Wave equation and Green's function (1/3)

- Scalar wave model:

$$\frac{1}{c^2(\boldsymbol{x})} \frac{\partial^2 u}{\partial t^2} - \Delta_{\boldsymbol{x}} u = n(t, \boldsymbol{x})$$

$n(t, \boldsymbol{x})$: source.
$c(\boldsymbol{x})$: propagation speed (parameter of the medium), assumed to be constant outside a domain with compact support.

- The time-dependent Green's function $G(t, \boldsymbol{x}, \boldsymbol{y})$ is the solution of

$$\frac{1}{c^2(\boldsymbol{x})} \frac{\partial^2 G}{\partial t^2} - \Delta_{\boldsymbol{x}} G = \delta(t)\delta(\boldsymbol{x} - \boldsymbol{y})$$

Assume that $G(t, \boldsymbol{x}, \boldsymbol{y}) = 0 \ \forall t < 0 \Longrightarrow$ unique solution (causal Green's function).
Emission from a point source at $\boldsymbol{y}$ emitting a Dirac pulse at time 0.

If the medium is homogeneous $c(\boldsymbol{x}) \equiv c_o$, then

$$G(t, \boldsymbol{x}, \boldsymbol{y}) = \frac{1}{4\pi|\boldsymbol{x} - \boldsymbol{y}|} \delta\Big(t - \frac{|\boldsymbol{x} - \boldsymbol{y}|}{c_o}\Big), \qquad t > 0$$

$\hookrightarrow$ spherical wave propagating at speed c_o.

Wave equation and Green's function (2/3)

- The time-harmonic Green's function

$$\hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = \int G(t, \boldsymbol{x}, \boldsymbol{y}) e^{i\omega t} dt$$

is the solution of the Helmholtz equation

$$\Delta \hat{G} + \frac{\omega^2}{c^2(\boldsymbol{x})} \hat{G} = -\delta(\boldsymbol{x} - \boldsymbol{y}),$$

with the Sommerfeld radiation condition ($c(\boldsymbol{x}) = c_o$ at infinity):

$$\lim_{|\boldsymbol{x}| \to \infty} |\boldsymbol{x}| \Big(\frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla_{\boldsymbol{x}} - i \frac{\omega}{c_o} \Big) \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = 0$$

If the medium is homogeneous $c(\boldsymbol{x}) \equiv c_o$, then

$$\hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = \frac{1}{4\pi |\boldsymbol{x} - \boldsymbol{y}|} e^{i \frac{\omega}{c_o} |\boldsymbol{x} - \boldsymbol{y}|}$$

Wave equation and Green's function (3/3)

- The solution of the wave equation with source $n(t, \boldsymbol{x})$

$$\frac{1}{c^2(\boldsymbol{x})} \frac{\partial^2 u}{\partial t^2} - \Delta_{\boldsymbol{x}} u = n(t, \boldsymbol{x})$$

has the form:

$$u(t, \boldsymbol{x}) = \iint G(t - s, \boldsymbol{x}, \boldsymbol{y}) n(s, \boldsymbol{y}) d\boldsymbol{y} ds$$

In the Fourier domain:

$$\hat{u}(\omega, \boldsymbol{x}) = \int u(t, \boldsymbol{x}) e^{i\omega t} dt$$

we have

$$\hat{u}(\omega, \boldsymbol{x}) = \int \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) \hat{n}(\omega, \boldsymbol{y}) d\boldsymbol{y}$$

Complement: Sommerfeld radiation condition (1/2)

- Consider the fundamental solution of the Helmholtz equation in $\mathbb{R}^3$:

$$\Delta_{\boldsymbol{x}} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) + \frac{\omega^2}{c^2(\boldsymbol{x})} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = -\delta(\boldsymbol{x} - \boldsymbol{y})$$

This equation has an infinite number of solutions.

- A solution is called radiating if it satisfies the Sommerfeld radiation condition:

$$\Big(\quad \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = \underset{|\boldsymbol{x}| \to \infty}{O} \big(\frac{1}{|\boldsymbol{x}|}\big) \quad \Big) \qquad \text{and} \qquad \big(\frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla_{\boldsymbol{x}} - i\frac{\omega}{c_o}\big) \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = \underset{|\boldsymbol{x}| \to \infty}{o} \big(\frac{1}{|\boldsymbol{x}|}\big)$$

uniformly in all directions ($c(\boldsymbol{x}) = c_o$ at infinity).

- Example: $c(\boldsymbol{x}) \equiv c_o$. There exist infinitely many solutions, in particular

$$\hat{G}_a(\omega, \boldsymbol{x}, \boldsymbol{y}) = \frac{1-a}{4\pi|\boldsymbol{x} - \boldsymbol{y}|} \exp\Big(i\frac{\omega}{c_o}|\boldsymbol{x} - \boldsymbol{y}|\Big) + \frac{a}{4\pi|\boldsymbol{x} - \boldsymbol{y}|} \exp\Big(-i\frac{\omega}{c_o}|\boldsymbol{x} - \boldsymbol{y}|\Big)$$

for some constant a. Only the solution with $a = 0$ satisfies the Sommerfeld radiation condition. It corresponds to a field radiating from $\boldsymbol{y}$. The other solutions are "unphysical". For example, the solution with $a = 1$ can be interpreted as energy coming from infinity and sinking at $\boldsymbol{y}$.

