

Practical Optimization Algorithms and Applications

Chapter V: Conjugate Gradient Methods

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The Linear Conjugate Gradient Method

Given an $n \times n$ symmetric positive definite matrix A , the following minimization problem:

$$\min \phi(x) \equiv \frac{1}{2}x^T Ax - b^T x, \quad (1)$$

can be stated equivalently as the problem of solving a linear system of equations

$$Ax = b. \quad (2)$$

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For future reference, we denote

$$\nabla \phi(x) = Ax - b \equiv r(x). \quad (3)$$

In particular at $x = x_k$, we have

$$r_k = Ax_k - b. \quad (4)$$

Definition

A set of nonzero vectors $\{p_0, p_1, \dots, p_t\}$ is said to be *conjugate* with respect to the symmetric positive definite matrix A if

$$p_i^T A p_j = 0, \quad \text{for all } i \neq j. \quad (5)$$

Definition

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- Any set of vectors satisfying this property is also linear independent.
- The importance of conjugacy lies in the fact that we can minimize $\phi(\cdot)$ in n steps by successively minimizing it along the individual directions in a conjugate set.

Conjugate Direction Methods

Consider the following *conjugate direction* method. Given a starting point $x_0 \in \mathbb{R}^n$ and a set of conjugate directions $\{p_0, p_1, \dots, p_{n-1}\}$, let us generate the sequence $\{x_k\}$ by setting

$$x_{k+1} = x_k + \alpha_k p_k, \quad (6)$$

where α_k is the one-dimensional minimizer of the quadratic function $\phi(\cdot)$ along $x_k + \alpha p_k$, given explicitly by

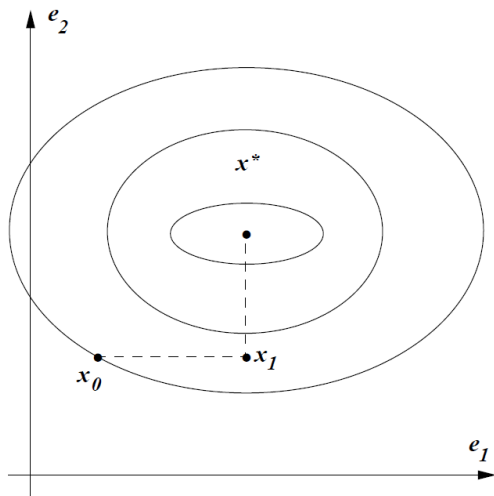
$$\alpha_k = -\frac{r_k^T p_k}{p_k^T A p_k}. \quad (7)$$

We have the following result.

Theorem

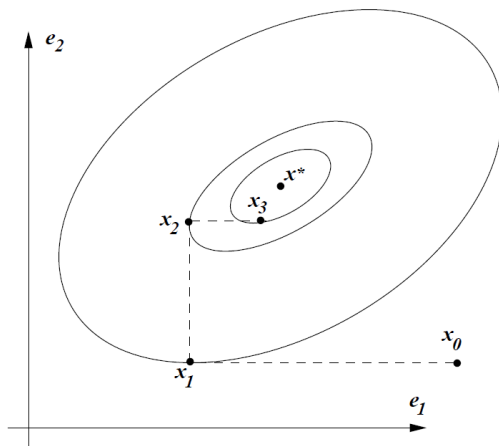
For any $x_0 \in \mathbb{R}^n$ the sequence $\{x_k\}$ generated by the conjugate direction algorithm (6), (7) converges to the solution x^ of the linear system (2) at most n steps.*

Figure 1: Demo



For a quadratic with a diagonal Hessian: Successive minimizations along the coordinate directions find its minimizer in n iterations.

Figure 2: Demo



For a general convex quadratic: Successive minimization along coordinate axes does not find the solution in n iterations.

Conjugate Direction Methods

We can recover the nice behavior of Figure 1 if we transform the problem to make A diagonal and then minimize along the coordinate directions.

