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

MINESnancy

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

Nelder-Mead algorithm

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

✓ A practical heuristic method when f is not differentiable
✗ **No guarantee of convergence to a local minimizer**

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

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

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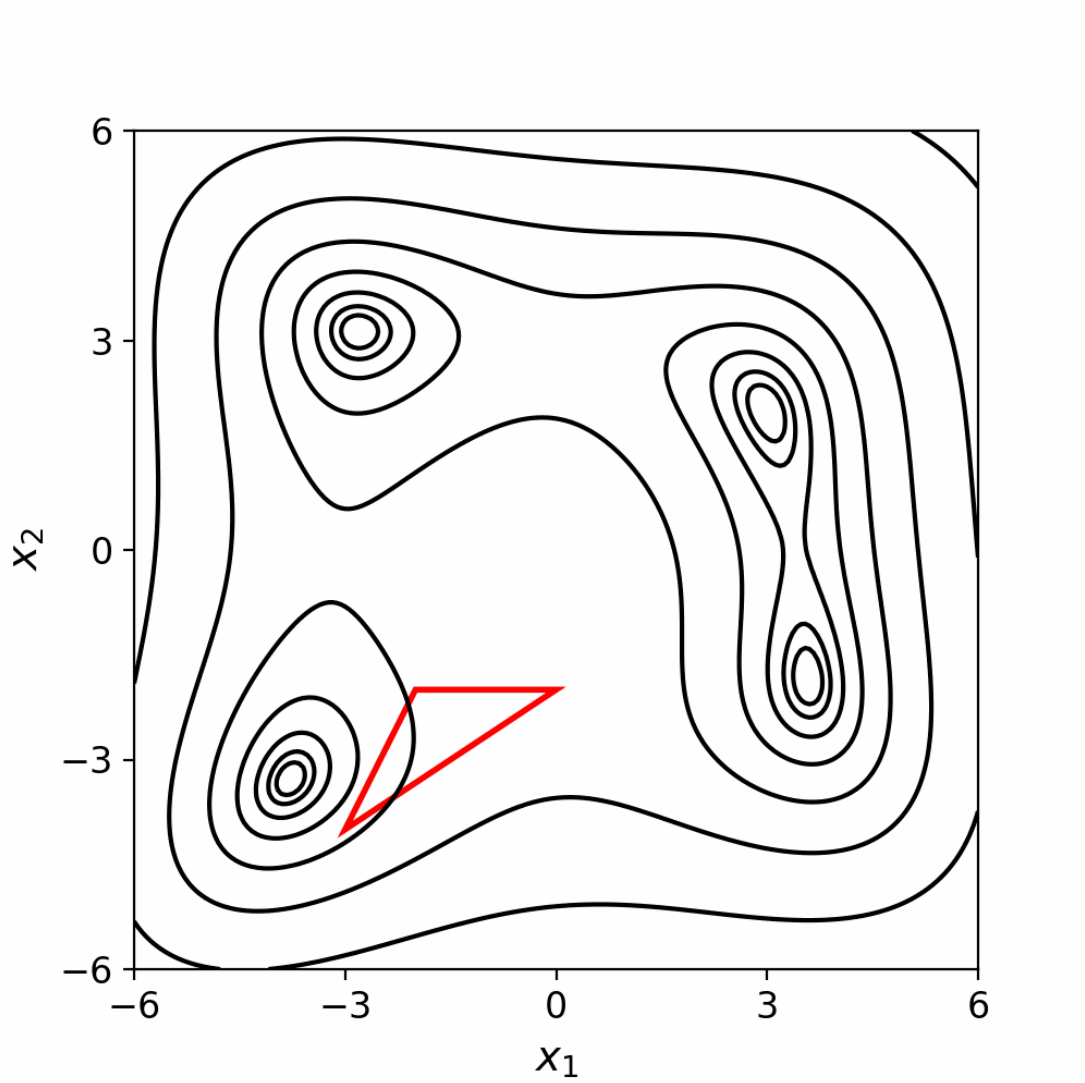
   reflection, expansion, contraction, shrinkage
5. Repeat the process until the simplex reaches a sufficiently small size

Example

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



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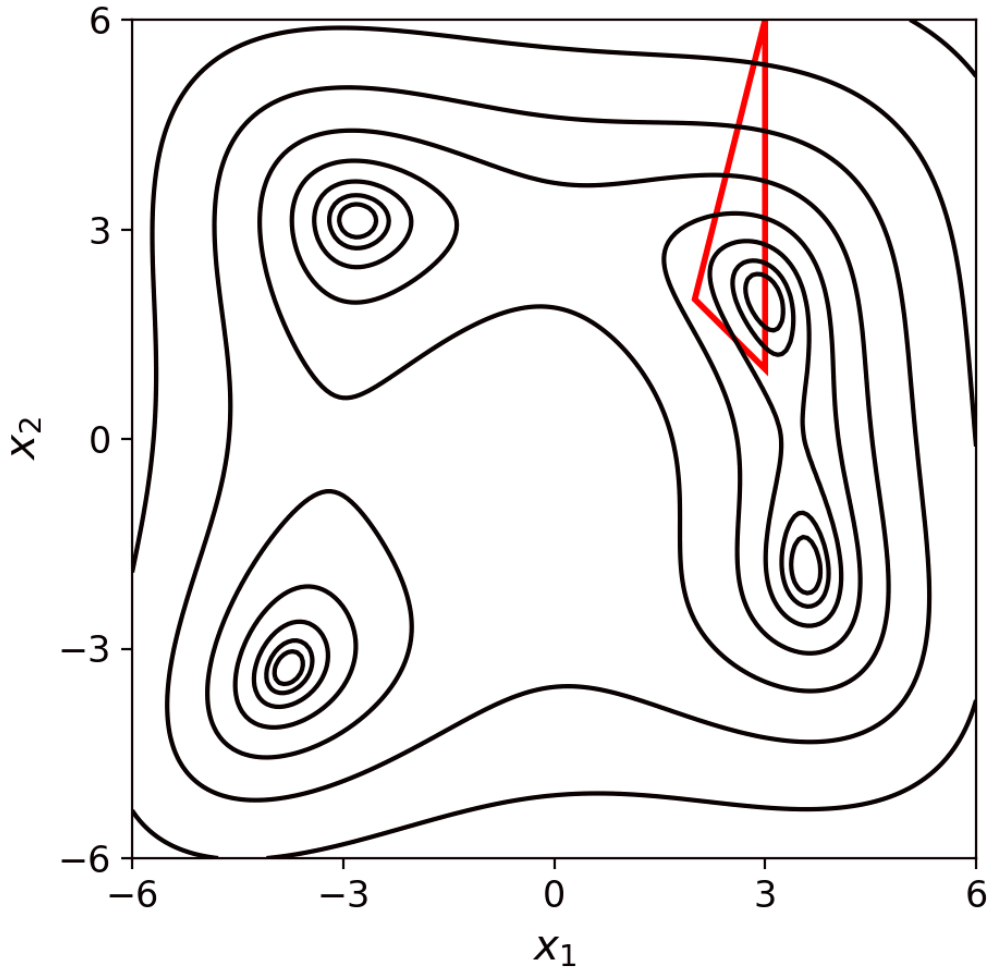
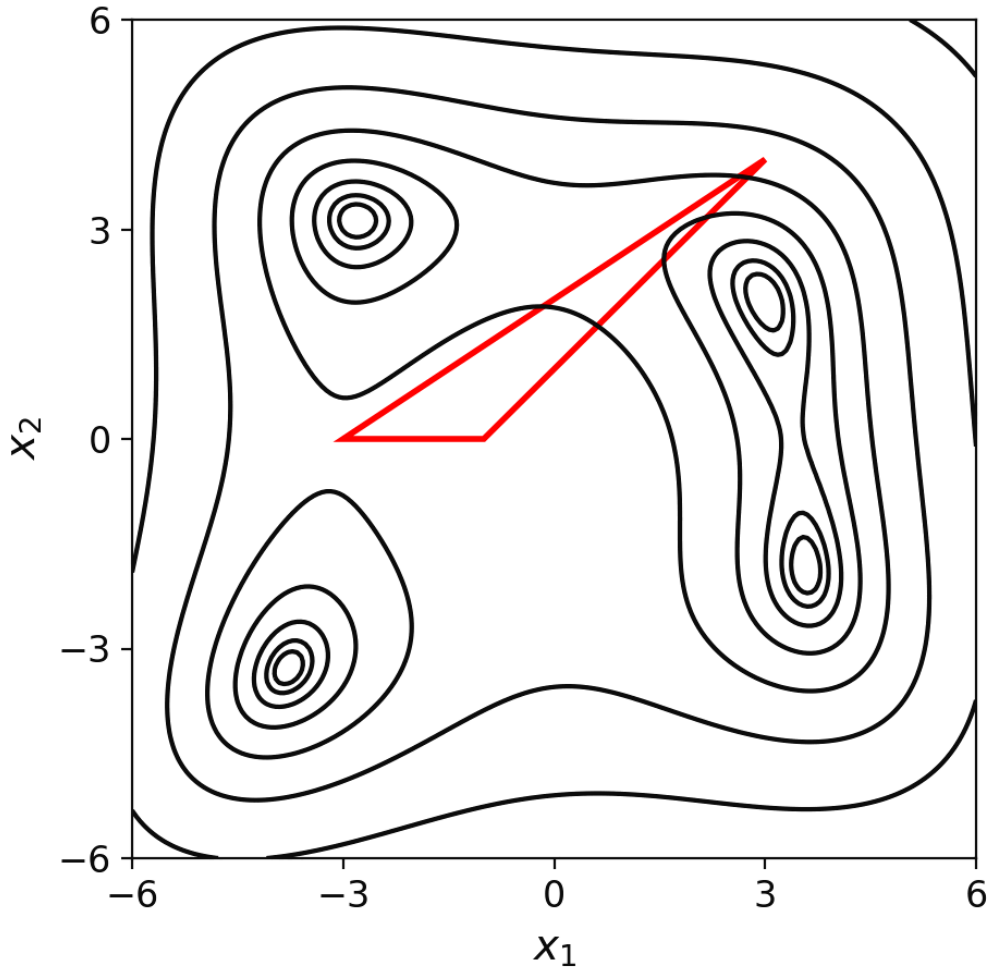


