Scientific Computing
Lecture 2

Introduction

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October 5, 2023

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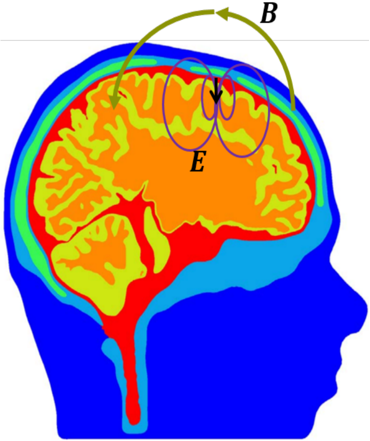
- This intro: example of simulation problem and occurring questions
- General form of SC problems: operator equation
- General classification of SC problems
- Spaces
- SLAE



- Neuronal currents occur inside the cortex.
- **Computational domain:** $\Omega \in \mathbb{R}^3$
- **Phenomenon:** generation of the electric potential by cortical currents.
- **Input:**
  - $\mathbf{J}(\mathbf{x})$ - current density
  - $\sigma(\mathbf{x}), \mathbf{x} \in \text{Head}$ - electric properties
- **Mathematical model:**

$$-div(\sigma \nabla U) = div\mathbf{J};$$

- **OUTPUT:** electric potential: $U(\mathbf{x})$.

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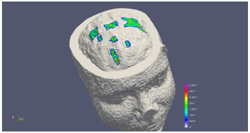
Problem 1: Infinite number of points

- How much points contains the complete number scale $\mathbb{R}$?
- How much points contains the interval $[0, 1] \subset \mathbb{R}$?
- How much points includes the head (computational domain)?
- Computers do not understand infinity.
- How can we use computers for calculations?

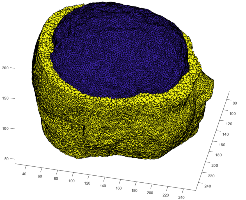
Answer: Divide et impera (lat).

Problem 2: Different properties of data

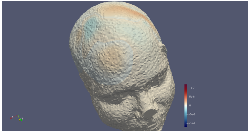
$\mathbf{J}(\mathbf{x})$ - current density inside the cortex:
Discontinuous.



$\sigma(\mathbf{x})$ - the conductivity of the tissues:
Discontinuous, piecewise-constant.



$u(\mathbf{x})$ - the electric potential:
Continuous, smooth function



Answer: Classify data by properties in order to formulate the final mathematical problem.

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Problems Classification

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Or use a microscope to hammer in nails.

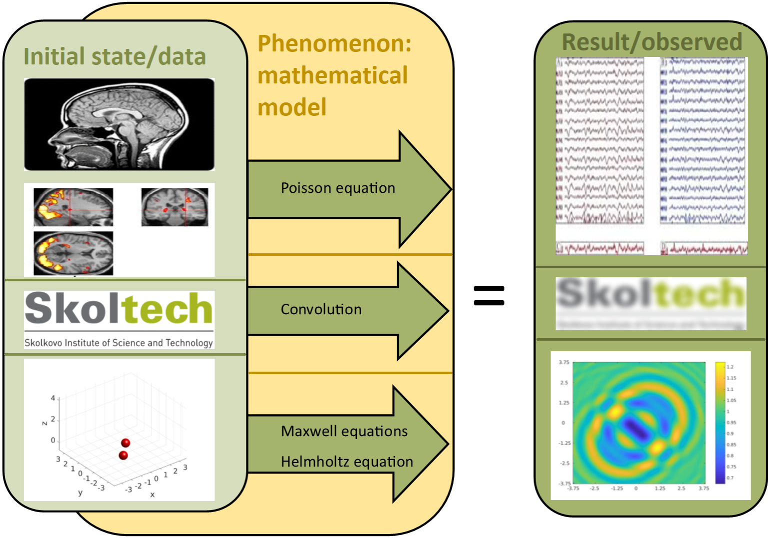
Classification allows:

- Not to reinvent the wheel
- Use proper methodology
- Understand the effective way to solve
- Understand the problem itself

General classification of Scientific Computing problems

- Forward and Inverse problems
- Well-posed and Ill-posed problems
- Static and Dynamic problems
- Deterministic and Stochastic problems
- Continuous and Discrete problems

Phenomena and data



- Or the operator equation: $A\mathbf{f} = \mathbf{b}$.
- The **Residual**: $L(\mathbf{f}, \mathbf{b}) \equiv A\mathbf{f} - \mathbf{b}$.
- $L(\mathbf{f}, \mathbf{b}) = 0$ - another form of equation.

- $\mathbf{f}$ represents some **input** wrt. phenomenon.
- A represents the **mathematical model** of the phenomenon under consideration. A affects at $\mathbf{f}$ resulting at $\mathbf{b}$. May be known, unknown or partially known. May depend on the subject $\mathbf{f}$, or be independent. May be 'virtual'.
- $\mathbf{b}$ represents the **output** wrt. phenomenon or the data observed after phenomenon occurred. Always depends on both **input data f** and **model** A or L.

The input data f could be:

- A vector or a matrix: **f** represents some distribution which defines some state of the phenomenon. Examples:
  - Spatial distribution of properties of the object of research: Electric activity (current density), intensity distribution, color distribution.
  - Spatial distribution of some parameters affecting the phenomenon output (density, solidity, conductivity etc).
  - Temporal distribution of boundary values for heat-transfer problem.
- A set of parameters of different nature, which are affecting on the model behavior. Examples:
  - Scanning electron microscopy: distribution of the electron probe density (function or matrix) comes together with its initial energy (value) and distribution of the density of the object under investigation.
  - Voltammetry: temporal dependence of the cathode current (a vector) comes together with parameters of the electrolyte.
- The input data/state may be changed by phenomenon, or keep unchanged.

