Mathematical Programming I:

Chapter 4 and Chapter 5

Sheets for the course, version: 22-05-2011
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The script is part of the book:
Faigle/Kern/Still, Algorithmic principles of Mathematical Programming.
on: ***http://wwwhome.math.utwente.nl/∼stillgj/priv/***

4. Convex sets, convex functions

4.1 Convex sets

Recall the definitions of closed, compact sets $P \subset \mathbb{R}^n$.

Def. A set $P \subset \mathbb{R}^n$ is called convex if

$$x, y \in P, \lambda \in [0, 1] \Rightarrow x + \lambda(y - x) \in P$$

Ex 4.1 Any intersection of closed convex sets is a closed convex set.

Def. Let H be a hyperplane $H = \{x \mid a^T x = \alpha\}$ (*with some* $0 \neq a \in \mathbb{R}^n$) and let $P \subset \mathbb{R}^n$, $y \notin P$. H is called a separating hyperplane wrt. P and y if:

$$a^T x \leq \alpha < a^T y \qquad \forall x \in P$$

Lem.4.1 $S \subseteq \mathbb{R}^n$ is an intersection of closed halfspaces $\Leftrightarrow$ for each y $\notin S$ there is a *separating hyperplane* w.r.t. S and y.

Th.4.1 Let $\emptyset \neq P \subseteq \mathbb{R}^n$ be closed convex, $y \notin P$. Then there is a separating hyperplane, i.e. there exists $0 \neq a \in \mathbb{R}^n, \ \alpha \in \mathbb{R}$ such that

$$a^T x \leq \alpha < a^T y \qquad \forall x \in P$$

Cor.4.1 $P \subseteq \mathbb{R}^n$ is closed, convex $\Leftrightarrow$ P is an intersection of (closed) halfspaces.

Def. $H = \{x \mid c^T x = \alpha\}$ $(0 \neq c)$ is *supporting* P at a point $x_0 \in P$ if:

$$c^T x \leq \alpha = c^T x_0 \qquad \forall x \in P$$

Th.4.2 Let $P \subseteq \mathbb{R}^n$ be closed, convex and $x_0 \in P$ a boundary point of P. Then there exists $c \neq 0$ such that:

$$c^T x \leq c^T x_0 \ \ (= \max_{x \in P} c^T x) \quad \forall x \in P$$

i.e. the hyperplane $H = \{x \mid c^T x = c^T x_0\}$ *supports* P *at* x_0.

The cone of positive semidefinite matrices.

Def. $K \subset \mathbb{R}^n$ is called a *convex cone* if:

$$x, y \in K, \quad \lambda_1, \lambda_2 \geq 0 \Rightarrow \lambda_1 x + \lambda_2 y \in K$$

Recall:

- $S^{n\times n} = \{X \in \mathbb{R}^{n\times n} \mid X^T = X\}$ symmetric matr.
- $K := \{X \in S^{n\times n} \mid a^T X a \geq 0 \ \forall a \in \mathbb{R}^n\}$ p.s.d. matr.

Rem.: K is a closed, convex cone.

Consider the program: with $C \subset \mathbb{R}^n$, convex, closed,

$$P_0 : \quad \max \ c^T x \quad \text{s.t.} \quad x \in C$$

By the Ellipsoid Method, P_0 can be solved *efficiently* if the check, $y \notin C$, and the construction of a separating hyperplane H wrt. C and y can be done *efficiently*.

Semidefinite programs: $c \in \mathbb{R}^n$, $B, A_i \in S^{n\times n}$

$$SDP: \quad \max \ c^T x \quad \text{s.t.} \quad B - \sum_{i=1}^{n} A_i x_i \succeq 0$$

Rem.: Given $Y \in S^{n\times n}$. Then the check, $Y \notin K$, and the construction of a separating hyperplane (in $S^{n\times n}$) wrt. K and Y can be done efficiently (by "Gauss").

4.2 Convex functions

Def. A function $f : K \to \mathbb{R}$, $K \subset \mathbb{R}^n$ a convex set, is called *convex* if for all $x, y \in K$ and $0 \le \lambda \le 1$ one has

$$f(\lambda x + (1-\lambda)y) \le \lambda f(x) + (1-\lambda) f(y) \; .$$

It is called *strictly convex* if for all $x, y \in K$, $0 < \lambda < 1$:

$$f(\lambda x + (1-\lambda)y) < \lambda f(x) + (1-\lambda) f(y)$$

Def. The epigraph of $f : K \to \mathbb{R}$ is given by:

$$\text{epi } f = \{(x, z) \mid z \ge f(x), x \in K\}$$

Ex.4.6 $f : K \to \mathbb{R}$ is convex if and only if epi f is convex.

Def. Let $r \geq 1,\ a_i \in \mathbb{R}^n,\ \lambda_i \geq 0,\ i = 1, \cdots, r;$ $\sum_{i=1}^r \lambda_i = 1$. Then

$$v = \sum_{i=1}^{r} \lambda_i a_i$$

is called a *convex combination* of the a_i's.

Given $V \subset \mathbb{R}^n$, the set of all convex combinations of vectors in V is called the *convex hull of V*,

$$\text{conv } V = \{\sum_{i=1}^{r} \lambda_i a_i \mid r \geq 1,\ a_i \in V,\ \lambda_i \geq 0,$$

$$i = 1, \cdots, r;\ \textstyle\sum_{i=1}^r \lambda_i = 1\}$$

Rem. conv V is the smallest convex set containing V.

