



Spectral Projected Gradient Methods: Review and Perspectives

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Abstract

Over the last two decades, it has been observed that using the gradient vector as a search direction in large-scale optimization may lead to efficient algorithms. The effectiveness relies on choosing the step lengths according to novel ideas that are related to the spectrum of the underlying local Hessian rather than related to the standard decrease in the objective function. A review of these so-called spectral projected gradient methods for convex constrained optimization is presented. To illustrate the performance of these low-cost schemes, an optimization problem on the set of positive definite matrices is described.

Keywords: spectral projected gradient methods, nonmonotone line search, large scale problems, convex constrained problems.

1. Introduction

A pioneering paper by [Barzilai and Borwein \(1988\)](#) proposed a gradient method for the unconstrained minimization of a differentiable function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ that uses a novel and nonstandard strategy for choosing the step length. Starting from a given $x^0 \in \mathbb{R}^n$, the Barzilai-Borwein (BB) iteration is given by

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

where the initial step length $\lambda_0 > 0$ is arbitrary and, for all $k = 1, 2, \dots$,

$$\lambda_k = \frac{s_{k-1}^\top s_{k-1}}{s_{k-1}^\top y_{k-1}}, \quad (2)$$

where $s_{k-1} = x^k - x^{k-1}$ and $y_{k-1} = \nabla f(x^k) - \nabla f(x^{k-1})$.

When $f(x) = \frac{1}{2}x^\top Ax + b^\top x + c$ is a quadratic function and A is a symmetric positive definite (SPD) matrix, then the step length (2) becomes

$$\lambda_k = \frac{\nabla f(x^{k-1})^\top \nabla f(x^{k-1})}{\nabla f(x^{k-1})^\top A \nabla f(x^{k-1})}. \quad (3)$$

Curiously, the step length (3) used in the BB method for defining x^{k+1} is the one used in the optimal Cauchy steepest descent method (Cauchy 1847) for defining the step at iteration k . Therefore, the BB method computes, at each iteration, the step that minimizes the quadratic objective function along the negative gradient direction but, instead of using this step at the k -th iteration, saves the step to be used in the next iteration. The main result in the paper by Barzilai and Borwein (1988) is to show the surprising result that for two-dimensional strictly convex quadratic functions the BB method converges R-superlinearly, which means that, in the average, the quotient between the errors at consecutive iterations tends asymptotically to zero. This fact raised the question about the existence of a gradient method with superlinear convergence in the general case. In 1990, the possibility of obtaining superlinear convergence for arbitrary n was discarded by Fletcher (1990), who also conjectured that, in general, only R-linear convergence should be expected. For more information about convergence rates see (Dennis and Schnabel 1983). Raydan (1993) established global convergence of the BB method for the strictly convex quadratic case with any number of variables. The nonstandard analysis presented in Raydan (1993) was later refined by Dai and Liao (2002) to prove the expected R-linear convergence result, and it was extended by Friedlander, Martínez, Molina, and Raydan (1999) to consider a wide variety of delayed choices of step length for the gradient method; see also Raydan and Svaiter (2002).

For the minimization of general (not necessarily quadratic) functions, a bizarre behavior seemed to discourage the application of the BB method: the sequence of functional values $f(x^k)$ did not decrease monotonically and, sometimes, monotonicity was severely violated. Nevertheless, it was experimentally observed (see, e.g., Fletcher 1990; Glunt, Hayden, and Raydan 1993) that the potential effectiveness of the BB method was related to the relationship between the step lengths and the eigenvalues of the Hessian rather than to the decrease of the function value. It was also observed (see, e.g., Molina and Raydan 1996) that, with the exception of very special cases, the BB method was not competitive with the classical Hestenes and Stiefel (1952) conjugate gradients (CG) algorithm when applied to strictly convex quadratic functions. On the other hand, starting with the work by Grippo, Lampariello, and Lucidi (1986), nonmonotone strategies for function minimization began to become popular when combined with Newton-type schemes. These strategies made it possible to define globally convergent algorithms without monotone decrease requirements. The philosophy behind nonmonotone strategies is that, frequently, the first choice of a trial point by a minimization algorithm hides a lot of wisdom about the problem structure and that such knowledge can be destroyed by the decrease imposition.

The conditions were given for the implementation of the BB method for general unconstrained minimization with the help of a nonmonotone strategy. Raydan (1997) developed a globally convergent method in 1997 using the Grippo-Lampariello-Lucidi (GLL) strategy (Grippo *et al.* 1986) and the BB method given by (1) and (2). He exhibited numerical experiments that showed that, perhaps surprisingly, the method was more efficient than classical conjugate gradient methods for minimizing general functions. These nice comparative numerical results were possible because, albeit the conjugate gradient method of Hestenes and Stiefel continued

to be the method of choice for solving strictly convex quadratic problems, its efficiency is hardly inherited by generalizations for minimizing general functions. Therefore, there existed a wide space for variations and extensions of the BB original method.

