Lecture 4: Unconstrained optimization algorithms

Michael Patriksson

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Method of choice

Consider the unconstrained optimization problem to

$$\underset{\mathbf{x}\in\mathbb{R}^n}{\text{minimize}}\ f(\mathbf{x}), \tag{1}$$

where $f \in C^0$ on $\mathbb{R}^n$ (f is continuous). Mostly, we assume that $f \in C^1$ holds (f is continuously differentiable), sometimes even C^2

- Size of the problem (n)?
- Are $\nabla f(\mathbf{x})$ and/or $\nabla^2 f(\mathbf{x})$ available; to what cost?
- What it is the goal? (Global/local minimum, stationary point?)
- What are the convexity properties of f?
- Do we have a good estimate of the location of a stationary point $\mathbf{x}^*$? (Can we use locally-only convergent methods?)

Example: curve fitting by least-squares

- Suppose we have m data points (t_i, b_i) believed to be related as

$$x_1 + x_2 \exp(x_3 t_i) + x_4 \exp(x_5 t_i) = b_i, \qquad i = 1, \ldots, m,$$

with unknown parameters $x_1, \ldots, x_5$. (Here, $\exp(x) = \mathrm{e}^x$.)
The best description minimizes the total "residual error," given by the norm of the residual

$$f_i(\mathbf{x}) := b_i - [x_1 + x_2 \exp(x_3 t_i) + x_4 \exp(x_5 t_i)], \qquad i = 1, \ldots, m$$

- Resulting optimization problem:

$$\min_{\mathbf{x} \in \mathbb{R}^5} f(\mathbf{x}) := \sum_{i=1}^{m} |f_i(\mathbf{x})|^2 = \sum_{i=1}^{m} (b_i - [x_1 + x_2 \exp(x_3 t_i) + x_4 \exp(x_5 t_i)])^2$$

- Very often solved problem type within numerical analysis and mathematical statistics

Typical algorithm

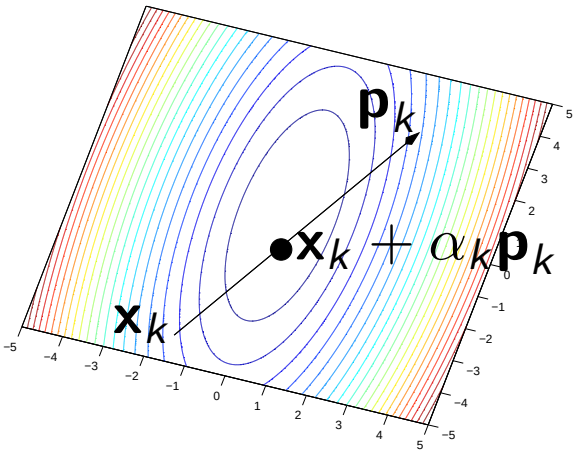
Step 0. *Starting point*: $\mathbf{x}_0 \in \mathbb{R}^n$. Set $k := 0$

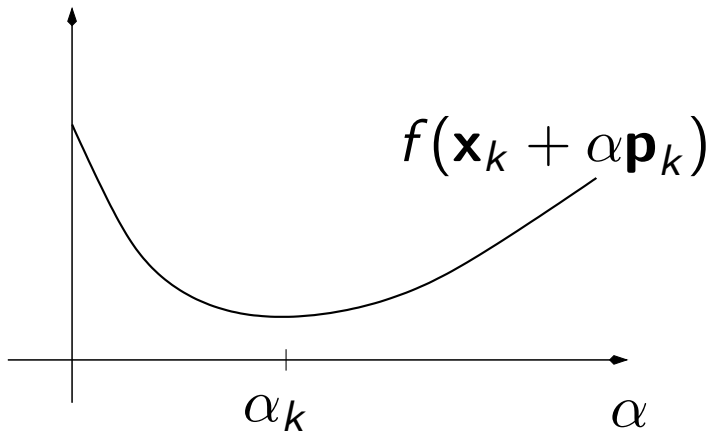
Step 1. *Search direction*: $\mathbf{p}_k \in \mathbb{R}^n$