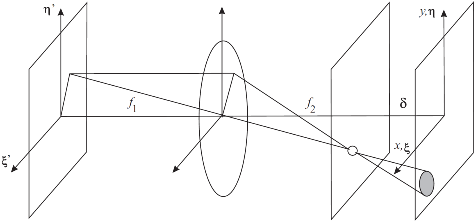
The mathematical description of the phenomenon is called the **Mathematical model**, or just **model**.

- The **model** represents the mathematical connection between the **input** and the **output**.
- The **model** may be both depend or do not depend on $\mathbf{x}$
  - *Example*: Heating of object, heat conductivity of which depends on the temperature. Input is initial heat distribution over the volume under study, model is heat equation, which depends on the initial heat distribution.
  - *Example*: Phenomenon of defocusing of flat screen obviously does not depend on the object it is affecting.
- The **model** may be an object of study; or both **model** and **input data** may be objects of study.
- The **model** may be represented as a differential, integral or matrix/tensor operator.

The output data

- The **output** is a result of application of a **model** on an **input data** .
- In simulation/modelling problems the **output** is the object of study.
- The **output** may be presented with vector of some properties.
- The **output** may be presented with some distribution.
- The **output** may be presented even with a number.
- The **output** may contain all of above.

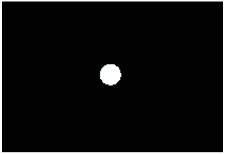
Example: defocused photographs



$$L(f, \mathbf{b}) \equiv K * f - \mathbf{b} = 0, \quad Af \equiv K * f.$$

Input (enter) $f(\mathbf{x})$

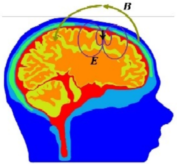
Output $b(\mathbf{x})$

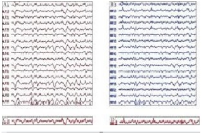


The law (kernel) $K(\mathbf{x}, \xi)$

Source: Yagola A.G., Koshev N.A. Restoration of smeared and defocused color images, Numerical Methods and Programming, V.9, 207-212, 2008 (in Russian)

Example: EEG/MEG





- **The input data:** Intracranial neuronal current distribution $\mathbf{J}(\mathbf{x})$
- **The Model (EEG): Poisson-like equation:**

$$L_{\text{EEG}}(\mathbf{J}, U) \equiv \nabla \cdot \big(\sigma(\mathbf{x}) \nabla U(\mathbf{x})\big) - \nabla \cdot \mathbf{J}(\mathbf{x}) = 0$$

- **The Model (MEG): Poisson-like equation:**

$$L_{\text{MEG}}(\mathbf{J}, \mathbf{B}) \equiv \nabla \times \mathbf{B} - \mu_0(\mathbf{J} - \sigma \nabla U) = 0$$

- **The Observed Data:** magnetic induction $\mathbf{B}(\mathbf{x}_k)$, or electric potential $U(\mathbf{x}_k)$, where x_k is a location of k^{th} sensor

Forward problems, Inverse problems

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General classification of Scientific Computing problems

- Forward and Inverse problems
- Well-posed and Ill-posed problems
- Static and Dynamic problems
- Deterministic and Stochastic problems
- Continuous and Discrete problems

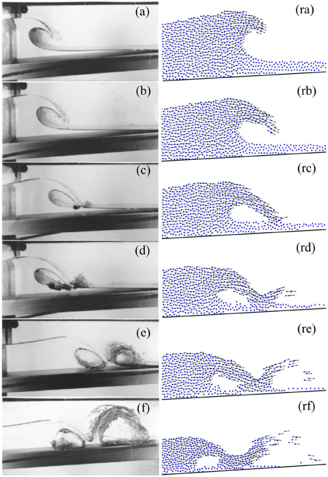
The main equation: $A\mathbf{f} = \mathbf{b}$ or $L(\mathbf{f}, \mathbf{b}) = 0$.

- Forward problem (simulation): find the vector $\mathbf{b}$, if the input data $\mathbf{f}$ and the model A or L are known.
- Inverse problem:
  - Assuming the output $\mathbf{b}$ and the model A to be known, find the **input data f**;
  - Assuming the output $\mathbf{b}$ and the **input data f** are known, define the model A;
  - Assuming the observed data $\mathbf{b}$ to be known, and the model A to be partially known, define $\mathbf{f}$ and complement the definition of the model A.

Forward problem: Applications

- **Studying the processes** Knowing basic principles and laws, it is possible to study more complicated processes, hard to understand from the analytical point of view.
- **Predictions** Knowing the basic rules and principles, it is possible to predict the further behaviour of the object of investigation.
- **Designing the processes:**
  - **Top-down approach (TD).** Knowing the objective process in general, it is possible simulate parts of it in order to optimize the process.
  - **Bottom-up approach (BU).** Knowing the simple interactions between the parts of a system, simulate the overall process.
- **Industrial design of objects: both top-down and bottom-up approaches.**

Forward problem: bottom-up approach



- **input data:** initial state of the system: $\mathbf{u}(t_0), \rho(t_0)$, fluid macroscopic parameters: ν.
- **The model:** Navier-Stokes (moving particles semi-implicit method, MPS):

