Numerical optimization

Mines Nancy - Fall 2024

session 4 – unconstrained optimization first and second-order descent methods

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Course material:

- arche.univ-lorraine.fr/course/view.php?id=74098
- github.com/jflamant/mines-nancy-fall24-optimization



Context

We aim to solve the unconstrained optimization problem

$$\min_{\mathbf{x} \in \mathbb{R}^N} f(\mathbf{x})$$

In many cases, it is not possible to find an explicit solution to the problem (as in the case of least squares).

Solution: iterative method(s) (algorithms)

We seek to find a minimizer of the problem iteratively:

- We fix one (or more) initial point $\mathbf{x}^{(0)} = \mathbf{x}_0$;
- At each iteration k, we obtain a new point $\mathbf{x}^{(k+1)}$ following an update, constructed from the function f to be minimized
- We repeat the process until a stopping criterion is satisfied

Outline

- **1** Gradient-free optimization: the Nelder-Mead algorithm
- ② Descent algorithms: general principles
- Gradient descent methods
- 4 Newton's Method
- **5** Quasi-Newton Methods
- 6 Nonlinear Least Squares
- Comparison: convergence rate vs. complexity

Gradient-free optimization algorithm \rightarrow It is enough to be able to evaluate the function $f(\mathbf{x})$

 \checkmark A practical heuristic method when f is not differentiable \checkmark No guarantee of convergence to a local minimizer

General idea for $f: \mathbb{R}^N \to \mathbb{R}$

1 Randomly select N+1 points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{N+1}$ in \mathbb{R}^N

Gradient-free optimization algorithm

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- 2 Construct the associated simplex (a convex polytope with N+1 vertices: a triangle in 2D, a tetrahedron in 3D...)

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- 3 Evaluate f at each vertex

- Gradient-free optimization algorithm
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- Perform a transformation of this simplex to make it "crawl" towards a (local) minimizer using operations of: reflection, expansion, contraction, shrinkage

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- 6 Repeat the process until the simplex reaches a sufficiently small size

Example

The Nelder-Mead algorithm can converge to a local minimizer ...

Example

The Nelder-Mead algorithm can converge to a local minimizer ...

Example

... but not always!

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Principle of descent algorithms

At iteration k, we construct

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}_k$$

where $\alpha_k \ge 0$ is the step size and \mathbf{d}_k is a direction.

Dream goal:

We want $\mathbf{x}^{(k)} \to \mathbf{x}^*$ with \mathbf{x}^* being a global minimizer of f.

 \rightarrow quite unlikely, since the function f is not necessarily convex.

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Realistic goal:

Construct $\mathbf{x}^{(k)} \to \mathbf{x}^*$ with \mathbf{x}^* being a local minimizer of f and require

• The sequence $\{\mathbf{x}^{(k)}\}$ describes a descent algorithm, i.e.,

$$f(\mathbf{x}^{(0)}) > f(\mathbf{x}^{(1)}) > \ldots > f(\mathbf{x}^{(k)}) > f(\mathbf{x}^{(k+1)}) > \ldots$$

 The algorithm stops when it no longer makes progress: at that point, a stopping criterion is defined.

How to choose \mathbf{d}_k

We want the sequence $\{\mathbf{x}^{(k)}\}$ to "decrease" the objective at each iteration,

$$f(\mathbf{x}^{(0)}) > f(\mathbf{x}^{(1)}) > \dots > f(\mathbf{x}^{(k)}) > f(\mathbf{x}^{(k+1)}) > \dots$$

We must choose \mathbf{d}_k as a descent direction.

Descent Condition
$$\nabla f(\mathbf{x}^{(k)})^{\mathsf{T}}\mathbf{d}_k < 0$$

A zoo of descent algorithms

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}_k$$

Choosing the direction $\mathbf{d}_k \rightarrow \text{leads}$ to different optimization algorithms.