Ex.4.9

(a) $C \subseteq \mathbb{R}^n$ **is convex if and only if for any choice** $r \geq 1$, $\mathbf{a}_i \in C,\ \lambda_i \geq 0,\ i = 1, \cdots, r;\ \sum_{i=1}^{r} \lambda_i = 1$ **we have**

$$\mathbf{x} = \sum_{i=1}^{r} \lambda_i \mathbf{a}_i \in C.$$

(b) **Given** $f:\ C \to \mathbb{R},\ C \subseteq \mathbb{R}^n$ **a convex set. Then,** f **is convex if and only if for any choice** $r \geq 1,\ \mathbf{a}_i \in C$, $\lambda_i \geq 0,\ i = 1, \cdots, r,\ \sum_{i=1}^{r} \lambda_i = 1$ **we have**

$$f\left(\sum_{i=1}^{r} \lambda_i \mathbf{a}_i\right) \leq \sum_{i=1}^{r} \lambda_i f(\mathbf{a}_i).$$

The following Lemma allows to (often) reduce convexity in $\mathbb{R}^n$ to convexity in $\mathbb{R}$.

<u>Lem.4.2</u> For $f : \mathcal{F} \to \mathbb{R}$ is convex if and only if for every $\mathbf{x}_0 \in \mathcal{F}$ and $\mathbf{h} \in \mathbb{R}^n$

$$p_{\mathbf{h}}(t) = f(\mathbf{x}_0 + t\mathbf{h})$$

is a convex function of t on the interval $I = \mathcal{F}_{\mathbf{h}}(\mathbf{x}_0) = \{t \in \mathbb{R} \mid \mathbf{x}_0 + t\mathbf{h} \in \mathcal{F}\}$.

<u>Lem.4.3</u> Let $f : (a, b) \to \mathbb{R}$ be convex and $x_0 \in (a, b)$. Then

$$\varphi(t) := \frac{f(x_0+t)-f(x_0)}{t} \qquad t \neq 0$$

is monotonically increasing in t. Moreover, the following one-sided limits exist:

$$f'_-(x_0) \;:=\; \lim_{t\uparrow 0} \frac{f(x_0+t)-f(x_0)}{t} \;\leq\; \lim_{t\downarrow 0} \frac{f(x_0+t)-f(x_0)}{t} \;=:\; f'_+(x_0)$$

Def. $f : \mathbb{R}^n \to \mathbb{R}$ **is Lipschitz-continuous at** $\mathbf{x}_0$ **if there is a neighborhood** $U_\varepsilon(\mathbf{x}_0) = \{\mathbf{x} \mid \|\mathbf{x} - \mathbf{x}_0\| < \varepsilon\}$ **(**$\varepsilon > 0$**) and some** $L \geq 0$ **such that**

$$|f(\mathbf{x}) - f(\mathbf{x}_0)| \leq L\,\|\mathbf{x} - \mathbf{x}_0\| \quad \forall \mathbf{x} \in U_\varepsilon(\mathbf{x}_0).$$

Th. 4.5 **Let** $f : (a, b) \to \mathbb{R}$ **be convex,** $x_0 \in (a, b)$**. Then** f **is Lipschitz continuous at** x_0**.**

Ex. **Convex functions** $f : K \to \mathbb{R}$ **need not be continuous at boundary points of** K**: The function**

$$f(x) = \begin{cases} 0\,, & 0 \leq x < 1 \\ 1\,, & x = 1 \end{cases}$$

is convex on $[0, 1]$ **but not continuous.**

Rem. **Convex functions on** (a, b) **need not be differentiable at** $x \in (a, b)$**, see e.g.,** $f(x) = |x|$**.**

Fact: Let $f : (a, b) \to \mathbb{R}$ be convex and differentiable on (a, b). Then by L.4.3 for any $x \in (a, b)$:

$$f(y) \geq f(x) + f'(x)(y - x) \quad \forall y \in (a, b)$$

Def: [*Generalization of the derivative*]
Let $f : (a, b) \to \mathbb{R}$ be convex on (a, b). $d \in \mathbb{R}$ is called ***subderivative*** of f at $x \in (a, b)$ if

$$f(y) \geq f(x) + d(y - x) \quad \forall y \in (a, b)$$

The set of all subderivatives of f at x is the ***subdifferential*** denoted by $\partial f(x)$.

Ex.4.11. (a) Let $f : (a, b) \to \mathbb{R}$ be convex. Then for all $x \in (a, b)$:

$$\partial f(x) = \{d \in \mathbb{R} \mid f'_-(x) \leq d \leq f'_+(x)\}.$$

Th. 4.6 Let $f : (a,b) \to \mathbb{R}$. Then

$$f \text{ is convex on } (a,b) \Leftrightarrow \partial f(x) \neq \emptyset \ \ \forall x \in (a,b)$$

For $f \in C^1$ this means:

$$f \text{ is convex} \quad \Leftrightarrow \quad f(y) \geq f(x) + f'(x)(y-x) \ \forall x, y$$

Th. 4.7 Let $f : (a,b) \to \mathbb{R}$ be differentiable. Then

f is convex on (a,b) $\quad \Leftrightarrow \quad$ $f'(x)$ is monot. increas. on (a,b)

Cor. 4.2 Let $f : (a,b) \to \mathbb{R}$ be twice differentiable. Then

f is convex on (a,b) $\quad \Leftrightarrow \quad$ $f''(x) \geq 0 \ \ \forall x \in (a,b)$

4.2.2 convex functions in n variables

In what follows: Let $f : U \to \mathbb{R}$, $U \subset \mathbb{R}^n$ convex, open.