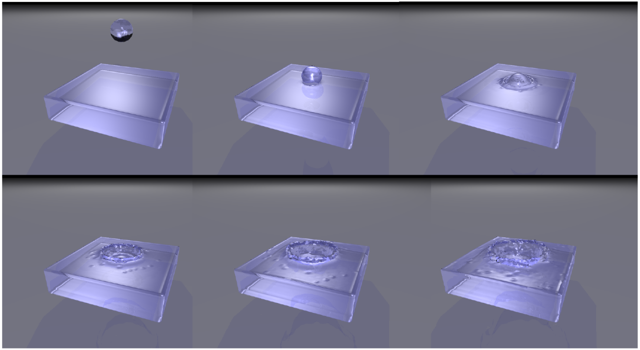
$$\frac{1}{\rho}\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{u} = 0$$

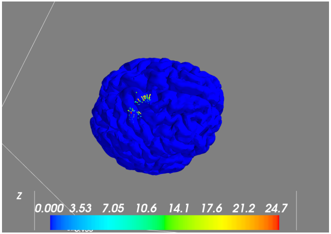
$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g}$$

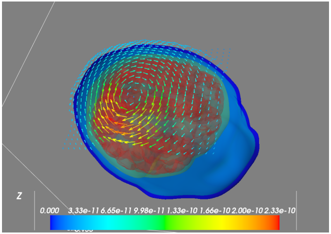
- **The output:** The state of the system at some moment T.
- Take a look at deep learning...

Source: Lizhu Wang et al., Improvement of moving particle semi-implicit method for simulation of progressive water waves. International Journal for Numerical Methods in Fluids, 2017.
Source: Jinning Li, Lianmin Zheng. DEEPWAVE: Deep Learning based Real-time Water Wave

Falling drop example: 200000 particles, 10000 time steps







- **input data:** Current density $\mathbf{J}(\mathbf{x}), \mathbf{x} \in$ Cortex; Conductivity $\sigma(\mathbf{x}), \mathbf{x} \in$ Head.
- **The model:** Poisson equations

$$\Delta \mathbf{B} = \nabla \times (\mathbf{J} - \sigma \nabla U), \mathbf{x} \in \text{Head},$$
$$\nabla \cdot (\sigma \nabla U) = \nabla \cdot \mathbf{J}, \mathbf{x} \in \text{Head}.$$

- **The output:** Magnetic induction $\mathbf{B}(\mathbf{x})$ at positions of N_s sensors $\tilde{\mathbf{x}} = \{\mathbf{x}_k, k = 1, ..., N_s\}$.

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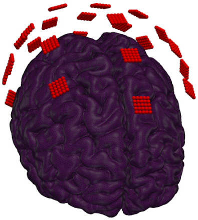
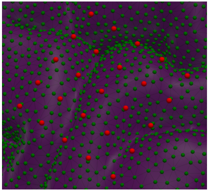
The Leadfield concept

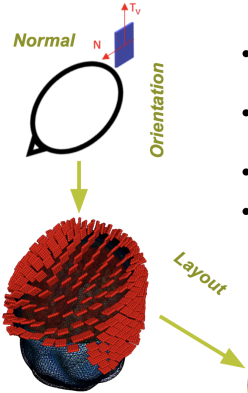


- Red points represent N_s coordinates $\boldsymbol{x}_m \in \mathbb{R}^3$ of sensors' integration points.
- The signal at integration points with the index $m : 0 \leq m \leq N_s$:

$$b_m \sim \frac{\mu_0}{4\pi} \int\limits_{\Omega} d\xi \frac{\nabla \times \big(\boldsymbol{j}(\boldsymbol{\xi}) - \sigma(\boldsymbol{\xi})\nabla u(\boldsymbol{\xi})\big)}{|\boldsymbol{x}_m - \boldsymbol{\xi}|^3}$$

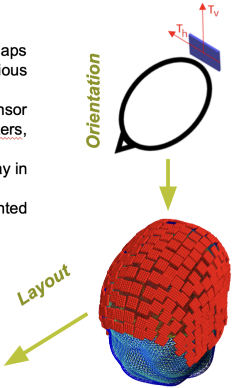
- Green points represent N possible sourcees (clusters) with coordinates $\boldsymbol{\xi}_k \in \Omega$.
- $\boldsymbol{j}(\boldsymbol{\xi}_k)$ - currents.
- Discretizing the above integral: $\boldsymbol{b} = L\boldsymbol{j}$

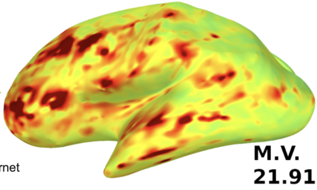




Analysis of the leadfield allows to:

- Compute cortical sensitivity and SNR maps for certain array of sensors of various orientations and sizes
- Estimate the systems of different sensor kinds: magnetometers, gradientometers, etc.
- Estimate total efficiency of a sensor array in terms information theory metrics.
- Create efficient low-channel task-oriented layouts for MEG/EEG

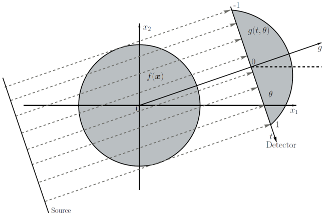


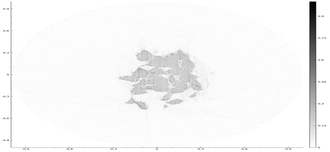


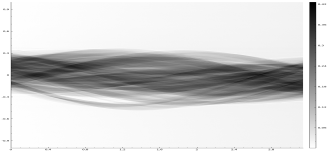
Source: Skidchenko, et al. "Yttrium-iron garnet magnetometer in MEG: Advance towards multi-channel arrays." *bioRxiv* (2022).

