MVE165/MMG630, Applied Optimization
Lecture 12
Unconstrained non-linear programming algorithms and the KKT conditions

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Contents, lectures 11–13

Solution methods for unconstrained optimization

- General iterative search method:
  1. Choose a starting solution, $\mathbf{x}^0 \in \Re^n$. Let $k = 0$
  2. Determine a seach direction $\mathbf{d}^k$
  3. Determine a step length, t_k, by solving:
  $$\min_{t \geq 0} \varphi(t) := f(\mathbf{x}^k + t \cdot \mathbf{d}^k)$$
  4. New iteration point, $\mathbf{x}^{k+1} = \mathbf{x}^k + t_k \cdot \mathbf{d}^k$
  5. If a termination criterion is fulfilled $\Rightarrow$ Stop!
     Otherwise: let $k := k + 1$ and return to step 2
- How choosing the search direction $\mathbf{d}^k$, the step length t_k, and the termination criterion?

Solution methods for unconstrained optimization

- General iterative search method:
  1. Choose a starting solution, $\mathbf{x}^0 \in \Re^n$. Let $k = 0$
  2. **Determine a seach direction $\mathbf{d}^k$**
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Search direction

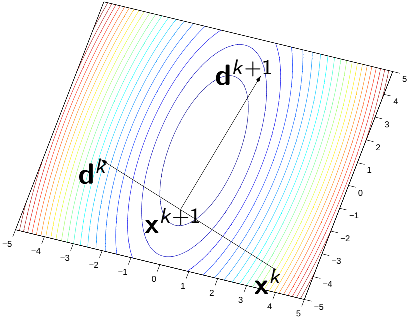
- Goal: $f(\mathbf{x}^{k+1}) < f(\mathbf{x}^k)$
- How does f change locally in a direction $\mathbf{d}^k$ at $\mathbf{x}^k$?
- Taylor expansion: $f(\mathbf{x}^k + t\mathbf{d}^k) = f(\mathbf{x}^k) + t\nabla f(\mathbf{x}^k)^{\mathrm{T}}\mathbf{d}^k + \mathcal{O}(t^2)$
- For sufficiently small $t > 0$:
  $\nabla f(\mathbf{x}^k)^{\mathrm{T}}\mathbf{d}^k < 0 \Rightarrow f(\mathbf{x}^k + t\mathbf{d}^k) < f(\mathbf{x}^k)$

$\Rightarrow$ **Definition:**
If $\nabla f(\mathbf{x}^k)^{\mathrm{T}}\mathbf{d}^k < 0$ then $\mathbf{d}^k$ is a descent direction for f at $\mathbf{x}^k$
If $\nabla f(\mathbf{x}^k)^{\mathrm{T}}\mathbf{d}^k > 0$ then $\mathbf{d}^k$ is an ascent direction for f at $\mathbf{x}^k$

- We wish to minimize (maximize) f over $\Re^n$:

$\Rightarrow$ Choose $\mathbf{d}^k$ as a descent (an ascent) direction from $\mathbf{x}^k$

An improving step



Figur: At $\mathbf{x}^k$, the descent direction $\mathbf{d}^k$ is generated. A step t_k is taken in this direction, producing $\mathbf{x}^{k+1}$. At this point, a new descent direction $\mathbf{d}^{k+1}$ is generated, and so on.

Solution methods for unconstrained optimization

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  3. **Determine a step length**, t_k, by solving:

$$\min_{t \geq 0} \varphi(t) := f(\mathbf{x}^k + t \cdot \mathbf{d}^k)$$

  4. New iteration point, $\mathbf{x}^{k+1} = \mathbf{x}^k + t_k \cdot \mathbf{d}^k$
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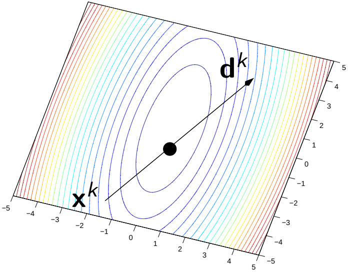
Step length—line search (minimization)