Conjugate Direction Methods

We can recover the nice behavior of Figure 1 if we transform the problem to make A diagonal and then minimize along the coordinate directions.

Suppose we transform the problem by defining new variables \hat{x} as

$$\hat{x} = S^{-1}x,$$

where S is the $n \times n$ matrix defined by

$$S = [p_0, p_1, \dots, p_{n-1}],$$

where $[p_0, p_1, \dots, p_{n-1}]$ is the set of conjugate directions with respect to A . The quadratic now becomes

$$\hat{\phi}(\hat{x}) \equiv \phi(S\hat{x}) = \frac{1}{2}\hat{x}^T(S^TAS)\hat{x} - (S^Tb)^T\hat{x},$$

By the conjugacy property, the matrix S^TAS is diagonal, so we can find the minimizing value of $\hat{\phi}$ by performing n one-dimensional minimizations along the coordinate directions of \hat{x} .

Conjugate Direction Methods

When the Hessian matrix is diagonal, each coordinate minimization correctly determines one of the components of the solution x^* . In other words, after k one-dimensional minimizations, the quadratic has been minimized on the subspace spanned by e_1, e_2, \dots, e_k . The following theorem proves this important result for the general case in which the Hessian of the quadratic is not necessarily diagonal.

Theorem (Expanding Subspace Minimization)

Let $x_0 \in \mathbb{R}^n$ be any starting point and suppose that the sequence $\{x_k\}$ is generated by the conjugate direction algorithm (6), (7). Then

$$r_k^T p_i = 0, \text{ for } i = 0, 1, \dots, k-1, \quad (8)$$

and x_k is the minimizer of $\phi(x) = \frac{1}{2}x^T Ax - b^T x$ over the set

$$\{x | x = x_0 + \text{span}\{p_0, p_1, \dots, p_{k-1}\}\}. \quad (9)$$

Conjugate Direction Methods

The fact that the current residual r_k is orthogonal to all previous search directions is a property that will be used extensively in the following.

The discussion so far has been general, in that it applies to a conjugate direction method based on any choice of the conjugate direction set $\{p_0, p_1, \dots, p_{n-1}\}$. There are many ways to choose the set of conjugate directions. For instance,

- the eigenvectors v_1, v_2, \dots, v_n of A are mutually orthogonal as well as conjugate with respect to A ;
- the Gram–Schmidt orthogonalization process can be modified to produce a set of conjugate directions rather than a set of orthogonal directions.

Basic Property of the Conjugate Gradient Method

The conjugate gradient method is a conjugate direction method with a very special property: In generating its set of conjugate vectors, it can compute a new vector p_k by using only the previous vector p_{k-1} . It does not need to know all the previous elements p_0, p_1, \dots, p_{k-2} of the conjugate set; p_k is automatically conjugate to these vectors.

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This remarkable property implies that the method requires **little storage and computation**.

Details of the Conjugate Gradient Method

Each direction p_k is chosen to be a linear combination of the steepest descent direction $-\nabla\phi(x_k)$ (which is the same as the negative residual r_k) and the previous direction p_{k-1} . We write

$$p_k = -r_k + \beta_k p_{k-1}, \quad (10)$$

where the scalar β_k is to be determined by the requirement that p_{k-1} and p_k must be conjugate with respect to A . By premultiplying (10) by $p_{k-1}^T A$ and imposing the condition $p_{k-1}^T A p_k = 0$, we find that

$$\beta_k = \frac{r_k^T A p_{k-1}}{p_{k-1}^T A p_{k-1}}.$$

It makes intuitive sense to choose the first search direction p_0 to be the steepest descent direction at the initial point x_0 . As in the general conjugate direction method, we perform successive one-dimensional minimizations along each of the search directions.

Algorithm 1 (CG-Preliminary Version).