General form $\mathbf{d}_k = -\mathbf{B}_k^{-1} \nabla f(\mathbf{x}^{(k)})$ where \mathbf{B}_k is symmetric and invertible

Examples

- Gradient Descent Method: $\mathbf{B}_k = \mathbf{I}_N$ (identity matrix)
- Newton's Method: $\mathbf{B}_k = \nabla^2 f(\mathbf{x}^{(k)})$ (Hessian of f)
- Quasi-Newton Methods: $\mathbf{B}_k \approx \nabla^2 f(\mathbf{x}^{(k)})$ (approx. Hessian)

How to define a stopping criterion ...

... or how to check that an algorithm has "converged". Idea: stop the algorithm when

criterion value at iteration $k \leq \varepsilon$

where ε is a (small) tolerance/precision set in advance (e.g., $\varepsilon = 10^{-6}$).

How to define a stopping criterion ...

... or how to check that an algorithm has "converged". Idea: stop the algorithm when

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where ε is a (small) tolerance/precision set in advance (e.g., ε = 10^{-6}).

Some Possible Criteria

- Change in objective function: $|f(\mathbf{x}^{(k+1)}) f(\mathbf{x}^{(k)})| \le \varepsilon$
- Change in solution: $\|\mathbf{x}^{(k+1)} \mathbf{x}^{(k)}\| \le \varepsilon$
- Gradient norm: $\|\nabla f(\mathbf{x}^{(k)})\| \le \varepsilon$

Preferably, we use a criterion calculated in relative terms, for example:

$$\frac{\left|f(\mathbf{x}^{(k+1)}) - f(\mathbf{x}^{(k)})\right|}{\left|f(\mathbf{x}^{(k)})\right|} \le \varepsilon \quad \text{or} \quad \frac{\left\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right\|}{\left\|\mathbf{x}^{(k)}\right\|} \le \varepsilon$$

in addition, a condition on the maximal number of iterations is often used to control the computational burden

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Gradient Descent Algorithm

Starting from an initial point $\mathbf{x}^{(0)} = \mathbf{x}_0$, iterate:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k \nabla f(\mathbf{x}^{(k)})$$

For proper choice of the step size α_k , $\mathbf{x}^{(k)}$ converges to a stationary point of f (a point \mathbf{x}^* such that $\nabla f(\mathbf{x}^*) = 0$).

Step size selection strategies

- Constant step size: set $\alpha_k = \alpha$ for all k;
- Optimal step size: at each iteration k, solve

$$\alpha_k = \underset{\alpha>0}{\operatorname{arg\,min}} f(\mathbf{x}^{(k)} - \alpha_k \nabla f(\mathbf{x}^{(k)}))$$

• Line search or backtracking methods.

Constant step size strategy

Constant step size gradient algorithm

Starting from an initial point $\mathbf{x}^{(0)} = \mathbf{x}_0$, iterate:

$$\mathbf{x}^{(\mathbf{k}+\mathbf{1})} = \mathbf{x}^{(k)} - \alpha \nabla f(\mathbf{x}^{(k)})$$

Intuitively,

- α too small \rightarrow very slow convergence
- α too large \rightarrow RISK OF DIVERGENCE

The step size α must be chosen to balance speed of convergence and convergence guarantees.

Constant step size strategy

Constant step size gradient algorithm

Starting from an initial point $\mathbf{x}^{(0)} = \mathbf{x}_0$, iterate:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha \nabla f(\mathbf{x}^{(k)})$$

Important Result: if f has an L-Lipschitz gradient, i.e.,

$$\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^N, \quad \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \le L \|\mathbf{x} - \mathbf{y}\|$$

Then, if

$$0 < \alpha < \frac{2}{I}$$

the algorithm converges to a stationary point of f.

more details on convergence results in future class

Optimal step size strategy

Optimal step size gradient algorithm

Starting from an initial point $\mathbf{x}^{(0)} = \mathbf{x}_0$, iterate:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k \nabla f(\mathbf{x}^{(k)})$$

where α_k is obtained by minimizing:

$$\alpha_k = \underset{\alpha \ge 0}{\operatorname{arg \, min}} f(\mathbf{x}^{(k)} - \alpha \nabla f(\mathbf{x}^{(k)}))$$

at each iteration.

