Block Relaxation Methods in Statistics

Jan de Leeuw

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Note

This book will be expanded/updated frequently and unpredictably. The directory deleeuwpdx.net/pubfolders/stress has a pdf version, the bib file, the complete Rmd file with the code chunks, the R and C source code, and whatever else is needed for perfect reproducibility. Suggestions for improvement of text and code are welcome. All text and code are in the public domain and can be copied and used by anybody in any way they like. Attribution will be appreciated, but is not required.

Just as an aside: “above” in the text refers to anything that comes earlier in the book and “below” refers to anything that comes later. This always confuses me, so I had to write it down. I also number *all* displayed equations. Equations are displayed if and only if they are important, are referred to in the text, or mess up the line spacing.

Preface

Many recent algorithms in computational statistics are variations on a common theme. In this book we discuss four such classes of algorithms. Or, more precisely, we discuss a single large class of algorithms, and we show how various well-known classes of statistical algorithms fit into this common framework. The types of algorithms we consider are, in logical order,

There is not much statistics, in the sense of data analysis or inference, in this book. It is almost exclusively about deterministic optimization problems (although we shall optimize a likelihood function or two). Some of our results have been derived in the statistical literature in the context of maximizing a multinomial or multinormal likelihood function. In most cases statisticians have developed their own results, not relying on the more comprehensive results in the optimization literature. We will try, from the start, to use existing results and apply them to our specific optimization methods.

There are many, many excellent books on optimization and mathematical programming. Without a doubt the canonical reference for statisticians is, and will be for many years to come, the book by Lange (2013). In particular his chapters 7,8, 9, and 12 have substantial overlap with this book. There is even more overlap with the book in progress *MM Optimization Algorithms* (Lange 2016 (in press)).

For the record, the books that have been most useful to me throughout my personal optimization career are Ortega and Rheinboldt (1970a), Ostrowski (1966), Rockafellar (1970), and, above all, Zangwill (1969). They were all published in a five year interval, at the end of the sixties. Around that time also started the ten-year period of my greatest intellectual curiosity and creativity.

Throughout the book we try to present our results in three different lan-

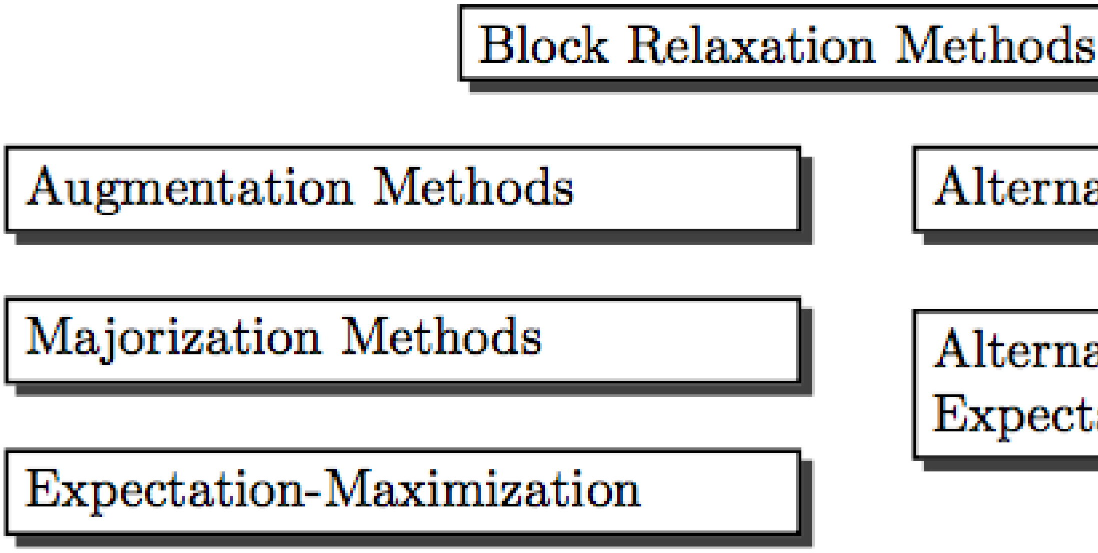


Figure 1: Algorithm Types

guages: the language of mathematics, the language of graphics, and the programming language `R`. We use `R` for all computations, tables, and figures (R Core Team 2016). In fact, all figures and tables are dynamically generated by chunks of `R` code using `knitr` (Xie 2015) and `bookdown` (Xie 2016) .

There are many examples throughout the book. They are usually presented in considerable and sometimes exasperating detail, with code, computations, and figures. I like to work on such examples, so please indulge me. It is nice to have an infinite number of pages available. The examples are mostly in separate subsections, so if you do not like them you can easily skip them.

In many cases the examples are simple one-dimensional optimization problems, which is maybe surprising, because the techniques we discuss are largely intended for high-dimensional problems. To further simplify the examples the functions involved are often cubic or quartic polynomials. Thus these small examples are not particularly representative for the types of applications we are interested in, but they are used to produce nice graphs, a more complete analysis, and illustrations of various general principles and properties. Also it sometimes makes sense to think of the polynomial examples as *models*, in the same sense in which the quadratic is a model for Newton's method.

Many of the remaining examples are taken from multivariate statistical analysis, which we define in the broadest possible sense. It includes data analysis using linear and bilinear algebra, and in particular it includes multidimensional scaling and cluster analysis. Given my history, it is probably not surprising that many examples have their origin in psychometrics, and more specifically in publications of researchers directly or loosely associated with the Data Theory group at Leiden University, starting in 1968. See Van der Heijden and Sijtsma (1996).

We take the point of view in this book that having global convergence of an iterative algorithm, i.e. convergence from an arbitrary starting point, is a desirable property. But it is neither necessary nor sufficient for the usefulness of the algorithm, because in addition one needs information about its speed of convergence. We try to give as much information as possible about *convergence speed* and *complexity* in our presentation of the examples.

It should be noted that this book is a corrected, updated, and expanded version of a twenty-five year old chapter in a conference proceedings volume (J. De Leeuw 1994). It will not be possible to erase all the traces of these humble beginnings. Specifically, references will often be to material from before 1994, and more recent work will probably be less completely covered.

Much of the material in this book is pasted together from published and unpublished papers and reports. This may lead to inconsistencies in the notation and to annoying duplications. Over time I will eliminate these blemishes as much as possible.

Items in the bibliography freely available on the internet are hyperlinked by title to external pdf files. This includes all published and unpublished works authored or co-authored by me. They can also be found in my bibliography of about 750 items, most of them linked to pdf files, on my server gifi.stat.ucla.edu.

Chapter 1

Introduction

1.1 Some History

The methods discussed in this book are special cases of what we shall call *block-relaxation methods*, although other names such as *decomposition* or *nonlinear Gauss-Seidel* or *ping-pong* or *seesaw* methods have also been used. There are many areas of applied mathematics where methods of this type have been discussed. Mostly, of course, in optimization and mathematical programming, but also in control and numerical analysis, and in differential equations.

In this section we shall give some informal definitions to establish our terminology. We will give some of the historical context, but the main historical and technical details will be discussed in subsequent chapters.

In a *block relaxation method* we minimize a real-valued function of several variables by partitioning the variables into blocks. We choose initial values for all blocks, and then minimize over one of the blocks, while keeping all other blocks fixed at their current values. We then replace the values of the active block by the minimizer, and proceed by choosing another block to become active. An iteration ofthe algorithm steps through all blocks in turn, each time keeping the non-active blocks fixed at current values, and each time replacing the active blocks by solving the minimization subproblems. If there are more than two blocks there are different ways to cycle through the blocks. If we use the same sequence of active blocks in each iteration then the block method is called *cyclic*.

In the special case in which blocks consist of only one coordinate we speak of the _ coordinate relaxation method_ or the *coordinate descent* (or *CD*) method. If we are maximizing then it is *coordinate ascent* (or *CA*). The cyclic versions are *CCD* and *CCA*.

Alternating Least Squares (or *ALS*) methods are block relaxation methods in which each minimization subproblem is a linear or nonlinear least squares problem. As far as we know, the term "Alternating Least Squares" was first used in J. De Leeuw (1968). There certainly were ALS methods before 1968, but the systematic use of these techniques in psychometrics and multivariate analysis started around that time. The inspiration clearly was the pioneering work of Kruskal (1964a), Kruskal (1964b) in nonmetric scaling. De Leeuw, Young, and Takane started the ALSOS system of techniques and programs around 1973 (see F. W. Young, De Leeuw, and Takane (1980)), and De Leeuw, with many others, at Leiden University started the Gifi system around 1975 (see Gifi (1990)).

ALS works well for fitting the usual linear, bilinear, and multilinear forms to data. Thus it covers much of classical multivariate analysis and its extensions to higher dimensional arrays. But pretty early on problems arose in Euclidean multidimensional scaling, which required fitting quadratic forms or, even worse, square roots of quadratic forms to data. Straightforward ALS could not be used, because the standard matrix calculations of least squares and eigen decomposition did not apply. Takane, Young, and De Leeuw (1977) circumvented the problem by fitting squared distances using cyclic coordinate descent, which only involved unidimensional minimizations.

Around 1975, however, De Leeuw greatly extended the scope of ALS by using *majorization*. This was first applied to Euclidean multidimensional scaling by J. De Leeuw (1977), but it became clear early on that majorization was a general technique for algorithm construction that also covered, for example, the EM algorithm, which was discovered around the same time (Dempster, Laird, and Rubin (1977)). In each iteration of a majorization algorithm we construct a *surrogate function* (Lange, Hunter, and Yang (2000)) or *majorization* (J. De Leeuw (1994), Heiser (1995)) that lies above the function we are minimizing and touches it in the current iterate. We then minimize this surrogate function to find an update of the current iterate, then construct a new majorization function in that update, and so on. The majorization function, if suitably chosen, can often be minimized using ALS techniques.

J. De Leeuw (1994) argues there is another important class of algorithms extending ALS. It is intermediate, since it is a special case of block relaxation and it contains majorization as a special case. In *augmentation methods* for the minimization of a real valued function we introduce an *augmentation*, which uses an additional vector of variables, with a surrogate function on the product of both sets, such that the original objective function is the minimum of the surrogate function over the augmenting block of variables. We then apply block relaxation to the augmented function.

Ortega and Rheinboldt majorization, Kantorovich, Toland duality, decomposition, quasi-linearization, Marshall-Olkin-Arnold, NIPALS, Moreau coupling functions

block relaxation is majorization

it suffices to study two blocks (in a sense)

1.2 Optimization Methods

Our block relaxation methods look for desirable points, which are usually fixed points of point-to-set maps. They minimize, in a vast majority of the applications, a *loss function* or *badness-of-fit function*, which is often derived from some general data analysis principle such as *Least Squares* or *Maximum Likelihood*. The desirable points are the local or global minimizers of this loss function.

Under certain conditions, which are generally satisfied in statistical applications, our block relaxation methods have *global convergence*, which means that the iterative sequences they generate converge to desirable points, no matter where we start them. They are generally *stable*, which means in this context that each step in the iterative process decreases the loss function value.

Under stronger, but still quite realistic, conditions our block relaxation methods exhibit linear convergence, i.e. the distance of the iterates to the desirable points decreases at the rate of a geometric progression. In many high-dimensional cases the ratio of the progression is actually close to one, which makes convergence very slow, and in some cases the ratio is equal to one and convergence is *sublinear*. We will also discuss stable block relaxation algorithms with *superlinear* convergence, but they are inherently more complicated. In addition we will discuss techniques to accelerate the convergence of block relaxation iterations.

In the optimization and mathematical programming literature, at least until recently, methods with linear convergence rates were generally deprecated or ignored. It was thought they were too slow to be of any practical relevance. This situation has changed for various reasons, all of them having to do with the way in which we now program and compute. Here "we" specifically means statisticians and data analysts, but the same reasons probably apply in other fields as well.

In the first place block relaxation methods often involve simple computations in each of their iterations. As a consequence they can tackle problems with a large number of variables, and they are often easily parallelized. In the second place, with the advent of personal computers it is not necessarily a problem any more to let an iterative process run for days in the background. Mainframe computer centers used to frown on such practices. Third, they are now many specific large problems characterized by a great deal of *sparseness*, which make block and coordinate methods natural alternatives because they can take this sparseness into account. And finally, simple computations in each of the steps make it easy to write ad hoc programs in interpreted special purpose languages such as `R`. Such programs can take the special structure of the problem they are trying to solve into account, and this makes them more efficient compared to general purpose optimization methods which may have faster convergence rates.

Statistics optimization R optimization

Chapter 2

Block Relaxation

2.1 Introduction

The history of block relaxation methods is complicated, because many special cases were proposed before the general idea became clear. I make no claim here to be even remotely complete, but I will try to mention at least most of the general papers that were important along the way.

It makes sense to distinguish the coordinate descent methods from the more general block methods. Coordinate descent methods have the major advantage that they lead to one-dimensional optimization problems, which are generally much easier to handle than multidimensional ones.

We start our history with iterative methods for linear systems. Even there the history is complicated, but it has been ably reviewed by, among others, Forsythe (1953), D. M. Young (1990), Saad and Van der Vorst (2000), Benzi (n.d.), and Axelsson (2010). The origins are in 19th century German mathematics, starting perhaps with a letter from Gauss to his student Gerling on December 26, 1823. See Forsythe (1950) for a translation. To quote Gauss: *"I recommend this method to you for imitation. You will hardly ever again eliminate directly, at least not when you have more than 2 unknowns. The indirect procedure can be done while half asleep, or while thinking about other things."* For discussion of subsequent contributions by Jacobi (1845), Seidel (1874), Von Mises and Pollackzek-Geiringer (1929), we refer to the excellent historical overviews mentioned before, and to the monumental textbooks by

Varga (1962) and D. M. Young (1971).

The next step in our history is the quadratic programming method proposed by Hildreth (1957). Coordinate descent is applied to the dual program, which is a simple quadratic problem with non-negativity constraints, originating from the Lagrange multipliers for the primal problem. Because the constraints are separable in the dual problem the technique can easily handle a large numbers of inequality constraints and can easily be parallelized. Hildreth already considered the non-cyclic greedy and random versions of coordinate descent. A nice historical overview of Hildreth's method and its various extensions is in Dax (2003).

Coordinate relaxation for convex functions, not necessarily quadratic, was introduced by D'Esopo (1959). in an important paper, followed by influential papers of Schechter (1962), Schechter (1968), Schechter (1970). The D'Esopo paper actually has an early version of Zangwill's general convergence theory, applied to functions that are convex in each variable separably and are minimized under separable bound constraints.

Ortega and Rheinboldt (1967), Ortega and Rheinboldt (1970b), Elkin (1968), Céa (1968), Céa (1970), Céa and Glowinski (1973), Auslender (1970), Auslender (1971), Martinet and Auslender (1974) Many of these papers present the method as a nonlinear generalization of the Gauss-Seidel method of solving a system of linear equations.

Modern papers on block-relaxation are by Abatzoglou and O'Donnell (1982) and by Bezdek et al. (1987).

So many more now Spall (2012), Beck and Tetruashvili (1913), Saha and Tewari (2013), Wright (2015)

In Statistics .. Statistical applications to mixed linear models, with the parameters describing the mean structure collected in one block and the parameters describing the dispersion collected in the second block, are in Oberhofer and Kmenta (1974). Applications to exponential family likelihood functions, cycling over the canonical parameters, are in Jensen, Johansen, and Lauritzen (1991). Applications in lasso etc.

2.2 Definition

Block relaxation methods are fixed point methods. A brief general introduction to fixed point methods, with some of the terminology we will use, is in the fixed point section 8.4 of the background chapter.

Let us thus consider the following general situation. We minimize a real-valued function f defined on the product-set $\mathcal{X} = \mathcal{X}_1 \otimes \mathcal{X}_2 \otimes \cdots \otimes \mathcal{X}_p$, where $\mathcal{X}_s \subseteq \mathbb{R}^{n_s}$.

In order to minimize f over $\mathcal{X}$ we use the following iterative algorithm.

Starter:	Start with $x^{(0)} \in \mathcal{X}$.
Step k.1:	$x_1^{(k+1)} \in \underset{x_1 \in \mathcal{X}_1}{\text{argmin}}\ f(x_1, x_2^{(k)}, \cdots, x_p^{(k)}).$
Step k.2:	$x_2^{(k+1)} \in \underset{x_2 \in \mathcal{X}_2}{\text{argmin}}\ f(x_1^{(k+1)}, x_2, x_3^{(k)}, \cdots, x_p^{(k)}).$
...	...
Step k.p:	$x_p^{(k+1)} \in \underset{x_p \in \mathcal{X}_p}{\text{argmin}}\ f(x_1^{(k+1)}, \cdots, x_{p-1}^{(k+1)}, x_p).$
Motor:	$k \leftarrow k + 1$ and go to $k.1$

Observe that we assume that the minima in the substeps exist, but they need not be unique. The argmin's are point-to-set maps, although in many cases they map to singletons. In actual computations we will always have to make a selection from the argmin.

We set $x^{(k)} := (x_1^{(k)}, \cdots, x_p^{(k)})$, and $f^{(k)} := f(x^{(k)})$. The map $\mathcal{A}$ that is the composition of the p substeps on an iteration satisfies $x^{(k+1)} \in \mathcal{A}(x^{(k)})$. We call it the *iteration map* (or the *algorithmic map* or *update map*). If $\mathcal{A}(x)$ is a singleton for all $x \in \mathcal{X}$, then we can write $x^{(k+1)} = \mathcal{A}(x^{(k)})$ without danger of confusion, and call $\mathcal{A}$ the *iteration function.*

If $\mathcal{A}$ is differentiable on $\mathcal{X}$ then we introduce some extra terminology and notation. The matrix $\mathcal{M}(x) := \mathcal{D}\mathcal{A}(x)$ of partial derivatives is called the *Iteration Jacobian* and its spectral radius $\rho(x) := \rho(\mathcal{D}\mathcal{A}(x))$, the eigenvalue of maximum modulus, is called the *Iteration Spectral Radius* or simply the *Iteration Rate.* Note that for a linear iteration $x^{(k+1)} = Ax^{(k)} + b$ we have $\mathcal{M}(x) = A$ and $\rho(x) = \rho(A)$.

The function `blockRelax()` in Code Segment 1 is a reasonable general `R` function for unrestricted block relation in which each $\mathcal{X}_s$ is all of $\mathbb{R}^{n_s}$. The arguments are the function to be minimized, the initial estimate, and the block structure. Both the initial estimate and the block structure are of length $n = \sum n_s$, and block structure is indicated by two elements having the same integer value if and only if they are in the same block. Each of the subproblems is solved by a call to the `optim()` function in `R`.

2.3 First Examples

Our first examples of block relaxation are linear least squares examples. There are obviously historical reasons to choose linear least squares, and in a sense they provide the simplest examples that allow us to illustrate various important calculations and results.

2.3.1 Two-block Least Squares

Suppose we have a linear least squares problems with two sets of predictors A_1 and A_2, and outcome vector b. Matrices A_1 and A_2 are $m \times n_1$ and $m \times n_2$, and the vector of regressions coefficients $x = (x_1 \mid x_2)$ is of length $n = n_1 + n_2$. Without loss of generality we assume $n_1 \leq n_2$.

Minimizing $f(x) = (b - A_1x_1 - A_2x_2)'(b - A_1x_1 - A_2x_2)$ is then conveniently done by block relaxation, alternating the two steps

$$\begin{aligned} x_1^{(k+1)} &= A_1^+(b - A_2x_2^{(k)}), \\ x_2^{(k+1)} &= A_2^+(b - A_1x_1^{(k+1)}). \end{aligned}$$

Here A_1^+ and A_2^+ are Moore-Penrose inverses.

