Large-scale inverse problems in geoscience

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Data Assimilation Summer School, Timisoara - 01/08/2019

Quiz

$$J = ||\mathbf{d} - \mathbf{G}\mathbf{m}||^2 + \lambda^2 ||\mathbf{D}\mathbf{m}||^2$$

How do you minimize this cost function *without* creating explicit matrices?

Goals

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- Basic of linear algebra (hopefully already...)

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- Python is **Slow** if you write is as C, it is not if you leverage its advanced libraries (numpy, scipy, tensorflow, pytorch, pycuda, dask...)

Course outline

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- Geophysical applications (EX5, EX6)

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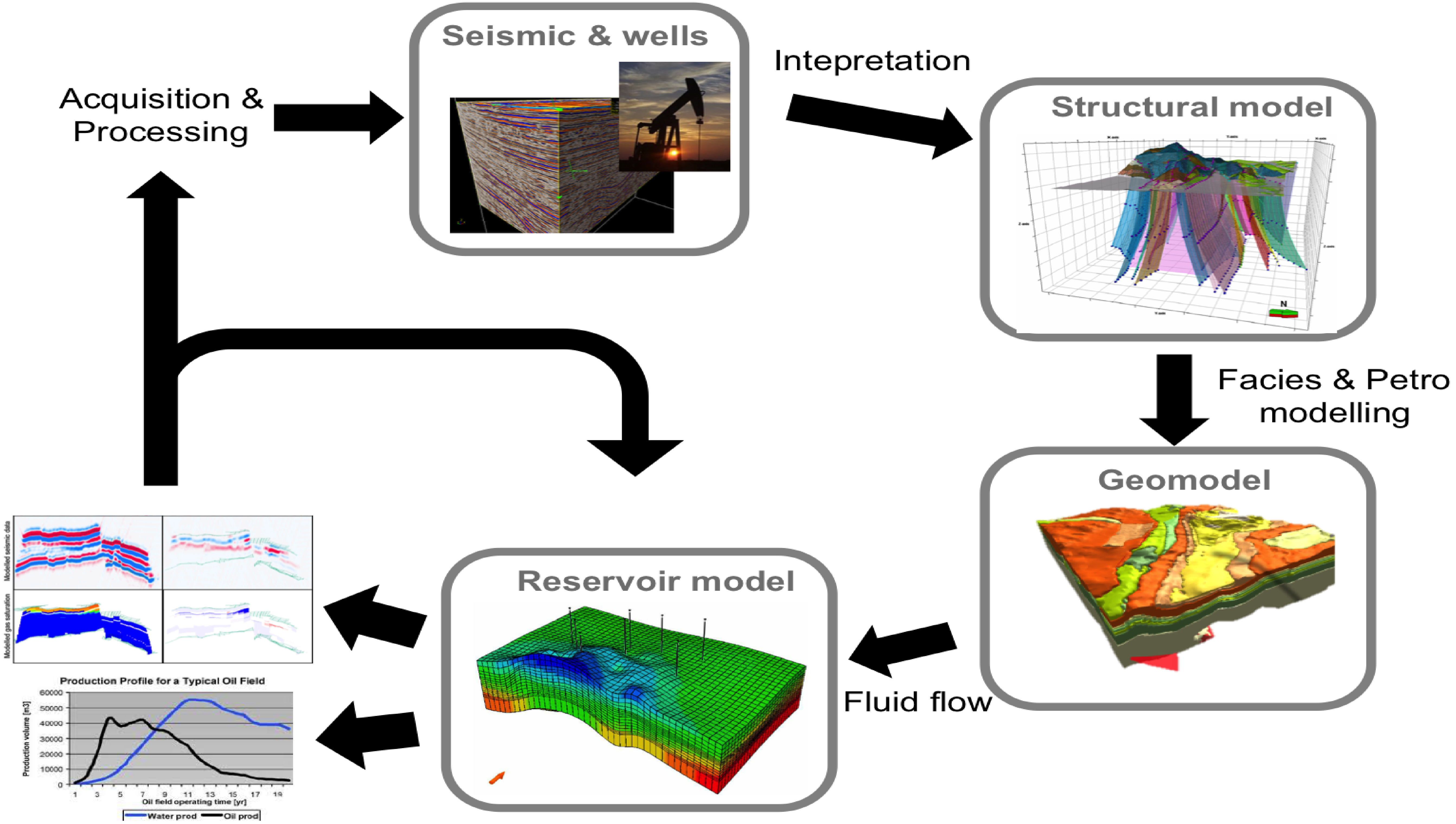
- Geophysical applications (EX5, EX6)
- Beyond single-machine inverse problems: GPUs, distributed...


