Introduction to the theory, numerical methods and applications of ill-posed problems
(lecture course)

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Introduction

- In the lecture course we will describe fundamentals of the theory of ill-posed problems so as numerical methods for their solution if different a priori information is available. For simplicity, only linear equations in normed spaces are considered.
Introduction

- Although, it is clear that all similar definitions can be introduced also for nonlinear problems in more general metric (even also topological) spaces.

- Numerous inverse problems can be found in different branches of physics (astrophysics, geophysics, spectroscopy, nuclear physics, etc.).
Introduction

- Mostly, these inverse problems are ill-posed. It means that small deviations of input data (due to experimental errors) can produce large errors in an approximate solution.
Introduction


Introduction

In 1963 Tikhonov formulated the definition of a regularizing algorithm. He and two other Russian mathematicians Mikhail Lavrentiev and Valentin Ivanov became founders of the modern theory of inverse and ill-posed problems.
Introduction
Introduction

- Now this theory is greatly developed throughout the world. The most eminent specialists in Sweden are Lars Elden from Linkoping and Larisa Beilina from Gothenburg.
Course literature


Course literature

Recommended reference literature


Recommended reference literature


Recommended reference literature


Well-posed and ill-posed problems

Let us consider an operator equation:

\[ Az = u, \]

where \( A \) is a linear operator acting from a Hilbert space \( Z \) into a Hilbert space \( U \). It is required to find a solution of the operator equation \( z \) corresponding to a given inhomogeneity (or right-hand side) \( u \).
Well-posed and ill-posed problems

The problem of solving the operator equation is called to be well-posed (according to Hadamard) if the following three conditions are fulfilled:

1) the solution exists \( \forall u \in U \);

2) the solution is unique;

3) if \( u_n \rightarrow u \), \( Az_n = u_n \), \( Az = u \), then \( z_n \rightarrow z \).
Well-posed and ill-posed problems

- Usually, a choice of the space of solutions (including a choice of the norm) is determined by requirements of an applied problem. A mathematical problem can be ill-posed or well-posed depending on a choice of a norm in a functional space.
Well-posed and ill-posed problems

- Lavrentiev’s example
- Condition 3) is fulfilled if
  - $\|z\|_A = \|Az\|$
  - A is an injective operator.
Elements of functional analysis

- Linear spaces
- Metric spaces
- Normed spaces
- Banach spaces
- Euclidean spaces
- Hilbert spaces
Elements of functional analysis

- **Example.** A finite-dimensional vector space $\mathbb{R}^n$ that is very well known from Linear algebra.
Elements of functional analysis

- **Example.** A space $C[a,b]$ of (real) functions defined and continuous on a segment $[a,b]$ with the norm:
  $$||y||_{C[a,b]} = \max\{|y(s)|, \quad s \in [a,b]\}.$$  
Convergence in this space is called **uniform** convergence.
Elements of functional analysis

- **Definition.** A sequence $x_n \in \mathbb{N}, n=1, 2, \ldots$ is called **fundamental** sequence if for any $\varepsilon > 0$ there exists a natural number $K$ such that for any $n \geq K$ and any natural number $p \ |x_{n+p} - x_n| \leq \varepsilon$.

- If any fundamental sequence converges then the normed space is called the **complete** space (or Banach space).
Elements of functional analysis

- Example. $\mathbb{R}^n$ and $C[a,b]$ are Banach spaces.
Elements of functional analysis

Example. A space $C^{(p)}[a,b]$ ($C^{(0)}[a,b] = C[a,b]$) of (real) functions defined and continuous with all derivatives up to $p$-th order ($p \geq 0$ – integer) on a segment $[a,b]$ with the norm:

$$\| y \|_{C^p[a,b]} = \sum_{k=0}^{p} \max_{s \in [a,b]} \{ |y^{(k)}(s)|, s \in [a,b] \}.$$ 

is a Banach space. Convergence in this space is called uniform convergence with all derivatives up to $p$-th order.
**Elements of functional analysis**

- **Definition.** A linear space is called the **Euclidean space** if for any two elements $x, y \in E$ is defined a real number $(x, y)$ (a **scalar product**) such that:

  1) for any $x, y \in E$ $(x, y) = (y, x)$;

  2) for any $x_1, x_2, y \in E$ $(x_1 + x_2, y) = (x_1, y) + (x_2, y)$;

  3) for any $x, y \in E$ and any real $\alpha$ $(\alpha x, y) = \alpha (x, y)$;

  4) for any $x \in E$ $(x, x) \geq 0$, and $(x, x) = 0$ if and only if $x = 0$. 
Elements of functional analysis

Example. A finite-dimensional vector space $\mathbb{R}^n$ is an Euclidean space with a scalar product $(x, y) = x_1y_1 + \ldots + x_ny_n$, where $x_1, \ldots, x_n; y_1, \ldots, y_n$; are components of vectors $x$ and $y$ respectively.
Elements of functional analysis

Example. A space of (real) functions defined and continuous on segment \([a, b]\) with a scalar product: for any continuous on \([a, b]\) functions \(y_1(x), y_2(x)\) define

\[
(y_1, y_2) = \int_a^b y_1(x)y_2(x)\,dx.
\]

This is the space \(L_2[a, b]\) with the norm

\[
\| y \| = \left( \int_a^b y^2(x)\,dx \right)^{1/2}.
\]

This Euclidean space is infinite-dimensional and is not complete.
Elements of functional analysis

**Definition.** An infinite-dimensional complete Euclidean space is called a **Hilbert space**.

Applying a space completion procedure any infinite-dimensional Euclidean space can be transformed in a Hilbert space. If apply this procedure to $\tilde{L}_2[a,b]$ we can get the Hilbert space $L_2[a,b]$. In order to describe elements of this space we should know not only the Riemann integral (known from Mathematical analysis) but also the Lebesgue integral.
Elements of functional analysis

We need also one of Sobolev’s spaces $W^1_2[a,b]$ (= $H^1[a,b]$). The scalar product in this space is defined as $(y_1, y_2) = \int_a^b y_1(x)y_2(x)\,dx + \int_a^b y_1'(x)y_2'(x)\,dx$, and the norm is equal to $\|y\| = \left(\int_a^b y^2(x)\,dx + \int_a^b (y'(x))^2\,dx\right)^{1/2}$. If derivatives are classic and integrals are Riemann ones then the space is an infinite-dimensional Euclidean space. If derivatives are generalized and integrals are Lebesgue ones then the space is a Hilbert space.
Elements of functional analysis

- Linear operators

**Example.** The Fredholm integral operator

\[ Ay = \int_{a}^{b} K(x, s)y(s)ds; \quad x, s \in [a, b]. \]

with a continuous kernel \( K(x, s) \) is a linear operator acting in the linear space of continuous on a segment \([a, b]\) continuous functions.
Elements of functional analysis

Definition. The norm of a linear operator $A$ is called

$$\|A\|_{N_1 \rightarrow N_2} = \sup_{\|y\|_{N_1} = 1} \|Ay\|_{N_2}$$

For simplicity, we will write $\|A\|_{N_1 \rightarrow N_2} = \|A\|$. 

Definition. If $\|A\| < +\infty$ then the operator $A$ is called bounded.

In finite-dimensional spaces any linear operator is bounded. In infinite-dimensional spaces it is not so.
Elements of functional analysis

Example. The space $C[0,1]$ is an infinite-dimensional space. Let us consider a differentiation operator $A = \frac{d}{ds}$ defined on the linear subspace of continuously differentiable functions in $C[0,1]$. The operator $A$ is unbounded. For the sequence $y_n = \cos ns; n=1, 2, \ldots$ we get: $\|y_n\| = \max_{s \in [0,1]} |\cos ns| = 1$, and $\|Ay_n(s)\| = |n \cdot \sin ns| \to \infty$ as $n \to \infty$. 
Definition. A sequence $y_n$, $n=1,2,...$, of elements of a normed space $N$ is called compact if any its subsequence has a convergent subsequence. If space $N$ is not Banach space, then it has a fundamental subsequence.
Elements of functional analysis

- **Definition.** A linear operator $A : N \rightarrow N$ is called **compact** if for any bounded sequence $i = 1, 2, \ldots$; elements of the sequence $z_n = Ay_n$ of elements in is compact.

- **Definition.** A linear compact operator is completely continuous.
Elements of functional analysis

- **Theorem.** Any completely continuous operator is bounded (consequently, continuous).

- In finite-dimensional spaces any linear operator is completely continuous. It is not true in infinite-dimensional spaces.
Elements of functional analysis

- **Example.** Let us consider the identity operator $I: Iy = y$ for any $y$. It is bounded but not compact.

- **Theorem.** Let $A$ be the Fredholm integral operator mapping from $L_2[a,b]$ into $L_2[a,b]$. Then $A$ is completely continuous.
Examples of ill-posed problems

The Fredholm integral equation of the 1st kind is a very well known sample of an ill-posed problem. Let an operator $A$ be of the form:

$$Az = \int_a^b K(x,s)z(s)ds = u(x), \quad x \in [c,d].$$

The integral operator $A$ is completely continuous (compact and continuous) while acting from $L_2[a,b]$ into $L_2[c,d]$. 
Examples of ill-posed problems

Let us suppose that the inverse operator is continuous. It is very easy to arrive to a contradiction. If $A$ is an injective operator then an inverse operator exists. Evidently, if an operator $B$ is continuous and an operator $A$ is completely continuous then the operator $BA$ is completely continuous.
Examples of ill-posed problems

$A^{-1}Az_n = z_n$

If inverse to $A$ operator is bounded then any bounded sequence is compact! It is not true in infinite-dimensional spaces.
Examples of ill-posed problems

- Infinite-dimensional range of a completely continuous operator \( R(A) \) is not closed! It is easy to prove using Banach’s Theorem. If the injective linear operator \( A \) is continuously mapping an infinite-dimensional Banach space on an infinite-dimensional Banach space then the inverse operator is continuous.
Examples of ill-posed problems

Sometimes a problem of solving an operator equation it is convenient to pose as problem of calculation of values of an unbounded and not everywhere defined operator $A^{-1}: z = A^{-1}u$. The simplest example is calculation of the differentiation operator: $z(x) = \frac{du}{dx}$. We showed before that this operator is unbounded and not everywhere defined if consider it is as a mapping from $C[0, 1]$ into $C[0, 1]$. The problem of calculation of values of this operator is not well-posed because the first and third conditions of well-posedness are not fulfilled.
Definition of the regularizing algorithm

Let us consider an operator equation:

\[ Az = u, \]

where \( A \) is an operator acting between normed spaces \( Z \) and \( U \). In 1963 A.N. Tikhonov formulated a famous definition of the regularizing algorithm (RA) that is a basic conception in the modern theory of ill-posed problems.
Definition of the regularizing algorithm

**Definition.** Regularizing algorithm (regularizing operator) $R(\delta, u_\delta) = R_\delta(u_\delta)$ is called an operator possessing two properties:

1) $R_\delta(u_\delta)$ is defined for any $\delta > 0$, $u_\delta \in U$, and is mapping $(0, +\infty) \times U$ into $Z$;

2) For any $z \in Z$ and for any $u_\delta \in U$ such that $Az = u$, $\|u - u_\delta\| \leq \delta$, $\delta > 0$,

$$z_\delta = R_\delta(u_\delta) \to z,$$
Definition of the regularizing algorithm

A problem of solving an operator equation is called to be regularizable if there exists at least one regularizing algorithm. Directly from the definition it follows that if there exists one regularizing algorithm then number of them is infinite.
At the present time, all mathematical problems can be divided into following classes:

- well-posed problems;
- ill-posed regularizable problems;
- ill-posed nonregularizable problems.
Definition of the regularizing algorithm

Not all ill-posed problems are regularizable, and it depends on a choice of spaces $Z$, $U$. Russian mathematician L.D. Menikhes constructed an example of an integral operator with a continuous closed kernel acting from $C[0,1]$ into $L_2[0,1]$ such that an inverse problem is nonregularizable.
Definition of the regularizing algorithm

An equivalent definition of the regularizing algorithm is following. Let be given an operator (mapping) $R_\delta(u_\delta)$ defined for any $\delta > 0$, $u_\delta \in U$, and reflecting $(0, +\infty) \times U$ into $Z$. An accuracy of solving an operator equation in a point $z \in Z$ using an operator $R_\delta(u_\delta)$ under condition that the right-hand side defined with an error $\delta > 0$ is defined as $\Delta(R_\delta, \delta, z) = \sup_{u_\delta \in U: \|u_\delta - u\| \leq \delta, A\delta = u} \|R_\delta u_\delta - z\|$. An operator $R_\delta(u_\delta)$ is called a regularizing algorithm (operator) if for any $z \in Z$ $\Delta(R_\delta, \delta, z) \rightarrow 0$. This definition is equivalent to the definition above.
Definition of the regularizing algorithm

Similarly, a definition of the regularizing algorithm can be formulated for a problem of calculating values of an operator (see the end of the previous section), that is for a problem of calculating values of mapping $G: D(G) \rightarrow Y$, $D(G) \subseteq X$ under condition that an argument of $G$ is specified with an error ($X$, $Y$ are metric or normed spaces). Of course, if $A$ is an injective operator then a problem of solving an operator equation can be considered as a problem of calculating values of $A^{-1}$.
Definition of the regularizing algorithm

It is very important to get an answer to the following question: is it possible to solve an ill-posed problem (i.e., to construct a regularizing algorithm) without knowledge of an error level $\delta$?

Evidently, if a problem is well-posed then a stable method of its solution can be constructed without knowledge of an error $\delta$. E.g., if an operator equation is under consideration then it can be taken $z_\delta = A^{-1}u_\delta \rightarrow z = A^{-1}u$ as $\delta \rightarrow 0$. It is impossible if a problem is ill-posed. A.B. Bakushinsky proved the following theorem for a problem of calculating values of an operator. An analogous theorem is valid for a problem of solving operator equations.
Definition of the regularizing algorithm

**Theorem.** If there exists a regularizing algorithm for calculating values of an operator $G$ on a set $D(G) \subseteq X$, and the regularizing algorithm does not depend on $\delta$ (explicitly), then an extension of $G$ from $D(G) \subseteq X$ to $X$ exists, and this extension is continuous on $D(G) \subseteq X$.

So, construction of regularizing algorithms not depending on errors explicitly is feasible only for well-posed on its domains problems.
Definition of the regularizing algorithm

■ The next very important property of ill-posed problems is impossibility of error estimation for a solution even if an error of a right-hand side of an operator equation or an error of an argument in a problem of calculating values of an operator is known. This basic result was also obtained by A.B. Bakushinsky for solving operator equations.
Definition of the regularizing algorithm

Theorem. Let \( \Delta(R_\delta, \delta, z) = \sup_{u_\delta \in U : \|u_\delta - u\| \leq \delta, A\delta = u} \| R_\delta u_\delta - z \| \leq \epsilon(\delta) \to 0 \) for any \( z \in D \subseteq Z \). Then a contraction of the inverse operator on the set \( AD : A^{-1}\big|_{AD \subseteq U} \) is continuous on \( AD \).