Given x_0 ;

Set $r_0 \leftarrow Ax_0 - b$, $p_0 \leftarrow -r_0$, $k \leftarrow 0$;

while $r_k \neq 0$, **do**

$$\alpha_k \leftarrow -\frac{r_k^T p_k}{p_k^T A p_k};$$

$$x_{k+1} \leftarrow x_k + \alpha_k p_k;$$

$$r_{k+1} \leftarrow Ax_{k+1} - b;$$

$$\beta_{k+1} \leftarrow \frac{r_{k+1}^T A p_k}{p_k^T A p_k};$$

$$p_{k+1} \leftarrow -r_{k+1} + \beta_{k+1} p_k;$$

$$k \leftarrow k + 1;$$

end while

Conjugate Gradient Method

Theorem

Suppose that the k -th iterate generated by the conjugate gradient method is not the solution point x^ . The following four properties hold:*

$$r_k^T r_i = 0, \quad \forall i = 0, \dots, k-1, \quad (11a)$$

$$\text{span}\{r_0, r_1, \dots, r_k\} = \text{span}\{r_0, Ar_0, \dots, A^k r_0\}, \quad (11b)$$

$$\text{span}\{p_0, p_1, \dots, p_k\} = \text{span}\{r_0, Ar_0, \dots, A^k r_0\}, \quad (11c)$$

$$p_k^T A p_i = 0, \quad \forall i = 0, 1, \dots, k-1. \quad (11d)$$

Therefore, the sequence $\{x_k\}$ converges to x^ in at most n steps.*

- The proof of this theorem relies on the fact that the first direction p_0 is the steepest descent direction $-r_0$; in fact, the result does not hold for other choices of p_0 .
- Since the gradients r_k are mutually orthogonal, the term “conjugate gradient method” is actually a misnomer. It is the search directions, not the gradients, that are conjugate with respect to A .

Conjugate Gradient Method

This theorem shows that

- the directions p_0, p_1, \dots, p_{n-1} are indeed conjugate, which implies termination in n steps;
- the residuals r_i are mutually orthogonal;
- each search direction p_k and residual r_k is contained in the Krylov subspace of degree k for r_0 , defined as

$$\mathcal{K}(r_0; k) \equiv \text{span}\{r_0, Ar_0, \dots, A^k r_0\}.$$

A Practical Form of the Conjugate Gradient Method

We can derive a slightly more economical form of the conjugate gradient method by using the results of above theorems.

From $r_k^T p_k = -r_k^T r_k$ and $r_{k+1} = r_k + \alpha_k A p_k$, we have

$$\alpha_k = \frac{r_k^T r_k}{p_k^T A p_k} \quad (12)$$

and

$$\beta_{k+1} = \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k} \quad (13)$$

A Practical Form of the Conjugate Gradient Method

Algorithm 2 (CG).

Given x_0 ;

Set $r_0 \leftarrow Ax_0 - b$, $p_0 \leftarrow -r_0$, $k \leftarrow 0$;

while $r_k \neq 0$, **do**

$$\alpha_k \leftarrow \frac{r_k^T r_k}{p_k^T A p_k};$$

$$x_{k+1} \leftarrow x_k + \alpha_k p_k;$$

$$r_{k+1} \leftarrow r_k + \alpha_k A p_k;$$

$$\beta_{k+1} \leftarrow \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k};$$

$$p_{k+1} \leftarrow -r_{k+1} + \beta_{k+1} p_k;$$

$$k \leftarrow k + 1;$$

end while

Rate of Convergence

Theorem

If A has only r distinct eigenvalues, the the CG iteration will terminate at the solution in at most r iterations.

Theorem

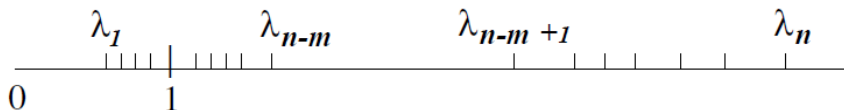
If A has eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \lambda_n$, we have that

$$\|x_{k+1} - x^*\|_A^2 \leq \left(\frac{\lambda_{n-k} - \lambda_1}{\lambda_{n-k} + \lambda_1} \right)^2 \|x_0 - x^*\|_A^2. \quad (14)$$

Above theorem can be used to predict the behavior of the CG method on specific problems.

