Iterative methods based on minimization techniques

We consider once again the problem of solving the linear system $Ax=b$. Suppose we can find a function $f: R^n \to R$ such that the solution x of $Ax=b$ is a (global) minimum of f. Then, any minimization algorithm can be use to approximate x. Of course, the minimization procedure should not lead to a problem more difficult than the solution of the original system and should converge with "reasonably" fast.

It turns out that if A is symmetric, positive definite, then an associated function f can be readily found.

Theorem Let A be an $n\times n$, symmetric, positive definite matrix. Then x is a solution of the linear system $Ax=b$ if and only if it is a global minimizer of the function $f(x): R^n \to R$ given by

$$f(x) = \frac{1}{2} x^T A x - b^T x .$$

Proof

Fix $x \in R^n$. Then, every vector $y \in R^n$ can be expressed as $y = x + \varepsilon v$ for some scalar ε and $v \in R^n$. We have

$$f(y) = f(x+\varepsilon v) = \frac{1}{2}(x+\varepsilon v)^T A (x+\varepsilon v) - b^T(x+\varepsilon v)$$

$$= \frac{1}{2} x^T A x - b^T x + \varepsilon \left[Ax - b \right] + \frac{1}{2}\varepsilon^2 v^T A v$$

$$= f(x) + \varepsilon v^T [Ax - b] + \frac{1}{2} \varepsilon^2 v^T A v.$$

Now if x solves $Ax = b$, then

$$f(y) = f(x) + \frac{1}{2} \varepsilon^2 v^T A v$$
$$\geq f(x), \qquad \forall y \in R^n$$

since A is s.p.d. . Hence x is a global minimizer of f.
Conversely, assume that x is a global minimum of f but that $Ax - b \neq 0$. We can find $v \neq 0$ such that $v^T [Ax - b] \equiv \alpha < 0$.
Thus

$$f(y) = f(x) + \varepsilon \alpha + \frac{1}{2} \varepsilon^2 v^T A v.$$
$$= f(x) + \varepsilon \left[\alpha + \frac{1}{2} \varepsilon v^T A v \right]$$

Since v is fixed and $\alpha < 0$, we can choose $\varepsilon > 0$ sufficiently small so that $\alpha + \frac{1}{2} \varepsilon v^T A v < 0$. This implies that $f(y) = f(x) +$ negative number

$\Rightarrow y = x + \varepsilon v \neq x$, $f(y) < f(x)$ which contradicts the fact that x is a global minimum of f. ■

Thus, in the special case where A is s.p.d., any minimization algorithm applied to the function $f(x) = \frac{1}{2} x^T A x - b^T x$, is in fact, an iterative algorithm for approximating the solution x of $Ax = b$.
One of the most simple minded (and slowest) methods is the steepest descent method

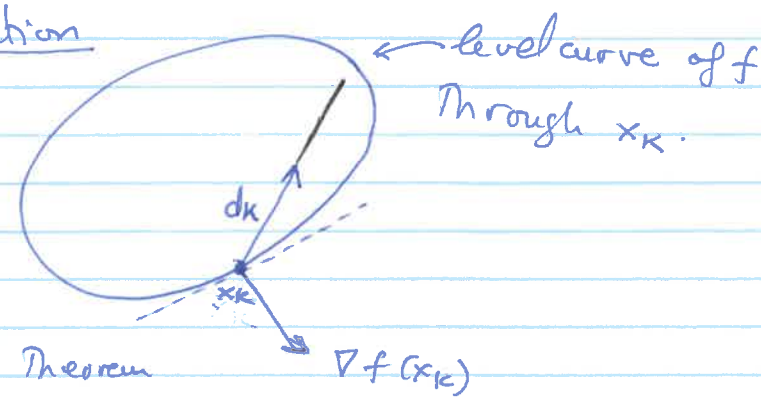
It is a special case of a class of <u>line search methods</u> which consist in replacing a minimization problem of the form

$$\underline{\text{Find } x \in \mathbb{R}^n} \quad \text{such that } f(x) = \inf_{v \in \mathbb{R}^n} f(v)$$

by a sequence of one-dimensional minimization problems along certain directions ("promising", "feasible", etc.)

