Scientific Computing
Lecture 6

Optimization

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Optimization

Motivation

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Deconvolution problem

The 2D deconvolution problem is the problem of finding $u(\mathbf{x})$ from the equation:

$$Au(\mathbf{x}) \equiv \int\limits_{B \in \mathbb{R}^2} K(\mathbf{x} - \xi) u(\xi) d\xi = f(\mathbf{x}).$$

- In case of finite and noisy functions u and K, the latter equation is ill-posed.
- The problem can be reduced to the optimization problem for the cost Tikhonov's functional

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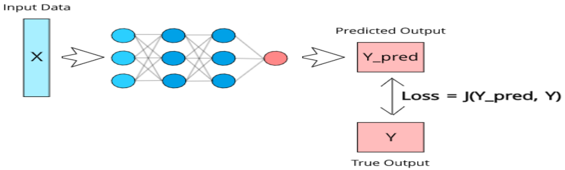
Deconvolution: regularization

The cost Tikhonov's functional:

$$M_\alpha[u] = ||Au - f||^2_{L_2(B)} + \alpha\Omega[u],$$

where the functional $\Omega[u]$ is a stabilizer.
To find an approximate solution, we need to **minimize** the functional above.

NN: Loss



- X - input
- Y - output (Ground True)
- $Y_{pred} \equiv Y_{pred}(\mathbf{w})$ - predicted output
- $\mathbf{w}$ - vector of all model weights

$$Loss(\mathbf{w}) = Error(Y_{pred}, Y); \quad \text{MSE Loss} = ||Y_{pred} - Y||^2_{L^2}$$

To restore the **the model** A, we need to **minimize** the loss function with respect to weights vector $\mathbf{w}$

Galerkin approach

- Represent (or approximate) the solution u with some weighted sum of functions
- Substitute the approximation or representation into the original equations
- **Minimize** the residual with respect to weights
- After the weights are calculated, reconstruct the approximate (or, sometimes, exact) solution, substituting the weights into your representation (or approximation) of it
- Be careful: the residual rarely being equal to zero, but it should be small!

Applications

- Optimal transport regulation
- Time-based distribution of the products from warehouses to stores
- Spatial optimal distribution of electronics within spacecraft or submarines
- Industrial optimization
- Information flows
- Neural networks and machine learning.

- Solution of large systems of algebraic equations (especially, ill-conditioned systems)
- Galerkin: Research of integral and differential equations. Minimization of the residual after application of the original operator to the approximated solution.
- Cost functionals: Solving integral and differential equations. Construction of the cost functional for the problem and providing its constrained or unconstrained optimization.
- Ill-posed problems: Solution of complex problems using certain functional spaces.
- Minimization of the coefficients within an artificial neural network.

Optimization

Basic concepts

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General problem statement

- H is some Hilbert space.
- Let $f : H \to \mathbb{R}$.
- **Optimization** or **Programming:**

$$u^* = \operatorname*{argmin}_{u \in U \subseteq H} f(u), \quad u^* = ?$$

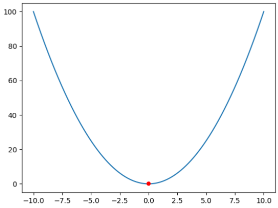
- **Linear Programming:** The function f is linear.
- **Nonlinear Programming:** The function f is non-linear.

Criteria and notations

- $f(u) : H \to \mathbb{R}$ - the function to be minimized.
- $u \in U \subseteq H$.
- **Unconstrained programming:** $U = H$.
- **Constrained programming:** $U \subset H$.
- $u^* = \operatorname*{argmin}_{u \in U} f(u)$ - the minimizer.
- $f^* = f(u^*) = \min_{u \in U} f(u)$ - the minimum.
- $U^* \subset U = \operatorname*{Argmin}_{u \in U} f(u)$ - the set of minimizers.