Sensitivity maps

- **Studying the object or its properties.** On the base of observed data and known connection between the data and observed information, it is possible to restore the properties (input data) of some object.
- **Studying the model.** Knowing the object properties, and observing some data, we can study the connection between the object and observed data, which we call 'model'.
- **Studying both object and the model.** On the base of observed data and **incomplete** knowledge of 'model', it is sometimes possible to restore both 'model' and properties of the object under investigation.







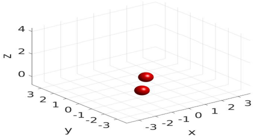
- **input data:** Feature distribution: $f(\mathbf{x})$.
- **The model:** The Radon transform

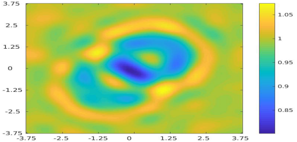
$$(Rf)(\theta, t) = \int_{\mathbb{R}^2} f(\mathbf{x})\delta(\mathbf{x}\cdot\xi - t)d\mathbf{x}$$

- **The output:** The sinogram

$$g(\theta, t) = Rf(\theta, t)$$

source: Eduardo Miqueles, Nikolay Koshev and Elias S. Helou. A Backprojection Slice Theorem for Tomographic Reconstruction. *IEEE TRANSACTIONS ON IMAGE PROCESSING*, 2017





- **input data:** Feature distribution (refractive index): $n(\mathbf{x})$
- **The model:** The Helmholtz

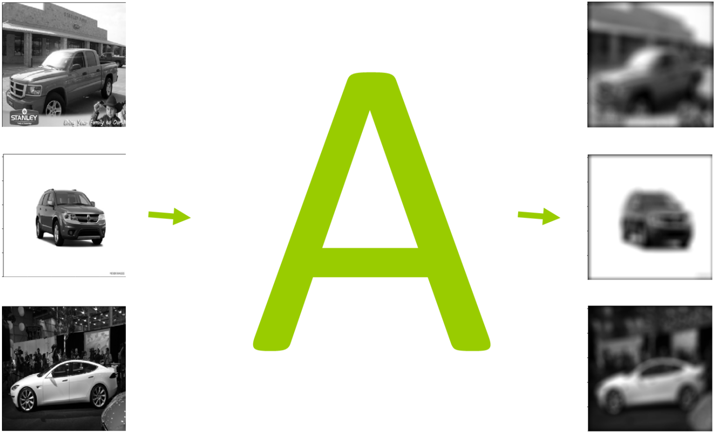
$$\Delta u(\mathbf{x}, k) + k^2 n^2(\mathbf{x}) u(\mathbf{x}, k) = 0.$$

- **The output:** The cell-phone camera photo as a boundary condition in the frame P:

$$u(\mathbf{x}, k) = f(\mathbf{x}, k), \quad \mathbf{x} \in P$$

Source: M.Klibanov, N.Koshev et al., A Numerical Method to Solve a Phaseless Coefficient Inverse Problem from a Single Measurement of Experimental Data. *SIAM J. IMAGING SCIENCES*, 2018.

Example: defocused photographs & NN



f(x)

b(x)

Example: defocused photographs & NN

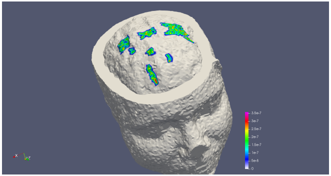
?

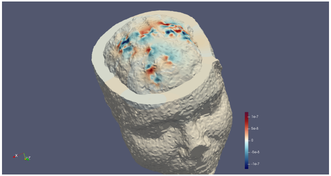
b(x)

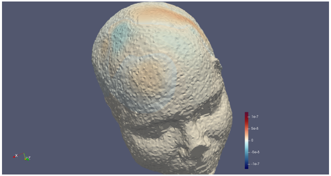
f(x)

The connection between forward and inverse problems

- The relativity of classification.
- Some inverse problems may be classified as forward (simulation) problems. Example: the Cauchy problem in EEG/MEG.
- The inverse problems are often being solved using the simulation. Iterative approaches are often based on comparison the simulation results on the base of the assumed object or partially known 'model'.







- Let $u(\mathbf{x})$ is a potential, and $\mathbf{J}(\mathbf{x})$ is the current density.
- **Forward Problem:** $\mathbf{J}(\mathbf{x}) \rightarrow u(\mathbf{x})$
- **Inverse Problem:** $u(\mathbf{x}) \rightarrow \mathbf{J}(\mathbf{x})$
- **And what about** $u(\mathbf{x}), x \in Scalp$ on scalp to $\rightarrow u(\mathbf{x}), x \in Cortex$ on the cortex (brain surface)? :)
- **Finally,** $5x = 10$ or $\frac{10}{5} = x$?

Source: N.Koshev et al., FEM-based Scalp-to-Cortex data mapping via the solution of the Cauchy problem. *arXiv preprint arXiv:1907.01504*, 2019

Two approaches

Solving **ANY** problem, we can **try** to find:

- **Explicit solution.** $A\mathbf{f} = \mathbf{b} \implies \mathbf{f} = A^{-1}\mathbf{b}$ (of course, if the operator A^{-1} exists).

  PROS: This scheme is very fast and, in case of well-posed problems, most accurate.

  CONS: This scheme is capable for cases when the inverse operator exists, stable and easy to find. Mostly it is the case of SOME **well-posed** problems.

- **Iterative approach.**
  - Chose the first approximation $\mathbf{f}_0$;
  - Construct an appropriate functional $M(\mathbf{f}_0) = F(L(\mathbf{f}_0, \mathbf{b}))$;
  - Change $\mathbf{f}_0$ to obtain $\mathbf{f}_1$ such that $M(\mathbf{f}_1) < M(\mathbf{f}_0)$;
  - Iterate.