Given x_k and a <u>direction</u> vector d_k, we say that d_k is a <u>feasible</u> direction at x_k if

$$\nabla f(x_k) \cdot d_k < 0.$$



Indeed, from Taylor's Theorem it follows that

$$f(x) = f(x_k) + \nabla f(x_k) \cdot (x - x_k) + O(\|x - x_k\|^2).$$

Suppose we restrict x to the half-line $x_k + \alpha d_k$, $\alpha > 0$. It then follows that

$$f(x_k + \alpha d_k) = f(x_k) + \alpha \nabla f(x_k) \cdot d_k + O(\alpha^2 \|d_k\|^2).$$

We see that there exists an open interval $(0, \epsilon)$ such that for $\alpha \in (0, \epsilon)$, $f(x_k + \alpha d_k) < f(x_k)$. In other words, it is possible to decrease the value of f in the direction of d_k, at least locally.

Of course nothing prevents us from posing the problem

(*) $$\boxed{\text{Find } \alpha_k > 0 \quad \text{such that } f(x_k + \alpha_k d_k) = \inf_{\alpha > 0} f(x_k + \alpha d_k).}$$

<u>If</u> such an α can be found, then we declare

$$x_{k+1} = x_k + \alpha_k d_k.$$

In the quadratic case, i.e. $f(x) = \frac{1}{2} x^T A x - b^T x$, where A is symmetric, positive definite, the one dimensional minimization problem (*) has a unique solution. Indeed, let $g: \mathbb{R} \to \mathbb{R}$ be given by

$$g(\alpha) = \frac{1}{2}(x_k + \alpha d_k)^T A (x_k + \alpha d_k) - (x_k + \alpha d_k)^T b$$

$$= \frac{1}{2} x_k^T A x_k + \alpha d_k^T A x_k + \frac{1}{2}\alpha^2 d_k^T A d_k - x_k^T b - \alpha d_k^T b.$$

From which we easily obtain

$$0 \equiv g'(\alpha_k) = \alpha_k d_k^T A d_k + d_k^T (A x_k - b)$$

$$\Rightarrow \boxed{\alpha_k = \frac{(b - A x_k)^T d_k}{d_k^T A d_k}}$$

Line-search Algorithm: The quadratic case

Given $x_0 \in \mathbb{R}^n$, and feasible directions d_k, $k \geq 0$

$$\begin{cases} x_{k+1} = x_k + \alpha_k d_k \\ \alpha_k = \dfrac{r_k^T d_k}{d_k^T A d_k}, \quad r_k = b - A x_k. \end{cases}$$

It can be shown that if one can guarantee feasible directions d_k satisfying

$$d_k^T \nabla f(x_k) < -\delta \qquad \forall k \geq 0,$$

Then the method is convergent.

The Method of steepest descent. We know that a function decreases fastest locally in the direction of $-\nabla f(x_k)$. Hence it makes sense to choose $\boxed{d_k = -\nabla f(x_k)}$

Thus

$$\boxed{\alpha_k = \frac{r_k^T A r_k}{r_k^T r_k}}$$

which brings us to the method of steepest descent for the quadratic function

$$\begin{cases} x_{k+1} = x_k + \alpha_k d_k, & k \geq 0. \\ d_k = r_k \equiv b - Ax_k = -\nabla f(x_k) \\ \alpha_k = \dfrac{r_k^T A r_k}{r_k^T r_k} \end{cases}$$

Convergence properties of the method of steepest descent.

We shall consider only the case of the quadratic function

$f(x) = \frac{1}{2} x^T A x$, with A being symmetric, positive definite.

Lemma The iterative process

$$x_{k+1} = x_k + \alpha_k r_k, \qquad r_k = b - Ax_k, \quad \alpha_k = \frac{r_k^T A r_k}{r_k^T r_k}$$

satisfies

$$E(x_{k+1}) = \left\{ 1 - \frac{(r_k^T r_k)^2}{(r_k^T A r_k)(r_k^T A^{-1} r_k)} \right\} E(x_k),$$

where the error functional $E: R^n \to R$ is given by

$$E(y) = \frac{1}{2}(x-y)^T A (x-y).$$

proof The proof is by direct computation. We have, setting $y_k = x_k - x$,

$$\frac{E(x_k)-E(x_{k+1})}{E(x_k)} = \frac{2\alpha_k r_k^T A r_k - \alpha_k^2 r_k^T A r_k}{y_k^T A y_k}.$$