- u^* is a **Global Minimizer** if $\forall u \in U \quad f(u) \geq f(u^*)$.
- u^* is a **Strict Global Minimizer** if $\forall u \in u \quad f(u) > f(u^*)$.
- Set $\bar{S}_r(u^*) = \{u \in H : ||u - u^*|| \leq r\}$ - a ball with the radius r.
- u^* is a **Local Minimizer** if $\exists r > 0 : f(u) \geq f(u^*) \quad \forall u \in U \cap \bar{S}_r(u^*)$
- u^* is a **Strict Local Minimizer** if $\exists r > 0 : f(u) > f(u^*) \quad \forall u \in U \cap \bar{S}_r(u^*)$

Local and Global minima



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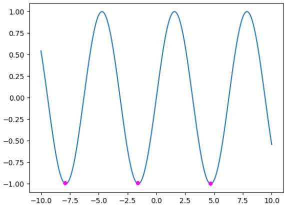

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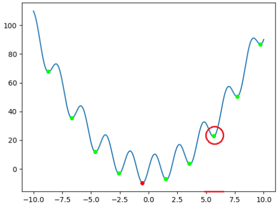

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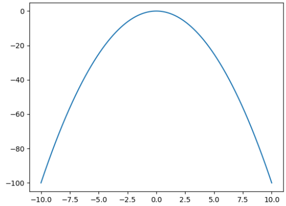

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Differentiable functionals

- The functional $f(u)$ is **differentiable** at the point u_0 if

$$f(u) = f(u_0) + \big(f'(u_0), u - u_0\big)_H + o\big(||u - u_0||_H\big)$$

- The operator f' is a **Strong derivative** (so-called the **Frechet derivative** or **The Gradient**).
- **Necessary condition of extremum:** Let the functional f to be differentiable at the point $u^* \in U$.
  If u^* is a local minimizer, than $f'(u^*) = 0$.

Differentiable functionals

- If the functional $f : H \to \mathbb{R}$, then $f'(u) \in H$.
- For example, let

$$f(\mathbf{x}) = ax_1^2 + bx_2^3; \quad \mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^2$$

- $f : \mathbb{R}^2 \to \mathbb{R}$
- $$f'(\mathbf{x}) = \left(2ax_1, 3bx_2^2\right)^T \in \mathbb{R}^2$$
- We can say the same about the higher-order Frechet derivatives.

Differentiable functionals

- The functional $f(u)$ is **twice differentiable** at the point u_0 if

$$f(u) = f(u_0) + \big(f'(u_0), u-u_0\big)_H + \frac{1}{2}\big(f''(u_0)(u-u_0), u-u_0\big)_H + o(||u-u_0||_H^2)$$

- The linear functional $f''(u_0) : H \to H$ is a **Second Frechet Derivative (SFD)**
- In finite dimensional case, the SFD is being defined with the Hessian
- Linear bounded operator A is **positively definite** if $\forall h \in H : (Ah, h) > 0$.
- **Sufficient condition of extremum:** Let the functional f to be twice differentiable at the point $u^* \in U$.
If $f'(u^*) = 0$ and $f''(u^*) > 0$ (positively definite), then u^* is a local minimizer

Convex set

The set U is a **Convex set** if $\forall u_1, u_2 \in U$ the interval connecting these points belongs fully to the set U:

$$[u_1, u_2] = \{u \in U : u = u_1 + \lambda(u_2 - u_1), \lambda \in [0, 1]\}$$

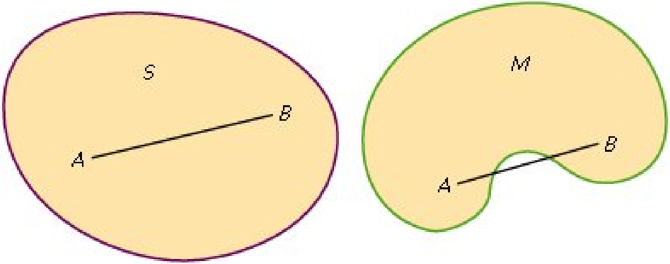
Examples:

