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OPTIMAL EXPERIMENTAL DESIGN AND QUADRATIC OPTIMIZATION

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ABSTRACT. A well known gradient-type algorithm for solving quadratic optimization problems is the method of Steepest Descent. Here the Steepest Descent algorithm is generalized to a broader family of gradient algorithms, where the step-length $\gamma_k$ is chosen in accordance with a particular procedure. The asymptotic rate of convergence of this family is studied. To facilitate the investigation we re-write the algorithms in a normalized form which enables us to exploit a link with the theory of optimum experimental design.

Introduction

The steepest descent algorithm in $\mathbb{R}^d$ has been shown to be equivalent to a special algorithm for updating measures on the real line, see, e.g., [4]. The connection is that when the steepest descent algorithm is applied to the minimization of the quadratic function

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

where $(x, y)$ is the inner product, it can be translated to the updating of measures in $[m, M]$ where

$$m = \inf_{\|x\|=1} (Ax, x), \quad M = \sup_{\|x\|=1} (Ax, x)$$

with $0 < m < M < \infty$; $m$ and $M$ are the smallest and largest eigenvalues of $A$, respectively. The research has developed from the well known result, due to Akaike [1], that for standard steepest descent the renormalized iterates $x_k/\|x_k\|$ converge to the two-dimensional space spanned by the eigenvectors corresponding to the eigenvalues $m$ and $M$.

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Let \( g(x) = Ax - y \) be the gradient of the objective function (1). The steepest
descent algorithm is \( x_{k+1} = x_k - \frac{(g_k, g_k)}{(g_k, g_k)} g_k \). Using the notation \( \gamma_k = \frac{(g_k, g_k)}{(g_k, g_k)} \),
we write the algorithm as \( x_{k+1} = x_k - \gamma_k g_k \). This can be rewritten in terms of
the gradients as
\[
g_{k+1} = g_k - \gamma_k A g_k .
\] (2)

The main objective of the paper is studying the family of algorithms (2)
where the step-length \( \gamma_k \) is chosen in a general way. To facilitate this study we
first rewrite the algorithm (2) in a different (normalized) form and then make
a connection with the theory of optimum experimental design.

Renormalized version of gradient algorithms

Let us convert (2) into a “renormalized” version. First note that
\[
(g_{k+1}, g_{k+1}) = (g_k, g_k) - 2\gamma_k (A g_k, g_k) + \gamma_k^2 (A^2 g_k, g_k) .
\] (3)

Letting \( r_k = \frac{(g_{k+1}, g_{k+1})}{(g_k, g_k)} \) and dividing (3) through by \( (g_k, g_k) \) gives
\[
r_k = 1 - 2\gamma_k \frac{(A g_k, g_k)}{(g_k, g_k)} + \gamma_k^2 \frac{(A^2 g_k, g_k)}{(g_k, g_k)} .
\] (4)

The value of \( r_k \) can be considered as a rate of convergence of algorithm (2)
at iteration \( k \). Other rates which are asymptotically equivalent to \( r_k \) can be
considered as well, see [4] for a discussion. The asymptotic rate of convergence
of the gradient algorithm (2) can be defined as \( R = \lim_{k \to \infty} (r_1 \cdots r_k)^{1/k} \). Of course,
this rate may depend on the initial point \( x_0 \) or, equivalently, on \( g_0 \).

To simplify the notation, we need to convert to moments and measures. Since
we assume that \( A \) is a positive definite \( d \)-dimensional square matrix, we can as-
sume, without loss of generality, that \( A \) is a diagonal matrix \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_d) \);
the elements \( \lambda_1, \ldots, \lambda_d \) are the eigenvalues of the original matrix such that
\( 0 < m = \lambda_1 \leq \ldots \leq \lambda_d = M \). Then for any vector \( g = (g(1), \ldots, g(d))^T \) we
can define
\[
\mu_\alpha(g) = \frac{(A^\alpha g, g)}{(g, g)} = \frac{\sum_i g(i, g)^\alpha}{\sum_j g(j, g)^\alpha} \lambda_i^\alpha .
\]