Using $r_k = A y_k$, we have

$$\frac{E(x_k)-E(x_{k+1})}{E(x_k)} = \frac{\frac{2(r_k^T r_k)^2}{r_k^T A r_k} - \frac{(r_k^T r_k)^2}{r_k^T A r_k}}{r_k^T A^{-1} r_k} = \frac{(r_k^T r_k)^2}{r_k^T A^{-1} r_k},$$

from which the result follows. ■

In order to obtain a bound on the rate of convergence, we need a bound on the r.h.s. of (1). The best bound is due to Kantorovich and his Lemma stated below.

<u>Lemma</u> (Kantorovich inequality) Let A be a symmetric, positive definite matrix. For any vector x there holds

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

where λ_1 and λ_n are respectively the smallest and largest eigenvalues of A.

<u>proof.</u>

Let the eigenvalues $\lambda_1, \dots, \lambda_n$ of A satisfy

$$0 < \lambda_1 \leq \lambda_2 \cdots \leq \lambda_n .$$

Since A is symmetric, A has a complete set of corresponding orthonormal eigenvectors $v_1, \dots, v_n$. Indeed, if $Q \equiv (v_1 | \cdots | v_n)$ then $Q^T A Q = \Lambda = \mathrm{diag}\{\lambda_1, \dots, \lambda_n\}$.

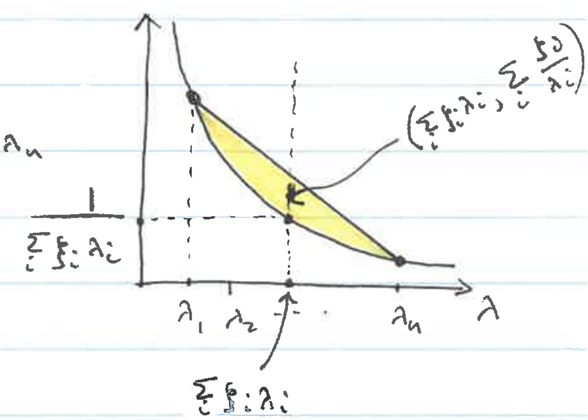
Now let $x = \sum_{i=1}^{n} \alpha_i v_i$. Then

$$\frac{(x^T x)^2}{(x^T A x)(x^T A^{-1} x)} = \frac{\left(\sum_{i=1}^{n} \alpha_i^2\right)^2}{\left(\sum_i \lambda_i \alpha_i^2\right)\left(\sum_i \lambda_i^{-1} \alpha_i^2\right)},$$

which can be written as

$$\frac{(x^T x)^2}{(x^T A x)(x^T A^{-1} x)} = \frac{\dfrac{1}{\sum \xi_i \lambda_i}}{\sum_i \left(\dfrac{\xi_i}{\lambda_i}\right)} \equiv \frac{\phi(\xi)}{\psi(\xi)}, \quad \text{where } \xi_i = \frac{\alpha_i^2}{\sum_j \alpha_j^2}.$$

(without loss, one could take $\sum_i \alpha_i^2 = 1$!!)



Note that $\sum_i \xi_i^2 = 1$.

$\Rightarrow$ $\sum_i \xi_i \lambda_i$ is a point between λ_1 and λ_n

Also, the point $\left(\sum_i \xi_i \lambda_i, \sum_i \frac{\xi_i}{\lambda_i}\right)$ is a convex combination of the points $(\lambda_1, \frac{1}{\lambda_1}), \ldots, (\lambda_n, \frac{1}{\lambda_n})$, hence it belongs to the convex hull of these pts., i.e. the shaded region. It also belongs to the same vertical line as $\left(\sum_i \xi_i \lambda_i, \frac{1}{\sum_i \xi_i \lambda_i}\right)$. Thus, an appropriate lower bound for $\frac{\phi(\xi)}{\psi(\xi)}$ is

$$\min_{\lambda_1 \le \lambda \le \lambda_n} \frac{\frac{1}{\lambda} \quad \leftarrow \text{pt. on curve}}{(\lambda_1 + \lambda_n - \lambda)/\lambda_1 \lambda_n \quad \leftarrow \text{pt. on line.}}$$

which is minimized at $\lambda = \frac{\lambda_1 + \lambda_n}{2}$ and has value there equal to $\frac{4 \lambda_1 \lambda_n}{(\lambda_1 + \lambda_n)^2}$.

