

Gradient algorithms for quadratic optimization with fast convergence rates

Luc Pronzato* and Anatoly Zhigljavsky †

Abstract We propose a family of gradient algorithms for minimizing a quadratic function $f(x) = (Ax, x)/2 - (x, y)$ in \mathbb{R}^d or a Hilbert space, with simple rules for choosing the step-size at each iteration. We show that when the step-sizes are generated by a dynamical system with ergodic distribution having the arcsine density on a subinterval of the spectrum of A , the asymptotic rate of convergence of the algorithm can approach the (tight) bound on the rate of convergence of a conjugate gradient algorithm stopped before d iterations, with $d \leq \infty$ the space dimension.

Key words: Chebyshev polynomials, conjugate gradient, Krylov space, logistic map, quadratic operator, steepest descent.

1 Introduction

Consider the problem of minimizing a quadratic function $f(\cdot)$ defined either on \mathbb{R}^d or a Hilbert space by

$$f(x) = \frac{1}{2}(Ax, x) - (x, y), \quad (1)$$

where (\cdot, \cdot) denotes the inner product. We assume that A is either a symmetric positive-definite matrix or a self-adjoint operator, with

$$0 < m = \inf_{(x,x)=1} (Ax, x) < M = \sup_{(x,x)=1} (Ax, x) < \infty.$$

If A is a matrix, then m and M are the smallest and largest eigenvalues of A , respectively.

Consider a general gradient algorithm with iterations of the form

$$x_{k+1} = x_k - \gamma_k g_k, \quad k = 0, 1, 2, \dots \quad (2)$$

where $g_k = \nabla f(x_k)$ is the gradient of the objective function $f(\cdot)$ at point x_k . For the objective function (1), $\nabla f(x) = Ax - y$. The iteration (2) can be rewritten in terms of the gradients as

$$g_{k+1} = g_k - \gamma_k A g_k. \quad (3)$$

In a series of papers [10, 11, 12] and the monograph [9] many gradient algorithms have been shown to be equivalent to special algorithms for updating measures on the interval $[m, M]$. The central idea is that of renormalization applied to the gradient. For simplicity the presentation is made for the finite dimensional case where A is a matrix, which can be assumed, without loss of generality, to be diagonal

*Laboratoire I3S, CNRS - UNS, Les Algorithmes - Bât. Euclide B, 2000 route des Lucioles - B.P. 121, F-06903 Sophia Antipolis Cedex, France (pronzato@i3s.unice.fr)

†School of Mathematics, Cardiff University, Senghennydd Road, Cardiff, CF24 4YH, UK (ZhigljavskyAA@cf.ac.uk)

$A = \text{diag}(\lambda_1, \dots, \lambda_d)$ with eigenvalues $m = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_d = M$. Extension to the Hilbert-space case will be considered in Section 5.

Write $z_k = g_k / \sqrt{(g_k, g_k)}$ for the normalized gradient at x_k and define

$$p_i^{(k)} = \{z_k\}_i^2 = \frac{\{g_k\}_i^2}{\sum_{j=1}^d \{g_k\}_j^2}, \quad i = 1, \dots, d,$$

as the i -th probability corresponding to vector z_k , where $\{v\}_i$ denotes the i -th component of vector v . Let ν_k denote the probability measure on the spectrum of A defined by the $p_i^{(k)}$'s, that is, $\nu_k(\lambda_i) = p_i^{(k)}$. The probability measure ν_{k+1} is defined by

$$p_i^{(k+1)} = \frac{\{g_{k+1}\}_i^2}{(g_{k+1}, g_{k+1})} \quad \text{for } i = 1, \dots, d.$$

Note that (3) gives

$$(g_{k+1}, g_{k+1}) = (g_k, g_k) - 2\gamma_k (Ag_k, g_k) + \gamma_k^2 (A^2 g_k, g_k), \quad (4)$$

so that

$$p_i^{(k+1)} = \frac{(1 - \gamma_k \lambda_i)^2}{(g_k, g_k) - 2\gamma_k (Ag_k, g_k) + \gamma_k^2 (A^2 g_k, g_k)} \{g_k\}_i^2 = \frac{(1 - \gamma_k \lambda_i)^2}{1 - 2\gamma_k \mu_1^{(k)} + \gamma_k^2 \mu_2^{(k)}} p_i^{(k)}, \quad (5)$$

where

$$\mu_\alpha^{(k)} = \mu_\alpha(\nu_k) = \frac{(A^\alpha g_k, g_k)}{(g_k, g_k)} \quad (6)$$

is the α -th moment of the measure ν_k . When two eigenvalues of A are equal, say $\lambda_j = \lambda_{j+1}$, the updating rules for $p_j^{(k)}$ and $p_{j+1}^{(k)}$ are identical so that the analysis of the behaviour of the algorithm remains the same when $p_j^{(k)}$ and $p_{j+1}^{(k)}$ are confounded. We may thus assume that all eigenvalues of A are distinct. Also, a zero weight remains equal to zero at all subsequent iterations, we thus assume that $\nu_0(\lambda_i) > 0$ for all i .

A common definition for the rate of convergence of the algorithm at iteration k is $r_k = (g_{k+1}, g_{k+1}) / (g_k, g_k)$. The rate for n iterations is

$$\prod_{k=0}^{n-1} r_k = \frac{(g_n, g_n)}{(g_0, g_0)};$$

therefore, the asymptotic rate of the algorithm can naturally be defined as

$$R = \lim_{n \rightarrow \infty} R_n, \quad \text{with } R_n = \left(\prod_{k=0}^{n-1} r_k \right)^{1/n}. \quad (7)$$

Of course, this rate may depend on the initial point x_0 or, equivalently, on g_0 . Other rates which are asymptotically equivalent to $\{r_k\}$ can be considered as well, see [12] and Remark 6.

The most familiar gradient algorithm is the steepest-descent algorithm, for which the step-size γ_k at iteration k is chosen so as to minimize $f(x_k - \gamma g_k)$ with respect to γ , which gives $\gamma_k = (g_k, g_k) / (Ag_k, g_k) = 1 / \mu_1^{(k)}$. Its asymptotic behaviour is well-known, see [1, 10]. In particular, its convergence is slow: the asymptotic rate R depends on the starting point but is never far from its worst value given by the Kantorovich bound

$$R_{\max} = \left(\frac{\rho - 1}{\rho + 1} \right)^2,$$

where $\rho = M/m$, the condition number of A . The asymptotic behaviour of the family of algorithms defined by $\gamma_k = \mu_\alpha^{(k)}/\mu_{\alpha+1}^{(k)}$ (which includes the method of minimum residues for $\alpha = 1$) is shown in [12] to be similar.

Obtaining a faster asymptotic rate of convergence for gradient algorithms requires to extend the possible choices for the step-size γ_k . Rewrite the updating rule (5) in terms of iteration applied to the probability measure ν_k ,

$$\nu_{k+1}(\lambda) = \frac{(1 - \gamma_k \lambda)^2}{1 - 2\gamma_k \mu_1^{(k)} + \gamma_k^2 \mu_2^{(k)}} \nu_k(\lambda) = \frac{(\lambda - \beta_k)^2}{\beta_k^2 - 2\beta_k \mu_1^{(k)} + \mu_2^{(k)}} \nu_k(\lambda), \quad (8)$$

where $\beta_k = 1/\gamma_k$ and $\nu_k(\lambda)$ is the weight assigned by the measure ν_k to the point λ . The roots β_k in (8) are the key control variables for a gradient algorithm. Different strategies for choosing β_k give different families of algorithms. Note that the only information about ν_k one has access to corresponds to its moments $\mu_\alpha^{(k)}$, $\alpha = 1, 2, \dots$. Many of the examples of algorithms presented in [6], with β_k a function of $\mu_1^{(k)}$ and $\mu_2^{(k)}$, exhibit a much faster asymptotic rate of convergence than R_{\max} (it seems that allowing β_k to depend on more moments $\mu_\alpha^{(k)}$ does not yield further improvement in the rate of convergence). Fast convergence (small R) is observed for algorithms that exhibit a chaotic-type behaviour in \mathbb{R}^d , which makes their theoretical study difficult. The same is true for some algorithms for which β_k is allowed to depend on moments of several previous measures ν_{k-i} , $i = 1, \dots, u$. For instance, in the Barzilai-Borwein algorithm [2], β_k is either $\mu_1^{(k-1)}$ or $\mu_2^{(k-1)}/\mu_1^{(k-1)}$.

