MVE165/MMG631
Linear and integer optimization with applications
Lecture 13
Overview of nonlinear programming

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Areas of applications, examples (Ch. 9.1)

Structural optimization

- Design of aircraft, ships, bridges, etc
- Decide on the material and the topology and thickness of a mechanical structure
- Minimize weight, maximize stiffness, constraints on deformation at certain loads, strength, fatigue limit, etc

Analysis and design of traffic networks

- Estimate traffic flows and discharges
- Detect bottlenecks
- Analyze effects of traffic signals, tolls, etc

Areas of applications, more examples (Ch. 9.1)

Least squares

Adaptation of data

Engine development, design of antennas or tyres, etc.

For each function evaluation a computationally expensive (time consuming) simulation may be needed

Maximize the volume of a cylinder

While keeping the surface area constant

Wind power generation

The energy content in the wind $\propto v^3$ (in Ass3a discretized measured data is used)

An overview of nonlinear optimization

General notation for nonlinear programs

$$\begin{aligned} \text{minimize}_{\mathbf{x}\in\Re^n} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g_i(\mathbf{x}) \leq 0, \quad i \in \mathcal{L}, \\ & h_i(\mathbf{x}) = 0, \quad i \in \mathcal{E}. \end{aligned}$$

Some special cases

- Unconstrained problems ($\mathcal{L} = \mathcal{E} = \emptyset$):

  $$\boxed{\text{minimize } f(\mathbf{x}) \text{ subject to } \mathbf{x} \in \Re^n}$$

- Convex programming: f convex, g_i convex, $i \in \mathcal{L}$, h_i linear, $i \in \mathcal{E}$.
- Linear constraints: g_i, $i \in \mathcal{L}$, and h_i, $i \in \mathcal{E}$
  - Quadratic programming: $\boxed{f(\mathbf{x}) = \mathbf{c}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}}$
  - Linear programming: $\boxed{f(\mathbf{x}) = \mathbf{c}^T\mathbf{x}}$

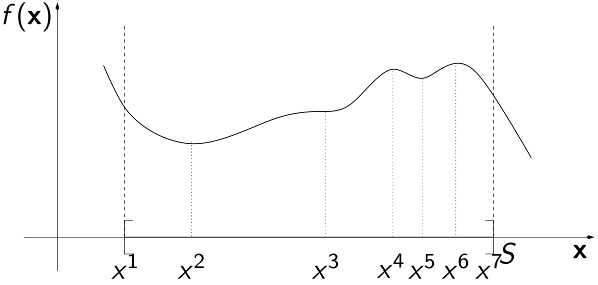
Properties of nonlinear programs

- The mathematical properties of nonlinear optimization problems can be very different
- *No* algorithm exists that solves *all* nonlinear optimization problems
- An optimal solution does *not* have to be located at an extreme point
- Nonlinear programs can be unconstrained

  What if a *linear program* has no constraints?
- f may be differentiable or non-differentiable

  E.g., the Lagrangean dual objective function; Ass3b
- *For convex problems*: Algorithms (typically) converge to an optimal solution
- Nonlinear problems can have *local* optima that are *not global* optima

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



Possible extremal points are

- boundary points of $S = [x^1, x^7]$ (i.e., $\{x^1, x^7\}$)
- stationary points, where $f'(\mathbf{x}) = 0$ (i.e., $\{x^2, \ldots, x^6\}$)
- discontinuities in f or f' DRAW!

