Optimization

Màster de Fonaments de Ciència de Dades

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Lecture IV. Alternating directions methods

Alternating directions methods

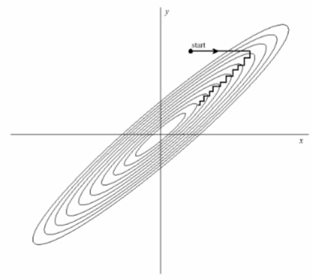
- The main purpose of the alternating directions methods is to accelerate the convergence of the descent methods and, in this way, reduce the total number of iterations.
- The basic tool for alternating directions methods, such as the gradient methods, is a 1-D minimization (Golden section, Fibonacci, Armijo,...)
- In the alternating directions methods, we start at a certain starting position $\boldsymbol{x}$, along a direction $\boldsymbol{d}$, and then minimize $f(\boldsymbol{x} + \alpha \boldsymbol{d})$ selecting the suitable value of α
- Next we use $\boldsymbol{x} + \alpha^* \boldsymbol{d}$ as the new starting position, choose a different direction, and minimize along that direction......
- Different alternating directions methods differ as to how the directions are chosen

Alternating directions methods

- The coordinate descent method: use n orthogonal unit vectors in turn:

$$\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n, \boldsymbol{e}_1, \boldsymbol{e}_2, \ldots$$

- This method has slow convergence, unless the unit vectors are well-oriented with respect to the valley in which there is $f(\boldsymbol{x}^*)$



- An advantage of the coordinate descent method is that it is well suited for parallel computation

Alternating directions methods

- We have already seen that, if we know the derivatives of f (i.e. we know ∇f), a good choice of the direction is $\boldsymbol{d} = -\nabla f / \|\nabla f\|$, which defines the steepest descent method
- With this procedure we always choose a new direction that is orthogonal to the previous direction:

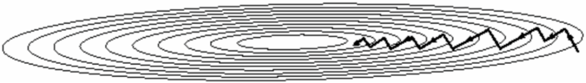
$$\boldsymbol{x}^{k+1} = \boldsymbol{x}^k - \alpha \nabla f(\boldsymbol{x}^k), \quad \Rightarrow$$

$$0 = \frac{df(x^{k+1})}{d\alpha} = \nabla f(\boldsymbol{x}^{k+1})^T \frac{d\boldsymbol{x}^{k+1}}{d\alpha} = -\nabla f(\boldsymbol{x}^{k+1})^T \nabla f(\boldsymbol{x}^k)$$

so

$$(\boldsymbol{d}^{k+1})^T \boldsymbol{d}^k = 0$$

- The performance isn't that good, because we can only ever take a right angle turn



Alternating directions methods

- Suppose that we are dealing with a 2-D problem, and that step k occurred along the y-axis, and led to position $\boldsymbol{x}^{k+1}$, at which

$$\frac{\partial f(\boldsymbol{x}^{k+1})}{\partial y} = 0$$

- The next step is along the x-axis: that step leads to a position $\boldsymbol{x}^{k+2}$, at which

$$\frac{\partial f(\boldsymbol{x}^{k+2})}{\partial x} = 0$$

- But if

$$\frac{\partial^2 f(\boldsymbol{x}^{k+2})}{\partial y \partial x} \neq 0$$

  $\partial f(\boldsymbol{x}^{k+2}) \, / \, \partial y$ will no longer be zero

- We really want to move along some direction other than the x-axis, such that $\partial f(\boldsymbol{x}^{k+2}) \, / \, \partial y$ remains zero

- Thus the optimum direction is not along ∇f but rather in a direction that preserves the minimization achieved in the previous step (and, in multi-dimensions, all previous steps)

Alternating directions methods. Conjugate directions

- Let $\boldsymbol{x}^k$, $\boldsymbol{x}^{k+1}$ and $\boldsymbol{x}^{k+2}$ be three consecutive points such that $\boldsymbol{x}^{k+1}$ is the minimum of f along $\boldsymbol{x}^k + \lambda \boldsymbol{d}^k$, and $\boldsymbol{x}^{k+2}$ is the minimum along $\boldsymbol{x}^{k+1} + \lambda \boldsymbol{d}^{k+1}$, where

$$\boldsymbol{d}^k = \frac{\boldsymbol{x}^{k+1} - \boldsymbol{x}^k}{\|\boldsymbol{x}^{k+1} - \boldsymbol{x}^k\|}, \quad \boldsymbol{d}^{k+1} = \frac{\boldsymbol{x}^{k+2} - \boldsymbol{x}^{k+1}}{\|\boldsymbol{x}^{k+2} - \boldsymbol{x}^{k+1}\|}$$

- By the definition of $\boldsymbol{x}^{k+1}$ and $\boldsymbol{x}^{k+2}$, we have that the directional derivatives

$$D_{\boldsymbol{d}^k} f(\boldsymbol{x}^{k+1}) = \nabla f(\boldsymbol{x}^{k+1})^T \boldsymbol{d}^k = 0, \quad D_{\boldsymbol{d}^{k+1}} f(\boldsymbol{x}^{k+2}) = \nabla f(\boldsymbol{x}^{k+2})^T \boldsymbol{d}^{k+1} = 0$$

- In addition, we would also like that

$$D_{\boldsymbol{d}^k} f(\boldsymbol{x}^{k+2}) = \nabla f(\boldsymbol{x}^{k+2})^T \boldsymbol{d}^k = 0$$

- To set this condition, consider the Taylor expansion

$$f(\boldsymbol{x} + \boldsymbol{\delta}) = f(\boldsymbol{x}) + \boldsymbol{\delta}^T \nabla f(\boldsymbol{x}) + \frac{1}{2} \boldsymbol{\delta}^T \nabla^2 f(\boldsymbol{x}) \boldsymbol{\delta} + \ldots$$

- Taking the gradient of the Taylor expansion, we obtain

$$\nabla f(\boldsymbol{x} + \boldsymbol{\delta}) = \nabla f(\boldsymbol{x}) + \nabla^2 f(\boldsymbol{x}) \boldsymbol{\delta} + \ldots$$

Alternating directions methods. Conjugate directions

- Since we want that

$$\nabla f(\boldsymbol{x}^{k+2})^T \boldsymbol{d}^k = (\boldsymbol{d}^k)^T \nabla f(\boldsymbol{x}^{k+2}) = 0,$$

  and, as we have just seen using Taylor expansion

$$\nabla f(\boldsymbol{x}^{k+2}) = \nabla f(\boldsymbol{x}^{k+1} + \boldsymbol{d}^{k+1}) = \nabla f(\boldsymbol{x}^{k+1}) + \nabla^2 f(\boldsymbol{x}^{k+1})\boldsymbol{d}^{k+1} + \dots$$

  the above condition requires

$$(\boldsymbol{d}^k)^T \left[\nabla f(\boldsymbol{x}^{k+1}) + \nabla^2 f(\boldsymbol{x}^{k+1})\boldsymbol{d}^{k+1}\right] \approx 0$$

- Since $(\boldsymbol{d}^k)^T \nabla f(\boldsymbol{x}^{k+1}) = 0$, because $\boldsymbol{x}^{k+1}$ was obtained by minimizing f along the $\boldsymbol{d}^k$, it follows that

$$(\boldsymbol{d}^k)^T \nabla^2 f(\boldsymbol{x}^{k+1})\boldsymbol{d}^{k+1} = 0$$

- If this last condition holds, we will say that $\boldsymbol{d}^k$ and $\boldsymbol{d}^{k+1}$ are conjugate with respect to $\nabla^2 f(\boldsymbol{x}^{k+1})$
- Clearly, this is different from steepest descent method, for which $(\boldsymbol{d}^k)^T \boldsymbol{d}^{k+1} = 0$

Alternating directions methods. Conjugate directions

- One basic idea for alternating directions methods is the one related to conjugate directions which is a generalization of orthogonality.
- Two vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ are said to be conjugate directions with respect to the $n \times n$ symmetric positive definite matrix A if

$$\boldsymbol{x}^T A \boldsymbol{y} = 0$$

- If A is symmetric positive definite matrix, then it has n orthogonal eigenvectors. These n vectors are also mutually conjugate, since

$$\boldsymbol{x}^T A \boldsymbol{y} = \boldsymbol{x}^T \lambda \boldsymbol{y} = \lambda \boldsymbol{x}^T \boldsymbol{y} = 0$$

  Thus, for every $n \times n$ symmetric positive definite matrix there is at least one set of n mutually conjugate directions

Conjugate directions

- **Remark**

  Let $\boldsymbol{d}_1, ..., \boldsymbol{d}_m$ $(m \leq n)$ be m nonzero vectors mutually conjugate with respect to A, then these vectors are linearly independent.