So, a uniform on \( z \) error estimation of an operator equation on a set \( D \subseteq Z \) exists then and only then if the inverse operator is continuous on \( AD \). The theorem is valid also for nonlinear operator equations, in metric spaces at that.
Definition of the regularizing algorithm

- From the definition of the regularizing algorithm it follows immediately if one exists then there is infinite number of them. While solving ill-posed problems, it is impossible to choose a regularizing algorithm that finds an approximate solution with the minimal error.
Definition of the regularizing algorithm

- It is impossible also to compare different regularizing algorithms according to errors of approximate solutions. Only including a priori information in a statement of the problem can give such a possibility, but in this case a reformulated problem is well-posed in fact. We will consider examples below.
Definition of the regularizing algorithm

Regularizing algorithms for operator equations in infinite dimensional Banach spaces could not be compared also according to convergence rates of approximate solutions to an exact solution as errors of input data tend to zero. The author of this principal result is V.A. Vinokurov.
Consider the results obtained by Vinokurov.

Let $A$ be a linear continuous injective operator acting in Banach space $Z$ and the inverse operator $A^{-1}$ be unbounded on $D(A^{-1})$. Suppose that $\varphi(\delta)$ is an arbitrary positive function such that $\varphi(\delta) \to 0$ as $\delta \to 0$, and $R$ is an arbitrary method to solve the problem.

The following equality holds for elements $\tilde{z}$ except maybe for a first category set in $Z$:

$$\lim_{\delta \to 0} \sup \left\{ \frac{\Delta(R, \delta, \tilde{z})}{\varphi(\delta)} \right\} = \infty$$

A uniform error estimate can only exist on a first category subset in $Z$. 
Definition of the regularizing algorithm

In conclusion of the section let formulate a definition of the regularizing algorithm in the case when an operator can also contain an error, i.e., instead of an operator $A$ it is given a bounded linear operator $A_h : A_h : \mathcal{Z} \to \mathcal{U}$, such that

$$\|A_h - A\| \leq h, \quad h \geq 0.$$  Briefly, let us note a pair of errors $\delta, h$ as $\eta = (\delta, h)$.  

Definition of the regularizing algorithm

Definition. Regularizing algorithm (regularizing operator)

$R(\eta, u_\delta, A_h) = R_\eta(u_\delta, A_h)$ is called an operator possessing two properties:

1) $R_\eta(u_\delta, A_h)$ is defined for any $\delta > 0$, $h \geq 0$, $u_\delta \in U$, $A_h \in L(Z, U)$, and is mapping $(0, +\infty) \times [0, +\infty) \times U \times L(Z, U)$ into $Z$;

2) for any $z \in Z$, for any $u_\delta \in U$ such that $Az = u$, $\|u - u_\delta\| \leq \delta$, $\delta > 0$ and for any $A_h \in L(Z, U)$ such that $\|A_h - A\| \leq h$, $h \geq 0$, $z = R_\eta(u_\delta, A_h) \underset{\eta \to 0}{\to} z$. 


Ill-posed problems on compact sets

Let us consider an operator equation:

\[ Az = u, \]

\( A \) is a linear injective operator acting between normed spaces \( Z \) and \( U \). Let \( \tilde{z} \) be an exact solution of an operator equation, \( A\tilde{z} = \tilde{u} \), \( \tilde{u} \) is an exact right-hand side, and it is given an approximate right-hand side such that \( \| \tilde{u} - u_\delta \| \leq \delta, \delta > 0 \).
Ill-posed problems on compact sets

A set \( Z_\delta = \{ z_\delta : \| A z_\delta - u_\delta \| \leq \delta \} \) is a set of approximate solutions of the operator equation. For linear ill-posed problems, \( \text{diam} Z_\delta = \sup \{ \| z_1 - z_2 \| : z_1, z_2 \in Z_\delta \} = \infty \) for any \( \delta > 0 \) since the inverse operator \( A^{-1} \) is not bounded.
Ill-posed problems on compact sets

- Tikhonov (1943) “On stability of inverse problems” (Soviet Mathematics Doklady)

**Theorem.** Let an injective continuous operator $A$ be mapping:

$$D \in Z \rightarrow AD \in U,$$

where $Z, U$ are normed spaces, $D$ is a compact. Then the inverse operator $A^{-1}$ is continuous on $AD$. 
Ill-posed problems on compact sets

Definition. An element $z_\delta \in D$ such that $z_\delta = \arg \min_{z \in D} \|Az - u_\delta\|$ is called a quasisolution of an operator equation on a compact $D$ ($z_\delta = \arg \min_{z \in D} \|Az - u_\delta\|$ means that $\|Az_\delta - u_\delta\| = \min \{\|Az - u_\delta\| : z \in D\}$).
Ill-posed problems on compact sets

A quasisolution exists but maybe is nonunique. Though, any quasisolution tends to an exact solution: \( z_\delta \to \bar{z} \) as \( \delta \to 0 \). In this case, knowledge of an error \( \delta \) is not obligatory. If \( \delta \) is known then:

1) any element \( z_\delta \in D \) satisfying an inequality: \( \|Az_\delta - u_\delta\| \leq \delta \), can be chosen as an approximate solution with the same property of convergence to an exact solution (\( \delta \)-quasisolution);
Ill-posed problems on compact sets

2) it is possible to find an error of an approximate solution solving an extreme problem:

\[
\text{find } \max \|z - z_\delta\| \text{ maximizing on all } z \in D \text{ satisfying an inequality:}
\]

\[
\|Ax - u_\delta\| \leq \delta \quad \text{(it is obviously that an exact solution satisfying the inequality).}
\]
Ill-posed problems on compact sets

If an operator $A$ is specified with an error then the definition of a quasisolution can be modified changing an operator $A$ to an operator $A_h$.

**Definition.** An element $z_\eta \in D$ such that $z_\eta = \arg \min_{z \in D} \| A_h z - u_\delta \|$ is called a quasisolution of an operator equation on a compact $D$.

Any element $z_\eta \in D$ satisfying an inequality: $\| A z_\eta - u_\delta \| \leq \delta + h \| z_\eta \|$ can be chosen as an approximate solution ($\eta$-quasisolution).
Extremal problems statement

As the main problem below, we will consider the following problem

(Problem (*)): 

To find \( \min f(x) = f^* \) if \( x \in X \subseteq H \), and an element \( x^* \epsilon X \) such that \( f(x^*) = f^* \).
Extremal problems statement

We denote:

\[ x^* = \arg \min \{ f(x) : x \in X \}, \quad f(x^*) = f^* = \min \{ f(x) : x \in X \}. \]

If the point of minimum is nonunique:

\[ X^* = \text{Argmin} \{ f(x) : x \in X \}. \]
Solvability of an extremal problem

Theorem (Weierstrass). Let $X$ be a compact in $H$, and a functional $f(x)$ continuous on $X$. Then there exists a point of a global minimum of $f(x)$ on $X$.

Corollary Let a functional $f(x)$ be lower semicontinuous on $X$, i.e.

$$
\forall x^{(0)} \in X, \forall x^{(n)} \in X, n = 1, 2, \ldots : x^{(n)} \to x^{(0)} \Rightarrow \lim_{n \to \infty} f(x^{(n)}) \geq f(x^{(0)}).$$

The Theorem is valid in this case also.
Solvability of an extremal problem

Definition. A functional $f(x)$ is called differentiable in a point $x^{(0)}$ of a Hilbert space $H$ if for any $x \in H$

$$f(x) = f(x^0) + (f'(x^0), x-x^0) + o(||x-x^0||).$$

Here $f'(x^{(0)}) \in X$ is called the Frechet derivative, or the gradient of a functional $f(x)$ in a point $x^{(0)}$.

In the finite-dimensional case ($H=\mathbb{R}^n$) a gradient is a vector, and its components are partial derivatives of a function of $n$ variables $f(x)$ in a point $x^{(0)}$. 
Solvability of an extremal problem

**Definition.** A functional $f(x)$ is called **twice differentiable** in a point $x^0$ if for any $x \in H$

$$f(x) = f(x^0) + (f''(x^0), x-x^0) + 1/2(f'''(x^0)(x-x^0), x-x^0) + o(||x-x^0||^2).$$

Here a bounded linear operator $f''(x^0) : H \to H$ called the **second Frechet derivative** of a functional $f(x)$ in a point $x^0$. In the finite-dimensional case
Solvability of an extremal problem

\[ f''(x^{(0)}) \] is given by the Hesse matrix (or Hessian). This matrix consists of second partial derivatives \[ \frac{\partial^2 f}{\partial x_i \partial x_j} \] in \( x^{(0)} \).

**Definition.** A linear bounded operator \( A: H \to H \) is called **nonnegatively definite** if for any \( h \in H \): \( (Ah, h) \geq 0 \), and **positively definite** if for any \( h \in H, h \neq 0 \): \( (Ah, h) > 0 \).
Solvability of an extremal problem

Following trivial results are known from Mathematical analysis. Here $H = \mathbb{R}^n$, and a functional $f(x)$ is a function of $n$ variables.

Theorem (necessary condition of local extremum). Let a functional $f(x)$ be differentiable in $x^* \in H$. If $x^*$ is a point of a local minimum then $f'(x^*) = 0$.

Theorem (necessary condition of local minimum). Let a functional $f(x)$ be twice differentiable in $x^* \in H$. If $x^*$ is a point of a local minimum, then $f'(x^*) = 0$ and $f''(x^*) \geq 0$ (nonnegatively definite).
Solvability of an extremal problem

Theorem (sufficient condition of local minimum). Let a functional $f(x)$ be twice differentiable in $x^* \in H$. If the gradient $f'(x^*) = 0$, the operator $f''(x^*) > 0$ (positively definite), then $x^*$ is a point of a local minimum.

These results are easily generalized on the infinite-dimensional case. The necessary conditions are the same, the sufficient condition should be strengthened.

The theorems are valid if the problem is with constraints, and $x^*$ is an interior point of $X$. 
Convex functionals

Definition. A set $X$ in a linear space is called convex if $\forall x^{(1)}, x^{(2)} \in X$ the segment $[x^{(1)}, x^{(2)}] = \{ x : x = \lambda x^{(2)} + (1-\lambda) x^{(1)} , \lambda \in [0,1] \} \subseteq X$.

Definition. A functional $f(x)$ defined on a convex set $X$ is called convex if $\forall x^{(1)}, x^{(2)} \in X \quad \forall \lambda \in [0,1] :$

$$f(\lambda x^{(1)} + (1-\lambda) x^{(2)}) \leq \lambda f(x^{(1)}) + (1-\lambda) f(x^{(2)}).$$

$\lambda x^{(1)} + (1-\lambda) x^{(2)}$, $\lambda \in [0,1]$ is called a convex combination of $x^{(1)}, x^{(2)}$. 
**Convex functionals**

**Definition.** A functional \( f(x) \) defined on a convex set \( X \) is called **strictly convex** if \( \forall x^{(1)}, x^{(2)} \in X, x^{(1)} \neq x^{(2)}, \forall \lambda \in (0,1) \)

\[
f(\lambda x^{(1)} + (1-\lambda)x^{(2)}) < \lambda f(x^{(1)}) + (1-\lambda)f(x^{(2)}).
\]

**Definition.** A functional \( f(x) \) defined on a convex set \( X \) of a Hilbert space is called **strongly convex** if there exists a constant \( \theta > 0 \) (constant of strong convexity) such that \( \forall x^{(1)}, x^{(2)} \in X \) \( \forall \lambda \in [0,1] \):}

\[
f(\lambda x^{(1)} + (1-\lambda)x^{(2)}) \leq \lambda f(x^{(1)}) + (1-\lambda)f(x^{(2)}) - \theta \lambda (1-\lambda) \| x^{(1)} - x^{(2)} \|^2.
\]
Convex functionals

A classification of extremal problems:

1) If $X$ is a convex set and $f(x)$ is a convex functional then (*) is a problem of convex programming (or convex optimization).
2) Often $X$ is defined by a system of equalities and inequalities:

$$X = \{ x \in P : g_i(x) \leq 0, i = 1, .., k, g_i(x) = 0, i = k + 1, .., m \}.$$  
Here $P$ is a set of direct constraints. Then (*) is a problem of **mathematical programming**. It is a problem of **convex programming** if $P$ is a convex set, functionals $g_i(x)$ in constraints of inequalities type are convex, and in constraints of equalities type they are affine. It follows from: 1) if $g(x)$ is a convex functional then the set $\{ x : g(x) \leq \beta \}$ ($\beta$ is a constant) is convex (or empty); 2) intersection of convex sets is convex or empty.
Convex functionals

3) (*) is a problem of linear programming if $H = \mathbb{R}^n$, $f(x) = a + (b, x)$ is a linear functional (more exactly, affine functional, but we will call linear), and all constraints produce a polyhedron (i.e. $P$ is a polyhedron, and all functionals $g_i(x)$ are linear). A linear programming problem is a special case of a convex programming problem. Using a necessary condition of minimum, it is easy to prove that a point of minimum (if it exists) is a vertex of the polyhedron.
Convex functionals

4) If $H = \mathbb{R}^n$, and $f(x) = a + (b, x) + \frac{1}{2}(Cx, x)$ (a quadratic functional), and constraints are linear then (*) is a problem of quadratic programming. Here $C$ is a symmetric matrix. If $C$ is nonnegatively definite the a problem of quadratic programming is a special case of a problem of convex programming.
Convex functionals

- **Theorem.** If (*) is a convex programming problem then any point of a local minimum is a point of the global minimum.
- Convex functionals have no local minima.
Convex functionals

Theorem. Let functional $f(x)$ be convex $H$ on a Hilbert space and differentiable in $x^* \in H$. If $f'(x^*) = 0$ then $x^*$ is a point of global minimum $f(x)$ on $H$.

Theorem. Let (*) be a solvable convex programming problem. Then the set of its solutions $X^* = \arg\min_{x \in X} f(x)$ is convex. If $f(x)$ is a strictly convex functional then $X^*$ contains an unique $x^*$. 
Solvability of a convex programming problem

- **Theorem.** A convex continuous (lower semicontinuous) functional $f(x)$ on a closed bounded convex set of a Hilbert space $H$ has a minimum point (i.e., a convex programming problem (*) is solvable).

- **Theorem (Weierstrass).** A weakly lower semicontinuous functional on a weak compact has a minimum point.
Solvability of a convex programming problem

- We need to prove two assertions only:
  - 1. A convex continuous (lower semicontinuous) functional is weakly lower semicontinuous.
  - 2. A closed bounded convex set of a Hilbert space is a weak compact.

- The theorem is true for reflexive Banach spaces only.
Solvability of a convex programming problem

Theorem. Let \( \{x^{(n)}\}_{n=1}^{\infty}, x^{(n)} \in H, \ x^{(n)} \to x \) weakly and \( \|x^{(n)}\| \to \|x\|. \) Then

\[ x^{(n)} \to x. \]

I.e., from weak convergence and convergence of norms follows strong convergence (H-property of Hilbert spaces).