Complement: Sommerfeld radiation condition (2/2)

• Consider the fundamental solution of the Helmholtz equation in $\mathbb{R}^3$:

$$\Delta_{\boldsymbol{x}} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) + \frac{\omega^2}{c^2(\boldsymbol{x})} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = -\delta(\boldsymbol{x} - \boldsymbol{y})$$

A solution is called radiating if it satisfies the Sommerfeld radiation condition

$$\lim_{|\boldsymbol{x}| \to \infty} |\boldsymbol{x}| \Big(\frac{\boldsymbol{x}}{|\boldsymbol{x}|} \cdot \nabla_{\boldsymbol{x}} - i \frac{\omega}{c_o} \Big) \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = 0$$

uniformly in all directions ($c(\boldsymbol{x}) = c_o$ at infinity).

• Theorem: The Helmholtz equation (with c bounded and constant outside a compact) has a unique radiating solution.

R. Courant and D. Hilbert, Methods of Mathematical Physics, Vol. 2, Chap. IV, Sec. 5.
B. Perthame and L. Vega, Geom. Funct. Anal. **17** 1685-1707 (2008).

Reciprocity

$$\hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}) = \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x})$$

Proof of reciprocity (1/2)

We consider the equations satisfied by the Green's function with the source at $\boldsymbol{y}_2$ and with the source at $\boldsymbol{y}_1$ ($\boldsymbol{y}_2 \neq \boldsymbol{y}_1$):

$$\Delta_{\boldsymbol{x}} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_2) + \frac{\omega^2}{c^2(\boldsymbol{x})} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_2) = -\delta(\boldsymbol{x} - \boldsymbol{y}_2)$$
$$\Delta_{\boldsymbol{x}} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_1) + \frac{\omega^2}{c^2(\boldsymbol{x})} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_1) = -\delta(\boldsymbol{x} - \boldsymbol{y}_1)$$

We multiply the first equation by $\hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_1)$ and subtract the second equation multiplied by $\hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_2)$:

$$\nabla_{\boldsymbol{x}} \cdot \Big[\hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_1) \nabla_{\boldsymbol{x}} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_2) - \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_2) \nabla_{\boldsymbol{x}} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_1) \Big]$$
$$= \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_2) \delta(\boldsymbol{x} - \boldsymbol{y}_1) - \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_1) \delta(\boldsymbol{x} - \boldsymbol{y}_2)$$

We next integrate over the ball $B(\mathbf{0}, L)$ which contains both $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ and use the divergence theorem:

$$\int_{\partial B(\mathbf{0}, L)} \boldsymbol{n} \cdot \Big[\hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_1) \nabla_{\boldsymbol{x}} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_2) - \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_2) \nabla_{\boldsymbol{x}} \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y}_1) \Big] d\sigma(\boldsymbol{x})$$
$$= \hat{G}(\omega, \boldsymbol{y}_1, \boldsymbol{y}_2) - \hat{G}(\omega, \boldsymbol{y}_2, \boldsymbol{y}_1)$$

where $\boldsymbol{n}$ is the unit outward normal to the ball $B(\mathbf{0}, L)$, which is $\boldsymbol{n} = \boldsymbol{x}/|\boldsymbol{x}|$.

Proof of reciprocity (2/2)

$$\int_{\partial B(\mathbf{0},L)} \boldsymbol{n} \cdot \Big[\hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}_1)\nabla_{\boldsymbol{x}}\hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}_2) - \hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}_2)\nabla_{\boldsymbol{x}}\hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}_1)\Big] d\sigma(\boldsymbol{x})$$
$$= \hat{G}(\omega,\boldsymbol{y}_1,\boldsymbol{y}_2) - \hat{G}(\omega,\boldsymbol{y}_2,\boldsymbol{y}_1)$$

where $\boldsymbol{n} = \boldsymbol{x}/|\boldsymbol{x}|$.

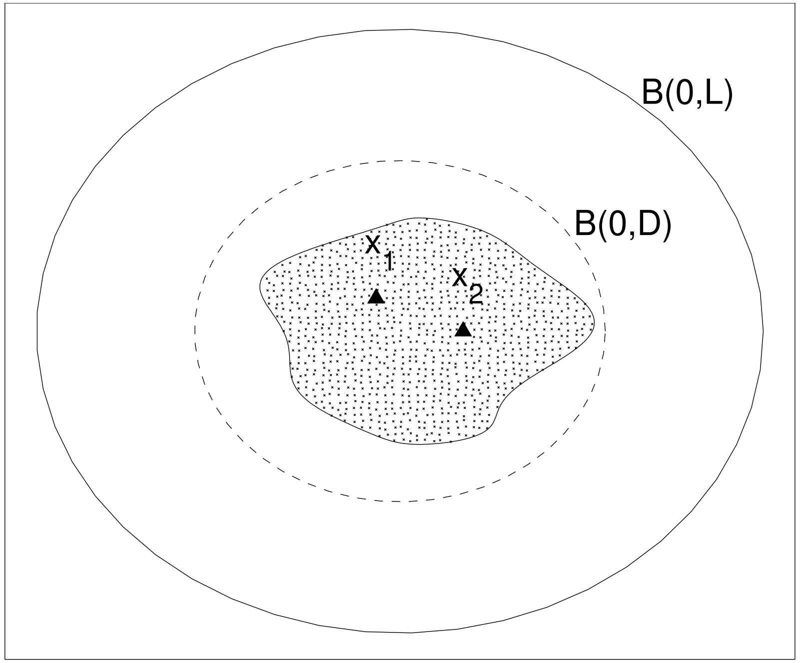
If $\boldsymbol{x} \in \partial B(\mathbf{0},L)$ and $L \to \infty$, then by the Sommerfeld radiation condition:

$$\boldsymbol{n} \cdot \nabla_{\boldsymbol{x}}\hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}) = i\frac{\omega}{c_o}\hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}) + o\Big(\frac{1}{L}\Big)$$