  If this was not the case, then we could write

  $$\boldsymbol{d}_m = \sum_{i=1}^{m-1} \alpha_i \boldsymbol{d}_i$$

  from which it follows that

  $$(\boldsymbol{d}_m)^T A \boldsymbol{d}_m = 0$$

  that contradics the fact that $\boldsymbol{d}_m \neq 0$ and that A is positive definite

Conjugate directions

- Let $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k$ be k linearly independent vectors, then we can construct k mutually conjugate directions $\boldsymbol{d}_1, \ldots, \boldsymbol{d}_k$, with respect to A, such that

$$< \boldsymbol{v}_1, \ldots, \boldsymbol{v}_k > = < \boldsymbol{d}_1, \ldots, \boldsymbol{d}_k >$$

The construction is similar to the Gram-Schmidt orthogonalization method. Define

$$\boldsymbol{d}_1 = \boldsymbol{v}_1, \qquad \boldsymbol{d}_{i+1} = \boldsymbol{v}_{i+1} - \sum_{m=1}^{i} \frac{\boldsymbol{v}_{i+1}^T A \boldsymbol{d}_m}{\boldsymbol{d}_m^T A \boldsymbol{d}_m} \boldsymbol{d}_m, \quad i = 1, \ldots, k-1$$

Note that $\boldsymbol{d}_m^T A \boldsymbol{d}_m \neq 0$ since A is positive definite. Clearly

$$\boldsymbol{v}_{i+1} \in < \boldsymbol{d}_1, \ldots, \boldsymbol{d}_{i+1} > \quad \text{and} \quad \boldsymbol{d}_{i+1} \in < \boldsymbol{v}_1, \ldots, \boldsymbol{v}_{i+1} >$$

so $< \boldsymbol{v}_1, \ldots, \boldsymbol{v}_{i+1} > = < \boldsymbol{d}_1, \ldots, \boldsymbol{d}_{i+1} >$

Now we need to proof that if $\boldsymbol{d}_1, \ldots, \boldsymbol{d}_i$ are mutually conjugate w.r.t. A, then $\boldsymbol{d}_{i+1}^T A \boldsymbol{d}_j = 0$ for $j = 1, \ldots, i$

$$\boldsymbol{d}_{i+1}^T A \boldsymbol{d}_j = \boldsymbol{v}_{i+1}^T A \boldsymbol{d}_j - \sum_{m=1}^{i} \frac{\boldsymbol{v}_{i+1}^T A \boldsymbol{d}_m}{\boldsymbol{d}_m^T A \boldsymbol{d}_m} \boldsymbol{d}_m^T A \boldsymbol{d}_j = \boldsymbol{v}_{i+1}^T A \boldsymbol{d}_j - \frac{\boldsymbol{v}_{i+1}^T A \boldsymbol{d}_j}{\boldsymbol{d}_j^T A \boldsymbol{d}_j} \boldsymbol{d}_j^T A \boldsymbol{d}_j = 0$$

since $\boldsymbol{d}_m^T A \boldsymbol{d}_j = 0$ except if $m = 1$

Conjugate directions

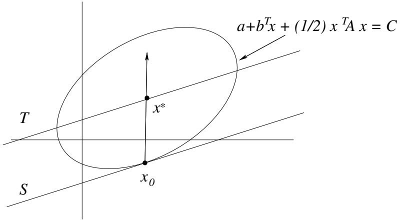
A geometric interpretation of conjugate vectors is the following. Let

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

with A a symmetric positive definite matrix, be a quadratic function with a global minimum at $\boldsymbol{x}^*$

$$\nabla f(\boldsymbol{x}^*) = 0 \quad \Rightarrow \quad \boldsymbol{x}^* = -A^{-1}\boldsymbol{b}$$

Then, the surfaces $f(\boldsymbol{x}) = c$ (constant) are generally ellipsoids with center at $\boldsymbol{x}^*$. Let $\boldsymbol{x}_0$ be a point satisfying $f(\boldsymbol{x}_0) = c$



Then the vector joining $\boldsymbol{x}_0$ and $\boldsymbol{x}^*$ is conjugate with respect to A to every vector in the tangent hyperplane to the ellipsoid at $\boldsymbol{x}_0$

Conjugate directions

Given a point $\mathbf{x}^0 \in \mathbb{R}^n$, the set of points satisfying

$$\mathbf{x} = \mathbf{x}^0 + \sum_{j=1}^{m} \alpha_j \mathbf{z}^j$$

where the $\mathbf{z}^j$ are m linearly independent vectors, and the α_j are arbitrary numbers, is an affine space or linear manifold generated by $\mathbf{x}^0$ and $\mathbf{z}^1, \ldots, \mathbf{z}^m$

Definition

Two affine spaces S and T ($S \neq T$) are parallel if they are generated by the same set of vectors $\mathbf{z}_1, \ldots, \mathbf{z}_m$ but at different points: $\mathbf{x}(S) \in S$, $\mathbf{x}(T) \in T$, and $\mathbf{x}(S) \neq \mathbf{x}(T)$.

Theorem

Let $\mathbf{x}^*(S)$ and $\mathbf{x}^*(T)$ be the points that minimize

$$f(\mathbf{x}) = \mathbf{a} + \mathbf{b}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T A\mathbf{x},$$

with A a symmetric positive definite matrix, in two parallel affine spaces S and T. Then $\mathbf{x}^*(S) - \mathbf{x}^*(T)$ and any direction $\mathbf{z}$ contained in S and T are conjugate w.r.t. A, this is

$$\mathbf{z}^T A[\mathbf{x}^*(S) - \mathbf{x}^*(T)] = 0$$

Conjugate directions. Proof of the theorem

Proof: Let $\boldsymbol{z}$ be a direction of S and T, then

$$\frac{d}{d\alpha}[f(\boldsymbol{x}^*(S) + \alpha \boldsymbol{z})]_{\alpha=0} = 0 \quad \Rightarrow \quad \boldsymbol{z}^T[A\boldsymbol{x}^*(S) + \boldsymbol{b}] = 0$$

$$\frac{d}{d\alpha}[f(\boldsymbol{x}^*(T) + \alpha \boldsymbol{z})]_{\alpha=0} = 0 \quad \Rightarrow \quad \boldsymbol{z}^T[A\boldsymbol{x}^*(T) + \boldsymbol{b}] = 0$$

so

$$\boldsymbol{z}^T A[\boldsymbol{x}^*(S) - \boldsymbol{x}^*(T)] = 0$$

$\square$

Remark:

$$\begin{aligned}
&\frac{d}{d\alpha}[f(\boldsymbol{x}^*(S) + \alpha \boldsymbol{z})] = \\
&= \frac{d}{d\alpha}\left[\boldsymbol{a} + \boldsymbol{b}^T x^*(S) + \alpha \boldsymbol{b}^T z + \frac{1}{2}\left((\boldsymbol{x}^*(S) + \alpha \boldsymbol{z})^T A(\boldsymbol{x}^*(S) + \alpha \boldsymbol{z})\right)\right] = \\
&= \boldsymbol{b}^T z + (x^*(S))^T A\boldsymbol{z} + \alpha \boldsymbol{z}^T A\boldsymbol{z}
\end{aligned}$$