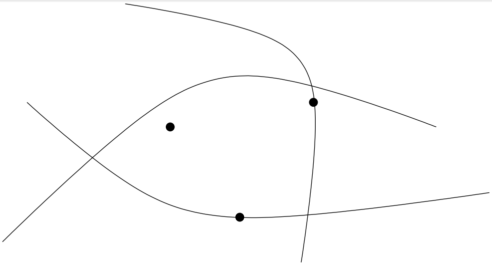
Boundary and stationary points (Ch. 10.0)

Boundary points

$\bar{\mathbf{x}}$ is a *boundary* point to the feasible set

$$S = \{\mathbf{x} \in \Re^n \mid g_i(\mathbf{x}) \leq 0, i \in \mathcal{L}\}$$

if $g_i(\bar{\mathbf{x}}) \leq 0$, $i \in \mathcal{L}$, and $g_i(\bar{\mathbf{x}}) = 0$ for at least one index $i \in \mathcal{L}$



Stationary points

$\bar{\mathbf{x}}$ is a *stationary* point to f if $\nabla f(\bar{\mathbf{x}}) = \mathbf{0}^n$ (for $n = 1$: if $f'(\bar{x}) = 0$)

Local and global minima (maxima) (Ch. 2.4)

Consider the nonlinear optimization problem to

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

Local minimum

- *In words:* A solution is a *local* minimum if it is *feasible* and no other feasible solution in a sufficiently *small neighbourhood* has a lower objective value
- *Formally:* $\bar{\mathbf{x}}$ is a local minimum if $\bar{\mathbf{x}} \in S$ and $\exists \varepsilon > 0$ such that $f(\bar{\mathbf{x}}) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \{\, \mathbf{y} \in S : \|\mathbf{y} - \bar{\mathbf{x}}\| \leq \varepsilon \,\}$ DRAW!!

Global minimum

- *In words:* A solution is a *global* minimum if it is *feasible* and no other feasible solution has a lower objective value
- *Formally:* $\bar{\mathbf{x}}$ is a global minimum if $\bar{\mathbf{x}} \in S$ and $f(\bar{\mathbf{x}}) \leq f(\mathbf{x})$ for all $\mathbf{x} \in S$

When is a local optimum also a global optimum? (Ch. 9.3)

The concept of convexity is essential

- Functions: convex (minimization), concave (maximization)
- Sets: convex (minimization and maximization)
- The minimization (maximization) of a convex (concave) function over a convex set is referred to as a convex optimization problem

Definition 9.5: Convex optimization problem

If f and g_i, $i \in \mathcal{L}$, are convex functions, then

$$\boxed{\text{minimize } f(\mathbf{x}) \text{ subject to } g_i(\mathbf{x}) \leq 0, \;\; i \in \mathcal{L}}$$

is said to be a *convex* optimization problem

Theorem 9.1: Global optimum

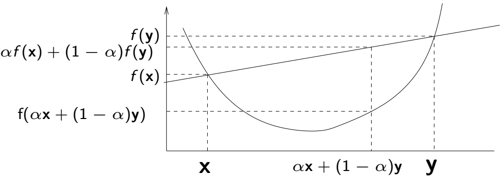
Let $\mathbf{x}^*$ be a *local* optimum of a convex optimization problem. Then $\mathbf{x}^*$ is also a *global* optimum

Convex functions

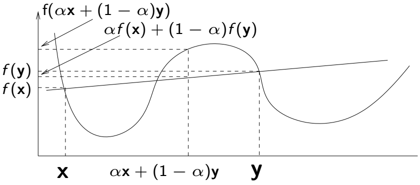
A function f is *convex* on S if, for any $\mathbf{x}, \mathbf{y} \in S$ it holds that

$$f(\alpha\mathbf{x} + (1-\alpha)\mathbf{y}) \leq \alpha f(\mathbf{x}) + (1-\alpha) f(\mathbf{y}) \quad \text{for all} \quad 0 \leq \alpha \leq 1$$

A CONVEX FUNCTION



A NON-CONVEX FUNCTION



The function f is *strictly convex* on S if, for any $\mathbf{x}, \mathbf{y} \in S$ such that $\mathbf{x} \neq \mathbf{y}$ it holds that

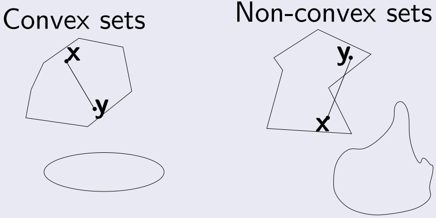
$$f(\alpha\mathbf{x} + (1-\alpha)\mathbf{y}) < \alpha f(\mathbf{x}) + (1-\alpha) f(\mathbf{y}) \quad \text{for all} \quad 0 < \alpha < 1$$

