = N \times \sigma^2$$

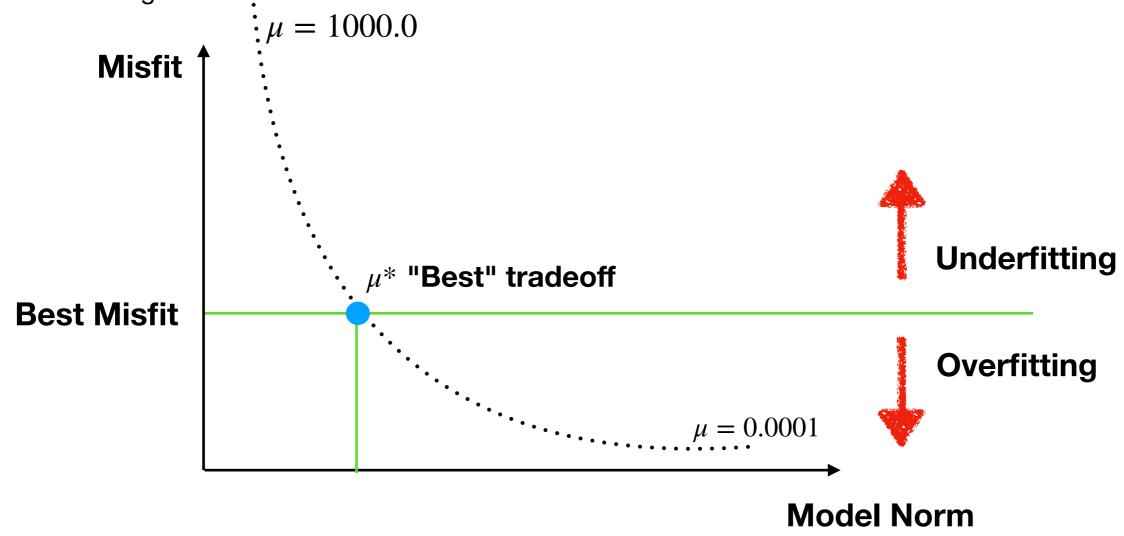


#### Underdetermined Problem with inaccurate data

#### **Minimum Norm Solution**

Underfitting: Observations are not properly fit. You are overestimating the amount of noise in the data. Solution norm decreases. Residuals are too large. There is probably some structure in the residuals.

Overfitting: Residuals become too small and therefore your estimated model produces data that fits the noise. As a consequence of the latter, the model can become unstable and the model norm is large.



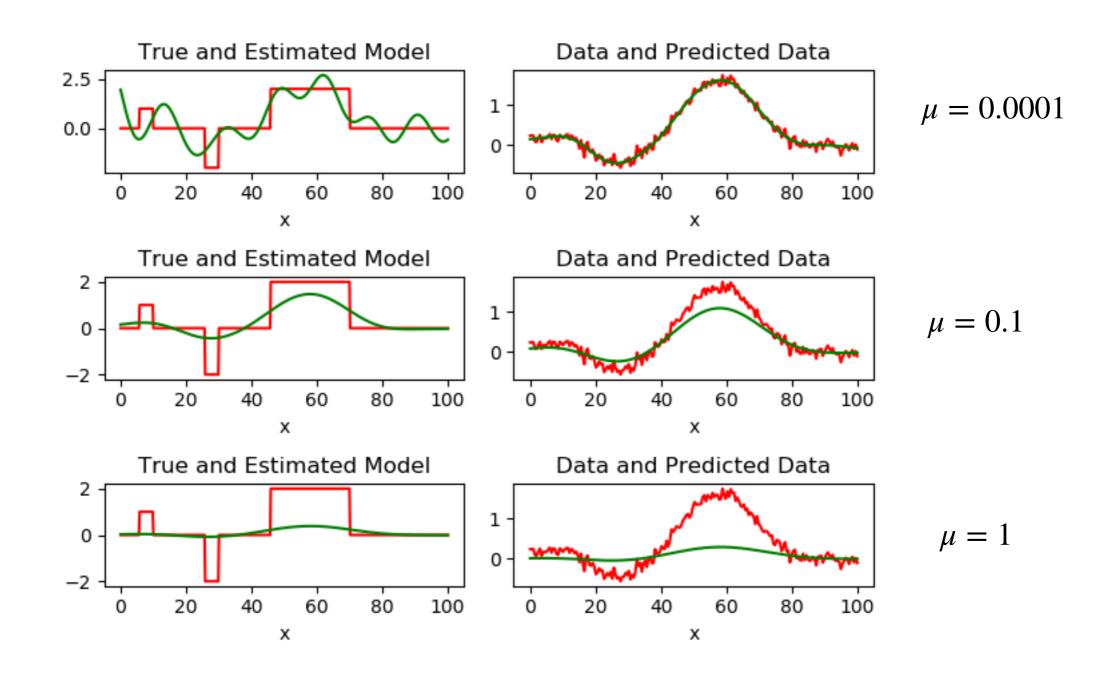
Cost 
$$J = \|\mathbf{d}_{obs} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{Wm}\|_{2}^{2}$$