Def. Let $f : U \to \mathbb{R}$ be convex on U. We call $d \in \mathbb{R}^n$ a *subgradient* of f at $x \in U$ if

$$f(y) \geq f(x) + d^T(y - x) \quad \forall y \in U$$

The set of all subgradients of f at x is the *subdifferential* denoted by $\partial f(x)$.
(*The concept of subgradient, subdifferential generalizes the derivative.*)

Prop.4.1 Let $f : U \to \mathbb{R}$ be such that $\partial f(\mathbf{x}) \neq \emptyset$ for all $\mathbf{x} \in U$. Then f is convex.

Th. 4.8 Let $f : U \to \mathbb{R}$ be differentiable. Then f is convex on U

$$\Leftrightarrow \quad f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})(\mathbf{y}-\mathbf{x}) \; \forall \mathbf{x}, \mathbf{y} \in U.$$

Cor. 4.3 Let $f : U \to \mathbb{R}$ be twice differentiable. Then

f is convex on U $\Leftrightarrow$ $\nabla^2 f(\mathbf{x})$ positive semidefinite $\forall \mathbf{x} \in U$.

Th.4.3 Let $V = \{v_1, \ldots, v_k\} \subset \mathbb{R}^n$ and let the function f : conv $V \to \mathbb{R}$ be convex. Then

$$\max_{x \in \text{conv } V} f(x) = \max_{1 \le j \le k} f(v_j)$$

Th. 4.9 Let $f : K \to \mathbb{R}$ be convex on the convex set $K \subset \mathbb{R}^n$. Then f is continuous on *int* K. More precisely, f is Lipschitz continuous in each interior point $\overline{x}$ of K.

Th. 4.10 Let $f : U \to \mathbb{R}$, $U \subset \mathbb{R}^n$ open. Then

$$f \text{ is convex on } U \Leftrightarrow \partial f \mathbf{x}) \neq \emptyset \ \ \forall \mathbf{x} \in U$$

Ex.4.19 Let $f : U \to \mathbb{R}$, ($U \subset \mathbb{R}^n$ open), be convex, $x \in U$. Then the subdifferential $\partial f(x)$ is (non-empty) convex and compact.

5. Unconstrained optimization

Minimization problem: Given $f : \mathcal{F} \subset \mathbb{R}^n \to \mathbb{R}$,

$$(P) \qquad \min_{\mathbf{x} \in \mathcal{F}} f(\mathbf{x})$$

Def. $\overline{x} \in \mathcal{F}$ **is a *global minimizer* of f (over $\mathcal{F}$) if**

$$f(\overline{x}) \le f(\mathbf{x}) \qquad \text{for all } x \in \mathcal{F} \; .$$

We call $\overline{x} \in \mathcal{F}$ a *local minimizer* of f if there is an $\epsilon > 0$ such that

$$f(\overline{x}) \le f(\mathbf{x}) \;\; \text{for all } \mathbf{x} \in \mathcal{F}, \; \|\mathbf{x} - \overline{x}\| \le \epsilon \; .$$

and a *strict local minimizer* if with an $\epsilon > 0$

$$f(\overline{x}) < f(\mathbf{x}) \;\; \text{for all } \mathbf{x} \in \mathcal{F}, \overline{x} \ne \mathbf{x}, \; \|\mathbf{x} - \overline{x}\| \le \epsilon \; .$$

In Nonlinear *(nonconvex)* Optimization we usually mean:

- **Find a local minimizer. (*Global minimization is "more difficult"*).**

CONCEPTUAL ALGORITHM: Choose $x_0 \in \mathbb{R}^n$. Iterate

- **step k:** Given $x_k \in \mathbb{R}^n$, find a new point x_{k+1} with
$$f(x_{k+1}) < f(x_k).$$

We hope that: $x_k \to \overline{x}$ with $\overline{x}$ a local mininimizer.

Definition Let $x_k \to \overline{x}$ for $k \to \infty$. The sequence (x_k) is:

- *linearly convergent* if with a constant $0 \leq C < 1$ and some $K \in \mathbb{N}$:

$$\|x_{k+1} - \overline{x}\| \leq C\|x_k - \overline{x}\|, \qquad \forall k \geq K.$$

C is called convergence factor.