  PROS: With the right construction of the functional $M(\mathbf{f})$, the iterative is capable to solve most of problems.
  CONS: The scheme demands to solve the **FORWARD** problem many times in order to calculate the values $M(\mathbf{f}_k)$, which makes it much slower. The accuracy for some kinds of problems may be lesser.
  This approach is being applied to most of **ill-posed** problems.

- X-ray tomography: both approaches are being used.
- Blurred images reconstruction: both approaches can be used.
- Blurred images (AI): iterative approach only.
- EEG/MEG forward problem: both approaches on dependence on approximation.
- Coefficient Inverse Problems: iterative approach only.

Classification of Scientific Computing problems

- Forward and Inverse problems
- Well-posed and Ill-posed problems
- Static and Dynamic problems
- Deterministic and Stochastic problems
- Continuous and Discrete problems

The object and data are connected with a law

The operator equation: $A\mathbf{f} = b$.

- $\mathbf{f}$ represents input (wrt. phenomenon) data. Can be initial state of the system or can define its properties.
- $\mathbf{b}$ represents result (wrt. phenomenon) data. Can be e.g. observed data.
- A represents the model, i.e. the mathematical description of the phenomenon affecting the input to obtain the result. May be known, unknown or partially known.

Well-posed problems
(as defined by Hadamard 1902)
A problem is **well-posed** if:

- A solution exists.
- The solution is unique.
- The solution depends continuously on the **input data**.

- Problems which do not fulfill these criteria are **ill-posed**.
- Well-posed problems have a good chance to be solved numerically with a stable algorithm.

Ill-posed problems

- Ill-posed problems play an important role in some areas. Most of **inverse problems** are ill-posed. But not all of them.
- Problem needs to be reformulated for numerical treatment.
- Add additional constraints to chose the right solution from set of possible solutions. For example, smoothness or sharpness of the solution.
- **Input data** need to be regularized / preprocessed.
- The **model** should be researched and complemented. Sometimes, it should also be regularized.
- Ill-posed problems demand a development of **stable** algorithm.

Ill-posed inverse problems

$$A\mathbf{f} = b, \quad \mathbf{f} \in F, \mathbf{b} \in B.$$

Thus, theoretically:

$$\mathbf{f} = A^{-1}\mathbf{b}.$$

- The inverse operator A^{-1} does not exist.
- The inverse operator A^{-1} is not defined on the whole set $B : AF \neq B$.
- The inverse operator A^{-1} is not continuous.
- The inverse operator A^{-1} is not defined uniquely.

Some examples of ill-posed problems

- Restoration of smoothed and defocused images: instability wrt. noises.
- Source localization in MEG/EEG: Underdetermined system, the inverse operator is not defined uniquely, infinite number of solutions; instability wrt. noises of measurements.
- Equation $x^2 = 4$: the inverse operator is not defined uniquely leading to existence of 2 solutions :)

Differentiation is ill-posed too

Let $f(x)$ be continuously differentiable, $x \in [0,1]$. Consider $f_\delta(x) = f(x) + n_\delta(x)$, where $n_\delta(x) = \delta sin(2\pi kx)$ - a high frequency noise. It is easy to show that:

$$||f(x) - f_\delta(x)||^2_{L^2[0,1]} = \delta^2.$$

On the other hand

$$\partial_x f_\delta(x) = \partial_x f(x) + 2\pi k\delta cos(2\pi kx),$$

and thus, $||\partial_x f(x) - \partial_x f_\delta(x)||^2_{L^2} = 2\pi^2\delta^2 k^2$. We can see that Assume the error $\delta = 0.01$ (1% error), and the frequency $k = 1000$. Thus,

$$||\partial_x f_\delta - \partial_x f||^2 \approx 10^3, \quad \text{while} \quad ||f - f_\delta||^2 = 10^{-4}$$

Classification of Scientific Computing problems

- Forward and Inverse problems
- Well-posed and Ill-posed problems
- Static and Dynamic problems
- Deterministic and Stochastic problems
- Continuous and Discrete problems

- **Static problem** is time-independent. In static problem, the observed data $\mathbf{b}$, the model A, and the input $\mathbf{f}$ do not depend on time.
- **Dynamic problem** is the problem, evolving in time. It means at least the observed data $\mathbf{b} \equiv \mathbf{b}(..., t)$. The model A and input $\mathbf{f}$ also can be time-dependent.
- **Quasi-static problem** is a dynamic problem which can be considered static at every moment of time (changes slowly or in a way such that previous's state *behavior* do not affect current step). Mathematically, it often means the derivative of the function of interest on time is small.
- Some dynamic problems can be considered as static problem.
- Some static problems may be also considered as dynamic.

Static problem simple example: the electric potential calculation

Dynamic problem: heat transfer

$$
\begin{aligned}
u_t(\mathbf{x}, t) - a^2 \Delta u(\mathbf{x}, t) - f(\mathbf{x}, t) = 0, \\
\mathbf{x} \in \Omega \subset \mathbb{R}^n, t > t_0 \geq 0, \\
u(\mathbf{x}, t_0) = \varphi(\mathbf{x}).
\end{aligned}
$$

- u - the temperature.
- a^2 - kinematic heat conductivity.
- $f(\mathbf{x}, t)$ - the heat source density.
- $\varphi(\mathbf{x})$ - initial state (temperature at the moment t_0.
- The heat transfer is definitely a dynamic problem.
- The initial (input) data $\varphi(x)$ does not depend on t;
- The model is time-dependent ($f(\mathbf{x}, t)$ depends on t).