Seismic & wells
Intepretation
Structural model
Acquisition &
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Production Profile for a Typical Oil Field
Production volume [m3]
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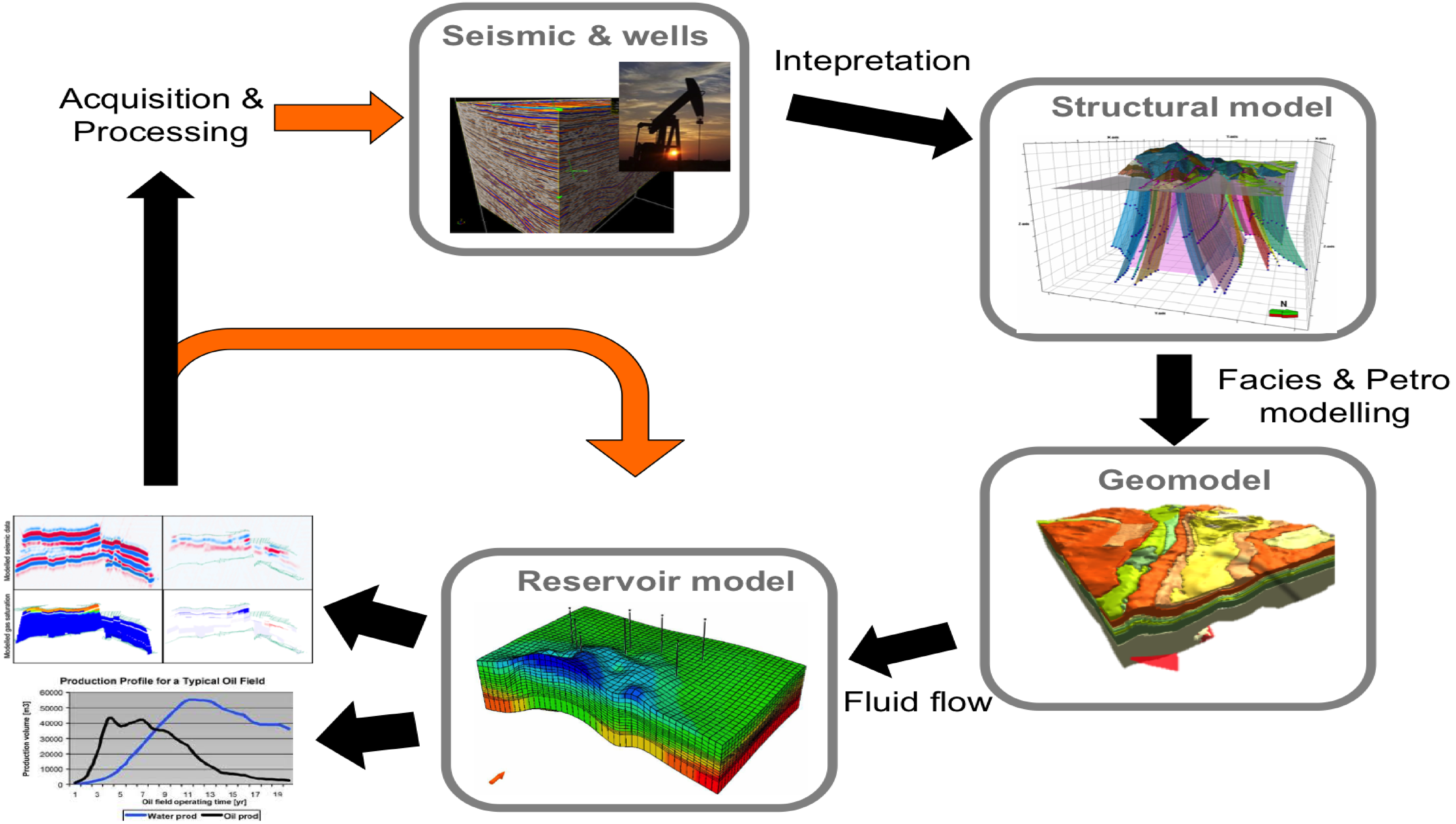
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Large... how large?

- Seismic processing:

$$n_S = n_R = 10^3, n_t = n_{fft} = 2 \cdot 10^3 \quad (dt = 4ms, t_{ma}$$

$$\rightarrow \mathbf{G} : n_S \cdot n_R \cdot n_{fft}^2 = 4 \cdot 10^{12} * 32bit = 128T$$

- Seismic inversion:

$$n_x = n_y = 10^3, n_z = 800 \quad (dz = 5m, z_{max} = 400$$

$$\rightarrow \mathbf{G} : n_x \cdot n_y \cdot n_z^2 = 6.4 \cdot 10^{11} * 32bit \sim 20T$$

Inverse problems

Fundamental theory developed in the '60/'70

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- Mathematicians: general theory, shared with other applications e.g., ML, data assimilation
- Seismologists: inference of subsurface properties/behaviours from large set of data
- Atmosferic scientists: more concerned with data assimilation through time

Inverse problems

References:

A. Tarantola, Inverse Problem Theory;

S. Kay, Fundamentals of statistical signal processing;

J. Claerbout, Basic Earth Imaging;

...

Forward model

$$\mathbf{d} = \mathbf{g}(\mathbf{m}) \quad / \quad \mathbf{d} = \mathbf{G}\mathbf{m}$$

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- **d**: observed data. Quantity that we can physicially measure - seismic, production, temperature, precipitation, MRI scan…

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- **m**: model. Quantity that we are interested to know and we think affects the data - rock properties, pressure, saturation, human organs...
- **G**: modelling operator. Set of equations that we think can explain the data by *nonlinear/linear combination* of model parameters - PDEs, seismic convolution model, camera blurring...