Conjugate gradient, s -step optimal, MINRES and other algorithms based on Krylov spaces do not use gradient directions for their successive iterations, see, e.g., [8]. However, when analyzing their behaviour, one can construct an equivalent sequence of iterations following the gradient directions with control variables β_k depending on k and on moments of previous measures ν_{k-i} , $i = 0, 1, 2, \dots$. The conjugate gradient algorithm in \mathbb{R}^d converges in d iterations. When d is large, preserving the conjugacy of successive directions is difficult and restarting the algorithm after each sequence of s iterations is recommended. This corresponds to the s -step optimal gradient algorithm, see [5, 13], which does not have finite convergence but whose guaranteed asymptotic rate of convergence is

$$R_s^* = \left(\frac{R_\infty^{s/2} + R_\infty^{-s/2}}{2} \right)^{-2/s} = T_s^{-2/s} \left(\frac{\rho + 1}{\rho - 1} \right) \quad (9)$$

where

$$R_\infty = \lim_{s \rightarrow \infty} R_s^* = \left(\frac{\sqrt{\rho} - 1}{\sqrt{\rho} + 1} \right)^2$$

and $T_s(\cdot)$ is the s -th Chebyshev polynomial:

$$T_s(t) = \cos[s \arccos(t)] = \frac{(t + \sqrt{t^2 - 1})^s + (t - \sqrt{t^2 - 1})^s}{2}.$$

In this paper we propose a family of gradient algorithms based on simple rules for choosing the sequence of control variables β_k . The main idea is to force $\nu_k(\lambda_j)$, $j = 2, \dots, d - 1$, to tend to zero as $k \rightarrow \infty$. The measure ν_k , which summarizes the state of the iterates at step k , is then almost fully characterized by $\nu_k(m)$, which facilitates the analysis of the asymptotic behaviour. Furthermore, we show that the sequence $\{\beta_k\}$ can be chosen independently of $\{\nu_k\}$ while ensuring that the asymptotic rate of convergence is arbitrarily close to R_∞ . This independence of $\{\beta_k\}$ on $\{\nu_k\}$ makes the algorithms at the same time simple and robust with respect to the precision of calculations. Also, the step-sizes $\gamma_k = 1/\beta_k$, $k = 1, 2, \dots$ are simpler to calculate than those of the steepest-descent algorithm. Convergence rates close

to R_∞ are obtained when the β_k 's are constructed so that their asymptotic distribution is close to a distribution with the arcsine density.

The worst-case rate R_s^* can be reached for the s -step optimal gradient when $d > s$, in the sense that there exist eigenvalues λ_i and initial point x_0 for the algorithm such that the rate of convergence after s iterations is exactly R_s^* (and the behavior in terms of renormalized gradient z_k is then periodic with period s), see [5, 13]. The same is true for the conjugate gradient algorithm: for $s < d$ there exist eigenvalues λ_i and a starting point x_0 such that the convergence rate after s iterations is exactly R_s^* .

If d is large (relative to the total number of iterations), s is not very large and the eigenvalues of A are well-spread in the spectral interval $[m, M]$, then the actual rates (per one matrix-vector multiplication) of the MINRES and other optimal methods based on the use of s -dimensional Krylov spaces are very close to R_s^* and are often larger than R_∞ . Bearing in mind that the asymptotic rates of the algorithms suggested below can be arbitrarily close to R_∞ and these algorithms are extremely simple and robust, these algorithms may be preferable to MINRES and other Krylov space based methods for large-scale quadratic optimization problems.

The paper is organized as follows. In Section 2 we show that for a suitable choice of the sequence $\{\beta_k\}$ the algorithm attracts to the plane spanned by the eigenvectors associated with $\lambda_1 = m$ and $\lambda_d = M$. In Section 3, we assume that the values of m and M are known and give the expression of the asymptotic rate of convergence of the algorithm in the case where the β_k 's are generated by pairs symmetric with respect to $(m + M)/2$. Several examples are presented, some with a rate arbitrarily close to R_∞ . The case where m and M are unknown is considered in Section 4 where a practical algorithm is suggested and some simulation results are presented. Finally, the infinite dimensional situation where $f(\cdot)$ is defined on a Hilbert space is considered Section 5.

2 Attraction of the sequence $\{\nu_k\}$ to the set of measures supported at m and M

Theorem 1 *Assume that $\beta_k > 0$, $\beta_k \notin \{m, M\}$ for all k and that the sequence $\{\beta_k\}$ has asymptotic distribution function $F(\beta)$ which is supported on an interval $[m', M']$ with $0 < m' \leq M' < \infty$. Suppose, moreover, that the limiting distribution satisfies*

$$\int \log(\beta - \lambda)^2 dF(\beta) < \max \left\{ \int \log(M - \beta)^2 dF(\beta), \int \log(\beta - m)^2 dF(\beta) \right\}, \quad \forall \lambda \in \{\lambda_2, \dots, \lambda_{d-1}\}. \quad (10)$$

Then, the gradient algorithm associated with the sequence $\{\beta_k\}$ is such that $\lim_{k \rightarrow \infty} \nu_k(\lambda_i) = 0$ for all $i = 2, \dots, d - 1$. Furthermore, there exist constants $C > 0, k_0 > 0$ and $0 \leq \theta < 1$ such that

$$\sum_{i=2}^{d-1} \nu_k(\lambda_i) \leq C\theta^k \text{ for } k > k_0. \quad (11)$$

Proof. The fact that the sequence $\{\beta_k\}$ has asymptotic distribution function $F(\beta)$ implies

$$\lim_{k \rightarrow \infty} \frac{1}{k} \sum_{j=0}^{k-1} h(\beta_j) = \int h(\beta) dF(\beta) \quad (12)$$

for any continuous function $h(\cdot)$ such that $\int |h(\beta)| dF(\beta) < \infty$, see [7]. Define

$$H_k(\lambda) = C_k (\lambda - \beta_0)^2 (\lambda - \beta_1)^2 \cdots (\lambda - \beta_{k-1})^2, \quad (13)$$

with C_k a normalizing constant such that $\nu_k(\lambda) = H_k(\lambda)\nu_0(\lambda)$ in (8), and assume that

$$\int \log(M - \beta)^2 dF(\beta) \leq \int \log(\beta - m)^2 dF(\beta) \quad (14)$$

(if this inequality is not met, m should be replaced with M in all considerations below). Define the sum

$$S_k(\lambda, m) = \frac{1}{k} \log \frac{H_k(\lambda)}{H_k(m)} = -\frac{1}{k} \sum_{j=0}^{k-1} \log(\beta_j - m)^2 + \frac{1}{k} \sum_{j=0}^{k-1} \log(\lambda - \beta_j)^2 \quad (15)$$

and consider the first sum $I_k(m) = (1/k) \sum_{j=0}^{k-1} \log(\beta_j - m)^2$ in the right-hand side of (15) and the related integral $I(m) = \int \log(\beta - m)^2 dF(\beta)$. Since the c.d.f. $F(\cdot)$ is supported on a bounded interval $[m', M']$ we have $I(m) < \infty$. The assumptions (10) and (14) imply $I(m) > -\infty$ and the property (12) then gives the convergence $I_k(m) \rightarrow I(m)$ as $k \rightarrow \infty$.

Consider now the second sum $I_k(\lambda) = (1/k) \sum_{j=0}^{k-1} \log(\beta_j - \lambda)^2$ in the right-hand side of (15) and the related integral $I(\lambda) = \int \log(\beta - \lambda)^2 dF(\beta)$. Since the c.d.f. $F(\cdot)$ is supported on a bounded interval, the integral $I(\lambda)$ is properly defined but may equal $-\infty$ (for example, if the c.d.f. $F(\cdot)$ has a discontinuity at the point λ). If $I(\lambda) = -\infty$ then as $k \rightarrow \infty$ the sum $I_k(\lambda)$ tends to $-\infty$ too. If $I(\lambda) > -\infty$ then either $I_k(\lambda) = -\infty$ for all k large enough (when at least one β_j is equal to λ) or (12) implies that $I_k(\lambda)$ tends to $I(\lambda)$ as $k \rightarrow \infty$.

Therefore, from (10), $S_k(\lambda, m)$ tends to a negative value (possibly $-\infty$) as $k \rightarrow \infty$. This implies that there exists $k_0 \geq 0$ and $\delta > 0$ such that for all $k \geq k_0$ and $\lambda \in \{\lambda_2, \dots, \lambda_{d-1}\}$

$$S_k(\lambda, m) = \frac{1}{k} \log \frac{H_k(\lambda)}{H_k(m)} \leq -\delta; \quad (16)$$

that is, $H_k(\lambda)/H_k(m) \leq \theta^k$, where $\theta = \exp(-\delta) < 1$. This yields $\sum_{i=2}^{d-1} \nu_k(\lambda_i) \leq \theta^k \left(\sum_{i=2}^{d-1} \nu_0(\lambda_i) \right) / \nu_0(m)$ for $k > k_0$, hence (11). The result $\lim_{k \rightarrow \infty} \nu_k(\lambda_i) = 0$ for $i = 2, \dots, d-1$ obviously follows from (11). ■

Remark 1 The sequence $\{\beta_k\}$ can be assumed random, for instance formed by independent and identically distributed random variables. In this case, all the statements are true with probability one. When the β_k 's are simply independent, with $\{F_k\}$ the sequence of corresponding distribution functions and $(1/k) \sum_{j=0}^{k-1} F_j$ converging weakly to F as k tends to infinity, one may refer to [3, Th. 2.5.3, p. 36] for a property similar to (12).

