Numerical Analysis – Lecture 3[1]

Method 1.11 (The steepest descent method). This method makes the choice $\boldsymbol{d}^{(k)} = -\boldsymbol{g}^{(k)}$ for every k that requires a search direction in the procedure of the previous section. It can be proved that, if the number of iterations is infinite, then the sequence $\boldsymbol{x}^{(k)}$, $k = 0, 1, 2, \ldots$, converges to the solution of the system $A\boldsymbol{x} = \boldsymbol{b}$ as required, but usually the speed of convergence is unacceptably slow. Fortunately, the use of *conjugate directions* provides an extension of the steepest descent method that performs very well for reasons that will be explained in the sequel.

Definition 1.12 (Conjugate directions). The vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$ are *conjugate* with respect to the positive-definite matrix A if they are nonzero and satisfy $\boldsymbol{u}^\top A\boldsymbol{v} = 0$.

The importance of conjugacy to Approach 1.10 depends on the identity $\boldsymbol{g}^{(k+1)} = \boldsymbol{g}^{(k)} + \omega^{(k)} A\boldsymbol{d}^{(k)}$, which is derived from $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \omega^{(k)}\boldsymbol{d}^{(k)}$ and from $\boldsymbol{g}^{(k)} = \nabla F(\boldsymbol{x}^{(k)}) = A\boldsymbol{x}^{(k)} - \boldsymbol{b}$:

$$\begin{aligned} A\boldsymbol{x}^{(k+1)} = A\boldsymbol{x}^{(k)} + \omega^{(k)} A\boldsymbol{d}^{(k)} \qquad &\Rightarrow \qquad (A\boldsymbol{x}^{(k+1)} - \boldsymbol{b}) = (A\boldsymbol{x}^{(k)} - \boldsymbol{b}) + \omega^{(k)} A\boldsymbol{d}^{(k)} \\ \Rightarrow\ \nabla F(\boldsymbol{x}^{(k+1)}) = \nabla F(\boldsymbol{x}^{(k)}) + \omega^{(k)} A\boldsymbol{d}^{(k)} \qquad &\Rightarrow \qquad \boldsymbol{g}^{(k+1)} = \boldsymbol{g}^{(k)} + \omega^{(k)} A\boldsymbol{d}^{(k)}. \end{aligned}$$

Hence, if $\boldsymbol{d}^{(k)}$ is conjugate to any vector $\boldsymbol{d}$ that satisfies $\boldsymbol{d}^\top \boldsymbol{g}^{(k)} = 0$, then $\boldsymbol{d}^\top \boldsymbol{g}^{(k+1)} = 0$ also holds. Thus the following algorithm provides ${\boldsymbol{d}^{(j)}}^\top \boldsymbol{g}^{(k+1)} = 0$, $j = 0, 1, 2, \ldots, k$, for every $k \in \mathbb{Z}_+$.

Algorithm 1.13 (The conjugate gradient method). This algorithm is of the form given in the second paragraph of Approach 1.10, where *(a)* $\boldsymbol{x}^{(0)}$ is arbitrary, *(b)* termination occurs if $\|\boldsymbol{g}^{(k)}\|$ is acceptably small, *(c)* every search direction satisfies the descent condition, and *(d)* the parameter $\omega^{(k)}$ in the formula $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \omega^{(k)}\boldsymbol{d}^{(k)}$ equals $-{\boldsymbol{d}^{(k)}}^\top \boldsymbol{g}^{(k)} / {\boldsymbol{d}^{(k)}}^\top A\boldsymbol{d}^{(k)}$. The search directions are the vectors

$$\boldsymbol{d}^{(0)} = -\boldsymbol{g}^{(0)} \qquad \text{and} \qquad \boldsymbol{d}^{(k)} = -\boldsymbol{g}^{(k)} + \beta^{(k)}\boldsymbol{d}^{(k-1)}, \quad k = 1, 2, 3, \ldots, \tag{1.6}$$

where $\beta^{(k)}$ is determined by the *conjugacy condition* ${\boldsymbol{d}^{(k)}}^\top A\boldsymbol{d}^{(k-1)} = 0$, which yields

$$\beta^{(k)} = \frac{{\boldsymbol{g}^{(k)}}^\top A\boldsymbol{d}^{(k-1)}}{{\boldsymbol{d}^{(k-1)}}^\top A\boldsymbol{d}^{(k-1)}}, \qquad k = 1, 2, 3, \ldots. \tag{1.7}$$

These directions obey the descent condition. Indeed, $\boldsymbol{g}^{(k+1)} = \boldsymbol{g}^{(k)} + \omega^{(k)} A\boldsymbol{d}^{(k)}$ and the value of $\omega^{(k)}$ give the important orthogonality property ${\boldsymbol{d}^{(k)}}^\top \boldsymbol{g}^{(k+1)} = 0$, so we have ${\boldsymbol{d}^{(k-1)}}^\top \boldsymbol{g}^{(k)} = 0$, $k = 1, 2, 3, \ldots$. It follows from (1.6) that the search direction of every iteration satisfies ${\boldsymbol{d}^{(k)}}^\top \boldsymbol{g}^{(k)} = -\|\boldsymbol{g}^{(k)}\|^2 < 0$, regardless of the values of the parameters (1.7).