Example

... but not always!



Outline

Principle of descent algorithms

At iteration k, we construct

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

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

Dream goal:
We want $\mathbf{x}^{(k)} \to \mathbf{x}^\star$ with $\mathbf{x}^\star$ being a global minimizer of f.
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Realistic goal:
Construct $\mathbf{x}^{(k)} \to \mathbf{x}^\star$ with $\mathbf{x}^\star$ 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,

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

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

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

A zoo of descent algorithms

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

Choosing the direction $\mathbf{d}_k \rightarrow$ 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

$$\text{criterion value at iteration } k \leq \varepsilon$$

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

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Some Possible Criteria

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

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

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

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

Outline

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 $\mathbf{x}^\star$ such that $\nabla f(\mathbf{x}^\star) = 0$).

Step size selection strategies

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

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

- 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:

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

Intuitively,

- α too small → very slow convergence
- α too large → 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.,

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

Then, if

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

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:

$$\alpha_k = \arg\min_{\alpha \geq 0} f(\mathbf{x}^{(k)} - \alpha \nabla f(\mathbf{x}^{(k)}))$$

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.

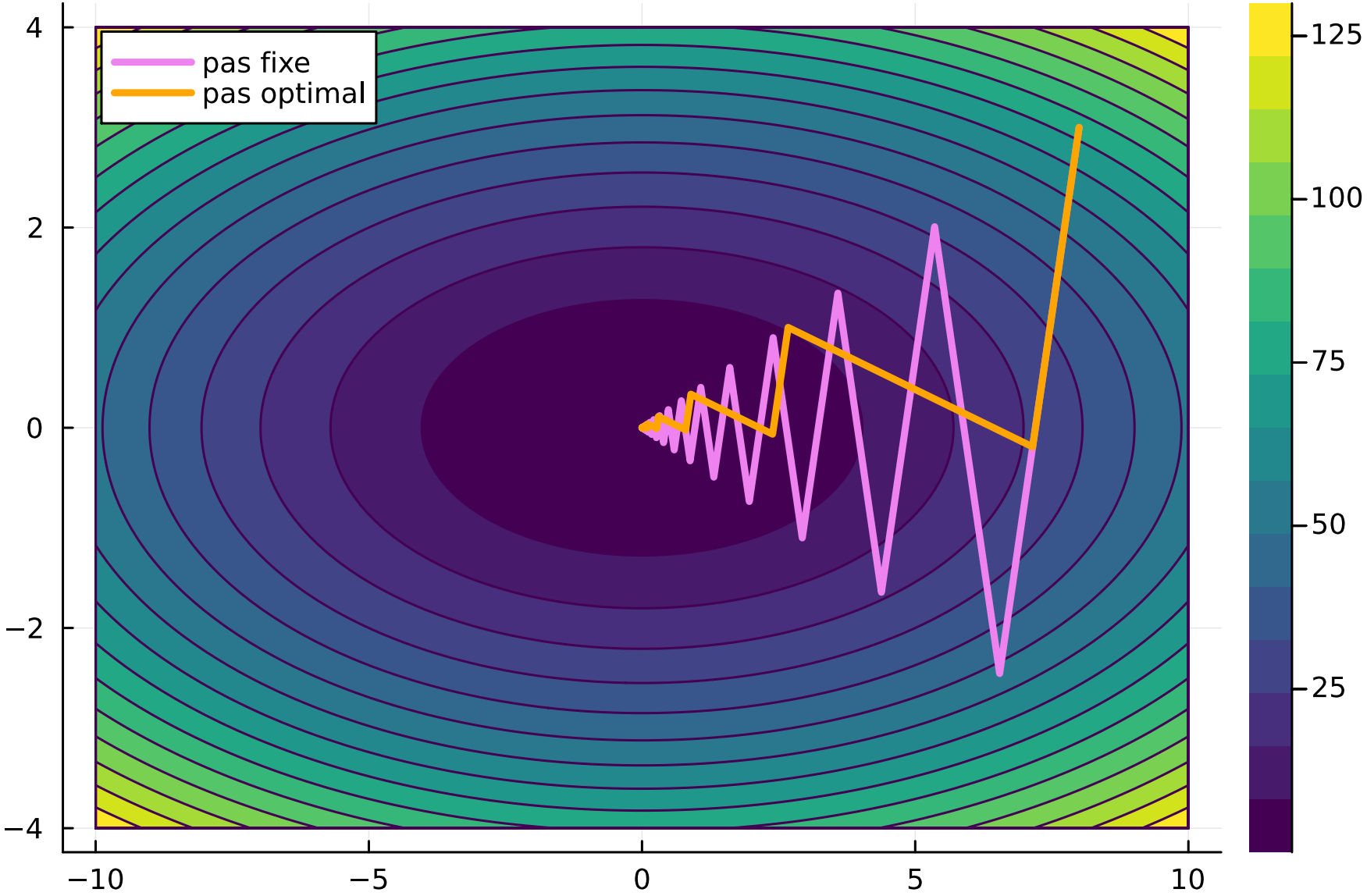
A 2D example

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

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 $\mathbf{x}^{(0)} = [\eta, 1]^\top$
4. Find the optimal step size for this iteration
5. 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 $\eta = 10$