Conjugate directions

Theorem

Let $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_m$ such that $\boldsymbol{z}_i \in \mathbb{R}^n$, $\boldsymbol{z}_i \neq 0$, $m \leq n$, and that they are m mutually conjugate directions with respect to the symmetric poisitive definite matrix A, then the minimum of the quadratic function

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

over the affine set generated by the point $\boldsymbol{x}_0 \in \mathbb{R}^n$ and the vectors $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_m$ will be found by searching along each of the conjugate directions only once

Conjugate directions. Proof of the theorem

Proof: The minimum will be a point $\mathbf{x}_0 + \alpha_1^* \mathbf{z}_1 + \ldots + \alpha_m^* \mathbf{z}_m$, such that the α_i^* minimize

$$f\left(\mathbf{x}_0 + \sum_{j=1}^{m} \alpha_j \mathbf{z}_j\right) = \mathbf{a} + \mathbf{b}^T \left(\mathbf{x}_0 + \sum_{j=1}^{m} \alpha_j \mathbf{z}_j\right) + \frac{1}{2}\left(\mathbf{x}_0 + \sum_{j=1}^{m} \alpha_j \mathbf{z}_j\right)^T A \left(\mathbf{x}_0 + \sum_{j=1}^{m} \alpha_j \mathbf{z}_j\right) =$$

$$= f(\mathbf{x}_0) + \sum_{j=1}^{m} \alpha_j \mathbf{z}_j^T \mathbf{b} + \sum_{j=1}^{m} \alpha_j \mathbf{z}_j^T A \mathbf{x}_0 + \frac{1}{2} \sum_{j=1}^{m} \alpha_j^2 \mathbf{z}_j^T A \mathbf{z}_j =$$

$$= f(\mathbf{x}_0) + \sum_{j=1}^{m} \left[\alpha_j \mathbf{z}_j^T (\mathbf{b} + A\mathbf{x}_0) + \frac{1}{2} \alpha_j^2 z_j^T A \mathbf{z}_j\right]$$

Since in the last expression there are no $\alpha_j \alpha_k$ terms with $j \neq k$, the optimal α_j are found minimizing each summand:

$$\min_{\alpha_j} \left[f(\mathbf{x}_0) + \alpha_j \mathbf{z}_j^T (\mathbf{b} + A\mathbf{x}_0) + \frac{1}{2} \alpha_j^2 \mathbf{z}_j^T A \mathbf{z}_j\right] = \min_{\alpha_j} f(\mathbf{x}_0 + \alpha_j \mathbf{z}_j), \quad j = 1, \ldots, m$$

□

Conjugate directions

Example. Consider the quadratic function

$$f(x,y) = 2x^2 + 6y^2 + 2xy + 2x + 3y + 3$$

that can also be written as

$$f(x,y) = \frac{1}{2} \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 4 & 2 \\ 2 & 12 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 2 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + 3$$

We choose $\boldsymbol{z}_1 = (1,0)^T$. A conjugate direction to $\boldsymbol{z}_1$ with respect to

$$A = \begin{pmatrix} 4 & 2 \\ 2 & 12 \end{pmatrix}$$

is $\boldsymbol{z}_2 = (-1/2, 1)^T$ since

$$\boldsymbol{z}_1^T A \boldsymbol{z}_1 = 4 \neq 0, \quad \boldsymbol{z}_2^T A \boldsymbol{z}_2 = 13 \neq 0, \quad \boldsymbol{z}_1^T A \boldsymbol{z}_2 = 0.$$

Let us find the minimum of f generated by the point $\boldsymbol{x}_0 = (0,0)^T$ and the vectors $\boldsymbol{z}_1$, $\boldsymbol{z}_2$.

Conjugate directions

Example (cont.)

Staring with the $\boldsymbol{z}_1$ direction, we want to minimize

$$f(\boldsymbol{x}_0 + \alpha_1 \boldsymbol{z}_1) = f(\alpha_1,\, 0) = 2\alpha_1^2 + 2\alpha_1 + 3.$$

The minima is achieved for $\alpha_1^* = -1/2$.

Proceeding now with the $\boldsymbol{z}_2$ direction, we need to minimize

$$f(\boldsymbol{x}_0 + \alpha_2 \boldsymbol{z}_2) = f(-\alpha_2/2,\, \alpha_2) = \frac{11}{2}\alpha_2^2 + 2\alpha_2 + 3.$$

The minima is achieved for $\alpha_2^* = -2/11$.

So, the minimum of f is then given by

$$\boldsymbol{x}^* = \boldsymbol{x}_0 + \alpha_1^* \boldsymbol{z}_1 + \alpha_2^* \boldsymbol{z}_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{2}{11}\begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix} = \begin{pmatrix} -\frac{9}{22} \\ -\frac{2}{11} \end{pmatrix}.$$

Conjugate gradient methods

Conjugate gradient methods generate a sequence

$$\boldsymbol{x}^k = \boldsymbol{x}^{k-1} + \alpha_k \boldsymbol{z}^k, \quad k = 1, 2, \ldots$$

- Suposse that the directions $\boldsymbol{z}^k$ are given, and let us see first how to compute the α_k.
- Define

$$F(\alpha_k) = f(\boldsymbol{x}^{k-1} + \alpha_k \boldsymbol{z}^k),$$

then, the value of α_k is chosen such that

$$\frac{dF(\alpha_k^*)}{d\alpha_k} = D_{\boldsymbol{z}^k} f(\boldsymbol{x}^{k-1} + \alpha_k^* \boldsymbol{z}^k) = (\boldsymbol{z}^k)^T \nabla f(\boldsymbol{x}^{k-1} + \alpha_k^* \boldsymbol{z}^k) = (\boldsymbol{z}^k)^T \nabla f(x^k) = 0$$

Conjugate gradient methods. Quadratic functions

Assume that f is the quadratic function

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

with A an $n \times n$ symmetric positive definite matrix. Then, from the identity

$$b + A\boldsymbol{x}^k = b + A\boldsymbol{x}^{k-1} + A(\boldsymbol{x}^k - \boldsymbol{x}^{k-1}),$$

it follows that the gradients of f ($\nabla f(\boldsymbol{x}) = \boldsymbol{b} + A\boldsymbol{x}$) at two consecutive points are related by

$$\nabla f(\boldsymbol{x}^k) = \nabla f(\boldsymbol{x}^{k-1}) + A(\boldsymbol{x}^k - \boldsymbol{x}^{k-1}).$$

If $\boldsymbol{x}^k = \boldsymbol{x}^{k-1} + \alpha_k \boldsymbol{z}^k$, we can obtain an explicit formula for α_k^* from the condition $dF(\alpha_k^*)/d\alpha_k = (\boldsymbol{z}^k)^T \nabla f(x^k) = 0$:

$$\begin{aligned} (\boldsymbol{z}^k)^T \nabla f(\boldsymbol{x}^k) &= (\boldsymbol{z}^k)^T \left(\nabla f(\boldsymbol{x}^{k-1}) + A(\boldsymbol{x}^k - \boldsymbol{x}^{k-1}) \right) \\ &= (\boldsymbol{z}^k)^T \left(\nabla f(\boldsymbol{x}^{k-1}) + \alpha_k^* A \boldsymbol{z}^k \right) = 0 \end{aligned}$$

$$\Rightarrow \quad \alpha_k^* = -\frac{(\boldsymbol{z}^k)^T \nabla f(\boldsymbol{x}^{k-1})}{(\boldsymbol{z}^k)^T A \boldsymbol{z}^k}.$$