Define

$$\begin{aligned} c &:= A_1^+b, \\ d &:= A_2^+b, \\ R &:= A_1^+A_2, \\ S &:= A_2^+A_1. \end{aligned}$$

Then the iterations are

$$\begin{aligned} x_1^{(k+1)} &= c - Rx_2^{(k)}, \\ x_2^{(k+1)} &= d - Sx_1^{(k+1)}. \end{aligned}$$

A solution $(\hat{x}_1, \hat{x}_2)$ of the least squares problem satisfies

$$\begin{aligned} \hat{x}_1 &= c - R\hat{x}_2, \\ \hat{x}_2 &= d - S\hat{x}_1, \end{aligned}$$

and thus

$$\begin{aligned} (x_1^{(k+1)} - \hat{x}_1) &= R(x_2^{(k)} - \hat{x}_2), \\ (x_2^{(k+1)} - \hat{x}_2) &= S(x_1^{(k+1)} - \hat{x}_1), \end{aligned}$$

and

$$\begin{aligned} (x_2^{(k+1)} - \hat{x}_2) &= SR(x_2^{(k)} - \hat{x}_2), \\ (x_1^{(k+1)} - \hat{x}_1) &= RS(x_1^{(k)} - \hat{x}_1). \end{aligned}$$

The matrices $SR = A_2^+ A_1 A_1^+ A_2$ and $RS = A_1^+ A_2 A_2^+ A_1$ have the same eigenvalues λ_s, equal to ρ_s^2, the squares of the canonical correlations of A_1 and A_2. Consequently $0 \leq \lambda_s \leq 1$ for all s. Specifically there exists a non-singular K of order n_1 and a non-singular L of order n_2 such that

$$\begin{aligned} K'A_1'A_1K &= I_1, \\ L'A_2'A_2L &= I_2, \\ K'A_1'A_2L &= D. \end{aligned}$$

Here I_1 and I_2 are diagonal, with the n_1 and n_2 leading diagonal elements equal to one and all other elements zero. D is a matrix with the non-zero canonical correlations in non-increasing order along the diagonal and zeroes everywhere else. This implies $R = KDL^{-1}$ and $S = LD'K^{-1}$, and consequently $RS = KDD'K^{-1}$ and $SR = LD'DL^{-1}$.

Let us look at the convergence speed of the $x_1^{(k)}$. The results for $x_2^{(k)}$ will be basically the same. Define

$$\delta^{(k)} \triangleq K^{-1}(x_1^{(k)} - \hat{x}_1)$$

It follows, using $RS = KDD'K^{-1}$, that $\delta^{(k)} = \Lambda^k\delta^{(0)}$, with the squared canonical correlations on the diagonal of $\Lambda = DD'$. If $\lambda_+ := \max_i \lambda_i > 0$ and $\mathcal{I} = \{i \mid \lambda_i = \lambda_+\}$ then

$$\frac{\delta_i^{(k)}}{\lambda_+^k} \rightarrow \begin{cases} \delta_i^{(0)} & \text{if } i \in \mathcal{I}, \\ 0 & \text{otherwise} \end{cases}$$

and thus

$$\frac{\|\delta^{(k+1)}\|}{\|\delta^{(k)}\|} \rightarrow \lambda^+.$$

This implies

$$\frac{\|x_1^{(k)} - \hat{x}_1\|}{\lambda^k} \rightarrow \|\sum_{i\in\mathcal{I}} \delta_i^{(0)} k_i\,\|$$

where the k_i are columns of K. In turn this implies

$$\frac{\|x_1^{(k+1)} - \hat{x}_1\|}{\|x_1^{(k)} - \hat{x}_1\|} \rightarrow \lambda.$$

2.3.2 Multiple-block Least Squares

Now suppose there are multiple blocks. We minimize the loss function

$$f(x) = \mathbf{SSQ}(b - \sum_{j=1}^m A_j x_j). \tag{2.1}$$

Block relaxation in this case is *Gauss-Seidel iteration*.

The update formula for the Gauss-Seidel method is

$$\beta_j^{(k+1)} = X_j'\left(y - \sum_{\ell=1}^{j-1} X_\ell \beta_\ell^{(k+1)} - \sum_{\ell=j+1}^{m} X_\ell \beta_\ell^{(k)}\right).$$

Define C_L to be the block triangular matrix with the blocks $X_j'X_\ell$ with $j > \ell$ of C below the diagonal, and C_U the block triangular matrix with the upper diagonal blocks $X_j'X_\ell$ with $j < \ell$. Thus $C_L + C_U + I = C$ and $C_L = C_U'$. Now

$$\beta^{(k+1)} = X'y - C_L\beta^{(k+1)} - C_U\beta^{(k)},$$

and thus

$$\beta^{(k+1)} = (I + C_L)^{-1}X'y - (I + C_L)^{-1}C_U\beta^{(k)}.$$

The least squares estimate $\hat{\beta}$ satisfies

$$\hat{\beta} = (I + C_L)^{-1}X'y - (I + C_L)^{-1}C_U\hat{\beta},$$

and thus

$$\beta^{(k+1)} - \hat{\beta} = -(I + C_L)^{-1}C_U(\beta^{(k)} - \hat{\beta}),$$

or

$$\beta^{(k)} - \hat{\beta} = \left[-(I + C_L)^{-1}C_U\right]^k(\beta^{(0)} - \hat{\beta}).$$

Code in Code Segment 2.

2.4 Generalized Block Relaxation

In some cases, even the supposedly simple minimizations within blocks may not have very simple solutions. In that case, we often use *generalized block relaxation*, which is defined by p maps $\mathcal{A}_s$ mapping $\mathcal{X}$ into (subsets of) $\mathcal{X}$. We have

$$\mathcal{A}_s(x) \in \{x_1\} \otimes \cdots \otimes \{x_{s-1}\} \otimes \mathcal{F}_s(x) \otimes \{x_{s+1}\} \otimes \cdots \otimes \{x_p\},$$

where $z \in \mathcal{F}_s(x$\$ implies

$$f(x_1, \cdots, x_{s-1}, z, x_{s+1}, \cdots, x_p) \leq f(x_1, \cdots, x_{s-1}, x_s, x_{s+1}, \cdots, x_p).$$

In ordinary block relaxation

$$\mathcal{F}_s(x) = \mathop{\mathbf{argmin}}_{z \in \mathcal{X}_s} f(x_1, \cdots, x_{s-1}, z, x_{s+1}, \cdots, x_p),$$

but in generalized block relaxation we could update x_s by taking one or more steps of a stable and convergent iterative algorithm for minimizing $f(x_1, \cdots, x_{s-1}, z, x_{s+1}, \cdots, x_p)$ over $z \in \mathcal{X}_s$.

###Rasch Model{#blockrelaxation:generalizedblockrelaxation:raschmodel}

In the item analysis model proposed by Rasch, we observe a binary $n \times m$ matrix $Y = \{y_{ij}\}$. The (unconditional) log-likelihood is

$$\mathcal{L}(x,z) = \sum_{i=1}^{n}\sum_{j=1}^{m} y_{ij}\log\pi_{ij}(x,z) + (1-y_{ij})\log(1-\pi_{ij}(x,z)),$$

with

$$\pi_{ij}(x,z) = \frac{\exp(x_i+z_j)}{1+\exp(x_i+z_j)}.$$

The negative log-likelihood can be written as

$$f(x,z) = \sum_{i=1}^{n}\sum_{j=1}^{m}\log\{1+\exp(x_i+z_j)\} - \sum_{i=1}^{n} y_{i\star}x_i - \sum_{j=1}^{m} y_{\star j}z_j,$$

where $\star$ indicates summation over an index. The stationary equations have the elegant form

$$\begin{aligned}\pi_{i\star}(x,z) &= y_{i\star}\\ \pi_{\star j}(x,z) &= y_{\star j}.\end{aligned}$$

The standard algorithm for the unconditional maximum likelihood problem (Wainer, Morgan, and Gustafsson (1980)) cycles through these two blocks of equations, using Newton's method at each substep. In this case Newton's method turns out to be

$$x_i^{(k+1)} = x_i^{(k)} - \frac{\pi_{i\star}(x^{(k)},z^{(k)}) - y_{i\star}}{\sum_{j=1}^{m}\pi_{ij}(x^{(k)},z^{(k)})(1-\pi_{ij}(x^{(k)},z^{(k)}))},$$

and similarly for $z_j^{(k+1)}$.

###Nonlinear Least Squares{#blockrelaxation:generalizedblockrelaxation:nonlinearleastsqua

Consider the problem of minimizing

$$\sum_{i=1}^{n}(y_i - \sum_{j=1}^{m}\phi_j(x_i,\theta)\beta_j)^2,$$

with the ϕ_j known nonlinear functions.

Again the parameters separate naturally into two blocks β and θ, and finding the optimal β for given θ is again linear regression.

The best way of finding the optimal θ for given β will typically depend on a more precise analysis of the problem, but one obvious alternative is to linearize the ϕ_j and apply Gauss-Newton.

##Block Order{#blockrelaxation:blockorder}

If there are more than two blocks, we can move through them in different ways. In analogy with linear methods such as Gauss-Seidel and Gauss-Jacobi, we distinguish *cyclic* and *free-steering* methods. We could select the block, for instance, that seems most in need of improvement. This is the *greedy* choice. We can pivot through the blocks in order, and start again when all blocks have been visited. Or we could go back in the reverse order after arriving at the last block. We can even choose blocks in *random order*, or use some other *chaotic* strategy.

We emphasize, however, that the methods we consider are all of the Gauss-Seidel type, i.e. as soon as we upgrade a block we use the new values in subsequent computations. We do not consider Gauss-Jordan type strategies, in which all blocks are updated independently, and then all blocks are replaced simultaneously. The latter strategy leads to fewer computations per cycle, but it will generally violate the monotonicity requirement for the loss function values.

We now give a formalization of these generalizations, due to Fiorot and Huard (1979) Suppose Δ_s are p point-to-set mappings of Ω into $\mathcal{P}(\Omega)$, the set of all subsets of Ω. We suppose that $\omega \in \Delta_s(\omega)$ for all $s = 1, \cdots, p$. Also define

$$\Gamma_s(\omega) \stackrel{\Delta}{=} \text{argmin}\{\psi(\overline{\omega}) \mid \overline{\omega} \in \Delta_s(\omega)\}.$$

There are now two versions of the generalized block-relaxation method which are interesting.

In the free-steering version we set

$$\omega^{(k+1)} \in \cup_{s=1}^{p} \Gamma_s(\omega^{(k)}).$$

This means that we select, from the p subsets defining the possible updates, one single update before we go to the next cycle of updates.

In the cyclic method we set

$$\omega^{(k+1)} \in \otimes_{s=1}^{p} \Gamma_s(\omega^{(k)}).$$

In a little bit more detail this means

$$\begin{aligned}
\omega^{(k,0)} &= \omega^{(k)},\\
\omega^{(k,1)} &\in \Gamma_s(\omega^{(k,0)}),\\
\cdots &\in \cdots,\\
\omega^{(k,p)} &\in \Gamma_s(\omega^{(k,p-1)}),\\
\omega^{(k+1)} &= \omega^{(k,p)}.
\end{aligned}$$

Since $\omega \in \Delta_s(\omega)$, we see that, for both methods, if $\xi \in \Gamma(\omega)$ then $\psi(\xi) \leq \psi(\omega)$. This implies that Theorem **??** continues to apply to this generalized block relaxation method.

A simple example of the Δ_s is the following. Suppose the G_s are arbitrary mappings defined on Ω. They need not even be real-valued. Then we can set

$$\Delta_s(\omega) \stackrel{\Delta}{=} \{\xi \in \Omega \mid G_s(\xi) = G_s(\omega)\}.$$

Obviously $\omega \in \Delta_s(\omega)$ for this choice of Δ_s.

There are some interesting special cases. If G_s projects on a subspace of Ω, then $\Delta(\omega)$ is the set of all ξ which project into the same point as ω. By defining the subspaces using blocks of coordinates, we recover the usual block-relaxation method discussed in the previous section. In a statistical context, in combination with the EM algorithm, functional constraints of the form

$$G_s(\overline{\omega}) = G_s(\omega)$$

were used by Meng and Rubin (1993). They call the resulting algorithm the ECM algorithm.

###Projecting Blocks{#blockrelaxation:blockorder:projectingblocks}

##Rate of Convergence{#blockrelaxation:rateofconvergence}

###LU-form{#blockrelaxation:rateofconvergence:luform}

In block relaxation methods, including generalized block methods, we update $x = (x_1, \cdots, x_n)$ to $y = (y_1, \cdots, y_n)$ by the rule

$$y_s = F_s(y_1, \cdots, y_{s-1}, x_s, x_{s+1}, \cdots, x_n).$$

Differentiation gives

$$\mathcal{D}_t y_s = \sum_{u<s} (\mathcal{D}_u F_s)(\mathcal{D}_t y_u) + \begin{cases} 0 & \text{if } t < s, \\ \mathcal{D}_t F_s & \text{if } t \geq s. \end{cases}. \tag{1}$$

It should be emphasized that in many cases of interest in F_s does not depend on x_s, so that $\mathcal{D}_s F_s = 0$ for all s. It is also important to realize that the derivatives, which we write without arguments in this section, are generally evaluated at points of the form $(y_1, \cdots, y_{s-1}, x_s, \cdots, x_p)$. At fixed points, however, $x_s = y_s$ for all s, and we can just write $\mathcal{D}_t y_s$ without ambiguity. And for our purposes the derivatives at fixed points are the interesting ones.

Now define

$$\mathcal{M} \triangleq \begin{bmatrix} \mathcal{D}_1 y_1 & \mathcal{D}_2 y_1 & \cdots & \mathcal{D}_n y_1 \\ \mathcal{D}_1 y_2 & \mathcal{D}_2 y_2 & \cdots & \mathcal{D}_n y_2 \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}_1 y_n & \mathcal{D}_2 y_n & \cdots & \mathcal{D}_n y_n \end{bmatrix},$$

and

$$\mathcal{N} \triangleq \begin{bmatrix} \mathcal{D}_1 F_1 & \mathcal{D}_2 F_1 & \cdots & \mathcal{D}_n F_1 \\ \mathcal{D}_1 F_2 & \mathcal{D}_2 F_2 & \cdots & \mathcal{D}_n F_2 \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}_1 F_n & \mathcal{D}_2 F_n & \cdots & \mathcal{D}_n F_n \end{bmatrix}.$$

Also

$$\mathcal{N}_L \triangleq \begin{bmatrix} 0 & 0 & \cdots & 0 \\ \mathcal{D}_1 F_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}_1 F_n & \mathcal{D}_2 F_n & \cdots & 0 \end{bmatrix},$$

and

$$\mathcal{N}_U \triangleq \begin{bmatrix} \mathcal{D}_1 F_1 & \mathcal{D}_2 F_1 & \cdots & \mathcal{D}_n F_1 \\ 0 & \mathcal{D}_2 F_2 & \cdots & \mathcal{D}_n F_2 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathcal{D}_n F_n \end{bmatrix},$$

so that $\mathcal{N} = \mathcal{N}_U + \mathcal{N}_L$. From (1)

$$\mathcal{M} = \mathcal{N}_L \mathcal{M} + \mathcal{N}_U,$$

or

$$\mathcal{M} = (I - \mathcal{N}_L)^{-1} \mathcal{N}_U.$$

This is the *Lower-Upper* or *LU form* of the derivative of the algorithmic map.

For two blocks $\mathcal{M}$ is equal to

$$\begin{bmatrix}\mathcal{D}_1F_1 & \mathcal{D}_2F_1\\(\mathcal{D}_1F_2)(\mathcal{D}_1F_1) & (\mathcal{D}_1F_2)(\mathcal{D}_2F_1)+\mathcal{D}_2F_2\end{bmatrix},$$

and if $\mathcal{D}_1F_1=0$ and $\mathcal{D}_2F_2=0$ this is

$$\begin{bmatrix}0 & \mathcal{D}_2F_1\\0 & (\mathcal{D}_1F_2)(\mathcal{D}_2F_1)\end{bmatrix}.$$

Thus the non-zero eigenvalues are the eigenvalues of $(\mathcal{D}_1F_2)(\mathcal{D}_2F_1)$.

###Product Form{#blockrelaxation:rateofconvergence:productform}

There is another way to derive the formulas from the previous section. We use the fact that the algorithmic map $\mathcal{A}$ is a composition of the form

$$\mathcal{A}(x)=\mathcal{A}_p(\mathcal{A}_{p-1}(\cdots(\mathcal{A}_1(x))),$$

where each $\mathcal{A}_s$ leaves all blocks, except block s, intact, and changes only the variables in block s, Thus

$$\mathcal{A}_s(x)=\begin{bmatrix}x_1\\\vdots\\x_{s-1}\\F_s(x_1,\cdots,x_p)\\x_{s+1}\\\vdots\\x_p\end{bmatrix}.$$

Blocks (u,v) of the matrix of partials is (surpressing the dependence on x again for the time being)

$$\{\mathcal{D}\mathcal{A}_s\}_{uv}\triangleq\begin{cases}\mathcal{D}_vF_u & \text{if } u=s,\\I & \text{if } u=v\neq p,\\0 & \text{otherwise.}\end{cases}$$

Again, in many cases of interest we have $\{\mathcal{D}\mathcal{A}\}_{uv}=0$ if $u=v=s$.

Now clearly, from the chain rule,

$$\mathcal{M} = \mathcal{D}\mathcal{A} = \mathcal{D}\mathcal{A}_p\mathcal{D}\mathcal{A}_{p-1}\cdots\mathcal{D}\mathcal{A}_1$$

This is the *product form* of the derivative of the algorithmic map.

For two blocks, and zero diagonal blocks, we have, as in the previous section,

$$\mathcal{M} = \mathcal{D}\mathcal{A}_2\mathcal{D}\mathcal{A}_1 = \begin{bmatrix} I & 0 \\ \mathcal{D}_1F_2 & 0 \end{bmatrix}\begin{bmatrix} 0 & \mathcal{D}_2F_1 \\ 0 & I \end{bmatrix} = \begin{bmatrix} 0 & \mathcal{D}_2F_1 \\ 0 & \mathcal{D}_1F_2\mathcal{D}_2F_1 \end{bmatrix}.$$

Thus the non-zero eigenvalues of $\mathcal{M}$ are the non-zero eigenvalues of $\mathcal{D}_1F_2\mathcal{D}_2F_1$.

In the general cases with p blocks computing eigenvalues of $\mathcal{M}$ we can use the result that the spectrum of $A_pA_{p-1}\cdots A_1$ is related in a straightforward fashion to the spectrum of the cyclic matrix

$$\Gamma(A_1,\cdots,A_p) \triangleq \begin{bmatrix} 0 & 0 & \cdots & 0 & A_p \\ A_1 & 0 & \cdots & 0 & 0 \\ 0 & A_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & A_{p-1} & 0 \end{bmatrix}.$$

In fact if λ is an eigenvalue of $\Gamma(A_1,\cdots,A_p)$ then λ^p is an eigenvalue of $A_pA_{p-1}\cdots A_1$, and if μ is a eigenvalue of $A_pA_{p-1}\cdots A_1$ then the p solutions of $\lambda^p = \mu$ are eigenvalues of $\Gamma(A_1,\cdots,A_p)$.