This can be considered as the \( \alpha \)th moment of a distribution with mass \( p_i = \frac{g(i)^2}{\sum_j g(j)^2} \)
at \( \lambda_i, i = 1, \ldots, d \). Using the notation \( \mu^{(k)}_\alpha = \mu_\alpha(g_k) \), where \( g_k \) are the iterates
in (2), we can rewrite (4) as
\[
r_k = 1 - 2\gamma_k \mu_1^{(k)} + \gamma_k^2 \mu_2^{(k)} .
\] (5)
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For the steepest descent algorithm $\gamma_k$ minimizes $f(x_k - \gamma g_k)$ over $\gamma$ and we have $\gamma_k = \frac{1}{\mu_1^{(k)}}$ and $r_k = \frac{\mu_2^{(k)}}{\mu_1^{(k)}} - 1$. Write $z_k = \frac{g_k}{\sqrt{(g_k, g_k)}}$ for the normalized gradient and recall that $p_i = \frac{g_i}{\sum_j g_j}$ is the $i$th probability corresponding to a vector $g$. The corresponding probabilities for the vectors $g_k$ and $g_{k+1}$ are

$$p_i^{(k)} = \frac{(g_k)^2_i}{(g_k, g_k)}$$

and

$$p_i^{(k+1)} = \frac{(g_{k+1})^2_i}{(g_{k+1}, g_{k+1})}$$

for $i = 1, \ldots, d$.

Now we are able to write down the re-normalized version of (2), which is the updating formula for $p_i$ ($i = 1, \ldots, d$):

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

$$= \frac{(1 - \gamma_k \lambda_i)^2}{1 - 2\gamma_k \mu_1^{(k)} + \gamma_k^2 \mu_2^{(k)}} p_i^{(k)}.$$  \hfill (6)

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.

A multiplicative algorithm for optimal design

Optimization in measure spaces covers a variety of areas and optimal experimental design theory is one of them. These areas often introduce algorithms which typically have two features: the measures are re-weighted in some way and the moments play an important role. Both features arise, as we have seen, in the above algorithms; see also [2], [3] and [5] for examples of other algorithms of this type.

In classical optimal design theory for the linear regression model $y_j = \alpha + \beta x_j + \varepsilon_j, x_j \in [m, M]$, one is interested in functionals of the moment matrix $M(\xi)$ of a design measure $\xi$:

$$M(\xi) = \begin{pmatrix} \mu_0 & \mu_1 \\ \mu_1 & \mu_2 \end{pmatrix},$$  \hfill (7)

where $\mu_\alpha = \mu_\alpha(\xi) = \int x^\alpha \, d\xi(x)$ are the $\alpha$th moments of the measure $\xi$ and $\mu_0 = 1$. 117
In the theory of optimum design the directional (Fréchet) derivative “towards” a discrete measure $\xi_x$ mass 1 at a point $x$ is of importance. This is

$$\frac{\partial}{\partial \alpha} \Phi \left( M \left[ (1 - \alpha) \xi + \alpha \xi_x \right] \right) |_{\alpha=0} = \text{tr} \left( \Phi(\xi) M(\xi_x) \right) - \text{tr} \left( \Phi(\xi) M(\xi) \right), \quad (8)$$

where

$$\Phi(\xi) = \frac{\partial \Phi}{\partial M} \bigg|_{M=M(\xi)} = \left( \begin{array}{cc} \frac{\partial \Phi}{\partial \mu_0} & \frac{1}{2} \frac{\partial \Phi}{\partial \mu_1} \\ \frac{1}{2} \frac{\partial \Phi}{\partial \mu_1} & \frac{\partial \Phi}{\partial \mu_2} \end{array} \right).$$

Here $\Phi$ is a functional on the space of $2 \times 2$ matrices usually considered as an optimality criterion to be maximized with respect to $\xi$. The first term on the right hand side of (8) is

$$\varphi(x, \xi) = \text{tr} \left( \Phi(\xi) M(\xi_x) \right) = \left( \begin{array}{c} 1 \\ x \end{array} \right) \Phi(\xi) \left( \begin{array}{c} 1 \\ x \end{array} \right) = \frac{\partial \Phi}{\partial \mu_0} + x \frac{\partial \Phi}{\partial \mu_1} + x^2 \frac{\partial \Phi}{\partial \mu_2}.$$  

A class of optimal design algorithms is based on the multiplicative updating of the weights of the current design measure $\xi^{(k)}$ with some function of $\varphi(x, \xi)$. We show below how algorithms in this class are related to the gradient algorithms (2) in their re-normalized form (6).