- The whole Hilbert space H
- Interval in $\mathbb{R}^1$
- Polyhedra in $\mathbb{R}^n$:

$$\{u \in \mathbb{R}^n : Au \leq b\} = \{u \in \mathbb{R}^n : (a_i, u) \leq b_i, i = 1, ..., n\}$$

  where a_i - vectors, b_i - numbers.
- The closed ball $\bar{S}_r(u_0)$

Convex set



Convex functional

- The functional $f(u)$, defined on convex set is a **Convex** if $u_1, u_2 \in U$ and $\forall \lambda \in [0,1]$:

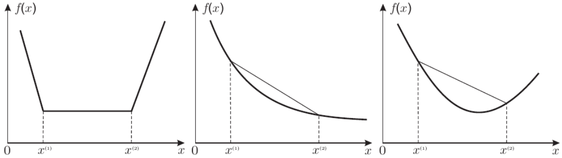
$$f(\lambda u_1 + (1-\lambda)u_2) \leq \lambda f(u_1) + (1-\lambda)f(u_2).$$

- If the inequality is strict, then the functional is **Strictly convex:**

$$f(\lambda u_1 + (1-\lambda)u_2) < \lambda f(u_1) + (1-\lambda)f(u_2).$$

- The functional is **Strongly Convex** if $\exists \theta > 0$ such that:

$$f(\lambda u_1 + (1-\lambda)u_2) \leq \lambda f(u_1) + (1-\lambda)f(u_2) - \theta\lambda(1-\lambda)||u_1 - u_2||^2$$



(a) Convex functional, (b) - strictly convex functional, (c) - strongly convex functional

- $f(x) = x^2$ is strongly convex
- $f(x) = x^4$ is strictly convex but not strongly convex
- $f(x) = ||x||$ is convex but not strongly or strictly convex
- $f(x) = ||x||^2 = (x, x)$, defined on the whole Hilbert space, is strongly convex.
- **It will be an exam question**

Programming problems in terms of convexity

$$u^* = \operatorname*{argmin}_{u \in U} f(u) - ?$$

- **Convex programming problem:** U is a convex set, and f is a convex functional.
  In Convex Programming, any local minimizer is a global minimizer!
- **Linear programming problem:** $H = \mathbb{R}^n$, the functional is linear: $f(x) = (b, x) + c$
  Linear programming is much easier than nonlinear
- **Quadratic programming problem:** $H = \mathbb{R}^n$, and the function takes the form:
  $$f(x) = \frac{1}{2}(Ax, x) + (b, x) + c,$$
  where the matrix A is a symmetric matrix.
  If the matrix A is nonnegative definite, then quadratic programming is a particular case of convex programming.

Optimization

Some aspects of will- and ill-posed problems

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Least Squares Fitting

System of Linear Algebraic Equations:

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

The residual:

$$\Phi(x) = ||Ax - b||^2 = (A^* Ax, x) - 2(A^* b, x) + (b, b).$$

$$\begin{aligned} \Phi'(x) &= 2(A^* Ax - A^* b), \\ \Phi''(x) &= 2A^* A \geq 0. \end{aligned}$$

Putting the gradient to zero, we obtain:

$$A^* Ax = A^* b$$

Pseudosolution

$$Ax = b \quad \Leftrightarrow \quad A^*Ax = A^*b$$

- In finite difference euclidian space the system $A^*Ax = A^*b$ have the solution for **any** b.
- The solution of this system is being called **Pseudosolution**
- If the original system has solution, then it coincides with the pseudosolution, and $\Phi(x) = \mu = 0$.
- If the original system is inconsistent $(\Phi(x) = \mu > 0)$, then the pseudosolution with minimal norm is called **Normal Pseudosolution:**

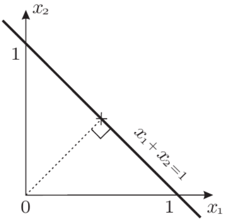
$$x = \min_{x:A^*Ax=A^*b} ||x||$$

Examples

- Consider the system:

$$\begin{cases} x_1 + x_2 = 1 \\ x_1 + x_2 = 1 \end{cases}$$

There are infinite number of solutions; the normal pseudosolution is $x_n = (1/2, 1/2)^T$.