- *quadratically convergent* if with a constant $c \geq 0$,

$$\|x_{k+1} - \overline{x}\| \leq c\|x_k - \overline{x}\|^2, \qquad k \in \mathbb{N}.$$

- *superlinear convergence* if

$$\lim_{k\to\infty} \frac{\|x_{k+1} - \overline{x}\|}{\|x_k - \overline{x}\|} = 0\ .$$

Geometry "of min $f(x)$": For $f \in C^1(\mathbb{R}^n, \mathbb{R})$

Consider the level set $N_\alpha = \{x \mid f(x) = \alpha\}$ (*for some $\alpha \in \mathbb{R}$*) and a point $\overline{x} \in N_\alpha$ with $\nabla f(\overline{x}) \neq 0$. Then:

In a neigborhood of $\overline{x}$ the solution set N_α is a C^1-manifold of dimension $n - 1$ and at $\overline{x}$ we have

$$\nabla f(\overline{x}) \quad \perp \quad N_\alpha$$

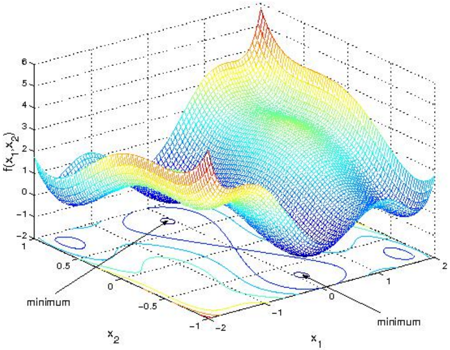
i.e., $\nabla f(\overline{x})$ is perpendicular to N_α and points into the direction where $f(x)$ has increasing values.

Notation: In this Chapter 5 of the "sheets" the gradient

$\nabla f(x)$ is always a column vector !!!!

Example: the 'humpback function'

$$\min \; x_1^2(4 - 2.1x_1^2 + \frac{1}{3}x_1^4) + x_1x_2 + x_2^2(-4 + 4x_2^2).$$



Two global minima: (0.089 -0.717) and (-0.0898 0.717), and four strict local minima.

5.1 Optimality conditions

Lem.5.1 [*Necessary optimality conditions*]
Let f be a C^2-function on $\mathbb{R}^n$. Then each local minimizer $\overline{x} \in \mathbb{R}^n$ of (P) satisfies:

(a) (First order condition) $\nabla f(\overline{x}) = 0$

(b) (Second order condition)

$$\mathbf{d}^T \nabla^2 f(\overline{x}) \mathbf{d} \geq 0 \quad \text{for all } \mathbf{d} \in \mathbb{R}^n.$$

(i.e. $\nabla^2 f(\overline{x}) \succeq 0$, posit.semi.def.)

Lem.5.2 [*Sufficient optimality conditions*] **Let f be a C^2-function on $\mathbb{R}^n$ and $\overline{x} \in \mathbb{R}^n$ such that**

$$\nabla f(\overline{x}) = 0 \quad \text{and} \quad \nabla^2 f(\overline{x}) \succ 0$$

Then $\overline{x}$ is a strict local minimizer of f.

Theoretical method: (based on optimality conditions)

- **Find a point $\overline{x}$ satisfying**

$$\nabla f(\overline{x}) = 0 \qquad \textit{(critical point)}$$

- **Check whether $\nabla^2 f(\overline{x}) \succ 0$.**

Minimization of convex functions

Th.4.4. **Let $f : \mathcal{F} \to \mathbb{R}$ be convex, $\overline{x} \in \mathcal{F}$. Then**

$$\overline{x} \text{ is loc. minim.} \quad \Rightarrow \quad \overline{x} \text{ is glob. minim.}$$

Moreover $\overline{x} \in \mathcal{F}$ is (global) minimizer if and only if

- $0 \in \partial f(\overline{\boldsymbol{x}})$ (*for general convex functions*)
- $0 = \nabla f(\overline{\boldsymbol{x}})$ (*for C^1 convex functions*)

5.2 Descent methods, steepest descent $(f \in C^1)$

Def. A vector $d_k \in \mathbb{R}^n$ is called a *descent direction* in x_k if

$$\nabla f(x_k)^T d_k < 0 \qquad (*)$$

Rem. If $(*)$ holds then for any $t > 0$ small enough:
$f(x_k + t d_k) < f(x_k)$

Abbreviation: $g(x) = \nabla f(x), \quad h(x) = \nabla^2 f(x),$
$$g_k = g(x_k), \qquad h_k = h(x_k)$$

Conceptual DESCENT METHOD: Choose a starting point $x_0 \in \mathbb{R}^n$ and $\epsilon > 0$. Iterate

step k: Given $x_k \in \mathbb{R}^n$, proceed as follows:

- if $||g(x_k)|| < \epsilon$, stop with $\overline{x} \approx x_k$.
- Choose a descent direction d_k in x_k: $\quad g_k^T d_k < 0$
- Find a solution t_k of the (one-dimens.) minimization problem

$$\min_{t \geq 0} f(x_k + t d_k) \quad \text{and put } x_{k+1} = x_k + t_k d_k. \qquad (**)$$

Rem. Minimization in $\mathbb{R}^n$ is reduced to (line) minimization in $\mathbb{R}$.