On paper, the strategy is ideal.

Main issue: calculating the optimal step size can be as difficult as the original problem and/or very computationally expensive.

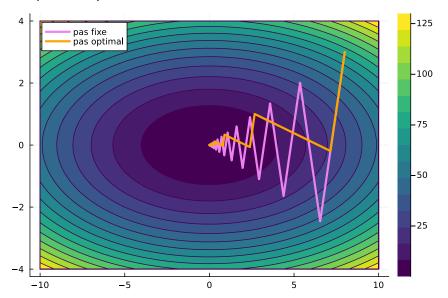
A 2D example

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}, \text{ with } \mathbf{Q} = \begin{bmatrix} 1 & 0 \\ 0 & \eta \end{bmatrix}, \eta > 0$$

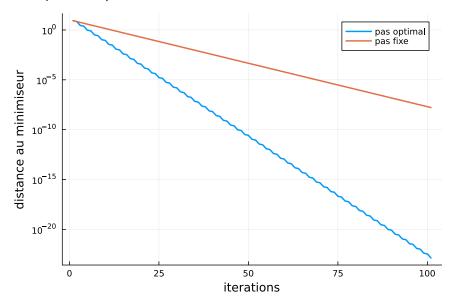
- **1** Calculate $\nabla f(\mathbf{x})$
- **2** Give the explicit expression for $\mathbf{x}^{(k+1)}$ in terms of $\mathbf{x}^{(k)}$
- **3** Give the expression for $\mathbf{x}^{(1)}$ in terms of α_0 for $\mathbf{x}^{(0)} = [\eta, 1]^T$
- Find the optimal step size for this iteration
- **6** Show that the iterations with optimal step size take the form:

$$x_1^{(k)} = \eta \left(\frac{\eta - 1}{\eta + 1}\right)^k \quad x_2^{(k)} = \left(-\frac{\eta - 1}{\eta + 1}\right)^k$$

Example for η = 10



Example for $\eta = 10$



Line search or backtracking strategies

We seek a step size α_k that sufficiently decreases the objective f:

$$\alpha_k \approx \underset{\alpha \geq 0}{\operatorname{arg \, min}} f(\mathbf{x}^{(k)} - \alpha \nabla f(\mathbf{x}^{(k)}))$$

 \rightarrow This is the most commonly used approach in practice, for which many "recipes" exist.

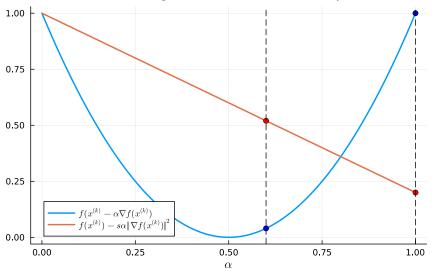
Example: backtracking for gradient algorithm

Fix $s \in (0,0.5)$ and $\eta \in (0,1)$ with an initial step size $\alpha = 1$.

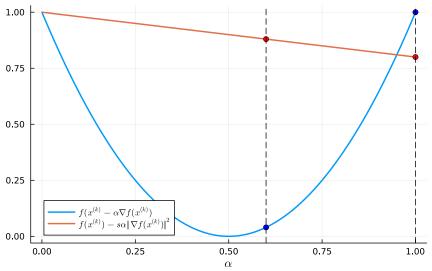
- 1: $\alpha \coloneqq 1$
- 2: while $f(\mathbf{x}^{(k)} \alpha \nabla f(\mathbf{x}^{(k)})) > f(\mathbf{x}^{(k)}) s\alpha \|\nabla f(\mathbf{x}^{(k)})\|^2$ do
- 3: $\alpha := \eta \alpha$
- 4: end while

Approximate step size strategies are constructed to ensure algorithm convergence.