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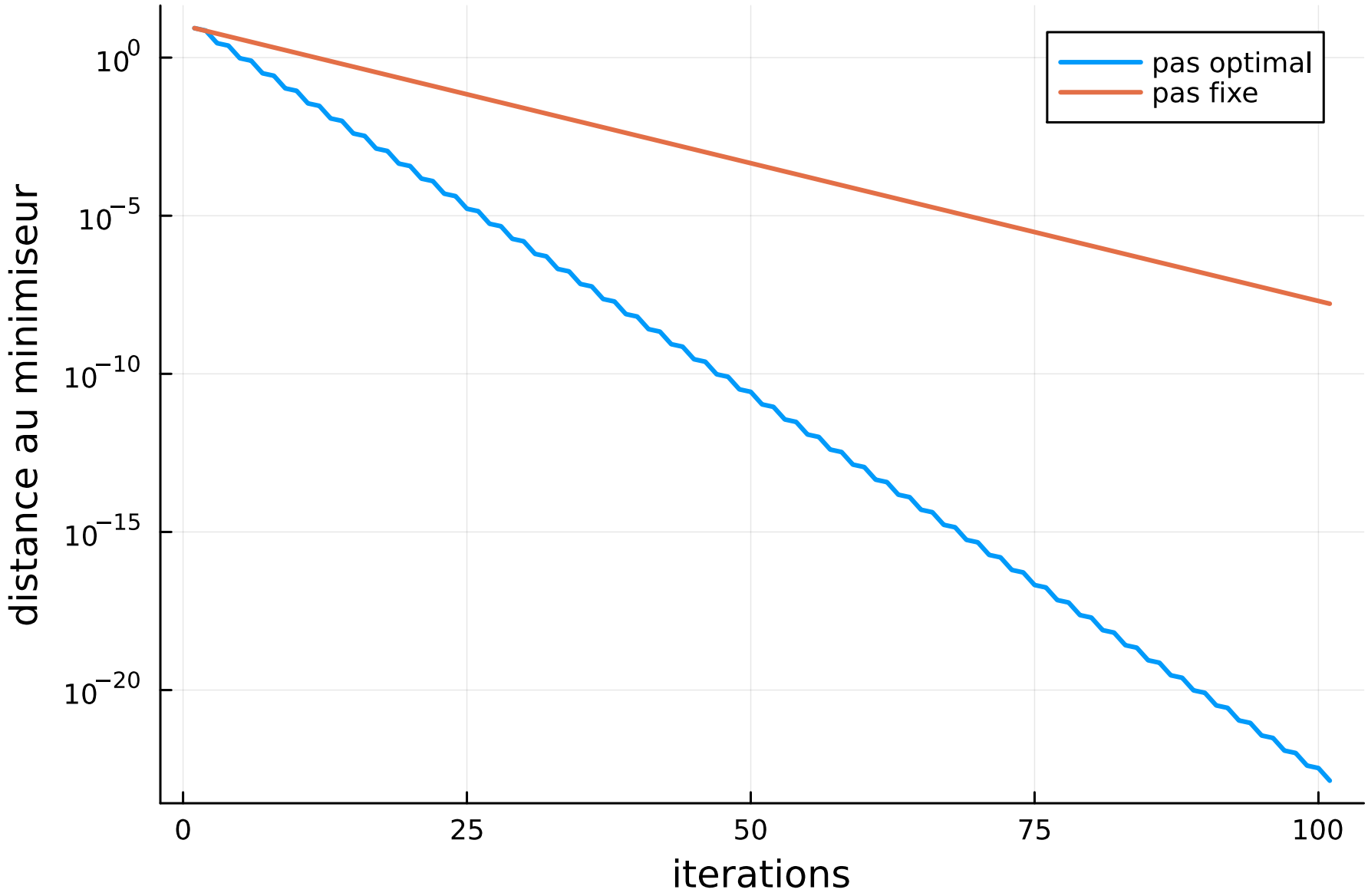


Line search or backtracking strategies

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

$$\alpha_k \approx \arg\min_{\alpha \geq 0} f(\mathbf{x}^{(k)} - \alpha \nabla f(\mathbf{x}^{(k)}))$$

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

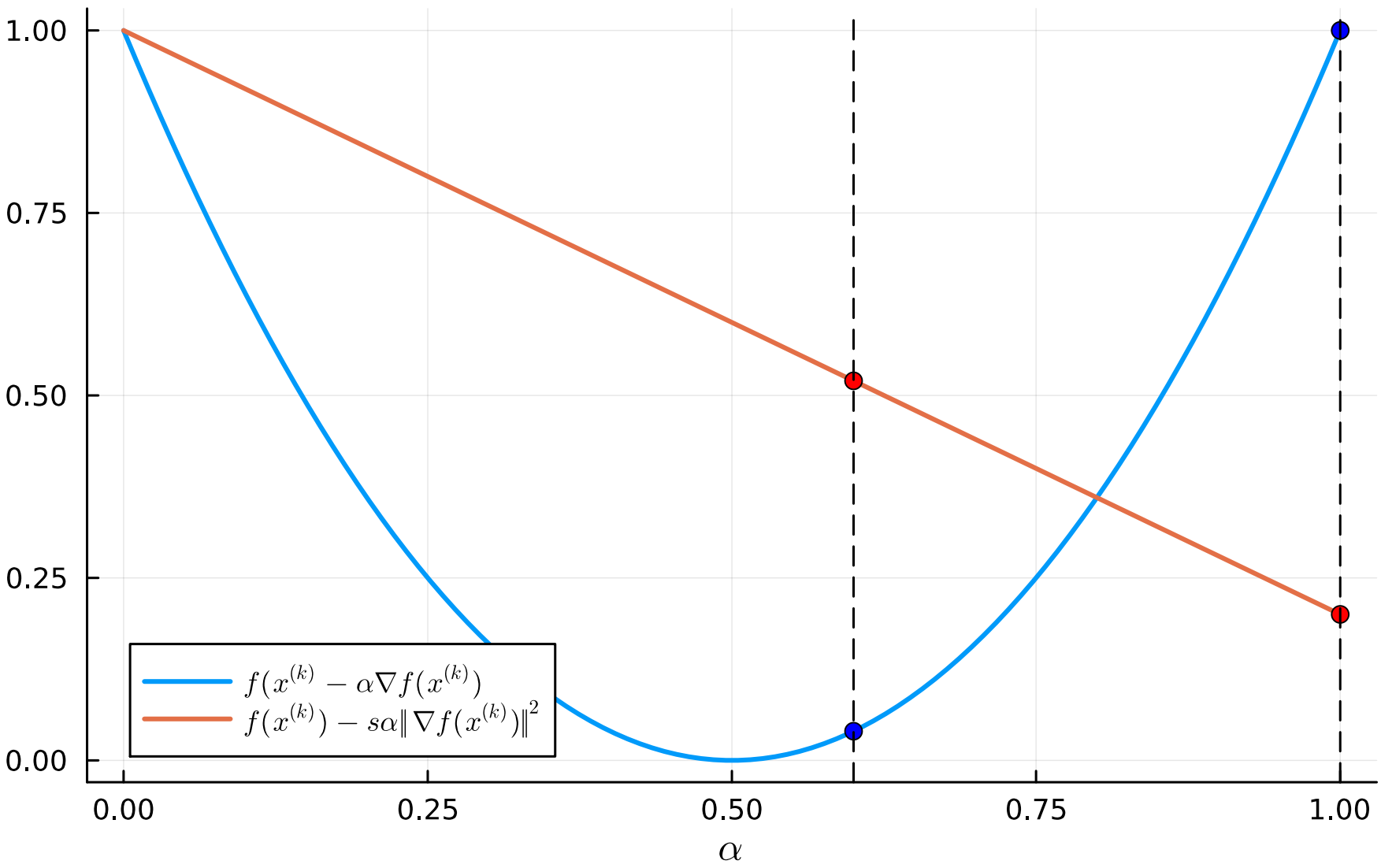
Example: backtracking for gradient algorithm

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

1: $\alpha := 1$
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: $\quad \alpha := \eta\alpha$
4: **end while**

Approximate step size strategies are constructed to ensure algorithm convergence.