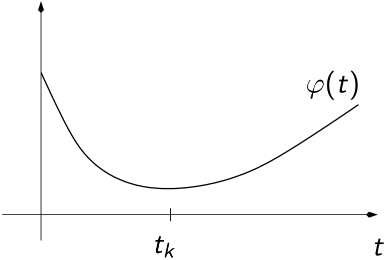
- Solve $\min_{t \geq 0} \varphi(t) := f(\mathbf{x}^k + t \cdot \mathbf{d}^k)$ where $\mathbf{d}^k$ is a descent direction from $\mathbf{x}^k$
- A minimization problem in one variable

$\Rightarrow$ Solution t_k

- Analytic solution: $\varphi'(t_k) = 0$
- Solution methods: e.g., Golden section method (reduce the interval of uncertainty, Chapter 13.2), Armijo's method (not in the book)
- In practice: Do not solve exactly, but to sufficient improvement of the function value: $f(\mathbf{x}^k + t_k \mathbf{d}^k) \leq f(\mathbf{x}^k) - \varepsilon$ for some $\varepsilon > 0$

Line search





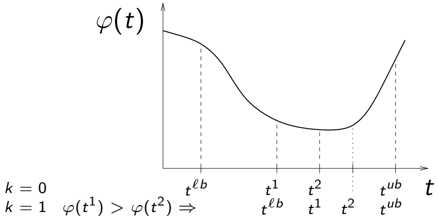
Figur: A line search in a descent direction.
t_k solves $\min_{t \geq 0} \varphi(t) := f(\mathbf{x}^k + t \cdot \mathbf{d}^k)$

Line search—the Golden section method

Based on narrowing down the interval in which t^* can lie

1. Let $t^{\ell b}$ be a lower bound on t^* (e.g. $= 0$) and t^{ub} be an upper bound on t^*
2. Choose $t^1 = t^{ub} - \alpha(t^{ub} - t^{\ell b})$, $t^2 = t^{\ell b} + \alpha(t^{ub} - t^{\ell b})$ where $\alpha \approx 0.618$ (the (inverted) golden ratio)
3. Evaluate $\varphi(t^1)$, $\varphi(t^2)$ and replace $t^{\ell b}$ or t^{ub} with t^1 or t^2
4. Terminate or return to 2.

$\Rightarrow$ whichever of $[t^{\ell b}, t^2]$ or $[t^1, t^{ub}]$ provides the next interval, its size will be α times the current



Solution methods for unconstrained optimization

- General iterative search method:
  1. Choose a starting solution, $\mathbf{x}^0 \in \Re^n$. Let $k = 0$
  2. Determine a seach direction $\mathbf{d}^k$
  3. Determine a step length, t_k, by solving:

     $$\min_{t \geq 0} \varphi(t) := f(\mathbf{x}^k + t \cdot \mathbf{d}^k)$$

  4. New iteration point, $\mathbf{x}^{k+1} = \mathbf{x}^k + t_k \cdot \mathbf{d}^k$
  5. If a **termination criterion** is fulfilled $\Rightarrow$ Stop!
     Otherwise: let $k := k + 1$ and return to step 2

Termination criteria

- Needed since $\nabla f(\mathbf{x}^k) = \mathbf{0}$ will never be fulfilled exactly
- Typical choices, where $\varepsilon_j > 0$, $j = 1, \dots, 4$
  (a) $\|\nabla f(\mathbf{x}^k)\| < \varepsilon_1$
  (b) $|f(\mathbf{x}^{k+1}) - f(\mathbf{x}^k)| < \varepsilon_2$
  (c) $\|\mathbf{x}^{k+1} - \mathbf{x}^k\| < \varepsilon_3$
- Often used in combination
- The search method only guarantees a stationary solution, whose character is determined by the properties of f (convexity, ...)