Therefore, for $L \to \infty$,

$$\hat{G}(\omega,\boldsymbol{y}_1,\boldsymbol{y}_2) - \hat{G}(\omega,\boldsymbol{y}_2,\boldsymbol{y}_1)$$
$$= i\frac{\omega}{c_o}\int_{\partial B(\mathbf{0},L)} \hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}_1)\hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}_2) - \hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}_2)\hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}_1) d\sigma(\boldsymbol{x})$$
$$= 0$$

The Helmholtz-Kirchhoff theorem



If the medium is homogeneous (velocity c_o) outside $B(\mathbf{0},D)$, then $\forall \boldsymbol{x}_1, \boldsymbol{x}_2 \in B(\mathbf{0},D)$ we have for $L \gg D$:

$$\hat{G}(\omega, \boldsymbol{x}_1, \boldsymbol{x}_2) - \overline{\hat{G}(\omega, \boldsymbol{x}_1, \boldsymbol{x}_2)} = \frac{2i\omega}{c_o} \int_{\partial B(\mathbf{0},L)} d\sigma(\boldsymbol{y}) \overline{\hat{G}(\omega, \boldsymbol{x}_1, \boldsymbol{y})} \hat{G}(\omega, \boldsymbol{x}_2, \boldsymbol{y})$$

Proof: second Green's identity and Sommerfeld radiation condition.

Useful for: scattering theory, time reversal experiment, and cross correlation.

Proof of Helmholtz-Kirchhoff theorem (1/2)

Consider

$$\Delta_{\boldsymbol{y}} \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2) + \frac{\omega^2}{c^2(\boldsymbol{y})} \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2) = -\delta(\boldsymbol{y} - \boldsymbol{x}_2)$$

$$\Delta_{\boldsymbol{y}} \overline{\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1)} + \frac{\omega^2}{c^2(\boldsymbol{y})} \overline{\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1)} = -\delta(\boldsymbol{y} - \boldsymbol{x}_1)$$

Multiply the first equation by $\overline{\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1)}$ and subtract the second equation multiplied by $\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2)$:

$$\begin{aligned} &\nabla_{\boldsymbol{y}} \cdot \Big[\overline{\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1)} \nabla_{\boldsymbol{y}} \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2) - \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2) \nabla_{\boldsymbol{y}} \overline{\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1)} \Big] \\ &= \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2) \delta(\boldsymbol{y} - \boldsymbol{x}_1) - \overline{\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1)} \delta(\boldsymbol{y} - \boldsymbol{x}_2) \\ &= \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2) \delta(\boldsymbol{y} - \boldsymbol{x}_1) - \overline{\hat{G}(\omega, \boldsymbol{x}_1, \boldsymbol{y})} \delta(\boldsymbol{y} - \boldsymbol{x}_2) \end{aligned}$$

using the reciprocity property $\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1) = \hat{G}(\omega, \boldsymbol{x}_1, \boldsymbol{y})$.

Integrate over the ball $B(\mathbf{0}, L)$ and use the divergence theorem:

$$\begin{aligned} &\int_{\partial B(\mathbf{0},L)} \boldsymbol{n} \cdot \Big[\overline{\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1)} \nabla_{\boldsymbol{y}} \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2) - \hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_2) \nabla_{\boldsymbol{y}} \overline{\hat{G}(\omega, \boldsymbol{y}, \boldsymbol{x}_1)} \Big] d\sigma(\boldsymbol{y}) \\ &= \hat{G}(\omega, \boldsymbol{x}_1, \boldsymbol{x}_2) - \overline{\hat{G}(\omega, \boldsymbol{x}_1, \boldsymbol{x}_2)} \end{aligned}$$

where $\boldsymbol{n}$ is the unit outward normal to the ball $B(\mathbf{0}, L)$, which is $\boldsymbol{n} = \boldsymbol{y}/|\boldsymbol{y}|$.

Proof of Helmholtz-Kirchhoff theorem (2/2)

$$\int_{\partial B(\mathbf{0},L)} \boldsymbol{n} \cdot \Big[\overline{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_1)} \nabla_{\boldsymbol{y}} \hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_2) - \hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_2) \nabla_{\boldsymbol{y}} \overline{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_1)} \Big] d\sigma(\boldsymbol{y})$$
$$= \hat{G}(\omega,\boldsymbol{x}_1,\boldsymbol{x}_2) - \overline{\hat{G}(\omega,\boldsymbol{x}_1,\boldsymbol{x}_2)}$$

where $\boldsymbol{n} = \boldsymbol{y}/|\boldsymbol{y}|$.
This equality can be viewed as an application of the second Green's identity.

The Green's function also satisfies the Sommerfeld radiation condition

$$\lim_{|\boldsymbol{y}|\to\infty} |\boldsymbol{y}| \Big(\frac{\boldsymbol{y}}{|\boldsymbol{y}|} \cdot \nabla_{\boldsymbol{y}} - \ i\frac{\omega}{c_o} \Big) \hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_1) = 0$$

uniformly in all directions $\boldsymbol{y}/|\boldsymbol{y}|$. Substitute $i(\omega/c_o)\hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_2)$ for $\boldsymbol{n} \cdot \nabla_{\boldsymbol{y}} \hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_2)$ in the surface integral over $\partial B(\mathbf{0},L)$, and $-i(\omega/c_o)\overline{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_1)}$ for $\boldsymbol{n} \cdot \nabla_{\boldsymbol{y}} \overline{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{x}_1)}$, which gives the desired result:

$$\hat{G}(\omega,\boldsymbol{x}_1,\boldsymbol{x}_2) - \overline{\hat{G}(\omega,\boldsymbol{x}_1,\boldsymbol{x}_2)} = \frac{2i\omega}{c_o} \int_{\partial B(\mathbf{0},L)} d\sigma(\boldsymbol{y}) \overline{\hat{G}(\omega,\boldsymbol{x}_1,\boldsymbol{y})} \hat{G}(\omega,\boldsymbol{x}_2,\boldsymbol{y})$$