The spectral projected gradient (SPG) method (Birgin, Martínez, and Raydan 2000, 2001, 2003b), for solving convex constrained problems, was born from the marriage of the global Barzila-Borwein (spectral) nonmonotone scheme (Raydan 1997) with the classical projected gradient (PG) method (Bertsekas 1976; Goldstein 1964; Levitin and Polyak 1966) which have been extensively used in statistics; see e.g., Bernaards and Jennrich (2005) and references therein. Indeed, the effectiveness of the classical PG method can be greatly improved by incorporating the spectral step length and nonmonotone globalization strategies; more details on this topic can be found in Bertsekas (1999). In Section 2, we review the basic idea of the SPG method and list some of its most important properties. In Section 3, we illustrate the properties of the method by solving an optimization problem on the convex set of positive definite matrices. In Section 4, we briefly describe some of the most relevant applications and extensions of the SPG method. Finally, in Section 5, we present some conclusions.

2. Spectral projected gradient (SPG) method

Quasi-Newton secant methods for unconstrained optimization (Dennis and Moré 1977; Dennis and Schnabel 1983) obey the recursive formula

$$x^{k+1} = x^k - \alpha_k B_k^{-1} \nabla f(x^k), \quad (4)$$

where the sequence of matrices $\{B_k\}$ satisfies the *secant equation*

$$B_{k+1} s_k = y_k. \quad (5)$$

It can be shown that, at the *trial point* $x^k - B_k^{-1} \nabla f(x^k)$, the affine approximation of $\nabla f(x)$ that interpolates the gradient at x^k and x^{k-1} vanishes for all $k \geq 1$.

Now assume that we are looking for a matrix B_{k+1} with a very simple structure that satisfies (5). More precisely, if we impose that

$$B_{k+1} = \sigma_{k+1} I,$$

with $\sigma_{k+1} \in \mathbb{R}$, then equation (5) becomes:

$$\sigma_{k+1} s_k = y_k.$$

In general, this equation has no solutions. However, accepting the least-squares solution that minimizes $\|\sigma s_k - y_k\|_2^2$, we obtain:

$$\sigma_{k+1} = \frac{s_k^\top y_k}{s_k^\top s_k}, \quad (6)$$

i.e., $\sigma_{k+1} = 1/\lambda_{k+1}$, where λ_{k+1} is the BB choice of step length given by (2). Namely, the method for unconstrained minimization is of the form $x^{k+1} = x^k + \alpha_k d_k$, where at each iteration,

$$d_k = -\lambda_k \nabla f(x^k),$$

$\lambda_k = 1/\sigma_k$, and formula (6) is used to generate the coefficients σ_k provided that they are bounded away from zero and that they are not very large. In other words, the method uses safeguards $0 < \lambda_{\min} \leq \lambda_{\max} < \infty$ and defines, at each iteration:

$$\lambda_{k+1} = \max \left\{ \lambda_{\min}, \min \left\{ \frac{s_k^\top s_k}{s_k^\top y_k}, \lambda_{\max} \right\}, \lambda_{\max} \right\}.$$

By the Mean-Value Theorem of integral calculus, one has:

$$y_k = \left[\int_0^1 \nabla^2 f(x^k + ts_k) dt \right] s_k.$$

Therefore, (6) defines a Rayleigh quotient relative to the average Hessian matrix $\int_0^1 \nabla^2 f(x_k + ts_k) dt$. This coefficient is between the minimum and the maximum eigenvalue of the average Hessian, which motivates the denomination of *spectral method* (Birgin *et al.* 2000).

Writing the secant equation as $H_{k+1}y_k = s_k$, which is also standard in the Quasi-Newton tradition, we arrive at a different spectral coefficient: $(y_k^\top y_k)/(s_k^\top y_k)$; see Barzilai and Borwein (1988) and Raydan (1993). Both this dual and the primal (6) spectral choices of step lengths produce fast and effective nonmonotone gradient methods for large-scale unconstrained optimization (Fletcher 2005; Friedlander *et al.* 1999; Raydan 1997). Fletcher (2005) presents some experimental considerations about the relationship between the nonmonotonicity of BB-type methods and their surprising computational performance; pointing out that the effectiveness of the approach is related to the eigenvalues of the Hessian rather than to the decrease of the function value; see also De Asmundis, Di Serafino, Riccio, and Toraldo (2013), Glunt *et al.* (1993), and Raydan and Svaiter (2002). A deeper analysis of the asymptotic behavior of BB methods and related methods is presented in Dai and Fletcher (2005). The behavior of BB methods has also been analyzed using chaotic dynamical systems (van den Doel and Ascher 2012). Moreover, in the quadratic case, several spectral step lengths can be interpreted by means of a simple geometric object: the Bézier parabola (Berlinet and Roland 2011). All of these interesting theoretical as well as experimental observations, concerning the behavior of BB methods for unconstrained optimization, justify the interest in designing effective spectral gradient methods for constrained optimization.