Example: backtracking



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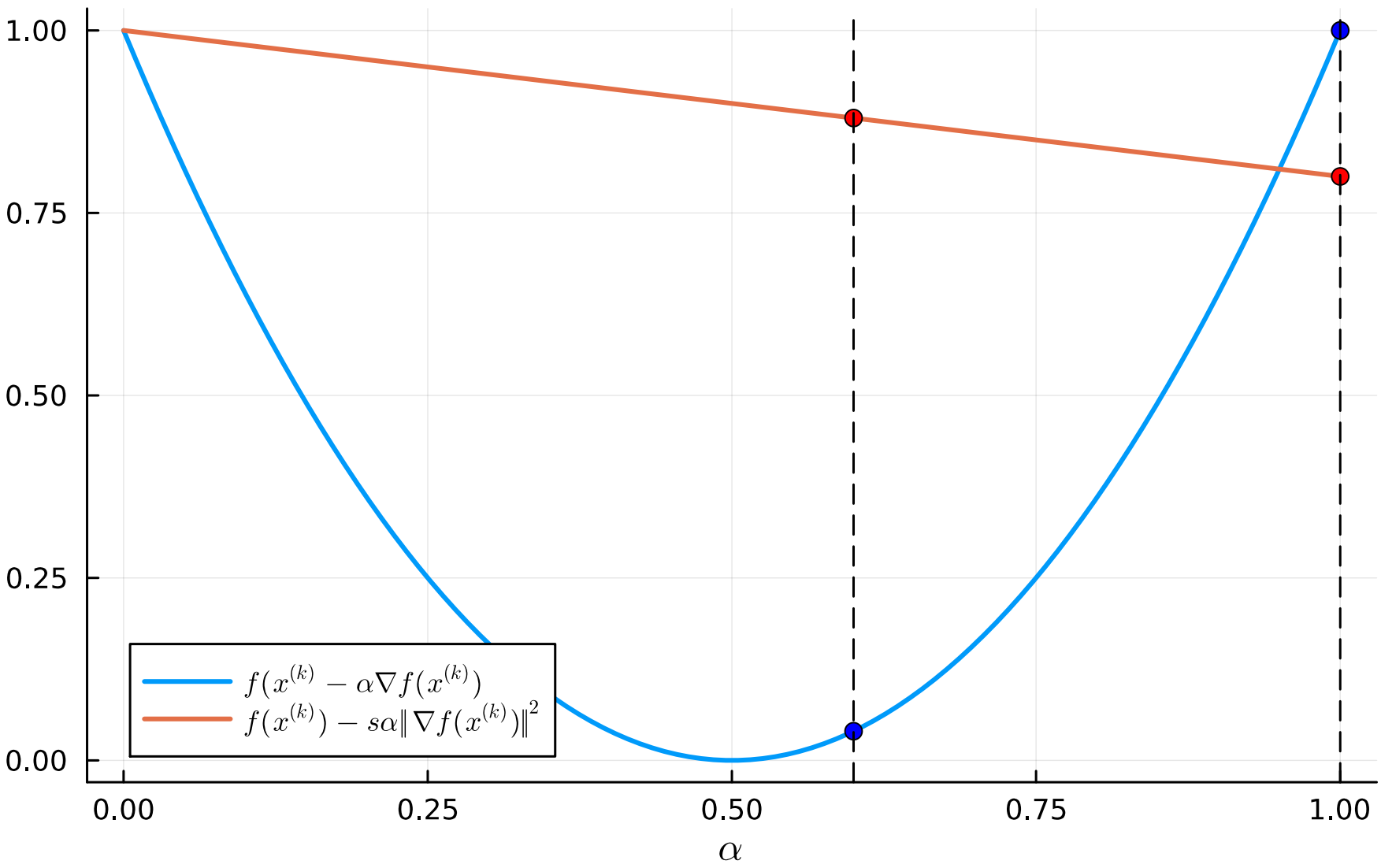

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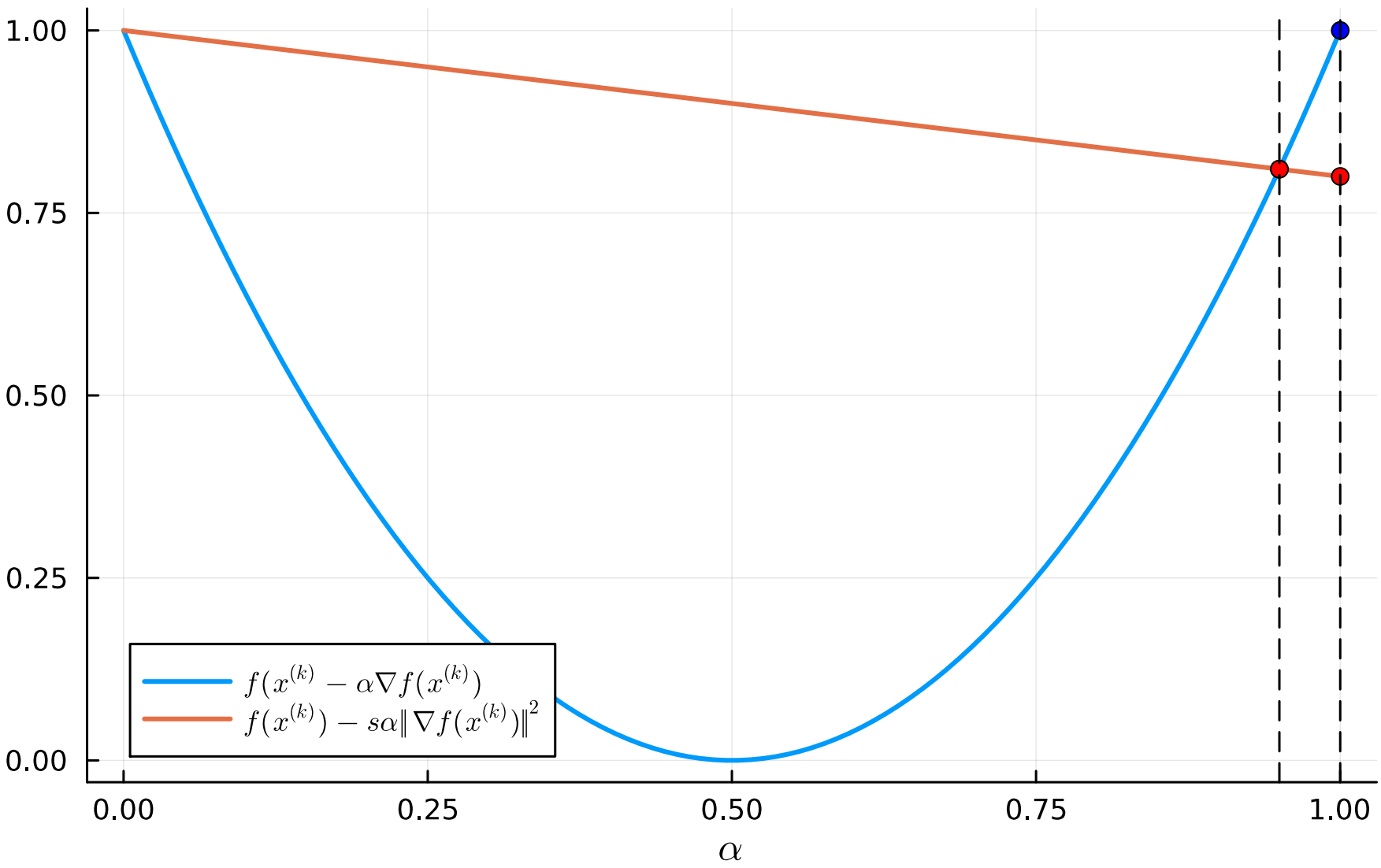