###Block Optimization Methods{#blockrelaxation:rateofconvergence:blockoptimizationmethods}

The results in the previous two sections were for general block modification methods. We now specialize to block relaxation methods for unconstrained differentiable optimization problems. The rate of convergence of block relaxation algorithms depends on the block structure, and on the matrix of second derivatives of the function f we are minimizing.

The functions F_s that update block s are defined implicitly by

$$\mathcal{D}_sf(x_1,x_2,\cdots,x_p) = 0.$$

From the implicit function theorem

$$\mathcal{D}_tF_s(x) = -[\mathcal{D}_{ss}f(x)]^{-1}\mathcal{D}_{st}f(x).$$

If we use this in the LU-form $\mathcal{M} = (I - B_L)^{-1}B_U$ we find

$$\mathcal{M}(x) = -\begin{bmatrix} \mathcal{D}_{11}f(x) & 0 & \cdots & 0 \\ \mathcal{D}_{21}f(x) & \mathcal{D}_{22}f(x) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}_{p1}f(x) & \mathcal{D}_{p2}f(x) & \cdots & \mathcal{D}_{pp}f(x) \end{bmatrix}^{-1} \begin{bmatrix} 0 & \mathcal{D}_{12}f(x) & \cdots & \mathcal{D}_{1p}f(x) \\ 0 & 0 & \cdots & \mathcal{D}_{2p}f(x) \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix},$$

If there are only two blocks the result simplifies to

$$\mathcal{M}(x) = -\begin{bmatrix} [\mathcal{D}_{11}f(x)]^{-1} & 0 \\ -[\mathcal{D}_{22}f(x)]^{-1}\mathcal{D}_{21}f(x)[\mathcal{D}_{11}f(x)]^{-1} & [\mathcal{D}_{22}f(x)]^{-1} \end{bmatrix} \begin{bmatrix} 0 & \mathcal{D}_{12}f(x) \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -[\mathcal{D}_{11}f(x)]^{-1}\mathcal{D}_{12}f(x) \\ 0 & [\mathcal{D}_{22}f(x)]^{-1}\mathcal{D}_{21}f(x)[\mathcal{D}_{11}f(x)]^{-1}\mathcal{D}_{12}f(x) \end{bmatrix}$$

Thus, in a local minimum, where the matrix of second derivatives is non-negative definite, we find that the largest eigenvalue of $\mathcal{M}(x)$ is like the largest squared canonical correlation ρ of two sets of variables, and is consequently less than or equal to one.

We also see that a sufficient condition for local convergence to a stationary point of the algorithm is that $\rho < 1$. This is always true for an isolated local minimum, because there the matrix of second derivatives is positive definite. If $\mathcal{D}^2f(x)$ is singular at the solution x, we find a canonical correlation equal to $+1$, and we do not have guaranteed linear convergence.

For the product form we find that

$$\mathcal{D}\mathcal{A}_s(x) = I - E_s[\mathcal{D}_{ss}f(x)]^{-1}E_s'\mathcal{D}^2f(x),$$

where E_s has blocks of zeroes, except for block s, which is the identity. Thus

$$\mathcal{M}(x) = \{I - E_s[\mathcal{D}_{ss}f(x)]^{-1}E_s'\mathcal{D}^2f(x)\} \times \cdots \times \{I - E_1[\mathcal{D}_{11}f(x)]^{-1}E_1'\mathcal{D}^2f(x)\}.$$

It follows that $\mathcal{M}(x)z = z$ for all z such that $\mathcal{D}^2f(x)z = 0$. Thus $\rho(\mathcal{M}(z)) = 1$ whenever $\mathcal{D}^2f(x)$ is singular.

For two blocks

$$\mathcal{M}(x) = \begin{bmatrix} I & 0 \\ -[\mathcal{D}_{22}f(x)]^{-1}\mathcal{D}_{21}f(x) & 0 \end{bmatrix} \begin{bmatrix} 0 & -[\mathcal{D}_{11}f(x)]^{-1}\mathcal{D}_{12}f(x) \\ 0 & I, \end{bmatrix}$$

which gives the same result as obtained from the LU-form.

The code in `blockRate.R` in Code Segment 3 computes $\mathcal{M}(x)$ in one of four ways. We can use the analytical form of the Hessian or compute it numerically, and we can use the LU-form or the product form. If we compute the Hessian numerically we give the function we are minimizing as an argument, if we use the Hessian analytically we pass a function for evaluating it at x.

###Block Newton Methods{#blockrelaxation:rateofconvergence:blocknewtonmethods}

In block Newton methods we update using

$$y_s = x_s - [\mathcal{D}_{ss}f(y_1,\cdots,y_{s-1},x_s,\ldots,x_p)]^{-1}\mathcal{D}_s f(y_1,\cdots,y_{s-1},x_s,\ldots,x_p)$$

It follows that at a point x where the derivatives vanish we have

$$\mathcal{D}_t F_s(x) = \delta^{st}I - [\mathcal{D}_{ss}f(x)]^{-1}\mathcal{D}_{st}f(x)$$

and in particular $\mathcal{D}_s F_s(x) = 0$. The iteration matrix $\mathcal{M}(x)$ is the same as the one in section **??**, and consequently the convergence rate is the same as well. We will again have the same rate if we make more than one Newton step in each block update.

Of course the single-step block Newton method does not guarantee decrease of the loss function, and consequently needs to be safeguarded in some way.

###Constrained Problems{#blockrelaxation:rateofconvergence:constrainedproblems}

Similar calculations can also be carried out in the case of constrained optimization, i.e. when the subproblems optimize over differentiable manifolds and/or convex sets. We then use the implicit function calculations on the Langrangean or Kuhn-Tucker conditions, which makes them a bit more complicated, but essentially the same. In the manifold case, for example, it suffices to replace the matrices $\mathcal{D}_{pq}$ by the matrices $H_p'\mathcal{D}_{pq}H_q$, where the matrices H_p contain a local linear coordinate system for Ω_p near the solution.

In this note we look at the special case in which f is differentiable, and the $\mathcal{X}_s$ are of the form

$$\mathcal{X}_s = \{x \in \mathbb{R}^{n_s} \mid G_s(x) = 0\}$$

for some differentiable vector-valued G_s.

The algorithm shows that the update y_s of block s is defined implicitly in terms of $y_1,\cdots,y_{s-1}$ and $x_{s+1},\cdots,x_p$ by the equations

$$\mathbf{D}_s f(y_1,\cdots,y_s,x_{s+1},\cdots,x_p) - \mathbf{D}G_s(y_s)\lambda_s = 0,$$

and

$$G_s(y_s) = 0.$$

The equations also implicitly define the vector λ_s of Lagrange multipliers.

Let us differentiate this again with respect to x. Define

$$\begin{aligned} H_{sr} &= \mathcal{D}^2_{sr} f, \\ U_{sr} &= \mathcal{D}_r y_s, \\ V_{sr} &= \mathcal{D}_r \lambda_s, \end{aligned}$$

as well as

$$W_s(\lambda) = \sum_{r=1} \lambda_r \mathcal{D}^2 g_{sr}$$

and

$$E_s = \mathcal{D}G_s.$$

From the first set of equations we find for all $r > 1$

$$\begin{bmatrix} H_{11} - W_1(\lambda) & -E_1 \\ E_1 & 0 \end{bmatrix} \begin{bmatrix} U_{1r} \\ V_{1r} \end{bmatrix} = \begin{bmatrix} -H_{1r} \\ 0 \end{bmatrix}.$$

which can easily be solved for U_{1r} and V_{1r}.

##Additional Examples{#blockrelaxation:additionalexamples}

###Canonical Correlation{#blockrelaxation:additionalexamples:canonicalcorrelation}

Canonical Correlation is a matrix problem in which the notion of blocks of variables is especially natural. The problem can be formulated in various ways, but we prefer a least squares formulation. We want to minimize

$$\sigma(A, B) \triangleq \mathbf{tr}\ (XA - ZB)'(XA - ZB)$$

over A and B. In order to avoid boring complications which merely lead to more elaborate notations we again suppose that $X'X = I$ and $Z'Z = I$.

Note that this problem is basically a multivariate version of the block least squares problem with $Y = 0$ in the previous example. There are some crucial differences, however. The fact that $Y = 0$ means that $A = B = 0$ trivially minimizes σ. Thus we need to impose some normalization condition such as $A'A = I$ and/or $B'B = I$ to exclude this trivial solution. Nevertheless, in our analysis we shall initially proceed without actually using normalization.

Start with $A^{(0)}$. To find the optimal $B^{(k)}$ for given $A^{(k)}$ we compute $R'A^{(k)} = B^{(k)}$, and then we update A with $RB^{(k)} = A^{(k+1)}$, where $R \overset{\Delta}{=} X'Z$, as before. Thus $A^{(k+1)} = R'RA^{(k)}$ and $A^{(k)} = (R'R)^k A^{(0)}$. Clearly $A^{(k)} \rightarrow 0$ if $R'R \lesssim I$, which implies convergence to the correct, but trivial, solution $A = B = 0$.

Suppose $R'R = K\Lambda K'$ is the eigen-decomposition and define $\Delta^{(k)} \overset{\Delta}{=} K'A^{(k)}$, so that $\Delta^{(k)} = \Lambda^k \Delta^{(0)}$. As in the previous example

$$\frac{\|\Delta^{(k)}\|}{\lambda_+^k} \rightarrow \|\tilde{\Delta}^{(0)}\|,$$

where $\tilde{\Delta}^{(0)}$ consists of the columns corresponding with the dominant eigenvalue. Again

$$\frac{\|\Delta^{(k+1)}\|}{\|\Delta^{(k)}\|} \rightarrow \lambda_+.$$

Now consider

$$\Xi^{(k)} = A^{(k)}((A^{(k)})'A^{(k)})^{-\frac{1}{2}} = \Lambda^k \Delta_0 (\Delta_0' \Lambda^{2k} \Delta_0)^{-\frac{1}{2}}$$

###Low Rank Approximation{#blockrelaxation:additionalexamples:lowrankapproximation}

Given an $n \times m$ matrix X we want to minimize

$$\sigma(A,B) = \text{tr }(X - AB')'(X - AB')$$

over the $n \times p$ matrices A and the $m \times p$ matrices B. In other words, we find the projection of X, in the Frobenius norm, on the set of matrices of rank less than or equal to p.

The block relaxation iterations are

$$\begin{aligned} B^{(k+1)} &= X'A^{(k)}((A^{(k)})'A^{(k)})^{-1} \\ A^{(k+1)} &= XB^{(k+1)}((B^{(k+1)})'B^{(k+1)})^{-1}, \end{aligned}$$

or

$$A^{(k+1)} = \left[XX'A^{(k)}((A^{(k)})'XX'A^{(k)})^{-1}(A^{(k)})'\right] A^{(k)}.$$

$$A^{(k)}(B^{(k+1)})' = P_A^{(k)}X,$$

$$A^{(k+1)}(B^{(k+1)})' = XP_B^{(k+1)},$$

It follows that $(A^{(k)})'(A^{(k+1)} - A^{(k)}) = 0$ and, thus, for all k

$$\|A^{(k+1)} - A^{(k)}\|^2 = \|A^{(k+1)}\|^2 - \|A^{(k)}\|^2 \geq 0.$$

Thus $||A^{(k)}||^2$ increases to a limit less than or equal to the upper bound α. Also

$$\sum_{i=1}^{k} \|A^{(i+1)} - A^{(i)}\|^2 = \|A^{(k+1)}\|^2 - \|A^{(0)}\|^2 \leq \alpha - \|A^{(0)}\|^2,$$

and consequently $\|A^{(i+1)} - A^{(i)}\|$ converges to zero.

Now suppose $\tilde{A}^{(k)} = A^{(k)}S$, with S nonsingular. Then $\tilde{B}^{(k+1)} = B^{(k+1)}S^{-t}$, and thus

$$\tilde{A}^{(k)}(\tilde{B}^{(k+1)})' = A^{(k)}(B^{(k+1)})'.$$

In addition $\tilde{A}^{(k+1)} = A^{(k+1)}S$, and thus

$$\tilde{A}^{(k+1)}(\tilde{B}^{(k+1)})' = A^{(k+1)}(B^{(k+1)})'.$$

Alternative

$$\begin{aligned} B^+ &= X'A, \\ A^+ &= XB^+((B^+)'B^+)^{-1} = XX'A(A'XX'A)^{-1}, \end{aligned}$$

$$\begin{aligned} B^+ &= X'A(A'XX'A)^{-\frac{1}{2}}, \\ A^+ &= XB^+ = XX'A(A'XX'A)^{-\frac{1}{2}}, \end{aligned}$$

$$A^+(B^+)' = X\{X'A(A'XX'A)^{-1}A'X\}$$

###Optimal Scaling with LINEALS{#blockrelaxation:additionalexamples:optimalscalingwith

Suppose we have m categorical variables, where variable j has k_j categories. Also suppose $C_{j\ell}$ are the $k_j \times k_\ell$ cross tables and D_j are the diagonal matrices with univariate marginals. Both the C_{jl} and the D_j are normalized so they add up to one.

A *quantification* of variable j is a k_j element vector y_j, normalized by $e'D_jy_j = 0$ and $y_j'D_jy_j = 1$. If we replace the categories of a variable by the corresponding elements of the quantification vector then the *correlation* between quantified variables j and ℓ is

$$\rho_{j\ell}(y_1,\cdots,y_m)\overset{\Delta}{=}y_j'C_{j\ell}y_\ell.$$

Of course $\rho_{j\ell}(y_1,\cdots,y_m) = \rho_{\ell j}(y_1,\cdots,y_m)$ for all j and ℓ, and $\rho_{jj}(y_1,\cdots,y_m)=1$ for all j.

The *correlation ratio* between variables j and ℓ is

$$\eta^2_{j\ell}(y_1,\cdots,y_m)\overset{\Delta}{=}y_j'C_{jl}D_\ell^{-1}C_{\ell j}y_j.$$

In general $\eta^2_{j\ell}(y_1,\cdots,y_m)\neq\eta^2_{\ell j}(y_1,\cdots,y_m)$, but still $\eta^2_{jj}(y_1,\cdots,y_m)=1$.

Statistical theory, and the Cauchy-Schwartz inequality, tell us that

$$\begin{aligned}\rho^2_{j\ell}(y_1,\cdots,y_m)&\leq\eta^2_{j\ell}(y_1,\cdots,y_m),\\ \rho^2_{j\ell}(y_1,\cdots,y_m)&\leq\eta^2_{\ell j}(y_1,\cdots,y_m),\end{aligned}$$

with equality if and only if

$$\begin{aligned}C_{\ell j}y_j&=\rho_{j\ell}(y_1,\cdots,y_m)D_\ell y_\ell,\\ C_{j\ell}y_\ell&=\rho_{j\ell}(y_1,\cdots,y_m)D_jy_j,\end{aligned}$$

i.e. if and only if the regressions between the quantified variables are both linear.

J. De Leeuw (1988) has suggested to find standardized quantifications in such a way that the loss function

$$f(y_1,\cdots,y_m)\sum_{j=1}^m\sum_{\ell=1}^m(\eta^2_{j\ell}(y_1,\cdots,y_m)-\rho^2_{j\ell}(y_1,\cdots,y_m))$$

is minimized. Thus we try to find quantifications of the variables that linearize all bivariate regressions. A block relaxation method to do just this is implemented in the `lineals` function of the `R` package `aspect` (Mair and De Leeuw (2010)). In `lineals` there is the additional option of requiring that the elements of the y_j are increasing or decreasing.

If we change quantification y_j while keeping all y_ℓ with $\ell\neq j$ at their current values, then we have to minimize

$$y_j'\left\{\sum_{\ell\neq j}C_{jl}\left[D_\ell^{-1}-y_\ell y_\ell'\right]C_{\ell j}\right\}y_j \tag{1}$$

over all y_j with $e'D_jy_j = 0$ and $y_j'D_jy_j = 1$. Thus each step in the cycle amounts to finding the eigenvector corresponding with the smallest eigenvalue of the matrix in (1).

###Multinormal Maximum Likelihood{#blockrelaxation:additionalexamples:multinormalma

The negative log-likelihood for a multinormal random sample is

$$f(\theta, \xi) = n \log \mathbf{det}(\Sigma(\theta)) + \sum_{i=1}^{n} (x_i - \mu(\xi))'\Sigma^{-1}(\theta)(x_i - \mu(\xi)).$$

The vector of means μ depends on the parameters ξ and the matrix of covariances Σ depends on θ. We assume the two sets of parameters are separated, in the sense that they do not overlap.

Oberhofer and Kmenta (1974) study this case in detail and give a proof of convergence, which is actually the expected special case of Zangwill's theorem.

Suppose we have a normal GLM of the form

$$\underline{y} \sim \mathcal{N}[X\beta, \sum_{s=1}^{p} \theta_s \Sigma_s]$$

where the Σ_s are known symmetric matrices. We have to estimate both β and θ, perhaps under the constraint that $\sum_{s=1}^{p} \theta_s \Sigma_s$ is positive semi-definite.

This can be done, in many case, by block relaxation. Finding the optimal β for given θ is just weighted linear regression. Finding the optimal θ for given β is more complicated, but the problem has been studied in detail by Anderson and others.

For further reference, we give the derivatives of the log-likelihood function for this problem.

$$\frac{\partial \mathcal{L}}{\partial \theta_s} = \text{tr } \Sigma^{-1}\Sigma_s - \text{tr } \Sigma^{-1}\Sigma_s\Sigma^{-1}S.$$

$$\frac{\partial^2 \mathcal{L}}{\partial \theta_s \partial \theta_t} = \text{tr } \Sigma^{-1}\Sigma_s\Sigma^{-1}\Sigma_t\Sigma^{-1}S + \text{tr } \Sigma^{-1}\Sigma_t\Sigma^{-1}\Sigma_s\Sigma^{-1}S - \text{tr } \Sigma^{-1}\Sigma_s\Sigma^{-1}\Sigma_t.$$

Taking expected values in Equation **??** gives

$$\mathbf{E}\left\{\frac{\partial^2 \mathcal{L}}{\partial \theta_s \partial \theta_t}\right\} = \text{tr } \Sigma^{-1}\Sigma_s\Sigma^{-1}\Sigma_t.$$

###Array Multinormals{#blockrelaxation:additionalexamples:arraymultinormals}

###Rasch Model{#blockrelaxation:additionalexamples:raschmodel}

The Rasch example has a rather simple structure for the second derivatives of the negative log-likelihood f defined in section @(blockrelaxation:generalizedblockrelaxation:raschmodel).

The elements of $\mathcal{D}_{12}f(x)$ are equal to $\pi_{ij}(x)(1-\pi_{ij}(x))$, while $\mathcal{D}_{11}f(x)$ is a diagonal matrix with the row sums of $\mathcal{D}_{12}f(x)$, and $\mathcal{D}_{22}f(x)$ is a diagonal matrix with the column sums.

This means that computing the eigenvalues of

$$[\mathcal{D}_{11}f(x)]^{-1}\mathcal{D}_{12}f(x)[\mathcal{D}_{22}f(x)]^{-1}\mathcal{D}_{21}f(x)$$

amounts, in this case, to a correspondence analysis of the matrix with elements $\pi_{ij}(x)(1-\pi_{ij}(x))$.The speed of convergence will depend on the maximum correlation, i.e. on the degree in which the off-diagonal matrix $\mathcal{D}_{12}f(x)$ deviates from independence.