The SPG method (Birgin *et al.* 2000, 2001, 2003b) is the spectral option for solving convex constrained optimization problems. As its unconstrained counterpart (Raydan 1997), the SPG method has the form

$$x^{k+1} = x^k + \alpha_k d_k, \tag{7}$$

where the search direction d_k has been defined in Birgin *et al.* (2000) as

$$d_k = P_\Omega(x^k - \lambda_k \nabla f(x^k)) - x^k,$$

P_Ω denotes the Euclidean projection onto the closed and convex set Ω , and λ_k is the spectral choice of step length (2). A related method with approximate projections has been defined in Birgin *et al.* (2003b). The feasible direction d_k is a descent direction, i.e., $d_k^\top \nabla f(x^k) < 0$ which implies that $f(x^k + \alpha d_k) < f(x^k)$ for α small enough. This means that, in principle, one could define convergent methods imposing sufficient decrease at every iteration. However, as in the unconstrained case, this leads to very inefficient practical results. A key feature is to accept the initial BB-type step length as frequently as possible while simultaneously guarantee

global convergence. For this reason, the SPG method employs a nonmonotone line search that does not impose functional decrease at every iteration. In Birgin *et al.* (2000, 2001, 2003b) the nonmonotone GLL (Grippo *et al.* 1986) search is used (see Algorithm 2.2 below). The global convergence of the SPG method, and some related extensions, can be found in Birgin *et al.* (2003b).

The nonmonotone sufficient decrease criterion, used in the SPG method, depends on an integer parameter $M \geq 1$ and imposes a functional decrease every M iterations (if $M = 1$ then GLL line search reduces to a monotone line search). The line search is based on a safeguarded quadratic interpolation and aims to satisfy an Armijo-type criterion with a sufficient decrease parameter $\gamma \in (0, 1)$. Algorithm 2.1 describes the SPG method in details, while Algorithm 2.2 describes the line search. More details can be found in Birgin *et al.* (2000, 2001).

Algorithm 2.1: Spectral projected gradient

Assume that a sufficient decrease parameter $\gamma \in (0, 1)$, an integer parameter $M \geq 1$ for the nonmonotone line search, safeguarding parameters $0 < \sigma_1 < \sigma_2 < 1$ for the quadratic interpolation, safeguarding parameters $0 < \lambda_{\min} \leq \lambda_{\max} < \infty$ for the spectral step length, an arbitrary initial point x^0 , and $\lambda_0 \in [\lambda_{\min}, \lambda_{\max}]$ are given. If $x^0 \notin \Omega$ then redefine $x^0 = P_{\Omega}(x^0)$. Set $k \leftarrow 0$.

1. *Stopping criterion*

If $\|P_{\Omega}(x^k - \nabla f(x^k)) - x^k\|_{\infty} \leq \varepsilon$ then stop declaring that x^k is an approximate stationary point.

2. *Iterate*

Compute the search direction $d_k = P_{\Omega}(x^k - \lambda_k \nabla f(x^k)) - x^k$, compute the step length α_k using Algorithm 2.2 (with parameters γ , M , σ_1 , and σ_2), and set $x^{k+1} = x^k + \alpha_k d_k$.

3. *Compute the spectral step length*

Compute $s_k = x^{k+1} - x^k$ and $y_k = \nabla f(x^{k+1}) - \nabla f(x^k)$. If $s_k^{\top} y_k \leq 0$ then set $\lambda_{k+1} = \lambda_{\max}$.

Otherwise, set $\lambda_{k+1} = \max\{\lambda_{\min}, \min\{s_k^{\top} s_k / s_k^{\top} y_k, \lambda_{\max}\}\}$. Set $k \leftarrow k + 1$ and go to Step 1.

Algorithm 2.2: Nonmonotone line search

Compute $f_{\max} = \max\{f(x_{k-j}) \mid 0 \leq j \leq \min\{k, M - 1\}\}$ and set $\alpha \leftarrow 1$.

1. *Test nonmonotone GLL criterion*

If $f(x^k + \alpha d_k) \leq f_{\max} + \gamma \alpha \nabla f(x^k)^{\top} d_k$ then set $\alpha_k \leftarrow \alpha$ and stop.

2. *Compute a safeguarded new trial step length*

Compute $\alpha_{\text{tmp}} \leftarrow -\frac{1}{2} \alpha^2 \nabla f(x^k)^{\top} d_k / [f(x^k + \alpha d_k) - f(x^k) - \alpha \nabla f(x^k)^{\top} d_k]$. If $\alpha_{\text{tmp}} \in [\sigma_1, \sigma_2 \alpha]$ then set $\alpha \leftarrow \alpha_{\text{tmp}}$. Otherwise, set $\alpha \leftarrow \alpha/2$. Go to Step 1.