Forward model

$$\mathbf{d} = \mathbf{g}(\mathbf{m}) \quad / \quad \mathbf{d} = \mathbf{G}\mathbf{m}$$

Unique and *easy* to compute, perhaps time consuming...

Inverse model

$$\mathbf{m} = \mathbf{g}^{-1}(\mathbf{d}) \quad / \quad \mathbf{m} = \mathbf{G}^{-1}\mathbf{d}$$

Nonunique and hard to *compute*, both expensive and unstable...

- **square** (N = M): rarely the case in real life. Solution:

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- **overdetermined** (N > M): most common case, robust to noise as more data poin than model parameters. Least-squares solution:

$$J = ||\mathbf{d} - \mathbf{G}\mathbf{m}||^2 \rightarrow \mathbf{m}_{est} = (\mathbf{G}^{\mathbf{H}}\mathbf{G})^{-1}\mathbf{G}^{\mathbf{H}}\mathbf{d}$$

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$$J = ||\mathbf{d} - \mathbf{Gm}||^2 \rightarrow \mathbf{m}_{est} = (\mathbf{G^H G})^{-1}\mathbf{G^H d}$$

- **underdetermined** (N < M): not ideal, but sometimes only option - e.g., MRI scar

  Least-squares solution:

$$J = ||\mathbf{m}||^2 \quad s.t \quad \mathbf{d} = \mathbf{Gm} \rightarrow \mathbf{m}_{est} = \mathbf{G^H}(\mathbf{GG^H})^{-}$$

  Sparse solution:

$$J = ||\mathbf{m}|| \quad s.t \quad \mathbf{d} = \mathbf{Gm}$$

Inversion in practice

Now that we know the analytical expressions, how do we find

$$\mathbf{G}^{-1} \quad (\mathbf{G}^{\mathbf{H}}\mathbf{G})^{-1} \quad (\mathbf{G}\mathbf{G}^{\mathbf{H}})^{-1}$$

Solutions studied in the fields of *Numerical analysis and Optimization*.

Two families of solvers:

Inversion in practice

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- **direct**: LU, QR, SVD...

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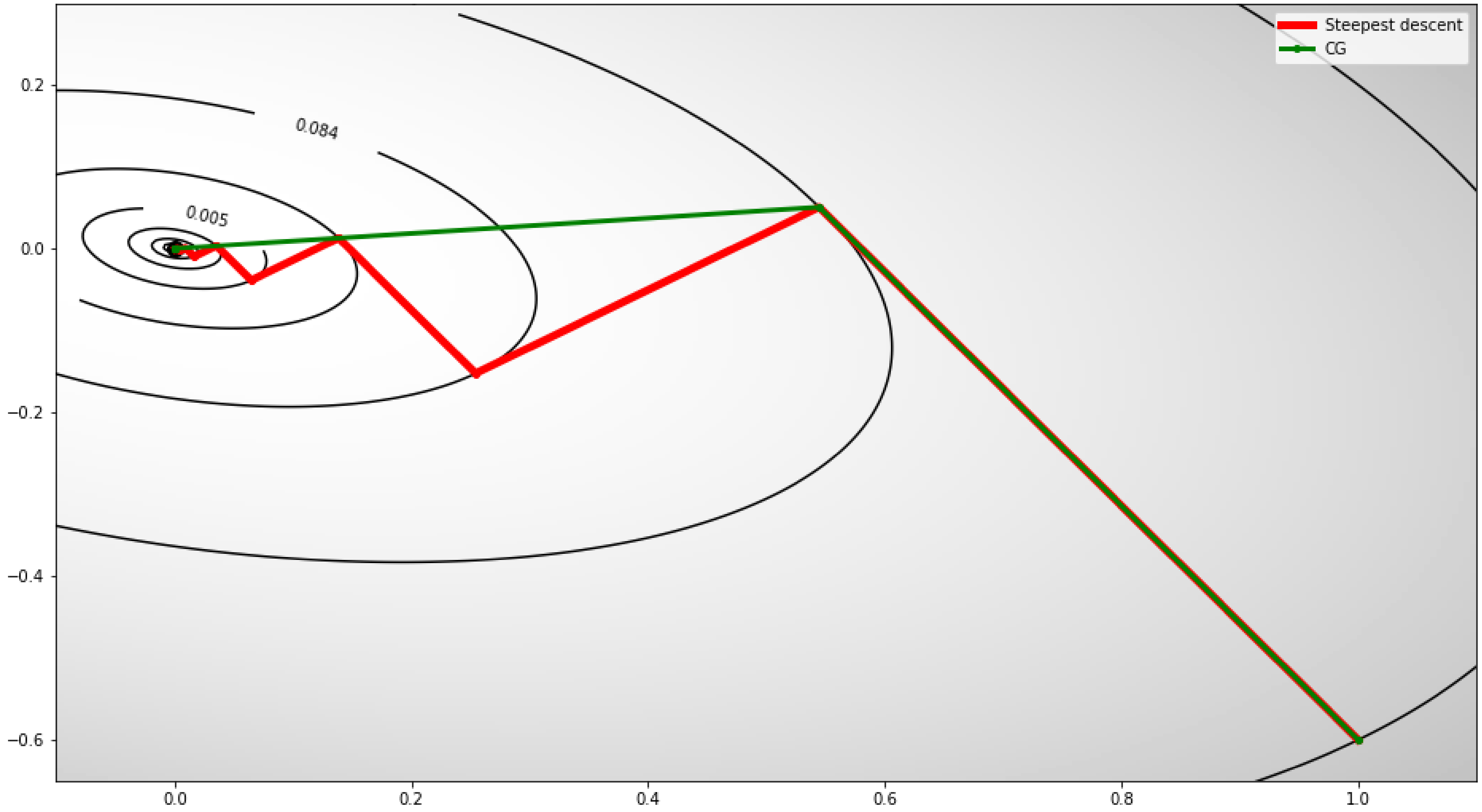
Two families of solvers:

- **direct**: LU, QR, SVD...
- **iterative**: gradient based methods - CG, LSQR, GMRES...

Inversion in practice



Let's practice EX1.

Why iterative?

$\mathbf{G}$ is too large to be inverted (or solved explicitely)

$\mathbf{G}$ is too large to be stored in memory

Take on message:

$$\mathbf{m}_{est} = \sum_{i=0}^{N_{iter}} f(\mathbf{G}, \mathbf{d}, \mathbf{m}_0) \qquad \mathbf{Gm}, \mathbf{G}^H\mathbf{d}, (\mathbf{m}^H\mathbf{m}, \mathbf{d}^H$$

Linear Operators

A piece of computer code that can perform *forward* and *adjoint* operations without the need to store an *explicit matrix*:

$$\mathbf{Gm}, \mathbf{G}^H\mathbf{d}$$

but how do we make sure that forward and adjoint are correctly implemented? --> **Dot-Test**

Ex: Diagonal

$$
\mathbf{D} = \begin{bmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \dots & & & \\ 0 & 0 & \dots & d_N \end{bmatrix}, \mathbf{D}^H = \begin{bmatrix} d_1 & 0 & \dots \\ 0 & d_2 & \dots \\ \dots & & \\ 0 & 0 & \dots \end{bmatrix}
$$

```
# forward
def _matvec(x)
    return self.diag * x
# adjoint
def _matvec(x)
    return self.diag * x
```

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Ex: Diagonal

Dot-Test: a correct implementation of forward and adjoint for a linear operator should verify the the following *equality* within a numerical tolerance:

$$(\mathbf{G} \cdot \mathbf{u})^H \mathbf{v} = \mathbf{u}^H (\mathbf{G}^H \cdot \mathbf{v})$$

Ex: First derivative

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$$\mathbf{D} = \begin{bmatrix} -1 & 1 & \dots & 0 & 0 \\ -0.5 & 0 & 0.5 & \dots & 0 \\ \dots & & & & \\ 0 & 0 & \dots & -1 & 1 \end{bmatrix}$$

```
def _matvec(x):
x, y = x.squeeze(), np.zeros(self.N, self.dtype)
y[1:-1] = (0.5 * x[2:] - 0.5 * x[0:-2]) / self.sampling
# edges
y[0] = (x[1] - x[0]) / self.sampling
y[-1] = (x[-1] - x[-2]) / self.sampling
```