##Some Counterexamples{#blockrelaxation:somecounterexamples}

###Convergence to a Saddle{#blockrelaxation:somecounterexamples:convergencetoasaddle}

Convergence, even it occurs, does not need to be towards a minimum. Consider

$$f(x,y)=\frac{1}{6}y^3-\frac{1}{2}y^2x+\frac{1}{2}yx^2-x^2+2x.$$

Perspective and contour plots of this function are in figures 2.1 and 2.2.

The derivatives are

$$\begin{aligned}\mathcal{D}_1f(x,y)&=(y-2)(x-\frac{1}{2}(y+2)),\\ \mathcal{D}_2f(x,y)&=\frac{1}{2}(x-y)^2,\end{aligned}$$

and

$$\mathcal{D}^2f(x,y)=\begin{bmatrix}y-2 & x-y\\ x-y & y-x\end{bmatrix}.$$

Start with $y^{(0)}>2$. Minimizing over x for given $y^{(k)}$ gives

$$x^{(k)}=\frac{1}{2}(y^{(k)}+2),$$

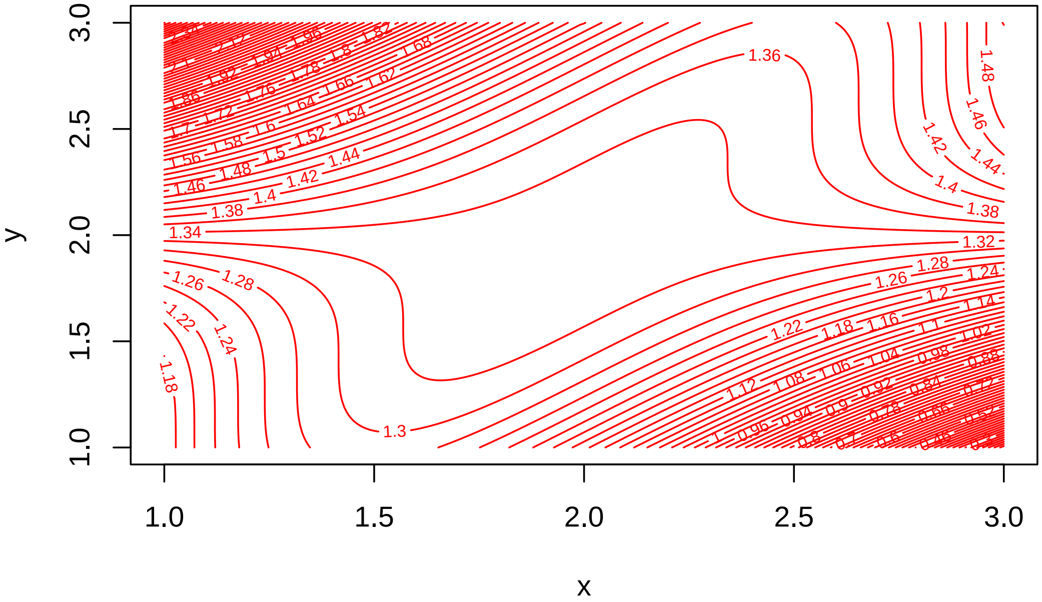


Figure 2.1: Contour Plot Bivariate Cubic

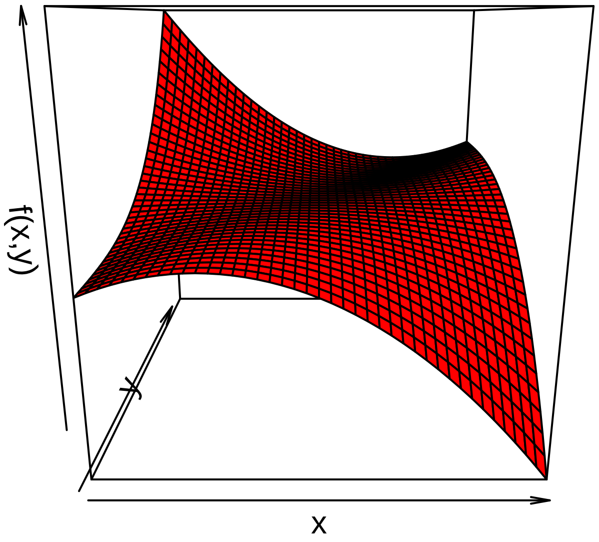


Figure 2.2: Perspective Plot Bivariate Cubic

and minimizing over y for given $x^{(k)}$ gives

$$y^{(k+1)} = x^{(k)}.$$

It follows that

$$\begin{aligned} x^{(k+1)} - 2 &= \frac{1}{2}(x^{(k)} - 2), \\ y^{(k+1)} - 2 &= \frac{1}{2}(y^{(k)} - 2). \end{aligned}$$

Thus both $x^{(k)}$ and $y^{(k)}$ decrease to two with linear convergence rate $\frac{1}{2}$. The function f has a saddle point at $(2, 2)$, and

$$\mathcal{D}^2 f(2,2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

###Convergence to Incorrect Solutions{#blockrelaxation:somecounterexamples:convergencetoincorrec

Convergence needs not be towards a minimum, even if the function is convex. This example is an elaboration of the one in Abatzoglou and O'Donnell (1982).

Let

$$f(a,b) = \max_{x\in[0,1]} \mid x^2 - bx - a \mid.$$

To compute $\min f(a,b)$ we do the usual Chebyshev calculations. If $h(x) \overset{\Delta}{=} bx + a$ and $g(x) \overset{\Delta}{=} x^2 - h(x)$ we must have $g(0) = \epsilon$, $g(y) = -\epsilon$ for some $0 < y < 1$ and $g(1) = \epsilon$. Moreover $g'(y) = 0$. Thus

$$\begin{aligned} -a &= \epsilon, \\ y^2 - by - a &= -\epsilon, \\ 1 - b - a &= \epsilon, \\ 2y - b &= 0. \end{aligned}$$

The solution is $b = 1$, $y = \frac{1}{2}$, $a = -\frac{1}{8}$, and $\epsilon = \frac{1}{8}$. Thus the best linear Chebyshev approximation to x^2 on the unit interval is $x - \frac{1}{8}$, which has function value $f(-\frac{1}{8}, 1) = \frac{1}{8}$,

Now use coordinate decent. Start with $b^{(0)} = 0$. Then

$$a^{(0)} = \underset{a}{\mathbf{argmin}}\, f(a,0) = \frac{1}{2}.$$

and

$$b^{(1)} = \mathop{\mathbf{argmin}}_{b} f(\frac{1}{2}, b) = 0.$$

Thus $b^{(1)} = b^{(0)}$, and we have convergence after a single cycle to a point $(a,b) = (\frac{1}{2}, 0)$ for which $f(\frac{1}{2}, 0) = \frac{1}{2}$.

This example can be analyzed in more in detail. First we compute the best constant (zero degree polynomial) approximation to $h(x) \overset{\Delta}{=} x^2 - bx$. The function h is a convex quadratic with roots at zero and b, with a mimimum equal to $-\frac{1}{4}b^2$ at $x = \frac{1}{2}b$.

We start with the simple rule that the best constant approximation is the average of the maximum and the minimum on the interval. We will redo the calculations later on, using a different and more general approach.

Case A: If $b \leq 0$ then h is non-negative and increasing in the unit interval, and thus $\mathop{\mathbf{argmin}}_{a} f(a,b) = \frac{1}{2}(h(0) + h(1)) = \frac{1}{2}(1 - b)$.

Case B: If $0 \leq b \leq 1$ then h attains its minimum at $\frac{1}{2}b$ in the unit interval, and its maximum at one, thus

$$\mathop{\mathbf{argmin}}_{a} f(a,b) = \frac{1}{2}(h(\frac{1}{2}b) + h(1)) = -\frac{1}{8}b^2 - \frac{1}{2}b + \frac{1}{2}$$

.

Case C: If $1 \leq b \leq 2$ then h still attains its minimum at $\frac{1}{2}b$ in the unit interval, but now the maximum is at zero, and thus $\mathop{\mathbf{argmin}}_{a} f(a,b) = \frac{1}{2}(h(\frac{1}{2}b) + h(0)) = -\frac{1}{8}b^2$.

Case D: If $b \geq 2$ then h is non-positive and decreasing in the unit interval, and thus again $\mathop{\mathbf{argmin}}_{a} f(a,b) = \frac{1}{2}(h(0) + h(1)) = \frac{1}{2}(1 - b)$.

We can derive the same results, and more, by using a more general approach. First

$$f(a,b) = \max\left\{\max_{0 \leq x \leq 1}(x^2 - a - bx), -\min_{0 \leq x \leq 1}(x^2 - a - bx)\right\}.$$

Since $x^2 - a - bx$ is convex, we see

$$f(a,b) = \max\left\{-a, 1 - a - b, -\min_{0 \leq x \leq 1}(x^2 - a - bx)\right\}.$$

Now $x^2 - a - bx$ has a minimum at $x = \frac{1}{2}b$ equal to $-a - \frac{1}{4}b^2$. This is the minimum over the closed interval if $0 \leq b \leq 2$, otherwise the minimum occurs at one of the boundaries. Thus

$$\min_{0\leq x\leq 1}(x^2 - a - bx) = \begin{cases} -a - \frac{1}{4}b^2 & \text{if } 0 \leq b \leq 2, \\ \min(-a, 1 - a - b) & \text{otherwise,} \end{cases}$$

and

$$f(a,b) = \begin{cases} \max\{1 - a - b, a + \frac{1}{4}b^2\} & \text{if } 0 \leq b \leq 1, \\ \max\{-a, a + \frac{1}{4}b^2\} & \text{if } 1 \leq b \leq 2, \\ \max\{|a|, |1 - a - b|\} & \text{otherwise.} \end{cases}$$

It follows that

$$\mathop{\mathbf{argmin}}_{a} f(a,b) = \begin{cases} \frac{1}{2} - \frac{1}{2}b - \frac{1}{8}b^2 & \text{if } 0 \leq b \leq 1, \\ -\frac{1}{8}b^2 & \text{if } 1 \leq b \leq 2, \\ \frac{1}{2}(1 - b) & \text{otherwise.} \end{cases}$$

It is more complicated to compute $\mathop{\mathbf{argmin}}_{b} f(a,b)$, because the corresponding Chebyshev approximation problem does not satisfy the Haar condition, and the solution may not be unique.

We make the necessary calculations, starting from the left. Define $g_1(b) \triangleq \max\{|a|, |1 - a - b|\}$. For $b \leq 0$ we have $f(a,b) = g_1(b)$. Define $b_- \triangleq (1 - a) - |a|$ and $b_+ \triangleq (1 - a) + |a|$. Then

$$g_1(b) = \begin{cases} (1 - a) - b & \text{if } b \leq b_-, \\ |a| & \text{if } b_1 < b < b+, \\ b - (1 - a) & \text{if } b \geq b_+. \end{cases}$$

Note that $b_+ > 0$ for all a. If $b_- < 0$ then g_1 has a minimum equal to $-b_-$ for all b in $[b_-, 0]$. Now $b_- < 0$ if and only if $a > \frac{1}{2}$. Thus for $a > \frac{1}{2}$ we have

$$\mathop{\mathbf{Arg\,min}}_{b} f(a,b) = [(1 - a) - |a|, 0].$$

Switch to $g_2(b) \triangleq \max\{1 - a - b, a + \frac{1}{4}b^2\}$. For $0 \leq b \leq 1$ we have $f(a,b) = g_2(b)$. We have $1 - a - b > a + \frac{1}{4}b^2$ if and only if $\frac{1}{4}b^2 + b + (2a - 1) < 0$. The discriminant of this quadratic is $2(1 - a)$, which means that if $a > 1$ we have $g_2(b) = a + \frac{1}{4}b^2$ everywhere. If $a < 1$ define b_- and b_+ as the two roots $-2 \pm 2\sqrt{2(1-a)}$ of the quadratic. Now

$$g_2(b) = \begin{cases} 1 - a - b & \text{if } b_- \leq b \leq b_+, \\ a + \frac{1}{4}b^2 & \text{otherwise.} \end{cases}$$

Clearly $b_- < 0$. If $a > \frac{1}{2}$ then also $b_+ < 0$ and thus $g_2(b) = a + \frac{1}{4}b^2$ on $[0,1]$. If $0 < b_+ < 1$ then g_2 has a minimum at b_+. Thus if $-\frac{1}{8} < a < \frac{1}{2}$ we have

$$\underset{b}{\mathbf{argmin}}\, f(a,b) = 2 + 2\sqrt{2(1-a)}.$$

Next $g_3(b) \overset{\Delta}{=} \max\{-a, a + \frac{1}{4}b^2\}$, which is equal to $f(a,b)$ for $1 \leq b \leq 2$. If $a > 0$ then $g_3(b) = a + \frac{1}{4}b^2$ everywhere. If $a < 0$ define b_- and b_+ as $\pm\sqrt{-8a}$. Then

$$g_3(b) = \begin{cases} -a & \text{if } b_- \leq b \leq b_+, \\ a + \frac{1}{4}b^2 & \text{otherwise.} \end{cases}$$

If $1 < b_+ < 2$ then we have a minimum of g_3 at b_+. Thus if $-\frac{1}{2} < a < -\frac{1}{8}$ we find

$$\underset{b}{\mathbf{argmin}}\, f(a,b) = \sqrt{-8a}.$$

And finally we get back to g_1 again at the right hand side of the real line. We have a minimum if $b_+ > 2$, i.e. $a < -\frac{1}{2}$. In that case

$$\underset{b}{\mathbf{Arg\,min}}\, f(a,b) = [2, (1-a) + |a|]$$

So, in summary,

$$\underset{b}{\mathbf{Arg\,min}}\, f(a,b) = \begin{cases} [(1-a) - |a|, 0] & \text{if } a > \frac{1}{2}, \\ \{2 + 2\sqrt{2(1-a)}\} & \text{if } -\frac{1}{8} < a < \frac{1}{2}, \\ \{\sqrt{-8a}\} & \text{if } -\frac{1}{2} < a < -\frac{1}{8}, \\ [2, (1-a) + |a|] & \text{if } a < -\frac{1}{2}. \end{cases}$$

We now have enough information to write a simple coordinate descent algorithm. Of course such an algorithm would have to include a rule to select from the set of minimizers if the minimers are not unique. In our `R` implementation in `ccd.R` we allow for different rules. If the minimizers are an interval, we always choose the smallest point, or always to largest point, or always the midpoint, or a uniform draw from the interval. We shall see in our example that these different options have a large influence on the approximation the algorithm converges too, in fact even on what the algorithm considers to be desirable points.

Insert ccd.R Here

We give the function that transforms

$$b^{(k)}$$

into

$$b^{(k+1)}$$

with the four different selection rules in Figure 1.

Insert upMe.R Here

The function is in red, the line $b^{(k+1)} = b^{(k)}$ in blue. Thus over most of the region of interest the algorithm does not change the slope, which means it converges in a single iteration to an incorrect solution. It needs more iterations only for the midpoint and random selection rules if started outside $[0, 2]$.

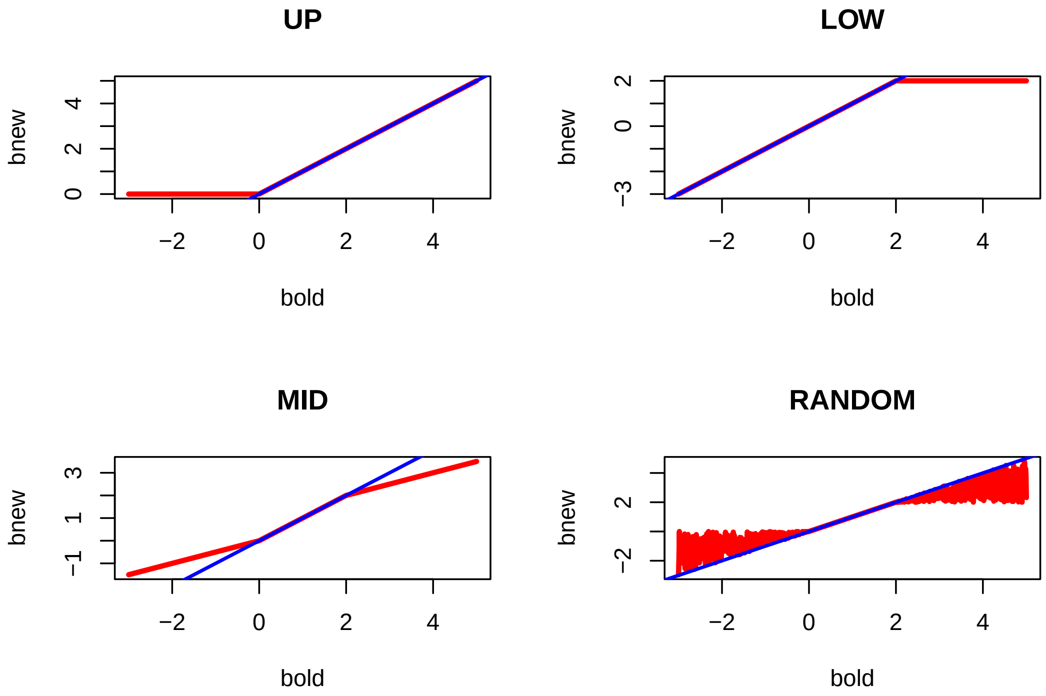


Figure 1: The UP, LOW, MID and RANDOM rules

###Non-convergence and Cycling{#blockrelaxation:somecounterexamples:nonconvergencean

Coordinate descent may not converge at all, even if the function is differentiable.

There is a nice example, due to Powell (1973). It is somewhat surprising that Powell does not indicate what the source of the problem is, using Zangwill's convergence theory. The reason seems to be that the mathematical programming community has decided, at an early stage, that linearly convergent algorithms are not interesting and/or useful. The recent developments in statistical computing suggest that this is simply not true.

Powell's example involves three variables, and the function

$$\psi(\omega)=\frac{1}{2}\omega' A\omega+\mathrm{dist}^2(\omega,\mathcal{K}),$$

where

$$a_{ij}=\begin{cases}-1 & \text{if } i\neq j,\\ 0 & \text{if } i=j,\end{cases}$$

and where $\mathcal{K}$ is the cube

$$\mathcal{K} = \{\omega \mid -1 \leq \omega_i \leq +1\},$$

The derivatives are

$$\mathcal{D}\psi = A\omega + 2(\omega - \mathcal{P}_{\mathcal{K}}(\omega)).$$

In the interior of the cube $\mathcal{D}\psi = A\omega$, which means that the only stationary point in the interior is the saddle point at $\omega = 0$. In general at a stationary point we have $(A + 2\mathcal{I})\omega = \mathcal{P}_{\mathcal{K}}(\omega))$, which means that we must have $u'\mathcal{P}_{\mathcal{K}}(\omega)) = 0$. The only points where the derivatives vanish are saddle points. Thus the only place where there can be minima is on the surface of the cube.

Also for $x = y = z = t > 1$ we see that $\psi(x, y, z) = -3t^2 + 3(t-1)^2 = 3 - 6t$, which is unbounded. For $x = y = t > 1$ and $z = -t$ we find

$$\psi(x, y, z) = -t^2 + 3(t-1)^2 = 2t^2 - 6t + 3.$$

This has its minimum -1.5 at $t = 1.5$ and it has a root at $t = \frac{1}{2}(3 + \sqrt{12}) = 4.9641$.

Let us apply coordinate descent. A search along the x-axis finds the optimum at $+1 + \frac{1}{2}(y+z)$ if $y + z > 0$ and at $-1 + \frac{1}{2}(y+z)$ if $y + z < 0$. If $y + z = 0$ the minimizer is any point in $[-1, +1]$.