- The system

$$\begin{cases} x_1 + x_2 = 1/2 \\ x_1 + x_2 = 3/2 \end{cases}$$

has no solutions at all; the pseudosolution, however, exists: $x_n = (1/2, 1/2)^T$

Well-posed problems in terms of optimization

- Let X, B be some Hilbert spaces.

$$Ax = b, x \in X, b \in B, A : X \to B, \tag{1}$$

- Consider the residual:

$$M(x) = ||Ax - b||_B^2, \quad x_m = \operatorname{argmin} M(x) \tag{2}$$

- If the operator A is **linear**, then the problem (2) is a **quadratic** optimization problem and has only the unique global minimizer.
- If the operator A is not linear, the programming problem still might be convex.
- If the problem (6) has an exact solution x^*, then the exact minimizer $x_m = x^*$.
- If the operator A has low condition number, then the minimizer x_m is stable.

Ill-posed problems in terms of optimization: pseudosolutions

Let X, B be some Hilbert spaces.

$$Ax = b, x \in X, b \in B, A : X \to B, \tag{3}$$

- If the solution of the above problem does not exist, the residual functional still has a minimum!
- The minimizer is called the **normal pseudosolution** and **always** exists.
- If the operator A is non-linear, there might be some number (up to infinity) of minimizers. The solution with minimal norm is also a **normal pseudosolution**.
- If due to some restrictions the solution exists but is outside of the solution scope, then, regularizing the functional, we can also chose the **normal pseudosolution**

Regularization

For the equation $Ax = b$ we form the residual $\Phi(x) = ||Ax - b||_B^2$. The cost Tiknonov's functional can be formed as follow:

$$M_\alpha(x) = ||Ax - b||_B^2 + \alpha\Omega(x),$$

where the functional Ω, defined on the subset of possible solutions space $X_1 \subset X$ is called regularization functional (or stabilizer), and should satisfy the following conditions:

- $\Omega(x) \geq 0, \quad \forall x \in X_1.$
- The element x^* (i.e., the exact solution) belongs to the support of the functional Ω: $x^* \in X_1$
- $\forall d > 0$, the set $F_{1,d} = \{x \in F_1 : \Omega(x) \leq d\}$ is a compact.

The approximate regularized solution:

$$x_\alpha = \underset{x \in F_1}{\operatorname{argmin}}\, M_\alpha(x)$$

Ill-conditioned problems: the instability

Let X, B be some Hilbert spaces, and A be a linear bounded operator.

$$Ax = b, x \in X, b \in B, A : X \to B, \tag{4}$$

Consider the residual:

$$\Phi(x) = ||Ax - b||_B^2$$

The Frechet derivative and necessary (in some cases - sufficient) condition for the minima at some element x:

$$A^*Ax - A * b = 0, \quad A^*Ax = A^*b.$$

The condition number: $cond(A) = ||A||||A^*||$. Probably, $||A^*||$ is big...
OR EVEN MIGHT NOT EXIST!

Let X, B be some Hilbert spaces, and A be a linear bounded operator.

$$Ax = b, x \in X, b \in B, A : X \to B, \tag{5}$$

Consider the Tikhonov's functional with the simplest stabilizer $\Omega = ||x||^2_{X_1}, X_1 \subset X$. In this case:

$$M(x) = ||Ax - b||^2_B + \alpha ||x||^2_B, \quad x_\alpha = \underset{x \in X}{\operatorname{argmin}} \, M(x)$$

Then

- The solution is a **normal pseudosolution**
- The minimizer exists, and it is unique if A is bounded linear operator
- The minimizer converges to the exact solution if errors $\to 0$ (stability).