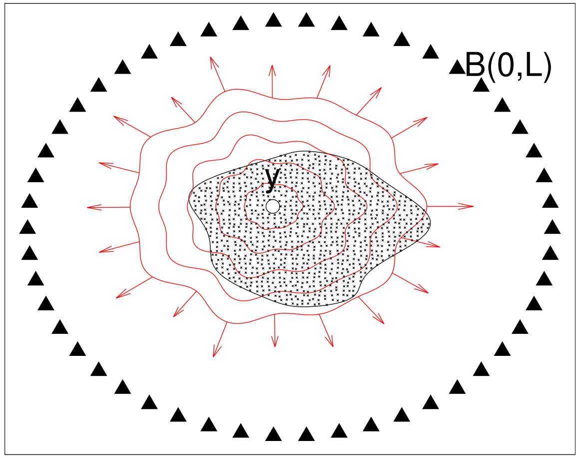
Time-reversal refocusing on a source (1/2)

First part:

A point source at $\boldsymbol{y}$ emits a pulse $f(t)$.

The waves are recorded at the surface $\partial B(\mathbf{0}, L)$:

$\hat{u}(\omega, \boldsymbol{x}) = \hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y})\hat{f}(\omega), \quad \boldsymbol{x} \in \partial B(\mathbf{0}, L)$



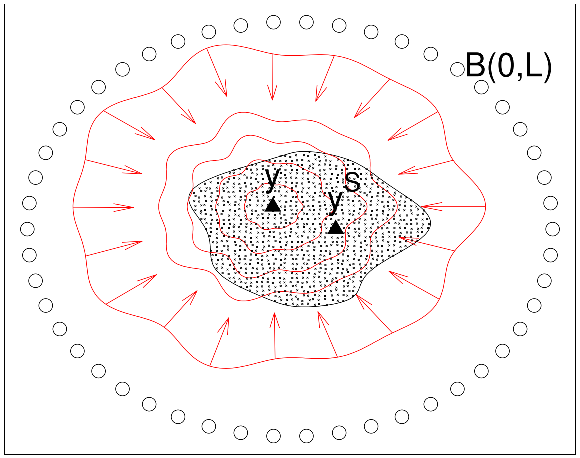
Second part:

The recorded signals are time-reversed

and sent back into the medium.

The signal received at $\boldsymbol{y}^S$ is

$$\hat{u}_{\mathrm{TR}}(\omega, \boldsymbol{y}^S) = \int_{\partial B(\mathbf{0},L)} d\sigma(\boldsymbol{x})\hat{G}(\omega, \boldsymbol{y}^S, \boldsymbol{x})\overline{\hat{G}(\omega, \boldsymbol{x}, \boldsymbol{y})\hat{f}(\omega)}$$



Time-reversal refocusing on a source (2/2)

The signal received at $\boldsymbol{y}^S$ is (using reciprocity: $\hat{G}(\omega,\boldsymbol{x},\boldsymbol{y}) = \hat{G}(\omega,\boldsymbol{y},\boldsymbol{x})$):

$$\hat{u}_{\rm TR}(\omega,\boldsymbol{y}^S) = \int_{\partial B(\boldsymbol{0},L)} d\sigma(\boldsymbol{x}) \overline{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{x})}\hat{G}(\omega,\boldsymbol{y}^S,\boldsymbol{x})\overline{\hat{f}(\omega)}$$

By Helmholtz-Kirchhoff identity:

$$\hat{G}(\omega,\boldsymbol{y},\boldsymbol{y}^S) - \overline{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{y}^S)} = \frac{2i\omega}{c_o}\int_{\partial B(\boldsymbol{0},L)} d\sigma(\boldsymbol{x}) \overline{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{x})}\hat{G}(\omega,\boldsymbol{y}^S,\boldsymbol{x})$$

we get

$$\hat{u}_{\rm TR}(\omega,\boldsymbol{y}^S) = \frac{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{y}^S) - \overline{\hat{G}(\omega,\boldsymbol{y},\boldsymbol{y}^S)}}{2i\omega/c_o}\overline{\hat{f}(\omega)} = \frac{c_o}{\omega}{\rm Im}\big(\hat{G}(\omega,\boldsymbol{y},\boldsymbol{y}^S)\big)\overline{\hat{f}(\omega)}$$

[Remember: $\boldsymbol{y}$ is the original source location].

In a three-dimensional homogeneous medium:

$$\hat{G}(\omega,\boldsymbol{y},\boldsymbol{y}^S) = \frac{1}{4\pi|\boldsymbol{y}-\boldsymbol{y}^S|}e^{i\frac{\omega|\boldsymbol{y}-\boldsymbol{y}^S|}{c_o}} \quad \Longrightarrow \quad \hat{u}_{\rm TR}(\omega,\boldsymbol{y}^S) = \frac{1}{4\pi}{\rm sinc}\Big(\frac{\omega|\boldsymbol{y}-\boldsymbol{y}^S|}{c_o}\Big)\overline{\hat{f}(\omega)}$$

$\hookrightarrow$ refocusing with a focal spot of diameter $\lambda/2 = \pi c_o/\omega$ (diffraction limit), ${\rm sinc}(s) = \frac{\sin(s)}{s}$.

Least-square inverse problems

Inverse problems

• We look for $\boldsymbol{m} \in \mathcal{X}$, the input parameters of a model, given the observed output $\boldsymbol{y} \in \mathcal{Y}$:

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{m}),$$

where $\boldsymbol{f} : \mathcal{X} \to \mathcal{Y}$, $\mathcal{X}$ and $\mathcal{Y}$ are abstract spaces (Banach).