This guarantees that the partial derivative with respect to x is zero. The other updates are given by symmetry. Thus, if we start from

$$(-1 - \epsilon, 1 + \frac{1}{2}\epsilon, -1 - \frac{1}{4}\epsilon),$$

with ϵ some small positive number, then we generate the following sequence.

$$\begin{bmatrix} (+1 + \frac{1}{8}\epsilon, & +1 + \frac{1}{2}\epsilon, & -1 - \frac{1}{4}\epsilon) \\ (+1 + \frac{1}{8}\epsilon, & -1 - \frac{1}{16}\epsilon, & -1 - \frac{1}{4}\epsilon) \\ (+1 + \frac{1}{8}\epsilon, & -1 - \frac{1}{16}\epsilon, & +1 + \frac{1}{32}\epsilon) \\ (-1 - \frac{1}{64}\epsilon, & -1 - \frac{1}{16}\epsilon, & +1 + \frac{1}{32}\epsilon) \\ (-1 - \frac{1}{64}\epsilon, & +1 + \frac{1}{128}\epsilon, & +1 + \frac{1}{32}\epsilon) \\ (-1 - \frac{1}{64}\epsilon, & +1 + \frac{1}{128}\epsilon, & -1 - \frac{1}{256}\epsilon) \end{bmatrix}$$

But the sixth point is of the same form as the starting point, with ϵ replaced by $\frac{\epsilon}{64}$. Thus the algorithm will cycle around six edges of the cube. At these edges the gradient of the function is bounded away from zero, in fact two of the partials are zero, the others are ±2. The function value is +1. The other two edges of the cube, i.e. $(+1,+1,+1)$ and $(-1,-1,-1)$ are the ones we are looking for, because there the function value is -3, the global minimum. At these two points all three partials are ±2.

Powell gives some additional examples which show the same sort of cycling behaviour, but are somewhat smoother.

###Sublinear Convergence{#blockrelaxation:somecounterexamples:sublinearconvergence}

Convergence can be sublinear.

$$\begin{aligned}
\psi(\omega,\xi)&=(\omega-\xi)^2+\omega^4,\\
\mathcal{D}_1\psi(\omega,\xi)&=2(\omega-\xi)+4\omega^3,\\
\mathcal{D}_2\psi(\omega,\xi)&=-2(\omega-\xi),\\
\mathcal{D}_{11}\psi(\omega,\xi)&=2+12\omega^2,\\
\mathcal{D}_{12}\psi(\omega,\xi)&=-2,\\
\mathcal{D}_{22}\psi(\omega,\xi)&=2.
\end{aligned}$$

It follows that coordinate descent updates $\omega^{(k)}$ by solving the cubic $\omega-\omega^{(k)}+2\omega^3=0$. The sequence converges to zero, and by l'Hopitål's rule

$$\lim_{k\rightarrow\infty}\frac{\omega^{(k+1)}}{\omega^{(k)}}=1.$$

This leads to very slow convergence. The reason is that the matrix of second derivatives of ψ is singular at the origin.

#Coordinate Descent{#coordinatedescent}

##Introduction{#coordinatedescent:introduction}

We discuss coordinate descent and ascent in a separate chapter, because it is a very important special case of block relaxation, with many really interesting examples.

##Convergence rate{#coordinatedescent:convergencerate}

The product form of the derivative of the algorithmic map for coordinate descent is

$$\mathcal{M}(x)=\left[I-\frac{e_pe_p'\mathcal{D}^2f(x)}{e_p'\mathcal{D}^2f(x)e_p}\right]\times\cdots\times\left[I-\frac{e_1e_1'\mathcal{D}^2f(x)}{e_1'\mathcal{D}^2f(x)e_1}\right],$$

where the e_s are unit vectors (all elements zero, except for element s, which is equal to one).

##Examples{#coordinatedescent:examples}

###The Cartesian Folium{#coordinatedescent:examples:thecartesianfolium}

The "folium cartesii' ' (letter of Descartes to Mersenne, August 23, 1638) is the function

$$f:\mathbb{R}^2\rightarrow\mathbb{R}$$

defined by

$$f(x,y)=x^3+y^3-3xy.$$

The gradient is

$$\mathcal{D}f(x,y)=\begin{bmatrix}3x^2-3y\\3y^2-3x\end{bmatrix},$$

and the Hessian is

$$\mathcal{D}^2f(x,y)=\begin{bmatrix}6x&-3\\-3&6y\end{bmatrix}.$$

It follows that $f(x,y)$ has a saddle point at $(0,0)$ and an isolated local minimum at $(1,1)$. These are the only two stationary points. At $(0,0)$ the eigenvalues of the Hessian are $+3$ and -3, at $(1,1)$ they are 9 and 3.

The Hessian is singular if and only if (x,y) is on the hyperbola $xy=\frac{1}{4}$. It is positive definite if and only if (x,y) is above the branch of the hyperbola in the positive orthant.

See Figure 1 for contour plots of sections of f on two different scales.

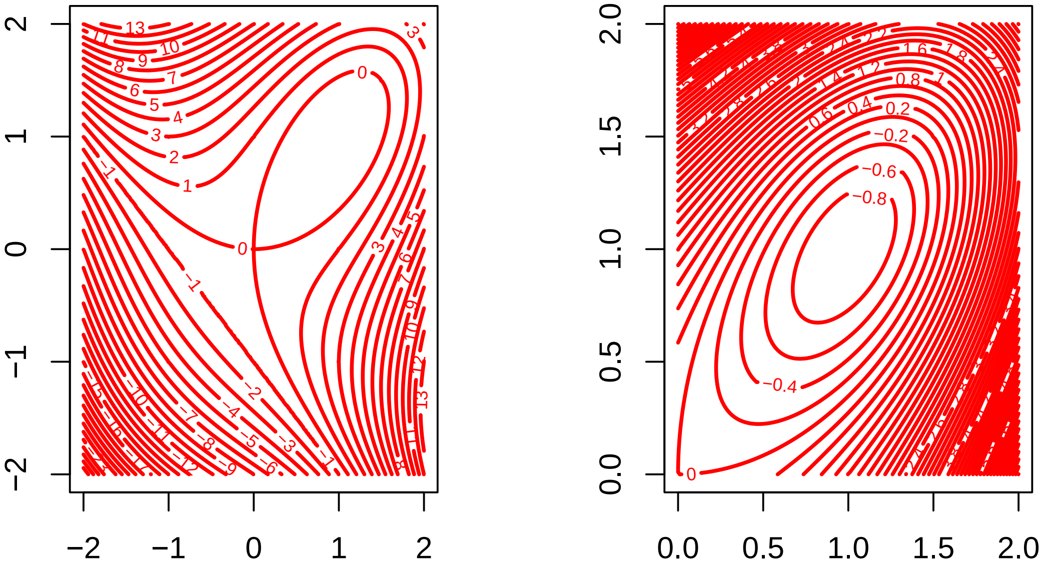


Figure 1: Folium, two scales, two sections

Now apply coordinate descent (J. De Leeuw (2007b)). The minimum over x for fixed y only exists if $y > 0$, in which case it is attained at $\sqrt{y}$. In the same way, the minimum over y for fixed $x > 0$ is attained at $\sqrt{x}$. Thus the algorithm is simply

$$
\begin{aligned}
x^{(k+1)} &= \sqrt{y^{(k)}},\\
y^{(k+1)} &= \sqrt{x^{(k+1)}},
\end{aligned}
$$

and the algorithmic map is

$$
\mathcal{A}(x,y) = \begin{bmatrix}\sqrt{y}\\ \sqrt[4]{y}\end{bmatrix}.
$$

The algorithm can only work if we start with $y^{(0)} > 0$. It then converges, linearly and monotonically, to $(1,1)$ with convergence rate $\frac{1}{4}$. If we start with $y^{(0)} \leq 0$ then $x^3 + (y^{(0)})^3 - 3xy^{(0)}$ is unbounded below and thus coordinate descent fails.

###A Family of Quadratics{#coordinatedescent:examples:afamilyofquadratics}

This example shows some of the properties of coordinate relaxation. We want to minimize

$$
\psi_\lambda(x,y) = \frac{1}{2}x^2 + \frac{1}{2}y^2 - \lambda xy.
$$

For each λ this is a quadratic in x and y. If we fix y and λ, the resulting function is a convex quadratic in x. And if we fix x and λ, the resulting function is a convex quadratic in y. Thus coordinate relaxation can always be carried out, with a unique minimum in each substep.

The partials are given by

$$\begin{aligned}\frac{\partial\psi_\lambda}{\partial x} &= x - \lambda y,\\ \frac{\partial\psi_\lambda}{\partial y} &= y - \lambda x,\end{aligned}$$

and the Hessian is the matrix

$$\begin{bmatrix}1 & -\lambda\\ -\lambda & 1\end{bmatrix}.$$

Thus the eigenvalues of the Hessian are $1+\lambda$ and $1-\lambda$.

If $-1 < \lambda < +1$ then the function has a unique isolated minimum equal to zero at $(0,0)$. If $\lambda = +1$ it has a minimum equal to zero on the line $x-y=0$ and if $\lambda = -1$ it has a minimum equal to zero on the line $x+y=0$. If $\lambda^2 > 1$ the unique stationary point at $(0,0)$ is a saddle point, and there are no minima or maxima.

Coordinate relaxation gives the algorithm

$$\begin{aligned}y^{(k+1)} &= \lambda x^{(k)} = \lambda^2 y^{(k)},\\ x^{(k+1)} &= \lambda y^{(k+1)} = \lambda^2 x^{(k)},\end{aligned}$$

or

$$\begin{aligned}x^{(k)} &= \lambda^{2k} x^{(0)},\\ y^{(k)} &= \lambda^{2k-1} x^{(0)}.\end{aligned}$$

Thus we have convergence to $(0,0)$ if and only if $\lambda^2 < 1$. In that case convergence is linear, with rate λ^2, Convergence is immediate, to $(x^{(0)}, x^{(0)})$ or $(x^{(0)}, -x^{(0)})$, if $\lambda^2 = 1$.

For the function values we have

$$\psi^{(k)} = \frac{1}{2}(1-\lambda^2)\lambda^{4k-2}[x^{(0)}]^2,$$

If $\lambda^2 > 1$ then the function values $\psi^{(k)}$ decrease, and diverge to $-\infty$. Also, $(x^{(k)}, y^{(k)})$ diverges to infinity. By defining $\tilde{\psi} = \exp\psi$, we easily change the problem into an equivalent one with the same iterates, for which function values converge to zero, but since $(x^{(k)}, y^{(k)})$ is the same sequence as before it still diverges to infinity.

Note that

$$\frac{\psi^{(k+1)}}{\psi^{(k)}} = \lambda^4,$$

while

$$\frac{x^{(k+1)}}{x^{(k)}} = \frac{y^{(k+1)}}{y^{(k)}} = \lambda^2.$$

Thus function values converge twice as fast as the coordinates of the solution vector.

###Loglinear Models{#coordinatedescent:examples:loglinearmodels}

Let

$$\mathcal{L}(\theta) = \sum_{k=1}^{K} n_k \log \lambda_k(\theta) - \lambda_k(\theta),$$

be a Poisson-log-likelihood with

$$\lambda_k(\theta) = \exp \sum_{j=1}^{m} x_{kj}\theta_j.$$

We see that

$$\mathcal{D}_j\mathcal{L}(\theta) = \sum_{k=1}^{n} n_k x_{kj} - \sum_{k=1}^{n} \lambda_k(\theta) x_{kj},$$

and

$$\mathcal{D}_{j\ell}\mathcal{L}(\theta) = -\sum_{k=1}^{n} \lambda_k(\theta) x_{kj} x_{k\ell}.$$

Thus the log-likelihood is concave. Normally we would apply a safe-guarded version of Newton's method, but here we want to illustrate CCA.

Now suppose $X = \{x_{kj}\}$ is a design-type matrix, with elements equal to 0 or 1. Let

$$\mathcal{K}_j \triangleq \{k \mid x_{kj} = 1\}.$$

Then the likelihood equations are

$$\sum_{k\in\mathcal{K}_j} n_k = \sum_{k\in\mathcal{K}_j} \lambda_k(\theta).$$

Solving each of these in turn is CCA (since we are maximizing), which is also known in this context as the *iterative propertional fitting* or *IPF* algorithm.

We have, using e_j for the coordinate directions,

$$\lambda_k(\theta+\tau e_j)=\begin{cases}\lambda_k(\theta) & \text{if } k\notin\mathcal{K}_j,\\ \mu\lambda_k(\theta) & \text{if } k\in\mathcal{K}_j,\end{cases}$$

with $\mu=\exp\tau$. This explains the name of the algorithm, because the λ_k in $\mathcal{K}_j$ are adjusted with the same proportionality factor.

Thus the optimal μ is simply

$$\mu=\frac{\sum_{k\in\mathcal{K}_j}n_k}{\sum_{k\in\mathcal{K}_j}\lambda_k(\theta)}.$$

This example can be extended to the case in which the elements of the design matrix are $-1,0$, and $+1$. We define

$$\mathcal{K}_j^+\triangleq\{k\mid x_{kj}=1\},$$

and

$$\mathcal{K}_j^-\triangleq\{k\mid x_{kj}=-1\}.$$

We now have to solve the quadratic equation

$$\mu^2\sum_{k\in\mathcal{K}_j^+}\lambda_k(\theta)-\mu\Delta_j-\sum_{k\in\mathcal{K}_j^-}\lambda_k(\theta)=0,$$

with

$$\Delta_j\triangleq\sum_{k\in\mathcal{K}_j^+}n_k-\sum_{k\in\mathcal{K}_j^-}n_k$$

for the proportionality factor. If $\mathcal{K}_j^-=\emptyset$ then

$$\mu=\frac{\sum_{k\in\mathcal{K}_j^+}n_k}{\sum_{k\in\mathcal{K}_j^+}\lambda_k(\theta)}$$

as before. If $\mathcal{K}_j^+=\emptyset$ then

$$\mu=\frac{\sum_{k\in\mathcal{K}_j^-}\lambda_k(\theta)}{\sum_{k\in\mathcal{K}_j^-}n_k}$$

If the positive and negative index sets are both nonempty, then the quadratic always has one positive and one negative root, and we select the positive one.

Basically the same CCA/IPF technique can also be applied if the elements of X are arbitrary integers. To avoid trivialities we assume each column of X has at least one non-zero element. In that case solving for μ amounts to solving a higher degree polynomial equation. Suppose the non-zero elements of column j of X are from a set $\mathcal{I}_j$ of integers. Elements of $\mathcal{I}_j$ can be positive or negative. Define

$$\begin{aligned}\overline{n}_{ij} &\triangleq \sum\{n_k \mid x_{kj} = i\},\\ \overline{\lambda}_{ij}(\theta) &\triangleq \sum\{\lambda_k(\theta) \mid x_{kj} = i\}.\end{aligned}$$

Also define

$$\Delta_j \triangleq \sum_{i\in\mathcal{I}_j} i\overline{n}_{ij}.$$

To find the optimal μ for coordinate j we must solve $g_j(\mu) = \Delta_j$, where

$$g_j(\mu) \triangleq \sum_{i\in\mathcal{I}_j} \mu^i i\overline{\lambda}_{ij}(\theta).$$

Note that $\mathcal{D}g_j(\mu) > 0$ for all $\mu > 0$, i.e. g_j is strictly increasing. Let i_j^+ be the maximum of the $i \in \mathcal{I}_j$ and let i_j^- be the minimum. We can distinguish three different behaviors of g_j on the positive reals.

1. If $i_j^- > 0$ then g_j increases from 0 to $+\infty$.
2. If $i_j^+ < 0$ then g_j increases from $-\infty$ to 0.
3. If $i_j^- < 0$ and $i_j^+ > 0$ then g_j increases from $-\infty$ to $+\infty$.

In all three cases there is a unique positive root of the equation $g_j(\mu) = \Delta_j$. To solve we note that if $i_j^- > 0$ we need to find the unique positive real root of a polynomial of degree i_j^+. If $i_j^+ < 0$ we solve the equation for $\frac{1}{\mu}$, again finding the unique positive real root of a polynomial of degree $-i_j^-$. In case 3, in which $\mathcal{I}_j$ has both negative and positive elements, we multiply both sides of the equation by $\mu^{-i_j{}^-}$ to get

$$\sum_{i\in\mathcal{I}_j} \mu^{i-i_j{}^-} i\overline{\lambda}_{ij}(\theta) = \Delta_j\mu^{-i_j{}^-},$$

which is a polynomial equation of degree $i_j^+ - i_j^-$, again with a single positive real root. I have written an `R` program for this general case. The function `polyLogLinF()` does the computations, the function `polyLogLin()` is the driver for the iterations.

Insert polyLoglin.R Here

Consider the example with

```
> x
      [,1] [,2] [,3] [,4]
 [1,]    1    1   -1    0
 [2,]    1    1    1    0
 [3,]    1    1   -1    0
 [4,]    1    2    1    0
 [5,]    1    2   -1    0
 [6,]    1    2    1   -1
 [7,]    1    3   -1   -1
 [8,]    1    3    1   -1
 [9,]    1    3   -1   -1
[10,]    1    0    1   -1
```

and `n` equal to `1:10`. We find, for the final iterations,

```
Iteration:   34 fold:    4.83068380 fnew:    4.83068066
Iteration:   35 fold:    4.83068066 fnew:    4.83067878
Iteration:   36 fold:    4.83067878 fnew:    4.83067765
Iteration:   37 fold:    4.83067765 fnew:    4.83067697
$lbd
 [1] 3.049407 2.988786 3.049407 2.925556 2.984896 7.968232 7.957861 7.799660
 [9] 7.957861 8.316384

$f
[1] 4.830677

$theta
[1]  1.12628967 -0.02138247 -0.01004005 -1.00197798
```

Note that if we say

```
polyLogLin(n,x+3)
```

then we find the same solution, although much more slowly,

```
Iteration:  428 fold:    4.83072092 fnew:    4.83071986
Iteration:  429 fold:    4.83071986 fnew:    4.83071882
Iteration:  430 fold:    4.83071882 fnew:    4.83071780
Iteration:  431 fold:    4.83071780 fnew:    4.83071681
$lbd
 [1] 3.049790 2.993221 3.049790 2.932093 2.987506 7.967771 7.952558 7.805050
 [9] 7.952558 8.303460

$f
[1] 4.830717

$theta
[1]  1.053848982 -0.020633792 -0.009361352 -0.999688396
```

###Rayleigh Quotient{#coordinatedescent:examples:rayleighquotient}

The problem is to minimize the Rayleigh quotient

$$\lambda(x)=\frac{x'Ax}{x'Bx}$$

over all x. Here A and B are known matrices, with B positive definite.

If we update x to $\tilde{x}=x+\theta e_i$, with e_i a unit vector, then

$$\lambda(\tilde{x})=\frac{\theta^2a_{ii}+2\theta x'a_i+x'Ax}{\theta^2b_{ii}+2\theta x'b_i+x'Bx}.$$

Think of this as a continous rational function γ of the single variable θ, which we have to minimize. Clearly γ has a horizontal asymptote, with

$$\lim_{\theta\rightarrow+\infty}\gamma(\theta)=\lim_{\theta\rightarrow-\infty}\gamma(\theta)=\frac{a_{ii}}{b_{ii}}.$$

Also

$$\mathcal{D}\gamma(\theta)=\frac{2Q(\theta)}{P^2(\theta)},$$

with

$$P(\theta) \overset{\Delta}{=} \theta^2 b_{ii} + 2\theta x'b_i + x'Bx,$$

and

$$Q(\theta) \overset{\Delta}{=} \theta^2(a_{ii}x'b_i - b_{ii}x'a_i) + \theta(a_{ii}x'Bx - b_{ii}x'Ax) + (x'a_ix'Bx - x'b_ix'Ax).$$

In addition

$$\mathcal{D}^2\gamma(\hat{\theta}) = 2\frac{P^2(\theta)\mathcal{D}Q(\theta) - Q(\theta)\mathcal{D}P^2(\theta)}{P^4(\theta)},$$

and thus $\mathbf{sign}(\mathcal{D}\gamma(\theta)) = \mathbf{sign}(Q(\theta))$ and at values where $Q(\theta) = 0$ we have $\mathbf{sign}(\mathcal{D}^2\gamma(\theta)) = \mathbf{sign}(\mathcal{D}Q(\theta))$.