Step 2. *Step length*: $\alpha_k > 0$ such that $f(\mathbf{x}_k + \alpha_k \mathbf{p}_k) < f(\mathbf{x}_k)$ holds

Step 3. Let $\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{p}_k$

Step 4. *Termination criterion*: If fulfilled, then stop! Otherwise, let $k := k + 1$ and go to step 1





Notes

- The figure was plotted using several thousands of function evaluations
- Never possible in reality! (And total waste of time)
- An "orienteering map" never exists
- Most algorithms are inherently *local*, only based on info at the current point $\mathbf{x}_k$, that is, $f(\mathbf{x}_k)$, $\nabla f(\mathbf{x}_k)$, and $\nabla^2 f(\mathbf{x}_k)$
- Possibly also on previous points passed
- An algorithm is a "near-sighted mountain climber" when trying to reach the summit (for a max problem!)
- The mountain climber is in a deep fog and can only check her barometer for the height and feel the steepness of the slope under her feet

Step 1: Search directions

- If $\nabla f(\mathbf{x}_k) \neq \mathbf{0}^n$, then $\mathbf{p} = -\nabla f(\mathbf{x}_k)$ is a descent direction for f at $\mathbf{x}_k$ (Part of necessary condition proof!)
- This *steepest descent direction* solves the problem to

$$\underset{\mathbf{p}\in\mathbb{R}^n:\|\mathbf{p}\|=1}{\text{minimize}} \ \nabla f(\mathbf{x}_k)^{\mathrm{T}}\mathbf{p}$$

- Suppose $\mathbf{Q} \in \mathbb{R}^{n\times n}$ is a symmetric, positive definite matrix. Then $\mathbf{p} = -\mathbf{Q}\nabla f(\mathbf{x}_k)$ is a descent direction for f at $\mathbf{x}_k$, because

$$\nabla f(\mathbf{x}_k)^{\mathrm{T}}\mathbf{p} = -\nabla f(\mathbf{x}_k)^{\mathrm{T}}\mathbf{Q}\nabla f(\mathbf{x}_k) < 0,$$

  due to the positive definiteness of $\mathbf{Q}$
- Special case: $\mathbf{Q} = \mathbf{I}^n$ yields steepest descent
- Special case: $\mathbf{Q}^{-1} = \nabla^2 f(\mathbf{x}_k)$, if the Hessian is positive definite. This is *Newton's method*

*Additional requirements

- Purpose: prevent the descent directions to deteriorate in quality, and prevent premature convergence
- Practical criteria:

$$|\nabla f(\mathbf{x}_k)^{\mathrm{T}}\mathbf{p}_k| \geq s_1\|\nabla f(\mathbf{x}_k)\|^2, \qquad \text{and} \quad \|\mathbf{p}_k\| \leq s_2\|\nabla f(\mathbf{x}_k)\|,$$

or

$$-\frac{\nabla f(\mathbf{x}_k)^{\mathrm{T}}\mathbf{p}_k}{\|\nabla f(\mathbf{x}_k)\| \cdot \|\mathbf{p}_k\|} \geq s_1, \qquad \text{and} \quad \|\mathbf{p}_k\| \geq s_2\|\nabla f(\mathbf{x}_k)\|$$

- Interpretations: $\nabla f(\mathbf{x}_k)^{\mathrm{T}}\mathbf{p}_k$ is the directional derivative of f at $\mathbf{x}_k$ in the direction of $\mathbf{p}_k$. Make sure it stays away from zero!
- Also, make sure that $\mathbf{p}_k$ stays bounded and that it tends to zero if and only if $\nabla f(\mathbf{x}_k)$ does
- These conditions hold for the above examples