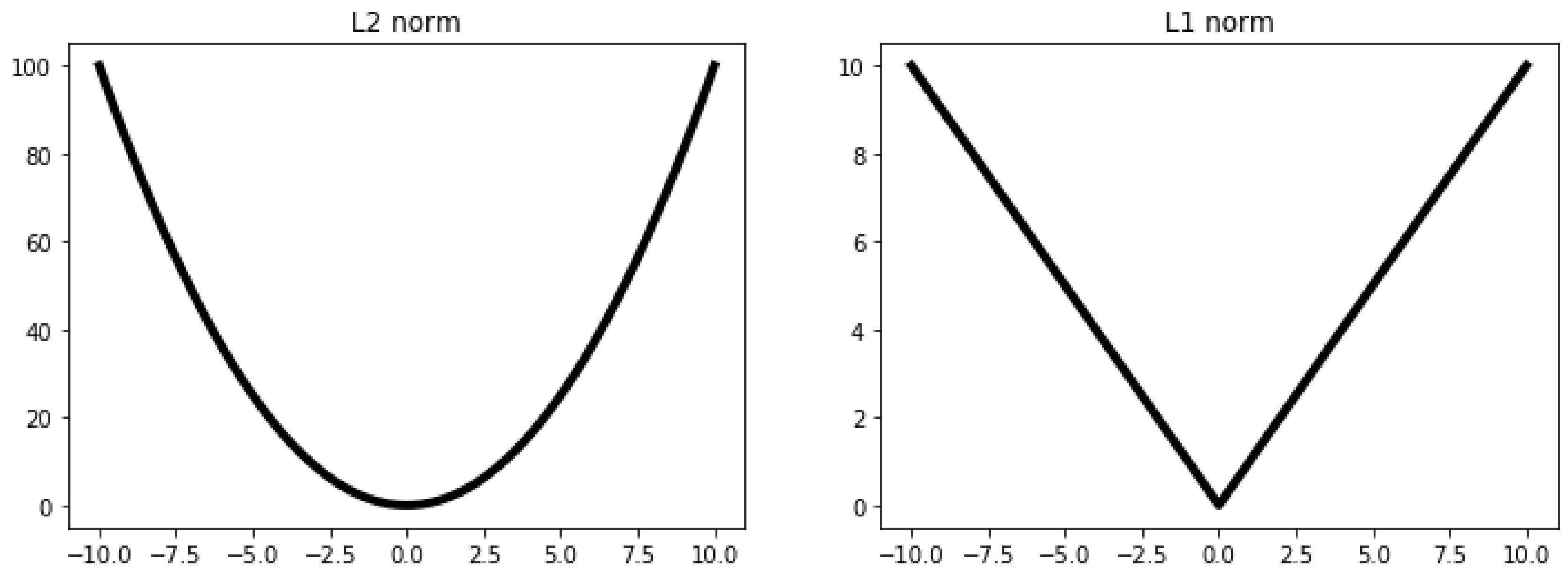
Ex: First derivative

$$\mathbf{D}^H = \begin{bmatrix} -1 & -0.5 & \dots & 0 & 0 \\ 1 & 0 & -0.5 & \dots & 0 \\ \dots & & & & \\ 0 & 0 & \dots & -0.5 & 1 \end{bmatrix}$$

```
def _rmatvec(x):
x, y = x.squeeze(), np.zeros(self.N, self.dtype)
y[0:-2] -= (0.5 * x[1:-1]) / self.sampling
y[2:] += (0.5 * x[1:-1]) / self.sampling
# edges
y[0] -= x[0] / self.sampling
y[1] += x[0] / self.sampling
y[-2] -= x[-1] / self.sampling
y[-1] += x[-1] / self.sampling
```

Let's practice EX2.

Solvers


L2 norm
L1 norm
100
80
60
40
20
0
10
8
6
4
2
0
−10.0 −7.5 −5.0 −2.5 0.0 2.5 5.0 7.5 10.0
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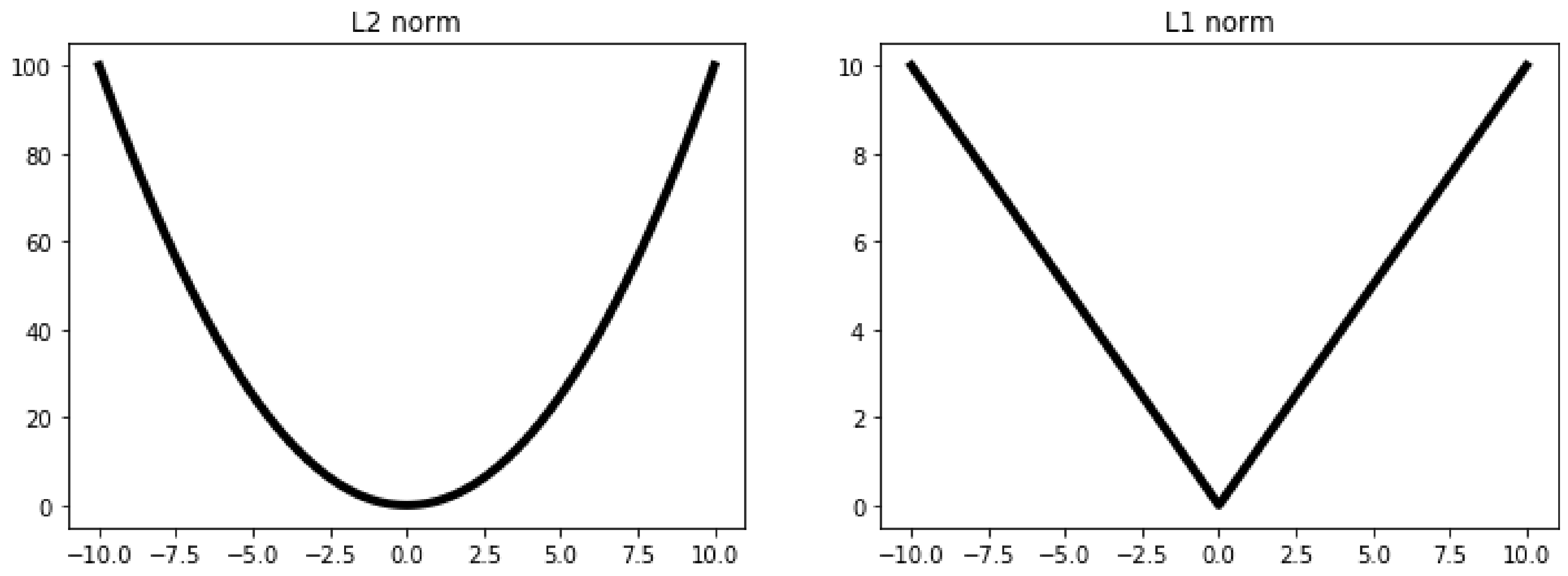
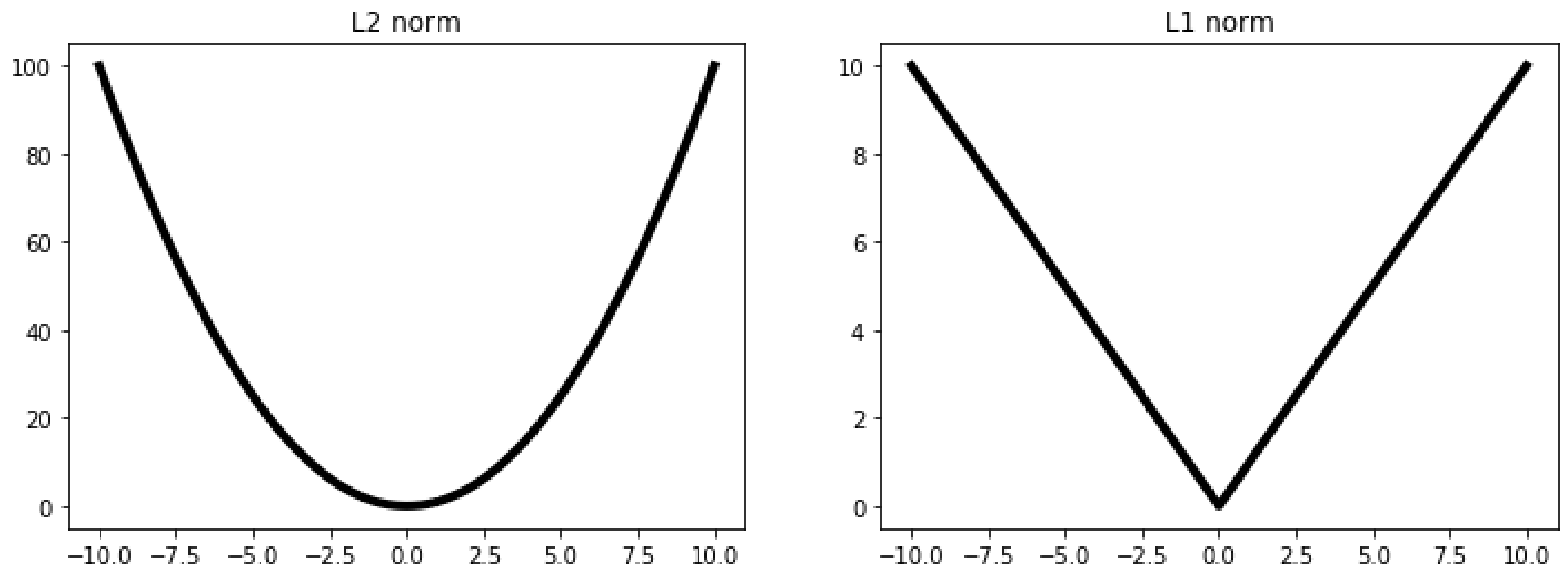
Solvers