- Solution  $\mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{W}^T \mathbf{W})^{-1} \mathbf{L}^T \mathbf{d}$
- Predicted data  $\mathbf{d}_{pred} = \mathbf{L}\mathbf{m}_{sol} = \mathbf{L}(\mathbf{L}^T\mathbf{L} + \mu \mathbf{W}^T\mathbf{W})^{-1}\mathbf{L}^T\mathbf{d}_{obs}$
- Predicted residuals  $\mathbf{r} = \mathbf{d}_{pred} \mathbf{d}$
- You can also show the following important identity:

$$\mathbf{m}_{sol} = (\mathbf{L}^T \mathbf{L} + \mu \mathbf{Q})^{-1} \mathbf{L}^T \mathbf{d} = \mathbf{Q}^{-1} \mathbf{L}^T (\mathbf{L} \mathbf{Q}^{-1} \mathbf{L}^T + \mu \mathbf{I})^{-1} \mathbf{d}$$

$$\mathbf{O} = \mathbf{W}^T \mathbf{W}$$

## Trade-off curves (for Damped least-squares)



### Changing the norm

### Edge preserving regularization (EPR)

- Avoid smoothing to preserve edges
- We adopt the ell-1 norm of the first order derivative of model parameters
- Make the derivative of the model sparse

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{D}_{1}\mathbf{m}\|_{1}$$

$$\underbrace{Error\ Norm} \qquad Model\ Norm$$

We ask  $u = D_1 m$  to be sparse

### The $L_1$ and the $L_2$ norms

$$\mathbf{u}: N \times 1 \longrightarrow \|\mathbf{u}\|_{2}^{2} = \mathbf{u}^{H}\mathbf{u} = \sum_{i=1}^{N} u_{i} u_{i}^{*} = \sum_{i=1}^{N} |u_{i}|^{2}$$

$$\mathbf{u}: N \times 1 \longrightarrow \|\mathbf{u}\|_1 = \sum_{i=1}^N |u_i|$$

Quadratic leads to close form solution (linear system of equations)