Newton's method

- Steepest descent is most often *not* a very good algorithm. Why?
- It fails to take into account more than information about ∇f
- A second-order Taylor approximation:

$$f(\mathbf{x}+\mathbf{p}) - f(\mathbf{x}) \approx \varphi_{\mathbf{x}}(\mathbf{p}) := \nabla f(\mathbf{x})^{\mathrm{T}}\mathbf{p} + \frac{1}{2}\mathbf{p}^{\mathrm{T}}\nabla^2 f(\mathbf{x})\mathbf{p}$$

Minimize $\varphi_{\mathbf{x}}$ over $\mathbf{p}$ by setting the gradient of $\varphi_{\mathbf{x}}(\mathbf{p})$ to zero:

$$\nabla_{\mathbf{p}}\varphi_{\mathbf{x}}(\mathbf{p}) = \nabla f(\mathbf{x}) + \nabla^2 f(\mathbf{x})\mathbf{p} = \mathbf{0}^n \iff \nabla^2 f(\mathbf{x})\mathbf{p} = -\nabla f(\mathbf{x})$$

- $n = 1$: $f'(x) + f''(x)p = 0 \implies p = -f'(x)/f''(x)$
- Provides descent if $f''(x) > 0$: $f'(x)p = -[f'(x)]^2/f''(x) < 0$
- Corresponding story in $\mathbb{R}^n$: $\mathbf{p} = -[\nabla^2 f(\mathbf{x})]^{-1}\nabla f(\mathbf{x})$, yields descent at non-stationary points if $\nabla^2 f(\mathbf{x})$ is positive definite!

Why do we not always choose Newton directions? I

- **Lack of positive definiteness.** $\nabla^2 f(\mathbf{x})$ is not positive definite (PD) (that is, some eigenvalue(s) is/are negative)
- Solution: add diagonal matrix so that the result is PD: if λ is an eigenvalue of $\nabla^2 f(\mathbf{x})$ then for any $\gamma \in \mathbb{R}$, $\lambda + \gamma$ is an eigenvalue of $\nabla^2 f(\mathbf{x}) + \gamma \mathbf{I}^n$; choose γ large enough to make $\lambda + \gamma > 0$ for all eigenvalues λ
- Note: If the value of γ is very large $\Longrightarrow$ direction $\approx$ steepest descent
- Name: *Levenberg–Marquardt*

Why do we not always choose Newton directions? II

- **Lack of enough differentiability.** If $f \notin C^2$, what do we do?
- $n = 1$: the *secant method*:

$$f''(x_k) \approx \frac{f'(x_k) - f'(x_{k-1})}{x_k - x_{k-1}}$$

- $n > 1$: *quasi-Newton*: choose approximate matrix $\mathbf{B}_k$ so that

$$\mathbf{B}_k(\mathbf{x}_k - \mathbf{x}_{k-1}) = \nabla f(\mathbf{x}_k) - \nabla f(\mathbf{x}_{k-1}),$$

$+$ additional choices (the above does not specify the entire matrix $\mathbf{B}_k$!), so that, for example, $\mathbf{B}_{k+1}$ can be computed easily from $\mathbf{B}_k$, and so that $\mathbf{B}_k$ is symmetric and positive definite

Why do we not always choose Newton directions? III

- **Computational burden.** It may be too much to ask for to solve a linear system many times when $n > 1000$ or so; it is enough to do *some* work on the linear system and still get a descent property. (See The Book, p. 275 for an example)

- There are many specific choices of matrices $\mathbf{B}_k$ that lead to a variety of *quasi-Newton* methods

Step 2: Line search

- Approximately solve the one-dimensional problem to

$$\underset{\alpha \geq 0}{\text{minimize}}\ \varphi(\alpha) := f(\mathbf{x}_k + \alpha \mathbf{p}_k)$$