Convex sets

A set S is convex if, for any $\mathbf{x}, \mathbf{y} \in S$ it holds that

$$\alpha\mathbf{x} + (1-\alpha)\mathbf{y} \in S \quad \text{for all} \quad 0 \leq \alpha \leq 1$$

Examples



Consider a set S defined by the intersection of $m = |\mathcal{L}|$ inequalities, where the functions $g_i : \Re^n \mapsto \Re$, $i \in \mathcal{L}$, as

$$S = \{\, \mathbf{x} \in \Re^n \mid g_i(\mathbf{x}) \leq 0, \;\; i \in \mathcal{L} \,\}$$

Theorems 9.2 & 9.3

If all the functions $g_i(\mathbf{x})$, $i \in \mathcal{L}$, are convex on $\Re^n$, then S is a convex set

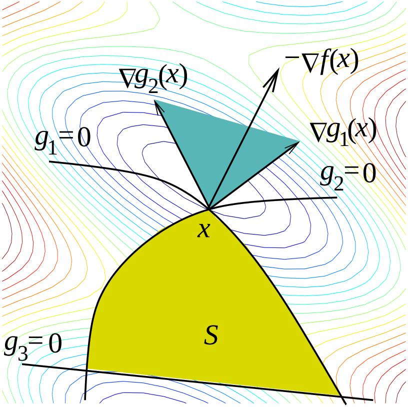
The Karush-Kuhn-Tucker conditions: necessary conditions for optimality

Let $S := \{ \mathbf{x} \in \Re^n \mid g_i(\mathbf{x}) \leq 0, i \in \mathcal{L} \}$

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

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

Geometry of the Karush-Kuhn-Tucker conditions



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

The Karush-Kuhn-Tucker conditions: sufficient for optimality under convexity

Assume that the functions $f, g_i : \Re^n \mapsto \Re$, $i \in \mathcal{L}$, are convex and differentiable, and let $S = \{ \mathbf{x} \in \Re^n \mid g_i(\mathbf{x}) \leq 0, i \in \mathcal{L} \}$

If the conditions (where $m = |\mathcal{L}|$)

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

hold, then $\mathbf{x}^* \in S$ is a global minimum of f over S

- The Karush-Kuhn-Tucker conditions can also be stated for optimization problems with equality constraints
- For unconstrained optimization KKT reads: $\nabla f(\mathbf{x}^*) = \mathbf{0}$
- For a quadratic program KKT forms a system of linear (in)equalities plus the complementarity constraints

The optimality conditions can be used to..

- verify an (local) optimal solution
- solve certain special cases of nonlinear programs (e.g. quadratic programs)
- 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?

- Is it an optimal solution?
- Derive: $\nabla f(\mathbf{x}) = (4x_1 + 2x_2 - 10, 2x_1 + 2x_2 - 10)^{\mathrm{T}}$, $\nabla g_1(\mathbf{x}) = (2x_1, 2x_2)^{\mathrm{T}}$, and $\nabla g_2(\mathbf{x}) = (3,1)^{\mathrm{T}}$

$$\begin{aligned} 4x_1^0 + 2x_2^0 - 10 + 2x_1^0\mu_1 + 3\mu_2 &= 0 \\ 2x_1^0 + 2x_2^0 - 10 + 2x_2^0\mu_1 + \mu_2 &= 0 \\ \mu_1((x_1^0)^2 + (x_2^0)^2 - 5) = \mu_2(3x_1^0 + x_2^0 - 6) &= 0 \\ \mu_1, \mu_2 &\geq 0 \end{aligned} \quad \Longleftrightarrow \quad \begin{aligned} 2\mu_1 + 3\mu_2 &= 2 \\ 4\mu_1 + \mu_2 &= 4 \\ 0\mu_1 = -\mu_2 &= 0 \\ \mu_1, \mu_2 &\geq 0 \end{aligned}$$