Static problem for evolving system

- Consider the equilibrium problem for the heat equation:

$$u_t(\mathbf{x},t) - a^2\Delta u(\mathbf{x},t) - f(\mathbf{x}) = 0,$$
$$\mathbf{x} \in \Omega \subset \mathbb{R}^n, t > t_0 \geq 0,$$
$$u(\mathbf{x},t_0) = \varphi(\mathbf{x}).$$
$$u_\Gamma = \mu(\mathbf{x}), \quad \Gamma = \partial\Omega.$$

  Find $u(\mathbf{x},\infty)$.
- It is proven that: $u(\mathbf{x},t) \to w(\mathbf{x}), \quad t \to \infty, \quad \forall\varphi(\mathbf{x})$, where $w(\mathbf{x})$ is the solution of the following stationary problem:

$$\Delta w(\mathbf{x}) = -f(\mathbf{x}), \quad , w(\mathbf{x})|_\Gamma = \mu(\mathbf{x}).$$

- Thus, equilibrium problems could be considered both as static and dynamic problems.

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Quasi-static problem: EEG/MEG

- Consider Maxwell equations:

$$\nabla \cdot \mathbf{E} = \rho/\epsilon_0, \quad \nabla \cdot \mathbf{B} = 0 \tag{1}$$

$$\nabla \times \mathbf{B} = \mu_0(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}), \quad \mathbf{J} = \sigma \mathbf{E} + (\epsilon - \epsilon_0)\frac{\partial \mathbf{E}}{\partial t}, \tag{2}$$

- Let $E = E_0(\mathbf{x}) exp(i2\pi ft)$, where f is frequency.
- Then: $\nabla \times \mathbf{B} = \mu_0(\sigma \mathbf{E} + (\epsilon - \epsilon_0)\frac{\partial \mathbf{E}}{\partial t} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t})$.
- Real values for the brain: $\sigma \approx 0.3, \epsilon = 10^5 \epsilon_0, f \approx 100$.
- Since the terms $\epsilon \frac{\partial \mathbf{E}}{\partial t}$ are much lesser than ohmic current $\sigma \mathbf{E}$, we may ignore them, considering the problem as quasistationary.

Source: Hämäläinen M, Hari R, Ilmoniemi RJ, Knuutila J, Lounasmaa OV. Magnetoencephalography: theory, instrumentation, and applications to noninvasive studies of the working human brain. Rev Modern Phys. 1993

Static or dynamic? Oscillations of the string

The wave (D'Alembert) equation:

$$\left(\Delta - \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right)u = 0, \quad a \leq x \leq b, u(a) = 0; \quad u(b) = 0.$$

Assume the solution can be presented in a form $u(x,t) = y(x) \cdot exp(i\omega t)$. After substitution to the equation above, we obtain the following ODE:

$$\frac{d}{dx}\left(p(x)\frac{dy(x)}{dx}\right) = -k^2 q(x) y(x), \quad y(a) = 0, y(b) = 0.$$

where $k = \omega/v$ is a wavenumber, ω - its frequency, and v is the speed.

Just one more axis!

Classification of Scientific Computing problems

- Forward and Inverse problems
- Well-posed and Ill-posed problems
- Static and Dynamic problems
- Deterministic and Stochastic problems
- Continuous and Discrete problems

Deterministic and Stochastic problems

- **Deterministic problems:** Model A, object $\boldsymbol{f}$ are not stochastic and do not include any randomness.
- **Stochastic problems:** At least, the object $\boldsymbol{f}$ is stochastic nature. The model A and observed data $\boldsymbol{b}$ can also be stochastic but unessential.
- Sometimes, stochastic nature caused by incomplete data on the model.
- The stochastic problems is sometimes a good way to study deterministic processes and its models.

Connection between deterministic and stochastic studies

- Knowing the stochastic observed data $\boldsymbol{b}$, obtained with known stochastic object $\boldsymbol{f}$, it is possible to study the model A.
- Example: electron microscope probe diffraction: from differential scattering cross-section of electrons to the model A by deterministic methods.
- Example: electron microscope probe diffraction: Monte-Carlo simulation for model A determination.

Classification of Scientific Computing problems

- Forward and Inverse problems
- Well-posed and Ill-posed problems
- Static and Dynamic problems
- Deterministic and Stochastic problems
- Continuous and Discrete problems

Continuous and Discrete problems

- **Continuous problems:** all functions, distributions and models are continuous; "smooth" motion of object.
- **Discrete problems:** Events occur at discrete times, discrete spatial nodes.
- Complicated continuous problems are often being considered as discrete for possibility of numerical methods application.
- Some discrete nature problems may be reduced to continuous problems in order to find analytical solution.

Scientific Computing
Lecture 2

Functional spaces

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October 5, 2023

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Space - a set of something with some added structure

- The simplest space: real number scale $\mathbb{R}$. Elements of this space: real numbers $x \in (-\infty, \infty)$.
- We are living at space consisting of 3D vectors $\mathbb{R}^3$. Each area of this space is a volume.
- All integers form the space $\mathbb{Z}$.
- All rational numbers $\frac{p}{q}, p, q \in \mathbb{Z}$ form the space $\mathbb{Q}$.
- Consider the interval $[a, b] \subset \mathbb{R}$ for certain a and b. All functions $f(x), x \in [a, b]$ form a space.