- **Least-squares**: regularized, preconditioned, bayesian



Solvers

- **Least-squares**: regularized, preconditioned, bayesian
- **L1**: sparsity promoting, blockiness promoting



Least-squares - Regularized inversion

Add information to the inverse problem --> mitigate *ill-posedness*

$$J = ||\mathbf{d} - \mathbf{G}\mathbf{m}||^2_{\mathbf{W}_d} + \sum_i \epsilon^2_{R_i} ||\mathbf{d}_{R_i} - \mathbf{R}_i \mathbf{m}||^2_{\mathbf{W}_{R_i}}$$

Least-squares - Regularized inversion

Add information to the inverse problem --> mitigate *ill-posedness*

```
def RegularizedInversion(G, Reg, d, dreg, epsR):
# operator
Gtot = VStack([G, epsR * Reg])
# data
dtot = np.hstack((d, epsR*dreg))
# solver
minv = lsqr(Gtot, dtot)[0]
```

Least-squares - Bayesian inversion

Add prior information to the inverse problem --> mitigate *ill-posedness*

$$J = ||\mathbf{d} - \mathbf{G}\mathbf{m}||^2_{\mathbf{C}_d^{-1}} + ||\mathbf{m}_0 - \mathbf{m}||^2_{\mathbf{C}_m^{-1}}$$

$$\begin{bmatrix} \mathbf{C}_d^{-1/2}\mathbf{G} \\ \mathbf{C}_m^{-1/2} \end{bmatrix} \mathbf{m} = \begin{bmatrix} \mathbf{C}_d^{-1/2}\mathbf{d} \\ \mathbf{C}_m^{-1/2}\mathbf{m}_0 \end{bmatrix} \rightarrow$$

$$\mathbf{m} = (\mathbf{G}^H\mathbf{C}_d^{-1}\mathbf{G} + \mathbf{C}_m^{-1})^{-1}(\mathbf{G}^H\mathbf{C}_d^{-1}\mathbf{d} + \mathbf{C}_m^{-1}\mathbf{m_0})$$

Least-squares - Bayesian inversion

Add prior information to the inverse problem --> mitigate *ill-posedness*

$$J = ||\mathbf{d} - \mathbf{G}\mathbf{m}||^2_{\mathbf{C}_d^{-1}} + ||\mathbf{m}_0 - \mathbf{m}||^2_{\mathbf{C}_m^{-1}}$$

$$\mathbf{m} = \mathbf{m_0} + \mathbf{C}_m\mathbf{R}^H(\mathbf{R}\mathbf{C}_m\mathbf{R}^H + \mathbf{C}_d)^{-1}(\mathbf{d} - \mathbf{R}\mathbf{m_0})$$