Remark 2 Typically, the spectrum of A is unknown. In that case, the condition (10) can be replaced with the more restrictive one

$$\int \log(\beta - \lambda)^2 dF(\beta) < \max \left\{ \int \log(M - \beta)^2 dF(\beta), \int \log(\beta - m)^2 dF(\beta) \right\}, \quad \forall \lambda \in (m, M). \quad (17)$$

Remark 3 If the distribution with c.d.f. $F(\cdot)$ is symmetric with respect to $(m + M)/2$, then we have $\int \log(M - \beta)^2 dF(\beta) = \int \log(\beta - m)^2 dF(\beta)$ and therefore the condition (17) simplifies to

$$\int \log(\beta - \lambda)^2 dF(\beta) < \int \log(\beta - m)^2 dF(\beta), \quad \forall \lambda \in (m, M). \quad (18)$$

Remark 4 Note that the support $[m', M']$ of the distribution with c.d.f. $F(\cdot)$ could be different from $[m, M]$ and does not have to be a subset of $[m, M]$.

Remark 5 The results of Theorem 1 also apply when β_k depends on the moments of previous measures ν_{k-i} , $i = 0, 1, 2 \dots$

Example 1 For the steepest-descent algorithm with $\beta_k = \mu_1^{(k)}$, the limiting measure for $\{\beta_k\}$ is the two-point measure assigning weights $1/2$ at z and $m + M - z$ for some $z \in (m, M)$. The condition (17) then simply expresses the property that two successive iterations (8) of the algorithm asymptotically give a larger increase of the weights at the endpoints m and M than at any other point in the interval (m, M) ; that is,

$$(z - m)^2 (M - z)^2 > (z - \lambda)^2 (m + M - z - \lambda)^2, \forall \lambda \in (m, M). \quad (19)$$

Since for all z the only maximum of $(z - \lambda)^2 (m + M - z - \lambda)^2$ with respect to $\lambda \in (m, M)$ is at $\lambda^* = (m + M)/2$, the inequality (19) can be rewritten as $(z - m)^2 (M - z)^2 > (z - \lambda^*)^2 (m + M - z - \lambda^*)^2$, which gives

$$z \in \left(\frac{1}{2}(m + M) - \frac{1}{2\sqrt{2}}(M - m), \frac{1}{2}(m + M) + \frac{1}{2\sqrt{2}}(M - m) \right). \quad (20)$$

This corresponds to the definition of the stability interval for the attractor in [10, 12]. A similar result holds for all gradient-type algorithms from the family considered in [12].

Example 2 If we choose $\beta_k = \sqrt{\mu_2^{(k)}}$, then the limiting measure for $\{\beta_k\}$ is the delta-measure concentrated at the point $\lambda^* = (m + M)/2$; as a consequence, the asymptotic rate for the related gradient algorithm is R_{\max} . Proof of these facts can be found in [4] and [6], Sect. 2.7.

3 Asymptotic rate for symmetrically placed control variables

3.1 Main result

Theorem 2 Assume that the conditions of Theorem 1 are satisfied and that, moreover, the control variables β_k are generated by symmetric pairs for large k ; that is, $\beta_{2j+1} = M + m - \beta_{2j}$ for all $j \geq j_0$, with $\beta_{2j} \in [m + \varepsilon, M - \varepsilon]$ for some $\varepsilon \in (0, (M - m)/2)$. Then, the asymptotic rate R satisfies

$$\log R = \int \log \left| \frac{(M - \beta)(\beta - m)}{\beta(m + M - \beta)} \right| dF(\beta) = \int \log \frac{(\beta - m)^2}{\beta^2} dF(\beta). \quad (21)$$

Proof. First note that dividing (4) through by (g_k, g_k) gives the following expression for the rate r_k ,

$$r_k = 1 - 2\gamma_k \frac{(Ag_k, g_k)}{(g_k, g_k)} + \gamma_k^2 \frac{(A^2 g_k, g_k)}{(g_k, g_k)} = 1 - 2\mu_1^{(k)}/\beta_k + \mu_2^{(k)}/\beta_k^2. \quad (22)$$

Consider a measure ν with weights p and $1 - p$ at m and M respectively, $0 < p < 1$. Apply two successive iterations (8) with control parameters β and $\beta' = m + M - \beta$ to this measure. The product of the two successive rates does not depend on p and is equal to $R_2^2(\beta) = (M - \beta)^2(\beta - m)^2/[\beta(m + M - \beta)]^2$.

According to Theorem 1, ν_k tends to be supported at m and M and the rate of convergence is exponential. We thus obtain for two successive iterations with control variables β_{2j} and $\beta_{2j+1} = m + M - \beta_{2j}$

$$R_2^2(\beta_{2j}) \left[1 - \frac{A\theta^{2j}}{R_2^2(\beta_{2j})} \right] < r_{2j}r_{2j+1} < R_2^2(\beta_{2j}) \left[1 + \frac{A\theta^{2j}}{R_2^2(\beta_{2j})} \right]$$

for some $A > 0$ and $j > k_0/2$, see Theorem 1. Since $\beta_{2j} \in [m + \varepsilon, M - \varepsilon]$, we have $R_2^2(\beta_{2j}) \geq R_2^2(m + \varepsilon) = \varepsilon(M - m - \varepsilon)/[(m + \varepsilon)(M - \varepsilon)] > 0$. Therefore,

$$\log R_2(\beta_{2j}) - B\theta^{2j} < \log \sqrt{r_{2j}r_{2j+1}} < \log R_2(\beta_{2j}) + B\theta^{2j},$$

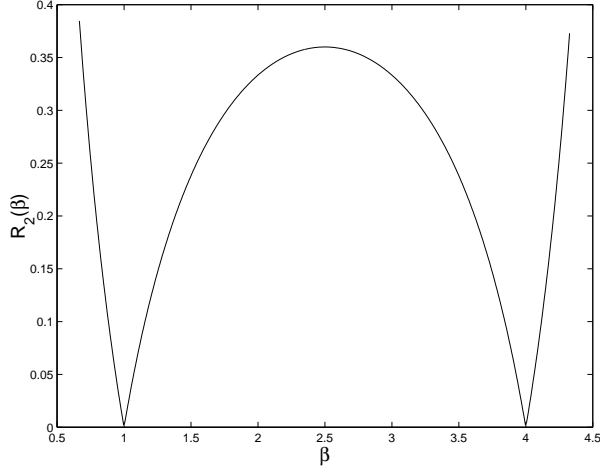


Figure 1: $R_2(\beta)$ for $m = 1$, $M = 4$

with $B = A/R_2^2(m + \varepsilon)$, for j large enough. Since $\sum_{j=0}^{\infty} \theta^{2j} = 1/(1 - \theta^2) < \infty$, we obtain from (12),

$$\log R = \lim_{k \rightarrow \infty} \frac{1}{k} \sum_{j=0}^{k-1} \log \sqrt{r_{2j} r_{2j+1}} = \int \log R_2(\beta) dF(\beta),$$

hence the first expression in (21). The second expression follows from the fact that the c.d.f. $F(\cdot)$ is symmetric with respect to $(m + M)/2$. \blacksquare

Example 3 Uniform density. Let the distribution with c.d.f. $F(\cdot)$ be uniform with density $p(\beta) = 1/(M' - m')$, $\beta \in [m', M']$, with $m' = m + \varepsilon$, $M' = M - \varepsilon$ and $0 < \varepsilon < (M - m)/2$. Then the asymptotic rate of convergence is

$$R_{\text{uniform}, \varepsilon} = \exp \left\{ \frac{1}{M' - m'} \int_{m'}^{M'} \log \frac{(\beta - m')^2}{\beta^2} d\beta \right\} = (M' - m')^2 \exp \left\{ -2 \frac{M' \log M' - m' \log m'}{M' - m'} \right\}. \quad (23)$$

Remark 6 One can easily check that the result stated in Theorem 2 holds for other definitions for the rate of convergence, see, e.g., [12, Th. 6]. For instance, the rate

$$r'_k = \frac{f(x_{k+1}) - f^*}{f(x_k) - f^*} = \frac{(A^{-1}g_{k+1}, g_{k+1})}{(A^{-1}g_k, g_k)},$$

where $f^* = \min_x f(x)$, can be written as

$$r'_k = 1 - 2/(\mu_{-1}^{(k)} \beta_k) + \mu_1^{(k)}/(\mu_{-1}^{(k)} \beta_k^2) \quad (24)$$

and the corresponding asymptotic rate $R' = \lim_{n \rightarrow \infty} \left(\prod_{k=0}^{n-1} r'_k \right)^{1/n}$ is equal to R which can be computed by (21).