In practice, it is usual to set $\lambda_{\min} = 10^{-30}$, $\lambda_{\max} = 10^{30}$, $\sigma_1 = 0.1$, $\sigma_2 = 0.9$, and $\gamma = 10^{-4}$. A typical value for the nonmonotone parameter is $M = 10$, although in some applications values ranging from 2 to 100 have been reported. However, the best possible value of M is problem-dependent and a fine tuning may be adequate for specific applications. It can only be said that $M = 1$ is not good because it makes the strategy to coincide with the classical monotone Armijo strategy (a comparison with this case can be found in Birgin *et al.* 2000) and that $M \approx \infty$ is not good either because in this case the decrease of the objective function is not controlled at all. Other nonmonotone techniques were also introduced (Grippo, Lampariello, and Lucidi 1991; Toint 1996; Dai and Zhang 2001; Zhang and Hager 2004; Grippo and Sciandrone 2002; La Cruz, Martínez, and Raydan 2006). Parameter $\lambda_0 \in [\lambda_{\min}, \lambda_{\max}]$ is arbitrary. In Birgin *et al.* (2000, 2001) it was considered

$$\lambda_0 = \max\{\lambda_{\min}, \min\{1/\|P_{\Omega}(x^0 - \nabla f(x^0)) - x^0\|_{\infty}, \lambda_{\max}\}\}, \quad (8)$$

assuming that x^0 is such that $P_{\Omega}(x^0 - \nabla f(x^0)) \neq x^0$. In Birgin *et al.* (2003b), at the expense of an extra gradient evaluation, it was used

$$\lambda_0 = \begin{cases} \max\{\lambda_{\min}, \min\{\bar{s}^{\top} \bar{s} / \bar{s}^{\top} \bar{y}, \lambda_{\max}\}\}, & \text{if } \bar{s}^{\top} \bar{y} > 0, \\ \lambda_{\max}, & \text{otherwise,} \end{cases}$$

where $\bar{s} = \bar{x} - x^0$, $\bar{y} = \nabla f(\bar{x}) - \nabla f(x^0)$, $\bar{x} = x^0 - \alpha_{\text{small}} \nabla f(x^0)$,

$$\alpha_{\text{small}} = \max\{\varepsilon_{\text{rel}} \|x^0\|_{\infty}, \varepsilon_{\text{abs}}\},$$

and ε_{rel} and ε_{abs} are relative and absolute small values related to the machine precision, respectively.

It is easy to see that SPG only needs $3n + O(1)$ double precision positions but one additional vector may be used to store the iterate with best functional value obtained by the method. This is almost always the last iterate but exceptions are possible. C/C++, Fortran 77 (including an interface with the **CUTEr**, Gould, Orban, and Toint 2003, test set), MATLAB, and Octave subroutines implementing the spectral projected gradient method (Algorithms 2.1 and 2.2) are available in the TANGO Project web page (<http://www.ime.usp.br/~egbirgin/tango/>). A Fortran 77 implementation is also available as Algorithm 813 of the ACM Collected Algorithms (<http://calgo.acm.org/>). An implementation of the SPG method in R (R Core Team 2014) is also available within the **BB** package Varadhan and Gilbert (2009). Recall that the method's purpose is to seek the least value of a function f of potentially many variables, subject to a convex set Ω onto which we know how to project. The objective function and its gradient should be coded by the user. Similarly, the user must provide a subroutine that computes the projection of an arbitrary vector x onto the feasible convex set Ω .

3. A matrix problem on the set of positive definite matrices

Optimization problems on the space of matrices, which are restricted to the convex set of positive definite matrices, arise in various applications, such as statistics, as well as financial mathematics, model updating, and in general in matrix least-squares settings (see e.g., Boyd and Xiao 2005; Escalante and Raydan 1996; Fletcher 1985; Higham 2002; Hu and Olkin 1991; Yuan 2012).

To illustrate the use of the SPG method, we now describe a classification scheme (see, e.g., [Kawalec and Magdziak 2012](#)) that can be written as an optimization problem on the convex set of positive definite matrices. Given a training set of labelled examples

$$D = \{(z_i, w_i), i = 1, \dots, m, z_i \in \mathbb{R}^q \text{ and } w_i \in \{1, -1\}\},$$

we aim to find a classifier ellipsoid $E(A, b) = \{y \in \mathbb{R}^q \mid y^\top A y + b^\top y = 1\}$ in \mathbb{R}^q such that $z_i^\top A z_i + b^\top z_i \leq 1$ if $w_i = 1$ and $z_i^\top A z_i + b^\top z_i \geq 1$, otherwise. Since such ellipsoid may not exist, defining $I = \{i \in \{1, \dots, m\} \mid w_i = 1\}$ and $O = \{i \in \{1, \dots, m\} \mid w_i = -1\}$, we seek to minimize the function given by

$$f(A, b) = \frac{1}{m} \left[\sum_{i \in I} \max\{0, z_i^\top A z_i + b^\top z_i - 1\}^2 + \sum_{i \in O} \max\{0, 1 - z_i^\top A z_i - b^\top z_i\}^2 \right]$$

subject to symmetry and positive definiteness of the $q \times q$ matrix A . Moreover, to impose closed constraints on the semi-axes of the ellipsoid, we define a lower and an upper bound

$$0 < \hat{\lambda}_{\min} \leq \lambda_i(A) \leq \hat{\lambda}_{\max} < +\infty$$

on the eigenvalues $\lambda_i(A)$, $1 \leq i \leq q$. Given a square matrix A , its projection onto this closed and convex set can be computed in two steps ([Escalante and Raydan 1996](#); [Higham 1988](#)). In the first step one symmetrizes A and in the second step one computes the QDQ^\top decomposition of the symmetrized matrix and replaces its eigenvalues by their projection onto the interval $[\hat{\lambda}_{\min}, \hat{\lambda}_{\max}]$.