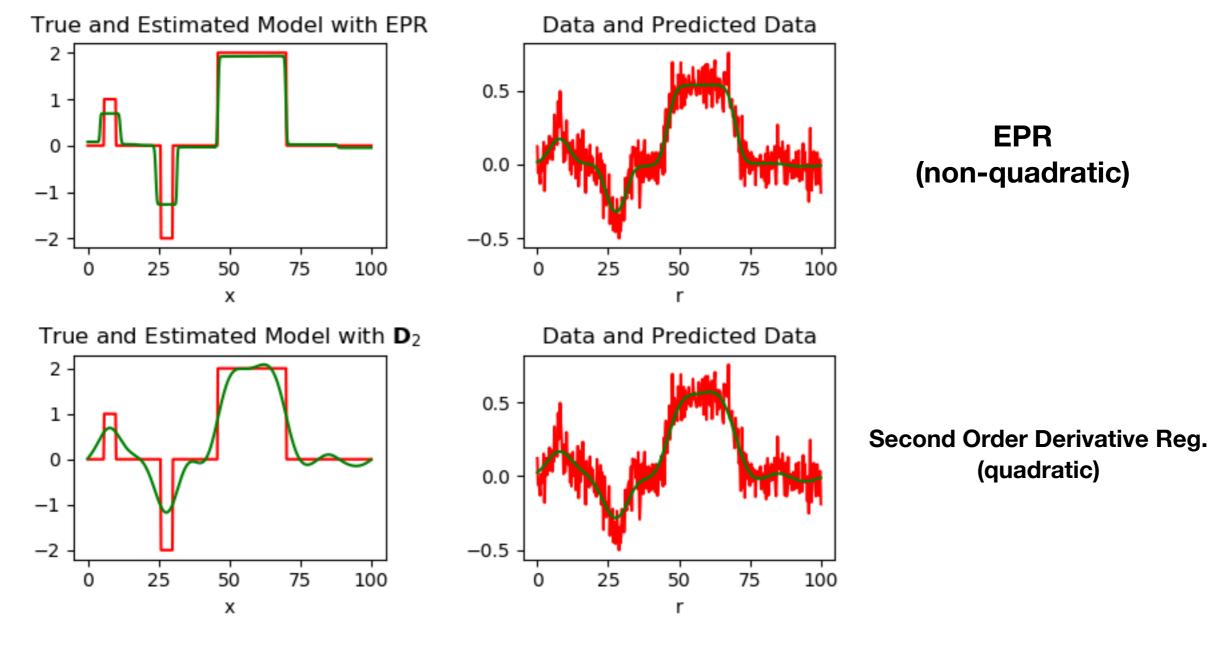
$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{Wm}\|_{2}^{2}$$

$$\underbrace{Error\ Norm} \qquad Model\ Norm$$

 EPR: Non-quadratic regularization leads to non-linear solution that tries to recover edges

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{D}_{1}\mathbf{m}\|_{1}$$

$$\underbrace{Error\ Norm} \qquad Model\ Norm$$



Non-quadratic regularization leads to non-linear solution

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{D}_{1}\mathbf{m}\|_{1}$$

$$\underbrace{Error\ Norm} \qquad Model\ Norm$$

Solution

$$\nabla J = 0 \rightarrow (\mathbf{L}'\mathbf{L} + \mu \mathbf{D}'_1 \mathbf{Q} \mathbf{D}_1)\mathbf{m} = \mathbf{L}'\mathbf{d}$$

• Where  $\mathbf{v} = \mathbf{D}_1 \, \mathbf{m}$ 

$$\mathbf{v} = \mathbf{D}_1 \,\mathbf{m} \qquad Q_{ii} = \frac{1}{|v_i|}$$

To avoid division by zero

$$Q_{ii} = \frac{1}{\epsilon + |v_i|}$$

Iterative re-weighted least-squares

$$\mathbf{m}^1 = \mathbf{m}_{initial}$$

For k=1 until convergence

$$\mathbf{v} = \mathbf{D}_1 \mathbf{m}$$

$$Q_{ii}^k = \frac{1}{\epsilon + |v_i^k|}$$

$$\mathbf{m}^{k+1} = (\mathbf{L}'\mathbf{L} + \mu \mathbf{D}_1'\mathbf{Q}^k\mathbf{D}_1)^{-1}\mathbf{L}'\mathbf{d}$$