Common special cases of search methods - SD

- **Steepest ascent (descent)** (*or Gradient search*)
  Let the search direction be (minus) the gradient:

  $$\mathbf{d}^k = +/-\nabla f(\mathbf{x}^k) \qquad\qquad (\text{max/min})$$

  PROS:
  - Requires only gradient information
  - Not so computationally demanding per iteration

  CONS:
  - (Very) Slow convergence towards a stationary point
  - Each direction $\mathbf{d}^k$ is perpendicular to the previous one $\mathbf{d}^{k-1}$ (if the line search is solved exactly)—the iterate sequence is zig-zagging

Common special cases of search methods - Newton

- **Newton's method**: Make use of second derivative information (curvature). Requires that f is twice continuously differentiable.
  - Taylor expansion of f around $\mathbf{x}$:
    $\varphi_{\mathbf{x}}(\mathbf{d}) := f(\mathbf{x}) + \nabla f(\mathbf{x})^{\mathrm{T}}\mathbf{d} + \frac{1}{2}\mathbf{d}^{\mathrm{T}}\nabla^2 f(\mathbf{x})\mathbf{d}$ $(\approx f(\mathbf{x}+\mathbf{d}))$
  - We wish to find a direction $\mathbf{d} \in \Re^n$ such that
    $\nabla_{\mathbf{d}}\varphi_{\mathbf{x}}(\mathbf{d}) = \nabla f(\mathbf{x}) + \nabla^2 f(\mathbf{x})\mathbf{d} = \nabla f(\mathbf{x}) + H_f(\mathbf{x})\mathbf{d} = \mathbf{0}^n$
    (a stationary point for $\varphi_{\mathbf{x}}$) $\Rightarrow$ $\mathbf{d}^k = -\mathbf{H}_f(\mathbf{x}^k)^{-1}\nabla f(\mathbf{x}^k)$
  - Observe that line search not needed, $t = 1$ (unit step)
  - Only look for stationary points $\Rightarrow$ $\mathbf{d}^k$ the same for min/max problems
  - If f is quadratic (i.e., $f(\mathbf{x}) = a + \mathbf{c}^{\mathrm{T}}\mathbf{x} + \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{Q}\mathbf{x}$), then Newtons method finds a stationary point in one iteration. Verify this!

Common special cases of search methods - Newton

PROS:

- Fast convergence

CONS:

- Convergens towards a stationary point only guaranteed if starting "sufficiently close" to one (If f is convex around the starting point $\mathbf{x}$ (i.e., $H_f(\mathbf{x})$ positive definite), then Newtons method converges towards a local minimum)
- Newton does not distinguish between different types of stationary points
- Requires more computations per iteration (matrix inversions)
- Does not always work (if $\texttt{det}(\mathbf{H}_f(\mathbf{x}^k)) = 0$)

Common special cases of search methods - Newton

PRACTICAL ADJUSTMENTS OF NEWTON'S METHOD:

- Start using steepest ascent, then change to Newton
- Use $\mathbf{d}^k = -\mathbf{Q}^k \nabla f(\mathbf{x}^k)$, where $\mathbf{Q}^k \approx \mathbf{H}_f(\mathbf{x}^k)^{-1}$ and $\mathbf{Q}^k$ positive (negative) definite (Quasi-Newton)
- Efficient updates of the inverse should be used
- Let $\mathbf{Q}^k = \left(\mathbf{H}_f(\mathbf{x}^k) +/- \mathbf{E}^k\right)^{-1}$ such that $\mathbf{Q}^k$ becomes positive/negative definite, e.g., $\mathbf{E}^k = \gamma \mathbf{I}$ (which shifts all the eigenvalues by $+/-\gamma$. This is called the *Levenberg-Marquardt modification*)

  Note: for large values of γ, this makes $\mathbf{d}^k$ resemble the steepest descent direction

Optimization over convex sets

Up to now, we have looked at unconstrained optimization. Now:

minimize $f(\mathbf{x})$ subject to $\mathbf{x} \in S$

where $S = \{ \mathbf{x} \in \Re^n \mid g_i(\mathbf{x}) \leq 0, i = 1, \dots, m \}$ is a convex set