Theorem 1.14 *(Properties of Algorithm 1.13). For every integer $k \geq 1$ until $\|\boldsymbol{g}^{(k)}\|$ is acceptably small, the conjugate gradient method enjoys the following properties.*
(1) *The linear space spanned by the gradients $\boldsymbol{g}^{(j)}$, $j = 0, 1, \ldots, k-1$, is the same as the linear space spanned by the search directions $\boldsymbol{d}^{(j)}$, $j = 0, 1, \ldots, k-1$;*
(2) *The conjugacy conditions ${\boldsymbol{d}^{(k-1)}}^\top A\boldsymbol{d}^{(j)} = 0$, $j = 0, 1, \ldots, k-2$, hold for $k \geq 2$;*
(3) *The gradients satisfy the orthogonality conditions ${\boldsymbol{g}^{(j)}}^\top \boldsymbol{g}^{(k)} = 0$, $j = 0, 1, \ldots, k-1$.*

Proof We use induction on $k \geq 1$, the assertions being easy to verify for $k = 1$: Indeed, **(1)** follows from $\boldsymbol{d}^{(0)} = -\boldsymbol{g}^{(0)}$, **(2)** is vacuous, and **(3)** follows from $\boldsymbol{d}^{(0)} = -\boldsymbol{g}^{(0)}$ and ${\boldsymbol{d}^{(k)}}^\top \boldsymbol{g}^{(k+1)} = 0$ when $k = 0$.

[1] Please email all corrections and suggestions to these notes to `A.Iserles@damtp.cam.ac.uk`. All handouts are available on the WWW at the URL `http://www.damtp.cam.ac.uk/user/na/PartII/Handouts.html`.

Therefore, assuming that the assertions are true for some $k \geq 1$, we ask if they remain true when k is increased by one.

The definition (1.6) of $\boldsymbol{d}^{(k)}$ and **(1)** of the inductive hypothesis imply that any vector in span of $\{\boldsymbol{g}^{(j)} : j = 0, 1, \ldots, k\}$ is also in span of $\{\boldsymbol{d}^{(j)} : j = 0, 1, \ldots, k\}$ and *vice versa*. Thus **(1)** is preserved when k is increased.

Turning to assertion **(2)**, the value of $\beta^{(k)}$ gives $\boldsymbol{d}^{(k)\top} A \boldsymbol{d}^{(k-1)} = 0$, so $\boldsymbol{d}^{(k)\top} A \boldsymbol{d}^{(j)} = 0$ is required for $j \in \{0, 1, \ldots, k-2\}$ when $k \geq 2$. Therefore, in view of the definition (1.6) of $\boldsymbol{d}^{(k)}$ and **(2)** of the inductive hypothesis, it is sufficient to establish $\boldsymbol{g}^{(k)\top} A \boldsymbol{d}^{(j)} = 0$, $j = 0, 1, \ldots, k-2$. Now, the formula $\boldsymbol{x}^{(j+1)} = \boldsymbol{x}^{(j)} + \omega^{(j)} \boldsymbol{d}^{(j)}$ and equation (1.4) yield $\boldsymbol{g}^{(j+1)} - \boldsymbol{g}^{(j)} = \omega^{(j)} A \boldsymbol{d}^{(j)}$, and we have noted $\omega^{(j)} > 0$. Therefore we require the conditions $\boldsymbol{g}^{(k)\top}(\boldsymbol{g}^{(j+1)} - \boldsymbol{g}^{(j)}) = 0$, $j = 0, 1, \ldots, k-2$. They are a consequence of assertion **(3)** of the inductive argument.