**End** 

#### Connection to sparsity

This cost function generates a sparse solution

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \quad \|\mathbf{m}\|_{1}$$

$$Error Norm \quad Model Norm$$

- Often used for Deconvolution
- Pre-stack data Reconstruction (Liu and Sacchi, 2004, Geophysics; Hermann, 2010, Geophysics)
- Radon Transfroms, etc etc etc (Sacchi & Ulrych, 1995, Geophysics)
- AVO Inversion (Alemie and Sacchi, 2011, Geophysics)

#### Connection to sparsity

Make m sparse:

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \quad \|\mathbf{m}\|_{1}$$

$$Error Norm \quad Model Norm$$

Make the derivative of m sparse = Make m blocky

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{D}_{1}\mathbf{m}\|_{1}$$

$$\underbrace{Error\ Norm} \qquad Model\ Norm$$

#### Sparsity (more to follow...)

- IRLS is the simplest solver one can imagine
  - Many new solvers in recent years
    - ISTA, FISTA, SALSA, SPG-L1, ADMM, L1-Magic, etc etc etc.. show Notes in Latex
    - I usually use IRLS or FISTA
    - ISTA/FISTA: Only need to know how to apply L and L' (on-the-flight)

#### PROBLEMS IN IMPLICIT FORM

#### Forward and Adjoint Operators

Two special operations (or operators?)

Forward : d = Lm

Conjugate transpose or adjoint :  $\tilde{\mathbf{m}} = \mathbf{L}' \mathbf{d}$ 

- L is a linear operator (Forward modelling operator).
- Why are them special?
  - Iterative solvers for large inverse problems only need to know how to evaluate  $L[\;\cdot\;]$  and  $L'[\;\cdot\;]$
  - I usually interpret operators as matrices. In reality, operators are codes applied on the flight
  - We will see these operators everywhere today

#### Forward and Adjoint Operators

For matrices

Forward: L

Conjugate transpose or adjoint :  $L' = L^T$ 

- Examples of parts (L, L')
  - Demigration, Migration
  - Radon Modeling  ${\mathscr R}$ , Radon adjoint  ${\mathscr R}'$
  - Sampling, Inserting zeros
  - Summation, Distribution or spraying
  - Fourier Synthesis  $\mathscr{F}$ , Fourier Analysis  $\mathscr{F}^H$

#### Steepest descent method

- Compute the gradient and iterate downhill until convergence
- Let's see the special role of L and L' in steepest descent optimization (or in any iterative optimization algorithm that only requires L and L')
- Simplify problem by considering minimization of quadratic cost  ${\cal J}$

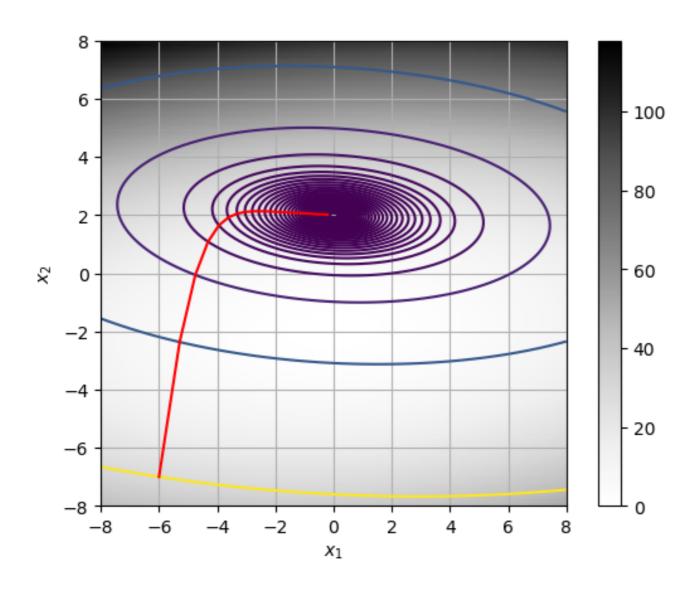
$$J = \|\mathbf{d} - \mathbf{Lm}\|_2^2$$

#### Steepest descent method

- Cost  $J = \|\mathbf{d} \mathbf{Lm}\|_2^2$
- Gradient  $\mathbf{g} = \nabla J = \mathbf{L}'(\mathbf{Lm} \mathbf{d})$
- Update  $\mathbf{m}^{k+1} = \mathbf{m}^k \alpha \mathbf{g}^k$
- Interesting, one can minimize J with a simple rule that does not involve inverting matrices. This is great because we can replace matrices by linear operators!!!!
- Aren't you excited?