Assume that our measure is discrete and concentrated on $[m, M]$. Assume also that $\frac{\partial \Phi(M)}{\partial \mu_2} > 0$; then $\varphi(x, \xi)$ has a well-defined minimum

$$c(\xi) = \min_{x \in \mathbb{R}} \varphi(x, \xi) = \frac{\partial \Phi}{\partial \mu_0} - B(\xi), \quad \text{where} \quad B(\xi) = \frac{1}{4} \left( \frac{\partial \Phi}{\partial \mu_1} \right)^2.$$

Let $\xi(x)$ be the mass at a point $x$ and define the re-weighting at $x$ by

$$\xi'(x) = \frac{\varphi(x, \xi) - c(\xi)}{b(\xi)} \xi(x), \quad (9)$$

where $b(\xi)$ is a normalizing constant

$$b(\xi) = \int_{m}^{M} (\varphi(x, \xi) - c(\xi)) \xi(\text{d}x) = \text{tr} \left[ M(\xi) \Phi(\xi) \right] - c(\xi).$$

Let us define $\gamma = \gamma(\xi) = \gamma(\mu_1, \mu_2)$ as

$$\gamma = \gamma(\xi) = -2 \frac{\partial \Phi}{\partial \mu_2}. \quad (10)$$

Then

$$\varphi(x, \xi) - c(\xi) = B(\xi) \left( 1 - \gamma(\xi)x \right)^2.$$
The normalization ensures that the measure $\xi'$ is a probability distribution. We obtain that the re-weighting formula (9) can be equivalently written as

$$\xi'(x) = \frac{(1 - \gamma x)^2}{1 - 2\gamma \mu_1 + \gamma^2 \mu_2} \xi(x).$$  \hspace{1cm} (11)

This is exactly the same as the general gradient algorithm in its renormalized form (6). To see that, we simply write the updating formula (11) iteratively

$$\xi^{(k+1)}(x) = \frac{(1 - \gamma_k x)^2}{1 - 2\gamma_k \mu_1^{(k)} + \gamma_k^2 \mu_2^{(k)}} \xi^{(k)}(x).$$

**Optimum design gives the worst rate of convergence**

Let $\Phi = \Phi(M(\xi))$ be an optimality criterion, where $M(\xi)$ is as in (7). Associate with it a gradient algorithm with step-length $\gamma(\mu_1, \mu_2)$ as given by (10).

Let $\xi^*$ be the optimum design for $\Phi$ on $[m, M]$; that is,

$$\Phi(M(\xi^*)) = \max_{\xi} \Phi(M(\xi))$$

where the maximum is taken over all probability measures supported on $[m, M]$. Note that $\xi^*$ is invariant for one iteration of the algorithm (11); that is, if $\xi = \xi^*$ in (11) then $\xi'(x) = \xi(x)$ for all $x \in \text{supp}(\xi)$.

In accordance with (5), the rate associated with the design measure $\xi$ is defined by

$$r(\xi) = 1 - 2\gamma \mu_1 + \gamma^2 \mu_2 = \frac{b(\xi)}{B(\xi)}.$$  \hspace{1cm}

Assume that the optimality criterion $\Phi$ is such that the optimum design $\xi^*$ is non-degenerate (that is, $\xi^*$ is not just supported at a single point). Note that if $\Phi(M) = -\infty$ for any singular matrix $M$, then this condition is satisfied.

Since the design $\xi^*$ is optimum, all directional derivatives are non-positive:

$$\frac{\partial}{\partial \alpha} \Phi\left[M\left((1 - \alpha)\xi^* + \alpha \xi(x)\right)\right]_{\alpha=0^+} \leq 0,$$

for all $x \in [m, M]$. Using (8), this implies

$$\max_{x \in [m, M]} \varphi(x, \xi^*) \leq t^* = \text{tr} \left[M(\xi^*) \frac{\partial}{\partial \xi} \Phi(\xi^*)\right].$$

Since $\varphi(x, \xi^*)$ is a quadratic convex function of $x$, this is equivalent to $\varphi(m, \xi^*) \leq t^*$ and $\varphi(M, \xi^*) \leq t^*$. As

$$\int_m^M \varphi(x, \xi^*)\xi^*(dx) = t^*$$
this implies that $\xi^*$ is supported at $m$ and $M$. Since $\xi^*$ is non-degenerate, $\xi^*$ has positive masses at both points $m$ and $M$ and

$$\varphi(m, \xi^*) = \varphi(M, \xi^*) = t^*.$$ 

As $\varphi(x, \xi^*)$ is quadratic in $x$ with its minimum at $\frac{1}{\gamma}$, this implies that

$$\gamma^* = \gamma(\mu_1(\xi^*), \mu_2(\xi^*)) = \frac{2}{(m + M)}.$$ 

The rate $v(\xi^*)$ is therefore

$$v(\xi^*) = \frac{b(\xi^*)}{B(\xi^*)} = \frac{t^* - c(\xi^*)}{B(\xi^*)} = (1 - m\gamma^*)^2 = (1 - M\gamma^*)^2 = R_{\text{max}},$$

where

$$R_{\text{max}} = \frac{(M - m)^2}{(M + m)^2}. \quad (12)$$

Assume now that the optimum design $\xi^*$ is degenerate and is supported at a single point $x^*$. Note that since $\varphi(x, \xi^*)$ is both quadratic and convex, $x^*$ is either $m$ or $M$. Since the optimum design is invariant in one iteration of the algorithm (11), $\gamma^*$ is constant and

$$\max_{\xi} r(\xi) = \max [(1 - m\gamma^*)^2, (1 - M\gamma^*)^2] \geq R_{\text{max}}$$

with the inequality replaced by an equality if and only if $\gamma^* = \frac{2}{(M+m)}$.