A Hilbert space is also strictly normed: \( \forall x, y, x \neq \lambda y, y \neq \lambda x : x + y \| \leq \|x\| + \|y\|. \)
Solvability of a convex programming problem

Theorem. Let $f(x)$ be a continuous strongly convex functional defined on a closed convex set $X$ of a Hilbert space $H$. Then $f(x)$ has a minimum point in $X$, and this point is unique.
Solvability of a convex programming problem

**Definition.** A sequence \( x^{(n)} \), \( n=1,2,... \), of elements of a set \( X \) is called a minimizing sequence if \( f(x^{(n)}) \rightarrow f(x^*) = f^* \).

**Definition.** A sequence \( x^{(n)} \), \( n=1,2,... \), of elements of a set \( X \) is called convergent to a minimum point if \( x^{(n)} \rightarrow x^* \).

**Theorem.** If a functional \( f(x) \) is strongly convex, then a minimizing sequence converges to a minimum point.
Criteria of convexity and strong convexity

In this and only this chapter for simplification of formulating theorems we note a convex functional as a strongly convex functional with constant $\theta = 0$.

**Theorem.** Let $f(x)$ be differentiable on a convex set $X \subseteq H$ functional, $H$ a Hilbert space. Then $f(x)$ is strongly convex with a constant $\theta \geq 0$ if and only if

$$\forall x, \hat{x} \in X \ f(x) \geq f(\hat{x}) + (f'(\hat{x}), x - \hat{x}) + \theta \|x - \hat{x}\|^2.$$
Criteria of convexity and strong convexity

**Theorem.** Let \( f(x) \) be a continuously differentiable functional defined on a convex set \( X \subseteq H \). Then \( f(x) \) is strongly convex with a constant \( \theta \geq 0 \) if and only if

\[
\forall x, \bar{x} \in X \quad (f'(x) - f'(\bar{x}), x - \bar{x}) \geq 2 \cdot \theta \cdot \|x - \bar{x}\|^2.
\]

**Theorem.** Let \( f(x) \) be a twice continuously differentiable functional, defined on a convex set \( X \) of a Hilbert space \( H \), and \( \text{int} \, X \neq \{\emptyset\} \). Then \( f(x) \) is strongly convex with a constant \( \theta \geq 0 \) if and only if \( \forall \bar{x} \in X, \forall h \in H \)

\[
(f''(\bar{x}) \cdot h, h) \geq 2 \cdot \theta \cdot \|h\|^2.
\]
Least square method. Pseudoinversion

Let us consider a system of linear algebraic equations (SLAE):

\[ Ax = b, \quad x \in \mathbb{R}^n, \quad b \in \mathbb{R}^m, \quad A: \mathbb{R}^n \to \mathbb{R}^m. \]

The system can be solvable or unsolvable. In the beginning of the XIX century, Gauss and Legendre independently proposed the least squares method. Instead of solving SLAE, they suggested to minimize a quadratic functional (discrepancy):

\[ \Phi(x) = \|Ax - b\|^2 = (A^* Ax, x) - 2 \cdot (A^* b, x) + (b, b), \]
Least square method.

Pseudoinversion

\[ \Phi'(x) = 2 \cdot (\hat{A}^* Ax - \hat{A}^* b) \]

\[ \Phi''(x) = 2 \cdot \hat{A}^* \hat{A} \geq 0 \]

System of normal equations

\[ \hat{A}^* Ax = \hat{A}^* b \]
Least square method. Pseudoinversion

If the system $Ax = b$ has a solution then it coincides with a solution of the system $A^*Ax = A^*b$. In this case, $\min_{x \in \mathbb{R}^n} \Phi(x) = \mu = 0$. But if $\min_{x \in \mathbb{R}^n} \Phi(x) = \mu > 0$, then the system $Ax = b$ has no solutions, though as it was shown above there exists a pseudosolution (maybe nonunique). The number $\mu$ is called a measure of incompatibility of the system $Ax = b$. 
Least square method. Pseudoinversion

Definition. A normal pseudosolution $x_n$ of the system $Ax = b$ is a pseudosolution with a minimal norm, i.e., it is a solution of extreme problem: find

$$\min_{x : A'Ax = A'b} \|x\|.$$ 

$$x_n = A^+ b$$
Least square method.  
Pseudoinversion

\[ A^\dagger = \lim_{\alpha \to 0^+} (A^* \cdot A + \alpha \cdot E)^{-1} \cdot A^* \]

Pseudoinverse to \( A \) operator
Least square method.

Pseudoinversion

If instead of a vector $b$ a vector $\tilde{b}$ is given such that: $\|\tilde{b} - b\| \leq \delta$, $\delta \geq 0$, and $x_n = A^+b$, $\tilde{x}_n = A^+\tilde{b}$, then $\|\tilde{x}_n - x_n\| \leq \|A^+\| \cdot \delta$ (it proves stability of a normal pseudosolution for disturbances in a right-hand side). So, the problem of finding a normal pseudosolution is well-posed if a pseudoinverse operator can be calculated exactly. But the problem of a pseudoinverse operator calculation can be ill-posed. It means that the problem to find $x_n = A^+b$ may be unstable for errors in $A$.
Minimizing sequences

Let us consider the problem: to find $x^* = \arg\min_{x \in X} f(x)$. The main approach to solve this problem is to construct an iterative process:

$$x^{(k+1)} = x^{(k)} + \alpha_k h^{(k)}, k = 0, 1, 2, \ldots, \quad x^{(0)} \text{ is an initial approximation, } h^{(k)} \text{ is a direction of minimization, } \alpha_k \text{ is a step along the direction of minimization.}$$
Minimizing sequences

The basic algorithm for constructing a sequence $x^{(k)}$ is following:

1. Assign $k=0$, define $x^{(0)}$.
2. Check stopping rules; if yes then go to 3, if no then go to 4.
3. Stop calculations.
4. Calculate $h^{(k)}$.
5. Calculate $\alpha_k$.
6. Calculate $x^{(k+1)}$.
7. Add 1 to $k$. Go to 2.
Minimizing sequences

We call a sequence $x^{(k)}$ to be minimizing if $f(x^{(k)}) \to f^* = \min_{x \in X} f(x)$. We need also $x^{(k)} \to x^* = \arg \min_{x \in X} f(x)$ (convergence of arguments). In this case, it is possible to estimate a rate of convergence. A sequence $x^{(k)}$ converges to $x^*$ with a linear rate if $\| x^{(k+1)} - x^* \| \leq q \| x^{(k)} - x^* \|$, $0 \leq q < 1$. If $\| x^{(k+1)} - x^* \| \leq q_k \| x^{(k)} - x^* \|$, $q_k \to 0$, $k \to \infty$, then convergence is superlinear. If $\| x^{(k+1)} - x^* \| \leq C \| x^{(k)} - x^* \|^2$, $C=\text{const}$, then convergence is quadratic.
Minimizing sequences

Mostly used stopping rules

1) $\| x^{(k+1)} - x^{(k)} \| \leq \varepsilon_1$;

2) $| f(x^{(k+1)}) - f(x^{(k)}) | \leq \varepsilon_2$;

3) $\| f'(x^{(k)}) \| \leq \varepsilon_3$, 
Minimizing sequences

Many minimization methods are so called descent methods. $h$ is a direction of descent of $f(x)$ if for sufficiently small positive $\alpha > 0$, $f(x + \alpha h) < f(x)$. We denote the set of directions of descent as $V(x, f)$. A minimization method is called a descent method if $h^{(k)} \in V(x^{(k)}, f)$. 
Minimizing sequences

Lemma. Let $f(x)$ be differentiable in a point $x \in H$. If $(f'(x), h) < 0$
then $h \in V(x, f)$. If $h \in V(x, f)$ then $(f'(x), h) \leq 0$.

In particular, if $h^{(k)} = -f'(x^{(k)})$ then it is a method of a gradient descent.
Minimizing sequences

\[ f(x^{(k)} + \alpha_k h^{(k)}) = \min_{\alpha \in \mathbb{R}^1} f(x^{(k)} + \alpha h^{(k)}) \]

\[ f(x) = \frac{1}{2} \langle Ax, x \rangle + \langle b, x \rangle \]

\[ \alpha_k = -\frac{\langle Ax^{(k)} + b, h^{(k)} \rangle}{\langle Ah^{(k)}, h^{(k)} \rangle} = -\frac{\langle f'(x^{(k)}), h^{(k)} \rangle}{\langle Ah^{(k)}, h^{(k)} \rangle} \]
Some methods for solving one-dimensional extremal problems

Golden section. At first, we shall find numbers $F_1$ и $F_2$ such that:

$$\frac{F_1}{F_2} = \frac{F_2}{1}, F_1 + F_2 = 1 \Rightarrow$$

$$F_1 = \frac{3 - \sqrt{5}}{2} \approx 0.38$$

$$F_2 = \frac{\sqrt{5} - 1}{2} \approx 0.62$$
Some methods for solving one-dimensional extremal problems

Quadratic approximation Let: $a_1 < c_1 < b_1$ and $f(c_1) < f(a_1); f(c_1) < f(b_1)$. 
Method of steepest descent

The method of steepest descent (or gradient descent) was proposed by Cauchy in the beginning of the 19th century. In this method:

$$h^{(k)} = -f'(x^{(k)}), \alpha_k = \arg \min f(x^{(k)} + \alpha h^{(k)}), 0 \leq \alpha < +\infty,$$

i.e. $\alpha_k$ is a solution of one-dimensional problem on a ray.
Method of steepest descent

Theorem. Let a functional $f(x)$ satisfy the following conditions:

1) It is defined, bounded from below and differentiable on a Hilbert space $H$.

2) For its gradient the Lipschitz condition holds:

$$\forall x, \hat{x} \in H : \| f'(x) - f'\hat{(x)} \| \leq M \| x - \hat{x} \|,$$

here $M > 0$ is a constant.

Then for any initial condition $x^{(0)}$ the sequence $x^{(k)}$ constructed, according to the method of steepest descent, has a property: $\lim_{k \to \infty} \| f'(x^{(k)}) \| = 0.$
Method of steepest descent

Remarks. 1) Any limit point of sequence $x^{(k)}$ is a stationary point of $f(x)$. If the functional is strongly convex, then it is a minimum point.

2) $\alpha_k$ is possible to calculate also by different methods. E.g., $\alpha_k = \frac{1}{2M}$, or if given $0 \leq \varepsilon \leq 1$, to choose $\alpha_k$ using the condition:

$$f(x^{(k)} - \alpha f''(x^{(k)}) - f(x^{(k)})) \leq -\varepsilon \alpha_k \| f'(x^{(k)}) \|^2.$$

3) The method of steepest descent for a strongly convex functional $f$ converges with a linear rate.
Conjugate gradient method

Let us consider a quadratic functional: 
\[ f(x) = \frac{1}{2} (Ax, x) + (b, x), \quad A = A^* > 0, \]
\[ x \in \mathbb{R}^n. \]

A problem: to find directions (vectors) in \( \mathbb{R}^n \): \( h^{(0)}, \ldots, h^{(n-1)} \in \mathbb{R}^n \), such that:
\[ f(x^{(n)}) = \min_{x \in \mathbb{R}^n} f(x) \quad \forall x^{(0)} \in \mathbb{R}^n; \]
\[ x^{(k+1)} = x^{(k)} + \alpha_k h^{(k)}; \quad \alpha_k = \arg\min f(x^{(k)} + \alpha h^{(k)}), \quad -\infty < \alpha < +\infty. \]
Conjugate gradient method

Definition. Two vectors $h', h'' \neq 0$ are conjugate (with respect to $A$) if

$$(Ah', h'') = 0.$$ 

Definition. Nonzero vectors $h^{(0)}, ..., h^{(k-1)} \in \mathbb{R}^n$ are conjugate (with respect to $A$) if

$$(Ah^{(i)}, h^{(j)}) = 0, \forall i \neq j; i, j = 0, ..., k - 1.$$ 

*
Conjugate gradient method

Theorem. If vectors $h^{(k)}, k = 0, \ldots, m-1 (m \leq n)$, are conjugate with respect to $A = A^* > 0$ and $\alpha_k$ are solutions one-dimensional minimization problem (see above), then

$$f(x^{(m)}) = \min_{x \in X_m} f(x), \quad X_m = \{x : x = x^{(0)} + \sum_{j=0}^{m-1} \lambda_j h^{(j)}\}, \quad \lambda_j \text{ are arbitrary real numbers.}$$

Remark. If $m = n$, then $f(x^{(n)}) = \min_{x \in \mathbb{R}^n} f(x)$. 
Let us describe a conjugate gradient method. An initial approximation $x^{(0)}$ is an arbitrary vector. $h^{(0)} = -f'(x^{(0)})$, $h^{(k)} = -f'(x^{(k)}) + \beta_{k-1} h^{(k-1)}$, $k \geq 1$. $f'(x) = Ax + b$.

$$\beta_{k-1} = \frac{(f'(x^{(k)}), Ah^{(k-1)})}{(h^{(k-1)}, Ah^{(k-1)})}.$$ 

Finally, $x^{(k+1)} = x^{(k)} + \alpha_k h^{(k)}$; $\alpha_k = \arg\min f(x^{(k)} + \alpha h^{(k)})$, $-\infty < \alpha < +\infty$. 

Conjugate gradient method
Conjugate gradient method

Lemma. Under conditions formulated above, vectors $h^{(0)},...,h^{(n-1)}$ are conjugate with respect to $A$, and a conjugate gradient method is a particular case of a conjugate direction method.

Theorem. A conjugate gradient method can find a minimum point of a quadratic functional $f(x) = \frac{1}{2} \cdot (Ax,x) + (b,x)$ ($A=A^* > 0$) in a finite-dimensional space $\mathbb{R}^n$ after no more than $n$ iterations.
Conjugate gradient method

A conjugate gradient method can be applied for minimizing a nonquadratic differentiable functional if a gradient of a functional satisfies a Lipschitz condition.

\[ x^{(0)} \in \mathbb{R}^n, \quad x^{(k+1)} = x^{(k)} + \alpha_k h^{(k)}, \quad \alpha_k = \arg \min_{\alpha \geq 0} f(x^{(k)} + \alpha h^{(k)}) \]

\[ h^{(0)} = -f'(x^{(0)}), \quad h^{(k)} = -f'(x^{(k)}) + \beta_{k-1} h^{(k-1)} \]
Conjugate gradient method

If

\[ \beta_{k-1} = \begin{cases} \frac{\|f'(x^{(k)})\|^2}{\|f'(x^{(k-1)})\|^2}, & k \neq 1, n+1, 2n+1, \ldots; \\ 0, & k = 1, n+1, 2n+1, \ldots, \end{cases} \]

then it is the Fletcher-Reeves method.
Conjugate gradient method

If

$$
\beta_{k-1} = \begin{cases} 
\frac{(f'(x^{(k)}), f'(x^{(k)}) - f'(x^{(k-1)}))}{\|f'(x^{(k-1)})\|^2}, & k \neq 1, n+1, 2n+1, \ldots, \\
0, & k = 1, n+1, 2n+1, \ldots, 
\end{cases}
$$

then it is the Polak-Ribiere method.
Newton’s method

Let $f(x)$ be a twice differentiable functional such that there exists a bounded linear operator $[f''(x)]^{-1}$ for any $x \in H$, $H$ is a Hilbert space.