• Example: calibration of a model.
We have:
- a parametric family of models $f_{\boldsymbol{m}} : \mathbb{R}^d \to \mathbb{R}$, parameterized by $\boldsymbol{m} \in \mathbb{R}^p$,
- a sample of observations $(\boldsymbol{x}_i, y_i)_{i=1}^n$ with $y_i = f_{\boldsymbol{m}^*}(\boldsymbol{x}_i)$(+noise), where $\boldsymbol{m}^*$ is unknown.

We want to determine the $\boldsymbol{m}$ that best fits the data.
Here $\mathcal{X} = \mathbb{R}^p$, $\mathcal{Y} = \mathbb{R}^n$, $\boldsymbol{y} = (y_i)_{i=1}^n$ and $\boldsymbol{f}(\boldsymbol{m}) = (f_{\boldsymbol{m}}(\boldsymbol{x}_i))_{i=1}^n$.

- A problem is ill-posed (in Hadamard's sense) if one of three following events occurs:
  - there is no solution,
  - the solution is not unique,
  - the solution is very sensitive to the data $\boldsymbol{y}$.

- In order to solve an inverse problem, the classical approach is to formulate a least-square minimization problem:

$$\underset{\boldsymbol{m}\in\mathcal{X}}{\operatorname{argmin}} \ \|\boldsymbol{y}-\boldsymbol{f}(\boldsymbol{m})\|_{\mathcal{Y}}^2.$$

This approach can fail:

- theres is no solution in $\mathcal{X}$,
- there are several minima,
- the solution is very sensitive to the data $\boldsymbol{y}$.

Linear inverse problems

- Here $\mathcal{X} = \mathbb{R}^p$, $\mathcal{Y} = \mathbb{R}^n$, $\boldsymbol{f}(\boldsymbol{m}) = \mathbf{A}\boldsymbol{m}$ with $\mathbf{A}$ a $n \times p$ matrix (with $n \geq p$). We look for

$$\mathcal{S} = \underset{\boldsymbol{m} \in \mathcal{X}}{\operatorname{argmin}} \|\boldsymbol{y} - \mathbf{A}\boldsymbol{m}\|^2$$

- Normal equations:

$$\boldsymbol{m} \in \mathcal{S} \text{ iff } \mathbf{A}^T \mathbf{A} \boldsymbol{m} = \mathbf{A}^T \boldsymbol{y}$$

where $\cdot^T$ stands for transpose (it would be the conjugate transpose in the complex case).
Remark: The normal equations concentrate the problem and the data.

- Use the SVD of $\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$. The rank r of $\mathbf{A}$ is the number of positive singular values. We have

$$\mathcal{S} = \mathbf{A}^+ \boldsymbol{y} + \mathrm{Ker}(\mathbf{A}) = \Big\{ \mathbf{A}^+ \boldsymbol{y} + \sum_{j=r+1}^{p} \alpha_j \boldsymbol{v}_j, \; \alpha_j \in \mathbb{R}, \; j = r+1, \ldots, p \Big\}$$

where $\mathbf{A}^+$ is the pseudo-inverse of $\mathbf{A}$:

$$\mathbf{A}^+ = \mathbf{V}\boldsymbol{\Sigma}^+ \mathbf{U}^T, \qquad \boldsymbol{\Sigma} = \mathrm{Diag}(\sigma_1^{-1}, \ldots, \sigma_r^{-1}, 0, \ldots, 0)$$

• Amongst all the solutions (elements of $\mathcal{S}$) we can determine the one with the minimal norm:

$$\boldsymbol{m}_{\mathrm{LS}} = \underset{\boldsymbol{m} \in \mathcal{S}}{\operatorname{argmin}} \ \|\boldsymbol{m}\|^2 = \mathbf{A}^{+}\boldsymbol{y}$$

If $\boldsymbol{y} = \sum_{j=1}^{n} \beta_j \boldsymbol{u}_j$ (where the $\boldsymbol{u}_j$ are the columns of $\mathbf{U}$), then we have

$$\|\boldsymbol{y} - \mathbf{A}\boldsymbol{m}_{\mathrm{LS}}\|^2 = \sum_{j=r+1}^{n} \beta_j^2$$

• If $\boldsymbol{y} = \mathbf{A}\boldsymbol{m}^{\mathrm{v}}$, $\boldsymbol{m}^{\mathrm{v}} = \sum_{j=1}^{p} m_j^{\mathrm{v}} \boldsymbol{v}_j$ (where the $\boldsymbol{v}_j$ are the columns of $\mathbf{V}$), then

$$\boldsymbol{m}_{\mathrm{LS}} = \sum_{j=1}^{r} m_j^{\mathrm{v}} \boldsymbol{v}_j$$

and

$$\|\boldsymbol{m}_{\mathrm{LS}} - \boldsymbol{m}^{\mathrm{v}}\|^2 = \sum_{j=r+1}^{p} (m_j^{\mathrm{v}})^2$$

$\rightarrow$ we can determine all coordinates of $\boldsymbol{m}^{\mathrm{v}}$ except those which are in $\mathrm{Ker}(\mathbf{A})$.

- If $\mathbf{A}$ has rank p then $\mathbf{A}^T\mathbf{A}$ is invertible and $\mathcal{S}$ is reduced to one point:

$$\hat{\boldsymbol{m}} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\boldsymbol{y}$$

Remark: $\mathrm{rg}(\mathbf{A}) = p$ iff $\mathrm{Ker}(\mathbf{A}) = \{\mathbf{0}\}$ iff $\mathbf{A}^T\mathbf{A}$ is invertible.