Steepest descent: (see Ex.5.7) use as descent direction

$$d_k = -\nabla f(x_k)$$

Ex.5.7 Assuming $\nabla f(x_k) \neq 0$, show that $d_k = -[\nabla f(x_k)]/\|\nabla f(x_k)\|$ solves the problem:

$$\min_{d \in \mathbb{R}^n} \nabla f(x_k)^T d \qquad \text{s.t.} \qquad \|d\| = 1$$

L.5.3 In the line-minimization step (**) we have

$$\nabla f(x_{k+1})^T d_k = 0$$

For the steepest descent method this means:

$$d_{k+1}^T d_k = 0 \qquad \textit{(ziggzagging)}$$

Th.5.1 [*Convergence result*] **Let $f \in C^1$. Apply the steepest descent method. If the iterates x_k converge, *i.e.,* $x_k \to \bar{x}$ then**

$$\nabla f(\bar{x}) = 0$$

Steepest descent applied to quadratic functions:

$q(\mathrm{x}) = \frac{1}{2}\mathrm{x}^T \mathrm{A}\mathrm{x}$, $\mathrm{A} \succ 0$, with (unique) minimizer $\bar{x} = 0$

Ex.5.8 **For quadratic functions the minimizer of $\min_{t \geq 0} f(x_k + td_k)$ is given by $t_k = -\frac{g_k^T d_k}{d_k^T A d_k}$.**

Th. 5.2 **Apply the steepest descent method to $q(\mathrm{x}) = \frac{1}{2}\mathrm{x}^T \mathrm{A}\mathrm{x}$, $\mathrm{A} \succ 0$. Then**

$$\sqrt{q(\mathrm{x}_{k+1})} \leq \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right) \sqrt{q(\mathrm{x}_k)}.$$

Here, $\lambda_{\min} > \mathbf{0}$ is the smallest and $\lambda_{\max} > \mathbf{0}$ the largest eigenvalue of **A**.

The proof is based on:

L. 5.4 *(Inequality of Kantorovich)* **Let A be a positive definite $n \times n$-matrix with eigenvalues $0 < \lambda_1 \le \ldots \le \lambda_n$. Then for any $x \in \mathbb{R}^n (x \neq 0)$:**

$$1 \ge \frac{(x^T x)^2}{(x^T A x)(x^T A^{-1} x)} \ge \frac{4\lambda_1 \lambda_n}{(\lambda_1 + \lambda_n)^2}.$$

Rem. **The next example shows that in general** *(even for min of quadratic functions)*, **the steepest descent method cannot be expected to converge better than *linearly*.**

Ex.5 .9. **Apply the steepest descent method to**

$$q(x) = x^T \begin{pmatrix} 1 & 0 \\ 0 & r \end{pmatrix} x \quad , \quad r \ge 1$$

Then with $x_0 = (r, 1)$ it follows

$$x_k = \left(\frac{r-1}{r+1}\right)^k (r, (-1)^k) \ .$$

(Linear convergence with factor $C = (r-1)/(r+1)$.)

5.3 Method of conjugate directions

Case: $f(x) = q(x) := \frac{1}{2}x^T Ax + b^T x$, $A \succ 0$ **(pd.)**

Idea. **Try to generate d_k's such that**
(*not only* $\nabla q(x_{k+1})^T d_k = 0$ *but*)

$$\nabla q(x_{k+1})^T d_j = 0 \quad \forall 0 \le j \le k$$

Then, after n steps we have

$$\nabla q(x_n)^T d_j = 0 \quad \forall 0 \le j \le n-1$$

and (*if the d_j's are lin. indep.*) $\nabla q(x_n) = 0$. So $x_n = -A^{-1}b$ is the minimizer of q.

L. 5.5 **Apply the descent method to $q(x)$. The following are equivalent:**

(i) $g_{j+1}^T d_i = 0$ for all $0 \le i \le j \le k$;

(ii) $d_j^T A d_i = 0$ for all $0 \le i < j \le k$.

Def. Vectors $d_0, \ldots, d_{n-1} \neq 0$ are called A-conjugate (or A-orthogonal) if: $d_j^T A d_i = 0 \quad \forall i \neq j$.

Ex. A collection of A-conjugate vectors $d_0, \ldots, d_{n-1} \neq 0$ in $\mathbb{R}^n$ are linearly independent.

Rem.: To obtain the conditions in L.5.5, simply try

$$d_k = -g_k + \alpha_k d_{k-1}$$

Then $d_k^T A d_{k-1} = 0$ implies $\alpha_k = \frac{g_k^T A d_{k-1}}{d_{k-1}^T A d_{k-1}}$.

Th.5.3 Apply the descent method to $q(x)$ with

$$d_k = -g_k + \alpha_k d_{k-1} \ , \quad \alpha_k = \frac{g_k^T A d_{k-1}}{d_{k-1}^T A d_{k-1}}$$

Then the d_k's are A-conjugate. In particular, the algorithm stops after *(at most)* n steps with the unique minimizer $\overline{x} = -A^{-1} b$ of q.

Conjugate Gradient Method

INIT: Choose $x_0 \in \mathbb{R}^n$, $\varepsilon > 0$, $d_0 := -g_0$;

ITER: WHILE $\|g_k\| \geq \varepsilon$ DO

BEGIN

Determine a solution t_k for the problem

$$(*) \qquad \min_{t \geq 0} f(x_k + t d_k)$$

Set $x_{k+1} = x_k + t_k d_k$.

Set $d_{k+1} = -g_{k+1} + \alpha_{k+1} d_k$.