Newton’s method produces the following minimizing sequence: $x^{(0)} \in H$ is an initial approximation: 

$x^{(n+1)} = x^{(n)} - [f''(x^{(n)})]^{-1} \cdot f'(x^{(n)})$, $n = 0, 1, ...$.
Remark. The sequence \( \{x^{(n)}\} \) in Newton’s method can be constructed in such way:

1) \( x^{(0)} \in H \);

2) \( x^{(n+1)} = \arg \min_{x \in H} f_n(x) \),

Here \( f_n(x) \equiv f(x^{(n)}) + (f'(x^{(n)}), x - x^{(n)}) + \frac{1}{2} (f''(x^{(n)})(x - x^{(n)}), x - x^{(n)}) \) is a quadratic approximation of \( f(x) \) in a point \( x^{(n)} \) according to a Taylor series.
Newton’s method

**Theorem.** Suppose that:

1) $f(x)$ is a twice differentiable strongly convex functional in $H$;

2) the second derivative $f''(x)$ satisfies the Lipschitz condition, i.e. there exists a constant $L \geq 0$ such that for any $x', x'' \in H$ \[ \| f''(x') - f''(x'') \| \leq L \| x' - x'' \| ; \]

3) the initial approximation is chosen such that $q \equiv \frac{L}{2\theta} \| x^{(0)} - x^{(0)} \| < 1$, here $\theta > 0$ is a constant of strong convexity.

Then:

1) $x^{(n)} \to x^* \in H$;

2) $\| x^{(n)} - x^* \| \leq \frac{2\theta}{L} \sum_{k=n}^{\infty} q^{2^k}$, $x^*$ is a solution of (*).
Newton’s method

An advantage of Newton’s method is a very high rate of convergence. Disadvantages are: 1) the method converges from a specially chosen initial approximation only; 2) it is necessary to invert a Hessian at each iteration. There exist modifications of the method.

If the functional is quadratic: \( f(x) = \frac{1}{2}(Ax, x) + (b, x) \), \( A = A^* > 0 \), then Newton’s method converges for one iteration starting from arbitrary initial approximation.
Zero-order methods

- Coordinate descent.
- Hooke-Jeeves method.
- Nelder-Mead method.
- Random search.
- Genetic algorithms.
Conditional gradient method

Let a differentiable functional \( f(x) \) be defined on a closed convex bounded set \( X \) in a Hilbert space \( H \). The conditional gradient method (or the Frank–Wolfe algorithm) produces two sequences \( \{x^{(n)}\} \subseteq X \) and \( \{\bar{x}^{(n)}\} \subseteq X \). An initial approximation \( x^{(0)} \in X \) is an arbitrary point in \( X \). After that we choose \( \bar{x}^{(0)} \) solving the problem

\[
(f' (x^{(n)}), \bar{x}^{(n)}) = \min_{x \in X} (f' (x^{(n)}), x)
\]

\((n=0)\), and construct

\[
x^{(n+1)} = x^{(n)} + \alpha_n (\bar{x}^{(n)} - x^{(n)})
\]

under condition that \( 0 \leq \alpha_n \leq 1 \). We repeat the process.
Conditional gradient method

**Theorem.** Let a functional $f(x)$ be defined on a closed convex bounded set $X \subseteq H$, and its gradient $f'(x)$ satisfies Lipschitz condition (i.e. there exists a constant $L > 0$ such that for any $x, y \in X$ $\| f'(x) - f'(y) \| \leq L \| x - y \|$). Let also parametrical steps $\alpha \in [0,1]$ be solutions of one-dimensional extremal problem:

$$f(x^{(n+1)}) = f(x^{(n)} + \alpha_n (\bar{x}^{(n)} - x^{(n)})) = \min_{0 \leq \alpha \leq 1} f(x^{(n)} + \alpha (\bar{x}^{(n)} - x^{(n)})).$$

Then for sequences $\{x^{(n)}\} \subseteq X$ and $\{\bar{x}^{(n)}\} \subseteq X$, defined above, following assertions are valid:
Conditional gradient method

1) \( \lim_{n \to +\infty} (f'(x^{(n)}))_\tau (x^{(n)} - x^{(n)}) = 0 \);

2) if the functional \( f(x) \) is convex, then \( \lim_{n \to +\infty} f(x^{(n)}) = f^* = \min_{x \in X} f(x) \);

3) if the functional \( f(x) \) is strongly convex, then the sequence \( \{x^{(n)}\} \subseteq X \) converges to \( x^* \in X \), the unique point of the global minimum of \( f(x) \) in \( X \), and

\[ \| x^{(n)} - x^* \| \leq \frac{C}{n}. \]
Projection of conjugate gradients method

We will describe the method of projection of conjugate gradients for minimization of a quadratic functional on the set of linear constraints in $\mathbb{R}^n$. Finite number of iterations is needed.

Let $J$ be a set of indexes, $c_J$ be a $m \times n$ matrix. Vectors $c^{(i)}, i \in J$ are its rows.

**Lemma.** If vectors $c^{(i)}, i \in J$ are linear independent, then the matrix $c_Jc_J^*$ is nondegenerated.
Projection of conjugate gradients method

Let us define \( P = C_j^*(C_j C_j^*)^{-1} C_j \). It is easy to see that
\[
PP = P, \quad P^* = P, \quad P(I - P) = (I - P)P = 0.
\]

The operator \( P : R^n \rightarrow R^n \) such that \( P^2 \equiv PP = P \) is called the projection operator. Obviously, \( I - P \) is the projection operator also. From written above, it is clear that \( PR^n \) and \( (I - P)R^n \) are orthogonal linear subspaces. So, \( P \) is the orthogonal projection operator on a subspace that is a linear shell of vectors \( c^{(i)}, i \in J \).
Projection of conjugate gradients method

We minimize a quadratic functional

\[ f(x) = \frac{1}{2} (Ax, x) + (b, x) \]

under linear constraints

\[ (c^{(i)}, x) - d_i = 0, \quad i \in J. \]

Here \( x, b, c^{(i)} \in \mathbb{R}^n \), \( d_i \) are numbers, \( n \times n \) matrix \( A \) is symmetric positively definite, \( J \) is a finite set of indexes.
Projection of conjugate gradients method

\[ x = x^{(0)} + (I - P) y. \]

Consider a function \( \varphi(y) = f(x^{(0)} + (I - P)y) \). Note that \( \varphi'(y) = (I - P)f'(x) \).

**Lemma.** Let \( \bar{y} \) be a point of global minimum of \( \varphi(y) \). Then \( \bar{x} = x^{(0)} + (I - P)\bar{y} \) is a point of minimum \( f(x) \) under linear constraints.
Projection of conjugate gradients method

**Theorem.** Minimization problem for a quadratic functional on the set of linear constraints can be solved for finite number of iterations using the method of projection of conjugate gradients. Starting from an initial approximation (satisfied constraints) $x^{(0)}$, we apply iterations:

\[
\begin{align*}
    h^{(0)} &= -(I - P)f'(x^{(0)}), \\
    x^{(k+1)} &= x^{(k)} + \alpha_k h^{(k)}, \\
    h^{(k)} &= -(I - P)f'(x^{(k)}) + \frac{\| (I - P)f'(x^{(k)}) \|^2}{\| (I - P)f'(x^{(k-1)}) \|^2} h^{(k-1)}, \\
    \alpha_k &= -\left( \frac{f'(x^{(k)}), h^{(k)}}{\langle p_k, Ah^{(k)} \rangle} \right), k = 0, 1, \ldots
\end{align*}
\]
Projection of conjugate gradients method

- If we have linear constraints of inequality type, the method can be applied also. It is a bit more complicated.
Numerical methods for solving ill-posed problems on special compact sets

Let us consider again an operator equation:

$$Az = u,$$

here $A$ is a linear bounded injective operator mapping a normed space $Z$ into a normed space $U$. Let $\tilde{z}$ be an exact solution of the operator equation, $A\tilde{z} = \tilde{u}$ is an exact right-hand side, $u_\delta$ is an approximate right-hand side such that

$$\|\tilde{u} - u_\delta\| \leq \delta, \; \delta > 0,$$

and $A_h : A_h : Z \to U$ is a linear bounded operator such that

$$\|A_h - A\| \leq h, \; h \geq 0.$$ We denote a pair of errors $\delta, h$ as $\eta=(\delta, h)$. 
Numerical methods for solving ill-posed problems on special compact sets

It is given that \( \bar{z} \in D, \ D \subseteq Z \) is a compact. Then we can consider as an approximate solution any \( z_\eta \in D \) that satisfies an inequality: \( \left\| A_h z_\eta - u_\delta \right\| \leq \delta + h \left\| z_\eta \right\| \)

(\( \eta \)-quasisolution), and \( z_\eta \to \bar{z} \) as \( \eta \to 0 \) at that.
Numerical methods for solving ill-posed problems on special compact sets

Suppose that it is known from a priori considerations that an exact solution of an operator equation is a monotonic on $[a,b]$ function (for definiteness, the function is nonincreasing) that is bounded from below and from above by constants $C_1$ and $C_2$. Without loss of generality, we suppose that $C_1=C>0$, $C_2=0$. We consider a set $Z \downarrow_c$ of nonincreasing functions $z(s)$ bounded by constants $C$ and $0$, i.e. $C \geq z(s) \geq 0 \quad \forall s \in [a,b]$. This set $Z \downarrow_c$ is a compact in $L_2[a,b]$, and thereby $z_\eta \to \bar{z}$ as $\eta \to 0$ in $L_2[a,b]$. This result can be reinforced if an exact solution is
Numerical methods for solving ill-posed problems on special compact sets

continuous on $[a, b]$, i.e. $\bar{z}(s) \in Z \downarrow_c \cap \mathbb{C}[a, b]$. In this case, regularized approximate solutions converge to the exact solution uniformly on any segment $[\gamma, \sigma] \subseteq (a, b)$. If the exact solution is piece-wise continuous then the convergence is uniform on any segment $[\gamma, \sigma] \subseteq (a, b)$ that doesn’t contain points of discontinuity of $\bar{z}$. Obviously, that the set $Z \downarrow_c$ is convex.
Bounded monotonic functions

- Let is a set of monotonic nonincreasing on \([a, b]\) functions is \(Z \downarrow_c\).
- Lemma. \(Z \downarrow_c\) is a compact in \(L_p[a,b]\), \(p>1\).
- The Lemma guarantees convergence of quasisolutions (or \(\eta\)-quasisolutions) to the exact solution in \(L_p[a,b]\), \(p>1\).
Bounded monotonic functions

Theorem (Goncharsky, Yagola). If the exact solution of the operator equation is a nonincreasing bounded monotonic continuous function then quasisolutions (or \(\eta\)-quasisolutions) converge to the exact solution uniformly on any segment \([\gamma, \sigma] \subseteq (a, b)\). If the exact solution is piecewise continuous then the convergence is uniform on any segment \([\gamma, \sigma] \subseteq (a, b)\) that doesn’t include the points of discontinuity of the exact solution (so called piecewise uniform convergence).
Numerical methods for solving ill-posed problems on special compact sets

Other sets under consideration are following: the set $\tilde{Z}_c$ of concave on $[a,b]$ functions bounded from above and from below by constants $C$ and $0$; the set $\bar{Z}_c$ of concave on $[a,b]$ monotonic (for definiteness, nonincreasing) functions bounded from above and from below by constants $C$ and $0$. Both these sets are compacts in $L_2[a,b]$, and the convergence of approximate solutions to the exact solution is uniform on any segment $[\gamma, \sigma] \subseteq (a,b)$.
Numerical methods for solving ill-posed problems on special compact sets

Let $Z = L_2[a,b]$, $U = L_2[c,d]$. Let us consider the quadratic functional (the discrepancy)

$$\Phi(z) = \|A_h z - u_\delta\|^2; \quad \Phi'(z) = 2(A_{h}^* A_{h} z - A_{h}^* u_\delta).$$

In order find a quasisolution $z_\eta \in D$ it is sufficient to minimize the discrepancy on the set $D$ using the stopping rule: $\Phi(z_\eta) \leq (\delta + h \|z_\eta\|)^2$. The conditional gradient method can be applied.
Numerical methods for solving ill-posed problems on special compact sets

After finite-dimensional approximation of sets $Z_{\downarrow C}, \tilde{Z}_{\downarrow C}, \bar{Z}_{\downarrow C}$ we can get sets $M_{\downarrow C}, \tilde{M}_{\downarrow C}, \bar{M}_{\downarrow C}$ respectively:

$$M_{\downarrow C} = \left\{ z : z \in \mathbb{R}^n, \begin{array}{l}
z_{i+1} - z_i \leq 0, i = 1 \ldots n - 1 \\
0 \leq z_i \leq C, i = 1 \ldots n \end{array} \right\}$$

$$\tilde{M}_{\downarrow C} = \left\{ z : z \in \mathbb{R}^n, \begin{array}{l}
z_{i+1} - 2z_i + z_{i+1} \leq 0, i = 2 \ldots n - 1 \\
0 \leq z_i \leq C, i = 1 \ldots n \end{array} \right\}$$

$$\bar{M}_{\downarrow C} = \left\{ z : z \in \mathbb{R}^n, \begin{array}{l}
z_{i+1} - 2z_i + z_{i+1} \leq 0, i = 2 \ldots n - 1 \\
z_{i-1} - 2z_i + z_{i+1} \leq 0, i = 2 \ldots n - 1 \\
0 \leq z_i \leq C, i = 1 \ldots n \end{array} \right\}$$

where $z_i = z(s_i)$, $\{s_i\}_{i=1}^n$ is an uniform grid on $[a, b]$ with a step $h_s$. 
Numerical methods for solving ill-posed problems on special compact sets

These sets $M \updownarrow_c, M \updownarrow_c, M_c$ are closed bounded and convex polyhedrons in $\mathbb{R}^n$, vertices of them $T^{(i)}$, $(1 \leq j \leq n)$ are following.