- If $\boldsymbol{y} = \mathbf{A}\boldsymbol{m}^{\mathrm{v}}$, then $\hat{\boldsymbol{m}} = \boldsymbol{m}^{\mathrm{v}}$. Great !
- If $\boldsymbol{y} = \mathbf{A}\boldsymbol{m}^{\mathrm{v}} + \boldsymbol{\varepsilon}$, then, using the SVD of $\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$, we get

$$\hat{\boldsymbol{m}} = \boldsymbol{m}^{\mathrm{v}} + \sum_{j=1}^{p} \frac{1}{\sigma_j}\varepsilon_j \boldsymbol{v}_j, \quad \varepsilon_j = \boldsymbol{u}_j^T \boldsymbol{\varepsilon}.$$

If $\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \sigma_{\mathrm{mes}}^2 \mathbf{I})$, then ε_j are i.i.d. with the distribution $\mathcal{N}(0, \sigma_{\mathrm{mes}}^2)$ and therefore

$$\mathbb{E}\big[\|\hat{\boldsymbol{m}} - \boldsymbol{m}^{\mathrm{v}}\|^2\big] = \sum_{j=1}^{p} \frac{\sigma_{\mathrm{mes}}^2}{\sigma_j^2}$$

$\rightarrow$ If $\mathbf{A}$ has a very small singular value, then the error blows up !

Regularization of ill-posed inverse problems

- A way to regularize the problem is to consider:

$$\underset{\boldsymbol{m}\in\mathcal{X}}{\operatorname{argmin}} \Big(\|\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{m})\|_{\mathcal{Y}}^2 + \|\boldsymbol{m} - \boldsymbol{m}_0\|_{\mathcal{X}'}^2 \Big),$$

with a norm $\|\cdot\|_{\mathcal{X}'}$ equal to or stronger than the norm $\|\cdot\|_{\mathcal{X}}$ and $\boldsymbol{m}_0 \in \mathcal{X}'$.

The penalization represents an a priori idea on the structure of the solution.

- Tikhonov regularization: $\|\cdot\|_{\mathcal{X}'} = \alpha\|\cdot\|_{\mathcal{X}}$ for some $\alpha > 0$.

A priori idea: the solution should not have a very large norm $\|\cdot\|_{\mathcal{X}}$.
If α is large enough, then the function to be minimized may become convex.
However: If α is too large, then the regularized problem becomes significantly different from the original problem.

- L^2 regularization (ridge regression).

Here $\mathcal{X} = \mathbb{R}^p$, $\mathcal{Y} = \mathbb{R}^n$, $\boldsymbol{f}(\boldsymbol{m}) = \mathbf{A}\boldsymbol{m}$ with $\mathbf{A}$ $n \times p$-matrix with $p \leq n$.
Let $\alpha > 0$. We look for

$$\underset{\boldsymbol{m}\in\mathcal{X}}{\operatorname{argmin}} \Big(\|\boldsymbol{y} - \mathbf{A}\boldsymbol{m}\|^2 + \alpha \|\boldsymbol{m}\|^2 \Big)$$

- Normal equations:

$$\boldsymbol{m} \in \mathcal{S}_\alpha \text{ iff } \big(\mathbf{A}^T\mathbf{A} + \alpha\mathbf{I}\big)\boldsymbol{m} = \mathbf{A}^T\boldsymbol{y}.$$

- There is a unique solution because $\mathbf{A}^T\mathbf{A} + \alpha\mathbf{I}$ is positive-definite:

$$\hat{\boldsymbol{m}}_\alpha = \big(\mathbf{A}^T\mathbf{A} + \alpha\mathbf{I}\big)^{-1}\mathbf{A}^T\boldsymbol{y}$$

- By using the SVD of $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$, we find

$$\hat{\boldsymbol{m}}_\alpha = \sum_{j=1}^{p} \frac{\sigma_j}{\sigma_j^2 + \alpha} y_j \boldsymbol{v}_j, \quad y_j = \boldsymbol{u}_j^T \boldsymbol{y}$$

$$\hat{\boldsymbol{m}}_\alpha = \sum_{j=1}^{p} \frac{\sigma_j}{\sigma_j^2 + \alpha} y_j \boldsymbol{v}_j, \quad y_j = \boldsymbol{u}_j^T \boldsymbol{y}$$

- If $\boldsymbol{y} = \mathbf{A}\boldsymbol{m}^{\mathrm{v}}$, with $\boldsymbol{m}^{\mathrm{v}} = \sum_{j=1}^{p} m_j^{\mathrm{v}} \boldsymbol{v}_j$, $m_j^{\mathrm{v}} = \boldsymbol{v}_j^T \boldsymbol{m}$, then $\boldsymbol{y} = \sum_{j=1}^{n} y_j \boldsymbol{u}_j$ with $y_j = \sigma_j m_j^{\mathrm{v}}$. Therefore

$$\hat{\boldsymbol{m}}_\alpha = \sum_{j=1}^{p} \frac{\sigma_j^2}{\sigma_j^2 + \alpha} m_j^{\mathrm{v}} \boldsymbol{v}_j$$

and the error is

$$\hat{\boldsymbol{m}}_\alpha - \boldsymbol{m}^{\mathrm{v}} = -\sum_{j=1}^{p} \frac{\alpha}{\sigma_j^2 + \alpha} m_j^{\mathrm{v}} \boldsymbol{v}_j$$

$$\|\hat{\boldsymbol{m}}_\alpha - \boldsymbol{m}^{\mathrm{v}}\|^2 = \sum_{j=1}^{p} \frac{\alpha^2}{(\sigma_j^2 + \alpha)^2} (m_j^{\mathrm{v}})^2$$

$\rightarrow$ It seems that we should take $\alpha = 0$!