Rate of Convergence

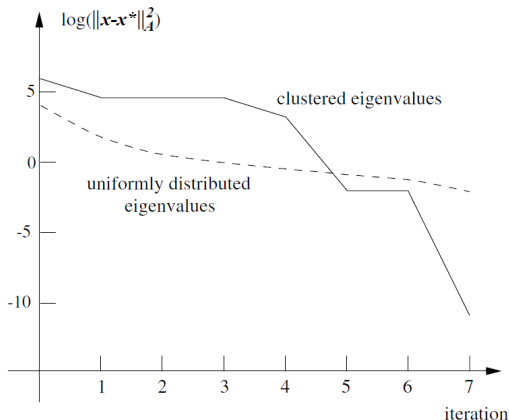
Suppose we have the situation plotted in the following figure, where the eigenvalues of A consist of m large values, with the remaining $n - m$ smaller eigenvalues clustered around 1.



If we define $\epsilon = \lambda_{n-m} - \lambda_1$, above theorem tells us that after $m + 1$ steps of the conjugate gradient algorithm, we have

$$\|x_{m+1} - x^*\|_A \approx \epsilon \|x_0 - x^*\|_A.$$

For a small value of ϵ , we conclude that the CG iterates will provide a good estimate of the solution after only $m + 1$ steps.



Performance of the conjugate gradient method on (a) a problem in which five of the eigenvalues are large and the remainder are clustered near 1, and (b) a matrix with uniformly distributed eigenvalues.

Preconditioning

We can accelerate the conjugate gradient method by transforming the linear system to improve the eigenvalue distribution of A . The key to this process, which is known as *preconditioning*, is a change of variables from x to \hat{x} via a nonsingular matrix C , that is,

$$\hat{x} = Cx.$$

The quadratic ϕ is transformed accordingly to

$$\hat{\phi}(\hat{x}) = \frac{1}{2}\hat{x}^T(C^{-T}AC^{-1})^{-1}\hat{x} - (C^{-T}b)^T\hat{x}.$$

If we use CG algorithm to minimize $\hat{\phi}$ or, equivalently, to solve the linear system

$$(C^{-T}AC^{-1})\hat{x} = C^{-T}b,$$

then the convergence rate will depend on the eigenvalues of the matrix $C^{-T}AC^{-1}$ rather than those of A . Therefore, we aim to choose C such that the eigenvalues of $C^{-T}AC^{-1}$ are more favorable for the convergence theory discussed above.

Algorithm 3 (Preconditioned CG).

Given x_0 , preconditioner M ;

Set $r_0 \leftarrow Ax_0 - b$;

Solve $My_0 = r_0$ for y_0 ;

$p_0 \leftarrow -r_0$, $k \leftarrow 0$;

while $r_k \neq 0$, **do**

$$\alpha_k \leftarrow \frac{r_k^T y_k}{p_k^T A p_k};$$

$$x_{k+1} \leftarrow x_k + \alpha_k p_k;$$

$$r_{k+1} \leftarrow r_k + \alpha_k A p_k;$$

Solve $My_{k+1} = r_{k+1}$;

$$\beta_{k+1} \leftarrow \frac{r_{k+1}^T y_{k+1}}{r_k^T y_k};$$

$$p_{k+1} \leftarrow -y_{k+1} + \beta_{k+1} p_k;$$

$$k \leftarrow k + 1;$$

end while

- The above algorithm does not make use of C explicitly, but rather the matrix $M = C^T C$, which is symmetric and positive definite by construction.
- If we set $M = I$ in above algorithm, we recover the standard CG method.
- The orthogonality property of the successive residuals becomes

$$r_i^T M^{-1} r_j = 0 \text{ for all } i \neq j.$$

- In terms of computational effort, the main difference between the preconditioned and unpreconditioned CG methods is the need to solve systems of the form $My = r$.