Vertices of $M \downarrow_c$:

$$T^{(0)} = 0,$$

$$T^{(j)}_i = \begin{cases} C, i \leq j, \\ 0, i > j, j = 1...n. \end{cases}$$
Numerical methods for solving ill-posed problems on special compact sets

Vertices of $\tilde{M} \downarrow_c$:

\[ T^{(0)} = 0, \]

\[ T^{(j)}_i = \begin{cases} C, & i \leq j, \\ \frac{n-i}{n-j} C, & i > j, \quad j = 1 \ldots n. \end{cases} \]
Numerical methods for solving ill-posed problems on special compact sets

Vertices of $\hat{M}_c$:

\[
T^{(0,0)} = 0,
\]

\[
T^{(i,j)}_k = \begin{cases} 
2C \frac{k - 1}{j - 1}, & k < j, \\
C, & i \leq k \leq j, \\
\frac{n - k}{n - j} C, & k > j, 1 \leq i \leq j \leq n.
\end{cases}
\]
Numerical methods for solving ill-posed problems on special compact sets

Let us consider the Fredholm integral equation of the 1st kind:

\[ A\mathbf{z} = \int_a^b K(x, s)z(s) = u(x), \]

where the kernel \( K(x, s) \) is nondegenerated, and it is a real continuous on \( \Pi = \{ a \leq x \leq b, c \leq s \leq d \} \) function. Instead of the exact right-hand side \( A\mathbf{z} = \mathbf{u} \) it is given \( \mathbf{u}_\delta : \| \mathbf{u} - \mathbf{u}_\delta \|_{L_2(\Pi)} \leq \delta \), and instead of \( K(x, s) \) it is given \( K_h(x, s) : \| K(x, s) - K_h(x, s) \|_{L_2(\Pi)} \leq h \). For simplicity, we choose uniform grids with steps \( h_x \) and \( h_s \) respectively \( \{ s_j \}_{j=1}^n \), on the segment \([a, b]\) and \( \{ x_i \}_{i=1}^m \) on the segment \([c, d]\).
Numerical methods for solving ill-posed problems on special compact sets

Then a finite-dimensional approximation of the discrepancy

$$\Phi(z) = \| A_h z - u_\delta \|_{L^2[a,b]}^2 = \int_a^b \left[ \int_a^b K_h(x,s)z(s)ds - u_\delta(x) \right]^2 dx$$

is a quadratic functional.

$$\hat{\Phi}(\hat{z}) = \sum_{i=1}^m \left[ \sum_{j=1}^n a_{ij} z_i h_s - u_i \right]^2 h_x,$$

where $a_{ij} = K_h(x_i,s_j)$, $\hat{z} = \{z_j\}_{j=1}^n$.

For its minimization on described above polyhedrons the conditional gradient method (or better the method of projection of conjugate gradients) can be applied.
Ill-posed problems with a source-wise represented solution

\[ A\bar{z} = \bar{u} \]  \hspace{1cm} (1)

\( A : Z \rightarrow U \) is a linear injective operator.

Assume the next \textit{a priori} information: \( \bar{z} \) is sourcewise represented with a linear compact operator \( B : V \rightarrow Z : \)

\[ \bar{z} = B\bar{v} \]  \hspace{1cm} (3)

Here \( V \) is a reflexive Banach space.

Suppose \( B \) is injective, \( A \) is known exactly, \( \|u_\delta - \bar{u}\| \leq \delta \).
Set $n = 1$ and define the set

$$Z_n = \{z \in Z : z = Bv, v \in V, \|v\| \leq n\}$$

Minimize the discrepancy $F(z) = \|Az - u_\delta\|$ on $Z_n$.

If $\min \{\|Az - u_\delta\| : z \in Z_n\} \leq \delta$, then the solution is found. Denote $n(\delta) = n$. Otherwise, we change $n$ to $n + 1$ and reiterate the process.

If $n(\delta)$ is found, then we define the approximate solution $z_{n(\delta)}$ of (1) as an arbitrary solution of the inequality

$$\|Az - u_\delta\| \leq \delta \quad z \in Z_{n(\delta)}$$
Theorem 1: The process described above converges: \( n(\delta) < \infty \). There exists \( \delta_0 > 0 \) (generally speaking, depending on \( \bar{Z} \)) such that \( n(\delta) = n(\delta_0) \) for \( \forall \delta \in (0, \delta_0] \). Approximate solutions \( z_{n(\delta)} \) strongly converge to \( \bar{Z} \) as \( \delta \to 0 \).

Proof The ball \( V_n = \{ v \in V : \| v \| \leq n \} \) is a bounded closed set in \( V \). The set \( Z_n \) is a compact in \( Z \) for any \( n \), since \( B \) is a compact operator. Due to Weierstrass theorem the continuous functional \( F(z) \) attains its exact lower bound on \( Z_n \).

Clearly, \( \bar{z} = B\bar{v} \in Z_N \), where

\[
N = \begin{cases} 
    \| \bar{v} \| & \text{is a positive integer} \\
    \| \bar{v} \| + 1 & \text{otherwise}
\end{cases}
\]

\( \lfloor \cdot \rfloor \) is the integer part of a number.
Therefore \( n(\delta) \) is a finite number and there is \( \delta_0 \) such that \( n(\delta) = n(\delta_0) \) for any \( \delta \in (0, \delta_0] \). The inequality \( n(\delta) \geq N \) for any \( \delta > 0 \) is evident. Thus, for all \( \delta \in (0, \delta_0] \) the approximate solutions \( z_n(\delta) \) belong to the compact set \( Z_n(\delta_0) \), and the method coincides with the quasisolutions method for all sufficiently small positive \( \delta \). The convergence \( z_n(\delta) \to \bar{z} \) follows from the general theory of ill-posed problems.

**Remark 1:** The method is a variant of the method of extending compacts (Ivanov, Dombrobskaya).
**Theorem 2:** For the method described above there exists an *a posteriori* error estimate. It means that a functional $\kappa(u_\delta, \delta)$ exists such that $\kappa(u_\delta, \delta) \to 0$ as $\delta \to 0$ and $\|z_{n(\delta)} - \overline{z}\| \leq \kappa(u_\delta, \delta)$ at least for all sufficiently small positive $\delta$.

**Remark 2:** The existence of the a posteriori error estimation follows from the following. If by $\overline{Z} \in Z$ we denote the space of sourcewise represented with the operator $B$ solutions of (1), then $\overline{Z} = \bigcup_{n=1}^{\infty} Z_n$. Since $Z_n$ is a compact set, then $\overline{Z}$ is a $\sigma$-compact space.
An *a posteriori* error estimate is not an error estimate in general meaning that is impossible in principle for ill-posed problems. But it becomes an upper error estimate of the approximate solution for “small” errors $\delta < \delta_0$, where $\delta_0$ depends on the exact solution $\bar{z}$.
Let $A$ be a linear injective completely continuous operator, and $Z$ and $U$ be Hilbert spaces. Consider the case when $\tilde{z} = (A^*A)^{p/2}\tilde{v}$, ($\tilde{v} \in Z$, $p = \text{const.} > 0$).

**Lemma 1** The operator $(A^*A)^{p/2}$ is completely continuous and injective from $Z$ into $Z$ for any $p > 0$.

For the case when $Z$ and $U$ are Hilbert spaces, $V = Z$, $A : Z \to U$ is a linear injective completely continuous operator, $B = (A^*A)^{p/2}$, and $p = \text{const.} > 0$, the following theorem holds.

**Theorem 3** (see [14,15]) For the case under consideration, the extending compacts method is the optimal regularizing algorithm in terms of the order of accuracy.

It is clear that, in the extending compacts method, we can replace the sequence $n = 1, 2, \ldots$ with any increasing sequence of positive numbers $r_1, r_2, \ldots, r_n, \ldots$ such that $\lim_{n \to \infty} r_n = +\infty$. 
The operators $A$ and $B$ are known with errors. Let there be linear operators $A_{h_A}, B_{h_B}$ such that $\|A_{h_A} - A\| \leq h_A, \|B_{h_B} - B\| \leq h_B$. Denote the vector of errors by $\eta \equiv (\delta, h_A, h_B)$. For any integer $n$ define a compact set $Z_{n,h_B} \equiv \{z \in Z : z = B_{h_B} v, v \in V, \|v\| \leq n\}$.

Find a minimal positive integer number $n = n(\eta)$ such that the inequality

$$\left\| A_{h_A} z - u_\delta \right\| \leq \delta + \left(h_A \left\| B_{h_B} \right\| + h_B \left\| A_{h_A} \right\| + h_A h_B \right) \cdot n(\eta)$$

has a nonempty set of solutions.

Then the *a posteriori* error estimation is

$$\kappa(u_\delta, A_{h_A}, B_{h_B}, \eta) \equiv h_B n(\eta) + \max \{\|z - z_{n(\eta)}\| : z \in Z_{n(\eta), h_B}\},$$

$$\left\| A_{h_A} z - u_\delta \right\| \leq \delta + \left(h_A \left\| B_{h_B} \right\| + h_B \left\| A_{h_A} \right\| + h_A h_B \right) \cdot n(\eta)$$
A posteriori error estimation

For some ill-posed problems it is possible to find a so-called *a posteriori* error estimation.

Let $A$ be an exact injective operator with closed graph and $Z$ be a $\sigma$-compact space.

Introduce a function $\kappa(u_\delta, \delta)$ such that $\forall \bar{z} \in Z$

$\exists \delta(\bar{z}) > 0$, $\forall \delta \in (0, \delta(\bar{z})]$, $\forall u_\delta \in U$, $\|u_\delta - \bar{u}\| \leq \delta$:

$$\|\bar{z} - R(u_\delta, \delta)\| \leq \kappa(u_\delta, \delta)$$

The function $\kappa(u_\delta, \delta)$ is an *a posteriori* error estimation for the problem (1), if $\kappa(u_\delta, \delta) \to 0$ as $\delta \to 0$
Tikhonov’s regularizing algorithm

Let \( Z, U \) be Hilbert spaces, \( D \subseteq Z \) be a closed convex set of \textit{a priori} constraints such that \( 0 \in D \), \( A, A_h \) be linear operators. On a set \( \{ A_h, u_\delta, \eta \} \) introduce the Tikhonov's functional:
\[
M^\alpha[z] = \|A_h z - u_\delta\|^2 + \alpha \|z\|^2
\]
where \( \alpha > 0 \) is a regularization parameter.
\[
\inf \left\{ M^\alpha[z] : z \in D \right\}
\]  \hspace{1cm} (2)

For any \( \alpha > 0, u_\delta \in U \) and bounded linear operator \( A_h \) the problem (2) is solvable and has a unique solution \( z_\eta^\alpha \in D \).
A priori choice of $\alpha$

A regularizing algorithm using the extreme problem (2) for $M^\alpha[z]$ : to construct $\alpha(\eta)$ such that $z^{\alpha(\eta)}_\eta \to \bar{z}$ as $\eta \to 0$ .

If $A$ is an injective operator, $\bar{z} \in D$ and $\alpha(\eta) \to 0$, 
\[
\frac{(h+\delta)^2}{\alpha(\eta)} \to 0 \text{ as } \eta \to 0 ,
\]
then $z^{\alpha(\eta)}_\eta \to \bar{z}$ as $\eta \to 0$ ,
i.e., there is the a priori choice of $\alpha$ .
Generalized discrepancy principle
(a posteriori choice of $\alpha$)

The incompatibility measure of (1) on $D$:
$$\mu_\eta(u_\delta, A_h) = \inf \left\{ \|A_h z - u_\delta\| : z \in D \right\}$$

Let it can be computed with an error $\kappa > 0$, i.e., instead of $\mu_\eta(u_\delta, A_h)$ there is $\mu^\kappa_\eta(u_\delta, A_h)$ such that
$$\mu_\eta(u_\delta, A_h) \leq \mu^\kappa_\eta(u_\delta, A_h) \leq \mu_\eta(u_\delta, A_h) + \kappa$$

The generalized discrepancy:
$$\rho^\kappa_\eta(\alpha) = \|A_h z^\alpha - u_\delta\|^2 - (\delta + h\|z^\alpha\|)^2 - (\mu^\kappa_\eta(u_\delta, A_h))^2$$

The generalized discrepancy $\rho^\kappa_\eta(\alpha)$ is continuous and monotonically non-decreasing for $\alpha > 0$. 
The generalized discrepancy principle to choose the regularization parameter:

1) If the condition \( \|u_\delta\|^2 > \delta^2 + (\mu_\eta^\kappa(u_\delta, A_h))^2 \) is not just, then \( z_\eta = 0 \) is an approximate solution of (1);

2) If the condition \( \|u_\delta\|^2 > \delta^2 + (\mu_\eta^\kappa(u_\delta, A_h))^2 \) is just, then the generalized discrepancy has a positive zero \( \alpha^* \) and \( z_\eta = z_\eta^\alpha \).

If \( A \) is an injective operator, then \( \lim_{\eta \to 0} z_\eta = \bar{z} \).

Otherwise, \( \lim_{\eta \to 0} z_\eta = z^* \), where \( \bar{z} \) is the normal solution of (1), i.e., \( \|z^*\| = \inf \{\|z\| : z \in D, Az = \bar{u}\} \).
If $A, A_h$ are bounded linear operators, $D$ is a closed convex set, $0 \in D$, $\bar{z} \in D$, the generalized discrepancy principle are equivalent to the generalized discrepancy method:

\[
\inf \left\{ \|z\| : z \in D, \|A_h z - u_\delta\|^2 \leq (\delta + h\|z\|)^2 + (\mu_\eta^\kappa (u_\delta, A_h))^2 \right\}
\]
Inverse problem for the heat conduction equation

\[
\begin{align*}
    w_t &= a^2 w_{xx}, \quad x \times t \in (0, l) \times (0, T) \\
    w(0, t) &= 0 \\
    w(l, t) &= 0
\end{align*}
\]

There is a function \( u_\delta(\xi) = w(\xi, T) \in L^2[0, l] \), we want to find \( z(x) = w(x, 0) \in W^1_2[0, l] \) such that \( z(x) \to \bar{z}(x) \) as \( \eta \to 0 \).

We can write that

\[
\|u(\xi)\|^2 = \int_0^l |u(\xi)|^2 d\xi, \quad \|z(x)\|^2 = \int_0^l \left( |z(x)|^2 + \left| \frac{\partial z(x)}{\partial x} \right|^2 \right) dx
\]
The problem may be written in the form of integral equation

\[ u(\xi) = \int_0^l G(\xi, x, T) z(x) \, dx \]

where \( G(\xi, x, t) \) is the Green function:

\[ G(\xi, x, t) = \sum_{n=1}^{+\infty} \frac{2}{l} \sin \left( \frac{\pi n \xi}{l} \right) \sin \left( \frac{\pi n x}{l} \right) \exp \left( -\left( \frac{\pi n a}{l} \right)^2 t \right) \]

The problem is solved for the parameters \( a = 1.0, T = 0.1, l = 1.0 \) , the function \( u_\delta(\xi) \) is taken such that \( \delta = 0.05 \cdot \| \overline{u}(\xi) \| \) .
The exact solution $\bar{z}(x)$ (---) and the approximate solution $z_\eta(x)$ (-----).
The Euler equation

The Tikhonov's functional $M^\alpha[z]$ is a strongly convex functional in a Hilbert space.

The necessary and sufficient condition for $z_\alpha^\eta$ to be a minimum point of $M^\alpha[z]$ on a set $D$ of a priori constraints is

$$\left(\left(M^\alpha[z_\alpha^\eta]\right)', z - z_\alpha^\eta\right) \geq 0 \quad \forall z \in D$$

If $z_\alpha^\eta$ is an interior point of $D$, then $(M^\alpha[z_\alpha^\eta])' = 0$, or

$$A_h^*A_h z_\alpha^\eta + \alpha z_\alpha^\eta = A_h^*u_\delta$$

We obtain the Euler equation.
Error-free methods

As the first example we consider so-called the “L-curve method” (P.C. Hansen). In this method the regularization parameter in Tikhonov functional $\alpha$ is selected as a point maximum curvature of the L-curve $\{(\ln||A_hz^\alpha - u_\delta||, \ln||z^\alpha||): \alpha > 0\}$.