Using Kantorovich's bound in (1) we get

<u>Theorem</u> (Steepest descent - quadratic case) Assume that A is s.p.d. Then for any $x_0 \in R^n$, the method of steepest descent converges to the unique minimum of

$$f(x) = \frac{1}{2} x^T A x - b^T x$$

i.e. the unique solution of the system $Ax = b$. Furthermore, with $E(x_k) = \frac{1}{2}(x_k - x)^T A (x_k - x)$, there holds

$$E(x_{k+1}) \le \left(\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}\right)^2 E(x_k), \qquad k = 0, 1, \ldots$$

$$= \left(\frac{1 - \lambda_1/\lambda_n}{1 + \lambda_1/\lambda_n}\right)^2 E(x_k). \qquad \blacksquare$$

<u>Remark</u> If the matrix A is such that $0 < \frac{\lambda_1}{\lambda_n} << 1$, then the ratio

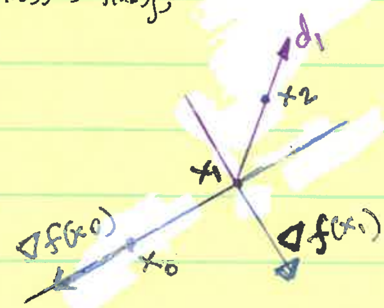
$$\frac{1 - \lambda_1/\lambda_n}{1 + \lambda_1/\lambda_n}$$ will be very close to 1

and consequently, convergence will be slow.

The Conjugate Gradient method

Let A be s.p.d. and let $f(x) = \frac{1}{2} x^T A x - b^T x$.

Given x_k, we define x_{k+1} as the solution of the minimization problem : Find $x_{k+1} \in x_k + G_k$; $G_k = \text{span}\{\nabla f(x_0), \ldots, \nabla f(x_k)\}$,



$$(*) \quad f(x_{k+1}) = \inf_{v \in G_k} f(x_k + v) .$$

$$= \inf_{v \in x_k + G_k} f(v)$$

Theorem Let A be $n \times n$ s.p.d.

(i) The algorithm is well-defined; i.e. for each $k \geq 0$, $(*)$ has a unique solution.

(ii) The successive gradients $\nabla f(x_0), \ldots \nabla f(x_k)$ are mutually orthogonal, i.e. $\nabla f(x_i) \cdot \nabla f(x_j) = 0$, $i \neq j$.

(iii) The algorithm terminates (in exact arithmetic) in at most n iterations.

proof

(i) First, we assume without loss of generality that $\nabla f(x_i) \neq 0$, $i = 0, \ldots, k$. For otherwise $\nabla f(x_i) = Ax_i - b = 0$ $\Rightarrow$ x_i is the solution.

Fix $z \in G_k$ to be appropriately chosen below so that $x_k + z$ is the solution of $(*)$. For $v \in G_k$, let $h = v - z$. Now,

$$f(x_k+v) = f(x_k+z+h) = \tfrac{1}{2}(x_k+z)^T A(x_k+z) + (x_k+z)^T A h + \tfrac{1}{2} h^T A h - b^T(x_k+z) - b^T h$$

$$\cdots(1) \qquad = f(x_k+z) + \left[(x_k+z)^T A h - b^T h\right] + \tfrac{1}{2} h^T A h$$

$$= f(x_k+z) + \left[Az + r_k\right]^T h + \tfrac{1}{2} h^T A h . \qquad (h = v - z)$$

<u>claim</u>: $f(x_k+z) = \inf_{v \in G_k} f(x_k+v) \iff (Az+r_k)^T w = 0 \quad \forall w \in G_k$.