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Nonlinear Conjugate Gradient Methods

- In place of the choice for the step length α_k (which minimizes ϕ along the search direction p_k), we need to perform a line search that identifies an approximate minimum of the nonlinear function f along p_k .
- The residual r , which is $\nabla\phi$ in linear CG algorithm, must be replaced by the gradient of the nonlinear objective f .

The Fletcher-Reeves Method

Algorithm 4 (FR).

Given x_0 ;

Evaluate $f_0 = f(x_0)$, $\nabla f_0 = \nabla f(x_0)$;

Set $p_0 \leftarrow -\nabla f_0$, $k \leftarrow 0$;

while $\nabla f_k \neq 0$, **do**

 Compute α_k and set $x_{k+1} = x_k + \alpha_k p_k$;

 Evaluate ∇f_{k+1} ;

$$\beta_{k+1}^{FR} \leftarrow \frac{\nabla f_{k+1}^T \nabla f_{k+1}}{\nabla f_k^T \nabla f_k};$$

$$p_{k+1} \leftarrow -\nabla f_{k+1} + \beta_{k+1}^{FR} p_k;$$

$$k \leftarrow k + 1;$$

end while

The Fletcher-Reeves Method

If the line search is exact or any inexact line search procedure that yields an α_k satisfying the following strong Wolfe conditions

$$f(x_k + \alpha_k p_k) \leq f(x_k) + c_1 \alpha_k \nabla f_k^T p_k \quad (15a)$$

$$|\nabla f(x_k + \alpha_k p_k)^T p_k| \leq c_2 |\nabla f_k^T p_k|, \quad (15b)$$

with $0 < c_1 < c_2 < \frac{1}{2}$ will ensure that all directions p_k are descent directions for the function f .

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with $0 < c_1 < c_2 < \frac{1}{2}$ will ensure that all directions p_k are descent directions for the function f .

♣ Goldstein conditions are not suitable for CG method.

Assumptions

- (i) The level set $\mathcal{L} := \{x | f(x) \leq f(x_0)\}$ is bounded;
- (ii) In some open neighborhood \mathcal{N} of \mathcal{L} , the objective function f is Lipschitz continuously differentiable.

These assumption imply that there is a constant $\bar{\gamma}$ such that

$$\|\nabla f(x)\| \leq \bar{\gamma}, \text{ for all } x \in \mathcal{L}. \quad (16)$$

Theorem (Al-Baali)

Suppose that Assumptions 1 holds, and that Algorithm 4 is implemented with a line search that satisfies the strong Wolfe conditions (15) with $0 < c_1 < c_2 < \frac{1}{2}$. Then

$$\liminf_{k \rightarrow \infty} \|\nabla f_k\| = 0. \quad (17)$$

Theorem

Suppose that FR algorithm is implemented with a step length α_k that satisfies the strong Wolfe conditions (15) with $0 < c_2 < \frac{1}{2}$. Then the method generates descent directions p_k that satisfy the following inequalities:

$$-\frac{1}{1-c_2} \leq \frac{\nabla f_k^T p_k}{\|\nabla f_k\|^2} \leq \frac{2c_2-1}{1-c_2} \text{ for all } k = 0, 1, \dots$$

Above theorem can be used to explain a weakness of the Fletcher-Reeves method. We will argue that if the method generates a bad direction and a tiny step, then the next direction and next step are also likely to be poor.