Conjugate gradient methods. Quadratic functions

Since

$$\begin{aligned} f(\boldsymbol{x}^k) &= f(\boldsymbol{x}^{k-1}) + (\boldsymbol{x}^k - \boldsymbol{x}^{k-1})^T \nabla f(\boldsymbol{x}^{k-1}) + \frac{1}{2}(\boldsymbol{x}^k - \boldsymbol{x}^{k-1})^T A (\boldsymbol{x}^k - \boldsymbol{x}^{k-1}) \\ &= f(\boldsymbol{x}^{k-1}) + \alpha_k^* (\boldsymbol{z}^k)^T \nabla f(\boldsymbol{x}^{k-1}) + \frac{1}{2}(\alpha_k^*)^2 (\boldsymbol{z}^k)^T A \boldsymbol{z}^k, \end{aligned}$$

and using the value obtained for α_k^* we get

$$f(\boldsymbol{x}^k) = f(\boldsymbol{x}^{k-1}) - \frac{(\boldsymbol{z}^k)^T \nabla f(\boldsymbol{x}^{k-1})}{(\boldsymbol{z}^k)^T A \boldsymbol{z}^k} (\boldsymbol{z}^k)^T \nabla f(\boldsymbol{x}^{k-1}) + \frac{1}{2} \left(\frac{(\boldsymbol{z}^k)^T \nabla f(\boldsymbol{x}^{k-1})}{(\boldsymbol{z}^k)^T A \boldsymbol{z}^k} \right)^2 (\boldsymbol{z}^k)^T A \boldsymbol{z}^k.$$

From which it follows that

$$f(\boldsymbol{x}^k) - f(\boldsymbol{x}^{k-1}) = -\frac{1}{2} \frac{\left[(\boldsymbol{z}^k)^T \nabla f(\boldsymbol{x}^{k-1}) \right]^2}{(\boldsymbol{z}^k)^T A \boldsymbol{z}^k} < 0,$$

so the conjugate gradient method applied to the quadratic function $f(\boldsymbol{x})$ is a descent method (assuming that the directions $\boldsymbol{z}^k$ are given).

Conjugate gradient methods. Choice of the directions

- We would like to do the choice of the directions $\boldsymbol{z}^i$ in such a way that the algorithm converges fast or, even better, that terminates in a finite number of steps when applied to minimizing a quadratic function.
- We have already seen that if the search directions $\boldsymbol{z}^k$ are mutually conjugate with respect to A, for $k = 1, \ldots, n$, then the point $\boldsymbol{x}^n$ will be the exact minimum of the quadratic function.
- The choice of the conjugate directions can be done in the following way:
  1. We start at a point $\boldsymbol{x}^0 \in \mathbb{R}^n$ and choose
  $$\boldsymbol{z}^1 = -\nabla f(\boldsymbol{x}^0)$$
  2. The next point, $\boldsymbol{x}^1$, is
  $$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \alpha_1^* \boldsymbol{z}^1$$
  where α_1^* has been computed with the formula given above
  3. We evaluate $\nabla f(\boldsymbol{x}^1)$ and set
  $$\boldsymbol{z}^2 = -\nabla f(\boldsymbol{x}^1) + \beta_{11} \boldsymbol{z}^1,$$
  where β_{11} is such that $\boldsymbol{z}^1$ and $\boldsymbol{z}^2$ will be A-conjugate, this is
  $$(\boldsymbol{z}^1)^T A \boldsymbol{z}^2 = (\boldsymbol{z}^1)^T A(-\nabla f(\boldsymbol{x}^1) + \beta_{11} \boldsymbol{z}^1) = 0,$$
  from which it follows
  $$\beta_{11} = \frac{(\boldsymbol{z}^1)^T A \nabla f(\boldsymbol{x}^1)}{(\boldsymbol{z}^1)^T A \boldsymbol{z}^1}.$$

Conjugate gradient methods. The algorithm (cont.)

4. Once $\boldsymbol{z}^2$ is known, we determine $\boldsymbol{x}^2 = \boldsymbol{x}^1 + \alpha_2^* \boldsymbol{z}^2$, with α_2^* computed with the formula given above.
5. We evaluate $\nabla f(\boldsymbol{x}^2)$ and the new direction will be
$$\boldsymbol{z}^3 = -\nabla f(\boldsymbol{x}^2) + \beta_{21} \boldsymbol{z}^1 + \beta_{22} \boldsymbol{z}^2,$$
with β_{21} and β_{22} such that $(\boldsymbol{z}^1)^T A \boldsymbol{z}^3 = (\boldsymbol{z}^2)^T A \boldsymbol{z}^3 = 0$.
6. In general, we get
$$\boldsymbol{z}^{k+1} = -\nabla f(\boldsymbol{x}^k) + \sum_{j=1}^{k} \beta_{kj} \boldsymbol{z}^j, \quad k = 0, ..., n-1.$$

If the function f is not quadratic, the computation of β_{ij} is long.

We shall show how the directions $\boldsymbol{z}^j$ can be generated more easily.

Conjugate gradient methods

The following result will be useful in the sequel

Theorem

Let $f(\boldsymbol{x}) = \boldsymbol{a} + \boldsymbol{b}^T\boldsymbol{x} + \frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}$ *and* $\boldsymbol{x}^0 \in \mathbb{R}^n$ *be given, and assume that the* m *nonzero vectors* $\boldsymbol{z}^1,\ldots,\boldsymbol{z}^m$, $\boldsymbol{z}^j \in \mathbb{R}^n$, $m \leq n$, *are mutually conjugate with respect to* A *(symmetric and positive definite).*

Starting at $\boldsymbol{x}^0$, *we move to* $\boldsymbol{x}^1,\ldots,\boldsymbol{x}^m$ *along* $\boldsymbol{z}^1,\ldots,\boldsymbol{z}^m$, *respectively, such that*

$$(\boldsymbol{z}^j)^T\nabla f(\boldsymbol{x}^j) = 0, \quad j = 1, \ldots, m,$$

then

$$(\boldsymbol{z}^j)^T\nabla f(\boldsymbol{x}^m) = 0, \quad j = 1, \ldots, m.$$

Proof: For $j = m$ the result is obvious

Since, as we have already seen, $\nabla f(\boldsymbol{x}^k) = \nabla f(\boldsymbol{x}^{k-1}) + A(\boldsymbol{x}^k - \boldsymbol{x}^{k-1})$, it follows that the gradient of f at any two points are related by

$$\begin{aligned}
\nabla f(\boldsymbol{x}^m) &= \nabla f(\boldsymbol{x}^{m-1}) + A(\boldsymbol{x}^m - \boldsymbol{x}^{m-1}) \\
&= \nabla f(\boldsymbol{x}^{m-2}) + A(\boldsymbol{x}^{m-1} - \boldsymbol{x}^{m-2}) + A(\boldsymbol{x}^m - \boldsymbol{x}^{m-1}) \\
&= \nabla f(\boldsymbol{x}^{m-2}) + A(\boldsymbol{x}^m - \boldsymbol{x}^{m-2}),
\end{aligned}$$

so

$$\nabla f(\boldsymbol{x}^m) = \nabla f(\boldsymbol{x}^j) + A(\boldsymbol{x}^m - \boldsymbol{x}^j), \quad j = 1, ..., m-1. \tag{1}$$

From $\boldsymbol{x}^j = \boldsymbol{x}^{j-1} + \alpha_j^* \boldsymbol{z}^j$, for $j = 1, ..., m$, it follows that

$$\boldsymbol{x}^m = \boldsymbol{x}^{m-1} + \alpha_m^* \boldsymbol{z}^m = \boldsymbol{x}^{m-2} + \alpha_{m-1}^* \boldsymbol{z}^{m-1} + \alpha_m^* \boldsymbol{z}^m = ...$$

so

$$\boldsymbol{x}^m - \boldsymbol{x}^j = \sum_{i=j+1}^{m} \alpha_i^* \boldsymbol{z}^i, \quad j = 0, ..., m-1$$

Conjugate gradient methods. Proof of the Theorem (cont.)