**Some special cases**

A few examples of gradient algorithms (2) worthy of mention are given below.

The steepest descent algorithm corresponds to the case when $\Phi(\xi)$ is the $D$-optimality criterion $\Phi(M(\xi)) = \mu_2 - \mu_1^2$ with a step length equal to $\gamma_k = \frac{1}{\mu_1^2}$. It is well-known that the asymptotic rate of the steepest descent algorithm is always close to the value $R_{\text{max}}$ defined in (12). The asymptotic behaviour of the steepest descent algorithm has already been extensively studied, see, e.g., [4].

The steepest descent algorithm with relaxation is also known in literature on optimization. For this algorithm, $\gamma_k = \frac{\varepsilon}{\mu_1^2},$ where $\varepsilon$ is some fixed positive number. This algorithm can be associated with the optimality criterion

$$\Phi(M(\xi)) = \varepsilon \mu_2 - \mu_1^2.$$ \quad (13)

It is known that for suitable values of the relaxation parameter $\varepsilon$ this algorithm has a faster convergence rate than the ordinary steepest descent algorithm. However, the reasons why this occurs were not previously known.
It can be shown that if the relaxation coefficient \( \varepsilon \) is either small \( \varepsilon < \frac{4Mm}{(m+M)^2} \) or large \( \varepsilon > 1 \), then for almost all starting points the algorithm asymptotically behaves as if it has started at the worst possible initial point. Equivalently, for these values of \( \varepsilon \) the sequence of designs converges to the optimal design for the criterion (13).

Moreover, if the relaxation parameter is either too small \( \varepsilon < \frac{2m}{m+M} \) or too large \( \varepsilon > \frac{2M}{m+M} \), then the rate of the steepest descent algorithm with relaxation becomes worse than \( R_{\text{max}} \), the worst-case rate of the standard steepest descent algorithm. This is related to the fact that for these values of \( \varepsilon \) the optimal design for the criterion (13) is degenerate (that is, it is concentrated at a single point). As a consequence, we also obtain a well-known result that if the value of the relaxation coefficient is either \( \varepsilon < 0 \) or \( \varepsilon > 2 \), then the steepest descent algorithm with relaxation diverges.

When \( \frac{4Mm}{(m+M)^2} < \varepsilon \leq 1 \) the relaxed steepest descent algorithm does not converge to the optimum design and its renormalized version (6) asymptotically exhibits either cyclic or chaotic behaviour. It is within this range of \( \varepsilon \) that improved asymptotic rates of convergence are observed. The behaviour of the asymptotic rate \( R \) is shown in Fig. 1, where we display the asymptotic rates in the case \( \frac{M}{m} = 10 \). In this figure we assume that \( d = 100 \) and all the eigenvalues are equally spaced. We have established numerically that the dependence on the dimension \( d \) is insignificant as long as \( d \geq 10 \). In addition, choosing equally spaced
eigenvalues is effectively the same as choosing eigenvalues uniformly distributed on \([m, M]\) and taking expected values of the asymptotic rates.

The convergence rates of all gradient-type algorithms depend on, amongst other things, the condition number \(\rho = \frac{M}{m}\). As one would expect, an increase in \(\rho\) gives rise to a worsening rate of convergence. Fig. 2 shows the effect of increasing the value of \(\rho\) on the rates of convergence for the steepest descent algorithm with relaxation coefficients \(\varepsilon = 0.9\) and \(\varepsilon = 0.99\).

Any optimization criterion \(\Phi(M(\xi))\) such that \(\frac{\partial \Phi}{\partial \mu^2} > 0\) creates an optimization algorithm of the form (2). Some of these algorithms can be very efficient. For example the family of \(\Phi_p\)-optimality criteria \(\Phi_p(M(\xi)) = (\text{tr} M^{-p}(\xi))^\frac{1}{p}\) creates very efficient optimization algorithms. Another useful generalization of the steepest descent algorithm is the family of so-called \(\alpha\)-root algorithms related to the criteria \(\Phi(M(\xi)) = \mu_2^\alpha - \mu_1^{2\alpha}\). For values of \(\alpha\) slightly larger than 1 the resulting optimization algorithms have been found to be extremely efficient.

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