$(\Rightarrow)$ Fix $w \in G_k$ and let $v = z + tw$, $t \in \mathbb{R}$. From ⊛

$$f(x_k+v) = f(x_k+z+tw) = f(x_k+z) + (Az+r_k)^T tw + \frac{t^2}{2} w^T A w .$$

It is easy to see that $(Az+r_k)^T w \geq 0$ for otherwise, by choosing $t > 0$ and sufficiently small, we get $f(x_k+v) < f(x_k+z)$ which contradicts the fact that x_k+z minimizes $f(x_k+\cdot)$ over G_k. Similarly, choosing $t<0$ and sufficiently small, we see that $(Az+r_k)^T w \leq 0$. Combining these two, we get $(Az+r_k)^T w = 0$. Since $w \in G_k$ was arbitrary, $(\Rightarrow)$ follows.

$(\Leftarrow)$ Suppose $(Az+r_k)^T w = 0$ $\forall w \in G_k$. Let $v \in G_k$, then with $h = v - z$, from ⊛ we get

$$f(x_k+v) = f(x_k+z) + \tfrac{1}{2} h^T A h$$
$$\geq f(x_k+z) \quad \text{since } A \text{ is s.p.d.}$$

Moreover, equality holds iff $h = 0$ i.e. $v = z$.

we shall next show that the equation

$$(2) \qquad (Az + r_k)^T w = 0 \qquad \forall\, w \in G_k$$

has a unique solution $z \in G_k$. Indeed, let $\{\phi_0, \dots, \phi_m\}$ $m \le k$ be a basis for G_k. writing $z = \sum_{j=0}^{m} \alpha_j \phi_j$, (**) becomes equivalent to the linear system

$$(3) \qquad M \vec{\alpha} = \vec{\rho}$$

where $\quad M_{ij} = \phi_i^T A \phi_j \quad , \qquad i,j = 0, \dots, m$

$$\rho_i = -r_k^T \phi_i \quad , \quad i = 0, \dots, m.$$

Since A is s.p.d., it is easy to see that M is s.p.d. $\Rightarrow$ $\vec{\alpha}$ and consequently z exist uniquely.

(ii) Note that $Az + r_k = Az + Ax_k - b = A(x_k + z) - b$
$= \nabla f(x_{k+1})$.

From (2), $\nabla f(x_{k+1}) \cdot w = 0 \quad \forall\, w \in G_k$, in particular
$\nabla f(x_{k+1}) \cdot \nabla f(x_j) = 0 \,, \qquad j = 0, \dots, k.$

(iii) Suppose that $\nabla f(x_i) \ne 0$, $\quad i = 0, \dots, n-1$.
Then from the above $\{\nabla f(x_0), \dots, \nabla f(x_{n-1})\}$ are lin. indep. since they are mutually orthogonal. This implies that $G_{n-1} = R^n \Rightarrow x_n = x$ since the two problems $f(x_n) = \inf_{v \in G_{n-1} = R^n} f(x_k + v)$ and $f(x) = \inf_{v \in R^n} f(v)$ are equivalent. ∎

Lemma Define the vectors Δ_ℓ, $\ell = 0, \dots, k$ by

$$\Delta_\ell = x_{\ell+1} - x_\ell \equiv \sum_{i=0}^{\ell} s_{i\ell} \nabla f(x_i)$$

where the (nonzero) vectors $\nabla f(x_i)$ are generated by the CG method. Then, $\Delta_0, \dots, \Delta_k$ are conjugate with respect to A, i.e.

$$\Delta_i^T A \Delta_j = 0 \quad , \quad i \neq j = 0, \dots, k.$$

proof.

We write $\nabla f(v+w) = A(v+w) - b = Av - b + Aw$
$= \nabla f(v) + Aw,$

and in particular, with $v = x_\ell$ and $w = \Delta_\ell \Rightarrow v + w = x_{\ell+1}$,

$$(*) \qquad \nabla f(x_{\ell+1}) = \nabla f(x_\ell) + A\Delta_\ell, \qquad 0 \le \ell \le k.$$

The vectors $\nabla f(x_\ell)$, $\ell = 0, \dots, k+1$ being orthogonal, we have

$$0 = \nabla f(x_\ell)^T \nabla f(x_{\ell+1}) = \| \nabla f(x_\ell) \|_2^2 + \nabla f(x_\ell)^T A \Delta_\ell, \quad \ell = 0, \dots, k.$$