In this way, we can write

$$\nabla f(\boldsymbol{x}^m) = \nabla f(\boldsymbol{x}^j) + A(\boldsymbol{x}^m - \boldsymbol{x}^j) = \nabla f(\boldsymbol{x}^j) + \sum_{i=j+1}^{m} \alpha_i^* A z^i, \quad j = 1, ..., m-1,$$

from which it follows that

$$(\boldsymbol{z}^j)^T \nabla f(\boldsymbol{x}^m) = (\boldsymbol{z}^j)^T \nabla f(\boldsymbol{x}^j) + \sum_{i=j+1}^{m} \alpha_i^* (\boldsymbol{z}^j)^T A \boldsymbol{z}^i = 0, \quad j = 1, ..., m-1.$$

since the first term of the right-hand side vanishes, according to the hypothesis, and the second term by the conjugacy of the $\boldsymbol{z}^j$.

$\square$

Corollary

If in the above theorem $m = n$, then $\nabla f(\boldsymbol{x}^n) = 0$ and x^n is the unconstrained minimum of f.

Proof: Since the $\boldsymbol{z}^j$ are linearly independent, from

$$\sum_{j=1}^{n} (\boldsymbol{z}^j)^T \nabla f(\boldsymbol{x}^j) = \sum_{j=1}^{n} \nabla f(\boldsymbol{x}^j)^T \boldsymbol{z}^j = 0,$$

it follows that $\nabla f(\boldsymbol{x}^n) = 0$. □

Conjugate gradient methods. Computation of the β_{ij} coefficients

- For the computation of the constants β_{ij} we will use the following remark: Let $\boldsymbol{\gamma}^i = \nabla f(\boldsymbol{x}^i) - \nabla f(\boldsymbol{x}^{i-1}), \quad i = 1, ..., n$

  If f is the previous quadratic function, then $\boldsymbol{\gamma}^i = A(\boldsymbol{x}^i - \boldsymbol{x}^{i-1})$.

- From now on we will assume that f is quadratic

- Recall that α_i^* is such that

$$\boldsymbol{x}^i = \boldsymbol{x}^{i-1} + \alpha_i^* \boldsymbol{z}^i \quad \Rightarrow \quad \boldsymbol{x}^i - \boldsymbol{x}^{i-1} = \alpha_i^* \boldsymbol{z}^i$$

- According to the definition of $\boldsymbol{\gamma}^i$, for $i = 1, ..., n$:

$$\boldsymbol{\gamma}^i = A(\boldsymbol{x}^i - \boldsymbol{x}^{i-1}) = \alpha_i^* A \boldsymbol{z}^i \quad \Rightarrow \quad (\boldsymbol{\gamma}^i)^T = \alpha_i^* (\boldsymbol{z}^i)^T A, \quad i = 1, ..., n$$

  so

$$(\boldsymbol{\gamma}^i)^T \boldsymbol{z}^j = \alpha_i^* (\boldsymbol{z}^i)^T A \boldsymbol{z}^j, \quad i = 1, ..., n, \quad j = 1, ..., n.$$

- If $\boldsymbol{z}^1, ..., \boldsymbol{z}^k$, $k \leq n$ are chosen to be mutually conjugate w.r.t. A, we get that for $i \neq j$.

$$(\boldsymbol{\gamma}^i)^T \boldsymbol{z}^j = 0, \quad i = 1, ..., k, \quad j = 1, ..., k, \quad i \neq j$$

We use these computations to obtain another expression of β_{11}.

Computation of the β_{ij} coefficients: β_{11}

Recall that

$$\begin{aligned}
\boldsymbol{z}^1 &= -\nabla f(\boldsymbol{x}^0) \\
\boldsymbol{z}^2 &= -\nabla f(\boldsymbol{x}^1) + \beta_{11}\boldsymbol{z}^1 \\
\gamma^1 &= \nabla f(\boldsymbol{x}^1) - \nabla f(\boldsymbol{x}^0)
\end{aligned}$$

so, according to the last result $((\gamma^i)^T \boldsymbol{z}^j = 0, \quad i \neq j)$

$$\begin{aligned}
0 &= (\gamma^1)^T \boldsymbol{z}^2 \\
&= (\gamma^1)^T [-\nabla f(\boldsymbol{x}^1) - \beta_{11}\nabla f(\boldsymbol{x}^0)] \\
&= -(\nabla f(\boldsymbol{x}^1) - \nabla f(\boldsymbol{x}^0))^T (\nabla f(\boldsymbol{x}^1) + \beta_{11}\nabla f(\boldsymbol{x}^0))
\end{aligned}$$

we get

$$\beta_{11} = \frac{(\nabla f(\boldsymbol{x}^1) - \nabla f(\boldsymbol{x}^0))^T \nabla f(\boldsymbol{x}^1)}{(\nabla f(\boldsymbol{x}^1) - \nabla f(\boldsymbol{x}^0))^T (-\nabla f(\boldsymbol{x}^0))}.$$

Computation of the β_{ij} coefficients: β_{11}

On the other hand, the value of α_k^* was chosen such that

$$\frac{df(\boldsymbol{x}^{k-1}+\alpha_k^*\boldsymbol{z}^k)}{d\alpha_k} = (\boldsymbol{z}^k)^T\nabla f(\boldsymbol{x}^{k-1}+\alpha_k^*\boldsymbol{z}^k) = (\boldsymbol{z}^k)^T\nabla f(\boldsymbol{x}^k) = 0$$

Recalling that

$$\boldsymbol{z}^1 \quad = \quad -\nabla f(\boldsymbol{x}^0)$$

it follows that

$$(\boldsymbol{z}^1)^T\nabla f(\boldsymbol{x}^1) = -(\nabla f(\boldsymbol{x}^0))^T\nabla f(x^1) = 0$$

so

$$\beta_{11} = \frac{(\nabla f(\boldsymbol{x}^1)-\nabla f(\boldsymbol{x}^0))^T\nabla f(\boldsymbol{x}^1)}{(\nabla f(\boldsymbol{x}^1)-\nabla f(\boldsymbol{x}^0))^T(-\nabla f(\boldsymbol{x}^0))} \quad \Rightarrow \quad \beta_{11} = \frac{(\nabla f(\boldsymbol{x}^1))^T\nabla f(\boldsymbol{x}^1)}{(\nabla f(\boldsymbol{x}^0))^T\nabla f(\boldsymbol{x}^0)}.$$

Computation of the β_{ij} coefficients

- The point x^2 is reached by minimizing along the conjugate directions z^1 and z^2.
- According to the last Theorem $((z^j)^T \nabla f(x^m) = 0, \quad j = 1, ..., m)$
$$(z^1)^T \nabla f(x^2) = 0, \quad (z^2)^T \nabla f(x^2) = 0.$$
- Substituting $z^1 = -\nabla f(x^0)$ and $z^2 = -\nabla f(x^1) + \beta_{11} z^1$ in these equalities, we get
$$(\nabla f(x^0))^T \nabla f(x^2) = 0, \quad (\nabla f(x^1))^T \nabla f(x^2) = 0. \tag{2}$$
- From $(\gamma^i)^T z^j = 0$ if $i \neq j$ (see page 28) and
$$\begin{aligned}
\gamma^1 &= \nabla f(x^1) - \nabla f(x^0), \\
\gamma^2 &= \nabla f(x^2) - \nabla f(x^1), \\
z^3 &= -\nabla f(x^2) + \beta_{21} z^1 + \beta_{22} z^2, \\
0 &= (\gamma^1)^T z^3 = (\nabla f(x^1) - \nabla f(x^0))^T (-\nabla f(x^2) + \beta_{21} z^1 + \beta_{22} z^2), \\
0 &= (\gamma^2)^T z^3 = (\nabla f(x^2) - \nabla f(x^1))^T (-\nabla f(x^2) + \beta_{21} z^1 + \beta_{22} z^2),
\end{aligned}$$
and the equalities (2), it follows that
$$\begin{aligned}
\beta_{21} &= 0, \\
\beta_{22} &= \frac{(\nabla f(x^2))^T \nabla f(x^2)}{(\nabla f(x^1))^T \nabla f(x^1)}.
\end{aligned}$$