Remark 7 The shape of $R_2(\beta)$ as a function of β shows that fast convergence is obtained for β close to m or M , see Figure 1, hence the interest of taking ε small in Theorem 2.

Remark 8 When ν_k is a two-point measure supported at m and M , two iterations of (8) with $\beta_{k+1} = M + m - \beta_k$ give $\nu_{k+2} = \nu_k$. Under the conditions of Theorem 2 the measure ν_k thus converges to a

measure $\bar{\nu}_k = p_k \delta_m + (1 - p_k) \delta_M$ supported at m and M , with p_{2j} tending to a constant p_∞ as j tends to infinity. The limiting distribution of the sequence $\{p_{2j+1}\}$ depends on $F(\cdot)$ and p_∞ , while the value of p_∞ depends on the initial measure ν_0 and the spectrum of A .

3.2 Finite collection of control variables

Assume that the points $\beta_0, \beta_1 \dots$ are generated in repeated groups $B = \{\beta_0, \dots, \beta_N\}$ of $N + 1$ points in (m, M) , $N \geq 0$. Additionally, the points in B are symmetric with respect to $(m + M)/2$. We may always assume that $\beta_0 \leq \dots \leq \beta_N$. In this case, if N is even then $\beta_{N/2} = (m + M)/2$. The condition (18) now becomes

$$\sum_{j=0}^N \log(\beta_j - \lambda)^2 < \sum_{j=0}^N \log(\beta_j - m)^2, \quad \forall \lambda \in (m, M). \quad (25)$$

If this condition is met then the asymptotic rate is

$$R = R_N = \left[\prod_{j=0}^N \frac{(\beta_j - m)^2}{\beta_j^2} \right]^{1/(N+1)}. \quad (26)$$

Example 4 *Uniform grid.* Assume that for some integer $N \geq 0$,

$$B = \{\beta_0, \dots, \beta_N\} \quad \text{with} \quad \beta_i = m + \frac{i + \frac{1}{2}}{N + 1} (M - m), \quad i = 0, 1, \dots, N. \quad (27)$$

It is easy to see that the condition (25) is met. The rate R_N computed by (26) is given by

$$R_N = \left(\frac{\Gamma^2(N + 3/2) \Gamma^2\left(\frac{m+M+2Nm}{2(M-m)}\right)}{\pi \Gamma^2\left(\frac{2NM+3M-m}{2(M-m)}\right)} \right)^{1/(N+1)},$$

where $\Gamma(\cdot)$ is the gamma-function. The value of R_N for $m = 1$, $M = 4$ is plotted in Figure 2 as a function of N . Asymptotically, as $N \rightarrow \infty$, R_N approaches $R_{\text{uniform},0}$ defined in (23) (with $R_{\text{uniform},0} \simeq 0.2232$ for $m = 1$, $M = 4$). Instead of using the β_i 's according to (27) for large N , one can generate the sequence $\{\beta_i\}$ using, for example, the Bernoulli shift:

$$H_B(t) = 2t \pmod{1}, \quad t \in (0, 1), \quad (28)$$

with β_0 randomly chosen in (m', M') , and for all $j = 0, 1, 2 \dots$

$$\beta_{2j+1} = M' + m' - \beta_{2j}, \quad \beta_{2j+2} = m' + (M' - m') H_B\left(\frac{\beta_{2j} - m'}{M' - m'}\right),$$

with $m' = m + \varepsilon$, $M' = M - \varepsilon$ and $0 < \varepsilon < (M - m)/2$.

Example 5 *Nearly optimal $N + 1$ points.* Consider first the case $N = 1$. When the condition (25) is satisfied, the asymptotic rate is $R_2 = |M - \beta| |\beta - m| / [\beta |m + M - \beta|]$, see the proof of Theorem 2. For $\beta \in [m, M]$, R_2 improves when $|\beta - (m + M)/2|$ increases and reaches its minimum value, zero, at $\beta \in \{m, M\}$, see Remark 7. Condition (25) imposes that β belongs to the interval (20), by choosing β sufficiently close to $(m + M)/2 \pm (M - m)/(2\sqrt{2})$ one makes the rate arbitrarily close to R_2^* , with R_s^* defined by (9).

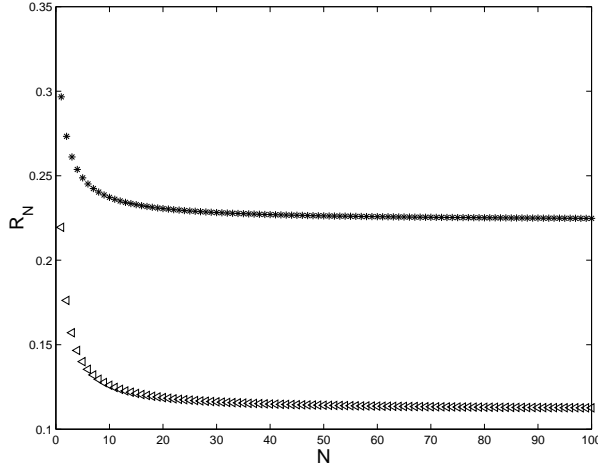


Figure 2: Asymptotic rate of convergence (26) for $m = 1$ and $M = 4$ when the β_j 's are on the uniform grid (stars) and when they correspond to Chebyshev points (triangles, $\varepsilon = 10^{-6}$)

Take now $N = 2$, with $\beta_0 = \beta$, $\beta_1 = (m + M)/2$ and $\beta_2 = m + M - \beta$. Similarly to the previous case, condition (25) imposes that β belongs to the interval $((m + M)/2 - \sqrt{3}(M - m)/4, (m + M)/2 + \sqrt{3}(M - m)/4)$, with the rate R_3 getting close to R_3^* for β close to $(m + M)/2 \pm \sqrt{3}(M - m)/4$.

By induction, one can show that the rate R_N can be made arbitrarily close to the value R_s^* defined by (9), with $s = N + 1$, when the $N + 1$ points β_i are suitably chosen and are constructed from the roots of Chebyshev polynomials. This construction is considered in the next example. (Note that the fact that R_N can be made arbitrarily close to R_{N+1}^* is not a coincidence: the worst case analysis of the s -step optimal gradient algorithm, which yields the rate R_s^* , corresponds to the situation where the β_i 's are rescaled roots of the s -th order Chebyshev polynomial, see [5].)

Example 6 *Chebyshev points.* Chebyshev points are defined by

$$t_k = \cos\left(\frac{\pi}{2} \frac{2k+1}{N+1}\right), \quad k = 0, \dots, N.$$

and correspond to the roots of $T_{N+1}(x) = \cos((N+1) \arccos x)$, the Chebyshev polynomials of the first kind. These points are symmetric on $(-1, 1)$. The asymptotic density of the points $\{t_k\}_0^N$, as $N \rightarrow \infty$, is $p(t) = 1/(\pi\sqrt{1-t^2})$, $t \in (-1, 1)$.

Define

$$\beta_k = \frac{m+M}{2} + \frac{M-m-2\varepsilon}{2} t_k, \quad k = 0, \dots, N,$$

where $0 < \varepsilon < (M - m)/2$. These points belong to the interval $(m + \varepsilon, M - \varepsilon)$ and are symmetric with respect to $(m + M)/2$. As $\varepsilon > 0$, the condition (25) holds. The rate R_N computed by (26) is plotted in Figure 2 as a function of N for $m = 1$, $M = 4$ and $\varepsilon = 10^{-6}$. Asymptotically, as $N \rightarrow \infty$, R_N approaches $R_{\arcsin, \varepsilon}$ defined below in (31).

3.3 Control variables with arcsine density on a subinterval of $[m, M]$

Let us assume that the distribution with c.d.f. $F(\cdot)$ has the density

$$p_\varepsilon(\beta) = \frac{1}{\pi\sqrt{(\beta - m')(M' - \beta)}}, \quad m' \leq \beta \leq M', \quad (29)$$

where $m' = m + \varepsilon$, $M' = M - \varepsilon$ and $0 < \varepsilon < (M - m)/2$. The density (29) is called the arcsine density on the interval $[m', M']$.