## Steepest descent (SD) method

Minimization of a quadratic cost by SD



 $x_{init} = [-6.0, -7.9]$ 

 $x_{final}=[-0.009,2.005]$ 

 $x_{true}=[0.0,2.0]$ 

K = 50 iterations at fixed step size

#### Steepest descent method

#### SD iterations:

Do until convergence 
$$\mathbf{m}^{k+1} = \mathbf{m}^k - \alpha (\mathbf{L}'(\mathbf{L}\mathbf{m}^k - \mathbf{d}))$$
 End Do

The above code can also be written as follows

Do until convergence
$$\mathbf{r}^k = (\mathbf{L}\mathbf{m}^k - \mathbf{d})$$

$$\mathbf{m}^{k+1} = \mathbf{m}^k - \alpha \mathbf{L}'(\mathbf{r}^k)$$

## Steepest descent method: Matrices are replaced by Linear Operators packed into Functions or Subroutines

Do until convergence

$$\mathbf{r}^{k} = (\mathbf{L}\mathbf{m}^{k} - \mathbf{d})$$
$$\mathbf{m}^{k+1} = \mathbf{m}^{k} - \alpha \mathbf{L}'(\mathbf{r}^{k})$$

**End Do** 

Do until convergence

$$\mathbf{r}^{k} = \mathbf{Do_{lt}}[\mathbf{m}^{k}, flag = f] - \mathbf{d}$$

$$\mathbf{m}^{k+1} = \mathbf{m}^{k} - \alpha \mathbf{Do_{lt}}[\mathbf{r}^{k}, flag = a]$$

**End Do** 

f: Forwarda: Adjoint or transpose

#### Operators on the flight

(Matrices are replaced by implicit form linear operators!!)

$$\mathbf{y} = \mathbf{L}\mathbf{x} - \mathbf{L} - \mathbf{x}$$

$$\tilde{\mathbf{x}} = \mathbf{L}'\mathbf{y} - \mathbf{L}' - \mathbf{y}$$

#### Operators on the flight

$$y = Lx$$
 — Do\_lt —  $x$ 

$$\tilde{\mathbf{x}} = \mathbf{L}'\mathbf{y} - \mathbf{Do_lt} - \mathbf{y}$$

*f:* Forward

a: Adjoint or transpose

## Why this is important?

- Migration and de-migration operators cannot be written as matrices. Least-squares migration requires the **Do\_It** approach.
- In addition, time-domain Radon transforms can not be written in explicit form. For Radon problems I also use the **Do\_It** approach.
- Reconstruction problems often entail using operators that cannot be written via explicit matrices (FFTs, Curvelet Frames, etc). In this case, we also adopt the **Do\_It** approach
- In general, multidimensional problems where m and d are not vectors can still be analyzed via linear algebra tools by providing simple rules that make linear operators behave like matrices

## **Dot-product test**

- How do you guarantee that the codes for the forward and adjoint operators behave like L and L'?
- Let's L be the forward operator and let's call B the tentative adjoint or transpose operator

$$\mathbf{y}_1 = \mathbf{L} \, \mathbf{x}_1 \,, \quad \mathbf{x}_2 = \mathbf{B} \, \mathbf{y}_2$$