Computation of the β_{ij} coefficients

In a similar way, we can also establish that

$$\begin{aligned} \beta_{kj} &= 0, \quad \text{for} \quad k \neq j \\ \beta_{kk} &= \frac{(\nabla f(\boldsymbol{x}^k))^T \nabla f(\boldsymbol{x}^k)}{(\nabla f(\boldsymbol{x}^{k-1}))^T \nabla f(\boldsymbol{x}^{k-1})}, \quad k = 1, ..., n \end{aligned}$$

thus

$$\boxed{\boldsymbol{z}^{k+1} = -\nabla f(\boldsymbol{x}^k) + \frac{(\nabla f(\boldsymbol{x}^k))^T \nabla f(\boldsymbol{x}^k)}{(\nabla f(\boldsymbol{x}^{k-1}))^T \nabla f(\boldsymbol{x}^{k-1})} \boldsymbol{z}^k.} \tag{3}$$

The conjugate gradient algorithm

1. Choose a starting point $\boldsymbol{x}^0 \in \mathbb{R}^n$.
2. Evaluate $\nabla f(\boldsymbol{x}^0)$ and set $\boldsymbol{z}^1 = -\nabla f(\boldsymbol{x}^0)$.
3. Move to $\boldsymbol{x}^1, \boldsymbol{x}^2, ..., \boldsymbol{x}^n$
$$\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \alpha^*_{k+1}\boldsymbol{z}^{k+1}$$
by minimizing $f(\boldsymbol{x})$ along the directions $\boldsymbol{z}^1, ..., \boldsymbol{z}^n$ computed according to
$$\boldsymbol{z}^{k+1} = -\nabla f(\boldsymbol{x}^k) + \frac{(\nabla f(\boldsymbol{x}^k))^T \nabla f(\boldsymbol{x}^k)}{(\nabla f(\boldsymbol{x}^{k-1}))^T \nabla f(\boldsymbol{x}^{k-1})}\boldsymbol{z}^k$$
4. If f is quadratic, then
$$\alpha^*_{k+1} = -\frac{(\boldsymbol{z}^{k+1})^T \nabla f(\boldsymbol{x}^k)}{(\boldsymbol{z}^{k+1})^T A \boldsymbol{z}^{k+1}}$$
and the procedure finishes after the first n minimizations.
5. After these n minimizations, restart the procedure by letting $\boldsymbol{x}^n$ and $-\nabla f(\boldsymbol{x}^n)$ be the new $\boldsymbol{x}^0$ and $\boldsymbol{z}^1$.
6. Repite the above two steps (3. and 4.) until
$$\|\nabla f(\boldsymbol{x}^k)\|^2 = (\nabla f(\boldsymbol{x}^k))^T \nabla f(\boldsymbol{x}^k) \leq \epsilon,$$
where ϵ is some predetermined small number.

The conjugate gradient algorithm. Example

Consider

$$f(\boldsymbol{x}) = \frac{3}{2}x^2 + \frac{1}{2}y^2 - xy - 2x,$$

so

$$\boldsymbol{a} = 0, \quad \boldsymbol{b} = \begin{pmatrix} -2 \\ 0 \end{pmatrix}, \quad A = \begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix}.$$

We take

$$\boldsymbol{x}^0 = \begin{pmatrix} -2 \\ 4 \end{pmatrix}, \quad \nabla f(\boldsymbol{x}^0) = \begin{pmatrix} -12 \\ 6 \end{pmatrix}, \quad \boldsymbol{z}^1 = -\nabla f(\boldsymbol{x}^0) = \begin{pmatrix} 12 \\ -6 \end{pmatrix}.$$

Minimizing $f(\boldsymbol{x}^0 + \alpha_1 \boldsymbol{z}^1)$ with respect to α_1 we get $\alpha_1^* = 5/17$ and

$$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \alpha_1^* \boldsymbol{z}^1 = \begin{pmatrix} 26/17 \\ 38/17 \end{pmatrix}, \quad \nabla f(\boldsymbol{x}^1) = \begin{pmatrix} 6/17 \\ 12/17 \end{pmatrix}.$$

So, we have

$$\boldsymbol{z}^2 = -\nabla f(\boldsymbol{x}^1) + \frac{(\nabla f(\boldsymbol{x}^1))^T \nabla f(\boldsymbol{x}^1)}{(\nabla f(\boldsymbol{x}^0))^T \nabla f(\boldsymbol{x}^0)} \boldsymbol{z}^1 = -\begin{pmatrix} 6/17 \\ 12/17 \end{pmatrix} + \frac{(6/17)^2 + (12/17)^2}{(-12)^2 + 6^2} \begin{pmatrix} 12 \\ -6 \end{pmatrix}$$

$$= -\begin{pmatrix} 90/289 \\ 210/289 \end{pmatrix}.$$

Minimizing $f(\boldsymbol{x}^1 + \alpha_2 \boldsymbol{z}^2)$ with respect to α_2 we get $\alpha_2^* = 17/10$. Consequently $\boldsymbol{x}^2 = \boldsymbol{x}^1 + \alpha_2^* \boldsymbol{z}^2 = (1, 1)^T$, which is the global minimum of the quadratic function f.

The conjugate gradient method. Exercises

Exercise 5. To be delivered before 11-XI-2018 as: `Ex05-YourSurname.pdf`

Solve the linear system

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

using the conjugate-gradient method.

Exercise 6. To be delivered before 18-XI-2018 as: `Ex06-YourSurname.pdf`

Consider the conjugate gradient method applied to the minimization of

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

where A is a positive definite and symmetric matrix.
Show that the iterate $\boldsymbol{x}^k$ minimizes f over

$$\boldsymbol{x}^0 + \ < \boldsymbol{v}^0, A\boldsymbol{v}^0, ..., A^{k-1}\boldsymbol{v}^0 >$$

where $\boldsymbol{v}^0 = \nabla f(\boldsymbol{x}^0)$, and $< v^0, A\boldsymbol{v}^0, ..., A^{k-1}\boldsymbol{v}^0 >$ is the subspace generated by $v^0, A\boldsymbol{v}^0, ..., A^{k-1}\boldsymbol{v}^0$

Powell's method

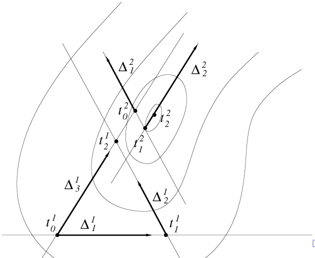
- We start presenting Powell's method as an empirical technique, later we will justify its underlying principles.
- The method does not require the computation of derivatives and, from now on, we will not assume that $f(\boldsymbol{x})$ is a quadratic function.
- The basic version of the method is as follows:

  1. Each stage the procedure consists of $\boldsymbol{n+1}$ successive 1-dimensional line searches.
  2. The first n searches are done along n linearly independent directions.
  3. The $(n+1)$th search is done along the direction connecting:
     - the obtained best point (obtained at the end of the n preceeding 1-dimensional line searches)
     - with the starting point of that stage
  4. After these searches, one of the first n directions is replaced by the $(n+1)$th direction, and a new stage begins.