Non-unique solutions. Choise principle

Let X, B be some Hilbert spaces, and A be a non-linear operator.

$$Ax = b, x \in X, b \in B, A : X \to B, \quad (6)$$

- Let $Q_\mu : \Phi(x) \equiv ||Ax - b|| \leq \mu$ - set of possible solutions.
- Use physical/chemical/economical/etc laws in order to make a constrains for the solution
- Two ways:
  - Use the constrained optimization of the residual $\Phi(x)$.
  - Construct a stabilizer $\Omega(x)$ such that on 'better' solution it reaches lesser values.
  - Example: Functional space with bounded total variation allows us to reconstruct blurred piecewise-constant functions.

Methods

Zero order methods list

- Coordinate descent
- Hook & Jeeves method
- Nelder-Mead method
- Random-Walk methods
- Genetic Algorithms

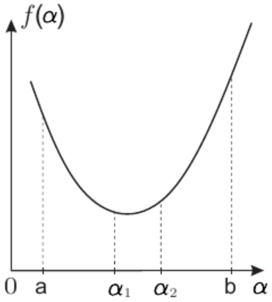
1D optimization: the Golden Section Method

$$x^* = \underset{x \in [a,b]}{\operatorname{argmin}} f(x).$$

1. Define the interval $[a, b]$ into three parts such that

$$\frac{b - \alpha_2}{b - a} = \frac{\alpha_1 - a}{b - a} = \xi \equiv \frac{2}{3 + \sqrt{5}} \approx 0.38.$$

2. Compare $f(a), f(b), f(\alpha_1), f(\alpha_2)$. Obvious, that we can exclude the interval not being attached to a point where $f(x)$ is minimal.
3. Repeat steps 1 and 2 until the length of the interval will be bigger than certain $\varepsilon > 0$.



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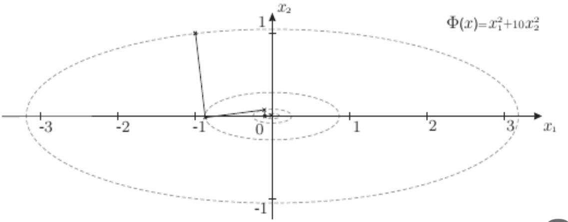
1D optimization: the quadratic approximation

$$x^* = \operatorname*{argmin}_{x \in [a,b]} f(x).$$

- Chose certain point $\alpha_1 \in [a, b]$ and calculate $f(a), f(b), f(\alpha_1)$
- Construct the parabola with these three points and find its minimizer α_{min}
- Denote $\alpha_2 = \alpha_{min}$.
- Throw out one of four points with, in which the value f is maximal
- Repeat the procedure.

$$x^* = \underset{x\in\Omega}{\operatorname{argmin}} f(x), \quad \Omega \subseteq H$$

- Let the functional f be differentiable.
- Chose initial approximation x_0 and calculate initial gradient $g_0 = f'(x_0)$.
- $x_1 = x_0 - \alpha_0 g_0$, where α_0 is parameter (step) to chose.
- $g_n = f'(x_n); \alpha_n = \underset{\alpha\geq 0}{\operatorname{argmin}} f(x_n + \alpha g_n); x_{n+1} = x_n - \alpha_n g_n$



Constant descent rate

Let the function $f(x)$ be:

- Limited from below $(f(x) \geq f^* > -\infty)$
- Differentiable: $\exists f'(x) \forall U$
- The gradient is Lipshitz-continuous with constant L: $||f'(x) - f'(y)|| \leq L||x - y||$

Then, if $0 < \alpha < 2/L$, the following is true:

- The gradient tend to zero with growing k:

$$\lim_{k \to \infty} f'(x_k) = 0$$

- The function $f(x_k)$ decays with k:

$$f(x_{k+1}) \leq f(x_k)$$

Steepest descent

The optimization problem:

$$x^* = \operatorname*{argmin}_{x \in \Omega} f(x), \quad \Omega \subseteq H$$

- Assume the function $f(x)$ be differentiable;
- Assume the function $f'(x)$ be continuous.