$$\hat{\boldsymbol{m}}_\alpha = \sum_{j=1}^{p} \frac{\sigma_j}{\sigma_j^2+\alpha} y_j \boldsymbol{v}_j, \quad y_j = \boldsymbol{u}_j^T \boldsymbol{y}$$

- If $\boldsymbol{y} = \mathbf{A}\boldsymbol{m}^{\rm v} + \boldsymbol{\varepsilon}$, with $\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \sigma_{\rm mes}^2 \mathbf{I})$, then we find

$$\hat{\boldsymbol{m}}_\alpha = \sum_{j=1}^{p} \frac{\sigma_j^2}{\sigma_j^2+\alpha} m_j^{\rm v} \boldsymbol{v}_j + \sum_{j=1}^{p} \frac{\sigma_j}{\sigma_j^2+\alpha} \varepsilon_j \boldsymbol{v}_j, \quad \varepsilon_j = \boldsymbol{u}_j^T \boldsymbol{\varepsilon}$$

Since ε_j are i.i.d. with the distribution $\mathcal{N}(0, \sigma_{\rm mes}^2)$,

$$\begin{aligned} \mathbb{E}\big[\|\hat{\boldsymbol{m}}_\alpha - \boldsymbol{m}^{\rm v}\|^2\big] &= \mathbb{E}\big[\|\hat{\boldsymbol{m}}_\alpha - \mathbb{E}[\hat{\boldsymbol{m}}_\alpha]\|^2\big] + \|\mathbb{E}[\hat{\boldsymbol{m}}_\alpha] - \boldsymbol{m}^{\rm v}\|^2 \\ &= \underbrace{\sum_{j=1}^{p} \frac{\sigma_j^2}{(\sigma_j^2+\alpha)^2} \sigma_{\rm mes}^2}_{variance} + \underbrace{\sum_{j=1}^{p} \frac{\alpha^2}{(\sigma_j^2+\alpha)^2} (m_j^{\rm v})^2}_{bias} \end{aligned}$$

→ The variance term does not blow up when there are small singular values, it is bounded by $p\sigma_{\rm mes}^2/(4\alpha)$ uniformly w.r.t. $(\sigma_j)_{j=1}^p$.
→ By allowing for a small bias, one can strongly reduce the variance.
↪ We look for adjusting the parameter α in order to minimize $\mathbb{E}\big[\|\hat{\boldsymbol{m}}_\alpha - \boldsymbol{m}^{\rm v}\|^2\big]$ (bias-variance trade-off).

$$\mathbb{E}\big[\|\hat{\boldsymbol{m}}_\alpha - \boldsymbol{m}^{\mathrm{v}}\|^2\big] = \sum_{j=1}^{p} \frac{\sigma_j^2}{(\sigma_j^2+\alpha)^2}\sigma_{\mathrm{mes}}^2 + \sum_{j=1}^{p} \frac{\alpha^2}{(\sigma_j^2+\alpha)^2}(m_j^{\mathrm{v}})^2$$

• The optimal α depends on $\boldsymbol{m}^{\mathrm{v}}$ and $\mathbf{A}$, it exists and it is positive.
→ one must regularize !

Proof (of positivity). The function $\alpha \mapsto \mathbb{E}\big[\|\hat{\boldsymbol{m}}_\alpha - \boldsymbol{m}^{\mathrm{v}}\|^2\big]$ is continuous, decaying close to 0,

$$\mathbb{E}\big[\|\hat{\boldsymbol{m}}_\alpha - \boldsymbol{m}^{\mathrm{v}}\|^2\big] = \Big[\sum_{j=1}^{p} \sigma_j^{-2}\sigma_{\mathrm{mes}}^2\Big] - \alpha\Big[2\sum_{j=1}^{p} \sigma_j^{-4}\sigma_{\mathrm{mes}}^2\Big] + O(\alpha^2), \quad \alpha \to 0^+,$$

and increasing at infinity:

$$\mathbb{E}\big[\|\hat{\boldsymbol{m}}_\alpha - \boldsymbol{m}^{\mathrm{v}}\|^2\big] = \Big[\sum_{j=1}^{p} (m_j^{\mathrm{v}})^2\Big] - \alpha^{-1}\Big[2\sum_{j=1}^{p} \sigma_j^2(m_j^{\mathrm{v}})^2\Big] + O(\alpha^{-2}), \quad \alpha \to +\infty.$$

• In practice (Morozov rule): choose α so that $\|\boldsymbol{y} - \mathbf{A}\hat{\boldsymbol{m}}_\alpha\|^2 \simeq \mathbb{E}[\|\boldsymbol{\varepsilon}\|^2] = n\sigma_{\mathrm{mes}}^2$.
→ do not try to adjust the model with an accuracy higher than the noise level (overfitting).

• L^0 regularization:

$$\underset{\boldsymbol{m}\in\mathcal{X}}{\operatorname{argmin}} \left(\|\boldsymbol{y} - \mathbf{A}\boldsymbol{m}\|^2 + \alpha \|\boldsymbol{m}\|_0 \right),$$

with $\|\boldsymbol{m}\|_0 = \sum_{j=1}^{p} \mathbf{1}_{m_j \neq 0} = \mathrm{Card}\{j = 1, \dots, p\,,\ m_j \neq 0\}$.

• We look for a *sparse* solution (parameter selection).

• The problem is numerically very challenging.

• L^1 regularization (lasso regression = Least Absolute Shrinkage and Selection Operator):

$$\underset{\boldsymbol{m}\in\mathcal{X}}{\operatorname{argmin}} \left(\|\boldsymbol{y} - \mathbf{A}\boldsymbol{m}\|^2 + \alpha \|\boldsymbol{m}\|_1 \right),$$

with $\|\boldsymbol{m}\|_1 = \sum_{j=1}^{p} |m_j|$.