We now distinguish three cases. 1. First, γ can be a constant function, everywhere equal to $\frac{a_{ii}}{b_{ii}}$. This happens only if $x = 0$ or $x = e_i$, which makes $Q(\theta) = 0$ for all θ. In this case we do not update, and just go to the next i. 2. Second, Q can have a zero quadratic term. If we make sure that $\frac{x'Ax}{x'Bx} < \frac{a_{ii}}{b_{ii}}$ then the unique solution of the linear equation $Q(\theta) = 0$ satisfies $\mathcal{D}^2\gamma(\theta) > 0$, and consequently corresponds with the unique minimum of γ. Updating x guarantees that we will have $\frac{x'Ax}{x'Bx} < \frac{a_{ii}}{b_{ii}}$ for all subsequent iterations. If we happen to start with or wind up in a point with a zero quadratic term and with $\frac{x'Ax}{x'Bx} > \frac{a_{ii}}{b_{ii}}$ then γ does not have a minimum and coordinate descent fails. 3. If Q is a proper quadratic then γ is either increasing at both infinities or decreasing at both infinities. In the first case, when Q is a convex quadratic, γ increases from the horizontal asymptote to the maximum, then decreases to the minimum, and then increases again to the horizontal asymptote. In the second case, with Q a concave quadratic, γ decreases from the horizontal asymptote to the minimum, then increases to the maximum, and then decreases again to the horizontal asymptote. In either case it has two extremes, one minimum and one maximum, corresponding to the roots of the quadratic Q. This also shows that if Q is a proper quadratic, then it always has two distinct real roots.

Here is some simple code to illustrate the cases distinguished above. We have a simple function to compute λ.

Insert fRayleigh.R Here

Case 2, with the zero quadratic term, and Case 3, the proper quadratic, are illustrated with

```
a <-  matrix (-1, 3, 3)
diag (a) <- 1
b <-  diag (3)
x <- c(1, 1, -1)
zseq <- seq (-8, 8, length = 100)
png("myOne.png")
plot (zseq, fRayleigh (zseq, 1, x, a, b),type="l",cex=3,col="RED",xlab="theta"
abline(h=a[1,1] / b[1,1])
dev.off()
x <- c(1,0,1)
png("myTwo.png")
plot (zseq, fRayleigh (zseq, 2, x, a, b),type="l",cex=3,col="RED",xlab="theta"
abline(h=a[2,2] / b[2,2])
dev.off()
```

For Case 2 we see that

$$\gamma$$

has no minimum, and CCD fails. For Case 3, which is of course the usual case, there are no problems.

Insert Figure 1 here

Insert Figure 2 here

The coordinate descent method can obviously take sparseness into account, and it can easily be generalized to separable constraints on the elements of x, such as non-negativity. Note that it also can be used to *maximize* the Rayleigh quotient, simply by taking the other root of the quadratic. Or, alternatively, we can interchange A and B.

Insert gevCCA.R Here

The second derivative of the Rayleigh quotient at a stationary point normalized by $x'Bx = 1$ is simply

$$\mathcal{D}^2\lambda(x) = 2(A - \lambda(x)B).$$

This is singular and thus the product form of the derative of the algorithmic map has largest eigenvalue equal to one, corresponding with the eigenvector

x. Singularity of the Hessian is due, of course, to the fact that λ is homogenous of degree zero, and rescaling x does not change the value of the objective function. We can use this to our advantage. Suppose we normalize x to $x'Bx = 1$, after each coordinate descent cycle. This will not change the function values computed by the algorithm, but is changes the algorithmic map. The derivative of the modified map is

$$\overline{\mathcal{M}}(x) = (I - yy'B)\mathcal{M}(x),$$

which has the same eigenvalues and eigenvectors as $\mathcal{M}(x)$, except for $\overline{\mathcal{M}}(x)x = 0$, while $\mathcal{M}(x)x = 1$.

###Squared Distance Scaling{#coordinatedescent:examples:squareddistancescaling}

In ALSCAL [Takane, Young, De Leeuw, 1977] we find multidimensional scaling solutions by minimizing the loss function *sstress*, defined by

$$\sigma_2(X) \triangleq \frac{1}{2}\sum_{i=1}^n\sum_{j=1}^n w_{ij}(\delta_{ij} - d_{ij}^2(X))^2.$$

Thus known dissimilarities δ_{ij} are approximated by squared Euclidean distances between points, which have coordinates in an $n \times p$ matrix X. Both dissimilarities $\Delta = \{\delta_{ij}\}$ and the weights $W = \{w_{ij}\}$ are non-negative, symmetric, and hollow. Thus

$$d_{ij}^2(X) = \sum_{s=1}^p (x_{is} - x_{js})^2.$$

Takane et al. discuss different block relaxation approaches to minimizing σ_2. Because the loss function is a multivariate quartic the stationary equations obtained by setting the partials equal to zero are a system of np cubic equations in np unknowns. So, at least theoretically, we could use algebraic methods to solve the stationary equations and find the global minimum of *sstress*. This corresponds with the case in which there is only a single block of coordinates, but in the ALSCAL context other blocks are introduced by optimally transforming the dissimilarities and by incorporating weights for individual difference MDS models. At the other extreme of the block relaxation spectrum we could introduce np blocks for the np coordinates, which means we would use coordinate descent. Takane et al. ultimately decide to use a generalized block relaxation method with n blocks of the p coordinates

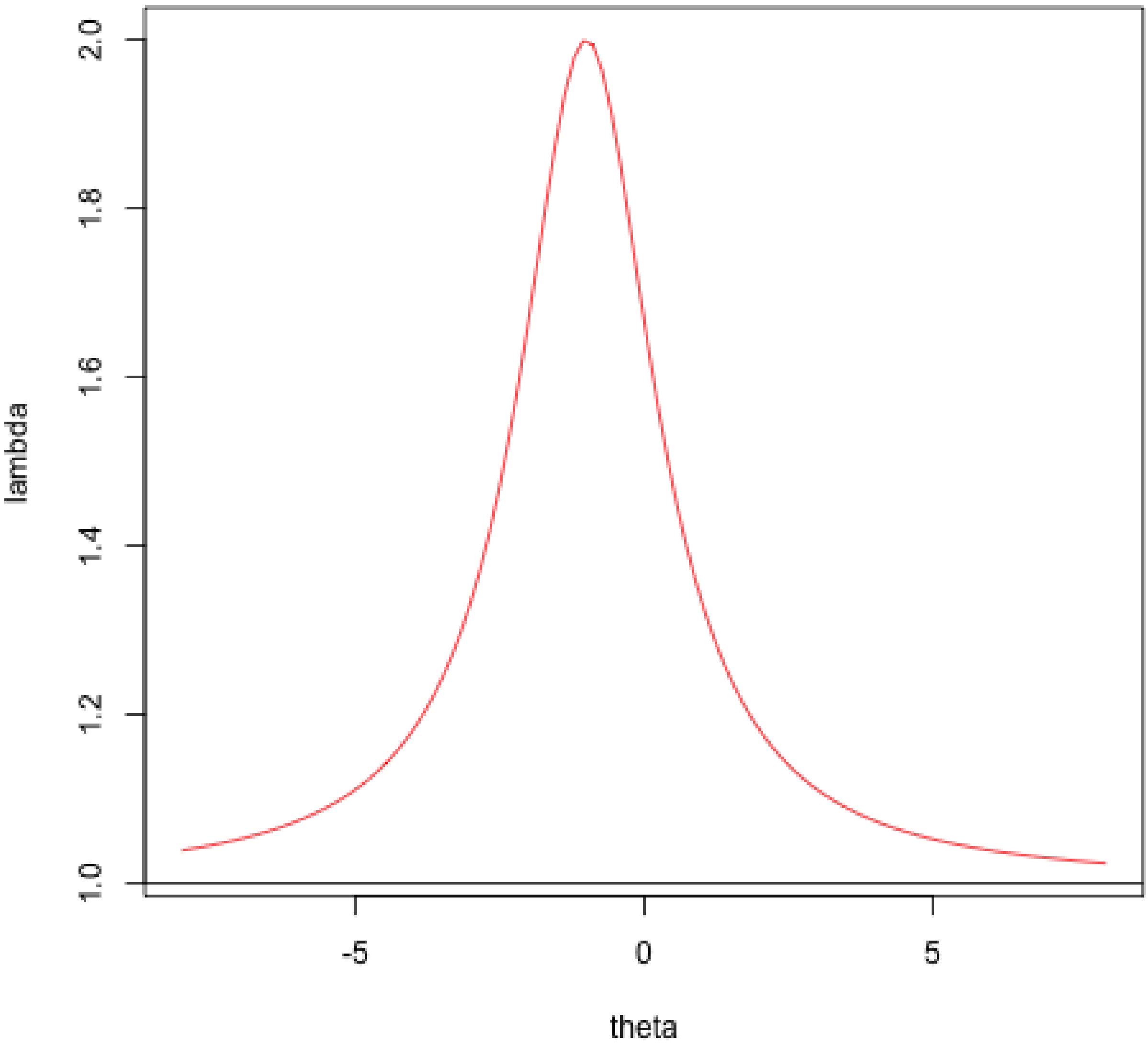


Figure 2.3: Case 2 – CCA Fails

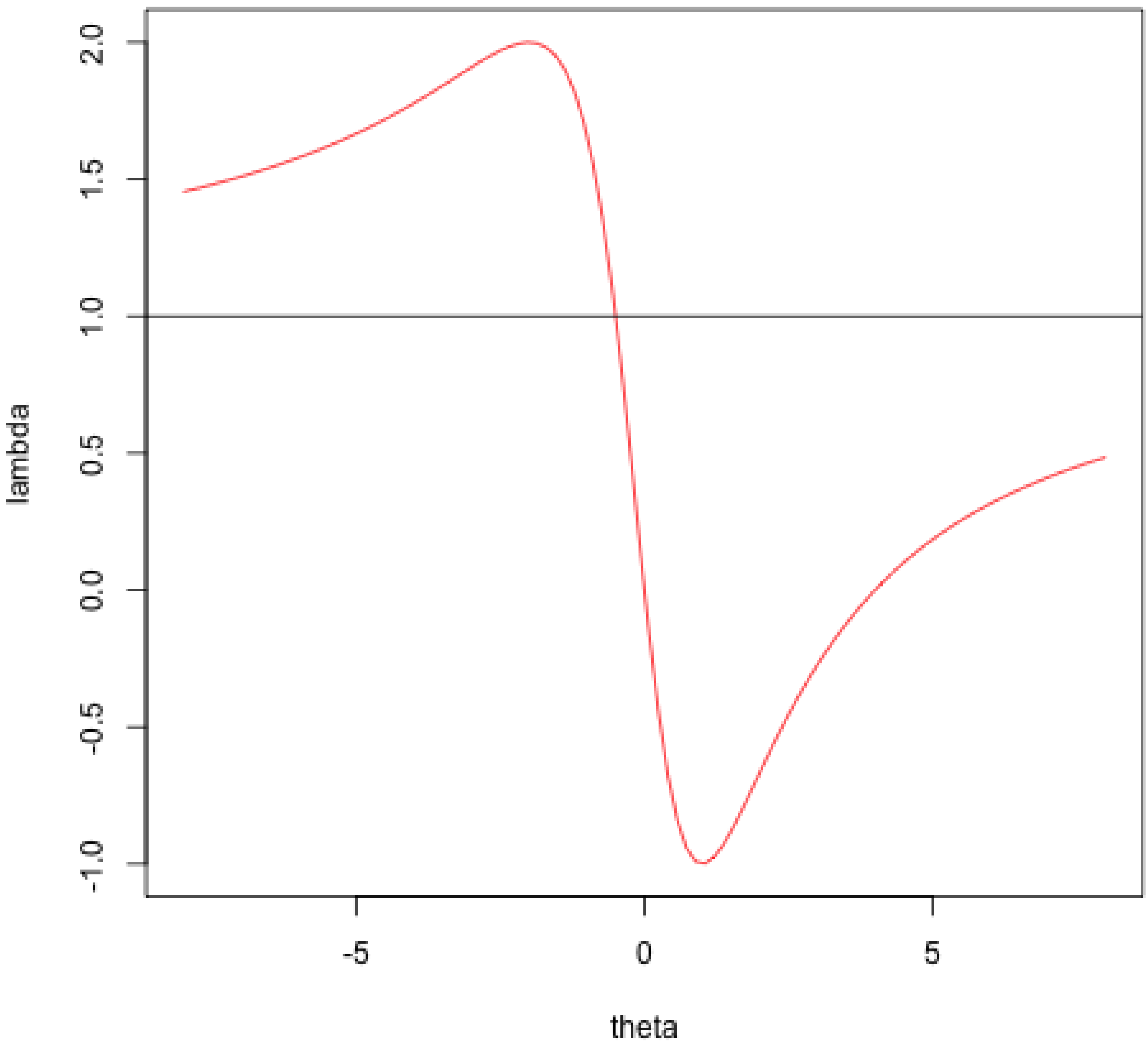


Figure 2.4: Case 3 – CCA Works

of a single point, with a safeguarded Newton method used to minimize over a single block.

In this section we study coordinate descent in detail. If we modify coordinate (k,t) then only the squared distances d_{ik}^2 and d_{ki}^2 with $i \neq k$ will change. Adding θ to x_{kt} with change d_{ik}^2 to $d_{ik}^2 - 2\theta(x_{it} - x_{kt}) + \theta^2$. Thus the part of *sstress* that depends on θ is

$$\sum_{i=1}^n w_{kj}((\delta_{kj} - d_{ik}^2) + 2\theta(x_{it} - x_{kt}) - \theta^2)^2.$$

Differentiating this and setting the derivative to zero gives the cubic equation

$$\sum_{i=1}^n w_{kj}((\delta_{kj} - d_{ik}^2) + 2\theta(x_{it} - x_{kt}) - \theta^2)((x_{it} - x_{kt}) - \theta) = 0$$

$$\begin{aligned}\sum_{i=1}^n w_{kj}(\delta_{kj} - d_{ik}^2)(x_{it} - x_{kt}) + 2\theta\sum_{i=1}^n w_{kj}(x_{it} - x_{kt})^2 - \theta^2\sum_{i=1}^n w_{kj}(x_{it} - x_{kt})\\ - \theta\sum_{i=1}^n w_{kj}(\delta_{kj} - d_{ik}^2) + 2\theta^2\sum_{i=1}^n w_{kj}(x_{it} - x_{kt}) - \theta^3\sum_{i=1}^n w_{kj}\end{aligned}$$

###Least Squares Factor Analysis{#coordinatedescent:examples:leastsquaresfactoranalysis}

#Alternating Least Squares{#alternatingleastsquares}

##Introduction{#alternatingleastsquares:introduction}

An *Alternating Least Squares* or *ALS* algorithm is defined as a block relaxation algorithm applied to a least squares loss function. Least squares loss functions are somewhat loosely defined. We will discuss what we have in mind, before giving some of the history of ALS methods.

We start with have a functions f of the form

$$f(x) = \sum_{j=1}^m \sum_{\ell=1}^m w_{j\ell} g_j(x) g_\ell(x),$$

where W is an $m \times m$ fixed positive semi-definite matrix of *weights*, and we minimize f over $x \in \mathcal{X}$.

One obvious property of least squares loss functions is that they are bounded below by zero, which means that a decreasing sequence of loss function values $f^{(k)} = f(x^{(k)})$, generated for example by an iterative algorithm, necessarily converges.

Alternating least squares methods by definition use block relaxation, so we introduce a block structure. As usual the block structure is designed to make the minimization subproblems relatively easy to solve. A first step towards simplicity is to

$$f(x_1, \cdots, x_p) = \sum_{j=1}^m \sum_{\ell=1}^m w_{j\ell} g_j(x_1, \cdots, x_p) g_\ell(x_1, \cdots, x_p),$$

which must be minimized over $x_s \in \mathcal{X}_s$, where $\mathcal{X} = \mathcal{X}_1 \otimes \cdots \otimes \mathcal{X}_p$. To make the problem interesting for block optimization we have separated the constraints on x into separate constraints on the n blocks x_i.

In many ALS examples there is additional structure. A familar special case has the form

$$f(x_1, x_2) = \sum_{j=1}^m \sum_{\ell=1}^m w_{j\ell}(g_j(x_1) - h_j(x_2))(g_\ell(x_1) - h_\ell(x_2))$$

Of course x_1 and x_2 can be further partitioned into blocks if that is convenient. Even more structure is introduced into the ALS problem when the functions g_j and h_j are polynomials or multilinear functions.

As explained in section 1.1 the term *Alternating Least Squares* was first used in J. De Leeuw (1968). There certainly were ALS methods before 1968. Examples are the missing data methods in factorial analysis of variance pioneered by Yayes (1933), the iterative principal factor analysis method of Thomson (1934), or the MINRES method for factor analysis by Harman and Jones (1966). The systematic use of ALS techniques in psychometrics and multivariate analysis started after the pioneering work of Kruskal (1964a), Kruskal (1964b), Kruskal (1965) in nonmetric multidimensional scaling. De Leeuw, Young, and Takane started the ALSOS system of techniques and programs around 1973 (see F. W. Young, De Leeuw, and Takane (1980)), and De Leeuw, with many others, at Leiden University started the Gifi system around 1975 (see Gifi (1990)).

##Close Relatives{#alternatingleastsquares:closerelatives}

###ALSOS{#alternatingleastsquares:closerelatives:alsos}

ALSOS algorithms are ALS algorithms in which one or more of the blocks defines transformations of variables.

$$f(x,z)=\sum_{j=1}^m\sum_{\ell=1}^m w_{j\ell}g_j(x_1,\cdots,x_p,z)g_\ell(x_1,\cdots,x_p,z).$$

Suppose we have n observations on two sets of variables x_i and y_i. We want to fit a model of the form

$$F_\theta(\Phi(x_i))\approx G_\xi(\Psi(y_i))$$

where the unknowns are the structural parameters θ and ξ and the transformations Φ and Ψ. In ALS we measure loss-of-fit by

$$\sigma(\theta,\xi,\Phi,\Psi)=\sum_{i=1}^n[F_\theta(\Phi(x_i))-G_\xi(\Psi(y_i))]^2.$$

This loss function is minimized by starting with initial estimates for the transformations, minimizing over the structural parameters, keeping the transformations fixed at their current values, and then minimizing over the transformations, with structural values kept fixed at their new values. These two minimizations are alternated, which produces a nonincreasing sequence of loss function values, bounded below by zero, and thus convergent. This is a version of the trivial convergence theorem.