The sequence of points $\{\beta_i\}$ can be generated using, for example, the logistic map

$$H_L(x) = 4x(1 - x), \quad x \in (0, 1), \quad (30)$$

with β_0 randomly chosen in (m', M') , and for all $j = 0, 1, 2, \dots$

$$\beta_{2j+1} = M' + m' - \beta_{2j}, \quad \beta_{2j+2} = m' + (M' - m')H_L\left(\frac{\beta_{2j} - m'}{M' - m'}\right).$$

Note that the control variables β_j are placed symmetrically in the interval $[m, M]$. We show below that the condition (17) holds for each $\varepsilon > 0$. According to (21), the asymptotic rate of convergence is then

$$R_{\arcsin, \varepsilon} = \exp\left\{\int_{m'}^{M'} \log\left(\frac{(\beta - m)^2}{\beta^2}\right) p_\varepsilon(\beta) d\beta\right\} \quad (31)$$

and we show below that

$$R_{\arcsin, \varepsilon} = \left(\frac{M - m + 2\sqrt{\varepsilon(M - m - \varepsilon)}}{M + m + 2\sqrt{(M - \varepsilon)(m + \varepsilon)}}\right)^2. \quad (32)$$

For $\varepsilon = 0$ this gives $R_{\arcsin, 0} = R_\infty = (\sqrt{\rho} - 1)^2 / (\sqrt{\rho} + 1)^2$ where $\rho = M/m$. However, we cannot choose $\varepsilon = 0$ as the condition (17) does not hold (we also show below that $I(\lambda) = \int \log(\beta - \lambda)^2 dF(\beta) = 2\log(M - m) - 4\log 2$ for $\lambda \in [m, M]$). Since the condition does hold for any $\varepsilon > 0$, the rate of the algorithm can be made arbitrarily close to R_∞ : for small $\varepsilon > 0$, we have

$$R_{\arcsin, \varepsilon} = R_\infty \left(1 + 4\sqrt{\varepsilon(M - m)}\right) + O(\varepsilon), \quad \varepsilon \rightarrow 0.$$

The rest of this section is devoted to the verification of (17) for $\varepsilon > 0$ and to the derivation of the formula (32) for the rate $R_{\arcsin, \varepsilon}$. Define the integral

$$J(z, m', M') = \int_{m'}^{M'} \frac{\log(\beta - z)^2}{\pi\sqrt{(\beta - m')(M' - \beta)}} d\beta, \quad (33)$$

where $-\infty < z < \infty$. The changes of variables $t = -1 + 2(\beta - m')/(M' - m')$ and $x = -1 + 2(z - m')/(M' - m')$ in the integral (33) give

$$J(z, m', M') = 2\log\frac{M' - m'}{2} + \frac{1}{\pi} I_x, \quad \text{where } I_x = \int_{-1}^1 \frac{\log(t - x)^2}{\sqrt{1 - t^2}} dt. \quad (34)$$

Assume first that $|x| \leq 1$. By changing the variable $t = \cos \phi$ in the integral I_x , we obtain

$$I_x = \int_0^\pi \frac{\log(\cos \phi - x)^2}{\sin \phi} \sin \phi d\phi = \int_0^\pi \log(\cos \phi - x)^2 d\phi.$$

As $\cos(\phi) = \cos(2\pi - \phi) \forall \phi$, we have $\int_0^\pi \log(\cos \phi - x)^2 d\phi = \int_\pi^{2\pi} \log(\cos \phi - x)^2 d\phi$, which implies $I_x = \frac{1}{2} \int_0^{2\pi} \log(\cos \phi - x)^2 d\phi$. As we assume $-1 \leq x \leq 1$ we can set $\psi = \arccos x$ (so that $x = \cos \psi$). Using now the identity $\cos \phi - \cos \psi = 2 \sin \frac{\psi - \phi}{2} \sin \frac{\phi + \psi}{2}$, we obtain

$$\begin{aligned} I_x &= \frac{1}{2} \int_0^{2\pi} \log(\cos \phi - \cos \psi)^2 d\phi = \frac{1}{2} \int_0^{2\pi} \log\left(2 \sin \frac{\phi - \psi}{2} \sin \frac{\phi + \psi}{2}\right)^2 d\phi \\ &= \frac{1}{2} \left[\int_0^{2\pi} 2 \log 2 d\phi + \int_0^{2\pi} \log\left(\sin \frac{\phi - \psi}{2}\right)^2 d\phi + \int_0^{2\pi} \log\left(\sin \frac{\phi + \psi}{2}\right)^2 d\phi \right] \\ &= 2\pi \log 2 + \left[\int_0^\pi \log(\sin^2(\phi - \psi/2)) d\phi + \int_0^\pi \log(\sin^2(\phi + \psi/2)) d\phi \right]. \end{aligned}$$

The function $t \rightarrow \sin^2 t$ is π -periodic and therefore for any ψ' we get

$$\int_0^\pi \log(\sin^2(\phi + \psi')) d\phi = \int_0^\pi \log(\sin^2(\phi)) d\phi = 2 \int_0^\pi \log(\sin \phi) d\phi.$$

This implies

$$I_x = 2\pi \log 2 + 4 \int_0^\pi \log(\sin \phi) d\phi = 2\pi \log 2 - 4\pi \log 2 = -2\pi \log 2, \quad \forall x \in [-1, 1]. \quad (35)$$

Assume now that $|x| \geq 1$. From (35) we have $I_1 = -2\pi \log 2$ and differentiating I_x we get

$$I'_x = \left(\int_{-1}^1 \frac{\log(x-t)^2}{\sqrt{1-t^2}} dt \right)' = \frac{2\pi}{\sqrt{x^2-1}}.$$

Therefore, for $x > 1$,

$$I_{-x} = I_x = I_1 + \int_1^x I'_z dz = -2\pi \log 2 + \int_1^x \frac{2\pi}{\sqrt{z^2-1}} dz = -2\pi \log 2 + 2\pi \log \left(\frac{x + \sqrt{x^2-1}}{2} \right). \quad (36)$$

Combining (35) and (36) we obtain

$$I_x = \int_{-1}^1 \frac{\log(t-x)^2}{\sqrt{1-t^2}} dt = \begin{cases} -2\pi \log 2 & \text{if } |x| \leq 1 \\ 2\pi \log(|x| + \sqrt{x^2-1}) - 2\pi \log 2 & \text{if } |x| \geq 1, \end{cases}$$

together with (34), it gives

$$J(z, m', M') = \begin{cases} 2 \log(M' - m') - 4 \log 2 & \text{if } m' \leq z \leq M' \\ 2 \log(M' - m') + 2 \log(|t_z| + \sqrt{t_z^2 - 1}) - 4 \log 2 & \text{if } z < m' \text{ or } z > M', \end{cases} \quad (37)$$

where $t_z = -1 + 2(z - m')/(M' - m')$. Therefore, $J(\lambda, m', M') < J(m, m', M') = J(M, m', M')$ for all λ in (m, M) and (17) is satisfied. The expression (32) for the rate $R_{\arcsin, \varepsilon}$ easily follows from (37) and the representation $R_{\arcsin, \varepsilon} = \exp[J(m, m', M') - J(0, m', M')]$ with $m' = m + \varepsilon$ and $M' = M - \varepsilon$.

4 Estimation of m, M and a practical algorithm

4.1 Estimation of m, M and asymptotic behavior in the non symmetric case

The values of m and M can be easily estimated in the first iterations of the algorithm (3), for instance by computing the first moment $\mu_1^{(j)}$ for several values of $j = 0, 1, 2, \dots$ and taking

$$m_k = \min\{\mu_1^{(j)}, j = 0, \dots, k\}, \quad M_k = \max\{\mu_1^{(j)}, j = 0, \dots, k\} \quad (38)$$

as estimates. We then necessarily have $m < m_k < M_k < M$ for $k \geq 1$.

Suppose that the estimation is stopped at some k_0 , that is, $m_k = m_{k_0}$ and $M_k = M_{k_0}$ for all $k > k_0$. Then, under the conditions of Theorem 1 with $m' = m_{k_0}$ and $M' = M_{k_0}$ we have $\sum_{i=2}^{d-1} \nu_k(\lambda_i) \leq C\theta^k$ for k larger than some k_1 and constants $C > 0$ and $0 \leq \theta < 1$. Suppose that the control variables are generated by pairs for $k > k_0$, as in Theorem 2, but with $\beta_{2k+1} = M_{k_0} + m_{k_0} - \beta_{2k}$, for all $k > k_0$.