The space X is called **linear** if:

- **Sum of elements** of X belongs to X.
- **Multiplication** of an element with an appropriate number maps to the same space.
- **Commutative property:** $x + y = y + x, \quad \forall x, y \in X$.
- **Zero element:** $\exists \theta \in X : x + \theta = x, \forall x \in X$.
- **Negative element:** $\forall x \in X, \exists (-x) \in X : x + (-x) = \theta$.
- **Linearity:**

$$
\begin{aligned}
&1 \cdot x = x, \quad \lambda(\mu x) = (\lambda\mu)x, \quad \forall \lambda, \mu \in \mathbb{R} \\
&(\lambda + \mu)x = \lambda x + \mu x, \quad \forall \lambda, \mu \in \mathbb{R}, \quad \forall x \in X \\
&\lambda(x + y) = \lambda x + \lambda y, \quad \forall x, y \in X, \forall \lambda \in \mathbb{R}
\end{aligned}
$$

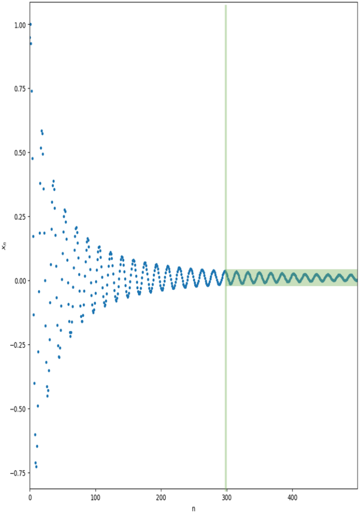
- Thus, all properties of **Linear space** are **linear** :)

Metric space

Space X is called **metric space** if there is a distance between two elements defined. The distance $\rho(x, y)$ is the functional mapping $X \to \mathbb{R}$, defined for $\forall x, y \in X$, and having the following properties:

- **Non-negativity:**
  $\rho(x, y) \geq 0$, and
  $\rho(x, y) = 0 \Rightarrow x \equiv y$.
- **Commutative property:**
  $\rho(x, y) = \rho(y, x)$.
- **Triangle inequality:**
  $\rho(x, y) + \rho(y, z) \geq \rho(x, z), \quad \forall x, y, z \in X$
- Metric space X with distance ρ sometimes being denoted with a pair (X, ρ).

Complete space



- *Fundamental sequence:* sequence $\{x_n\}_{n=1}^{\infty} \in X$ is fundamental if $\forall \varepsilon, \exists N$: $\rho(x_n, x_m) < \varepsilon, \forall n, m > N$
- Picture on the left: fundamental sequence $x_n = \frac{sin(\alpha n)}{n^2} \to 0$
- X is a **complete** space if for *every* fundamental sequence $x_n \in X$, the element $x = \lim_{n\to\infty} \in X$.
- Example: space $(\mathbb{Q}, d(x, y) = |x - y|)$ is not complete.

Normed space

Linear space X is a normed space if $\forall x \in X$ there is the functional $||x|| : X \to \mathbb{R}$ defined:

- **Non-negativity:** $||x|| \geq 0, \quad ||x|| = 0 \Rightarrow x = \theta.$
- **Triangle inequality:**$||x + y|| \leq ||x|| + ||y||, \quad \forall x, y \in X.$
- **Multiplication with a number:** $||\lambda x|| = |\lambda| \cdot ||x||, \quad \forall x \in X, \forall \lambda \in \mathbb{R}.$

Some properties:

- Each normed space is a metric space with $\rho(x, y) = ||x - y||$.
- If $y = \theta$, then $\rho(x, \theta) = ||x - \theta|| = ||x||$. Thus, a norm can be considered a distance to origin.
- Normed and complete space X is called **Banach space**
- **Cauchy-Schwartz inequality:** $||x \cdot y|| \leq ||x|| \cdot ||y||$

Banach space H is called a **Hilbert space**, if for $\forall x, y \in H$ is defined a functional $H \to \mathbb{R}$ (**Scalar product**), satisfying the following points:

- **Non-negativity of 'square':** $(x, x) > 0, \quad \forall x \neq \theta.$
- **Commutative property:** $(x, y) = (y, x).$
- **Linearity:** $(x + y, z) = (x, z) + (y, z), \quad \forall x, y, z \in H.$
- **Linearity:** $(\lambda x, y) = \lambda(x, y), \quad \forall x, y \in H$ and $\forall \lambda \in \mathbb{R}.$
- **Norm is formed with inner product:** $||x||^2 \equiv ||x||_H^2 = (x, x), \quad \forall x \in H.$
- Every inner product defined within a Banach space forms a Hilbert space and thus, connected to a concrete space. Notation: $(x, y)_H$.

- **Linear Space:** linear properties.
- **Metric Space:** space with distance between elements.
- **Normed Space:** space with norm of element.
- **Complete Space:** Fundamental sequence converges to element of the space.
- **Banach Space:** Normed complete space.
- **Hilbert Space:** Banach space with scalar product.
- **Each Hilbert Space is:**
  - Normed
  - Metric
  - Complete

Examples of concrete spaces

- $\mathbb{R}^n: \quad x = (x_1, ..., x_n)^T, \quad (x, y) = \sum_{k=1}^{n} x_k y_k,$
  $||x|| = \left(\sum_{k=1}^{n} x_k^2 \right)^{\frac{1}{2}}.$
- $C[a, b]$ space. Consists of continuous real-valued functions $x(t), t \in [a, b]$. $||x||_C = max(|x(t)|), t \in [a, b]$. This space is Banach space.
- $C^m[a, b]$ space. Consists of m-times continuously differentiable functions $x(t), t \in [a, b]$.

$$||x||_{C^m} = ||x||_C + \sum_{k=1}^{m} ||x^{(k)}||_C.$$

Examples of spaces: the L_p space

- $L_p[a,b]$: The Lebesgue space:
  $x(t), \quad t \in [a,b]$.

$$||x||_{L_p} = \left(\int_a^b |x(t)|^p dt \right)^{1/p}$$

- $L_2[a,b]$ (Hilbert space) $\leftarrow$

$$(x,y)_{L_2} = \int_a^b x(t)y(t)dt, \quad x,y \in L_2[a,b].$$

- n-dimensional case: let $T \in \mathbb{R}^n$ be a closed bounded set.