But this method cannot be used for the solution of ill-posed problems because the L-curve doesn’t depend on $h$ and $\delta$ (see the theorem). Everybody can easily prove that this method is inapplicable to solving the simplest finite-dimensional well-posed problems (e.g., equation $z=1$).
Another very popular “error free” method is GCV – the generalized cross-validation method (G. Wahba), where $\alpha(A_h, u_\delta)$ is found as the point of the global minimum of the function

$$G(\alpha) = \|(A_hA_h^* + \alpha I)^{-1}u_\delta\| [\text{tr}(A_hA_h^* + \alpha I)^{-1}]^{-1}, \ \alpha \geq 0.$$ 

This method is not applicable for the solution of ill-posed problems including ill-posed systems of linear algebraic equations (see the theorem above). It is possible construct well-posed systems of linear algebraic equations the GCV method failed for their solution. Let $Z = U = \mathbb{R}^2$,

$$u = \left(\begin{array}{c} -2 \\ -1 \end{array}\right), \quad A = \left(\begin{array}{cc} 1 & 1 \\ 1 & 2 \end{array}\right)$$
Here \( h > 0 \). Very easy to calculate the GCV solution \( z_{gcv} \) and prove that it converges to \((-1/3, -1/3)^*\) instead of \( z^e = (-3, 1)^* \) when \( h \to 0 \).

A lot of other examples could be found in a paper by

Publications on error-free methods


Incompatible ill-posed problems

Let us consider an operator equation:

\[ Az = u \]

where \( z \in D \subseteq Z \) is a convex closed set, \( 0 \in D \), \( u \in U \), \( Z \) and \( U \) are Hilbert spaces, \( A \) is a linear bounded operator. If \( u = \bar{u} \), a solution of the equation, maybe, does not exist, but we suppose that there exists \( \bar{z} \in D \) such that minimizes the discrepancy:

\[ \bar{u} = \inf_{z \in D} \| Az - \bar{u} \| \geq 0. \]
\( \overline{\mu} \) is called the **incompatibility measure** of the operator equation with exact data \( \overline{u} \) and \( A \). If \( \overline{\mu} > 0 \), then \( \overline{z} = \arg \min_{z \in D} \| Az - \overline{u} \| \) (или \( \| A\overline{z} - \overline{u} \| = \overline{\mu} \), \( \overline{z} \in D \)) is called the **pseudosolution** (or quasisolution). If \( \overline{Z} = \{ z : z \in D, \| Az - \overline{u} \| = \overline{\mu} \} \) contains more than one element, then \( \overline{Z} \) is convex and closed. Consequently, there exists the unique element \( \overline{z} = \arg \min_{z \in \overline{Z}} \| z \| \) that is called the **normal pseudosolution**. If \( \overline{\mu} = 0 \), then a pseudosolution is a solution of the operator equation, and a normal pseudosolution is a normal solution.
Let us try to construct an algorithm for stable approximation to the normal pseudosolution of the incompatible operator equation if we are given approximate data: \( \{A_h, u_\delta, \eta\} \), here \( \eta = (\delta, h) \), \( \delta > 0 \), \( h \geq 0 \), \( \| u_\delta - \overline{u} \| \leq \delta \), \( \| A_h - A \| \leq h \) (\( \overline{\mu} = 0 \) we will consider as a particular case).

We will consider an upper estimate for the incompatibility measure:

\[
\overline{\mu}_\eta (u_\delta, A_h) = \inf_{\mathbf{z} \in \mathcal{D}} \left( \delta + h \| \mathbf{z} \| + \| A_h \mathbf{z} - u_\delta \| \right).
\]
Lemma. Under formulated above conditions \( \tilde{\mu}_\eta(u_\delta, A_h) \geq \mu \), and

\[ \lim_{\eta \to 0} \tilde{\mu}_\eta(u_\delta, A_h) = \mu. \]

We denote the minimizer of Tikhonov’s functional \( M^\alpha[z] \) as \( z^\alpha \) and introduce the generalized discrepancy: \( \tilde{\rho}_\eta(\alpha) = \left\| A_h z^\alpha_\eta - u_\delta \right\|^2 - \left( \delta + h \left\| z^\alpha_\eta \right\| + \tilde{\mu}_\eta(u_\delta, A_h) \right)^2. \)
If $\tilde{\mu}_\eta(u_\delta, A_h)$ is calculated with an error $k \geq 0$, then the generalized discrepancy is

$$\hat{\rho}_\eta^k(\alpha) = \|A_h z_\eta^\alpha - u_\delta\|^2 - (\delta + h \|z_\eta^\alpha\| + \tilde{\mu}_\eta(u_\delta, A_h))^2,$$

where $\tilde{\mu}_\eta(u_\delta, A_h) \leq \tilde{\mu}_\eta^k(u_\delta, A_h) \leq \tilde{\mu}_\eta(u_\delta, A_h) + k$, $\tilde{\mu}_\eta^k(u_\delta, A_h) \geq \overline{\mu}$, and $\tilde{\mu}_\eta^k(u_\delta, A_h) \to \overline{\mu}$ as $\eta \to 0$ if $k = k(\eta) \to 0$ as $\eta \to 0$. 
The generalized discrepancy has following properties:

1) \( \tilde{\rho}^k_\eta(\alpha) \) is continuous and nondecreasing for \( \alpha > 0 \);

2) \( \lim_{\alpha \to +\infty} \tilde{\rho}^k_\eta(\alpha) = \|u_\delta\|^2 - \left(\delta + \tilde{\mu}^k_\eta(u_\delta, A_h)\right)^2 \);

3) \( \lim_{\alpha \to 0+0} \tilde{\rho}^k_\eta(\alpha) \leq \left(\mu_\eta(u_\delta, A_h)\right)^2 - \left(\delta + \tilde{\mu}^k_\eta(u_\delta, A_h)\right)^2 < 0. \)

4) If \( \|u_\delta\| > \delta + \tilde{\mu}^k_\eta(u_\delta, A_h) \), then \( \exists \alpha^* > 0: \tilde{\rho}^k_\eta(\alpha^*) = 0 \), that is equivalent to 
\[ \|A_hz^{\alpha^*_\eta} - u_\delta\| = \delta + h\|z^{\alpha^*_\eta}\| + \tilde{\mu}^k_\eta(u_\delta, A_h) ; \quad z^{\alpha^*_\eta} \text{ is unique.} \]
Modified GDP: we are given \( \{A_h, u_\delta, \eta\} \). We calculate

\[
\tilde{\mu}_\eta^k(u_\delta, A_h) = \inf_{z \in D} \left( \delta + h \|z\| + \|A_h z - u_\delta\| \right) + k = \tilde{\mu}_\eta(u_\delta, A_h) + k, \quad k \geq 0, \quad k = k(\eta) \to 0 \text{ as } \eta \to 0. \]

If \( \|u_\delta\| > \delta + \tilde{\mu}_\eta^k(u_\delta, A_h) \) is not true, then \( z_\eta = 0 \); in the opposite case we shall find \( \alpha^* \) and calculate \( z_\eta = z^*_\eta \).
Theorem. $\lim_{\eta \to 0} z_\eta = \bar{z}$, where $\bar{z}$ is the normal pseudosolution of the operator equation.

Modified GDP is equivalent to Modified GDM:

$$\inf \| z \|, \quad z \in \{ z \in D, \| A_h z - u_\delta \| \leq \delta + h \| z \| + \tilde{\mu}_\eta^k (u_\delta, A_h) \}.$$
Numerical methods for the solution of Fredholm integral equations of the first kind

Suppose that we are given the Fredholm integral equation of the first kind:

\[ A z = \int_{a}^{b} K(x, s) z(s) \, ds = u(x), \]
where the kernel $K(x,s)$ is not degenerated and is real and continuous on $\Pi = \{a \leq x \leq b, c \leq s \leq d\}$. We choose $U = L_2[c,d]$ and $Z = W^1_2[a,b]$. In this case, we can guarantee convergence of regularized approximations in $W^1_2[a,b]$, and uniform convergence (in $C[a,b]$). We do not know the exact right-hand side $A\vec{z} = \vec{u}$, and we are given $u_\delta : \|\vec{u} - u_\delta\|_{L_2[c,d]} \leq \delta$, and instead of $K(x,s)$ we know $K_h(x,s) : \|K(x,s) - K_h(x,s)\|_{L_2(\Pi)} \leq h$. For simplicity, we introduce uniform grids with steps $h_x$ and $h_s$: on the segment $[a,b]$ the grid $\{s_j\}_{j=1}^n$, and on the segment $[c,d]$ the grid $\{x_i\}_{i=1}^m$. 
Then the discrepancy functional

\[
\Phi(z) = \left\| A_h z - u_\delta \right\|^2_{L_2[a,b]} = \int_a^b \left[ \int_a^b K_h(x, s) z(s) ds - u_\delta(x) \right]^2 dx
\]

can be approximated by the quadratic functional

\[
\hat{\Phi}(\hat{z}) = \sum_{i=1}^m \left[ \sum_{j=1}^n a_{ij} z_j h_x - u_i \right]^2 h_x,
\]

where \( a_{ij} = K_h(x_i, s_j), \) \( \hat{z} = \{z_j\}_{j=1}^n \). Some methods for minimization of this functional if a priori information is available were described earlier.
Finite-dimensional approximation of Tikhonov’s functional

\[ M^\alpha[z] = \left\| A_h z - u_\delta \right\|^2_{L_2[a,b]} + \alpha \left\| z \right\|^2_{W^1_2[a,b]} + \int_a^b \int_a^b K_h(x,s)z(s)ds - u_\delta(x) \right\| dx + \]

\[ + \alpha \left[ \int_a^b z^2(s)ds + \int_a^b (z'(s))^2 ds \right] \]

can be written as following:

\[ \hat{M}^\alpha[\hat{z}] = \sum_{i=1}^m \left[ \sum_{j=1}^n a_{ij} \hat{z}_j h_s - u_i \right] h_s + \alpha \sum_{j=1}^n \hat{z}_j^2 h_s + \alpha \sum_{j=2}^n (\hat{z}_j - \hat{z}_{j-1})^2 / h_s. \]
It is a quadratic functional defined on $\mathbb{R}^n$. If linear constraints are available, then for its minimization different methods can be used, e.g., the method of projection of conjugate gradients.

If no constraints, then we can get a system of linear algebraic equations: $(\hat{M}^a[z])' = 0$. For its solution it can be used different numerical methods including the Cholesky decomposition.
Convolution type equations

1D convolution type equation is following:

\[ Az = \int_{-\infty}^{\infty} K(x-s)z(s)ds = u(x), \quad -\infty < x < +\infty. \]
We suppose that the functions in the equation satisfy requirements:

\[ K(y) \in L_1(R^1) \cap L_2(R^1), \]
\[ u(x) \in L_2(R^1), \]
\[ z(s) \in W^1_2(R^1), \]

- \( A \) is an injective operator (the kernel \( K \) is closed).
- No constraints \( D = Z \).
- For \( \bar{u} \) there exists an unique solution \( A\bar{z} = \bar{u} \) in \( W^1_2(R^1) \).

We are given approximate data \( u_\delta \) and the integral operator of the convolution type \( A_h \) (with the kernel \( K_h \)), \( \delta > 0 \), \( h \geq 0 \) such that:

\[ \| u_\delta - \bar{u} \|_{L_2} \leq \delta; \]
\[ \| A - A_h \|_{W^1_2 \rightarrow L_2} \leq \| A - A_h \|_{L_2 \rightarrow L_2} \leq h. \]
Let us consider Tikhonov’s functional:

\[ M^\alpha [z] = \| A_n z - u_\delta \|_{L_2}^2 + \alpha \| z \|_{W^1_2}^2. \]

If we choose the regularization parameter in appropriate way (e.g., using GDP), we can guarantee convergence regularized approximations to the exact solution in $W^1_2(R^1)$, and, consequently, for any segment $[a,b]$:

\[ \left\| z^\alpha_\eta (s) \right\|_{C[a,b]} \xrightarrow{\eta \to 0} \left\| z(s) \right\|_{C[a,b]}. \]
Let us find $z^\alpha_\eta(s)$. We define direct and inverse Fourier transforms for $f(x) \in L_2(R^1)$ as:

$$\tilde{f}(\omega) = \int_{-\infty}^{+\infty} f(x)e^{i\omega x} \, dx; \quad f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{f}(\omega)e^{-i\omega x} \, d\omega.$$

Using the convolution theorem, the Plancherel equality and varying $M^\alpha$ over $W_2^1(R^1)$, we obtain:

$$z^\alpha_\eta(s) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{K}_h^*(\omega)\tilde{u}_\delta(\omega)e^{-i\omega x} \frac{\tilde{K}_h(\omega)\tilde{K}_h(\omega) + \alpha(\omega^2 + 1)}{\tilde{K}_h^*(\omega)\tilde{K}_h(\omega) + \alpha(\omega^2 + 1)} \, d\omega,$$

where $\tilde{K}_h(\omega), \tilde{u}_\delta$ are the Fourier transforms of $K_h(s), u_\delta$, and $\tilde{K}_h^*(\omega) = \tilde{K}_h(-\omega)$. 

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If we substitute the Fourier transform of $\tilde{u}_\delta(x)$ in the expression for $z_\eta^\alpha(s)$, we obtain:

$$z_\eta^\alpha(s) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} K^\alpha(x-s)\tilde{u}_\delta(x)dx,$$

where:

$$K^\alpha(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{\tilde{K}^\ast_h(\omega)e^{i\omega t}}{\tilde{K}^\ast_h(\omega)\tilde{K}_h(\omega) + \alpha(\omega^2 + 1)} d\omega.$$
Consider the case when the solution and the kernel have local supports. We remind that the support of a function $f(x)$ is the set $\text{Supp} f = \{x \in \mathbb{R}^1 : f(x) \neq 0\}$.