Its optimality conditions are that

$$\varphi'(\alpha^*) \geq 0, \qquad \alpha^* \cdot \varphi'(\alpha^*) = 0, \qquad \alpha^* \geq 0,$$

that is,

$$\nabla f(\mathbf{x}_k + \alpha^* \mathbf{p}_k)^{\mathrm{T}} \mathbf{p}_k \geq 0, \quad \alpha^* \cdot \nabla f(\mathbf{x}_k + \alpha^* \mathbf{p}_k)^{\mathrm{T}} \mathbf{p}_k = 0, \quad \alpha^* \geq 0,$$

holds

- If $\alpha^* > 0$, then $\varphi'(\alpha^*) = 0$ holds $\Longrightarrow \nabla f(\mathbf{x}_k + \alpha^* \mathbf{p}_k)^{\mathrm{T}} \mathbf{p}_k = 0$
- The search direction $\mathbf{p}_k$ then is orthogonal to the gradient of f at the point $\mathbf{x}_k + \alpha^* \mathbf{p}_k$

Step 2: An illustration

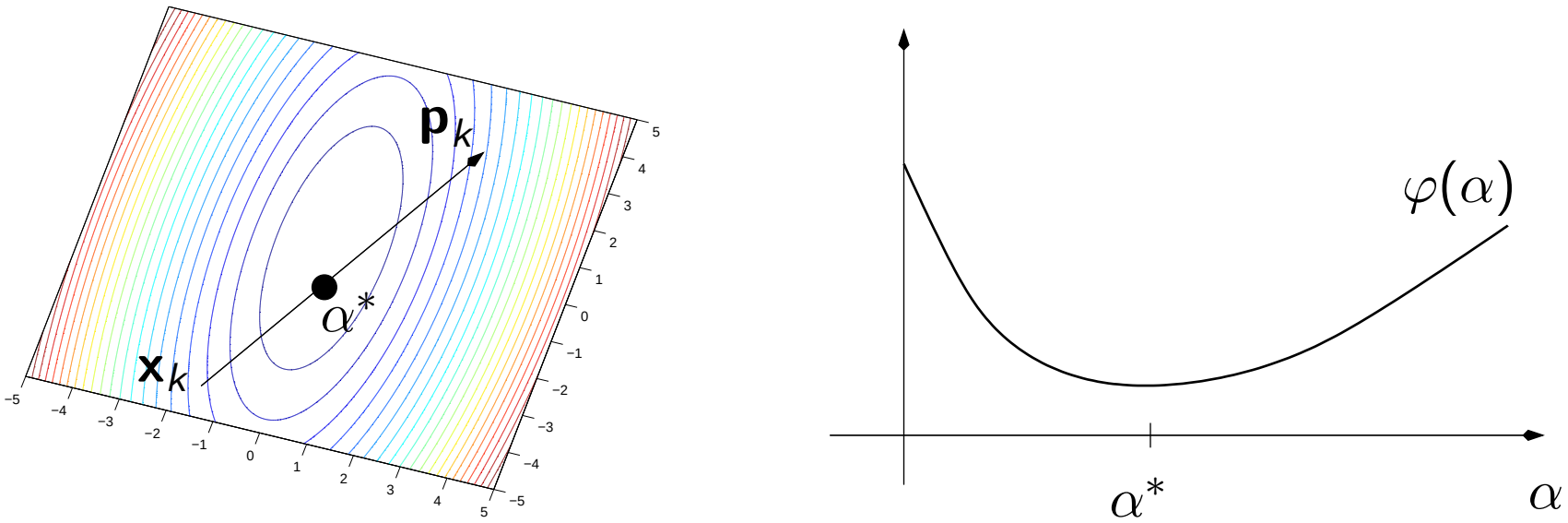


Figure: A line search in a descent direction

Approximate line search

- No point solving the one-dimensional problem exactly! Why? The optimum to the entire problem lies elsewhere!
- *Interpolation*: Use $f(\mathbf{x}_k), \nabla f(\mathbf{x}_k), \nabla f(\mathbf{x}_k)^{\mathrm{T}}\mathbf{p}_k$ to model a quadratic function approximating f along $\mathbf{p}_k$. Minimize it by using the analytic formula for quadratics
- *Newton's method*: Repeat the improvements gained from a quadratic approximation: $\alpha := \alpha - \varphi'(\alpha)/\varphi''(\alpha)$
- *Golden section*: Derivative-free method that shrinks an interval wherein a solution to $\varphi'(\alpha) = 0$ lies