If $M_{k_0} + m_{k_0} = M + m$, Theorem 2 applies and the asymptotic rate R satisfies (21). For instance, if the β_k 's are generated as in Section 3.3, and have the arcsine density on $[m_{k_0}, M_{k_0}]$, the asymptotic rate is $R_{\arcsin, \varepsilon}$ with $\varepsilon = m_{k_0} - m = M - M_{k_0}$. Consider now the standard situation where $M_{k_0} + m_{k_0} \neq M + m$

and suppose that $M - M_{k_0} > m_{k_0} - m$. The asymptotic distribution of the β_k 's, symmetric in $[m_{k_0}, M_{k_0}]$, is then biased towards m and $\nu_k(m)$ tends to zero when $k \rightarrow \infty$. Following the same line as in the proof of Theorem 2, we obtain that the product of rates at two successive iterations for the delta measure at M , with control parameters respectively β and $\beta' = M_{k_0} + m_{k_0} - \beta$, is $R_2^2 = (M - \beta)^2(M - \beta')^2/(\beta\beta')^2$. The asymptotic rate then satisfies

$$\log R = \int \log \left| \frac{(M - \beta)(M + \beta - M_{k_0} - m_{k_0})}{\beta(M_{k_0} + m_{k_0} - \beta)} \right| dF(\beta).$$

Similarly, supposing that $M - M_{k_0} < m_{k_0} - m$ gives an asymptotic distribution of the β_k 's biased towards M , so that $\nu_k(m)$ tends to 1 as $k \rightarrow \infty$, and the asymptotic rate satisfies

$$\log R = \int \log \left| \frac{(\beta - m)(M_{k_0} + m_{k_0} - \beta - m)}{\beta(M_{k_0} + m_{k_0} - \beta)} \right| dF(\beta).$$

Now, note that $\nu_k(m) \rightarrow 0$ implies that $\mu_1^{(k)} \rightarrow M$ and $\nu_k(m) \rightarrow 1$ implies that $\mu_1^{(k)} \rightarrow m$, $k \rightarrow \infty$, so that maintaining the adaptation of the estimation of m_k and M_k by (38) ensures that $m_k \rightarrow m$ and $M_k \rightarrow M$ as $k \rightarrow \infty$. This permits to recover the same asymptotic rates as Section 3.3, even in situations where m and M are unknown. Since the estimated values m_k and M_k quickly converge to m and M , see for instance Figure 3, we need to generate the control variable β_k in $[m_k + \varepsilon, M_k - \varepsilon]$ at iteration k . A practical algorithm is given below.

4.2 An algorithm based on the arcsine density

A possible algorithm is then as follows.

- Choose τ as a small positive number (e.g., $\tau = 10^{-6}$), set $z_0 = 0$;
 - for $k = 0, 1$, set $\beta_k = \mu_1^{(k)}$ (steepest-descent) and set $m_1 = \min\{\mu_1^{(0)}, \mu_1^{(1)}\}$, $M_1 = \max\{\mu_1^{(0)}, \mu_1^{(1)}\}$;
 - for $k > 1$, set $\varepsilon_k = \tau(M_{k-1} - m_{k-1})$ and generate the β_k 's by pairs:
 - for $k = 2j$, set $z_j = \{\varphi + z_{j-1}\}$ and $\beta_{2j} = m_k + \varepsilon_k + (\cos(\pi z_j) + 1)(M_k - m_k - 2\varepsilon_k)/2$, where $\{t\}$ denotes the fractional part of t and $\varphi = (\sqrt{5} - 1)/2 \simeq 0.61803$;
 - for $k = 2j + 1$, set $\beta_{2j+1} = M_k + m_k - \beta_{2j}$;
- set $m_k = \min\{m_{k-1}, \mu_1^{(k)}\}$, $M_k = \max\{M_{k-1}, \mu_1^{(k)}\}$.

The sequence $z_1, z_2 \dots$ is such that $z_j = \{j\varphi\}$ so that the sequence is asymptotically uniform on $[0, 1]$, see, e.g., [7]. This implies that the asymptotic distribution of the sequence β_k has the arcsine density on $[m + \varepsilon, M - \varepsilon]$ where $\varepsilon = \tau(M - m)$. From (32), the rate of the algorithm satisfies

$$\lim_{n \rightarrow \infty} R_n = R_{\arcsin, \tau(M-m)} = R_\infty(1 + 4\sqrt{\tau}) + \mathcal{O}(\tau), \quad \tau \rightarrow 0.$$

The dynamical system $z_j = \{j\varphi\}$ generates a sequence in $[0, 1]$ with much better uniformity characteristics than sequences generated by the Bernoulli shift (28). Since the logistic map (30) corresponds to a transformation of the Bernoulli shift, the construction above, based on $z_j = \{j\varphi\}$, produces a sequence of control variables β_k with better distribution characteristics than sequences generated with (30).

Figures 3, 4 and 5 illustrate the typical behavior of the algorithm above in a large-dimensional badly conditioned problem. In the example presented, $d = 1000$, $m = 1$, $M = \rho = 1000$ and the eigenvalues λ_i

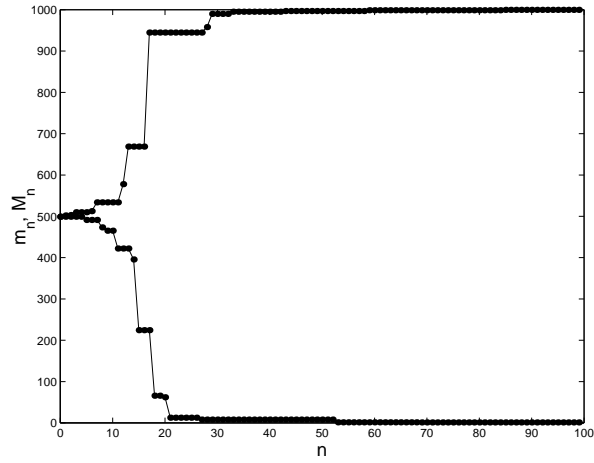


Figure 3: Convergence of the estimates m_n and M_n as functions of n ($m = 1$, $M = 1000$, $d = 1000$)

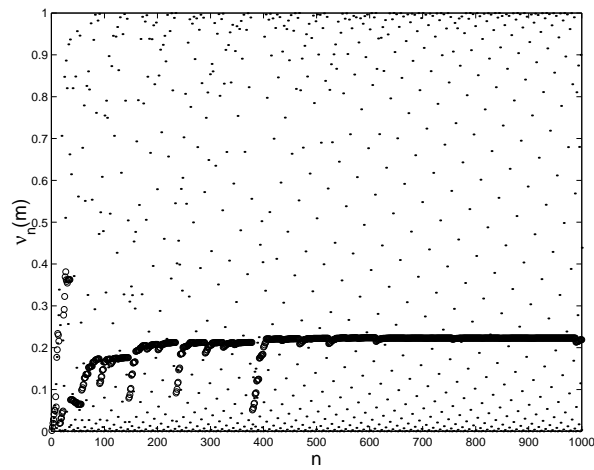


Figure 4: Values $\nu_n(m)$ as functions of n ; circles for $n = 2j$, dots for $n = 2j + 1$ ($\rho = 1000$, $d = 1000$)

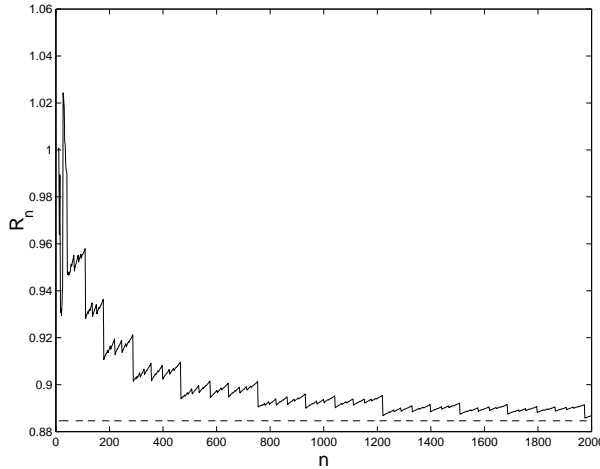


Figure 5: Rate of convergence R_n , see (7), as a function of n ; the limiting value $R_{\arcsin, \tau(M-m)}$ is indicated by the dashed line ($m = 1, M = 1000, d = 1000, \tau = 10^{-6}$)

are random and uniformly distributed on the interval $[m, M]$ (one would obtain exactly the same plots if the eigenvalues were equally-spaced on $[m, M]$).

In terms of complexity of calculations, only the multiplications of d -dimensional vectors by the $d \times d$ matrix A are expensive. The steepest descent algorithm requires the calculation of $\beta_k = \mu_2^{(k)} / \mu_1^{(k)} = (Ag_k, Ag_k) / (Ag_k, g_k)$ at iteration k . Having computed g_k and Ag_k , one may notice that next gradient g_{k+1} can be obtained as $g_{k+1} = g_k - (1/\beta_k)Ag_k$, so that only the computation of Ag_{k+1} is expensive at iteration $k + 1$. However, a long sequence of iterations of this type may produce an accumulation of rounding errors, and it is rather recommended to recalculate g_{k+1} from x_{k+1} by $g_{k+1} = Ax_{k+1} - y$, see (1). This then requires two multiplications by A at each steepest-descent iteration.