Form the two inner products

$$\mathbf{y}_{2}^{T}\mathbf{y}_{1} = \mathbf{y}_{2}\mathbf{L}\mathbf{x}_{1} \qquad \langle \mathbf{y}_{2}, \mathbf{y}_{1} \rangle = \langle \mathbf{y}_{2}, \mathbf{L}\mathbf{x}_{1} \rangle$$

$$\mathbf{x}_{1}^{T}\mathbf{x}_{2} = \mathbf{x}_{1}\mathbf{B}\mathbf{y}_{2} \qquad \langle \mathbf{x}_{1}, \mathbf{x}_{2} \rangle = \langle \mathbf{x}_{1}\mathbf{B}\mathbf{y}_{2} \rangle$$

More general notation

#### **Dot-product test**

 Notice, the definition of the inner product can be extended to multidimensional array

For vectors

$$\mathbf{y}_2^T \mathbf{y}_1 = \mathbf{sum}(y_2. * y_1)$$

For ND-arrays

$$<\mathbf{y}_{2},\mathbf{y}_{1}>=\mathbf{sum}(y_{2}[:].*y_{1}[:])$$

#### **Dot-product test**

The two inner products are equal

$$\mathbf{y}_2^T \mathbf{y}_1 = \mathbf{y}_2 \mathbf{L} \mathbf{x}_1 \qquad \mathbf{x}_1^T \mathbf{x}_2 = \mathbf{x}_1 \mathbf{B} \mathbf{y}_2$$

If and only if  $\mathbf{B} = \mathbf{L}'$ 

Therefore, one can write a code for L and a code for L', do the dot-product test and if the two product are equal then one can say that L and L' (packed by the function **Do\_It**) behave like a matrix and transpose multiplications, respectively. Then you can safely use all you know about linear algebra to solve an inverse problem!

#### Dot-product test in practice

```
# Dot product test example using operators rather than matrices
# Fourier DFT matrices and its Hermitian Transpose are replaced by
# on-the-flight FFTs
M = 512
x1 = randn(M)
y1 = fft(x1)
y2 = randn(M)
                          => Why I have multiplied by M?
x2 = M*ifft(y2)
dot_x = x1'*x2
dot_y = y1'*y2
println(dot_x)
println(dot_y)
```

using LinearAlgebra, FFTW

#### **Conjugate Gradients**

- It is more efficient to use the Conjugate Gradient (CG) method than SD.
- I will not discuss CG but it basically amounts to also applying on the flight the operators L and L' in each iteration (step)
- The Conjugate Gradient algorithm is quite popular so you can find one in C,Fortran, Matlab, Python, etc by just doing a google search.
- CG minimizes the general quadratic cost function:

$$J = \|\mathbf{d} - \mathbf{Lm}\|_2^2$$

#### Concatenation of operators

Forward

$$L = ABC$$

Adjoint

$$L' = C'B'A'$$

 Dot product test must work for individual operators (codes) and then it will work for L and L'

 When using iterative methods (SD or CG), I prefer not to worry about matrices of weights

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{Wm}\|_{2}^{2}$$

Therefore, I like to use the following change of variables

$$Wm = u \rightarrow Pu = m$$

$$J = \|\mathbf{d} - \mathbf{LPu}\|_{2}^{2} + \mu \|\mathbf{u}\|_{2}^{2}$$

Minimize with iterative solver

$$J = \|\mathbf{d} - \mathbf{LPu}\|_{2}^{2} + \mu \|\mathbf{u}\|_{2}^{2}$$

With **Do\_It** operators:

Forward: LP

Adjoint : P'L'

In this example, I use SD to minimize

$$J = \|\mathbf{d} - \mathbf{LPu}\|_{2}^{2} + \mu \|\mathbf{u}\|_{2}^{2}$$

Do until convergence

$$\mathbf{r}^{k} = (\mathbf{L}\mathbf{P}\mathbf{u}^{k} - \mathbf{d})$$

$$\mathbf{u}^{k+1} = \mathbf{u}^{k} - \alpha(\mathbf{P}'\mathbf{L}'(\mathbf{r}^{k}) + \mu \mathbf{u}^{k})$$