The number of variables n of the problem is $n = q(q + 1)$, corresponding to the q^2 elements of matrix $A \in \mathbb{R}^{q \times q}$ plus the elements of $b \in \mathbb{R}^q$. Variables correspond to the column wise representation of A plus the elements of b .

3.1. Coding the problem

The problem will be solved using the implementation of the SPG method that is part of the R package **BB** [Varadhan and Gilbert \(2009\)](#) as subroutine `spg`. Using the SPG method requires subroutines to compute the objective function, its gradient, and the projection of an arbitrary point onto the convex set. The gradient is computed once per iteration, while the objective function may be computed more than once. However, the nonmonotone strategy of the SPG method implies that the number of function evaluations per iteration is in general near one. There is a practical effect associated with this property. If the objective function and its gradient share common expressions, they may be computed jointly in order to save computational effort. This is the case of the problem at hand. Therefore, subroutines to compute the objective function and its gradient, that will be named `evalf` and `evalg`, respectively, are based on a subroutine named `evalfg` that, as its name suggests, computes both at the same time. Every time `evalf` is called, it calls `evalfg`, returns the computed value of the objective function and saves its gradient. When subroutine `evalg` is called, it returns the saved gradient. This is possible because the SPG method possesses the following property: every time the gradient at a point x is required, the objective function was already evaluated at point x and that point was the last one at which the objective function was evaluated. Therefore, the code of subroutines that compute the objective function and its gradient is given by

```
R> evalf <- function(x) {
+   r <- evalfg(x)
+   gsaved <- r$g
+   r$f
+ }
```

and

```
R> evalg <- function(x) {
+   gsaved
+ }
```

Both subroutines return values effectively computed by the subroutine `evalfg` given by

```
R> evalfg <- function(x) {
+   n <- length(x)
+   A <- matrix(x, nrow = nmat, ncol = nmat)
+   b <- x[seq(length = nmat, from = nmat^2 + 1, by = 1)]
+   fparc <- apply(p, 2, function(y) {
+     return(t(y) %*% A %*% y + b %*% y)
+   }) - 1.0
+   I <- which((t == "i" & fparc > 0.0) | (t == 'o' & fparc < 0.0))
+   if (length(I) > 0) {
+     f <- sum(as.array(fparc[I])^2)/np
+     g <- (as.vector(apply(as.matrix(p[, I]), 2, function(y) {
+       return(c(as.vector(y %*% t(y)), y) )
+     }) %*% (2.0 * as.array(fparc[I]))))/np
+   } else {
+     f <- 0.0
+     g <- rep(0.0, n)
+   }
+   list(f = f, g = g)
+ }
```

The subroutine that computes the projection onto the feasible convex set is named `proj` and is given by

```
R> proj <- function(x) {
+   A <- matrix(x, nrow = nmat, ncol = nmat)
+   A <- 0.5 * (t(A) + A)
+   r <- eigen(A, symmetric = TRUE)
+   lambda <- r$values
+   V <- r$vectors
+   lambda <- pmax(lowerl, pmin(lambda, upperl))
+   A <- V %*% diag(lambda) %*% t(V)
+   x[seq(length = nmat^2, from = 1, by = 1)] <- as.vector(A)
+   x
+ }
```

Note that subroutine `proj` uses subroutine `eigen` to compute eigenvalues and eigenvectors.

3.2. Numerical experiments

Numerical experiments were conducted using R version 2.14.1 on a 2.67GHz Intel Xeon CPU X5650 with 8GB of RAM memory and running GNU/Linux operating system (Ubuntu 12.04 LTS, kernel 3.2.0-33).

In the numerical experiments, we considered the default parameters of the SPG mentioned in Section 2. Regarding the initial spectral step length, we considered the choice given by (8) and for the stopping criterion we arbitrarily fixed $\varepsilon = 10^{-6}$. The nonmonotone line search parameter was arbitrarily set as $M = 100$.

Four small two-dimensional illustrative examples were designed. In the four examples we considered $q = 2$ and $m = 10,000$ random points $z_i \in \mathbb{R}^q$ uniformly distributed within the box $[-100, 100]^q$; and we fixed the suitable values $\hat{\lambda}_{\min} = 10^{-4}$ and $\hat{\lambda}_{\max} = 10^4$. In the first example, label $w_i = 1$ is given to the points inside a circle with radius 70 centered at the origin (see Figure 1(a)). If the reader is able to see the figure in colors, points labelled with $w_i = 1$ (i.e., inside the circle) are depicted in blue while points outside the circle (with $w_i = -1$) are depicted in red. Examples in Figures 1(b-d) correspond to a square of side 70 centered at the origin, a rectangle with height equal to 70 and width equal to 140 centered at the origin, and a triangle with corners $(-70, 0)$, $(0, -70)$, and $(70, 70)$, respectively.