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

Example, continued

OK, the Karush-Kuhn-Tucker conditions hold

Is the solution 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 and $f(\mathbf{x}^0) = -20$

General iterative search method for unconstrained optimization (Ch. 2.5.1)

1. Choose a starting solution, $\mathbf{x}^0 \in \Re^n$. Let $k = 0$
2. Determine a search direction $\mathbf{d}^k$
3. If a termination criterion is fulfilled $\Rightarrow$ Stop!
4. Determine a step length, t_k, by solving:

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

5. New iteration point, $\mathbf{x}^{k+1} = \mathbf{x}^k + t_k \cdot \mathbf{d}^k$
6. Let $k := k + 1$ and return to step 2

How choose *search directions* $\mathbf{d}^k$, *step lengths* t_k, and *termination criteria*?

Goal: $f(\mathbf{x}^{k+1}) < f(\mathbf{x}^k)$ (minimization)

- How does f change locally in a direction $\mathbf{d}^k$ at $\mathbf{x}^k$?
- Taylor expansion (Ch. 9.2):
  $f(\mathbf{x}^k + t\mathbf{d}^k) = f(\mathbf{x}^k) + t\nabla f(\mathbf{x}^k)^{\mathrm{T}}\mathbf{d}^k + \mathcal{O}(t^2)$
- For sufficiently small $t > 0$:
  $f(\mathbf{x}^k + t\mathbf{d}^k) < f(\mathbf{x}^k) \quad \Rightarrow \quad \nabla f(\mathbf{x}^k)^{\mathrm{T}}\mathbf{d}^k < 0$

$\Rightarrow$

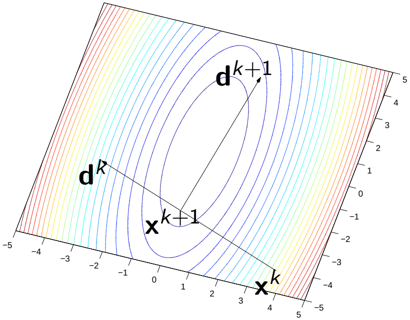
Definition

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, etc.

General iterative search method for unconstrained optimization (Ch. 2.5.1)

1. Choose a starting solution, $\mathbf{x}^0 \in \Re^n$. Let $k = 0$
2. Determine a search direction $\mathbf{d}^k$
3. If a termination criterion is fulfilled $\Rightarrow$ Stop!
4. Determine a step length, t_k, by solving:

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

5. New iteration point, $\mathbf{x}^{k+1} = \mathbf{x}^k + t_k \cdot \mathbf{d}^k$
6. Let $k := k + 1$ and return to step 2

Step length—line search (minimization) (Ch. 10.4)

- 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: $\varphi'(t_k) = 0$ (seldom possible to derive)

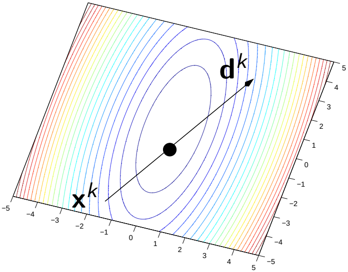
Numerical solution methods

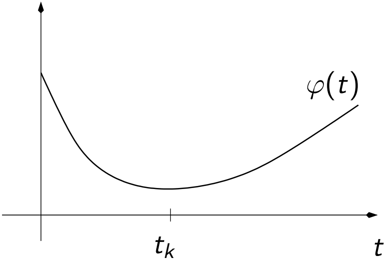
- The golden section method (reduce the interval of uncertainty)
- The bi-section method (reduce the interval of uncertainty)
- Newton-Raphson's method
- Armijo's method

In practice

Do not solve exactly, but to a 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 $\min_{t \geq 0} \varphi(t) := f(\mathbf{x}^k + t \cdot \mathbf{d}^k)$