**End** 

$$\mathbf{m}_{sol} = \mathbf{P}\mathbf{u}$$

W and P should behave like the inverse of each other

$$Wm = u \rightarrow Pu = m$$

Then

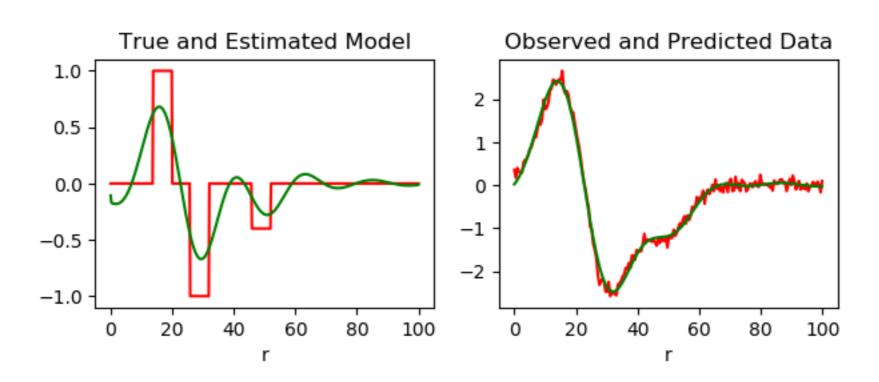
W is a high-pass operator (applies roughening)

P is low-pass operator (applies smoothing)

Oldie but goodie: S. Ronen, D. Nichols, R. Bale, and R. Ferber, "Dealiasing DMO: Good-pass, bad-pass, and unconstrained", SEG Technical Program Expanded Abstracts 1995. January 1995, 743-746

## Preconditioning (SD)

$$\mathbf{P} = \frac{1}{2} \begin{pmatrix} 2 & 1 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 1 & 2 \end{pmatrix}$$



## My favourite CG (CGLS)

I prefer to use a CG algorithm that minimizes the so called Standard Form

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{m}\|_{2}^{2}$$

```
function ConjugateGradients(d,operators,parameters;Niter=10,mu=0)
  r = copy(d)
                                                                         g = L'r
  g = LinearOperator(r,operators,parameters,adj=true)
  m = zero(g)
  s = copy(g)
  gamma = InnerProduct(g,g)
  for iter = 1: Niter
     t = LinearOperator(s,operators,parameters,adj=false)
                                                                          t = Ls
     delta = InnerProduct(t,t) + mu*InnerProduct(s,s)
     alpha = gamma/delta
     m = m + alpha*s
     r = r - alpha*t
     g = LinearOperator(r,operators,parameters,adj=true)
                                                                          \mathbf{g} = \mathbf{L}'\mathbf{r}
     g = g - mu^*m
     gamma0 = copy(gamma)
     gamma = InnerProduct(g,g)
     beta = gamma/gamma0
     s = beta*s + g
   end
  return m
end
```

https://github.com/SeismicJulia/SeisReconstruction.jl/blob/master/src/Tools/ConjugateGradients.jl

# Advantages of CGLS to minimize the standard form

You can turn a general problem with quadratic regularization into its standard form and use the previous page CGLS algorithm

$$J = \|\mathbf{d} - \mathbf{Lm}\|_{2}^{2} + \mu \|\mathbf{Wm}\|_{2}^{2}$$



$$J = \|\mathbf{d} - \mathbf{LPu}\|_{2}^{2} + \mu \|\mathbf{u}\|_{2}^{2}$$
, with,  $\mathbf{u} = \mathbf{Pm}$ 

$$P = W^{-1} \leftarrow to discuss$$

#### Advantages of CGLS to minimize the standard form

You can also concatenate linear operators

$$J = \|\mathbf{W}_d[\mathbf{d} - \mathbf{ABm}]\|_2^2 + \mu \|\mathbf{W}_m \mathbf{m}\|_2^2$$



$$J = \|\mathbf{d}_{w_d} - \mathbf{W}_d \mathbf{A} \mathbf{B} \mathbf{P}_m \mathbf{u}\|_2^2 + \mu \|\mathbf{u}\|_2^2, \text{ with, } \mathbf{u} = \mathbf{P}_m \mathbf{m}, \mathbf{d}_{w_d} = \mathbf{W}_d \mathbf{d}$$

operators = 
$$[\mathbf{W}_d, \mathbf{A}, \mathbf{B}, \mathbf{P}_m]$$

LinearOperator(Input,operators,parameters,adj=false)