END

Ex.5.10 Under the assumptions of Th.5.3, show that the iteration point x_{k+1} is the (global) minimizer of the quadratic function q on the affine subspace

$$S_k = \{x_0 + \gamma_0 d_0 + .. + \gamma_k d_k \mid \gamma_0, .., \gamma_k \in \mathbb{R}\}$$

Case: non-quadratic functions $f(x)$

Note that for quadratic function $f = q$ we have:

$$\alpha_{k+1} = \frac{g_{k+1}^T A d_k}{d_k^T A d_k} = \frac{g_{k+1}^T (g_{k+1} - g_k)}{d_k^T (g_{k+1} - g_k)}$$

$$= \frac{g_{k+1}^T (g_{k+1} - g_k)}{\|g_k\|^2} = \frac{\|g_{k+1}\|^2}{\|g_k\|^2}$$

So, for non-quadratic $f(x)$, in the CG-method, we can use the formulas:

Hestenes-Stiefel (1952): $\alpha_{k+1} = \dfrac{g_{k+1}^T (g_{k+1} - g_k)}{d_k^T (g_{k+1} - g_k)}$

Fletcher-Reeves (1964): $\alpha_{k+1} = \dfrac{\|g_{k+1}\|^2}{\|g_k\|^2}$

Polak-Ribiere (1969): $\alpha_{k+1} = \dfrac{g_{k+1}^T (g_{k+1} - g_k)}{\|g_k\|^2}$

Application to sparse systems $Ax = b, \quad A \succeq 0$

Def. $A = (a_{ij})$ is sparse if less than

α% of the a_{ij}-s are $\neq 0$ with *(say)* $\alpha \leq 5$

CG-method: apply the CG-method to

$$\min \frac{1}{2}x^T A x - b^T x \quad \text{with solution } \overline{x} = A^{-1}b$$

Conjugate Gradient Meth. for Lin. Systems

INIT: Choose $x_0 \in \mathbb{R}^n$ and $\varepsilon > 0$ and set $d_0 = -g_0$;

ITER: WHILE $\|g_k\| \geq \varepsilon$ DO

BEGIN

Set $x_{k+1} = x_k + t_k d_k$ with $t_k = -\dfrac{g_k^T d_k}{d_k^T A d_k}$

Set $g_{k+1} = g_k + t_k A d_k$

Set $d_{k+1} = -g_{k+1} + \alpha_{k+1} d_k$ with $\alpha_{k+1} = \dfrac{g_{k+1}^T g_{k+1}}{g_k^T g_k}$.

END

Rem. Complexity: $\approx \frac{\alpha}{100} n^2$ flop's per ITER.

5.4 Line minimization

In the general descent method (see Ch.5.2) we have to repeatedly solve:

$$\min_{t \geq 0} \; h(t) \quad \text{with } h(t) = f(x_k + td_k)$$

where $h'(0) < 0$.

This can be done by:

- ***'exact line minimization'*** **of numerical analysis** *e.g.*, **bisection, golden section, Newton-, secant method**
- **or better by** ***'inexact line search'*** *Goldstein-, Goldstein-Wolfe test*

5.5 Newton's method:

Basis method *using* $\nabla f(x), \nabla^2 f(x)$*; is (locally) quadratically convergent.*

Newtons's Iteration: For solving $F(x) = 0$

with $F : \mathbb{R}^n \to \mathbb{R}^n$ *(a system of n equations in n unknowns)*

$$\boxed{x_{k+1} \;=\; x_k - [\nabla F(x_k)]^{-1} F(x_k)}$$

Th.5.4 (***local convergence of Newton's method***)

Given $F : \mathbb{R}^n \to \mathbb{R}^n$, $F \in C^2$ **such that**

$$F(\overline{x}) = 0 \quad \text{and} \quad \nabla F(\overline{x}) \text{ is non-singular.}$$

Then the Newton iteration x_k **converges quadratically to** $\overline{x}$ **for any** x_0 **sufficiently close to** $\overline{x}$**.**

'Newton' for solving : min $f(x)$ or $F(x) := \nabla f(x) = 0$.

$$x_{k+1} = x_k - [\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

(local) quadratic convergence if: $f \in C^3$, $\nabla f(\overline{x}) = 0$ with $\nabla^2 f(\overline{x})$ non-singular.

Problems: Newton for min $f(x)$

- $x_k \to \overline{x}$ possibly a loc. maximizer.
- $x_k \to x_{k+1}$ with *increasing "f"*

Newton descent method: The 'Newton direction'

$$d_k = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

is a *descent direction* ($g_k^T d_k < 0$) if (*assume* $\nabla f(x_k) \neq 0$):

$$[\nabla^2 f(x_k)]^{-1} \text{ or equivalently } \nabla^2 f(x_k)$$

is positive definite.

Algorithm: *(Levenberg-Marquardt variant)*

step k: **Given $x_k \in \mathbb{R}^n$ with $g_k \neq 0$.**

1. **determine $\sigma_k > 0$ such that $(\nabla^2 f(x_k) + \sigma_k I) \succ 0$,**

   compute $d_k = -\big(\nabla^2 f(x_k) + \sigma_k I\big)^{-1} g_k \quad (*)$

2. **Find a minimizer t_k of** $\min_{t \geq 0} f(x_k + t d_k)$

   and put $x_{k+1} = x_k + t_k d_k$.