General iterative search method for unconstrained optimization

1. Choose a starting solution, $\mathbf{x}^0 \in \Re^n$. Let $k = 0$
2. Determine a search direction $\mathbf{d}^k$
3. If a termination criterion is fulfilled $\Rightarrow$ Stop!
4. Determine a step length, t_k, by solving:

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

5. New iteration point, $\mathbf{x}^{k+1} = \mathbf{x}^k + t_k \cdot \mathbf{d}^k$
6. 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 ($\varepsilon_j > 0$, $j = 1, \ldots, 4$)

(a) $\|\nabla f(\mathbf{x}^k)\| < \varepsilon_1$

(b) $|f(\mathbf{x}^{k+1}) - f(\mathbf{x}^k)| < \varepsilon_2$

(c) $\|\mathbf{x}^{k+1} - \mathbf{x}^k\| < \varepsilon_3$

(d) $t_k < \varepsilon_4$

These are often combined

The search method only guarantees a stationary solution, whose properties are determined by the properties of f (convexity, ...)

Constrained optimization: Penalty methods

Consider both inequality and equality constraints

$$\begin{aligned} \text{minimize}_{\mathbf{x}\in\Re^n} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g_i(\mathbf{x}) \leq 0, \quad i \in \mathcal{L}, \\ & h_i(\mathbf{x}) = 0, \quad i \in \mathcal{E}. \end{aligned} \tag{1}$$

Drop the constraints and add terms in the objective that *penalize infeasibile solutions*

$$\text{minimize}_{\mathbf{x}\in\Re^n} \quad F_\mu(\mathbf{x}) := f(\mathbf{x}) + \mu \sum_{i\in\mathcal{L}\cup\mathcal{E}} \alpha_i(\mathbf{x}) \tag{2}$$

where $\mu > 0$ and $\alpha_i(\mathbf{x}) = \begin{cases} = 0 & \text{if } \mathbf{x} \text{ satisfies constraint } i \\ > 0 & \text{otherwise} \end{cases}$

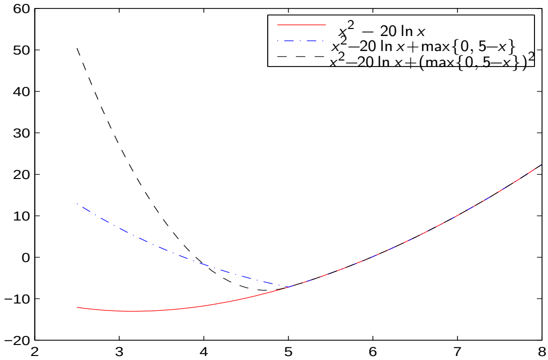
Common penalty functions (which of these are differentiable?)

$i \in \mathcal{L}$: $\quad \alpha_i(\mathbf{x}) = \max\{0, g_i(\mathbf{x})\} \quad$ or $\quad \alpha_i(\mathbf{x}) = (\max\{0, g_i(\mathbf{x})\})^2$

$i \in \mathcal{E}$: $\quad \alpha_i(\mathbf{x}) = |h_i(\mathbf{x})| \quad$ or $\quad \alpha_i(\mathbf{x}) = |h_i(\mathbf{x})|^2$

Squared and non-squared penalty functions

minimize $\left(x^2 - 20\ln x\right)$ subject to $x \geq 5$

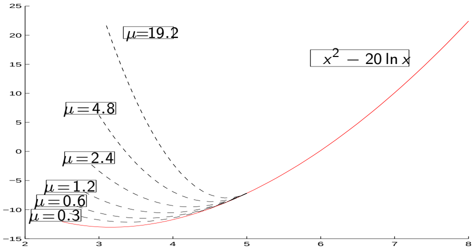


Figur: Squared and non-squared penalty function. g_i differentiable $\Longrightarrow$ squared penalty function differentiable