The first ALS example is due to Kruskal (1965). We have a factorial ANOVA, with, say, two factors, and we minimize

$$\sigma(\phi,\mu,\alpha,\beta)=\sum_{i=1}^n\sum_{j=1}^m[\phi(y_{ij})-(\mu+\alpha_i+\beta_j)]^2.$$

Kruskal required ϕ to be monotonic. Minimizing loss for fixed ϕ is just doing an analysis of variance, minimizing loss over ϕ for fixed μ,α,β is doing a *monotone regression*. Obviously also some normalization requirement is needed to exclude trivial zero solutions.

This general idea was extended by De Leeuw, Young, and Takane around 1975 to

$$\sigma(\phi;\psi_1,\cdots,\psi_m)=\sum_{i=1}^n[\phi(y_i)-\sum_{s=1}^p\psi_j(x_{ij})]^2.$$

This ALSOS work, in the period 1975-1980, is summarized in F. W. Young, De Leeuw, and Takane (1980). Subsequent work, culminating in the book by Gifi (1990) generalized this to ALSOS versions of principal component analysis, path analysis, canonical analysis, discriminant analysis, MANOVA, and so on. The classes of transformations over which loss was minimized were usually step-functions, splines, monotone functions, or low-degree polynomials. To illustrate the use of more sets in ALS, consider

$$\sigma(\psi_1,\cdots,\psi_m;\alpha,\beta)=\sum_{i=1}^n\sum_{j=1}^m(\psi_j(x_{ij})-\sum_{s=1}^p\alpha_{is}\beta_{js})^2.$$

This is principal component analysis (or partial singular value decomposition) with optimal scaling. We can now cycle over three sets, the transformations, the component scores α_{is} and the component loadings β_{js}. In the case of monotone transformations this alternates monotone regression with two linear least squares problems.

###ACE{#alternatingleastsquares:closerelatives:ace}

The ACE methods, developed by Breiman and Friedman (1985), minimize over all *smooth* functions.

A problem with ACE is that smoothers, at least most smoothers, often do not minimize a loss function, or the same loss function as is used for the remaining parameters.

In any case, ACE is less general than ALS, because not all least squares problems can be interpreted as computing conditional expectations.

Another obviously related area in statistics is the Generalized Additive Models discussed extensively by Hastie and Tibshirani (1990).

###NIPALS and PLS{#alternatingleastsquares:closerelatives:nipalsandpls}

##Rate of Convergence{#alternatingleastsquares:rateofconvergence}

The least squares loss function, in the most general form we consider here, is

$$f(x)=\frac{1}{2}\sum_{j=1}^m\sum_{\ell=1}^m w_{j\ell}g_j(x)g_\ell(x),$$

with W a fixed symmetric positive semi-definite matrix of weights.

Thus

$$\mathcal{D}f(x)=\sum_{j=1}^m\sum_{\ell=1}^m w_{j\ell}g_j(x)\mathcal{D}g_\ell(x),$$

and

$$\mathcal{D}^2f(x)=\sum_{j=1}^m\sum_{\ell=1}^m w_{j\ell}\left\{g_j(x)\mathcal{D}^2g_\ell(x)+\mathcal{D}g_j(x)(\mathcal{D}g_\ell x)'\right\}.$$

Note: Older piece follows (fix) 03/12/15

It is easy to apply the general results from the previous sections to ALS. The results show that it is important that the solutions to the subproblems are unique. The least squares loss function has some special structure in its second derivatives which we can often exploit in a detailed analysis. If

$$\sigma(\omega,\xi)=\sum_{i=1}^n(f_i(\omega)-g_i(\xi))^2,$$

then

$$\mathcal{D}^2\sigma=\begin{bmatrix}S_1&0\\0&S_2\end{bmatrix}+\begin{bmatrix}G'G&-G'H\\-H'G&H'H\end{bmatrix},$$

with G and H the Jacobians of f and g, and with S_1 and S_2 weighted sums of the Hessians of the f_i and g_i, with weights equal to the least squares residuals at the solution. If S_1 and S_2 are small, because the residuals are small, or because the f_i and g_i are linear or almost linear, we see that the rate of ALS will be the canonical correlation between G and H.

##Examples{#alternatingleastsquares:examples}

###Homogeneity Analysis{#alternatingleastsquares:examples:homogeneityanalysis}

###Fixed Rank Approximation{#alternatingleastsquares:examples:fixedrankapproximation}

###Multilinear Fitting{#alternatingleastsquares:examples:multilinearfitting}

2.4.1 MCR-ALS

###Scaling and Splitting{#alternatingleastsquares:examples:scalingandsplitting}

Early on in the development of ALS algorithms some interesting complications where discovered. Let us consider canonical correlation analysis with optimal scaling. There we want to minimize

$$\sigma(X,Y,A,B)=\text{tr }(XA-YB)'(XA-YB),$$

where the X and the Y are optimally scaled or transformed variables. This problem is analyzed in detail in Van der Burg and De Leeuw (1983). This seems like a perfectly straightforward ALS problem. It can be formulated as a problem with the two blocks (X, Y) and (A, B), or as a problem with the four blocks X, Y, A, B. But no matter how one formulates it, a normalization must be chosen to prevent trivial solutions. In the spirit of canonical analysis it makes sense to require $A'X'XA = \mathcal{I}$ or $B'Y'YB = \mathcal{I}$. Both sets of conditions basically lead to the same solution, but in the intermediate iterations the normalization condition creates a problem, because it involves elements from two different blocks. Also, although $A'X'XA = \mathcal{I}$ is a simple constraint on A for given X, it is not such a simple constraint on X for given $A.

The solution to this dilemma, basically due to Takane, is to constrain either (X, A) or (Y, B), always update the unconstrained block, and switch normalizations after each update. Global convergence (at least of loss function values) is guaranteed by the following analysis.

Theorem 1:

$$\min_A \min_{B'Y'YB=\mathcal{I}} \sigma(X, Y, A, B) = \min_{A'X'XA=\mathcal{I}} \min_B \sigma(X, Y, A, B) = \sum_{s=1}^{p}(1-\rho_s^2(X, Y)).$$

Proof:

$$\min_A \sigma(X, Y, A, B) = \text{ tr } B'Y'YB - B'Y'X(X'X)^{-1}X'YB,$$

and minimizing the right-hand side over $B'Y'YB = \mathcal{I}$ clearly proves the first part of the Theorem. The second part goes the same. **QED**

#Augmentation and Decomposition Methods

##Introduction

We take up the historical developments. Alternating Least Squares was useful for many problems, but it some cases it was not powerful enough to do the job. Or, to put it differently, the subproblems were still too complicated to be efficiently solved a large number of times. In order to solve some additional least squares problems, we can use *augmentation*. We first illustrate this with some examples.

The examples show that augmentation is somewhat of an art (like integration). The augmentation is in some cases not obvious, and there are no mechanical rules. The idea of adding variables that augment the problem to a simpler one is very general. It is also at the basis, for instance, of the Lagrange multiplier method.

##Definition

Formalizing augmentation is straightforward. Suppose f is a real valued function, defined for all $x\in\mathcal{X}$, where $\mathcal{X}\subseteq\mathbb{R}^n$. Suppose there exists another real valued function g, defined on $\mathcal{X}\otimes\mathcal{Y}$, where $\mathcal{Y}\subseteq\mathbb{R}^m$, such that

$$f(x)=\min_{y\in\mathcal{Y}} g(x,y).$$

We also suppose that minimizing f over $\mathcal{X}$ is *hard* while minimizing g over $\mathcal{X}$ is *easy* for all $y\in\mathcal{Y}$. And we suppose that minimizing g over $y\in\mathcal{Y}$ is also *easy* for all $x\in\mathcal{X}$. This last assumption is not too far-fatched, because we already know what the value at the minimum is.

I am not going to define *hard* and *easy*. What may be easy for you, may be hard for me.

Anyway, by augmenting the function we are in the block-relaxation situation again, and we can apply our general results on global convergence and linear convergence. The results can be adapted to the augmentation situation.

Note: augmentation duality.

$$h(y)=\min_{x\in\mathcal{X}} g(x,y)$$

then

$$\min_{x\in\mathcal{X}} f(x)=\min_{x\in\mathcal{X}}\min_{y\in\mathcal{Y}} g(x,y)=\min_{y\in\mathcal{Y}}\min_{x\in\mathcal{X}} g(x,y)=\min_{y\in\mathcal{Y}} h(y).$$

##Rate of Convergenc

Because of the structure of f we know that $\mathcal{D}f(x)=\mathcal{D}_1g(x,y(x))$, where $y(x)$ is defined implicitly by $f(x)=g(x,y(x))$, or more explicitly by

$$y(x)=\mathop{\mathbf{argmin}}_{y\in\mathcal{Y}} g(x,y),$$

or, in the unconstrained and differentiable case,

$$\mathcal{D}_2g(x,y(x))=0.$$

Differentiating again gives

$$\mathcal{D}^2 f(x) = \mathcal{D}_{11}g(x,y(x)) - \mathcal{D}_{12}g(x,y(x))[\mathcal{D}_{22}g(x,y(x))]^{-1}\mathcal{D}_{21}g(x,y(x)),$$

It follows that

$$\mathcal{M}(x) = \mathcal{I} - [\mathcal{D}_{11}g(x,y(x))]^{-1}\mathcal{D}^2 f(x).$$

This shows how the iteration matrix does not depend (directly) on the derivatives of g with respect to y, and can be interpreted as one minus the curvature of the function at the minimum, relative to the curvature of the augmentation function.

##Half-Quadratic Methods

Half-quadratic or *HQ* methods are used heavily in image restoration and reconstructions problems. They were introduced in two different but related forms in Geman and Reynolds [1992] and Geman and Yang [1995].

$$f(x) = \|Ax - z\|_2^2 + \beta \sum_{i\in\mathcal{I}} \phi(u_i'x - v_i)$$

potential funcion, regularization function. edge-preserving requires non-quadratic potential function typically U is a discrete version of a differential operator, such as a first or second-order difference matrix

$$g(x,y) = \|Ax - z\|_2^2 + \beta \sum_{i=1}^{r} \frac{b_i}{2}\|\mathcal{D}_i x\|_2^2 + k(b_i)$$

$$k(b) := \sup_{t\in\mathcal{R}} \left\{-\frac{1}{2}bt^2 + h(t)\right\}.$$

By convex conjugacy

$$h(t) = \inf_{b\in\mathcal{R}} \left\{\frac{1}{2}bt^2 + k(b)\right\}$$

and the infimum is attained at

$$b = \begin{cases} h''(0^+) & \text{if } t = 0, \\ \frac{h'(t)}{t} & \text{if } t \neq 0. \end{cases}$$

##Examples

###Yates Augmentation

A linear least squares problem is *balanced* if the design matrix A is orthogonal. In the balanced case the problem of minimizing

$$f(x) = (b - Ax)'(b - Ax) \tag{1}$$

is easily solved, with solution $x = A'b$. Computing x does not involve any matrix inversion. In the case of a balanced factorial design it simply involves computing means of rows, columns, slices, and so on.

If some elements of b are missing then we can partition A and b into a missing and non-missing part as in

$$A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \qquad b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix},$$

with A_1 and b_1 the non-missing part, and minimize

$$f(x) = (b_1 - A_1x)'(b_1 - A_1x).$$

Now $A_1'A_1 = I - A_2'A_2 < I$, and the optimal x can no longer be computed with a simple matrix multiplication.

If one want to avoid matrix inversion, then we can use the basic approach suggested by Yayes (1933). We define the augmentation g by

$$g(x, z) = (b_1 - A_1x)'(b_1 - A_1x) + (z - A_2x)'(z - A_2x).$$

Because $f(x) = \min_z g(x, z)$ this leads to an easy block relaxation algorithm.

$$\begin{aligned} z^{(k+1)} &= A_2x^{(k)}, \\ x^{(k+1)} &= A_1'b_1 + A_2'z^{(k+1)}. \end{aligned}$$

This gives

$$\begin{aligned} z^{(k+1)} &= A_2A_1'b_1 + A_2A_2'z^{(k)}, \\ x^{(k+1)} &= A_1'b_1 + A_2'A_2x^{(k)}. \end{aligned}$$

As we have shown in section blockrelaxation:twoblockleastsquares this implies an iteration radius equal to the largest eigenvalue of $A_2'A_2$.

Note that Yates augmentation can be used to transform any linear least squares problem to a balanced problem, even if there are no missing data.

In minimizing $f(x)$ of (1) we first check if $A'A \lesssim I$. If this is the case, there is no need to normalize. If we do not have $A'A \lesssim I$ we start by dividing A by $\tau(A) = \sqrt{\mathbf{tr}\ A'A}$. This new normalized A, say $\tilde{A}$, now satisfies $\tilde{A}'\tilde{A} \lesssim I$. Then find any G such that $\tilde{A}'\tilde{A} + G'G = I$, and iterate according to

$$\begin{aligned} z^{(k+1)} &= Gx^{(k)}, \\ x^{(k+1)} &= \tilde{A}'b + G'z^{(k+1)}, \end{aligned}$$

which amounts to

$$x^{(k+1)} = \tilde{A}'b + (I - \tilde{A}'\tilde{A})x^{(k)}.$$

The iteration radius is

$$\kappa = 1 - \frac{\lambda_{\min}(A'A)}{\mathbf{tr}\ A'A}.$$

We can do better if we compute $\tilde{A}$ by dividing A by its trace norm, i.e. its largest singular value. Then

$$\kappa = 1 - \frac{\lambda_{\min}(A'A)}{\lambda_{\max}(A'A)}.$$

There is `R` code for Yates augmentation in the file `yates.R`.

Insert yates.R Here

###Optimal Scaling with ORDINALS

In LINEALS (section x.x.x) we try to find quantifications of the variables that linearize all bivariate regressions. J. De Leeuw (1988) has suggested to find standardized quantifications in such a way that the loss function

$$f(y) = \sum\sum_{j \neq \ell} \left\{ y_j' C_{jl} D_\ell^{-1} C_{\ell j} y_j - y_j' C_{jl} y_\ell y_\ell' C_{\ell j} y_j \right\} \tag{1}$$

is minimized.

A more general loss function is

$$g(y,z) = \sum\sum_{j \neq \ell} (z_{jl} - D_j^{-1} C_{j\ell} y_\ell)' D_j (z_{jl} - D_j^{-1} C_{j\ell} y_\ell), \tag{2}$$

which must be minimized over both y and z. The z_{jl} are $m(m-1)$ vectors, called *regression targets*, and target z_{jl} has k_j elements.

To see that this loss function generalizes (1) suppose we constrain z by requiring that $z_{j\ell}$ is proportional to y_j, i.e. $z_{j\ell} = r_{jl}y_j$. Then, using $y_j'D_jy_j = 1$,

$$g(y, R) = \sum\sum_{j\neq\ell} r_{jl}^2 - 2\sum\sum_{j\neq\ell} r_{j\ell}y_j'C_{j\ell}y_\ell + \sum\sum_{j\neq\ell} y_\ell'C_{\ell j}D_j^{-1}C_{j\ell}y_\ell.$$

This is minimized over R by $r_{j\ell} = y_j'C_{j\ell}y_\ell$, and the minimum is precisely the loss function (1). Thus $f(y) = \min_R g(y, R)$, and g is an augmentation of f. Block relaxation for g alternates minimization over R for fixed y, which we have shown to be easy, and minimization over y for fixed R, which is a modified eigenvalue problem of the kind discussed in BRAS3, section x.x.x. This is not necessarily simpler than the direct minimum eigenvalue problem for minimizing f in section x.x.x.

The major advantage from augmenting f is that it now becomes simple to incorporate quite general restrictions on the $z_{j\ell}$. For example, they can be required to be monotone with the original data, or a spline transformation, or a monotone spline. Or a mixture of these options. Thus we can constrain each individual regression functions $D_j^{-1}C_{j\ell}y_\ell$ to have one of a pre-determined number of shapes.

In `ordinals.R` we implement the three standard options of the Gifi system. A vector y_j is treated as nominal, ordinal, or numerical. If it is nominal then it is unconstrained, except for the normalization. In that case the $z_{j\ell}$ are also unconstrained for all ℓ. If y_j is treated as ordinal is must be monotone with the data, and so must all $z_{j\ell}$. And a numerical y_j must be linear with the data, together with its targets $z_{j\ell}$. Of course if all variables are numerical there is nothing to optimize, and we just compute correlations. If all variables are nominal there is nothing to optimize either, because we immediately get zero loss from any starting point.

Insert ordinals.R Here

###Least Squares Factor Analysis

In LS factor analysis we want to minimize

$$\sigma(A) = \sum_{i=1}^m\sum_{j=1}^m w_{ij}(r_{ij} - \sum_{s=1}^p a_{is}a_{js})^2,$$

with

$$w_{ij} = \begin{cases} 0, & \text{if } i = j, \\ 1, & \text{if } i \neq j. \end{cases}$$

We augment by adding the *communalities*, i.e. the diagonal elements of R as variables, and by using ALS over A and the communalities. For a complete R, minimizing over A just means computing the p dominant eigenvalues-eigenvectors. This algorithm dates back to the thirties, when it was proposed by Thomson and others.

Think of this as an algorithm for updating communalities. We have

$$H^{(k+1)} = \mathbf{diag}(I - R_p^{(k)})$$

where $R_p^{(k)}$ is the best rank p approximation to $R - H^{(k)}$.

###Squared Distance Scaling

Suppose we want to minimize

$$\sigma(X) = \sum_{i=1}^m \sum_{j=1}^m (\delta_{ij} - d_{ij}^2(X))^2,$$

with $d_{ij}^2(X) = (x_i - x_j)'(x_i - x_j)$ squared Euclidean distance. An augmentation algorithm for this problem, modestly called ELEGANT, was designed by J. De Leeuw (1975). That paper was never published and the manuscript is probably lost, but the algorithm was described, discussed, and applied by both Takane (1977) and Browne (1987).

We augment σ to

$$\sigma(X, \eta) = \sum_{i=1}^m \sum_{j=1}^m \sum_{k=1}^m \sum_{\ell=1}^m (\eta_{ijk\ell} - (x_i - x_j)'(x_k - x_\ell))^2,$$

where we require $\eta_{ijij} = \delta_{ij}$ while the other $\eta_{ijk\ell}$ are free. Define $C \overset{\Delta}{=} XX'$ and assume that X is column-centered, i.e. C is doubly-centered. The augmentation works because

$$\sum_{i=1}^m \sum_{j=1}^m \sum_{k=1}^m \sum_{\ell=1}^m \left((x_i - x_j)'(x_k - x_\ell)\right)^2 = 4n^2 \mathbf{tr}\ C^2.$$

Also

$$\sum_{i=1}^m \sum_{j=1}^m \sum_{k=1}^m \sum_{\ell=1}^m \eta_{ijk\ell}(x_i - x_j)'(x_k - x_\ell) = \mathbf{tr}\ UC,$$

where

$$u_{ij} \overset{\Delta}{=} \sum_{k=1}^m \sum_{\ell=1}^m (\eta_{ikj\ell} - \eta_{i\ell kj} - \eta_{kij\ell} + \eta_{\ell ikj}).$$

Thus we can minimize the augmented loss function over X for fixed $\eta_{ijk\ell}$ by minimizing $\mathbf{tr}\ (\frac{1}{4n^2}U - XX')^2$. This means computing the p largest eigenvalues and corresponding eigenvectors of U.