In this case the equation has a form:

$$A_z \equiv \int_0^{2a} K(x-s)z(s)ds = u(x), \ 0 \leq x \leq 2a.$$
We assume the following conditions:

\[ A: W_2^l[0,2a] \rightarrow L_2[0,2a], \quad \text{Supp}_K(y) \subseteq \left[-\frac{l}{2}, \frac{l}{2}\right], \quad \text{Supp}_z(x) \subseteq \left[a-\frac{l_z}{2}, a+\frac{l_z}{2}\right], \]

\[ a, l > 0, l_z \geq 0, 2l + l_z \leq 2a. \]

Under these conditions we define to be equal zero \( K(y) \) on \([-a,a]\) and \( z(s) \) on \([0,2a]\), and after that define their periodical continuation on \( \mathbb{R}^1 \) with the period \( T = 2a \). In this case, the right-hand side \( u(x) \) has the support in \([0,2a]\), and has also a periodical continuation on \( \mathbb{R}^1 \) with the period \( T = 2a \).
We now introduce uniform grids: \( x_k = s_k = k \Delta x, \Delta x = \frac{2\alpha}{n}, k = 0, n-1 \), where \( n \) is even. For simplicity we approximate the equation by the rectangle formula:

\[
\sum_{j=0}^{n-1} K(x_k - s_j) z(s_j) \Delta x = u(x_k).
\]
Put \( K(x_k - s_j) = K_{k-j} \), \( z(s_j) = z_j \), \( u(x_k) = u_k \). We define the discrete Fourier direct and inverse transforms for functions (vectors) of a discrete variable \( k \) that are periodic with the period \( (f_{k+n} = f_k) \):

\[
\hat{f}_m = \sum_{k=0}^{n^{-1}} f_k e^{-i\omega_m x_k} , \quad f_k = \frac{1}{n} \sum_{m=0}^{n^{-1}} \hat{f}_m e^{i\omega_m x_k} , \quad \text{где} \quad \omega_m = \frac{2\pi}{T} , \quad k, m = 0, n-1.
\]
It is easy to check Plancherel’s equality and the convolution theorem for the discrete Fourier transform:

\[ \sum_{k=0}^{n-1} f_k^2 = \frac{1}{n} \sum_{k=0}^{n-1} \tilde{f}_m^2, \]

\[ \sum_{k=0}^{n-1} \sum_{j=0}^{n-1} K_{k-j} z_j e^{\alpha_m x_k} = \tilde{K}_m \tilde{z}_m \Delta x \]
We approximate Tikhonov’s functional:

\[ M^\alpha[z] = \sum_{k=0}^{n-1} \sum_{j=0}^{n-1} (K_{k-j}z_j \Delta x - u_k)^2 \Delta x + \alpha \sum_{k=0}^{n-1} z_k^2 \Delta x + \alpha \sum_{k=0}^{n-1} z'(x_k)^2 \Delta x. \]

Using Plancherel’s equality, the convolution theorem and the equality

\[ \tilde{z}'(x_k) = i\omega_k \tilde{z}(x_k), \]

we obtain:

\[ M^\alpha[z] = \frac{\Delta x}{n} \sum_{m=1}^{n-1} \left( |\tilde{K}_m|^2 z^*_m z_m \Delta x^2 - 2\Delta x \tilde{K}_m^* z^*_m \tilde{u}_m + |\tilde{u}_m|^2 + \alpha(1 + \omega^2) z^*_m z_m \right). \]
The minimum of this functional is attained on the vector with the discrete Fourier transform coefficients

\[
\tilde{z}_m = \frac{\tilde{K}_m^* \tilde{u}_m \Delta x}{|\tilde{K}_m^*| \Delta x^2 + \alpha \left( \left( \frac{\pi m}{a} \right)^2 + 1 \right)}, \quad m = 0, n-1.
\]

Applying the inverse discrete Fourier transform, we find the regularized solution. If \( n = 2^k \), FFT (fast Fourier transform) can be used.

In 2D case we should use 2D discrete Fourier transform.
Examples and Applications
Functions convex along lines parallel to coordinate axes

Consider an n-dimensional Euclidean space $\mathbb{R}^n$, $n < \infty$.

A set $\Omega \subset \mathbb{R}^n$ is convex along all lines parallel to coordinate axes if $\forall i \in [1,n] \ \forall x_1, x_2 \in \Omega$ such that

\[
x_1 = (a^1, \ldots, a^{i-1}, x_1^i, a^{i+1}, \ldots, a^n),
\]
\[
x_2 = (a^1, \ldots, a^{i-1}, x_2^i, a^{i+1}, \ldots, a^n)
\]

and $\forall \lambda \in (0,1): x_3 = \lambda x_1 + (1-\lambda) x_2 \in \Omega$. 
A cross is an example of a set convex along coordinate axes
A function \( z(x) \) on \( \Omega \) is convex downwards along all lines parallel to an \( i \)-th coordinate axis if \( \forall x_1, x_2 \in \Omega \) such that

\[
x_1 = (a^1, \ldots, a^{i-1}, x_1^i, a^{i+1}, \ldots, a^n),
\]

\[
x_2 = (a^1, \ldots, a^{i-1}, x_2^i, a^{i+1}, \ldots, a^n)
\]

and \( \forall \lambda \in (0,1) \):

\[
z(\lambda x_1 + (1-\lambda) x_2) \leq \lambda z(x_1) + (1-\lambda) z(x_2)
\]
Let $n^* \in [0,n]$. Consider functions $z(x)$ given on $\Omega$. By $M_{n^*}^{n}(\Omega)$ define the set of functions $z(x)$ that are convex downwards along all lines parallel to $n^*$ first coordinate axes and convex upwards along all lines parallel to $(n-n^*)$ last coordinate axes.

Assume there exist finite numbers $C_L$ and $C_U$ such that $\forall x \in \Omega$ and $\forall z(x) \in M_{n^*}^{n}(\Omega)$: $C_L \leq z(x) \leq C_U$. 
Theorem 1.: Let there be a sequence \( \{z_m\} \) and an element \( z \) such that \( \forall m \in 1, \ldots, +\infty: z_m \in M_{n^*}(\Omega), z \in L^p(\Omega), p > 1, \|z_m - z\|_{L^p(\Omega)} \to 0 \) as \( m \to +\infty \), where \( \Omega \) is an open bounded set. Then from the sequence \( \{z_m\} \) a subsequence \( \{z_m^{(k)}\} \) may be taken that converges to a function \( \tilde{z} \in M_{n^*}(\Omega) \) at any point of \( \Omega \) and \( \tilde{z} = z \) in \( L^p(\Omega) \).

Corollary 1.: \( M_{n^*}(\Omega) \) is a compact set in \( L^p(\Omega) \).

Corollary 2.: The sequence \( \{z_m(x)\} \) considered in Theorem 2.1 converges to the function \( \tilde{z}(x) \) at any point of \( \Omega \).
Theorem 2.: Let $\|z_m - z\|_{L^p(\Omega)} \to 0$ as $m \to \infty$, where $z_m, z \in M^n_{n^*}(\Omega)$, $p \geq 1$ and $\Omega$ is an open bounded set. Then the sequence $\{z_m\}$ converges to $z$ uniformly on any closed set $\nu \subset \Omega$. 
Let $D=[a_1, b_1] \times [a_2, b_2] \times \ldots \times [a_n, b_n]$. On each segment $[a_i, b_i]$, we define a grid $X_i = \{x_{i,j}\}_{j=1}^{n_i}$ such that $a_i = x_{i,1} < x_{i,2} < \ldots < x_{i,n_i} = b_i$. Let $X = X_1 \times X_2 \times \ldots \times X_n$. A vector of indices $J=(j_1, j_2, \ldots, j_n)$ for a grid point with coordinates $(x_1^{j_1}, x_2^{j_2}, \ldots, x_n^{j_n})$. Then the point is written as $x_J$.

For any $x \in D$ there is a set $B_J = [x_1^{j_1}, x_1^{j_1+1}] \times \ldots \times [x_n^{j_n}, x_n^{j_n+1}]$: $x \in B_J$. As an approximation of a function $z(x)$ we use a function $z_N(x)$ that is linear on grid values of $z(x)$ at vertices of $B_J$. 

After finite dimensional approximation we obtain a set $\mathcal{Z}_M$ which is a polytope.

If $x_1, x_2, x_3$ are grid points that belong to a line parallel to an $i$-th coordinate axis and there is no another grid point between them, then for a uniform grid $X_i$: $-z_1 + 2z_2 - z_3 \leq 0$ ($i \leq n^*$) or $z_1 - 2z_2 + z_3 \leq 0$ (otherwise). ($z_k = z(x_k)$)
Error estimation

1) Find the minimum and the maximum values for each coordinate of $Z_M^\eta$. Denote them by $z_i^l$ and $z_i^u$, $1 \leq i \leq n$. They form vectors $\hat{z}^l$, $\hat{z}^u$.

2) Secondly, using $\hat{z}^l$, $\hat{z}^u$ we construct functions $z_i^l(x)$ and $z_i^u(x)$ close to $Z_M^\eta$ such that $\forall z \in Z_M^\eta: z_i^l(x) \leq z(x) \leq z_i^u(x)$.

Therefore, we should minimize a linear function on a convex set. We may approximate the set by a convex polyhedron and solve a linear programming problem. The simplex-method or the method to cut convex polyhedra may be used. We also may construct the sequence $W_0 \supset W_1 \supset \ldots \supset W_m$ of convex polyhedrons contained the point of minimum.
Let $D=\left[0,d_1\right] \times \left[0,d_2\right]$}, $d_1$, $d_2<+\infty$, and for $w(x,y,t)$ there are the heat conduction equation and zero boundary conditions:

$$\frac{\partial w}{\partial t} = a^2 \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right)$$

$$w(0, y, t) = 0 \quad w(d_1, y, t) = 0$$
$$w(x,0,t) = 0 \quad w(x,d_2,t) = 0$$

Denote $z(x,y)=w(x,y,0)$, $u(x,y)=w(x,y,T)$, $0<T<+\infty$. Therefore

$$u(x,y)=\int\int G(x, y, \xi, \eta, T) \ z(\xi, \eta) \ d\xi d\eta.$$
Assume the exact solution $z \in M^2_0(D)$. We set $n_1 = n_2 = 11$, $d_1 = d_2 = 1.0$, the grids are uniform, $a = 1.0$, $T=0.001$. As the exact solution the function $z(x,y) = \sin(\pi x) \cdot \sin(\pi y)$ is taken. The approximate right-hand side we take as $u_\delta = \bar{u}$. The error of finite dimensional approximation $\Delta = 0.01 \cdot ||\bar{u}|| \approx 0.005$.

In the figure there is an upper function $z^U(x,y)$ that bounds all approximate solutions. To construct it we use additional grid values. We find that $||z^U - z^L|| = 0.212$ ($\approx 0.424 \cdot ||z||$).
Linear ill-posed problems on sets of convex functions on two-dimensional sets

This case is more complicated. It is possible to prove that the set of bounded convex 2D functions is a compact in $L^p(\Omega)$. A set $\Omega \subset \mathbb{R}^n$ is closed bounded set. So we can find a quasisolution and its error estimation.

The detailed description of the algorithm so as the algorithm of the previous paragraph can be found in our joint publications with Valery Titarenko.
Electron microscopy

Fig. 1
Fig. 2
$A\varphi = I_\delta^{om}$, \hspace{1cm} (1)

where

$A\varphi = \int_0^\rho K(\rho z, \gamma)\varphi(\rho z)d\rho z$.

$\delta > 0$ – error of assignment of the right part of the equation (1), i.e. $\|I_\delta^{rel} - I^{rel}\| \leq \delta$, $A\varphi = \overline{I}^{rel}$, $I^{rel} = \frac{I}{I(0)}$ - relative intensity.
At that it is enough to find such an element $\varphi_{\delta}$, that

$$F[\varphi_{\delta}] \leq \delta^2.$$  

At finite-difference approximation set $Z$ transforms into set

$$\hat{Z} = \left\{ \begin{array}{ll} 
\varphi_{i-1} - 2\varphi_i + \varphi_{i+1} \leq 0, & i = 2, \ldots, N_{infl} - 1 \\
\varphi_{i-1} - 2\varphi_i + \varphi_{i+1} \geq 0, & i = N_{infl} + 1, \ldots, N_{\rho z} - 1 \\
\varphi_i \geq 0, & i = 1, 2, \ldots, N_{\rho z} 
\end{array} \right\}.$$  

(4)
Let $T^{(j)}$, $j=0,1,...,m (m = N_{\rho z})$ – apexes of a convex limited polyhedron $\hat{Z}$.

Lemma. Let $\varphi \in \hat{Z}$. Then the unique representation is correct

$$\varphi = \sum_{j=1}^{m} a_j T^{(j)},$$

at that $a_j \geq 0, j = 1,2,...,m$. 
Let us examine operator $T$ from $\mathbb{R}^m$ in $\mathbb{R}^m$, determined by the formula

$$T\xi = \sum_{j=1}^{m} \xi_j T^{(j)}, \quad \xi \in \mathbb{R}^m.$$ 

It is obvious, that $TR^m = \hat{Z}$ and $T^{-1}\hat{Z} = R^m$,

Where $R^m_+$ - set of vectors $R^m_+ \subset \mathbb{R}^m$, that have all non-negative coordinates $\xi \in \mathbb{R}^m_+$, if $\xi_j \geq 0, j = 1,2,\ldots,m$.

Let us examine function $Y(\xi) = f(T\xi)$, determined on set $R^m_+$.

We need to find such an element $\xi_\delta \in \mathbb{R}^m_+$, that $Y(\xi_\delta) \leq \delta^2$. The approximate solution of the original problem is found then by the formula $\varphi_\delta = T\xi_\delta$. 

$$T\xi = \sum_{j=1}^{m} \xi_j T^{(j)}, \quad \xi \in \mathbb{R}^m.$$
\[ \phi(\rho Z) \]
INVERSE PROBLEM OF CATHODOLUMINESCENCE MICROSCOPY
The Scheme of Installation

1. Focused electrical probe
2. Object under investigation
3. Region of generation of nonequilibrium carriers
4. Ellipsoidal mirror
5. Diaphragm with detector
Problem

Develop method for determination of optoelectrical local properties of cathodoluminescence objects with resolution of micrometer part, having at our disposal the set of measurements of intensity values. Describe the scheme of experiment, mathematical statement and the method of solution of the problem, which is ill-posed. The interaction of focused electrical probe with cathodoluminescence substance was modulated. An alternative method of microtomography in cathodoluminescence mode is presented. The solution is based on confocal ellipsoidal mirror [Phang J.C.H, Chan D.C.H.]. The photon rays transport in luminescence volume of specimen and ellipsoid are calculated.
We have to solve the next inverse problem: define the internal quantum yield of the material 
\[ \eta(s), \ s \in [0, R_0] \]
from Fredholm integral equation of the first kind:
\[
I(x) = \int_0^{R_0} K_1(x, s)\eta(s)\,ds, \ x - \text{the deflection of the object in respect to the mirror} \]
\[ I(x) \in L_2[x_{\min}, x_{\max}] \quad \eta(s) \in [0, R_0] \]
where \( I(x) \)- intensity, measured in experiment, as function of deflection of the object in vertical direction,
\( s \)-the distance from the surface of the object,
\( R_0 \)-maximal depth of penetration of electrons into the object,
\( K_1(x, s) \)-some continuous function, which was calculated by numerical methods (the physical sense of is that \( K_1(x, s)ds \) is the contribution into the total intensity the layer with center on the depth \( s \) and thickness \( ds \)).
A Priori Information

Let it is known that the solution of the problem is sourcewise represented with help of completely continuous integral operator:

\[ \eta(s) = \int_{0}^{R_0} K_2(s, \xi) \eta_0(\xi) d\xi, \quad s \in [0, R_0] \]

where

\[ K_2(s, \xi) = \begin{cases} \cos((s - \xi)1/2 \pi/2), & |s - \xi| \leq 2, \\ 0, & \text{otherwise} \end{cases} \]

We shall consider that:

\[ \eta_0(s) \in L_2[0, R_0] \quad \eta_0(s) \in L_2[0, R_0] \]

For solving the problem under such a priori information the method of extending compacts, which was described above, is used.
Model Calculations Results
An Inverse Problem of Nuclear Physics
Experiment:

Fig.1: 1 - the target for producing bremsstrahlung beam, 2 - the sample under consideration, D – detector.