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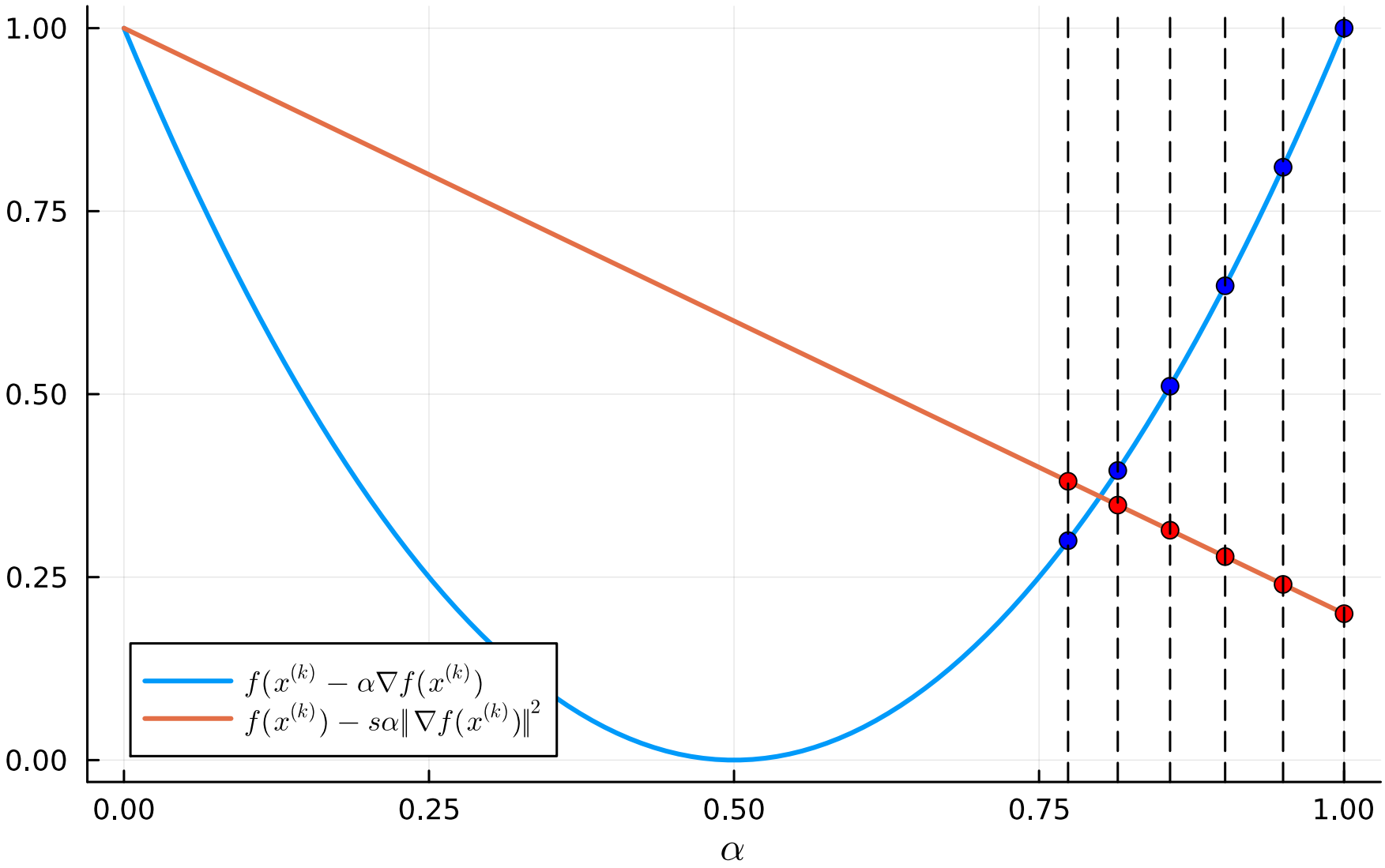
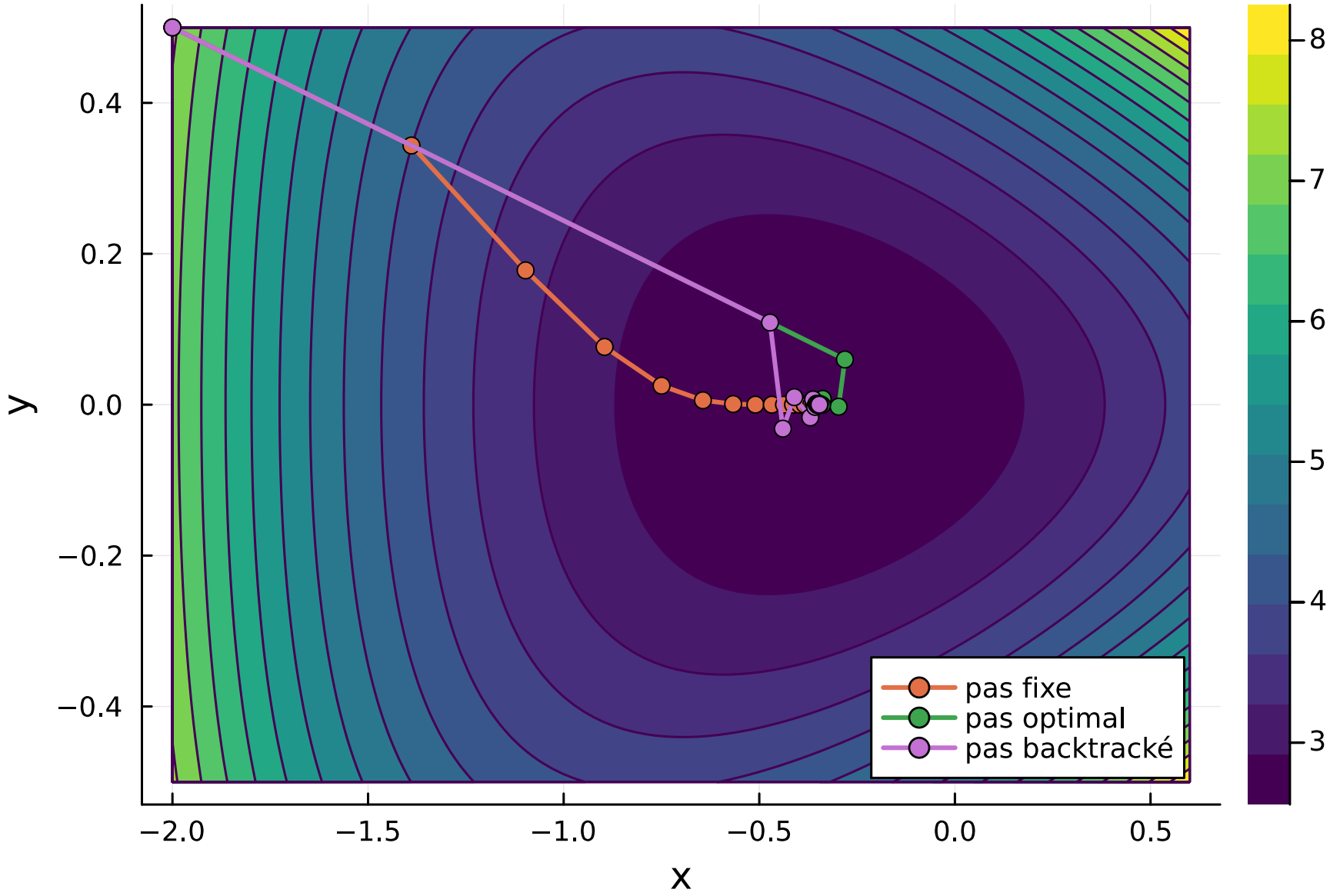