In the algorithm above, iteration k only requires the calculation of the gradient $g_k = Ax_k - y$, and thus only one multiplication by A . Notice that the estimation of m_k and M_k through the moments $\mu_1^{(j)} = (Ag_j, g_j) / (g_j, g_j)$, see (38), does not require the calculation of Ag_j at step k . Indeed, allowing a delay of one step in the estimation, we have $(g_j, g_{j+1}) = (g_j, g_j - (1/\beta_j)Ag_j)$ so that $\mu_1^{(j)}$ is obtained at next step from

$$\mu_1^{(j)} = \beta_j \left[1 - \frac{(g_j, g_{j+1})}{(g_j, g_j)} \right].$$

Also, one may observe in Figure 3 that the convergence of m_n and M_n to m and M respectively is very fast, so that the estimation can be stopped after a few iterations. On the whole, it makes iterations with the algorithm above about twice simpler than steepest-descent iterations (even when m and M are estimated), with much faster convergence.

5 Hilbert space case

In the Hilbert-space case, A is a self-adjoint operator and its spectrum \mathcal{S}_A is a closed subset of the interval $[m, M]$ of the real line, with $m, M \in \mathcal{S}_A$. Let E_λ be the spectral family associated with A and define the measure $\nu_k = d(E_\lambda z_k, z_k)$, $m \leq \lambda \leq M$, with $z_k = g_k / \sqrt{(g_k, g_k)}$ the normalized gradient at x_k . We have $(z_k, z_k) = 1 = \int_m^M \nu_k(d\lambda)$ and ν_k is a probability measure on the Borel sets of $(0, \infty)$, satisfying

$\nu_k([m, M]) = 1$ for all k and with moments still defined by (6). One iteration of a gradient algorithm with control variable β_k thus gives in terms of ν_k

$$\nu_{k+1}(\mathcal{A}) = \frac{\int_{\mathcal{A}} (\lambda - \beta_k)^2 \nu_k(d\lambda)}{\beta_k^2 - 2\beta_k \mu_1^{(k)} + \mu_2^{(k)}},$$

for \mathcal{A} any measurable subset of $[m, M]$, see (8). The properties obtained for the finite dimensional case remain valid and only a few adaptations are required.

Theorem 3 *Assume that the sequence $\{\beta_k\}$ has asymptotic distribution function $F(\beta)$ which is supported on an interval $[m', M'] = [m + \varepsilon, M - \varepsilon]$ with $0 < \varepsilon < (M - m)/2$. Suppose, moreover, that $I(\lambda) = \int \log(\beta - \lambda)^2 dF(\beta)$ is a continuous function of λ on (m', M') and that*

$$I(\lambda) < \max \left\{ \int \log(M - \beta)^2 dF(\beta), \int \log(\beta - m)^2 dF(\beta) \right\}, \quad \forall \lambda \in (m', M'), \quad (39)$$

and that $\nu_0\{[m, m + \gamma]\} > 0$ and $\nu_0\{(M - \gamma, M]\} > 0$ for all $\gamma > 0$. Then, the measure ν_k converges to a two-point measure supported at m and M , in the sense that there exists k_0 such that, for any function $g(\lambda)$ continuous on $[m, M]$ and any $\delta > 0$, there exists $\gamma > 0$ such that

$$\max \left\{ \left| \int_m^C g(\lambda) \nu_k(d\lambda) - g(m) \int_m^C \nu_k(d\lambda) \right|, \left| \int_C^M g(\lambda) \nu_k(d\lambda) - g(M) \int_C^M \nu_k(d\lambda) \right| \right\} < \delta + C_\gamma \alpha_\gamma^k, \quad k > k_0,$$

where $C = (m + M)/2$ and $C_\gamma > 0$, $\alpha_\gamma \in (0, 1)$ are constants depending on γ . If, moreover, the control variables β_k are generated by symmetric pairs for large k , that is, $\beta_{2j+1} = M + m - \beta_{2j}$ for all $j \geq j_0$, then the asymptotic rate R satisfies (21).

Proof. The proof of convergence of ν_k to a two-point measure follows the same arguments as for Theorem 1. Suppose that $F(\cdot)$ satisfies (14). We still have for the first term of the sum $S_k(\lambda, m)$ defined by (15)

$$I_k(m) = \frac{1}{k} \sum_{j=0}^{k-1} \log(\beta_j - m)^2 \rightarrow I(m) = \int \log(\beta - m)^2 dF(\beta), \quad k \rightarrow \infty.$$

Concerning the second term $I_k(\lambda) = (1/k) \sum_{j=0}^{k-1} \log(\beta_j - \lambda)^2$ we need now a bound uniform in λ , that is, we need to show that

$$\forall \epsilon > 0, \exists K_0 \text{ such that: } \sup_{\lambda \in (m', M')} I_k(\lambda) - I(\lambda) < \epsilon, \quad \forall k > K_0. \quad (40)$$

Take a ball $\mathcal{B}(\lambda_1, \delta) = \{\lambda : |\lambda - \lambda_1| \leq \delta\}$ and consider $\bar{a}_\delta(\beta) = \sup_{\lambda \in \mathcal{B}(\lambda_1, \delta)} \log(\beta - \lambda)^2$, which is an increasing function of δ , $\bar{a}_\delta(\beta) = 2 \log(|\beta - \lambda_1| + \delta)$. We have

$$\lim_{\delta \rightarrow 0} \int \bar{a}_\delta(\beta) dF(\beta) = \int \left[\lim_{\delta \rightarrow 0} \bar{a}_\delta(\beta) \right] dF(\beta) = I(\lambda_1)$$

and therefore, there exists $\delta_1 = \delta_1(\lambda_1)$ such that $\int \bar{a}_\delta(\beta) dF(\beta) < I(\lambda_1) + \epsilon/3$ for $\delta < \delta_1$. Now,

$$\sup_{\lambda \in \mathcal{B}(\lambda_1, \delta)} I_k(\lambda) \leq (1/k) \sum_{j=0}^{k-1} 2 \log(|\beta_j - \lambda| + \delta) < \int \bar{a}_\delta(\beta) dF(\beta) + \epsilon/3$$

for all k larger than some $K_1 = K_1(\lambda_1, \delta)$. Also, from the continuity of $I(\lambda)$, there exists $\delta_2 = \delta_2(\lambda_1)$ such that $\inf_{\lambda \in \mathcal{B}(\lambda_1, \delta)} I(\lambda) > I(\lambda_1) - \epsilon/3$ for $\delta < \delta_2$. Altogether it gives $\sup_{\lambda \in \mathcal{B}(\lambda_1, \delta)} I_k(\lambda) - I(\lambda) < \epsilon$ for

$\delta < \delta_0(\lambda_1) = \min(\delta_1, \delta_2)$ and $k > K_1$. It only remains to cover $[m', M']$ with a finite number of such balls $\mathcal{B}(\lambda_i, \delta)$, with $\delta < \min_i \delta_0(\lambda_i)$ to obtain the result (40). Since $\log(\beta - \lambda)^2$ is a decreasing (resp. increasing) function of λ in $[m, m']$ (resp. in $[M', M]$), together with the condition (39) it implies that for any set $\mathcal{S} \subset (m, M)$, $\limsup_{k \rightarrow \infty} \sup_{\lambda \in \mathcal{S}} S_k(\lambda, m) \leq -\delta$ for some $\delta = \delta(\mathcal{S}) > 0$. Therefore, there exists k_0 such that, $\forall k > k_0$, $\sup_{\lambda \in (m', M')} H_k(\lambda)/H_k(m) \leq \theta_\varepsilon^k$ where $\theta_\varepsilon = \exp(-\delta_\varepsilon) < 1$.