• For "good" matrices **A** (satisfying the RIP - Restricted Isometry Property), the solution of the L^1-regularized problem is the same as the solution of the L^0-regularized problem.

• The problem is numerically challenging (not differentiable function), but not impossible (in particular, when the solution is sparse).

Bayesian approach of inverse problems

• Principle: We do not look for a unique answer, but a probability measure on $\mathcal{X}$ which gives the likelihood of the states $\boldsymbol{m}$ given $\boldsymbol{y}$.

• We assume that:
- $\mathcal{X} = \mathbb{R}^p$ and $\mathcal{Y} = \mathbb{R}^n$.
- We have a priori information on the most likely states $\boldsymbol{m}$ in the form of an a priori distribution on $\mathcal{X}$ with density π_0 (w.r.t. the Lebesgue measure on $\mathcal{X}$).
- The observations are noisy:

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{m}) + \boldsymbol{\eta},$$

where $\boldsymbol{\eta}$ is a random variable taking values in $\mathcal{Y}$ with density ρ (w.r.t. the Lebesgue measure on $\mathcal{Y}$).

$\rightarrow$ The likelihood (distribution of $\boldsymbol{y}$ given $\boldsymbol{m}$) has density $\rho(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{m}))$.

$\rightarrow$ Bayes theorem: the a posteriori distribution of $\boldsymbol{m}$ given $\boldsymbol{y}$ has density:

$$\pi_{\boldsymbol{y}}(\boldsymbol{m}) = \frac{\rho(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{m}))\pi_0(\boldsymbol{m})}{\int_{\mathbb{R}^p} \rho(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{m}'))\pi_0(\boldsymbol{m}')d\boldsymbol{m}'}.$$

Bayesian approach - Gaussian case

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{m}) + \boldsymbol{\eta}$$

• We assume, moreover, that the a priori distribution of $\boldsymbol{m}$ is $\mathcal{N}(\boldsymbol{m}_0, \boldsymbol{\Sigma}_0)$ and that the distribution of $\boldsymbol{\eta}$ is $\mathcal{N}(\boldsymbol{0}, \boldsymbol{\Gamma})$, with invertible real matrices $\boldsymbol{\Sigma}_0$ and $\boldsymbol{\Gamma}$.

$$\pi^0(\boldsymbol{m}) = \frac{1}{(2\pi)^{p/2}\mathrm{Det}(\boldsymbol{\Sigma}_0)^{1/2}} \exp\Big(-\frac{1}{2}(\boldsymbol{m}-\boldsymbol{m}_0)^T \boldsymbol{\Sigma}_0^{-1}(\boldsymbol{m}-\boldsymbol{m}_0)\Big)$$

• The a posteriori distribution of $\boldsymbol{m}$ given $\boldsymbol{y}$ has density:

$$\pi_{\boldsymbol{y}}(\boldsymbol{m}) \approx \exp\Big(-\frac{1}{2}\|\boldsymbol{y}-\boldsymbol{f}(\boldsymbol{m})\|_{\boldsymbol{\Gamma}}^2 - \frac{1}{2}\|\boldsymbol{m}-\boldsymbol{m}_0\|_{\boldsymbol{\Sigma}_0}^2\Big),$$

where

$$\|\boldsymbol{y}\|_{\boldsymbol{\Gamma}}^2 = \boldsymbol{y}^T\boldsymbol{\Gamma}^{-1}\boldsymbol{y} = (\boldsymbol{\Gamma}^{-1/2}\boldsymbol{y})^T\boldsymbol{\Gamma}^{-1/2}\boldsymbol{y} = \|\boldsymbol{\Gamma}^{-1/2}\boldsymbol{y}\|^2.$$

• The Maximum A Posteriori (MAP) (mode of the a posteriori distribution of $\boldsymbol{m}$ given $\boldsymbol{y}$) is:

$$\underset{\boldsymbol{m}\in\mathbb{R}^p}{\mathrm{argmin}} \Big(\|\boldsymbol{y}-\boldsymbol{f}(\boldsymbol{m})\|_{\boldsymbol{\Gamma}}^2 + \|\boldsymbol{m}-\boldsymbol{m}_0\|_{\boldsymbol{\Sigma}_0}^2\Big).$$

$\hookrightarrow$ We recover the L^2-regularized minimization problem.

Bayesian approach - Laplace case

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{m}) + \boldsymbol{\eta}$$

- We assume, moreover, that the a priori distribution of $\boldsymbol{m}$ is a Laplace distribution with density

$$\pi^0(\boldsymbol{m}) = \lambda^p \exp\Big(-\frac{\lambda}{2}\|\boldsymbol{m}\|_1\Big)$$

with $\lambda > 0$, and that the distribution of $\boldsymbol{\eta}$ is $\mathcal{N}(\mathbf{0}, \boldsymbol{\Gamma})$.

- The a posteriori distribution of $\boldsymbol{m}$ given $\boldsymbol{y}$ has density

$$\pi_{\boldsymbol{y}}(\boldsymbol{m}) \approx \exp\Big(-\frac{1}{2}\|\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{m})\|_{\boldsymbol{\Gamma}}^2 - \frac{\lambda}{2}\|\boldsymbol{m}\|_1\Big).$$

- The Maximum A Posteriori (MAP) is:

$$\underset{\boldsymbol{m}\in\mathbb{R}^p}{\operatorname{argmin}} \Big(\|\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{m})\|_{\boldsymbol{\Gamma}}^2 + \lambda\|\boldsymbol{m}\|_1\Big).$$

$\rightarrow$ We recover the L^1-regularized minimization problem. We understand (from the cusp of the Laplace density) that the MAP favors the solutions with entries equal to 0.