Comparison of step size strategies



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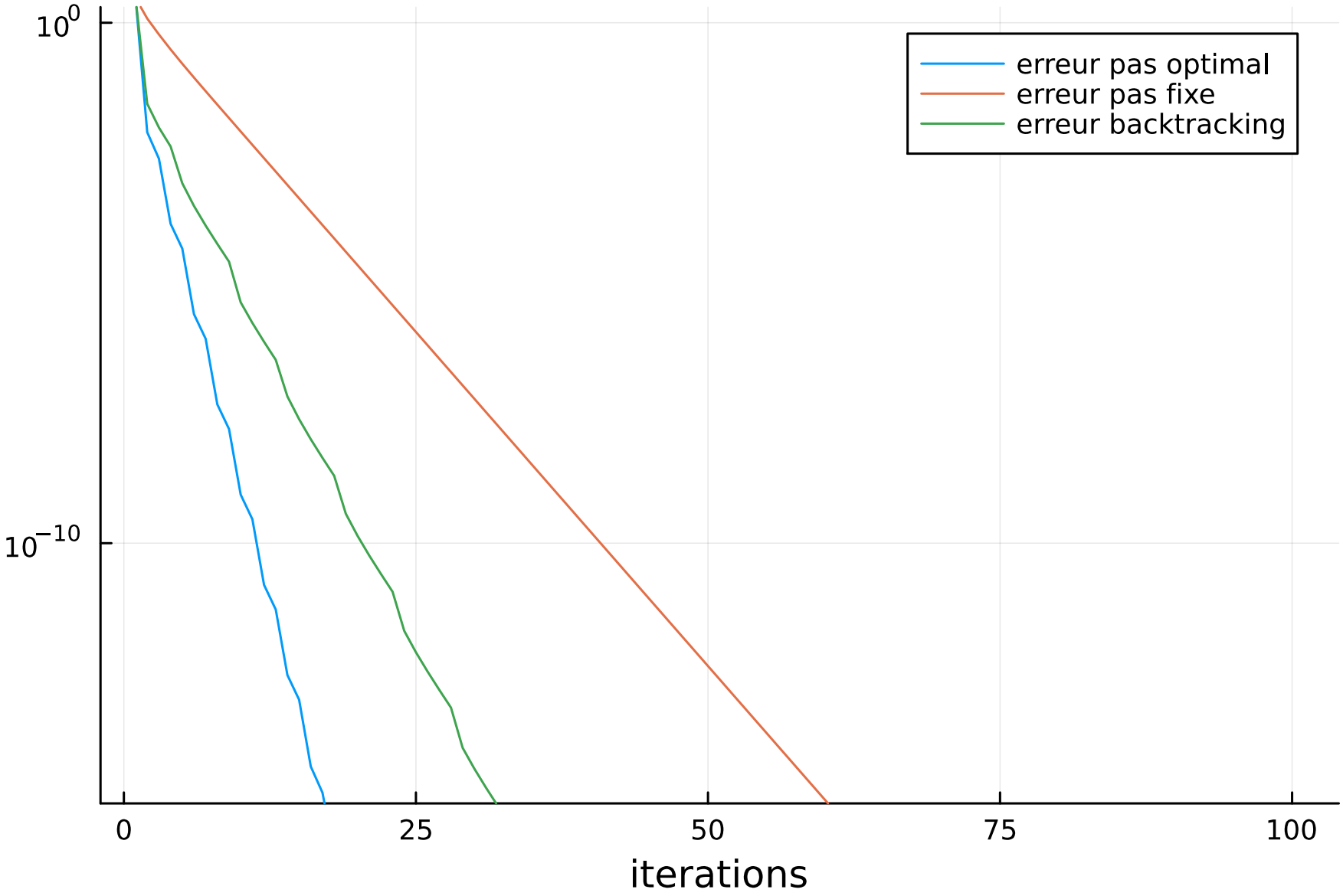


Outline

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:

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

Step-size selection strategies

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

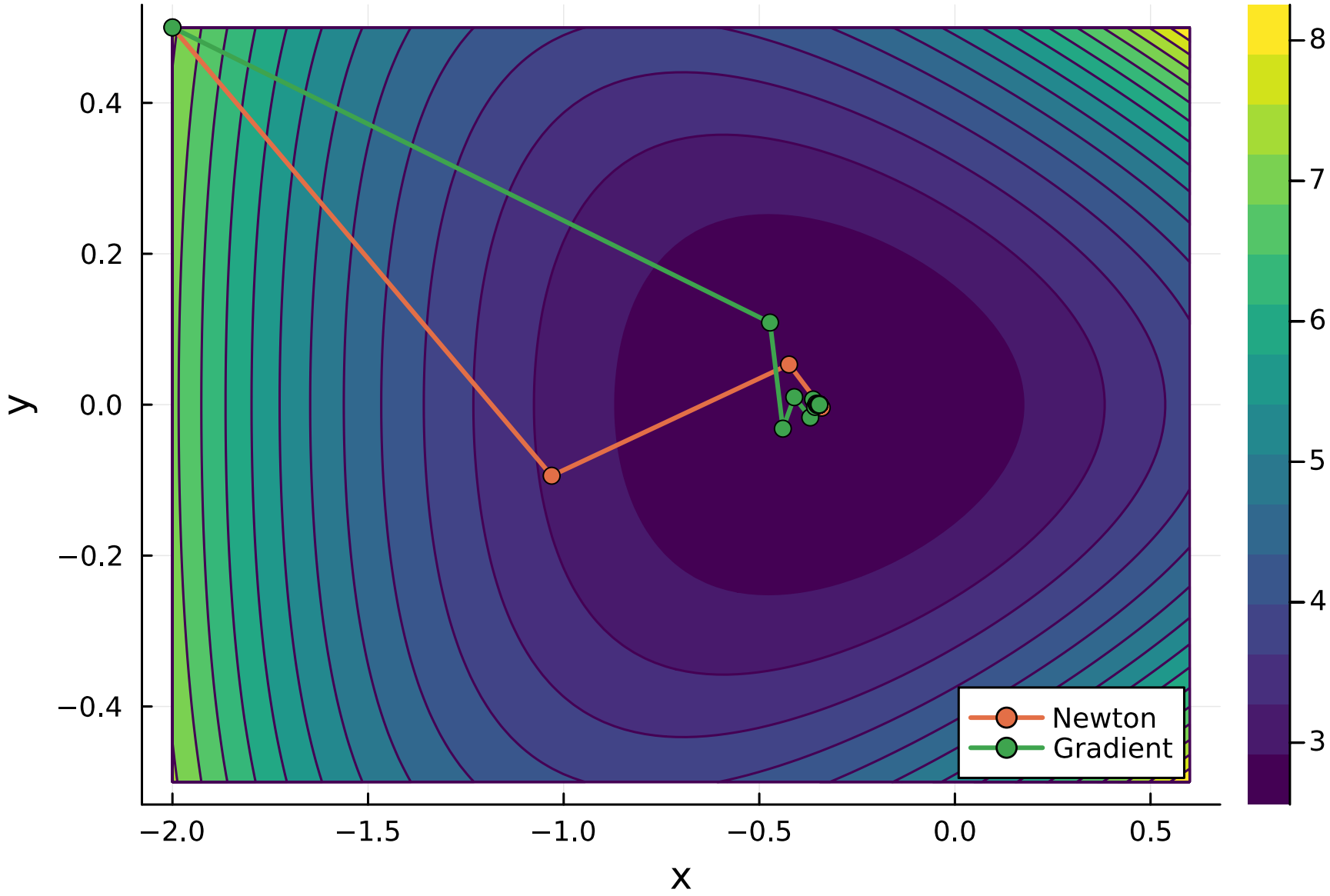
The return of the 2D unconstrained QP example

We consider the function

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

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
4. What can we deduce from this?