The kth stage of Powell's method

The kth stage of the method is given by the following steps:

1. Let $\boldsymbol{x}_B^{k-1} = \boldsymbol{t}_0^k \in \mathbb{R}^n$ be the starting point of the kth stage and $\Delta_1^k,\dots,\Delta_n^k$, n linearly independent directions. *(for $n = 2$, $k = 1$, start with $\boldsymbol{t}_0^1$, Δ_1^1, Δ_2^1)*
2. Determine θ_j^*, per $j = 1, \dots, n$ (*for $n = 2$, k=1, determine θ_1^* and θ_2^**) such that
$$f(\boldsymbol{t}_{j-1}^k + \theta_j^* \Delta_j^k) = \min_{\theta_j} f(\boldsymbol{t}_{j-1}^k + \theta_j \Delta_j^k),$$
and define
$$\boldsymbol{t}_j^k = \boldsymbol{t}_{j-1}^k + \theta_j^* \Delta_j^k, \quad j = 1, \dots, n.$$
(for $n = 2$, $k = 1$, define $\boldsymbol{t}_1^1 = \boldsymbol{t}_0^1 + \theta_1^* \Delta_1^1, \quad \boldsymbol{t}_2^1 = \boldsymbol{t}_1^1 + \theta_2^* \Delta_2^1$)
3. The new search directions are
$$\Delta_j^{k+1} = \Delta_{j+1}^k, \quad j = 1, \dots, n-1, \quad \Delta_n^{k+1} = \Delta_{n+1}^k = \boldsymbol{t}_n^k - \boldsymbol{t}_0^k.$$
(for $n = 2$, $k = 1$, the new directions are $\Delta_1^2 = \Delta_2^1$, $\Delta_2^2 = \Delta_3^1 = \boldsymbol{t}_2^1 - \boldsymbol{t}_0^1$)

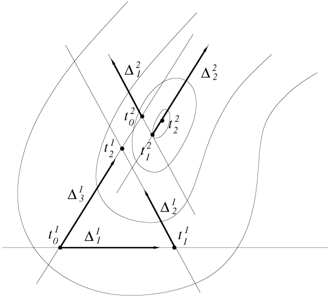


The kth stage of Powell's method

4. Find θ^*_{n+1} such that

$$f(\boldsymbol{t}^k_n + \theta^*_{n+1}(\boldsymbol{t}^k_n - \boldsymbol{t}^k_0)) = \min_{\theta_{n+1}} f(\boldsymbol{t}^k_n + \theta_{n+1}(\boldsymbol{t}^k_n - \boldsymbol{t}^k_0)),$$

(for $n = 2$, $k = 1$, find θ^*_3 s.t. $f(\boldsymbol{t}^1_2 + \theta^*_3 \Delta^2_2) = \min_{\theta_3} f(\boldsymbol{t}^1_2 + \theta_3 \Delta^2_2),$)



5. Take as new initial point

$$\boldsymbol{x}^k_B = \boldsymbol{t}^{k+1}_0 = \boldsymbol{t}^k_n + \theta^*_{n+1}(\boldsymbol{t}^k_n - \boldsymbol{t}^k_0).$$

(for $n = 2$, $k = 1$, take as initial point $\boldsymbol{x}^1_B = t^2_0 = \boldsymbol{t}^1_2 + \theta^*_3 \Delta^2_2$)

6. If $\|\boldsymbol{x}^{k-1}_B - \boldsymbol{x}^k_B\| < \epsilon$ ($\epsilon > 0$ fixed) stop, otherwise proceed to stage $k+1$.

Powell's method. Example 1 (first step)

Let

$$f(x, y) = \frac{3}{2}x^2 + \frac{1}{2}y^2 - xy - 2x,$$

which has a minimum at $(1,\ 1)$.

1. We start with

$$\boldsymbol{x}_B^0 = \boldsymbol{t}_0^1 = \begin{pmatrix} -2 \\ 4 \end{pmatrix}, \quad \Delta_1^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \Delta_1^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

2. The first minimization is in the Δ_1^1 direction

$$\min_{\theta_1} f(\boldsymbol{t}_0^1 + \theta_1 \Delta_1^1) = \min_{\theta_1} \left\{ \frac{3}{2}(-2+\theta_1)^2 + \frac{1}{2}4^2 - (-2+\theta_1)4 - 2(-2+\theta_1) \right\}$$

$$\Rightarrow \quad \theta_1^* = 4, \quad \Rightarrow \quad t_1^1 = (2,\ 4)^T$$

3. Now we minimize in the Δ_2^1 direction

$$\min_{\theta_2} f(\boldsymbol{t}_1^1 + \theta_2 \Delta_2^1) = \min_{\theta_2} \left\{ \frac{3}{2}2^2 + \frac{1}{2}(4+\theta_2)^2 - 2(4+\theta_2) - 4 \right\}$$

$$\Rightarrow \quad \theta_2^* = -2, \quad \Rightarrow \quad t_2^1 = (2,\ 2)^T$$

4. Consequently, the new direction is

$$\Delta_3^1 = t_2^1 - t_0^1 = \begin{pmatrix} 2-(-2) \\ 2-4 \end{pmatrix} = \begin{pmatrix} 4 \\ -2 \end{pmatrix}$$

Powell's method. Example 1 (first step)

5. Next we minimize along the new direction Δ_3^1

$$\min_{\theta_3} f(\boldsymbol{t}_2^1 + \theta_3 \Delta_3^1) =$$

$$= \min_{\theta_3} \left\{ \frac{3}{2}(2+4\theta_3)^2 + \frac{1}{2}(2-2\theta_3)^2 - (2+4\theta_3)(2-2\theta_3) - 2(2+4\theta_3) \right\}$$

$$\Rightarrow \quad \theta_3^* = -2/17, \quad \Rightarrow \quad x_B^1 = t_0^2 = \begin{pmatrix} 2-8/17 \\ 2+4/17 \end{pmatrix} = \begin{pmatrix} 26/17 \\ 38/17 \end{pmatrix}$$

This concludes the first iteration of the algorithm. The first two search directions of the second iteration are

$$\Delta_1^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \Delta_2^2 = \begin{pmatrix} 4 \\ -2 \end{pmatrix}.$$

Powell's method. Example 1 (second step)

6. The first minimization is in the Δ_1^2 direction

$$\min_{\theta_1} f(\boldsymbol{t}_0^2 + \theta_1 \Delta_1^2) = \min_{\theta_1} \left\{ \frac{3}{2}\left(\frac{26}{17}\right)^2 + \frac{1}{2}\left(\frac{38}{17} + \theta_1\right)^2 - \frac{26}{17}\left(\frac{38}{17} + \theta_1\right) - \frac{52}{17} \right\}$$

$$\Rightarrow \quad \theta_1^* = -12/17, \quad \Rightarrow \quad \boldsymbol{t}_1^2 = (26/17,\ 26/17)^T.$$

7. The second minimization is in the Δ_2^2 direction

$$\min_{\theta_2} f(\boldsymbol{t}_1^2 + \theta_2 \Delta_2^2) =$$

$$= \min_{\theta_2} \left\{ \frac{3}{2}\left(\frac{26}{17} + 4\theta_2\right)^2 + \frac{1}{2}\left(\frac{26}{17} - 2\theta_2\right)^2 - \left(\frac{26}{17} + 4\theta_2\right)\left(\frac{26}{17} - 2\theta_2\right) - 2\left(\frac{26}{17} + 4\theta_2\right) \right\}$$

$$\Rightarrow \quad \theta_2^* = -18/289, \quad \Rightarrow \quad t_2^2 = (370/289,\ 478/289)^T.$$

8. The new direction is

$$\Delta_3^2 = t_2^2 - t_0^2 = \begin{pmatrix} -72/289 \\ -168/289 \end{pmatrix}.$$

9. Finally, when we compute $\min_{\theta_3} f(\boldsymbol{t}_2^2 + \theta_3 \Delta_3^2) = \ldots$ we get

$$\theta_3^* = 9/8, \quad x_B^2 = (1,\ 1)^T.$$

That is, the exact minimum of the quadratic function is found in two iterations

Powell's method. Example 2

In the above example the directions $\Delta_{1,2}^k$ $(k = 1, 2)$ were linearly independent. This condition is important, as is shown in the next example.