Since $\nabla f(x_\ell) \neq 0$, it follows that $\Delta_\ell \neq 0$. Also, for $k \ge 1$, from (*)

$$0 = \nabla f(x_{\ell+1})^T \nabla f(x_i) = \underbrace{\nabla f(x_\ell)^T \nabla f(x_i)}_{0} + \nabla f(x_i)^T A \Delta_\ell$$

$$= \nabla f(x_i)^T A \Delta_\ell, \qquad 0 \le i < \ell \le k.$$

So, for $0 \le i < \ell \le k$,

$$\Delta_i^T A \Delta_\ell = \left(\sum_{j=0}^{i} s_{ji} \nabla f(x_j) \right)^T A \Delta_\ell = 0.$$

We have thus shown that each Δ_ℓ is A-conjugate to the previous Δ's. This effectively concludes the proof. ∎

It is easy to show that the (nonzero) vectors $\Delta_0, \dots$ are linearly independent. Hence we may write

$$\left[\Delta_0 \,\middle|\, \Delta_1 \,\middle|\, \cdots \,\middle|\, \Delta_k\right] = \left[\nabla f(x_0) \,\middle|\, \nabla f(x_1) \cdots \,\middle|\, \nabla f(x_k)\right] \overbrace{\begin{bmatrix} \delta_{00} & \delta_{01} & \cdots & \delta_{0k} \\ & \delta_{11} & \cdots & \delta_{1k} \\ & O & \ddots & \\ & & & \delta_{kk} \end{bmatrix}}^{D}.$$

By linear independence of the sets $\{\Delta_0, \dots, \Delta_k\}$ and $\{\nabla f(x_0), \dots, \nabla f(x_k)\}$, the (upper triangular) matrix D is invertible $\Rightarrow \delta_{\ell\ell} \neq 0, \quad \ell = 0, \dots, k$.

Now we make the simple but important observation that

$$f(x_{k+1}) = \inf_{v \in G_k} f(x_k + v) = f(x_k + \Delta_k)$$

$$= \inf_{\alpha \in R} f(x_k + \alpha d_k)$$

where d_k is any nonzero vector in the direction of Δ_k.

So, if we knew the right direction d_k, we could compute x_{k+1} as the solution of the one-dimensional search problem

$$f(x_{k+1}) = \inf_{\alpha \in R} f(x_k + \alpha d_k)$$

$$\Rightarrow \alpha_k = - \frac{\nabla f(x_k)^T d_k}{d_k^T A d_k} = - \frac{r_k^T d_k}{d_k^T A d_k}.$$

So, we try to find a simple formula for d_k!

we choose

$$d_\ell \equiv \frac{1}{\delta_{\ell\ell}} \Delta_\ell = \sum_{j=0}^{\ell} \frac{\delta_{j\ell}}{\delta_{\ell\ell}} \nabla f(x_j) \equiv \sum_{j=0}^{\ell} \lambda_{j\ell} \nabla f(x_j)$$

$\lambda_{j\ell} = \dfrac{\delta_{j\ell}}{\delta_{\ell\ell}}, \quad \lambda_{\ell\ell} = 1$

Now, using ⊛ in previous lemma, for $0 \le l \le k-1$

$$0 = d_k^T A \Delta_l = d_k^T \left(\nabla f(x_{l+1}) - \nabla f(x_l) \right)$$

or

$$0 = \sum_{i=0}^{k} \lambda_{ik} \nabla f(x_i)^T \left(\nabla f(x_{l+1}) - \nabla f(x_l) \right)$$

$$\Rightarrow \quad - \lambda_{lk} \| \nabla f(x_l) \|_2^2 + \lambda_{l+1,k} \| \nabla f(x_{l+1}) \|_2^2 = 0, \quad l = 0, \ldots, k-1.$$

Summing this identity from i to $k-1$, we get

$$- \lambda_{ik} \| \nabla f(x_i) \|_2^2 + \overset{=1}{\lambda_{kk}} \| \nabla f(x_k) \|_2^2 = 0, \quad 0 \le i \le k-1$$

$$\Rightarrow \quad \boxed{\lambda_{ik} = \frac{\| \nabla f(x_k) \|_2^2}{\| \nabla f(x_i) \|_2^2}, \quad i = 0, \ldots, k-1}$$