Example: Non-Quadratic Case



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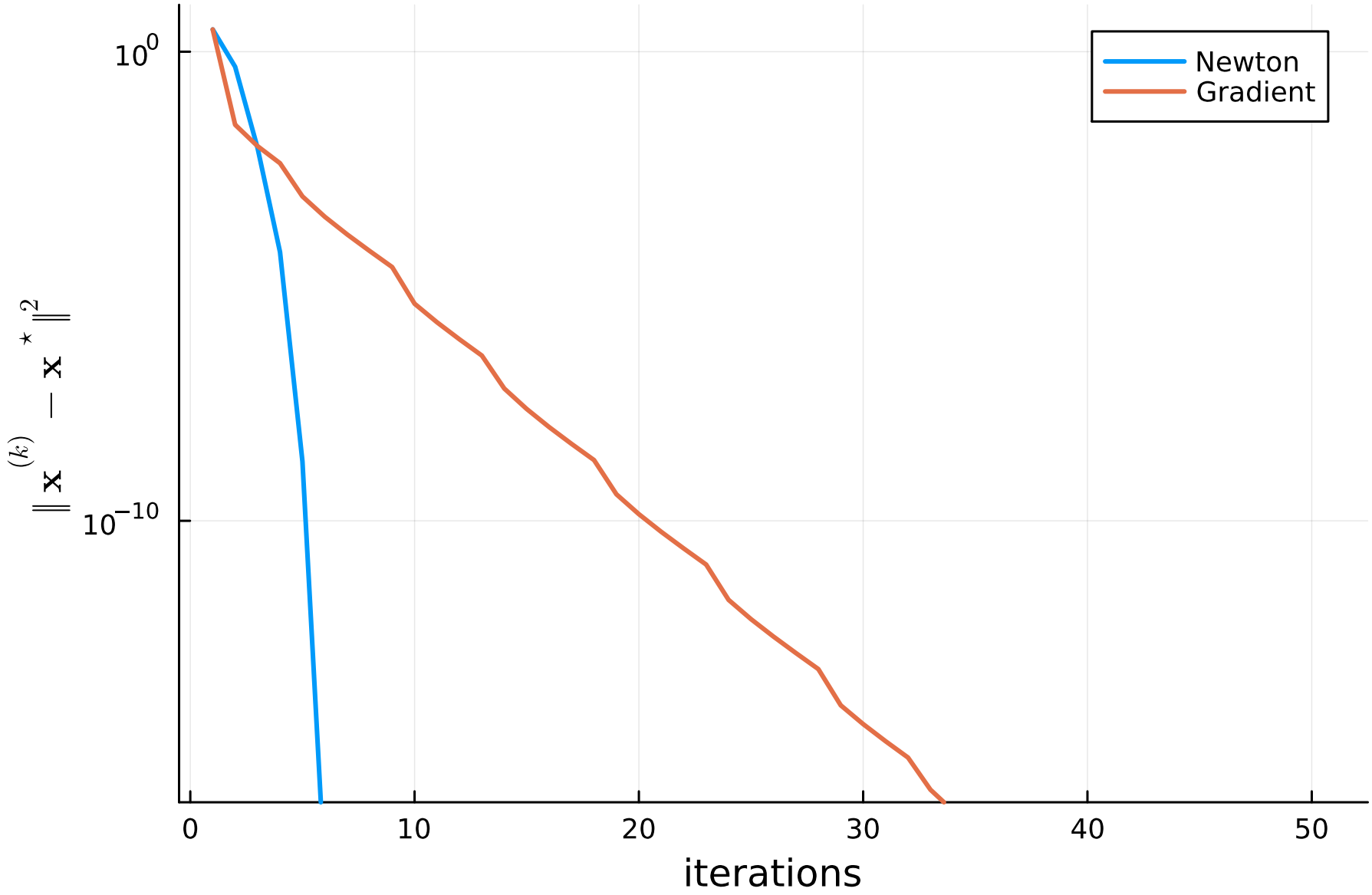


Outline

Motivation

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

- Computing Newton's step involves calculating and inverting the Hessian matrix $\nabla^2 f(\mathbf{x}^{(k)})$, 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

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

An update rule $\rightarrow$ 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

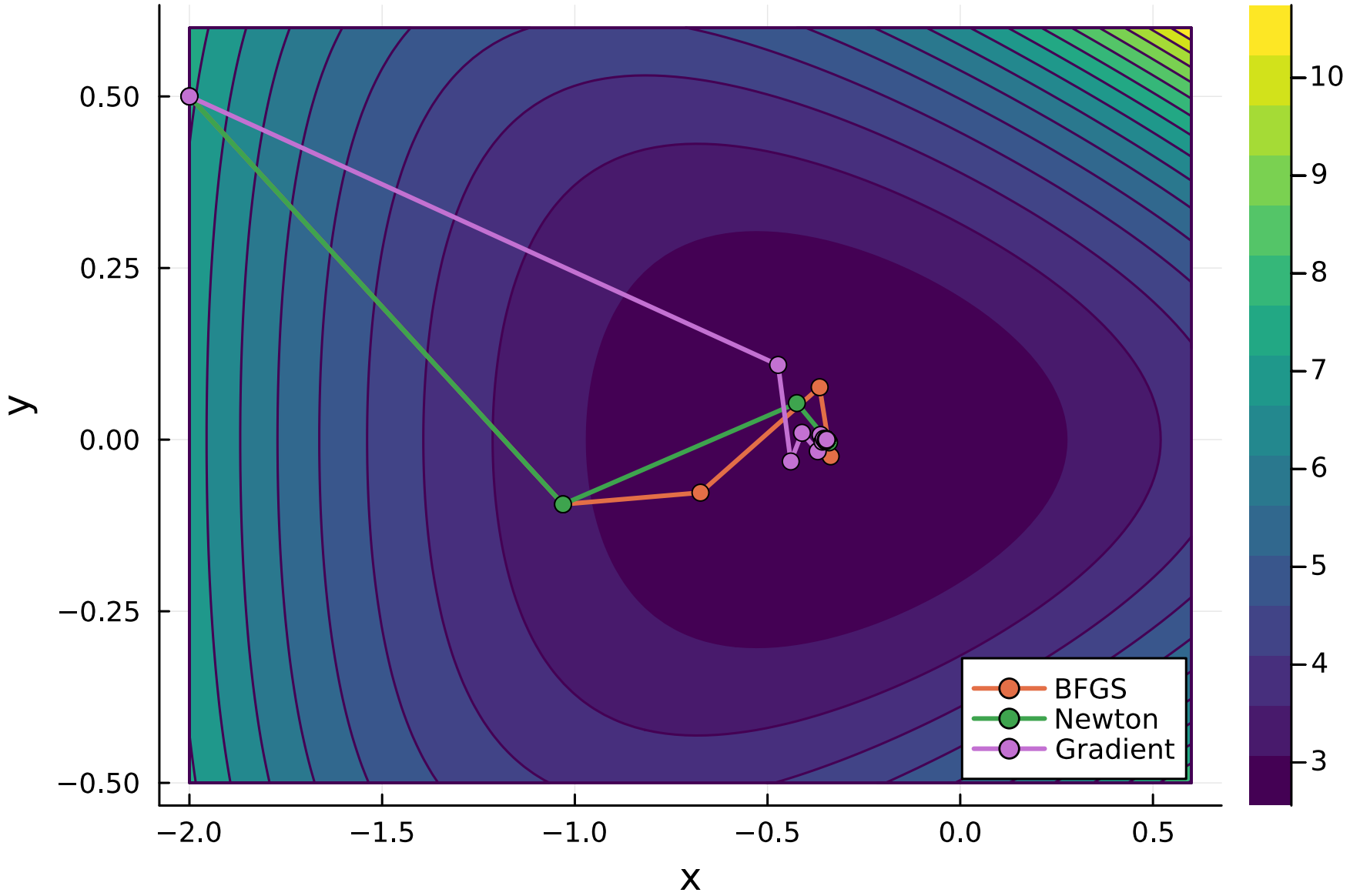
$$\mathbf{s}_k = -\alpha_k \mathbf{H}_k \nabla f(\mathbf{x}^{(k)}), \quad \mathbf{y}_k = \nabla f(\mathbf{x}^{(k+1)}) - \nabla f(\mathbf{x}^{(k)}), \quad \rho_k = \frac{1}{\mathbf{s}_k^\top \mathbf{y}_k}$$