Consider now a function $g(\lambda)$ continuous on $[m, M]$ and define

$$\Delta_k = \left| \int_m^C g(\lambda) \nu_k(d\lambda) - g(m) \int_m^C \nu_k(d\lambda) \right|,$$

where $C = (m + M)/2$. We show below that

$$\forall \delta > 0, \exists \gamma > 0 \text{ such that } \Delta_k < \delta + 2 \frac{D_g}{\int_m^{m+\gamma} \nu_0(d\lambda)} \alpha_\gamma^k \text{ for all } k > k_0, \quad (41)$$

for some $\alpha_\gamma < 1$, where $D_g = \max_{\lambda \in [m, C]} |g(\lambda) - g(m)|$. We have $\Delta_k < \int_m^C |g(\lambda) - g(m)| \nu_k(d\lambda) = \Delta_{k,1} + \Delta_{k,2} + \Delta_{k,3}$, with

$$\Delta_{k,1} = \int_m^{m+2\gamma} |g(\lambda) - g(m)| \nu_k(d\lambda), \quad \Delta_{k,2} = \int_{m+2\gamma}^{m'} |g(\lambda) - g(m)| \nu_k(d\lambda), \quad \Delta_{k,3} = \int_{m'}^C |g(\lambda) - g(m)| \nu_k(d\lambda),$$

$\gamma < \varepsilon/2$. From the continuity of $g(\lambda)$, we can take γ small enough to have $\Delta_{k,1} < \delta \int_m^{m+2\gamma} \nu_k(d\lambda) \leq \delta$. Next, $\Delta_{k,2} < D_g \int_{m+2\gamma}^{m'} \nu_k(d\lambda) = D_g \int_{m+2\gamma}^{m'} H_k(\lambda) \nu_0(d\lambda)$ with $H_k(\lambda)$ defined by (13). Since $\beta_k \in [m', M']$ for all k , $H_k(\lambda)$ is a decreasing function of λ for $\lambda \in [m, m']$, and for $m + 2\gamma < \lambda < m'$ it satisfies

$$H_k(\lambda) < H_k(m + 2\gamma) < H_k(m + \gamma) \left(\frac{M - m - \varepsilon - 2\gamma}{M - m - \varepsilon - \gamma} \right)^{2k}.$$

Since $\int_m^{m+\gamma} \nu_k(d\lambda) = \int_m^{m+\gamma} H_k(\lambda) \nu_0(d\lambda) \geq H_k(m + \gamma) \int_m^{m+\gamma} \nu_0(d\lambda)$, we obtain

$$\Delta_{k,2} < \frac{D_g}{\int_m^{m+\gamma} \nu_0(d\lambda)} \left[\frac{M - m - \varepsilon - 2\gamma}{M - m - \varepsilon - \gamma} \right]^{2k}.$$

We also obtain for the last term,

$$\Delta_{k,3} < D_g \int_{m'}^C H_k(\lambda) \nu_0(d\lambda) < D_g \theta_\varepsilon^k H_k(m) \int_{m'}^C \nu_0(d\lambda) < D_g \theta_\varepsilon^k H_k(m) \text{ for } k > k_0.$$

For $\lambda \in [m, m']$ we have $H_k(\lambda)/H_k(m) \geq (m' - \lambda)^{2k}/\varepsilon^{2k}$ so that

$$1 \geq \int_m^{m+\gamma} \nu_k(d\lambda) \geq H_k(m) \int_m^{m+\gamma} [(m' - \lambda)/\varepsilon]^{2k} \nu_0(d\lambda) > H_k(m) [(\varepsilon - \gamma)/\varepsilon]^{2k} \int_m^{m+\gamma} \nu_0(d\lambda).$$

Therefore, for $k > k_0$,

$$\Delta_{k,3} < \frac{D_g}{\int_m^{m+\gamma} \nu_0(d\lambda)} \left[\frac{\theta_\varepsilon \varepsilon^2}{(\varepsilon - \gamma)^2} \right]^k.$$

We have $\theta_\varepsilon \varepsilon^2 / (\varepsilon - \gamma)^2 < 1$ for $\gamma < \varepsilon(1 - \sqrt{\theta_\varepsilon})$ so that (41) is satisfied for $\alpha_\gamma = \max\{\theta_\varepsilon \varepsilon^2 / (\varepsilon - \gamma)^2, (M - m - \varepsilon - 2\gamma)^2 / (M - m - \varepsilon - \gamma)^2\}$ and $\alpha_\gamma < 1$ for γ small enough. One can show a similar property for $\Delta'_k = \left| \int_C^M g(\lambda) \nu_k(d\lambda) - g(M) \int_C^M \nu_k(d\lambda) \right|$.

Finally, we apply the property above to $g(\lambda) = \lambda$ and $g(\lambda) = \lambda^2$ and, following the same line as in the proof of Theorem 2, we then obtain for the product of rates at two successive iterations with control variables β_{2j} and $\beta_{2j+1} = m + M - \beta_{2j}$:

$$R_2^2(\beta_{2j}) \left[1 - \frac{A_\gamma \alpha_\gamma^{2j} + B\delta}{R_2^2(\beta_{2j})} \right] < r_{2j} r_{2j+1} < R_2^2(\beta_{2j}) \left[1 + \frac{A_\gamma \alpha_\gamma^{2j} + B\delta}{R_2^2(\beta_{2j})} \right],$$

for some $A_\gamma > 0$, $B > 0$ and $j > k_0/2$. Therefore,

$$\log R_2(\beta_{2j}) - A'_\gamma \alpha_\gamma^{2j} - B'\delta < \log \sqrt{r_{2j} r_{2j+1}} < \log R_2(\beta_{2j}) + A'_\gamma \alpha_\gamma^{2j} + B'\delta,$$

with $A'_\gamma = A_\gamma/R_2^2(m + \varepsilon)$ and $B' = B/R_2^2(m + \varepsilon)$, for j large enough. Since $\sum_{j=0}^{\infty} \alpha_\gamma^{2j} = 1/(1 - \alpha_\gamma^2) < \infty$, we obtain from (12),

$$\left| \log R - \int \log R_2(\beta) dF(\beta) \right| = \left| \lim_{k \rightarrow \infty} \frac{1}{k} \sum_{j=0}^{k-1} \log \sqrt{r_{2j} r_{2j+1}} - \int \log R_2(\beta) dF(\beta) \right| < B'\delta.$$

Since δ is arbitrary, the asymptotic rate of convergence is thus the same as in the finite dimensional case. ■

Remark 9 Note that the condition $I(\lambda)$ being a continuous function of λ is satisfied for all examples considered in Section 3. It is also satisfied when the distribution function $F(\cdot)$ has density $\phi(\cdot)$ with derivative $\phi'(\cdot)$ uniformly bounded on (m', M') . Indeed, one can write $I(\lambda) = \int_{\lambda-M'}^{\lambda-m'} \phi(\lambda-t) \log t^2 dt$ which has derivative $I'(\lambda) = \phi(m') \log(\lambda - m')^2 - \phi(M') \log(\lambda - M')^2 + \int_{m'}^{M'} \phi'(t) \log(\lambda - t)^2 dt$; this derivative is bounded, which implies the continuity of $I(\lambda)$.

References

- [1] H. Akaike. On a successive transformation of probability distribution and its application to the analysis of the optimum gradient method. *Ann. Inst. Statist. Math. Tokyo*, 11:1–16, 1959.
- [2] J. Barzilai and J.M. Borwein. Two-point step size gradient methods. *IMA Journal of Numerical Analysis*, 8:141–148, 1988.
- [3] H.J. Bierens. *Topics in Advanced Econometrics*. Cambridge University Press, Cambridge, 1994.
- [4] Y. H. Dai and X. Q. Yang. A new gradient method with an optimal stepsize property. *Comput. Optim. Appl.*, 33(1):73–88, 2006.
- [5] G.E. Forsythe. On the asymptotic directions of the s -dimensional optimum gradient method. *Numerische Mathematik*, 11:57–76, 1968.
- [6] R. Haycroft, L. Pronzato, H.P. Wynn, and A.A. Zhigljavsky. Studying convergence of gradient algorithms via optimal experimental design theory. In L. Pronzato and A.A. Zhigljavsky, editors, *Optimal Design and Related Areas in Optimization and Statistics*, pages 13–37. Springer, 2009.
- [7] L. Kuipers and H. Niederreiter. *Uniform Distribution of Sequences*. Wiley, New York, 1974.
- [8] D.G. Luenberger. *Introduction to Linear and Nonlinear Programming*. Addison-Wesley, Reading, Massachusetts, 1973.

- [9] L. Pronzato, H.P. Wynn, and A.A. Zhigljavsky. *Dynamical Search*. Chapman & Hall/CRC, Boca Raton, 2000.
- [10] L. Pronzato, H.P. Wynn, and A.A. Zhigljavsky. Renormalised steepest descent in Hilbert space converges to a two-point attractor. *Acta Applicandae Mathematicae*, 67:1–18, 2001.
- [11] L. Pronzato, H.P. Wynn, and A.A. Zhigljavsky. An introduction to dynamical search. In P.M. Pardalos and H.E. Romeijn, editors, *Handbook of Global Optimization*, volume 2, chapter 4, pages 115–150. Kluwer, Dordrecht, 2002.
- [12] L. Pronzato, H.P. Wynn, and A.A. Zhigljavsky. Asymptotic behaviour of a family of gradient algorithms in \mathbb{R}^d and Hilbert spaces. *Mathematical Programming*, A107:409–438, 2006.
- [13] L. Pronzato, H.P. Wynn, and A.A. Zhigljavsky. A dynamical-system analysis of the optimum s -gradient algorithm. In L. Pronzato and A.A. Zhigljavsky, editors, *Optimal Design and Related Areas in Optimization and Statistics*, pages 39–80. Springer, 2009.