Thus we have found the direction $d_k = \sum_{i=0}^{k} \lambda_{ik} \nabla f(x_i)$.
It turns out that there exists a 3-term recursive formula for the d_k's. Indeed,

$$d_k = \sum_{i=0}^{k-1} \frac{\| \nabla f(x_k) \|_2^2}{\| \nabla f(x_i) \|_2^2} \nabla f(x_i) + \nabla f(x_k) \qquad (\lambda_{kk} = 1)$$

$$= \nabla f(x_k) + \frac{\| \nabla f(x_k) \|_2^2}{\| \nabla f(x_{k-1}) \|_2^2} \left\{ \sum_{j=0}^{k-2} \frac{\| \nabla f(x_{k-1}) \|_2^2}{\| \nabla f(x_j) \|_2^2} \nabla f(x_j) + \nabla f(x_{j-1}) \right\}$$

$$= \nabla f(x_k) + \frac{\| \nabla f(x_k) \|_2^2}{\| \nabla f(x_{k-1}) \|_2^2} d_{k-1}.$$

Thus, the directions $d_0, \ldots$ can be calculated as follows:

$$d_0 = \nabla f(x_0)$$

$$d_l = \nabla f(x_l) + \frac{\| \nabla f(x_l) \|_2^2}{\| \nabla f(x_{l-1}) \|_2^2} d_{l-1}, \quad l = 1, \ldots, k.$$

Conjugate Gradient Method

Given $x_0 \in \mathbb{R}^n$ we set $d_0 = -\nabla f(x_0) = b - Ax_0 = r_0$

If $\nabla f(x_0) = 0$, the algorithm terminates since $\nabla f(x_0) = Ax_0 - b$.

Otherwise, let

$$\alpha_0 = \frac{d_0^T \nabla f(x_0)}{d_0^T A d_0} \quad \text{and} \quad x_1 = x_0 + \alpha_0 d_0 .$$

Assume, by induction, that $x_1, d_1, \ldots, d_{k-1}, x_k$ are available which assumes that $\nabla f(x_\ell) \neq 0$, $\ell = 0, \ldots, k-1$.

If $\nabla f(x_k) = 0$, the algorithm terminates.

Otherwise, let

$$d_k = -\nabla f(x_k) + \frac{\|\nabla f(x_k)\|_2^2}{\|\nabla f(x_{k-1})\|_2^2} d_{k-1}$$

and

$$\alpha_k = \frac{d_k^T \nabla f(x_k)}{d_k^T A d_k}$$

and

$$x_{k+1} = x_k + \alpha_k d_k .$$

This is efficiently implemented as

Algorithm 10.2.1 (Conjugate Gradient)

$k = 0$

$r_0 = b - Ax_0$

while $k < 10000$ or $\|e_k\|_A \leq \epsilon \|e_0\|_A$

$\quad k = k+1$

$\quad$ if $k = 1$

$\quad\quad p_1 = r_0$

$\quad$ else

$\quad\quad \beta_k = r_{k-1}^T r_{k-1} / r_{k-2}^T r_{k-2}$

$\quad\quad p_k = r_{k-1} + \beta_k p_{k-1}$

$\quad$ end

$\quad q_k = A p_k$

$\quad \alpha_k = r_{k-1}^T r_{k-1} / p_k^T q_k$

$\quad x_k = x_{k-1} + \alpha_k p_k$

$\quad r_k = r_{k-1} - \alpha_k q_k$

end

$x = x_k$

$$\left(\begin{aligned} \Rightarrow \quad & -Ax_{k+1} = -Ax_k - \alpha_k q_k \\ & \underbrace{b - Ax_{k+1}}_{r_{k+1}} = \underbrace{b - Ax_k}_{r_k} - \alpha_k q_k \end{aligned} \right)$$

Theorem Let A be s.p.d. and let $\{x_k\}_{k\geq 0}$ be generated by the CG method above. Then,

$$\|e_k\|_A \leq 2 \left(\frac{1 - \sqrt{\lambda_1/\lambda_n}}{1 + \sqrt{\lambda_1/\lambda_n}} \right)^k \|e_0\|_A , \quad k \geq 0$$

where $\|x\|_A = (x^T A x)^{1/2}$. $\square$

Note that this is a global estimate and reduction of the error is not guaranteed at every step.