Passing through the first target the accelerated electrons produce the bremsstrahlung beam (γ-rays). The bremsstrahlung spectrum is continuous. The sample 2 is bombarded by the γ-rays. The scattered γ-rays are detected.
Nuclear reaction: \( \gamma + ^{63}_{29}Cu \rightarrow ^{62}_{29}Cu + n \)

Constraints:

- **A priori**: \( 0 \leq \sigma(E_\gamma) \leq 90, \ E_\gamma \in [10, 24.1] \)
- **A posteriori**:
  - \( \sigma(E_\gamma), \ E_\gamma \in [10, 16] \): is a monotone nondecreasing function
  - \( \sigma(E_\gamma), \ E_\gamma \in [16, 18] \): is a convex upwards function
  - \( \sigma(E_\gamma), \ E_\gamma \in [18, 24.1] \): is a monotone nonincreasing function
Fig. 2: (• • •) – the approximate cross section from the Center of Data of Photonuclear experiments (http://depni.sinp.msu.ru/cdfe/);

(• • •) – the approximate solution found by Tikhonov regularization;

(−) – the functions $\sigma_{low}(E_\gamma)$, $\sigma_{upper}(E_\gamma)$ bounded the set of approximate solutions from below and from above.
Experimental data processing

- Nuclear reaction: \( \gamma + \overset{34}{16}S \rightarrow \overset{33}{15}P + p \)

- Constraints:
  - **A priori:** \( 0 \leq \sigma(E_\gamma) \leq 45, \ E_\gamma \in [12.3, 25.3] \)
  - **A posteriori:**
    - \( \sigma(E_\gamma), \ E_\gamma \in [12.3, 16] \) is a monotone nondecreasing function
    - \( \sigma(E_\gamma), \ E_\gamma \in [16, 17] \) is a convex upwards function
    - \( \sigma(E_\gamma), \ E_\gamma \in [17, 18.5] \) is a monotone nonincreasing function
    - \( \sigma(E_\gamma), \ E_\gamma \in [18.5, 20] \) is a convex downwards function
    - \( \sigma(E_\gamma), \ E_\gamma \in [20, 22] \) is a monotone nondecreasing function
    - \( \sigma(E_\gamma), \ E_\gamma \in [22, 23] \) is a convex upwards function
    - \( \sigma(E_\gamma), \ E_\gamma \in [23, 25.3] \) is a monotone nonincreasing function
Fig. 3: (• • •) – the approximate cross section
from the Center of Data of Photonuclear
experiments;

(• • •) – the approximate cross section found
by Tikhonov regularization;

(─ ) – the functions $\sigma^{\text{low}}(E_\gamma)$, $\sigma^{\text{upper}}(E_\gamma)$
bounded the set of approximate solutions
from below and from above.
The system QSO 2237+0305, known as the “Einstein Cross”: 4 quasar images against the background of the lensing galaxy. Several observation were carried out using the Huble Space Telescope and Nordic Optical Telescope.
Model of Kernel

Star

PSF (Kernel) profile

Approximation of the star from the frame with 2-dimensional Gauss profile

FWHM ~ 5 pixels

Kernel

Residuals
Tikhonov Regularization

- Ill-posed problem
- Smoothing function:
  \[ M^\alpha[z] = \| k * z - u_\delta \|^2_U + \alpha \cdot \Omega(z) \]
- Solution \[ z^\alpha \] :
  \[ M^\alpha[z^\alpha] = \inf \{ M^\alpha[z] : z \in Z \} \]
- Regularization parameter \( \alpha \) from discrepancy principle:
  \[ \| k * z^\alpha - u_\delta \|_U \approx \delta, \alpha > 0 \]
A priori information

True Image = Galaxy + Quasar Components

\[ z(x, y) = g(x, y) + \sum_{k=1}^{K} I_k \delta(x-a_k, y-b_k) \]

\( K=4 \), number of quasar components

\( K=5 \), number of quasar components + galaxy nuclear
A priori information

• Nonnegativity of the solution, $z_{ij} \geq 0$

• Galaxy: assumption about smoothness

$$\Omega(g) = \| g \|_G^2 ; G \equiv \{ L_2, W_21, BV \}$$

• Galaxy model

$$\Omega(g) = \left\| g - g_{\text{model}} \right\|_G^2$$

g_{\text{model}}(r) = I(0) \exp\{-b_n \ (r/r_e)^{1/n}\}$

$$_{\text{generalized de Vaucouleurs profile (Sersic’s model)}}$$

$b_n = 2n - 0.324$ for $1 \leq n \leq 4$
A priori information

Sourcewise representation:

\[ z = R[z'] \equiv r \ast z' \]

Total PSF = Source PSF \ast Final PSF

\[ k = s \ast r \]

\[ z(x, y) = \sum_{k=1}^{K} a_k r(x - b_k, y - c_k) + g(x, y) \]
Results: $L_2$

$\Omega(g) = \left\| g - g_{sersic} \right\|_2^2$
Results: $L_2$

Galaxy

Error distribution
Results: $W_{21}$

$\Omega(g) = \left\| g - g_{sersic} \right\|_{W_{21}}^2$
Results: $W_{21}$

Galaxy

Error distribution
Results: MCS

\[ \text{kernel} = s \ast r \]

\[ \Omega(g) = \left\| g - r \ast g \right\|_{L2}^2 \]
Results: MCS

- Quasar components
- Galaxy
Results: MCS

Quasar components

Error distribution
Results: TV

\[ \Omega(g) = \sum_{m=1}^{N-1} \sum_{n=1}^{N-1} \left| g_{m+1,n+1} - g_{m+1,n} - g_{m,n+1} + g_{m,n} \right| \]

Observed image

Deconvolved image
Results: TV

Quasar components

Galaxy
Using parallel computing for solving multidimensional ill-posed problems
1. Introduction

1.1. An example of a multi-dimensional ill-posed problem

The inverse problem is to identify the permanent magnetization \( \mathbf{M} \) (both strengths and directions) using measurements of the magnetic flux density \( \mathbf{B} \).

The equation describing the magnetic field \( \mathbf{B}_i \) induced by sources of magnetic fields \( \mathbf{M}_j \), located at a distance \( r_{ij} \) from the sensor \( i \), is defined as

\[
\mathbf{B}_i = \sum_{j=1}^{J} \frac{\mu_0}{4\pi} \left[ \frac{3(\mathbf{M}_j \cdot \mathbf{r}_{ij}) \mathbf{r}_{ij}}{|\mathbf{r}_{ij}|^5} - \frac{\mathbf{M}_i}{|\mathbf{r}_{ij}|^3} \right]
\]
1. Introduction

1.1. An example of a multi-dimensional ill-posed problem

1. General mathematical formulation of the problem

In other words, the source of the magnetic field with magnetic moment $\mathbf{M}$, located at a point with radius vector $\mathbf{q}$, creates at point with radius vector $\mathbf{q}$ a magnetic field with induction $\mathbf{B}$:

$$\mathbf{B}_q(\mathbf{r}) = \frac{\mu_0}{4\pi} \left[ \frac{3((\mathbf{r} - \mathbf{q}), \mathbf{M} (\mathbf{q}))}{|\mathbf{r} - \mathbf{q}|^5} (\mathbf{r} - \mathbf{q}) - \frac{\mathbf{M} (\mathbf{q})}{|\mathbf{r} - \mathbf{q}|^3} \right]$$

The total field of the ship can be expressed by the integral

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int_V \left[ \frac{3((\mathbf{r} - \mathbf{q}), \mathbf{M} (\mathbf{q}))}{|\mathbf{r} - \mathbf{q}|^5} (\mathbf{r} - \mathbf{q}) - \frac{\mathbf{M} (\mathbf{q})}{|\mathbf{r} - \mathbf{q}|^3} \right] dV_q$$

But this statement of the problem is computationally very difficult.
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1.1. An example of a multi-dimensional ill-posed problem

1. Some different types of simplifications of the numerical model for the assigned problem

- 1D-problem: Dividing the ship into subdivisions with constant values of magnetization
- 2D-problem: Approximation the hull of the ship by an ellipsoid
- 2D-problem: Approximation the hull of the ship by polyhedrons
- 2D-problem: Approximation the hull of the ship by a plane

But all these simplifications can be applied only in specific cases (not in general)
1. Introduction

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3. Inverse problem without any simplifications

But if we do not have any *a priori* information about the investigated object we cannot use mentioned simplifications. In this case we have to solve the problem “in general” that is very difficult to perform on common PC.

For example, how can 67 500 parameters be inverted efficiently?

The answer is only one: we have to use parallel computing.
2. Using parallel computing

2.1. The main idea of parallel computing

Parallel computing is a form of computation in which many calculations are carried out simultaneously, operating on the principle that large problems can often be divided into smaller ones, which are then solved concurrently (“in parallel”). Parallel computation can be performed on multi-processor clusters or on multi-core computers having multiple processing elements within a single machine.

But not every problem can be parallelized efficiently.
2. Using parallel computing

2.2. Parallel computing limitations

The speed-up of a program as a result of parallelization is observed as **Amdahl’s law**

\[
S = \frac{1}{(1 - P) + \frac{P}{N}}
\]

- \(S\) -- the speed-up of the program (as a factor of its original sequential runtime)
- \(N\) -- number of processors
- \(P\) -- the fraction of the program that is parallelizable.

It will be shown that parallelizable fraction for multidimensional Fredholm integral equation of the 1st kind is \(~ 99,(9)\)% that gives us high effectiveness.
3. Parallelization of multidimensional ill-posed problems

3.1. Formulation of the problem

The total field of the ship expressed by the integral

$$\vec{B}(\vec{r}) = \frac{\mu_0}{4\pi} \int_V \left[ \frac{3((\vec{r} - \vec{q}), \vec{M}(\vec{q}))}{|\vec{r} - \vec{q}|^5} (\vec{r} - \vec{q}) - \frac{\vec{M}(\vec{q})}{|\vec{r} - \vec{q}|^3} \right] dV_q$$

can be replaced by an equivalent 3D integral equation

$$\vec{B}(x_s, y_s, z_s) = \int_V K(x_s, y_s, z_s, x, y, z) \vec{M}(x, y, z) \, dv$$

and then, after change of variables,

$$\vec{B}(s, t, r) = \int_{L_x}^{R_x} \int_{L_y}^{R_y} \int_{L_z}^{R_z} K(s, t, r, x, y, z) \vec{M}(x, y, z) \, dx \, dy \, dz$$
3. Parallelization of multidimensional ill-posed problems

3.2. Finite-difference approximation of the functional and its gradient

When we solve minimization problem by conjugate gradient method, it is necessary to calculate values of the functional $F^\alpha \left[ \bar{M} \right]$ and its gradient $\text{grad } F^\alpha \left[ \bar{M} \right]$

Finite-difference approximation of the Tikhonov functional is

$$F^\alpha \left[ \bar{M} \right] = \sum_{j_1=1}^{N_x} \sum_{j_2=1}^{N_y} \sum_{j_3=1}^{N_z} \sum_{n=1}^{3} h_s h_t h_r \left[ \sum_{i_1=1}^{N_x} \sum_{i_2=1}^{N_y} \sum_{i_3=1}^{N_z} \sum_{m=1}^{3} h_x h_y h_z K_{j_1j_2j_3i_1i_2i_3}^{nm} M_{i_1i_2i_3}^{m} - B_{j_1j_2j_3}^{n} \right]^2 + \alpha \Omega \left[ \bar{M} \right]$$

Finite-difference approximation of its gradient is

$$\left( \text{grad } F^\alpha \left[ \bar{M} \right] \right)_{i_1i_2i_3}^m = \frac{\partial F^\alpha (M_{i_1i_2i_3}^m)}{\partial M_{i_1i_2i_3}^m} =$$

$$= 2h_x h_y h_z \sum_{j_1=1}^{N_x} \sum_{j_2=1}^{N_y} \sum_{j_3=1}^{N_z} \sum_{n=1}^{3} h_s h_t h_r \left[ \sum_{l_1=1}^{N_x} \sum_{l_2=1}^{N_y} \sum_{l_3=1}^{N_z} \sum_{m=1}^{3} h_x h_y h_z K_{j_1j_2j_3l_1l_2l_3}^{nm} M_{l_1l_2l_3}^{m} - B_{j_1j_2j_3}^{n} \right] + \alpha \frac{\partial \Omega (M_{i_1i_2i_3}^m)}{\partial M_{i_1i_2i_3}^m}$$

Structure of algorithm allows to divide the large problem into smaller ones which are then solved “in parallel”.

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3. Parallelization of multidimensional ill-posed problems

3.3. One possible scheme of paralleling

Paralleling of the functional is consider on the example $N_x = N_y = N_z = N_s = N_t = N_r = 2$, steps $h_x, h_y, h_z, h_s, h_t, h_r$ and smoothing functional $\Omega$ are skipped for simplicity.

$$F^\alpha[M] = \sum_{j_1=1}^{2} \sum_{j_2=1}^{2} \sum_{j_3=1}^{3} \left[ \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \sum_{m=1}^{3} K^{nm}_{j_1j_2j_3i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^n_{j_1j_2j_3} \right]^2$$

$$= \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \left[ K^{1m}_{111i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^1_{j_1j_2j_3} \right]^2 + \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \left[ K^{2m}_{111i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^2_{j_1j_2j_3} \right]^2 + \ldots + \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \left[ K^{1m}_{212i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^1_{j_1j_2j_3} \right]^2 + \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \left[ K^{1m}_{222i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^1_{j_1j_2j_3} \right]^2$$

$$= \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \left[ K^{1m}_{111i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^1_{j_1j_2j_3} \right]^2 + \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \left[ K^{2m}_{111i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^2_{j_1j_2j_3} \right]^2 + \ldots + \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \left[ K^{1m}_{212i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^1_{j_1j_2j_3} \right]^2 + \sum_{i_1=1}^{2} \sum_{i_2=1}^{2} \sum_{i_3=1}^{3} \left[ K^{1m}_{222i_1i_2i_3} M^{m}_{i_1i_2i_3} - B^1_{j_1j_2j_3} \right]^2$$
3. Parallelization of multidimensional ill-posed problems

3.3. One possible scheme of paralleling II

The scheme of calculating the value of the functional for a) zero process, b) non-zero processes.

\[ N = N_s \times N_t \times N_r \]
3. Parallelization of multidimensional ill-posed problems

3.3. One possible scheme of paralleling III

The scheme of calculating value of the gradient of the functional for: a) zero process; b) non-zero processes.
3. Parallelization of multidimensional ill-posed problems

3.4. Some examples of calculations

Results of restoring 100x15x15x3 = 67500 magnetization parameters. Time of calculation is ~29 hours on 256 processors (Intel Xeon E5472 3.0 GHz).
4. Conclusion

The proposed method can be efficiently applied for solving multidimensional Fredholm integral equations of the 1\textsuperscript{st} kind in many areas of physics were it is necessary to solve inverse problems such as:

- radiophysics
- optics
- acoustics
- spectroscopy
- geophysics
- tomography
- image processing
- etc.

The testing calculations were performed on the Computing Cluster of the Moscow State University.

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