Let

$$f(x, y, z) = (x - y + z)^2 + (-x + y + z)^2 + (x + y - z)^2,$$

that has a minimum at $(x^*, y^*, z^*) = (0,\ 0,\ 0)$. Start Powell's method with

$$x_B^0 = \begin{pmatrix} 1/2 \\ 1 \\ 1/2 \end{pmatrix}, \quad \Delta_1^1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \Delta_2^1 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \Delta_3^1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The results of the first three steps are

j	Δ_j^1	t_j^1	$f(t_j^1)$
0	–	$(1/2,\ 1,\ 1/2)$	2
1	Δ_1^1	$(1/2,\ 1,\ 1/2)$	2
2	Δ_3^1	$(1/2,\ 1/3,\ 1/2)$	$2/3$
3	Δ_3^1	$(1/2,\ 1/3,\ 5/18)$	$42/81$

The new direction is

$$\boldsymbol{t}_3^1 - \boldsymbol{t}_0^1 = \begin{pmatrix} 1/2 \\ 1/3 \\ 5/18 \end{pmatrix} - \begin{pmatrix} 1/2 \\ 1 \\ 1/2 \end{pmatrix} = \begin{pmatrix} 0 \\ -2/3 \\ -2/9 \end{pmatrix}$$

Powell's method. Example 2 (cont.)

The new search directions are

$$\Delta_1^2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \Delta_2^2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \Delta_3^2 = \begin{pmatrix} 0 \\ -2/3 \\ -2/9 \end{pmatrix}.$$

Thus, the first component of all forthcoming points reached will remain equal to $1/2$, and the true optimum at $(x^*, y^*, z^*) = (0,\ 0,\ 0)$ can never be reached.

Powell's method for quadratic functions

Let us show how the properties about conjugate directions can be used to prove termination of Powell's method in a finite number of steps for quadratic functions.

Assume that:

- The function f is quadratic and A is a symmetric positive define matrix.
- The initial point is $\boldsymbol{x}_B^0 \in \mathbb{R}^n$.
- The initial directions $\Delta_1^1, \ldots, \Delta_n^1$ are linearly independent.

After the steps of the first stage, we have:

- The $n+1$ points: $t_0^1, \ldots, t_n^1$.
- A new direction $\Delta_n^2 = \boldsymbol{z}^1 = \boldsymbol{t}_n^1 - \boldsymbol{t}_0^1$. We assume that $\boldsymbol{t}_n^1 \neq \boldsymbol{t}_0^1$.
- A new starting point $\boldsymbol{t}_0^2 = \boldsymbol{t}_n^1 + \theta_{n+1}^* \Delta_n^2 = \boldsymbol{x}_B^1$.
- The point $\boldsymbol{x}_B^1 = \boldsymbol{t}_0^2$, is a minimum of f in the Δ_n^2 direction.

Powell's method for quadratic functions

- Because of the properties of the conjugate directions (see Theorem in page 13), the direction $\boldsymbol{z}^2 = \boldsymbol{t}_n^2 - \boldsymbol{t}_0^2$ is conjugate to $\boldsymbol{z}^1$ with respect to A.
- After k steps of the procedure, we have generated k non-zero directions $\boldsymbol{z}^1,\dots,\boldsymbol{z}^k$ mutually conjugate w.r.t. A.
- If the directions $\Delta_1^k,\dots,\Delta_{n-k}^k$, $\boldsymbol{z}^1,\dots,\boldsymbol{z}^k$ are linearly independent, then $\boldsymbol{z}^{k+1} = \boldsymbol{t}_n^{k+1} - t_0^{k+1}$ will be conjugate to $\boldsymbol{z}^1,\dots,\boldsymbol{z}^k$.
- After completing n stages all the search directions are mutually conjugate w.r.t. A and the minimum of f over $\mathbb{R}^n$ has been reached.

  Recall that for a quadratic function, if a point in $\mathbb{R}^n$ is optimal in n mutually conjugate t directions, then it must be the global optimum of the function (see Theorem in page 15).

Avoiding linearly dependent search directions

We can modify Powell's method to avoid linearly dependent search directions.

The new method does not possess the quadratic termination property, but has a satisfactory performance.

Let

- $\boldsymbol{x}_B^{k-1} = \boldsymbol{t}_0^k$ be the starting point of the kth stage.
- $\Delta_1^k, \ldots, \Delta_n^k$, n linearly independent directions.

Then

- Find $\boldsymbol{t}_j^k$ for $j = 1, ..., n$, the minima of f along the directions $\Delta_1^k, \ldots, \Delta_n^k$.
- Set $\Delta_{n+1}^k = \boldsymbol{t}_n^k - \boldsymbol{t}_0^k$.
  - If $\|\boldsymbol{t}_n^k - \boldsymbol{t}_0^k\| < \epsilon$, stop.
  - Otherwise, find α_{n+1}^* such that

$$f(\boldsymbol{t}_0^k + \alpha_{n+1}^* \Delta_{n+1}^k) = \min_{\alpha_{n+1}} f(\boldsymbol{t}_0^k + \alpha_{n+1} \Delta_{n+1}^k),$$

    and let $\boldsymbol{t}_0^{k+1} = \boldsymbol{x}_B^k = \boldsymbol{t}_0^k + \alpha_{n+1}^*.$

Avoiding linearly dependent search directions

- If $\|\boldsymbol{x}_B^k - \boldsymbol{x}_B^{k-1}\| < \epsilon$, stop (convergence).
- Otherwise find the index m such that

$$f(\boldsymbol{t}_{m-1}^k) - f(\boldsymbol{t}_m^k) = \max_{j=1,\dots,n} \{f(\boldsymbol{t}_{j-1}^k) - f(t_j^k)\},$$

(largest function decreese).

  - If

$$|\alpha_{n+1}^*| < \left(\frac{f(\boldsymbol{t}_0^k) - f(\boldsymbol{t}_0^{k+1})}{f(\boldsymbol{t}_{m+1}^k) - f(\boldsymbol{t}_m^k)} \right)^{1/2}, \qquad (4)$$

    set $\Delta_j^{k-1} = \Delta_j^k$, $j = 1, \dots, n$.
    In other words, the search directions of the $(k+1)$th stage are the same as in the kth stage.

  - If (4) does not hold, set

$$\begin{aligned} \Delta_j^{k-1} &= \Delta_j^k, \quad j = 1, \dots, m-1, \\ \Delta_j^{k-1} &= \Delta_{j+1}^k, \quad j = m, \dots, n, \end{aligned}$$

    and proceed to stage $k+1$.

Avoiding linearly dependent search directions. Example 2 (cont.)

Consider again the problem of Example 2.

$$f(x, y, z) = (x - y + z)^2 + (-x + y + z)^2 + (x + y - z)^2.$$

The first steps are the same as before. We can see that the largest function decrease is obtained by going from t_1^1 to t_2^1, hence $m = 2$.
We have

$$\Delta_4^1 = (0,\ -2/3,\ -2/9)^T.$$

We find that $\alpha_4^* = 9/8$ minimizes

$$f(1/2,\ 1 - (2/3)\alpha_4,\ 1/2 - (2/9)\alpha_4) \quad \Rightarrow$$

$$\boldsymbol{t}_0^2 = (1/2,\ 1,\ 1/2)^T + (9/8)(0,\ -2/3,\ -2/9)^T = (1/2,\ 1/4,\ 1/4)^T \quad \Rightarrow f(\boldsymbol{t}_0^2) = 1/2.$$

Now

$$\left(\frac{f(\boldsymbol{t}_0^1) - f(\boldsymbol{t}_0^2)}{f(\boldsymbol{t}_1^1) - f(\boldsymbol{t}_2^1)} \right)^{1/2} = \left(\frac{2 - 1/2}{2 - 2/3} \right)^{1/2} = (9/8)^{1/2}.$$

Since $\alpha_4^* > (9/8)^{1/2}$, we see that (4) does not hold. Accordingly, the new directions will be the independents vectors

$$\begin{aligned} \Delta_1^2 &= (1,\ 0,\ 0)^T, \\ \Delta_2^2 &= (0,\ 0,\ 1)^T, \\ \Delta_3^2 &= (0,\ -(2/3),\ -(2/9))^T. \end{aligned}$$