Armijo rule, I

- Idea: quickly generate a step α which provides "sufficient" decrease in f. Note: $f(\mathbf{x}_k + \alpha \mathbf{p}_k) \approx f(\mathbf{x}_k) + \alpha \cdot \nabla f(\mathbf{x}_k)^{\mathrm{T}} \mathbf{p}_k$, valid for small values of $\alpha > 0$
- Requirement: we get a decrease in f which is at least a *fraction* of that predicted in the right-hand side above. Let $\mu \in (0, 1)$ be this fraction. Acceptable step lengths are $\alpha > 0$ satisfying

$$\varphi(\alpha) - \varphi(0) \leq \mu \alpha \varphi'(0), \tag{2a}$$

that is,

$$f(\mathbf{x}_k + \alpha \mathbf{p}_k) - f(\mathbf{x}_k) \leq \mu \alpha \nabla f(\mathbf{x}_k) \mathbf{p}_k \tag{2b}$$

Armijo rule, II

- Can add condition making α also large enough (*Wolfe*)

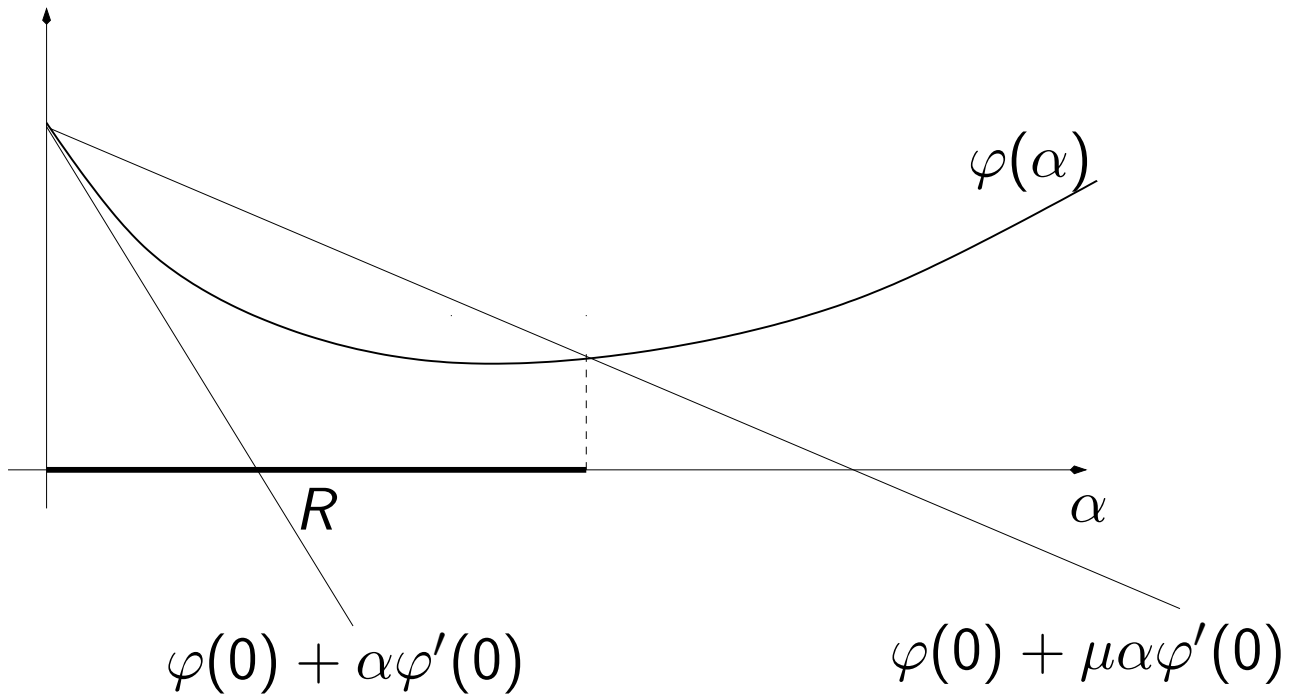


Figure: The interval (R) accepted by the Armijo step length rule

*Typical convergence result

- *Suppose $f \in C^1$, and for the starting point $\mathbf{x}_0$ the level set $\operatorname{lev}_f(f(\mathbf{x}_0)) = \{\mathbf{x} \in \mathbb{R}^n \mid f(\mathbf{x}) \leq f(\mathbf{x}_0)\}$ is bounded. Consider the iterative algorithm, with the following choices for each k:*
  - *$\mathbf{p}_k$ satisfies the second sufficient descent condition (see *-slide above);*
  - *$\|\mathbf{p}_k\| \leq M$, where M is some positive constant; and*
  - *the Armijo step length rule is used*

  Then, the sequence $\{\mathbf{x}_k\}$ is bounded, the sequence $\{f(\mathbf{x}_k)\}$ is descending, lower bounded and therefore converges, and every limit point of $\{\mathbf{x}_k\}$ is stationary
- For convex f much stronger convergence properties:

  Optimum exists $\iff$ $\{\mathbf{x}_k\}$ converges to an optimal solution

  (Theorem established later for a more general algorithm)

Step 4: Termination criteria