Squared penalty functions

- In practice: Start with a low value of $\mu > 0$ and increase the value as the computations proceed
- **Example:** $\boxed{\text{minimize } (x^2 - 20 \ln x) \text{ subject to } x \geq 5}$ $\quad (*)$

$$\Rightarrow \boxed{\text{minimize } \left(x^2 - 20 \ln x + \mu(\max\{0, 5 - x\})^2\right)} \qquad (**)$$

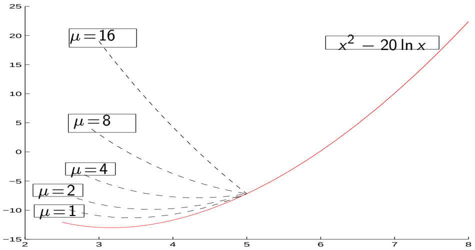


Figur: Squared penalty function: $\nexists \mu < \infty$ such that an optimal solution for $(**)$ is optimal (feasible) for $(*)$

Non-squared penalty functions

- In practice: Start with a low value of $\mu > 0$ and increase the value as the computations proceed
- **Example:** $\boxed{\text{minimize } \left(x^2 - 20\ln x\right) \text{ subject to } x \geq 5}$ $\quad (+)$

$$\Rightarrow \boxed{\text{minimize } \left(x^2 - 20\ln x + \mu \max\{0, 5 - x\}\right)} \qquad (++)$$



Figur: Non-squared penalty function: For $\mu \geq 6$ the optimal solution for $(++)$ is optimal (and feasible) for $(+)$

Constrained optimization: Barrier methods

Consider only inequality constraints

$$\begin{aligned} \text{minimize}_{\mathbf{x}\in\Re^n} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g_i(\mathbf{x}) \leq 0, \quad i \in \mathcal{L} \end{aligned} \tag{3}$$

- Drop the constraints and add terms in the objective that *prevents from approaching the boundary* of the feasible set

$$\text{minimize}_{\mathbf{x}\in\Re^n} \quad F_\mu(\mathbf{x}) := f(\mathbf{x}) + \mu \sum_{i\in\mathcal{L}} \alpha_i(\mathbf{x}) \tag{4}$$

where $\mu > 0$ and $\alpha_i(\mathbf{x}) \to +\infty$ as $g_i(\mathbf{x}) \to 0$ (as constraint i approaches being active)

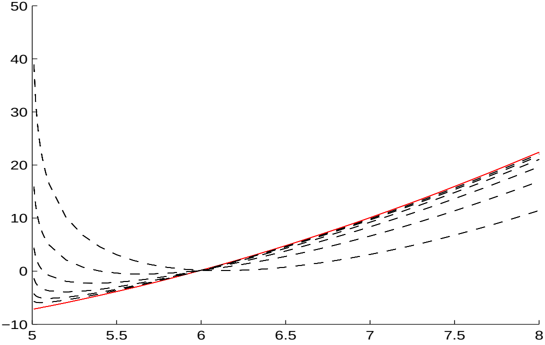
Common barrier functions

$$\alpha_i(\mathbf{x}) = -\ln[-g_i(\mathbf{x})] \quad \text{or} \quad \alpha_i(\mathbf{x}) = \frac{-1}{g_i(\mathbf{x})}$$

Logarithmic barrier functions

- Choose $\mu > 0$ and decrease it as the computations proceed
- **Example:** $\boxed{\text{minimize} \quad \left(x^2 - 20 \ln x\right) \text{ subject to } x \geq 5}$

$$\Rightarrow \quad \boxed{\text{minimize}_{\,x>5} \left(x^2 - 20 \ln x - \mu \ln(x-5)\right)}$$



Fractional barrier functions

- Choose $\mu > 0$ and decrease it as the computations proceed
- **Example:** $\boxed{\text{minimize } \left(x^2 - 20 \ln x\right) \text{ subject to } x \geq 5}$

$\Rightarrow$ $\boxed{\text{minimize}_{\,x>5} \left(x^2 - 20 \ln x + \frac{\mu}{x-5}\right)}$