The sequence of operations needed to solve the first example is given by:

```
R> library("BB")
R> nmat <- 2
R> np <- 10000
R> set.seed(123456)
R> p <- matrix(runif(nmat * np, min = -100.0, max = 100.0),
+   nrow = nmat, ncol = np)
R> t <- apply(p, 2, function(y) {
+   if (sum(y^2) <= 70.0^2) return("i") else return("o")
+ })
R> lowerl <- rep(1.0e-04, nmat)
R> upperl <- rep(1.0e+04, nmat)
R> n <- nmat^2 + nmat
R> set.seed(123456)
R> x <- runif(n, min = -1.0, max = 1.0)
R> ans <- spg(par = x, fn = evalf, gr = evalg, project = proj, method = 1,
+   control = list(M = 100, maxit = 10000, maxfeval = 100000, ftol = 0.0,
+   gtol = 1.e-06))
```

In the code above, `nmat` represents the dimension q of the space, `np` is the number of points m , and `p` saves the m randomly generated points $z_i \in \mathbb{R}^q$. For each point, `t` saves the value of w_i that, instead of -1 and 1 , is represented by 'i' that means inside and 'o' that means outside the circle centered at the origin with radius 70. `lowerl` and `upperl` represent, respectively, the lower and the upper bounds $\hat{\lambda}_{\min}$ and $\hat{\lambda}_{\max}$ for the eigenvalues of matrix A . Finally, the number of variables `n` of the optimization problem and a random initial guess $\mathbf{x} \in [-1, 1]^n$

are computed and the `spg` subroutine is called. The other three examples can be solved substituting the command that defines `t` by

```
R> t <- apply(p, 2, function(y) {
+   if (length(y) == sum(-70.0 <= y & y <= 70.0))
+     return("i") else return("o")
+ })
```

or

```
R> t <- apply(p, 2, function(y) {
+   if (-70.0 <= y[1] & y[1] <= 70.0 & -35.0 <= y[2] & y[2] <= 35.0)
+     return("i") else return("o")
+ })
```

or

```
R> t <- apply(p, 2, function(y) {
+   if (2.0 * y[1] - y[2] <= 70.0 & -y[1] + 2.0 * y[2] <= 70.0 &
+     -y[1] - y[2] <= 70.0) return("i") else return("o")
+ })
```

respectively.

Figure 1 shows the solutions to the four illustrative examples. The problem depicted on Figure 1(a) corresponds to a problem with known global solution at which the objective function vanishes, and the graphic shows that the global solution is correctly found by the method. The remaining three examples clearly correspond to problems at which the global minimum is strictly positive. Moreover, problems depicted on Figure 1(b) and 1(c) are symmetric problems whose solutions are given by ellipses with their axes parallel to the Cartesian axes, while Figure 1(d) displays a solution with a rotated ellipse.

Table 1 presents a few figures that represent the computational effort needed by the SPG method to solve the problems. Figures in the table show that the stopping criterion was satisfied in the four cases and that, as expected, the ratio between the number of functional evaluations and the number of iterations is near unity, stressing the high rate of acceptance of the trial spectral step length along the projected gradient direction. A short note regarding the reported CPU times is in order. A Fortran 77 version of the SPG method (available in <http://www.ime.usp.br/~egbirgin/>) was also considered to solve the same four problems. Equivalent solutions were obtained using CPU times three orders of magnitude smaller than the ones required by the R version of the method. From the required total CPU time, approximately 99% is used to compute the objective function and its gradient. This observation is in complete agreement with the fact that SPG iterations have a time complexity $O(n)$ while the objective function and gradient evaluations have time complexity $O(nm)$, and that, in the considered examples, we have $n = q(q + 1) = 6$ and $m = 10,000$. In this scenario, coding the problem subroutines (that computes the objective function f , its gradient, and the projection onto the convex feasible set Ω) in R and developing an interface to call a compiled Fortran 77 version of `spg` is not an option. On the other hand, when the execution of the subroutines that define the problem is inexpensive compared to the linear algebra involved in an iteration of the optimization method, coding the problem subroutines in an interpreted language