Behavior of the Fletcher-Reeves Method

Let θ denote the angle between p_k and $-\nabla f_k$, defined by

$$\cos \theta_k = \frac{-\nabla f_k^T p_k}{\|\nabla f_k\| \|p_k\|}.$$

Suppose that p_k is a poor search direction, in the sense that it makes an angle of nearly $\pi/2$ with $-\nabla f_k$, that is, $\cos \theta_k \approx 0$. By multiplying both sides of the relationship in the above theorem by $\|\nabla f_k\|/\|p_k\|$, we obtain

$$\frac{1 - 2c_2}{1 - c_2} \frac{\|\nabla f_k\|}{\|p_k\|} \leq \cos \theta_k \leq \frac{1}{1 - c_2} \frac{\|\nabla f_k\|}{\|p_k\|}, \text{ for all } k = 0, 1, \dots.$$

From these inequalities, we deduce that $\cos \theta_k \approx 0$ if and only if

$$\|\nabla f_k\| \ll \|p_k\|.$$

Behavior of the Fletcher-Reeves Method

Since p_k is almost orthogonal to the gradient, it is likely that the step from x_k to x_{k+1} is tiny, that is, $x_{k+1} \approx x_k$. If so, we have $\nabla f_{k+1} \approx \nabla f_k$, and therefore

$$\beta_{k+1}^{FR} \approx 1,$$

By using this approximation together with $\|\nabla f_{k+1}\| \approx \|\nabla f_k\| \ll \|p_k\|$, we conclude that

$$p_{k+1} \approx p_k,$$

so the new search direction will improve little (if at all) on the previous one. It follows that if the condition $\cos \theta_k \approx 0$ holds at some iteration k and if the subsequent step is small, a long sequence of unproductive iterates will follow.

The Polak-Ribière Method

There are many variants of the Fletcher-Reeves method that differ from each other mainly in the choice of the parameter β_k . An important variant, proposed by Polak and Ribière, defines this parameter as follows:

$$\beta_{k+1}^{PR} = \frac{\nabla f_{k+1}^T (\nabla f_{k+1} - \nabla f_k)}{\|\nabla f_k\|^2}. \quad (18)$$

We refer the algorithm in which β_{k+1}^{PR} replaces β_{k+1}^{FR} in Algorithm 4 as Algorithm PR.

- Algorithm PR and Algorithm PR are identical when f is a strongly convex quadratic function and the line search is exact, since the gradients are mutually orthogonal, and so $\beta_{k+1}^{PR} = \beta_{k+1}^{FR}$.
- When applied to general nonlinear functions with inexact line searches, however, the behavior of the two algorithms differs markedly. Numerical experience indicates that Algorithm PR-CG tends to be the more robust and efficient of the two.

Behavior of the Polak-Ribière Method

If the search direction p_k satisfies $\cos \theta_k \approx 0$ for some k , and if the subsequent step is small, it follows by substituting $\nabla f_k \approx \nabla f_{k+1}$ into the PR formula, we get $\beta_{k+1}^{PR} \approx 0$. So the new search direction p_{k+1} will be close to the steepest descent direction $-\nabla f_{k+1}$ and $\cos \theta_{k+1}$ will be close to 1. Therefore, Algorithm PR-CG essentially performs a restart after it encounters a bad direction.

The Polak-Ribière Method's Variant: PR+

For Algorithm PR-CG, the strong Wolfe conditions (15) do not guarantee that p_k is always a descent direction.

Theorem

Consider the Polak-Ribière method (18) with an ideal line search. There exists a twice continuously differential objective function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ and starting point $x_0 \in \mathbb{R}^3$ such that the sequence of gradients $\{\nabla f_k\}$ is bounded away from zero.

If we define the β parameter as

$$\beta_{k+1}^+ = \max\{\beta_{k+1}^{PR}, 0\}. \quad (19)$$

which gives an algorithm called Algorithm PR+, then a simple adaptation of the strong Wolfe conditions ensures that the descent property holds.

The FR-PR Formula

It is possible to guarantee global convergence for any parameter β_k satisfying the bound

$$|\beta_k| \leq \beta_k^{FR}, \quad \forall k = 2.$$

This fact suggest the following modification of the PR method. For all $k \geq 2$ let

$$\beta_k = \begin{cases} -\beta_k^{FR} & \text{if } \beta_k^{PR} < -\beta_k^{FR} \\ \beta_k^{PR} & \text{if } |\beta_k^{PR}| \leq \beta_k^{FR} \\ \beta_k^{FR} & \text{if } \beta_k^{PR} > \beta_k^{FR}. \end{cases}$$

The algorithm based on this strategies will be denoted by FR-PR.