Ex. ***[connection with the 'trust region method']***
Consider the quadratic Taylor approximation of f near x_k:

$$q(x) := f(x_k) + \nabla f(x_k)^T (x - x_k) + \frac{1}{2}(x - x_k)^T \nabla^2 f(x_k)(x - x_k)$$

Compute the descent step d_k according to $(*)$ *(Levenberg-Marquardt)* **and put $x_{k+1} = x_k + d_k$, $\tau := \|d_k\|$.**
Show that x_{k+1} is a local minimizer of the *trust region problem*: $\min \; q(x) \quad \text{s.t.} \quad \|x - x_k\| \leq \tau$

Disadvantage of the Newton methods:

- $\nabla^2 f(x_k)$ needed
- work per step: linear system
  $F_k x = b_k$ $\approx n^3$ flop's

5.6 The Gauss-Newton Method

min $f(x)$ for the case: (*nonlinear least square*)

$$f(x) = \frac{1}{2}\|r(x)\|^2 = \frac{1}{2}\sum_{i=1}^{m} r_i^2(x) \ .$$

with • $r_i \in C^2(\mathbb{R}^n, \mathbb{R})$ • $m \geq n$.

derivatives of f:

$$\begin{aligned} \nabla f(\mathrm{x}) &= \nabla r(\mathrm{x}) \cdot r(\mathrm{x}) \\ \nabla^2 f(\mathrm{x}) &= \nabla r(\mathrm{x})[\nabla r(\mathrm{x})]^T + \sum_{i=1}^{m} r_i(\mathrm{x}) \nabla^2 r_i(\mathrm{x}). \end{aligned}$$

The method uses the first order approximation $A(x) = \nabla r(\mathrm{x})[\nabla r(\mathrm{x})]^T$ of $\nabla^2 f(x)$: (*and iterates*)

$$x_{k+1} = x_k - [A(x_k)]^{-1} \nabla f(x_k) \ .$$

5.7 Quasi-Newton method

Algorithm *which only uses* $\nabla f(x_k)$*; needs* $\mathcal{O}(n^2)$ *flop's per step; and is "Newton like" superlinear convergent.*

Consider the descent method with:

$$d_k = -H_k g_k$$

desired properties for H_k:

- i $H_k \succ 0$
- ii $H_{k+1} = H_k + E_k$ **simple update rule**
- iii **for quadratic f $\to$ conjugate directions d_j**
- iv **the *Quasi-Newton condition*:**

$$(x_{k+1} - x_k) = H_{k+1}(g_{k+1} - g_k)$$

Notation: $\delta_k := (x_{k+1} - x_k)$, $\gamma_k := (g_{k+1} - g_k)$

Quasi-Newton Method

INIT: Choose some $x_0 \in \mathbb{R}^n$, $H_0 \succ 0$, $\varepsilon > 0$

ITER: WHILE $\|g_k\| \geq \varepsilon$ DO

BEGIN

Set $d_k = -H_k g_k$,

Determine a solution t_k for the problem

$$\min_{t \geq 0} f(x_k + td_k)$$

Set $x_{k+1} = x_k + t_k d_k$ and update

$H_{k+1} = H_k + E_k$.

END

For the *update* E_k try: with $\alpha, \beta, \mu \in \mathbb{R}$

$$E_k = \alpha uu^T + \beta vv^T + \mu(uv^T + vu^T) \quad (*)$$

where $u := \delta_k, \; v := H_k \gamma_k$

Note that E_k is symmetric with rank ≤ 2.

L.5.6 **Apply the Quasi-Newton method to $q(x) = \frac{1}{2}x^T Ax + b^T x$, $A \succ 0$ with**

E_k of the form (*) and

H_{k+1} satisfying iv: $\delta_k = H_{k+1}\gamma_k$

Then the directions d_j are A-conjugate :

$$d_j^T A d_i = 0 \qquad 0 \le i < j \le k$$

Last step: Find α, β, μ in (*) such that (iv) holds. This leads to the following *update.*

***Broyden family*: with $\Phi \in \mathbb{R}$**

$$H_{k+1} = H_k + \frac{\delta_k \delta_k^T}{\delta_k^T \gamma_k} - \frac{H_k \gamma_k \gamma_k^T H_k}{\gamma_k^T H_k \gamma_k} + \Phi\, w w^T \quad (**)$$

where $w := \left(\frac{\delta_k}{\delta_k^T \gamma_k} - \frac{H_k \gamma_k}{\gamma_k^T H_k \gamma_k} \right) (\gamma_k^T H_k \gamma_k)^{\frac{1}{2}}.$

As special cases we obtain:

$\Phi = 0$, the *DFP-method* (1963)
(Davidon, Fletcher, Powell)

$\Phi = 1$, the *BFGS-method* (1970)
(Broyden, Fletcher, Goldfarb, Shanno)

The next lemma finally shows that property i): $H_k \succ 0$ is preserved.

L.5.7 In the Quasi-Newton method, if we use (**) with $\Phi \geq 0$, then

$$H_k \succ 0 \quad \Rightarrow \quad H_{k+1} \succ 0$$

5.8 Minimization of nondifferentiable f

5.8.1 Subgradient method (f convex)

Problem: $\min_{x \in \mathbb{R}^n} f(x)$, where f is nondifferentiable but convex.

Idee: In a descent method replace the *search direction* $d_k = -\nabla f(x_k)$ by $d_k = -g_k \in -\partial f(x_k)$.