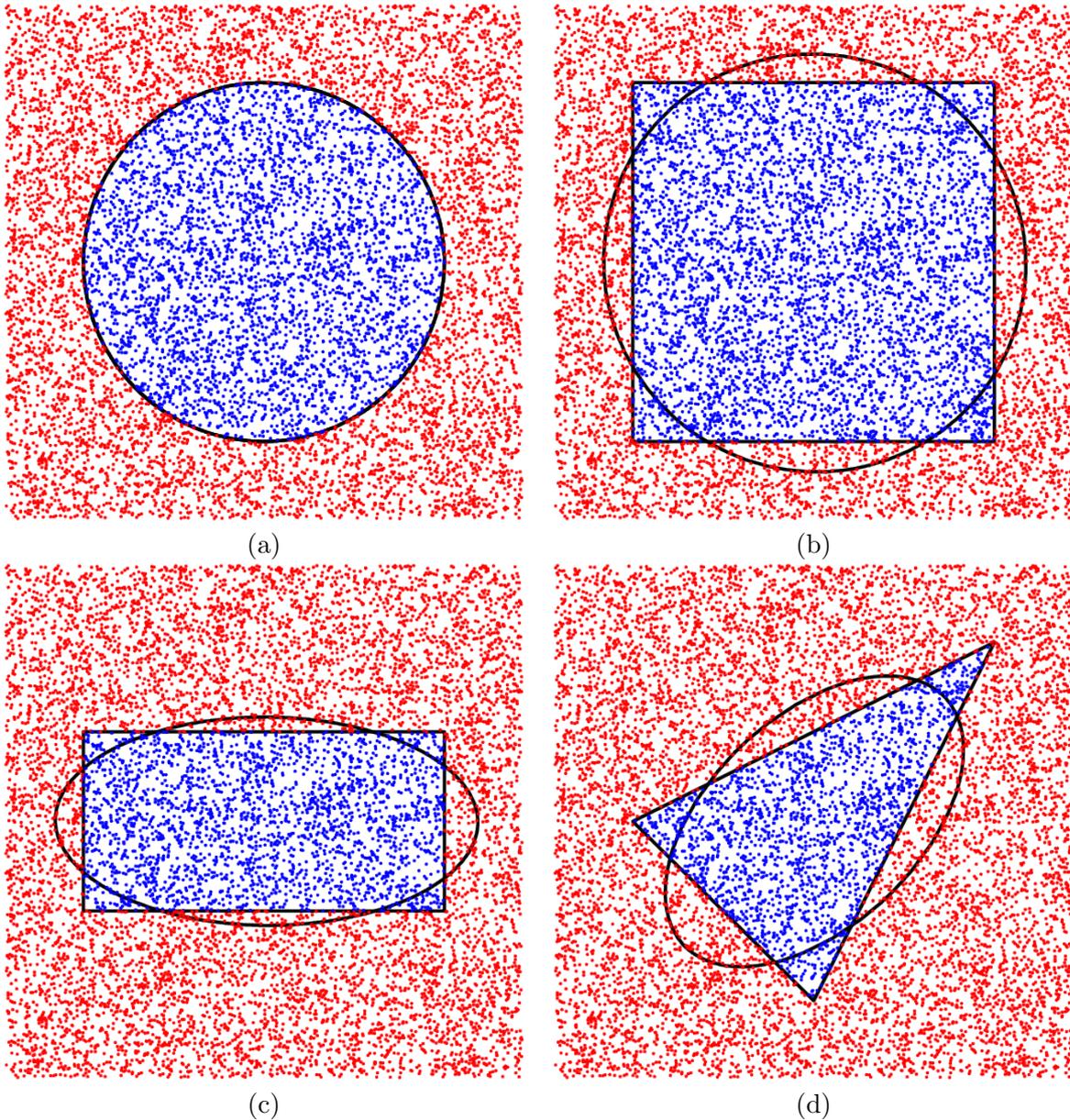


Figure 1: Solutions to four small two-dimensional illustrative examples.

like R and developing interfaces to optimization methods developed in compiled languages might be an adequate choice. This combination may jointly deliver (a) the fast development supplied by the usage of the user preferred language to code the problem subroutines and (b) the efficiency of powerful optimization tools developed in compiled languages especially suited to numeric computation and scientific computing. This is the case of, for example, the optimization method **Algencan** (Andreani, Birgin, Martínez, and Schuverdt 2007, 2008) (see also the TANGO Project web page: <http://www.ime.usp.br/~egbirgin/tango/>) for non-linear programming problems, coded in Fortran 77 and with interfaces to R, AMPL, C/C++, **CUTEr**, Java, MATLAB, Octave, Python, and TCL.

Problem	Iterations	Evaluations	$f(x^*)$	$\ P_{\Omega}(x^* - \nabla f(x^*)) - x^*\ _{\infty}$	CPU time
Circle	3307	3440	1.195192e-13	3.4e-07	1003.92
Square	1761	1907	2.352849e-03	7.9e-07	597.43
Rectangle	7269	8177	1.036716e-03	8.9e-07	2174.63
Triangle	7193	7753	6.512737e-03	9.9e-07	2199.36

Table 1: Performance of the R version of SPG in the four small two-dimensional illustrative examples.

4. Applications and extensions

As a general rule, the SPG method is applicable to large-scale convex constrained problems in which the projection onto the feasible set can be inexpensively computed. Moreover, the scenario is also beneficial to the application of the SPG method whenever the convex feasible set is hard to describe with nonlinear constraints or when the nonlinear constraints that are needed to describe the convex feasible set have an undesirable property (e.g., being too many, being highly nonlinear, or having a dense Jacobian). A clear example of this situation is the problem that illustrates the previous section. Comparisons with other methods for the particular case in which the feasible set is an n -dimensional box can be found in Birgin *et al.* (2000); Birgin and Gentil (2012).