- Lesson 1: Cannot terminate based on the exact optimality conditions, because $\nabla f(\mathbf{x}) = \mathbf{0}^n$ rarely happens!
- Recommended:
  1. $\|\nabla f(\mathbf{x}_k)\| \leq \varepsilon_1(1 + |f(\mathbf{x}_k)|)$, $\varepsilon_1 > 0$ small;
  2. $f(\mathbf{x}_{k-1}) - f(\mathbf{x}_k) \leq \varepsilon_2(1 + |f(\mathbf{x}_k)|)$, $\varepsilon_2 > 0$ small; and
  3. $\|\mathbf{x}_{k-1} - \mathbf{x}_k\| \leq \varepsilon_3(1 + \|\mathbf{x}_k\|)$, $\varepsilon_3 > 0$ small
- Why? Need to cover cases of very steep and very flat functions
- May need to use ∞-*norm*: $\|\mathbf{x}\|_\infty := \max_{1 \leq j \leq n} |x_j|$, for large n
- Problem with the scaling of the problem: If

$$\mathbf{x}_{k-1} = (56.8894238, 0.045278842, 0.0000001798781)^{\mathrm{T}},$$
$$\mathbf{x}_k = (56.8897234, 0.045267545, 0.0000004629675)^{\mathrm{T}};$$
$$\|\mathbf{x}_{k-1} - \mathbf{x}_k\|_\infty = \|(-0.0002996, 0.000011297, -0.0000002830894)^{\mathrm{T}}\|_\infty = 0.0002996$$

- Small absolute error but large relative error!

Why is the C^1 property important? I

- Suppose f is only in C^0, not C^1. Example:

$$f(\mathbf{x}) := \underset{i \in \{1,\ldots,m\}}{\text{maximum}} \{\mathbf{c}_i^{\mathrm{T}} \mathbf{x} + b_i\}, \qquad \mathbf{x} \in \mathbb{R}^n$$

- This is a piece-wise linear and convex function (see next page)
- It is differentiable almost everywhere, but *not* at the optimal solution!
- Ignoring non-differentiability may lead to the convergence to a non-optimal point. In other words, methods for minimizing non-differentiable function cannot only rely on gradient values
- Convex functions always has *subgradients*, corresponding to all the possible slopes of the function
- For more on subgradients and their use in algorithms, see Chapter 6 on Lagrangian duality!