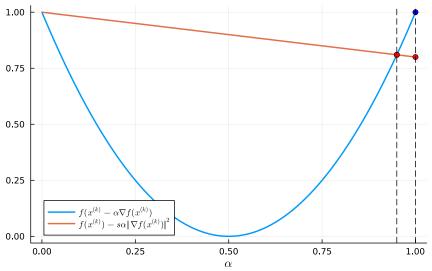
backtracking line search, $s=0.2,\,\eta=0.6$



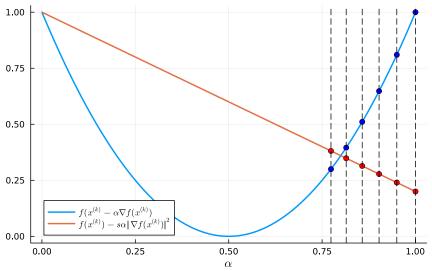
backtracking line search, $s=0.05,\,\eta=0.6$



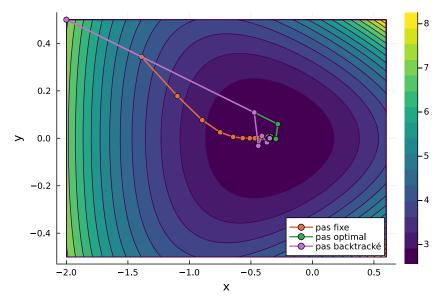
backtracking line search, $s=0.05,\,\eta=0.95$



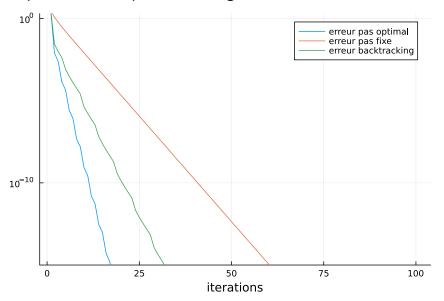
backtracking line search, s = 0.2, $\eta = 0.95$



Comparison of step size strategies



Comparison of step size strategies



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Newton's Algorithm

Starting from an initial point $\mathbf{x}^{(0)} = \mathbf{x}_0$, iterate

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k \left[\nabla^2 f(\mathbf{x}^{(k)}) \right]^{-1} \nabla f(\mathbf{x}^{(k)})$$

The quantity $\mathbf{d}_k = -\left[\nabla^2 f(\mathbf{x}^{(k)})\right]^{-1} \nabla f(\mathbf{x}^{(k)})$ is indeed a descent direction as long as the Hessian of f at $\mathbf{x}^{(k)}$ is positive definite:

$$\nabla f(\mathbf{x}^{(k)})^{\mathsf{T}} \mathbf{d}_{k} = -\nabla f(\mathbf{x}^{(k)})^{\mathsf{T}} \left[\nabla^{2} f(\mathbf{x}^{(k)}) \right]^{-1} \nabla f(\mathbf{x}^{(k)}) < 0$$

Step-size selection strategies

- constant step-size: we fix $\alpha_k = \alpha$ for all k (often $\alpha = 1$);
- possible use of backtracking.

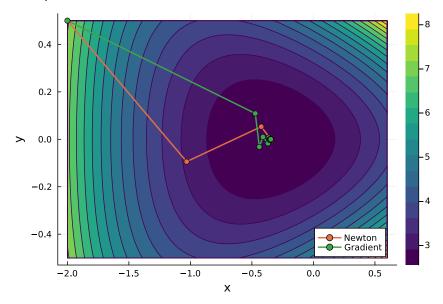
The return of the 2D unconstrained QP example

We consider the function

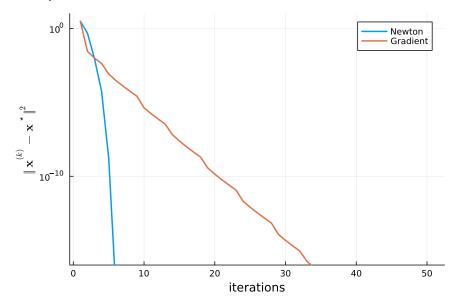
$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathsf{T}}\mathbf{Q}\mathbf{x} - \mathbf{b}^{\mathsf{T}}\mathbf{x}, \text{ with } \mathbf{Q} > 0$$

- **1** Compute $\nabla f(\mathbf{x})$ and deduce the minimizer of f
- **2** Compute $\nabla^2 f(\mathbf{x})$
- **3** Give the explicit expression of $\mathbf{x}^{(k+1)}$ as a function of $\mathbf{x}^{(k)}$ for Newton's method with constant step-size
- What can we deduce from this?