Since its appearance, the SPG method has been useful for solving real applications in different areas, including optics (Andrade, Birgin, Chambouleyron, Martínez, and Ventura 2008; Azofeifa, Clark, and Vargas 2005; Birgin, Chambouleyron, and Martínez 1999b; Birgin, Chambouleyron, Martínez, and Ventura 2003a; Chambouleyron, Ventura, Birgin, and Martínez 2009; Curiel, Vargas, and Barrera 2002; Mulato, Chambouleyron, Birgin, and Martínez 2000; Murphy 2007; Ramirez-Porras and Vargas-Castro 2004; Vargas 2002; Vargas, Azofeifa, and Clark 2003; Ventura, Birgin, Martínez, and Chambouleyron 2005), compressive sensing (van den Berg and Friedlander 2008, 2011; Figueiredo, Nowak, and Wright 2007; Loris, Bertero, Mol, Zanella, and Zanni 2009), geophysics (Bello and Raydan 2007; Birgin, Biloti, Tygel, and Santos 1999a; Cores and Loreto 2007; Deidda, Bonomi, and Manzi 2003; Zeev, Savasta, and Cores 2006), statistics (Borsdorf, Higham, and Raydan 2010; Varadhan and Gilbert 2009), image restoration (Benvenuto, Zanella, Zanni, and Bertero 2010; Bonettini, Zanella, and Zanni 2009; Bouhamidi, Jbilou, and Raydan 2011; Guerrero, Raydan, and Rojas 2013), atmospheric sciences (Jiang 2006; Mu, Duan, and Wang 2003), chemistry (Francisco, Martínez, and Martínez 2006; Birgin, Martínez, Martínez, and Rocha 2013), and dental radiology (Kolehmainen *et al.* 2006, 2007). The SPG method has also been combined with several schemes for solving scientific problems that appear in other areas of computational mathematics, including eigenvalue complementarity (Júdice, Raydan, Rosa, and Santos 2008), support vector machines (Cores, Escalante, Gonzalez-Lima, and Jiménez 2009; Dai and Fletcher 2006; Serafini, Zanghirati, and Zanni 2005), non-differentiable optimization (Crema, Loreto, and Raydan 2007), trust-region globalization (Maciel, Mendonça, and Verdiell 2013), generalized Sylvester equations (Bouhamidi *et al.* 2011), nonlinear monotone equations (Zhang and Zhou 2006), condition number estimation (Brás, Hager, and Júdice 2012), optimal control (Birgin and Evtushenko 1998), bound-constrained minimization (Andreani, Birgin, Martínez, and Schuverdt 2010; Andretta, Birgin, and Martínez 2005; Birgin and Martínez 2001, 2002), nonlinear programming (Andreani *et al.* 2007, 2008; Andreani, Birgin, Martínez, and Yuan 2005; Andretta, Birgin, and Martínez 2010; Birgin and Martínez 2008; Diniz-Ehrhardt, Gomes-

Ruggiero, Martínez, and Santos 2004; Gomes-Ruggiero, Martínez, and Santos 2009), non-negative matrix factorization (Li, Liu, and Zheng 2012), and topology optimization (Tavakoli and Zhang 2012). Moreover, alternative choices of the spectral step length have been considered and analyzed for solving some related nonlinear problems. A spectral approach has been considered to solve large-scale nonlinear systems of equations using only the residual vector as search direction (Grippio and Sciandrone 2007; La Cruz and Raydan 2003; La Cruz *et al.* 2006; Varadhan and Gilbert 2009; Zhang and Zhou 2006). Spectral variations have also been developed for accelerating the convergence of fixed-point iterations, in connection with the well-known EM algorithm which is frequently used in computational statistics (Roland and Varadhan 2005; Roland, Varadhan, and Frangakis 2007; Varadhan and Roland 2008).

The case in which the convex feasible set of the problem to be solved by SPG is defined by linear equality and inequality constraints has been considered in Birgin *et al.* (2003b), Andreani *et al.* (2005), Martínez, Pilotta, and Raydan (2005), and Andretta *et al.* (2010). A crucial observation is that this type of set is not necessarily one in which it is easy to project. Projecting onto a polytope requires to solve a convex quadratic programming problem, for which there exist many efficient algorithms, especially when the set exhibits additional structure. To perform this task, the **BB** package relies on the method introduced in Goldfarb and Idnani (1983), implemented in the package **quadprog** (Weingessel 2013). An important observation is that the dual of such a problem is a concave box-constrained problem, which allows the use of specialized methods to solve them (see Andreani *et al.* 2005). In the large-scale case, it is important to have the possibility of performing the projection only approximately. The SPG theory for that case have been extensively developed in Birgin *et al.* (2003b).

5. Conclusions

The SPG method is nowadays a well-established numerical scheme for solving large-scale convex constrained optimization problems when the projection onto the feasible set can be performed efficiently. The attractiveness of the SPG method is mainly based on its simplicity. No sophisticated linear codes are required, no additional linear algebra packages are needed and the user can code its own version of the method with a relatively small effort. In this review, we presented the basic ideas behind the SPG method, discussed some of its most relevant properties, and discussed recent applications and extensions. In addition, we illustrated how the method can be applied to a particular matrix problem for which the feasible convex set is *easily* described by a subroutine that computes the projection onto it.

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