Least-squares - Bayesian inversion

Add prior information to the inverse problem --> mitigate *ill-posedness*

```
def BayesianInversion(G, d, Cm, Cd):
# operator
Gbayes = G * Cm * G.H + Cd
# data
dbayes = d - G * m0
# solver
minv = m0 + Cm * G.H * lsqr(Gbayes, dbayes)[0]
```

Least-squares - Preconditioned inversion

Limit the range of plausible models --> mitigate *ill-posedness*

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

$$\mathbf{m} = \mathbf{Pp}$$

Least-squares - Preconditioned inversion

Limit the range of plausible models --> mitigate *ill-posedness*

```
def PreconditionedInversion(G, P, d):
# operator
Gtot = G * P
# solver
minv = lsqr(Gtot, d)[0]
```

Sparsity

Introduce L1 norms to cost function

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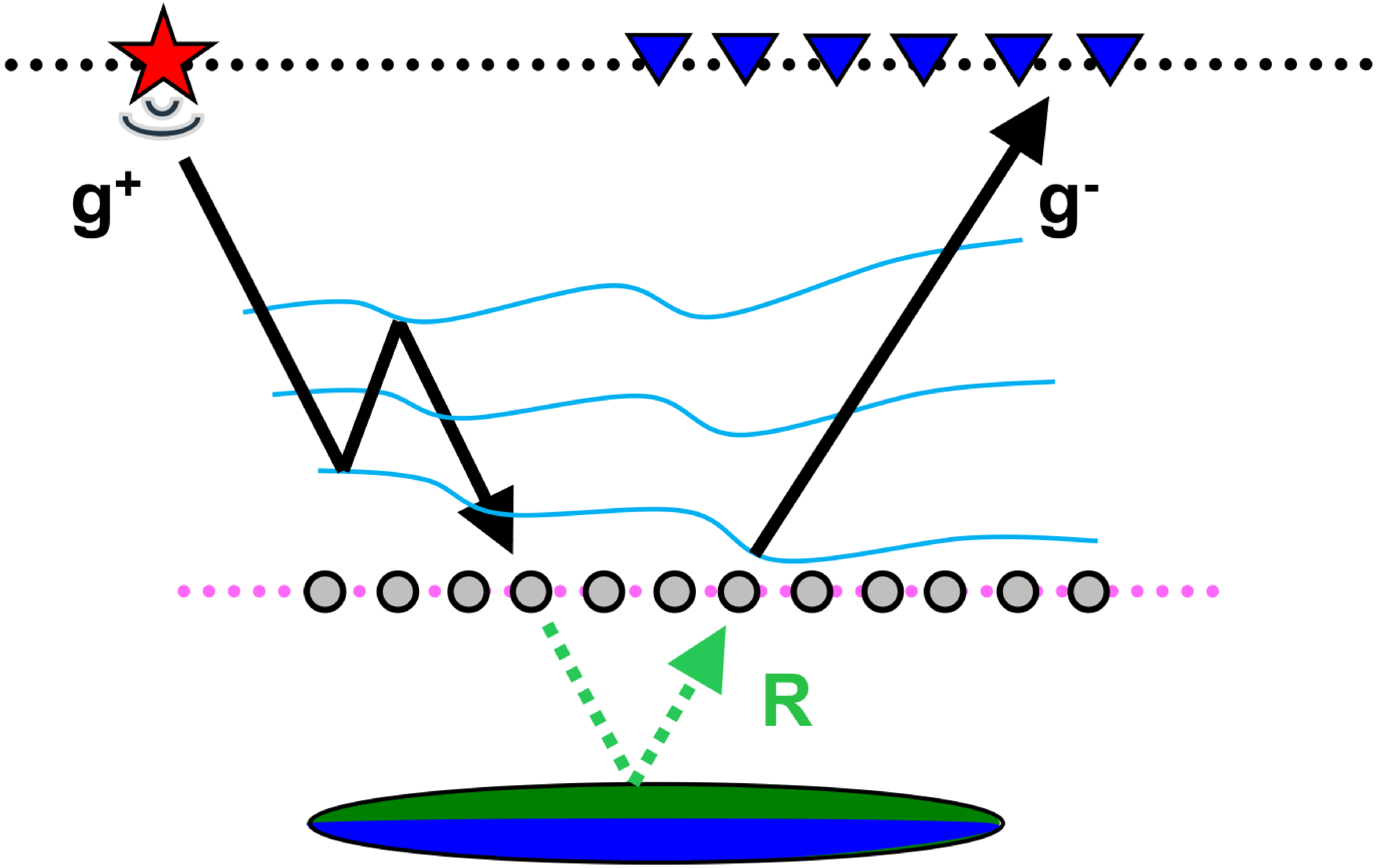
Let's practice EX3-EX4.