Why is the C^1 property important? II

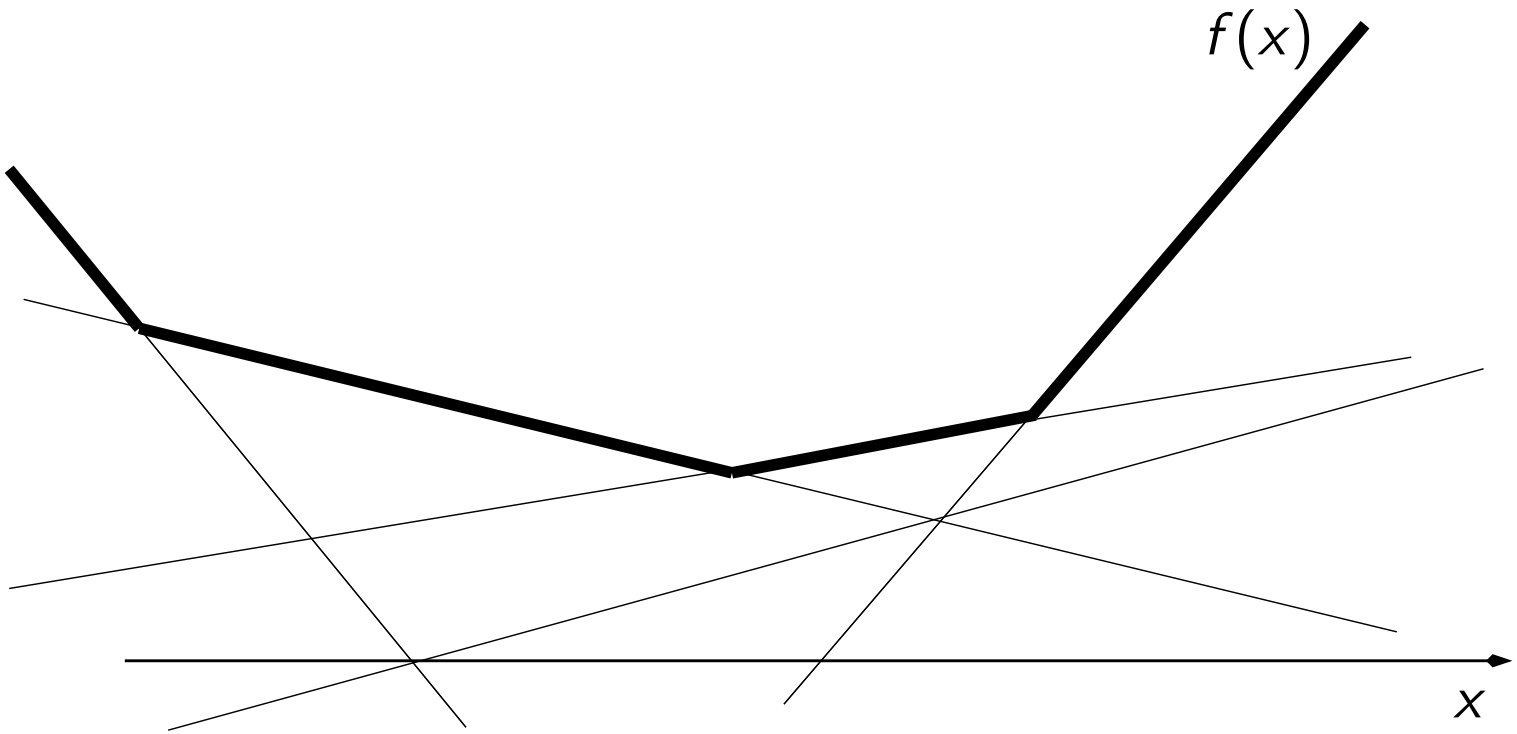
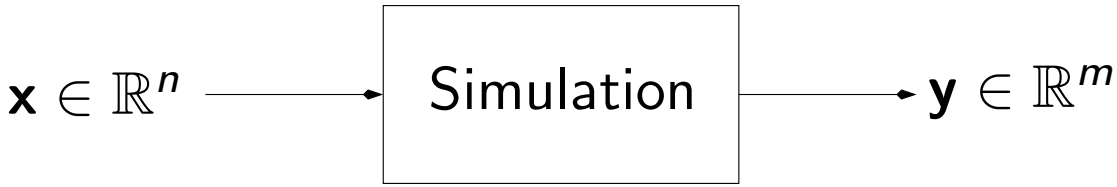