Quadratic Termination and Restarts

A modification that is often used in nonlinear conjugate gradient procedures is to restart the iteration at every n steps by setting $\beta_k = 0$, that is, by taking a steepest descent step. Restarting serves to periodically refresh the algorithm, erasing old information that may not be beneficial. We can even prove a strong theoretical result about restarting: It leads to n -step quadratic convergence, that is,

$$\|x_{k+n} - x^*\| = O(\|x_k - x^*\|^2). \quad (20)$$

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$$\|x_{k+n} - x^*\| = O(\|x_k - x^*\|^2). \quad (20)$$

Though above result is interesting from a theoretical viewpoint, it may not be relevant in a practical context, because nonlinear conjugate gradient methods can be recommended only for solving problems with large n . In such problems restarts may never occur, since an approximate solution is often located in fewer than n steps.

Quadratic Termination and Restarts

Since the gradients are mutually orthogonal when f is a quadratic function. A restart is performed whenever two consecutive gradients are far from orthogonal, as measured by the test

$$\frac{|\nabla f_k^T \nabla f_{k-1}|}{\|\nabla f_k\|^2} \geq \nu \quad (21)$$

where a typical value for the parameter ν is 0.1.

The parameters in the strong Wolfe conditions (15) were chosen to be $c_1 = 10^4$ and $c_2 = 0.1$. The iterations were terminated when

$$\|\nabla f_k\|_\infty < 10^{-5}(1 + |f_k|),$$

or after 10,000 iterations (the latter is denoted by a *).

Numerical Performance

Problem	n	Alg FR it/f-g	Alg PR it/f-g	Alg PR+ it/f-g	mod
CALCVAR3	200	2808/5617	2631/5263	2631/5263	0
GENROS	500	*	1068/2151	1067/2149	1
XPOWSING	1000	533/1102	212/473	97/229	3
TRIDIA1	1000	264/531	262/527	262/527	0
MSQRT1	1000	422/849	113/231	113/231	0
XPOWELL	1000	568/1175	212/473	97/229	3
TRIGON	1000	231/467	40/92	40/92	0

Iterations and function/gradient evaluations required by three nonlinear conjugate gradient methods on a set of test problems.

The Hestenes-Stiefel Formula

In the case where the objective is quadratic and the line search is exact, There are many other choices for β_{k+1} that coincide with the Fletcher-Reeves formula β_{k+1} .

The Hestenes-Stiefel formula, which defines

$$\beta_{k+1}^{HS} = \frac{\nabla f_{k+1}^T (\nabla f_{k+1} - \nabla f_k)}{(\nabla f_{k+1} - \nabla f_k)^T p_k}. \quad (22)$$

gives rise to an algorithm (called Algorithm HS) that is similar to Algorithm PR, both in terms of its theoretical convergence properties and in its practical performance.

Other variants of the CG method have recently been proposed. Such as

$$\beta_{k+1}^{DY} = \frac{\nabla f_{k+1}^T \nabla f_{k+1}}{(\nabla f_{k+1} - \nabla f_k)^T p_k}, \quad (23)$$

which possess attractive theoretical and computational properties. This choice guarantee that p_k is a descent direction, provided the steplength α_k satisfies the Wolfe conditions. The CG algorithm based on (23) appear to be competitive with the PR method.

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- The *linear* conjugate gradient method was proposed by Hestenes and Stiefel in the 1950s as an iterative method for solving linear systems with positive definite coefficient matrices.
- The first *nonlinear* conjugate method was introduced by Fletcher and Reeves in the 1960s.
- For recent survey on CG methods see the book of Dai and Yuan and works of Hager and Zhang.

Thanks for your attention!