Example: Non-Quadratic Case



Example: Non-Quadratic Case



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Motivation

Despite its numerous advantages, Newton's method suffers from two disadvantages:

- Computing Newton's step involves calculating and inverting the Hessian matrix ∇²f(x^(k)), which becomes very costly in high dimensions;
- The Hessian matrix $\nabla^2 f(\mathbf{x}^{(k)})$ is not always positive definite, so it's not always possible to calculate its inverse.

Solution: Quasi-Newton Methods

We replace the Hessian matrix with an approximation $\mathbf{B}_k \approx \nabla^2 f(\mathbf{x}^{(k)})$, so that the iterations become:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k \mathbf{B}_k^{-1} \nabla f(\mathbf{x}^{(k)})$$

Principle of Quasi-Newton Methods

We aim to recursively estimate the matrices \mathbf{B}_k (or \mathbf{H}_k) such that

$$\mathbf{B}_k \approx \nabla^2 f(\mathbf{x}^{(k)})$$
 or $\mathbf{H}_k \approx \left[\nabla^2 f(\mathbf{x}^{(k)})\right]^{-1}$

An update rule → a quasi-Newton method

Some examples

- Broyden-Fletcher-Goldfarb-Shanno (BFGS): the most popular
- L-BFGS: memory-efficient BFGS
- Symmetric rank-one (SR1)
- Davidon–Fletcher–Powell (DFP)
- ..

Broyden-Fletcher-Goldfarb-Shanno (BFGS)

At iteration k,

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k \mathbf{H}_k \nabla f(\mathbf{x}^{(k)})$$

We define

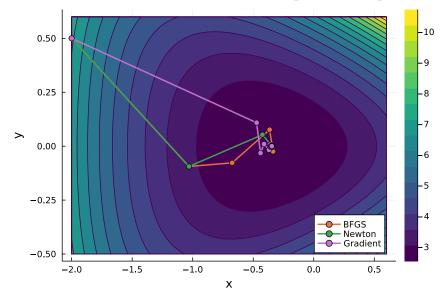
$$\mathbf{s}_{k} = -\alpha_{k} \mathbf{H}_{k} \nabla f(\mathbf{x}^{(k)}), \quad \mathbf{y}_{k} = \nabla f(\mathbf{x}^{(k+1)}) - \nabla f(\mathbf{x}^{(k)}), \quad \rho_{k} = \frac{1}{\mathbf{s}_{k}^{\mathsf{T}} \mathbf{y}_{k}}$$

Update of \mathbf{H}_k in BFGS

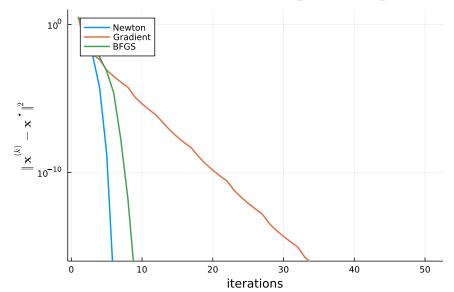
$$\mathbf{H}_{k+1} = \left(\mathbf{I}_{N} - \rho_{k} \mathbf{s}_{k} \mathbf{y}_{k}^{\mathsf{T}}\right) \mathbf{H}_{k} \left(\mathbf{I}_{N} - \rho_{k} \mathbf{y}_{k} \mathbf{s}_{k}^{\mathsf{T}}\right) + \rho_{k} \mathbf{s}_{k} \mathbf{s}_{k}^{\mathsf{T}}$$

Step-size α_k is chosen using a line search technique (e.g., backtracking).