- **Definition** FEASIBLE DIRECTION
  If $\mathbf{x} \in S$, then $\mathbf{d} \in \Re^n$ is a feasible direction from $\mathbf{x}$ if a small step in this direction does not lead outside the set S

  Formally: $\mathbf{d}$ defines a feasible direction at $\mathbf{x} \in S$ if

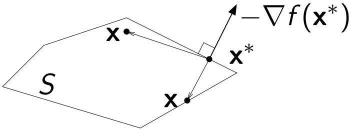
  $$\exists \delta > 0 \text{ such that } \mathbf{x} + t\mathbf{d} \in S \text{ for all } t \in [0, \delta]$$

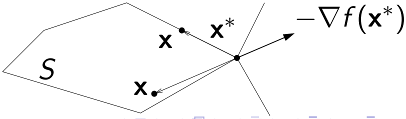
- **Definition** ACTIVE CONSTRAINTS
  The active constraints at $\mathbf{x} \in S$ are those that are fulfilled with equality, i.e., $\mathcal{I}(\mathbf{x}) = \{ i = 1, \dots, m \mid g_i(\mathbf{x}) = 0 \}$
- DRAW!!

Optimality conditions

- **Definition** FEASIBLE DIRECTIONS FOR LINEAR CONSTRAINTS
  Suppose that $g_i(\mathbf{x}) = \mathbf{a}_i^{\mathrm{T}}\mathbf{x} - b_i$, $i = 1, \dots, m$. Then, the set of feasible directions at $\mathbf{x}$ is $\{\, \mathbf{d} \in \Re^n \mid \mathbf{a}_i^{\mathrm{T}}\mathbf{d} \leq 0, i \in \mathcal{I}(\mathbf{x}) \,\}$
- **Necessary optimality conditions**
  If $\mathbf{x}^* \in S$ is a local minimum of f over S then $\nabla f(\mathbf{x}^*)^{\mathrm{T}}\mathbf{d} \geq 0$ holds for all feasible directions $\mathbf{d}$ at $\mathbf{x}^*$
  (i.e., at $\mathbf{x}^*$ there are no feasible descent directions)
- **Necessary and sufficient optimality conditions**
  Suppose S is non-empty and convex and f convex. Then,

$$\begin{aligned} &\mathbf{x}^* \text{ is a global minimum of } f \text{ over } S \\ \Leftrightarrow\ &\nabla f(\mathbf{x}^*)^{\mathrm{T}}(\mathbf{x} - \mathbf{x}^*) \geq 0 \text{ holds for all } \mathbf{x} \in S \end{aligned}$$



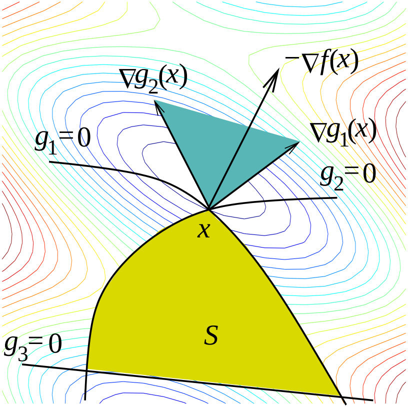


Necessary conditions for optimality

Assume that the functions $g_i : \Re^n \mapsto \Re$, $i = 1, \ldots, m$, are convex and differentiable and that there exists a point $\bar{\mathbf{x}} \in S$ such that $g_i(\bar{\mathbf{x}}) < 0$, $i = 1, \ldots, m$. Further, assume that $f : \Re^n \mapsto \Re$ is differentiable. If $\mathbf{x}^* \in S$ is a local minimum of f over S, then there exists a vector $\boldsymbol{\mu} \in \Re^m$ such that

$$\begin{aligned}
\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \mu_i \nabla g_i(\mathbf{x}^*) &= \mathbf{0}^n \\
\mu_i g_i(\mathbf{x}^*) &= 0, \qquad i = 1, \ldots, m \\
g_i(\mathbf{x}^*) &\leq 0, \qquad i = 1, \ldots, m \\
\boldsymbol{\mu} &\geq \mathbf{0}^m
\end{aligned}$$

Geometry of the Karush-Kuhn-Tucker conditions



Figur: Geometric interpretation of the Karush-Kuhn-Tucker conditions. At a local minimum, minus the gradient of the objective can be expressed as a non-negative linear combination of the gradients of the active constraints at this point.