Update of $\mathbf{H}_k$ in BFGS

$$\mathbf{H}_{k+1} = \left(\mathbf{I}_N - \rho_k \mathbf{s}_k \mathbf{y}_k^\top\right) \mathbf{H}_k \left(\mathbf{I}_N - \rho_k \mathbf{y}_k \mathbf{s}_k^\top\right) + \rho_k \mathbf{s}_k \mathbf{s}_k^\top$$

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

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



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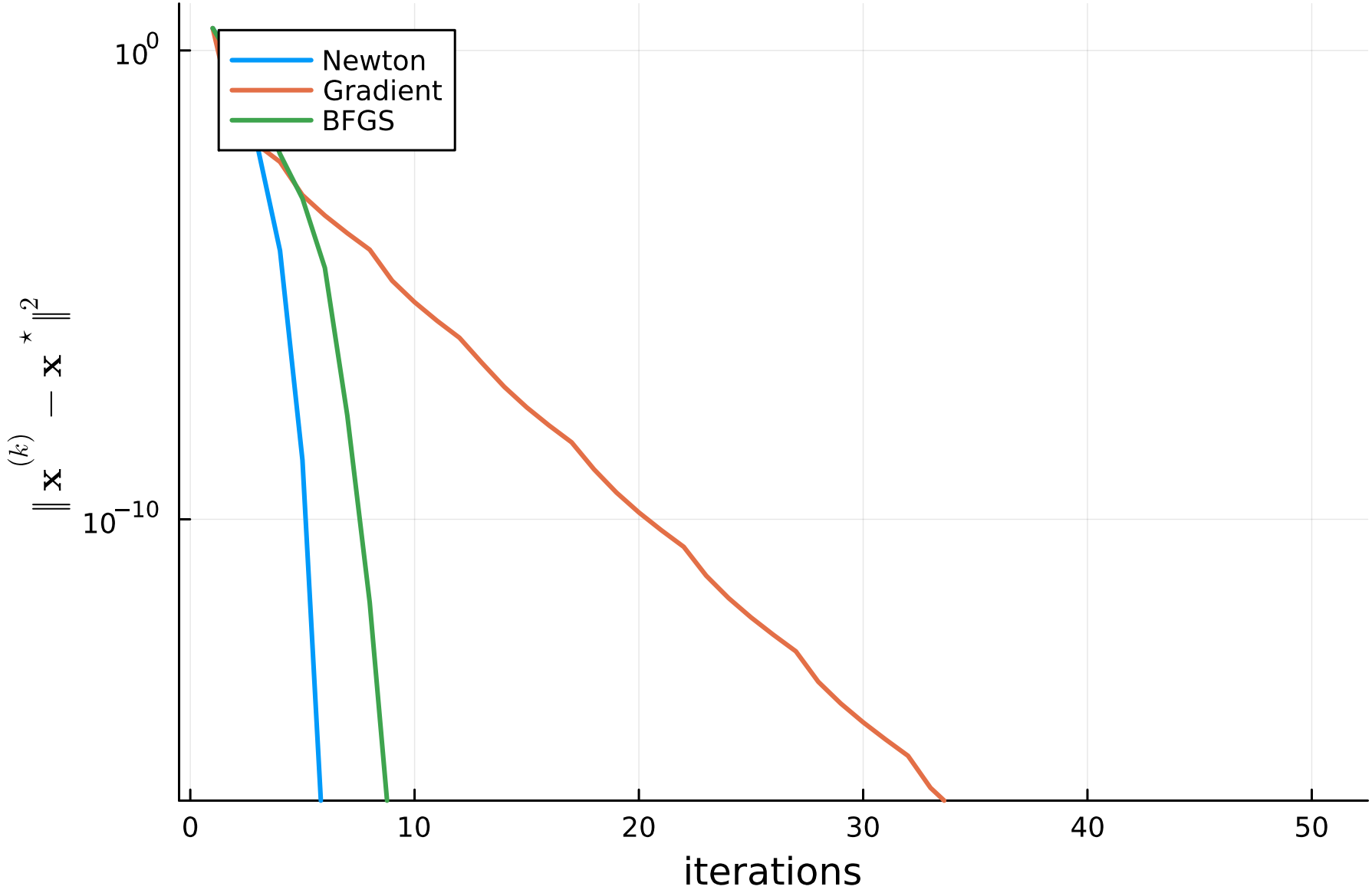

Outline

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

$$R(\mathbf{x}) = (r_1(\mathbf{x}), r_2(\mathbf{x}), \ldots, r_M(\mathbf{x}))^\top$$

We can rewrite the problem as

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

Remark

if $\mathbf{R}(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b}$, 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

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

Hessian of f

$$\begin{aligned}\nabla^2 f(\mathbf{x}) &= \sum_{j=1}^{M} \nabla r_j(\mathbf{x}) \nabla r_j(\mathbf{x})^\top + \sum_{j=1}^{M} r_j(\mathbf{x}) \nabla^2 r_j(\mathbf{x}) \\ &= \mathbf{J}(\mathbf{x})^\top \mathbf{J}(\mathbf{x}) + \sum_{j=1}^{M} r_j(\mathbf{x}) \nabla^2 r_j(\mathbf{x})\end{aligned}$$

Why is this interesting?

In many applications:

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

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

  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 $\mathbf{B}_k = \mathbf{J}(\mathbf{x}^{(k)})^\top \mathbf{J}(\mathbf{x}^{(k)})$

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

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

Levenberg-Marquardt Method

Can also be interpreted as a quasi-Newton method

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

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

where λ_k is a regularization parameter.

$\rightarrow$ Algorithm commonly used in practice for nonlinear least squares problems.

Outline

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

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

  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

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

- Linear convergence:

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

- Super-linear convergence:

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

- 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 $\mathbf{a}^\top \mathbf{b}$ with $\mathbf{a}, \mathbf{b} \in \mathbb{R}^N$ $\mathcal{O}(N)$ flops
- Matrix-vector product $\mathbf{Ab}$ 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

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

- 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

- 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

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!