The **Steepest gradient descent**:

$$x_{n+1} = x_n - \alpha_n g_n$$

$$\alpha_n = \operatorname*{argmin}_{\alpha \geq 0} \varphi_k(\alpha), \quad \varphi_k(\alpha) = f\left(x_n - \alpha f'(x_n)\right)$$

- If $f(x)$ is quadratic function $f(x) = (Ax, x) + (b, x)$, then:

$$\alpha_n = \frac{||f'(x_n)||^2}{(Af'(x_n), f'(x_n))}$$

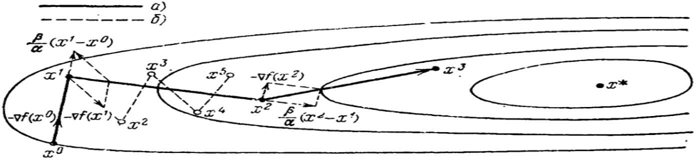
Heavy ball method

- Within the current iteration, the gradient descent does not use the information obtained in earlier iterations.
- **Multistep (s-step) methods**: $x_{n+1} = \varphi_n(x_n, x_{n-s-1})$

The heavy-ball method:

$$x_{n+1} = x_n - \alpha f'(x_n) + \beta(x_n - x_{n+1})$$

- Good for ill-conditioned problems.



Conjugate gradients method

One more two-step method:

$$x_{n+1} = x_n - \alpha_n f'(x_n) + \beta_n(x_n - x_{n-1}),$$

where

$$\{\alpha_n, \beta_n\} = \underset{(\alpha,\beta)}{\operatorname{argmin}}\, f\left(x_n - \alpha f'(x_n) + \beta(x_n - x_{n-1})\right)$$

In case of $f(x) = (Ax, x)/2 - (b, x)$ (quadratic):

$$\alpha_n = \frac{||r_n||^2(Ap_n, p_n) - (r_n, p_n)(Ar_n, p_n)}{(Ar_n, r_n)(Ap_n, p_n) - (Ar_n, p_n)^2}, \quad r_n = f'(x_n) = Ax_n - b,$$

$$\beta_n = \frac{||r_n||^2(Ar_n, p_n) - (r_n, p_n)(Ar_n, r_n)}{(Ar_n, r_n)(Ap_n, p_n) - (Ar_n, p_n)^2}, \quad p_n = x_n - x_{n-1}$$

Conjugate gradients method

- The method uses two previous approximations instead of only one. To initiate the CGM, the point x_1 can be obtained using any x_0 with the steepest descent method.
- The functions $r_n = f'(x_n)$ are pairwise orthogonal: $(r_n, r_k) = 0, \forall n \neq k$.
- The directions p_n are conjugate: $(Ap_n, p_k) = 0, \forall n \neq k$.
- In case of quadratic programming, the CGM allows to reach minimum at n iterations.
- Good for a 'big' quadratic tasks!

Another form of the CGM:

$$x_{n+1} = x_n + \alpha_n p_n, \quad \alpha_n = \operatorname*{argmin}_{\alpha} f(x_n + \alpha p_n),$$

$$p_n = r_n + \beta_n p_{n-1}, \quad \beta_n = \frac{||r_n||^2}{||r_{n-1}||^2},$$

$$r_n = f'(x_n), \beta_0 = 0$$

Optimization

Examples

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Image deblurring task

The problem:

$$Af \equiv K * f = u, \quad x \in B$$

The cost Tikhonov's functional:

$$M_\alpha[u] = ||Af - u||^2 + \alpha\Omega[f],$$

where the functional $\Omega[f]$ is a stabilizer.

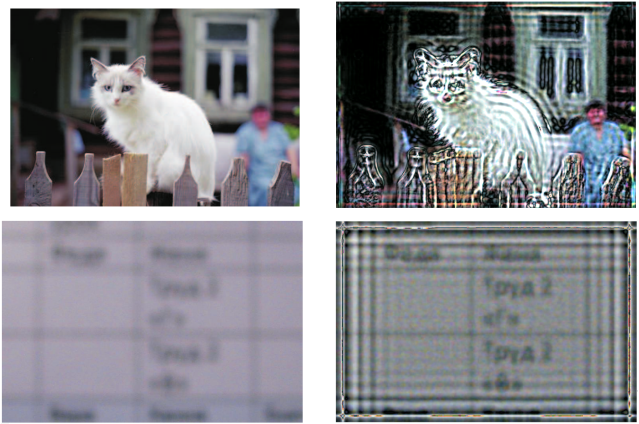
The cost Tikhonov's functional:

$$M_\alpha[z] = ||Az - u||^2 + \alpha\Omega[z],$$

where the functional $\Omega[z]$ is a stabilizer.