Sufficient conditions under convexity

Assume that the functions $f, g_i : \Re^n \mapsto \Re$, $i = 1, \dots, m$, are convex and differentiable. If the conditions

$$
\begin{aligned}
\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \mu_i \nabla g_i(\mathbf{x}^*) &= \mathbf{0}^n \\
\mu_i g_i(\mathbf{x}^*) &= 0, \qquad i = 1, \dots, m \\
\boldsymbol{\mu} &\geq \mathbf{0}^m
\end{aligned}
$$

hold, then $\mathbf{x}^* \in S$ is a global minimum of f over $S = \{\, \mathbf{x} \in \Re^n \mid g_i(\mathbf{x}) \leq 0, i = 1, \dots, m \,\}$.

The Karush-Kuhn-Tucker conditions can also be stated for optimization problems with equality constraints

The optimality conditions can be used to

- verify an (local) optimal solution
- solve certain special cases of nonlinear programs (e.g. quadratic)
- algorithm construction
- derive properties of a solution to a non-linear program

Example

$$\begin{array}{lrcl} \text{minimize} & f(\mathbf{x}) := 2x_1^2 + 2x_1x_2 + x_2^2 - 10x_1 - 10x_2 \\ \text{subject to} & x_1^2 + x_2^2 & \leq & 5 \\ & 3x_1 + x_2 & \leq & 6 \end{array}$$

- Is $\mathbf{x}^0 = (1, 2)^{\mathrm{T}}$ a Karush-Kuhn-Tucker point?
- An optimal solution?
- $\nabla f(\mathbf{x}) = (4x_1 + 2x_2 - 10, 2x_1 + 2x_2 - 10)^{\mathrm{T}}$, $\nabla g_1(\mathbf{x}) = (2x_1, 2x_2)^{\mathrm{T}}$, $\nabla g_2(\mathbf{x}) = (3, 1)^{\mathrm{T}}$

$$\Rightarrow \begin{bmatrix} 4x_1^0 + 2x_2^0 - 10 + 2x_1^0\mu_1 + 3\mu_2 = 0 \\ 2x_1^0 + 2x_2^0 - 10 + 2x_2^0\mu_1 + \mu_2 = 0 \\ \mu_1((x_1^0)^2 + (x_2^0)^2 - 5) = \mu_2(3x_1^0 + x_2^0 - 6) = 0 \\ \mu_1, \mu_2 \geq 0 \end{bmatrix} \Leftrightarrow$$

$$\begin{bmatrix} 2\mu_1 + 3\mu_2 = 2 \\ 4\mu_1 + \mu_2 = 4 \\ 0\mu_1 = -\mu_2 = 0 \\ \mu_1, \mu_2 \geq 0 \end{bmatrix}$$

$$\Rightarrow \mu_2 = 0 \quad \Rightarrow \quad \mu_1 = 1 \geq 0$$

Example, continued

- The Karush-Kuhn-Tucker conditions hold.
- Optimal? Check convexity!
- $\nabla^2 f(\mathbf{x}) = \begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix}$, $\nabla^2 g_1(\mathbf{x}) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$, $\nabla^2 g_2(\mathbf{x}) = \mathbf{0}^{2\times 2}$

$\Rightarrow$ f, g_1, and g_2 are convex $\Rightarrow \mathbf{x}^0 = (1,2)^{\mathrm{T}}$ is an optimal solution $f(\mathbf{x}^0) = -20$