Output =  $W_d A B P_m$  Input

LinearOperator(Input,operators,parameters,adj=true)

Output =  $P'_m B' A' W'_d Input$ 

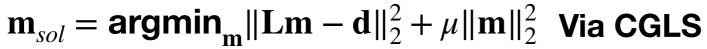
#### Example: Time-domain Parabolic Radon Transform

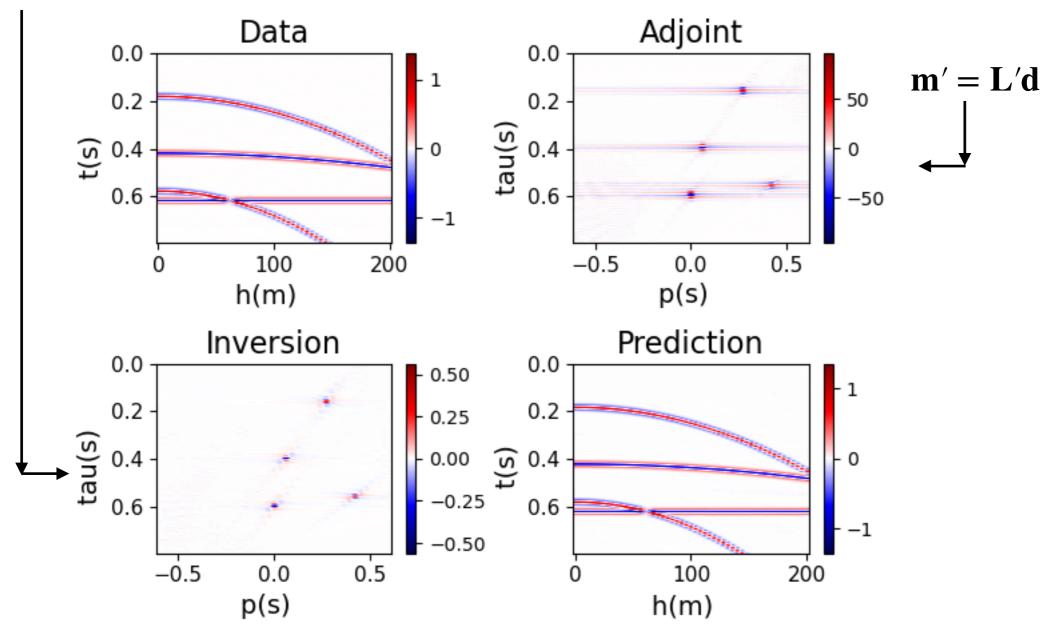
- Notebook: ConjugateGradient\_in\_SeisReconstruction.ipynbin
- Compute reflections with parabolic moveout and then use CG to retrieve the Radon domain coefficient that model the reflections.
- Radon adjoint and forward operators:

$$m'(\tau, p) = \sum_{h} d(t = \tau + pg(h), h) \rightarrow \mathbf{m}' = \mathbf{L}'\mathbf{d}$$
  
 $d(t, h) = \sum_{h} m(\tau = t - pg(h)) \rightarrow \mathbf{d} = \mathbf{Lm}$ 

- Linear RT g(h) = h, p : Slope
- Parabolic RT  $g(h) = (h/h_{max})^2, p$ : Residual moveout at far offset

#### Example: Time-domain Parabolic Radon Transform





#### CGLS\_versus\_SD\_example.ipynb

Comparison of SD and CGLS path for a simple problem with two unknown where one can visualize the cost function