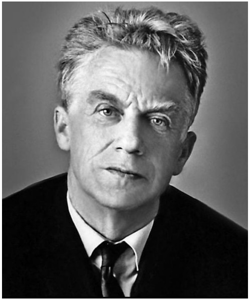
$$(x,y)_{L_2(T)} = \int_T x(t)y(t), \quad t \in T.$$

Henri Lebesgue
(1875-1941)

Examples of spaces: Sobolev spaces

- $T \in \mathbb{R}^n$ is a bounded closed domain.
- If function $x(t) \in L_p(T)$, and all its derivatives up to l^{th} order also belong to $L_p(T)$, then function belongs to Sobolev space W_p^l.
- $W_2^1 \equiv H^1$ case: $\leftarrow$

$$||x||^2_{H^1} = ||x||^2_{L_2(T)} + \sum_{r=1}^{n} ||\frac{\partial x}{\partial t_r}||^2_{L_2(T)}.$$



Sergei Sobolev
(1908-1989)

Scientific Computing
Lecture 3

SLAE

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Systems of linear equations

$$Au = f$$

- A is a matrix of the system
- u is a vector to be found
- f is the right-hand side (vector)

Properties of the matrix

- Condition number $\kappa(A)$ defines the system to be well- or ill-conditioned.
- Dense or sparse
- Symmetric or not
- Positively or negatively definite

Ill-conditioned problems

- Ill-conditioned problems are the simplest example of ill-posed problems. Forward problems are sometimes also ill-conditioned and, therefore, ill-posed.
- $\implies$ Small changes (errors, noise) in data lead to large errors in the solution.
- Can occur if continuous problems are solved approximately on a numerical grid.
  PDE $\implies$ algebraic equation in a form $A\mathbf{f} = \mathbf{b}$
- Condition number of matrix A (for normal matrices):
  $$\kappa(A) = \frac{|\lambda_{max}(A)|}{|\lambda_{min}(A)|},$$
  where $\lambda_{max}(A)$ and $\lambda_{min}(A)$ are maximal and minimal eigenvalues of A.
- Well conditioned problems have a low condition number.

Ill-conditioned problems

- Consider the system for a pair $\mathbf{f} = (x_1, x_2)^T$:

$$A\mathbf{f} = \mathbf{b}, \quad A = \begin{pmatrix} 1 & 1 \\ 1 & 1.001 \end{pmatrix}, \quad \mathbf{b} = (2, 2)^T \Leftrightarrow \begin{cases} x_1 + x_2 = 2 \\ x_1 + 1.001x_2 = 2. \end{cases}$$

- The system has a solution $(2, 0)^T$.
- Now let the $\mathbf{b} = (2, 2.001)^T$ instead of $\mathbf{b} = (2, 2)^T$. The solution is $(1, 1)^T$...
- The condition number is $\kappa(A) = 4004.0010$.

Methods of SLAE solution

- Direct methods:
  - Gauss methods
  - Tridiagonal matrix algorithm
  - LU-decomposition
  - And many other methods...
- Iterative methods:
  - Jacobi method
  - Seidel method
  - Multigrid method
  - Successive over-relaxation
  - Conjugate and biconjugate gradients
  - And many other methods...

Performance of some methods

Method	Computational complexity
Gauss method	$O(N^3)$
Tridiagonal method	$O(N^{2.5})$
Jacobi's and Seidel's method	$O(N^2 log\frac{1}{\varepsilon})$
Successive over-relaxation	$O(N^{\frac{3}{2}} log\frac{1}{\varepsilon})$
Lower-bound estimate	$O(N)$.

'Bad' systems

$$Au = f.$$

- **Ill-conditioned** systems. The solution is unstable with respect to errors in the right-hand-side f.
- **Overdetermined systems**. The system may be inconsistent (do not have solutions).
- **Underdetermined systems**. Such systems have more than one solution.

The regularization:

$u_\alpha = argmin\left(||Au - f||^2 + \alpha||u||^2_?\right)$ - the approximate solution.

The space "?" should be chosen using reasoning!

Questions (Lecture 2)

- What is the mathematical model of the phenomenon? How can it be represented in the operator form? Describe all parts of the latter in terms of possible representation.
- What is the forward problem, and what is inverse problem? What is the difference between them? Reason on relativity of this classification. Explain with examples.
- List several applications of both Forward and Inverse problems. Justify on why the concrete problem is Forward or Inverse.
- Give the definitions and describe with examples the Top-Down and Bottom-Up approaches.
- Give the definitions and describe with examples two direct and iterative approaches to solution of any problem.
- List three points J.Hadamard proposed to consider in order to classify problems in terms of well- and ill-posedness. What do these points mean mathematically?
- List the possible issues for the inverse operator in case of ill-posed problems.
- What does the continuous dependence of the solution on input means? Prove that derivative of noised function might depend discontinuously on the small error (noises) of the function to be differentiated.
- What is ill-conditioned problem? Define it mathematically and give reasoning on behaviour of the solution with respect to changes in input data. Give any example of ill-conditioned problem. Explain it.
- Which additional research and additional steps should or might be done in case of ill-posed problems? Reason on all possibilities you know.
- Define static and dynamic problems. Give at least two examples of each and explain these examples. List the cases in which a dynamic problem may be considered to be a static one. Explain these cases.
- Write the definitions of deterministic and stochastic problems. Give at least two examples of each kind. Explain, why these examples can be considered as static or dynamic. Provide an example of the problem, which can be considered both in deterministic and stochastic ways. Explain the example.