1. $\Omega[z] = ||z||^2_{H^1}$. The solution of a quadratic functional can be found analytically.
2. $\Omega[z] = ||z||_{TV}$. In this case, the cost functional is not quadratic and requires iterative minimization. The minimization was provided using the method of Conjugated Gradients Projections (MCGP).

Quadratic optimization



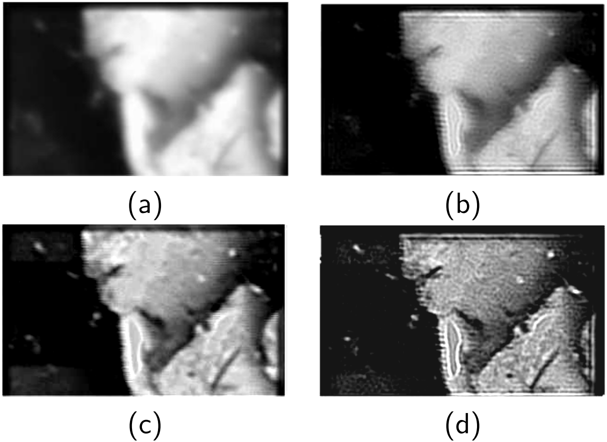
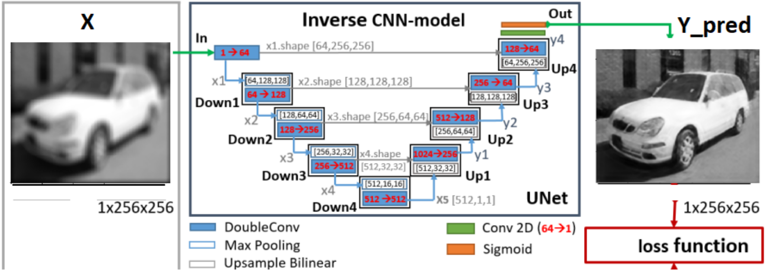


Figure: Results of image reconstruction in SEM BE: (a) - the enter data, (b) - reconstruction on H^1 Sobolev's space, analytical solution, (c) - reconstruction on TV Bounded Total Variations functional space, (MCGP, zero first approximation), (d) - reconstruction on TV with the result on H^1 taken as a first approximation for MCGP

NN: Gradient Descent



L1 loss

BCE loss

MSE loss

NN: Gradient Descent

Software

Optimization

- NLOPT (C++,Python)
- ALGIP (C++,C#)
- Dlib (C++)
- IPOPT (C++)
- SciPy (Python)

Differential equations solver

- FEniCS & DOLFIN (C++,Python)
- OpenFOAM

Molecular dynamics

- Abalone
- AMBER
- Gromacs
- LAMMPS
- NAMD

FEM Meshing

- CGAL and CGAL-based products
- FEniCS
- HyperMesh
- Iso2Mesh (Matlab/Octave)
- FreeSurfer (Encephalography)

S.Rykovanov, A.Vishnyakov: Parallel Computing in Mathematical Modeling and Data-Intensive Applications

S.Rykovanov: High Performance Python Lab

S.Rykovanov: High Performance Computing and Modern Architectures

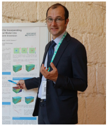
I.Zacharov: Introduction to Linux and Supercomputers

Numerical methods & Modeling

SLAE: I.Oseledets: Numerical Linear Algebra

Data Structures: G.Kucherov: Efficient Algorithms and Data Structures

PDE N.Yavich: Advanced Solvers for Numerical PDEs



Modeling: A.Shapeev: Numerical Modeling

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Thank you for your attention!