Figure: A piece-wise linear convex function

Minimizing implicit functions, I

- Common in engineering and natural science applications that f is not explicitly given but through a simulation:



- The wish is to minimize a function of both $\mathbf{x}$ and $\mathbf{y}$: $f(\mathbf{x}, \mathbf{y})$; find the vector $\mathbf{x}$ that gives the best *response* $\mathbf{y}$ for f
- The form of the response $\mathbf{y} = \mathbf{y}(\mathbf{x})$ from the input $\mathbf{x}$ is normally unknown
- Cannot differentiate $\mathbf{x} \mapsto f(\mathbf{x}, \mathbf{y}(\mathbf{x}))$
- Two distinct possibilities!

Minimizing implicit functions, II

- (1) *Numerical differentiation* of f by using a difference formula:
- Let $\mathbf{e}_i = (0, 0, \ldots, 0, 1, 0, \ldots, 0)^{\mathrm{T}}$ be the unit vector in $\mathbb{R}^n$. Then,

$$\begin{aligned} f(\mathbf{x} + \alpha \mathbf{e}_i) &= f(\mathbf{x}) + \alpha \mathbf{e}_i^{\mathrm{T}} \nabla f(\mathbf{x}) + (\alpha^2/2) \mathbf{e}_i^{\mathrm{T}} \nabla^2 f(\mathbf{x}) \mathbf{e}_i + \ldots \\ &= f(\mathbf{x}) + \alpha \partial f(\mathbf{x}) / \partial x_i + (\alpha^2/2) \partial^2 f(\mathbf{x}) / \partial x_i^2 + \ldots \end{aligned}$$

- So, for small $\alpha > 0$,

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \frac{f(\mathbf{x} + \alpha \mathbf{e}_i) - f(\mathbf{x})}{\alpha} \quad \text{(forward difference)}$$

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \frac{f(\mathbf{x} + \alpha \mathbf{e}_i) - f(\mathbf{x} - \alpha \mathbf{e}_i)}{2\alpha} \quad \text{(central difference)}$$

Minimizing implicit functions, III

- Value of α typically set to a function of the machine precision; too large $\longrightarrow$ bad approximation of the partial derivative; too small $\longrightarrow$ numerical cancellation
- May work well *if* the simulation is *accurate*, otherwise bad derivative information. Requires *cheap* simulations!
- (2) *Derivative-free methods* are available. (Not counting subgradient methods, because they demand f to be convex!) Either builds explicit *models* $\hat{f}$ of the objective function from evaluations of f at test points, or evaluates f at grid points that are moved around, shrunk or expanded. *Names and terms: Nelder–Mead, Pattern search, surrogate models, radial basis functions, . . .*
- Check hand-out!

Methods based on interpolating/approximating f

- Alternative: create explicit algebraic (e.g., polynomial) model $\tilde{f}$ based on visited points $\mathbf{x}_k$; solve this problem with gradient methods; evaluate its optimum in the real problem (i.e., perform a simulation); update $\tilde{f}$ with the new information $\Longrightarrow$ minimizes the number of simulations!
- Recent application: diesel engine optimization for Volvo Powertrain and Volvo Car Corporation
- Optimize fuel consumption, keep soot/nitrogen emissions at an acceptable level
- Simulations hard (42 hours each) and response contains noise
- New method developed based on approximate (surrogate) models