

Minimization in \mathbb{R}^N : Gradient Methods

Let us consider a functional $\mathcal{J}(\mathbf{X}) : \mathbb{R}^N \mapsto \mathbb{R}$, defined as $\mathcal{J}(\mathbf{X}) = \frac{1}{2}\mathbf{X} \cdot [\underline{\mathcal{C}}\mathbf{X}] + \mathbf{B}_0 \cdot \mathbf{X}$, where $\underline{\mathcal{C}}$ is a $N \times N$ matrix and \mathbf{B}_0 is a vector of size N . For example

$$\underline{\mathcal{C}} = -(N+1) \begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 1 & -2 & 1 \\ 0 & \cdots & 0 & 1 & -2 \end{pmatrix} \quad \text{and} \quad \mathbf{B}_0 = - \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ (N+1) \end{pmatrix}$$

and in this case the minimum of \mathcal{J} is $\mathbf{U} \in \mathbb{R}^N$ with $U_j = \frac{j}{N+1}$. In order to solve the minimization problem in \mathbb{R}^N it is defined, step by step from a given vector \mathbf{V}^0 (for example $\mathbf{V}^0 \equiv \mathbf{0}$), positions $\mathbf{V}^k \in \mathbb{R}^N$ such as $\mathcal{J}(\mathbf{V}^{k+1}) \leq \mathcal{J}(\mathbf{V}^k)$

For the gradient methods

$$\mathbf{V}^{k+1} = \mathbf{V}^k + \alpha_k \mathbf{d}^k \quad \text{where} \quad \mathbf{d}^k = -\nabla \mathcal{J}(\mathbf{V}^k).$$

In the current case, the gradient can be computed either analytically or numerically.

Gradient method with Constant step $\alpha_k = \alpha$. In a fortran program, compute \mathbf{V}_α^K , for $N = 200$, $K = N/2$, using values $\alpha = 10, 1, 10^{-1}, 10^{-2}, \dots$, For the defined example, plot $\|\mathbf{U} - \mathbf{V}_\alpha^K\|$ as a function of α and define, in this case, an approximated convergence criteria.

Gradient method with optimal step. For a given vector \mathbf{V}_k and a descent direction $\mathbf{d}_k \in \mathbb{R}^N$, we define a functional $f_k(\rho) : \mathbb{R} \mapsto \mathbb{R}$ as $f_k(\rho) = \mathcal{J}(\mathbf{V}_k + \rho \mathbf{d}_k)$. Then for the optimal step, α_k is the minimum of $f_k(\rho)$ on an interval $[0, b]$ with $0 < b$. In a fortran program, compute \mathbf{V}_b^K , for $N = 200$, $K = N/2$, using values $b = 10^{-2}, 10^{-1}, 1, 10^2, 10^3, \dots$, For the defined example, plot $\|\mathbf{U} - \mathbf{V}_b^K\|$ as a function of b .

Gradient method with optimal step and equality constraint. In this item we consider the minimization in a sub-space \mathcal{E} defined by vector \mathbf{O}_e the normal \mathbf{n} with $\|\mathbf{n}\| \neq 0 : \mathcal{X} \in \mathcal{E} \iff (\mathcal{X} - \mathbf{O}_e) \cdot \mathbf{n} = 0$. Propose a modification of the optimal step method to approximate the minimum of J on \mathcal{E} .

Gradient method with optimal step and inequality constraint. In this item we consider the minimization in a half space \mathcal{E} defined by vector \mathbf{O}_e the normal \mathbf{n} with $\|\mathbf{n}\| \neq 0 : \mathcal{X} \in \mathcal{E} \iff (\mathcal{X} - \mathbf{O}_e) \cdot \mathbf{n} \geq 0$. Propose a modification of the optimal step method to approximate the minimum of J on \mathcal{E} .

Gradient method with optimal step and strict inequality constraint. What about the case of \mathcal{E} defined by vector \mathbf{O}_e the normal \mathbf{n} with $\|\mathbf{n}\| \neq 0 : \mathcal{X} \in \mathcal{E} \iff (\mathcal{X} - \mathbf{O}_e) \cdot \mathbf{n} > 0$?

for the minimization of $f_k(\rho)$ use the Dichotomous or the GoldSection algorithm.