Seismic redatuming



Seismic redatuming

Integral relation:

$$g^{-}(t, x_s, x_v) = \mathscr{F}^{-1}\left(\int_S g^{+}(f, x_s, x_r)\mathscr{F}(R(t, x_r, x_v)\right.$$

Discretized relation:

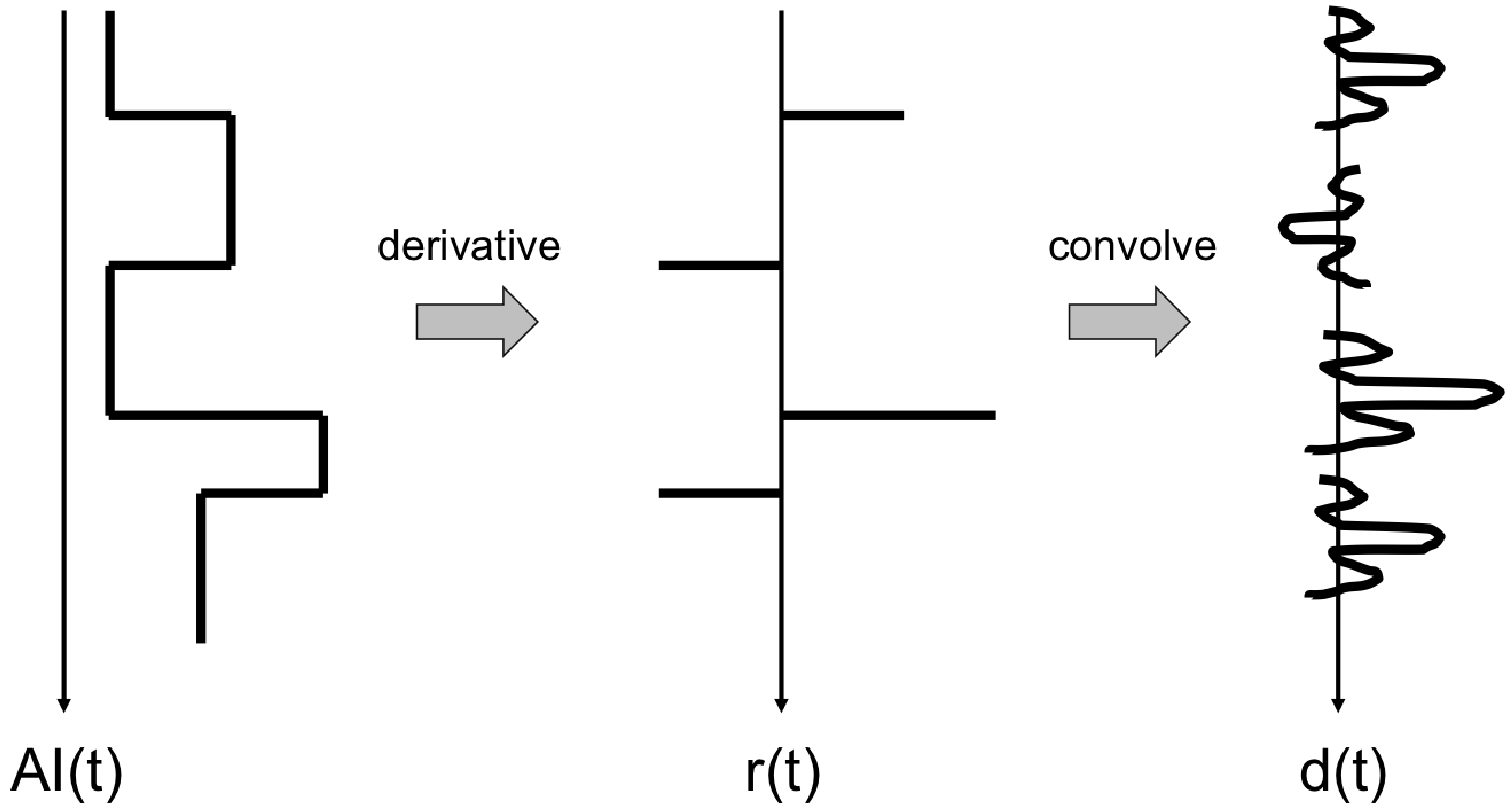
$$\mathbf{G}^{-} = \hat{\mathbf{G}}^{+}\mathbf{R}$$

where:

$$\hat{\mathbf{G}}^{+} = \mathbf{F}^{H}\mathbf{G}^{+}\mathbf{F}$$

Let's practice EX5.

Seismic inversion



Seismic inversion

Integral relation:

$$d(t) = w(t) * \frac{d(ln(AI(t)))}{dt}$$

Discretized relation:

$$\mathbf{d} = \mathbf{WDai}$$

where **D** is a derivative operator and **W** is a convolution operator.

Let's practice EX6.

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- Solving large-scale inverse problems can be daunting --> *Divide and conquer* paradigm
- Focus on fast operators as well as on advanced solvers
- Various paradigms (deterministic, bayesian..) can share same frameworks

Beyond laptop usage - GPUs

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Beyond laptop usage - GPUs

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- Several operators are convolution filters in disguise --> leverage ML libraries
- Seismic inversion example: **d** = **W D m**, **W**: convolution with w, **D**: derivative = convolution with [-1, 1]
    - *TensorFlow*, **PyTorch**, Cupy, PyCuda...

Beyond laptop usage - Distributed computing

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    - Joblib, mpi4py, **Dask**...