Subgradient Steepest Descent

INIT: Choose $\mathbf{x}_0 \in \mathbb{R}^n$

ITER: WHILE $\mathbf{0} \notin \partial f(\mathbf{x}_k)$ DO

BEGIN

Choose a $\mathbf{g}_k \in \partial f(\mathbf{x}_k)$, set $\mathbf{d}_k = -\mathbf{g}_k / \|\mathbf{g}_k\|$

Determine a solution t_k for the problem

$$(*) \qquad \min_{t \geq 0} f(\mathbf{x}_k + t\mathbf{d}_k)$$

Set $\mathbf{x}_{k+1} = \mathbf{x}_k + t_k \mathbf{d}_k$.

END

Problem:

- $\mathbf{0} \neq -\mathbf{g}_k \in -\partial f(x_k)$ **is possibly *not a descent* direction**

- **possibly converges to a non-optimal $\overline{x}$ (where f is not differentiable)**

However For convex *f* with $\mathbf{d}_k = -\mathbf{g}_k/\|\mathbf{g}_k\| \neq 0$ and any minimizer $\overline{x}$ we have:

$$\mathbf{d}_k^T(\overline{x} - \mathbf{x}_k) \geq \frac{f(\mathbf{x}_k) - f(\overline{x})}{\|\mathbf{g}_k\|} > 0$$

i.e., $\mathbf{d}_k$ and $(\overline{x} - \mathbf{x}_k)$ form an acute angle.

L.5.8 $f : \mathbb{R}^n \to \mathbb{R}$ **convex, $\overline{x}$ a minimizer, $\mathbf{0} \neq \mathbf{g}_k \in \partial f(\mathbf{x}_k)$. Then for** $0 < t_k \leq \mathbf{d}_k^T(\overline{x} - \mathbf{x}_k)$, $\mathbf{x}_{k+1} = \mathbf{x}_k + t_k\mathbf{d}_k$**:**

$$\|\mathbf{x}_{k+1} - \overline{x}\|^2 \leq \|\mathbf{x}_k - \overline{x}\|^2 - t_k\mathbf{d}_k^T(\overline{x} - \mathbf{x}_k)$$

Subgradient Method
INIT: Choose $\mathbf{x}_0 \in \mathbb{R}^n$ and 'steps' $t_k > 0$
ITER: Choose a $\mathbf{g}_k \in \partial f(\mathbf{x}_k)$.
(If $\mathbf{g}_k = \mathbf{0}$, STOP)
Set $\mathbf{d}_k = -\mathbf{g}_k/\|\mathbf{g}_k\|$ and $\mathbf{x}_{k+1} = \mathbf{x}_k + t_k\mathbf{d}_k$.

Step-size t_k?: (Without line-minimization). Choose a sequence $t_k > 0$ *a-priori* such that

$$(\star) \qquad \lim_{k\to\infty} t_k = 0 \quad \text{and} \quad \sum_{k=0}^{\infty} t_k = \infty \ .$$

Th.5.6 $f : \mathbb{R}^n \to \mathbb{R}$ convex with (at least one) minimizer $\overline{x}$. Choose $t_k > 0$ such that $(\star)$ holds. Then the subgradient method generates points $\mathbf{x}_0, \mathbf{x}_1, \ldots$ such that

$$\min\{f(\mathbf{x}_0), \ldots, f(\mathbf{x}_k)\} \to \quad f(\overline{x}) \qquad (k \to \infty)$$

Convergence: is ***sub-linear*** **!!!**

Better convergence if the minimum value $\bar{f} = f(\bar{\mathbf{x}})$ of f is known and if $\bar{\mathbf{x}}$ is a *strict minimizer of order* 1**:** *i.e.* **there exists some constant $L > 0$ such that**

$$(\star) \qquad f(\mathbf{x}) - f(\bar{\mathbf{x}}) \geq L\|\mathbf{x} - \bar{\mathbf{x}}\| \quad \forall x \in \mathbb{R}^n$$

Th.5.7 **If $f : \mathbb{R}^n \to \mathbb{R}$ is convex and ($\star$) holds for the minimizer $\bar{\mathbf{x}} \in \mathbb{R}^n$, then the subgradient method with step sizes**

$$t_k = \frac{f(\mathbf{x}_k) - f(\bar{\mathbf{x}})}{\|\mathbf{g}_k\|} \quad \left(\geq L\frac{\|\mathbf{x}_k - \bar{\mathbf{x}}\|}{\|\mathbf{g}_k\|} \right)$$

converges linearly to $\bar{\mathbf{x}}$.

5.8.2 "Lipschitz minimization", global minimizer.

Problem: $\min_{x \in \mathcal{F}} f(x)$, with $\mathcal{F} \subset \mathbb{R}^n$, compact, where $f \in C^0$ is non-convex.

Bad news. Even for $f : [0,1] \to \mathbb{R}$ ***"without some global information"***:
No upper bounds for the *"complexity"* can be given for the computation of an ε-approximation x for a *global minimizer* $\overline{x}$ of f, i.e.,

$$f(x) \leq f(\overline{x}) + \varepsilon$$

However a (known) Lipschitz-constant L, i.e.,

$$|f(\mathbf{x}) - f(\mathbf{y})| \leq L \, \|\mathbf{x} - \mathbf{y}\| \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{F}$$

yields such a global information.
Based on the knowledge of L an exhaustive search can be done to find an ε-approximation.