Example: Non-Quadratic Case $(\mathbf{H}_0 = \left[\nabla^2 f(\mathbf{x}^{(0)})\right]^{-1})$



Example: Non-Quadratic Case $(\mathbf{H}_0 = \left[\nabla^2 f(\mathbf{x}^{(0)})\right]^{-1})$



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Nonlinear Least Squares

General Form

$$\min_{\mathbf{x} \in \mathbb{R}^N} f(\mathbf{x}) := \frac{1}{2} \sum_{j=1}^M r_j(\mathbf{x})^2, \quad r_j : \mathbb{R}^N \to \mathbb{R}$$

Let us define

$$R(\mathbf{x}) = (r_1(\mathbf{x}), r_2(\mathbf{x}), \dots, r_M(\mathbf{x}))^{\mathsf{T}}$$

We can rewrite the problem as

$$\min_{\mathbf{x} \in \mathbb{R}^N} f(\mathbf{x}) \coloneqq \frac{1}{2} \| R(\mathbf{x}) \|_2^2, \quad R(\mathbf{x}) : \mathbb{R}^N \to \mathbb{R}^M$$

Remark

if R(x) = Ax - b, this reduces to a linear least squares problem.

Nonlinear Least Squares: Jacobian Matrix

The particular form of $f(\mathbf{x})$ can be exploited to construct efficient algorithms.

Key Tool: Jacobian Matrix of $\mathbf{R}: \mathbb{R}^N \to \mathbb{R}^M$

$$\mathbf{J}(\mathbf{x}) = \begin{bmatrix} \frac{\partial r_1}{\partial x_1} & \cdots & \frac{\partial r_1}{\partial x_N} \\ \frac{\partial r_2}{\partial x_1} & \cdots & \frac{\partial r_2}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial r_M}{\partial x_1} & \cdots & \frac{\partial r_M}{\partial x_N} \end{bmatrix} = \begin{bmatrix} \nabla r_1(\mathbf{x})^\top \\ \nabla r_2(\mathbf{x})^\top \\ \vdots \\ \nabla r_M(\mathbf{x})^\top \end{bmatrix} \in \mathbb{R}^{M \times N}$$

Gradient and Hessian Expressions

Using the Jacobian matrix allows for a simple expression of the gradient and Hessian of $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{R}(\mathbf{x})\|_2^2$.

Gradient of f

$$\nabla f(\mathbf{x}) = \sum_{j=1}^{M} r_j(\mathbf{x}) \nabla r_j(\mathbf{x}) = \mathbf{J}(\mathbf{x})^{\mathsf{T}} \mathbf{R}(\mathbf{x})$$

Hessian of f

$$\nabla^{2} f(\mathbf{x}) = \sum_{j=1}^{M} \nabla r_{j}(\mathbf{x}) \nabla r_{j}(\mathbf{x})^{\top} + \sum_{j=1}^{M} r_{j}(\mathbf{x}) \nabla^{2} r_{j}(\mathbf{x})$$
$$= \mathbf{J}(\mathbf{x})^{\top} \mathbf{J}(\mathbf{x}) + \sum_{j=1}^{M} r_{j}(\mathbf{x}) \nabla^{2} r_{j}(\mathbf{x})$$

Why is this interesting?

In many applications:

- Computing the Jacobian J(x) is inexpensive (or easy to obtain)
- The gradient is directly obtained from $\nabla f(\mathbf{x}) = \mathbf{J}(\mathbf{x})^{\mathsf{T}} \mathbf{R}(\mathbf{x})$
- Often, the second term in the Hessian can be neglected (especially near the solution), so that

$$\nabla^2 f(\mathbf{x}) \approx \mathbf{J}(\mathbf{x})^{\mathsf{T}} \mathbf{J}(\mathbf{x})$$

meaning the Hessian can be computed without second derivatives.