It remains to justify $\boldsymbol{g}^{(j)\top} \boldsymbol{g}^{(k+1)} = 0$, $j = 0, 1, \ldots, k$, which is equivalent to $\boldsymbol{d}^{(j)\top} \boldsymbol{g}^{(k+1)} = 0$, $j = 0, 1, \ldots, k$, because **(1)** is preserved when k is increased. The case $j = k$ is covered by $\boldsymbol{d}^{(k)\top} \boldsymbol{g}^{(k+1)} = 0$. Moreover, the old assertions **(1)** and **(3)** give $\boldsymbol{d}^{(j)\top} \boldsymbol{g}^{(k)} = 0$, $j = 0, 1, \ldots, k-1$. Therefore it is sufficient to show $\boldsymbol{d}^{(j)\top}(\boldsymbol{g}^{(k+1)} - \boldsymbol{g}^{(k)}) = 0$, $j = 0, 1, \ldots, k-1$, which is equivalent to $\boldsymbol{d}^{(j)\top} A \boldsymbol{d}^{(k)} = 0$, $j = 0, 1, \ldots, k-1$, because of $\boldsymbol{g}^{(k+1)} - \boldsymbol{g}^{(k)} = \omega^{(k)} A \boldsymbol{d}^{(k)}$ and $\omega^{(k)} > 0$. It follows from the symmetry of A and the new assertion **(2)** that the proof is complete. □

Corollary 1.15 *(A termination property). If Algorithm 1.13 is applied in exact arithmetic, then, for any $\boldsymbol{x}^{(0)} \in \mathbb{R}^n$, termination occurs after at most n iterations.*

Proof Assertion **(3)** of Theorem 1.14 states that $\boldsymbol{g}^{(k)}$, $k = 0, 1, 2, \ldots$, is a sequence of mutually orthogonal vectors. Therefore at most n of them can be nonzero, so $\|\boldsymbol{g}^{(k)}\|$ is acceptably small for some iteration number $k \leq n$. □

Standard Form 1.16 (Reformulation of the conjugate gradient method). We now simplify and reformulate Algorithm 1.13. Specifically, we let $\boldsymbol{x}^{(0)}$ be the zero vector and we write $-\boldsymbol{r}^{(k)}$ instead of $\boldsymbol{g}^{(k)}$, where $\boldsymbol{r}^{(k)}$ is the *residual* $\boldsymbol{b} - A\boldsymbol{x}^{(k)}$. Furthermore, because $\boldsymbol{g}^{(k)} - \boldsymbol{g}^{(k-1)}$ is a multiple of $A\boldsymbol{d}^{(k-1)}$, we write the parameter (1.7) as

$$\beta^{(k)} = \frac{\boldsymbol{g}^{(k)\top}(\boldsymbol{g}^{(k)} - \boldsymbol{g}^{(k-1)})}{\boldsymbol{d}^{(k-1)\top}(\boldsymbol{g}^{(k)} - \boldsymbol{g}^{(k-1)})} = \frac{\|\boldsymbol{g}^{(k)}\|^2}{\|\boldsymbol{g}^{(k-1)}\|^2},$$

which depends on the orthogonality of $\boldsymbol{g}^{(k)}$ to $\boldsymbol{g}^{(k-1)}$ and $\boldsymbol{d}^{(k-1)}$, proved above, and on the property $\boldsymbol{d}^{(k-1)\top} \boldsymbol{g}^{(k-1)} = -\|\boldsymbol{g}^{(k-1)}\|^2$. Thus Algorithm 1.13 takes the following form.

1. Set $\boldsymbol{x}^{(0)} = \boldsymbol{0}$, $\boldsymbol{r}^{(0)} = \boldsymbol{b}$, $k = 0$ and $\boldsymbol{d}^{(0)} = \boldsymbol{r}^{(0)}$;
2. Stop if $\|\boldsymbol{r}^{(k)}\|$ is acceptably small;
3. If $k \geq 1$, set $\boldsymbol{d}^{(k)} = \boldsymbol{r}^{(k)} + \beta^{(k)} \boldsymbol{d}^{(k-1)}$, where $\beta^{(k)} = \|\boldsymbol{r}^{(k)}\|^2 / \|\boldsymbol{r}^{(k-1)}\|^2$;
4. Calculate the matrix vector product $\boldsymbol{v}^{(k)} = A\boldsymbol{d}^{(k)}$ and $\omega^{(k)} = \|\boldsymbol{r}^{(k)}\|^2 / \boldsymbol{d}^{(k)\top} \boldsymbol{v}^{(k)}$;
5. Apply the formulae $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \omega^{(k)} \boldsymbol{d}^{(k)}$ and $\boldsymbol{r}^{(k+1)} = \boldsymbol{r}^{(k)} - \omega^{(k)} \boldsymbol{v}^{(k)}$;
6. Increase k by one, and then go back to **2.**

The total work is usually dominated by the number of iterations, multiplied by the time it takes to compute $\boldsymbol{v}^{(k)} = A\boldsymbol{d}^{(k)}$. It follows from Corollary 1.15 that the conjugate gradient algorithm is highly suitable when most of the elements of A are zero, i.e. when A is *sparse.*