- → We exploit these properties to construct algorithms:
 - Gauss-Newton method
 - Levenberg-Marquardt method

Algorithms for nonlinear least squares

Gauss-Newton Method

This is a quasi-Newton method with $\mathbf{B}_k = \mathbf{J}(\mathbf{x}^{(k)})^{\mathsf{T}}\mathbf{J}(\mathbf{x}^{(k)})$

At iteration k, $(\alpha_k = 1)$:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \left[\mathbf{J}(\mathbf{x}^{(k)})^{\mathsf{T}}\mathbf{J}(\mathbf{x}^{(k)})\right]^{-1} \nabla f(\mathbf{x}^{(k)})$$

Levenberg-Marquardt Method

Can also be interpreted as a quasi-Newton method

At iteration k, $(\alpha_k = 1)$, we set $\mathbf{C}_k = \mathbf{J}(\mathbf{x}^{(k)})^{\mathsf{T}}\mathbf{J}(\mathbf{x}^{(k)})$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - [\mathbf{C}_k + \lambda_k \operatorname{diag}(\mathbf{C}_k)]^{-1} \nabla f(\mathbf{x}^{(k)})$$

where λ_k is a regularization parameter.

→ Algorithm commonly used in practice for nonlinear least squares problems.

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How to choose an algorithm for a given problem?

For a given problem, choosing an algorithm can depend on:

 Convergence rate: It indicates how fast the iterates approach their limit, measured by the distance

$$\varepsilon_k = \|\mathbf{x}^{(k)} - \mathbf{x}^{\star}\|_2$$
 where \mathbf{x}^{\star} is a local minimizer

The rate of convergence is *asymptotic*, meaning it appears as $k \to \infty$.

 Numerical complexity: It measures the computational cost associated with an algorithm (usually, the cost per iteration).

Different types of convergence

Distance to a local minimizer

$$\varepsilon_k = \|\mathbf{x}^{(k)} - \mathbf{x}^*\|_2$$
 where \mathbf{x}^* is a local minimizer

• Linear convergence:

$$\frac{\varepsilon_{k+1}}{\varepsilon_k} \underset{k \to \infty}{\to} \mu, \quad 0 < \mu < 1$$

• Super-linear convergence:

$$\frac{\varepsilon_{k+1}}{\varepsilon_k} \to 0$$

• Quadratic convergence:

$$\frac{\varepsilon_{k+1}}{\varepsilon_k^2} \underset{k \to \infty}{\to} \mu, \quad 0 < \mu < 1$$

Computational complexity

The complexity is measured in flops = number of elementary operations (addition, multiplication)

Complexity of basic operations

- Dot product $\mathbf{a}^{\mathsf{T}}\mathbf{b}$ with $\mathbf{a},\mathbf{b}\in\mathbb{R}^{N}$ $\mathcal{O}(N)$ flops
- Matrix-vector product $\mathbf{A}\mathbf{b}$ with $\mathbf{A} \in \mathbb{R}^{M \times N}, \mathbf{b} \in \mathbb{R}^{N}$ $\mathcal{O}(MN)$ flops
- Matrix-matrix product \mathbf{AB} with $\mathbf{A} \in \mathbb{R}^{M \times N}, \mathbf{B} \in \mathbb{R}^{N \times P}$ $\mathcal{O}(MNP)$ flops
- Matrix inversion \mathbf{A}^{-1} with $\mathbf{A} \in \mathbb{R}^{N \times N}$ $\mathcal{O}(N^3)$ flops

The overall complexity of a sequence of operations can sometimes be difficult to calculate or may not be sufficient to characterize the computational cost (issues related to memory footprint / swapping, in particular)

Properties of some algorithms

$$\min_{\mathbf{x} \in \mathbb{R}^N} f(\mathbf{x})$$

Gradient method with constant step size

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha \nabla f(\mathbf{x}^{(k)})$$

- Complexity: $\mathcal{O}(N)$ per iteration
- Linear convergence rate [under some conditions]
- Newton's method

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k \left[\nabla^2 f(\mathbf{x}^{(k)}) \right]^{-1} \nabla f(\mathbf{x}^{(k)})$$

- Complexity: $\mathcal{O}(N^3)$ per iteration
- Quadratic convergence rate [under some conditions]

more on convergence in the dedicated lecture

After the holidays

Class of 05/11/24

- ~ 30 min course exam
- ~ 2h30 TP on first and second-order descent methods

Course exam details

- simple questions on the content of sessions 1-4
- short answers and justifications required
- no documents
- doing examples from the lectures slides can be useful!