Minimizing the augmented loss over the $\eta_{ijk\ell}$ for fixed X is

$$\eta_{ijk\ell}^{(k)} = \begin{cases} \delta_{ij} & \text{if } (i,j) = (k,\ell), \\ (x_i^{(k)} - x_j^{(k)})'(x_k^{(k)} - x_\ell^{(k)}) & \text{otherwise.} \end{cases}$$

This is enough information to get the ALS algorithm going. The "elegance" so far is reducing a problem involving multivariate quartics to a sequence of eigenvalue problems. It is distinctly unelegant, however, that the computations need four-dimensional arrays. But it turns out these can easily be gotten rid of. We use

$$\sum_{i=1}^m\sum_{j=1}^m\sum_{k=1}^m\sum_{\ell=1}^m \eta_{ijk\ell}^{(k)}(x_i - x_j)'(x_k - x_\ell) = 2\mathbf{tr}\ C\left(2n^2C^{(k)} + B(X^{(k)})\right),$$

where

$$B(X^{(k)}) \triangleq \sum_{i=1}^m\sum_{j=1}^m(\delta_{ij} - d_{ij}^2(X^{(k)}))A_{ij}$$

and $A_{ij} \triangleq (e_i - e_j)(e_i - e_j)'$. Thus we find $X^{(k+1)}$ by computing eigenvalues and eigenvectors of $C^{(k)} + \frac{1}{2n^2}B(X^{(k)})$ and no intermediate computation or storage of the $\eta_{ijk\ell}$ is required.

###Linear Mixed Model

This example is taken from a paper of J. De Leeuw and Liu (1993), which describes the algorithm in detail. We simply give a list of results that show augmentation at work. We maximize a multinormal likelihood, not a least squares criterium.

Result: If $A = B + TCT'$, with $B, C > 0$, $y'A^{-1}y = \min_x (y - Tx)'B^{-1}(y - Tx) + x'C^{-1}x$.

Result: If $A = B + TCT'$, with $B, C > 0$,

$$\log\det A = \log\det B + \log\det C + \log\det C^{-1} + T'B^{-1}T.$$

Result: If $A = B + TCT'$ then

$$\begin{aligned}\log\det A + y'A^{-1}y = \min_x\ &\log\det B + \log\det C + \\ &+ \log\det C^{-1} + T'B^{-1}T + \\ &\qquad + (y - Tx)'B^{-1}(y - Tx) + x'C^{-1}x.\end{aligned}$$

Result: If $T > 0$ then

$$\log\det T = \min_{S>0} \log\det S + \text{ tr } S^{-1}T - p,$$

with the unique minimum attained at $S = T$.

We can use these four results to augment the original maximum likelihood problem.

$$\begin{aligned}\log\det A + y'A^{-1}y = \min_{x,S>0}\ &\log\det B + \log\det C + \\ &+ \log\det S + \text{ tr } S^{-1}(C^{-1} + T'B^{-1}T) + \\ &\qquad + (y - Tx)'B^{-1}(y - Tx) + x'C^{-1}x.\end{aligned}$$

Minimize over x, S, B, C using block-relaxation. The conditional minimizers are

$$\begin{aligned}S &= C^{-1} + T'B^{-1}T,\\ C &= S^{-1} + xx',\\ B &= TS^{-1}T' + (y - Tx)(y - Tx)',\\ x &= (T'B^{-1}T + C^{-1})^{-1}T'B^{-1}y.\end{aligned}$$

##Decomposition Methods

The following theorem is so simple it's almost embarassing. Nevertheless it seems to have some important applications to algorithm construction.

Theorem: Suppose $G : X \otimes Y \Rightarrow Z$ and f is an extended real-valued function. Then

$$\inf_{z\in\overline{Z}} f(z) = \inf_{x\in X} \inf_{y\in Y} f(G(x, y)),$$

where $\overline{Z} = G(X,Y)$. Moreover if the infimum on the right is attained in $(\hat{x},\hat{y})$, then the infimum on the left is attained in $\hat{z} = G(\hat{x},\hat{y})$.

Proof: In the eating (see below).**QED**

Here are some quick examples. First take $G(x,y) = x - y$. Then

$$\begin{aligned}\inf_z f(z) &= \inf_{x\geq 0}\inf_{y\geq 0} f(x-y) = \\ &= \inf_x \inf_y f(x-y).\end{aligned}$$

Now take $G(x,\lambda) = \lambda x$, with λ a scalar and x a vector,

$$\begin{aligned}\inf_z f(z) &= \inf_{\lambda\geq 0}\inf_{x'x=1} f(\lambda x) = \\ &= \inf_\lambda \inf_{x'x=1} f(\lambda x) = \\ &= \inf_\lambda \inf_x f(\lambda x).\end{aligned}$$

If $G(x,\lambda) = \frac{x}{\lambda}$, with $\lambda \neq 0$ and $x'x = 1$, then $\overline{Z}$ is the set of all vectors $z \neq 0$. Thus

$$\inf_{z\neq 0} f(z) = \inf_{\lambda\neq 0}\inf_{x'x=1} f(\frac{x}{\lambda}).$$

Somewhat less trivially, for a symmetric matrix argument A,

$$\inf_A f(A) = \inf_{\mathbf{dg}(\Lambda)=\Lambda} \quad \inf_{K'K=I} \; f(K\Lambda K').$$

Observe we can always interchange the two infimum operations, because $\inf_{x\in X}\inf_{y\in Y} = \inf_{y\in Y}\inf_{x\in X}$. Because f is extended real valued, the infimum always exists, although it may be $-\infty$.

###Quadratic Form on a Sphere

We now discuss an actual example. Consider the problem of minimizing the function

$$f(z) = \frac{(z-b)'A(z-b)+c}{z'z},$$

over $z \neq 0$, where we make no assumptions on the matrix A, the vector b, and the scalar c. Instead of going the usual route of differentiating and solving the stationary equations, we use the decomposition approach.

Define

$$g(x,\lambda) = \frac{(\lambda x - b)'A(\lambda x - b)+c}{\lambda^2 x'x},$$

or, letting $\theta = \lambda^{-1}$,

$$g(x,\theta) = \frac{\theta^2(b'Ab + c) - 2\theta b'Ax + x'Ax}{x'x},$$

Then

$$\inf_{z\neq 0} f(z) = \inf_{x'x=1} \inf_{\theta\geq 0} g(x,\theta),$$

but also

$$\inf_{z\neq 0} f(z) = \inf_{x'x=1} \inf_{\theta} g(x,\theta).$$

If $x'x = 1$ then

$$\inf_{\theta} g(x,\theta) = \inf_{\theta} \theta^2(b'Ab + c) - 2\theta b'Ax + x'Ax.$$

We distinguish three cases.

- If $b'Ab + c > 0$ the minimum is attained at

  $$\hat{\theta} = \frac{b'Ax}{b'Ab + c}$$

  and the minimum is equal to $x'\overline{A}x$, where

  $$\overline{A} = A - \frac{Abb'A}{b'Ab + c}.$$

  It follows that in this case $\min_z f(z)$ is the smallest eigenvalue of $\overline{A}$, written as $\kappa(\overline{A})$. If $\overline{x}$ is the corresponding unit-length eigenvector, then the minimizer of $f(z)$ is

  $$\hat{z} = \frac{b'Ab + c}{b'A'\overline{x}}\,\overline{x}.$$

- If $b'Ab + c < 0$ the minimum is not attained and $\inf_\theta g(x,\theta) = -\infty$ for each x. Thus $\inf_z f(z) = -\infty$ as well.

- If $b'Ab + c = 0$ then we must distinguish two sub-cases. If $b'Ax = 0$ then $\min_\theta g(x,\theta) = x'Ax$. If $b'Ax \neq 0$ then $\inf_\theta g(x,\theta) = -\infty$ again. Thus if $b'Ab + c = 0$ we have $\inf_z f(z) = -\infty$, unless both $c = 0$ and $Ab = 0$, in which sub-case we have $\min_z f(z)$ equal to $\kappa(A)$, the smallest eigenvalue of A and the minimizer equal to any corresponding eigenvector.

Of course if $Ab = 0$ we have $\overline{A} = A$. Thus

$$\inf_z f(z) = \begin{cases} \kappa(\overline{A}) & \text{if } (b'Ab + c > 0) \text{ or } (Ab = 0 \text{ and } c = 0), \\ -\infty & \text{otherwise.} \end{cases}$$

Now start with the alternative decomposition

$$\min_{z \neq 0} f(z) = \min_{x'x=1} \min_{\theta \geq 0} \theta^2(b'Ab + c) - 2\theta b'Ax + x'Ax.$$

We want to show that although the intermediate calculations are different, the result is the same.

- If $b'Ab + c > 0$ and $b'Ax \geq 0$ then $\min_\theta g(x,\theta) = x'\overline{A}x$, as before. But if $b'Ab + c > 0$ and $b'Ax < 0$ the minimum is attained at $\hat{\theta} = 0$, and $\min_\theta g(x,\theta) = x'Ax$. Because $\kappa(\overline{A})$ is less than or equal to $\kappa(A)$, we still have $\min_z f(z)$ equal to the smallest eigenvalue of $\overline{A}$.
- If $b'Ab + c < 0$ we still have $\inf_z f(z) = -\infty$.
- If $b'Ab + c = 0$ we distinguish three sub-cases. If $b'Ax = 0$ then $\min_\theta g(x,\theta) = x'Ax$, as before. If $b'Ax\ 0$ then $\inf_\theta g(x,\theta) = -\infty$. And if $b'Ax < 0$ the minimum is attained at $\hat{\theta} = 0$ and equal to $x'Ax$. Again we have $\inf_z f(z) = -\infty$, unless both $c = 0$ and $Ab = 0$, when $\min_z f(z)$ is equal to $\kappa(A)$.

We have solved the problem by using the decompositions~(**??**) and~(**??**). But we can also interchange the order of the infimums and use

$$\inf_{z \neq 0} f(z) = \inf_{\theta \geq 0} \inf_{x'x=1} g(x,\theta),$$

or

$$\inf_{z \neq 0} f(z) = \inf_{\theta} \inf_{x'x=1} g(x,\theta).$$

Let's look at the problem $\min_{x'x=1} g(x,\theta)$. For a minimum we must have $x = \theta(A - \mu I)^{-1}Ab$, where the Lagrange multiplier μ is chosen such that $\theta^2 b'A(A - \mu I)^{-2}Ab = 1$. At the minimum

$$\min_{x'x=1} g(x,\theta) = \\ \theta^2[(b'Ab+c)-2b'A(A-\mu I)^{-1}Ab+b'A(A-\mu I)^{-1}A(A-\mu I)^{-1}Ab]$$

###Multidimensional Unfolding

Now a data analysis example. In least-squares-squared metric unfolding (LSSMU) we must minimize

$$\sigma(X,Y)=\sum_{i=1}^n\sum_{j=1}^m w_{ij}(\delta_{ij}^2-[x_i'x_i+y_j'y_j-2x_i'y_j])^2.$$

over the $n\times p$ and $m\times p$ configuration matrices X and Y. This has been typically handled by block decomposition. The $(n+m)p$ unknowns are partitioned into a number of subsets. Block relaxation algorithms then cycle through the subsets, minimizing over the parameters in the subset while keeping all parameters fixed at their current values. One cycle through the subsets is one iteration of the algorithm.

In ALSCAL (Takane, Young, and De Leeuw (1977))) coordinate descent is used, which means that the blocks consist of a single coordinate. There are $(n+m)p$ blocks. Solving for the optimal coordinate, with all other fixed, means minimizing a quartic, which in turn means finding the roots of a cubic. The algorithm converges to a stationary point which is a global minimum with respect to each coordinate separately. An alternative algorithm, proposed by Browne (1987), uses the $n+m$ points as blocks. Each substep is again an easy unidimensional minimization. Their algorithm converges to a stationary point which is a global minimum with respect to each point. Generally it is considered to be desirable to have fewer blocks, both to increase the speed of convergence and to restrict the class of local minima we can converge to.

Let us use our basic theorem to construct a four-block algorithm for LSSMU. Minimizing~(**??**) is the same as minimizing

$$\sigma(X,Y,\alpha,\beta)=\sum_{i=1}^n\sum_{j=1}^m w_{ij}(\delta_{ij}^2-[\alpha_i^2+\beta_j^2-2\alpha_i\beta_j x_i'y_j])^2$$

over $\alpha,\beta,X,$ and Y, where the configuration matrices X and Y are constrained by $\mathbf{diag}(XX')=I$ and $\mathbf{diag}(YY')=I$.

The algorithm starts with values $\Theta^{(0)} = (\alpha^{(0)}, \beta^{(0)}, X^{(0)}, Y^{(0)})$ satisfying the constraints. Suppose we have arrived at $\Theta^{(k)}$. We then update

$$\begin{aligned} \alpha^{(k+1)} &= \underset{\alpha}{\mathbf{argmin}} \quad \sigma(X^{(k)}, Y^{(k)}, \alpha, \beta^{(k)}), && (2.2)\\ \beta^{(k+1)} &= \underset{\beta}{\mathbf{argmin}} \quad \sigma(X^{(k)}, Y^{(k)}, \alpha^{(k+1)}, \beta), && (2.3)\\ X^{(k+1)} &= \underset{\mathbf{diag}(XX')=I}{\mathbf{argmin}} \quad \sigma(X, Y^{(k)}, \alpha^{(k+1)}, \beta^{(k+1)}), && (2.4)\\ Y^{(k+1)} &= \underset{\mathbf{diag}(YY')=I}{\mathbf{argmin}} \quad \sigma(X^{(k+1)}, Y, \alpha^{(k+1)}, \beta^{(k+1)}). && (2.5) \end{aligned}$$

This gives $\Theta^{(k+1)}$. It is understood that in each of the four substeps of~(**??**) we compute the global minimum, and if the global minimum happens to be nonunique we select any of them. We also remark that, as with any block relaxation method having more than two blocks, there are many variations on this basic scheme. We can travel through the substeps in a different order, we can change the order in each cycle, we can pass through the substeps in random order, we can cycle through the first two substeps a number of times before going to the third and fourth, and so on. Each of these strategies has its own overall convergence rate, and further research would be needed to determine what is best.

Let us look at the subproblems a bit more in detail to see how they can be best solved. Expanding~(**??**) and organizing terms by powers of α gives

$$\begin{aligned} \sigma(X, Y, \alpha, \beta) = &\sum_{i=1}^n \alpha_i^4 \sum_{j=1}^m w_{ij} + \\ &- \sum_{i=1}^n \alpha_i^3 \sum_{j=1}^m w_{ij}\beta_j c_{ij} + \\ &+ \sum_{i=1}^n \alpha_i^2 \sum_{j=1}^m w_{ij}(4\beta_j^2 c_{ij}^2 + 2\beta_j^2 - 2\delta_{ij}^2) + \\ &- \sum_{i=1}^n \alpha_i^2 \sum_{j=1}^m 4w_{ij}\beta_j^3 c_{ij} + \\ &+ \sum_{i=1}^n \sum_{j=1}^m w_{ij}(\delta_{ij}^4 + \beta_j^4 + 4\delta_{ij}^2 c_{ij} - 2\delta_{ij}^2\beta_j^2), \end{aligned}$$

where $c_{ij} = x_i' y_j$. This is a sum of n univariate quartic polynomials, which can be minimized separately to give the global minimum over α. Obviously the same applies to minimization over β.

For minimization over X and Y we define

$$\begin{aligned} r_{ij} &= \frac{\delta_{ij}^2 - [\alpha_i^2 + \beta_j^2]}{2\alpha_i\beta_j}, \\ w_{ij} &= 4\alpha_i^2\beta_j^2 w_{ij}. \end{aligned}$$

Then

$$\sigma(X, Y, \alpha, \beta) = \sum_{i=1}^n \sum_{j=1}^m w_{ij}[r_{ij} - x_i'y_j]^2.$$

Expanding and collecting terms gives

$$\sigma(X, Y, \alpha, \beta) = \sum_{i=1}^n \psi_i(x_i)$$

with

$$\psi_i(x_i) = f_i - 2x_i'g_i + x_i'H_ix_i)$$

and

$$\begin{aligned} f_i &= \sum_{j=1}^m w_{ij}r_{ij}^2, \\ g_i &= \sum_{j=1}^m w_{ij}r_{ij}y_j, \\ H_i &= \sum_{j=1}^m w_{ij}y_jy_j'. \end{aligned}$$

Again this is the sum of n separate functions ψ_i, quadratics in this case, which can be minimized separately for each x_i. By symmetry, we have the same strategy to minimize over Y.

Minimizing over x_i, under the constraint $x_i'x_i = 1$, leads to the secular equation problem discussed in the Appendix. Since typically p is two or at most three, the subproblems are very small indeed and can be solved efficiently.

#Majorization Methods

##Introduction

The next step (history again) was to find *systematic ways* to do augmentation (which is an art, remember). We start with examples.

An early occurrence of majorization, in the specific context of finding a suitable step size for descent methods, is in Ortega and Rheinboldt (1970b)). They call this approach the *Majorization Principle*, which exists alongside other step size principles such as the *Curry-Altman Principle*, the *Goldstein Principle*, and the *Minimization Principle*.

Suppose we have a current solution $x^{(k)}$ and a descent direction $p^{(k)}$. Consider the function

$$g(\alpha) := f(x^{(k)} - \alpha p^{(k)}).$$

Suppose we can find a function h such that $g(\alpha) \leq h(\alpha)$ for all $0 < \alpha < \overline{\alpha}$ and such that $g(0) = h(0)$. Now set

$$\alpha^{(k)} := \mathop{\mathbf{argmin}}_{0 \leq \alpha \leq \overline{\alpha}} h(\alpha).$$

Then the sandwich inequality says

$$g(\alpha^{(k)}) \leq h(\alpha^{(k)}) \leq h(0) = g(0),$$

and thus $f(x^{(k)} - \alpha^{(k)} p^{(k)}) \leq f(x^{(k)})$.

Ortega and Rheinboldt point out that if the derivative of f is Hölder continuous, i.e. if for some $0 < \lambda \leq 1$

$$\|\mathcal{D}f(x) - \mathcal{D}f(y)\| \leq \gamma \|x - y\|^{\lambda},$$

then we can choose

$$h(\alpha) = h(0) - \alpha \langle p^{(k)}, \mathcal{D}f(x^{(k)}) \rangle + \frac{\gamma}{1+\lambda}(\alpha \|p^{(k)}\|)^{1+\lambda},$$

which implies

$$\alpha^{(k)} = \frac{1}{\|p^{(k)}\|} \left[\frac{\langle p^{(k)}, \mathcal{D}f(x^{(k)}) \rangle}{\gamma \|p^{(k)}\|} \right]^{\frac{1}{\lambda}}.$$

##Definitions

###Majorization at a Point

Suppose f and g are real-valued functions on $\mathcal{X} \subseteq \mathbb{R}^n$. We say that g *majorizes* f *over* $\mathcal{X}$ *at* $y \in \mathcal{X}$ if

- $g(x) \geq f(x)$ for all $x \in \mathcal{X}$,

- $g(y) = f(y)$.

If the first condition can be replaced by

- $g(x) > f(x)$ for all $x \in \mathcal{X}$ with $x \neq y$,

we say that majorization at $y \in \mathcal{X}$ is *strict*.

Equivalently majorization is strict if the second condition can be replaced by

- $g(x) = f(x)$ if and only if $x = y$.

Since we formulate all optimization problems we encounter as minimization problems, we only use *majorization*, not *minorization*. But just for completeness, if g majorizes f at y over $\mathcal{X}$, then f *minorizes* g at y over $\mathcal{X}$.

We will see plenty of examples as we go on, but for now a simple one suffices. Figure 1 shows the logarithm on $\mathbb{R}^+$ strictly majorized at $+1$ by the linear function $g : x \rightarrow x - 1$.

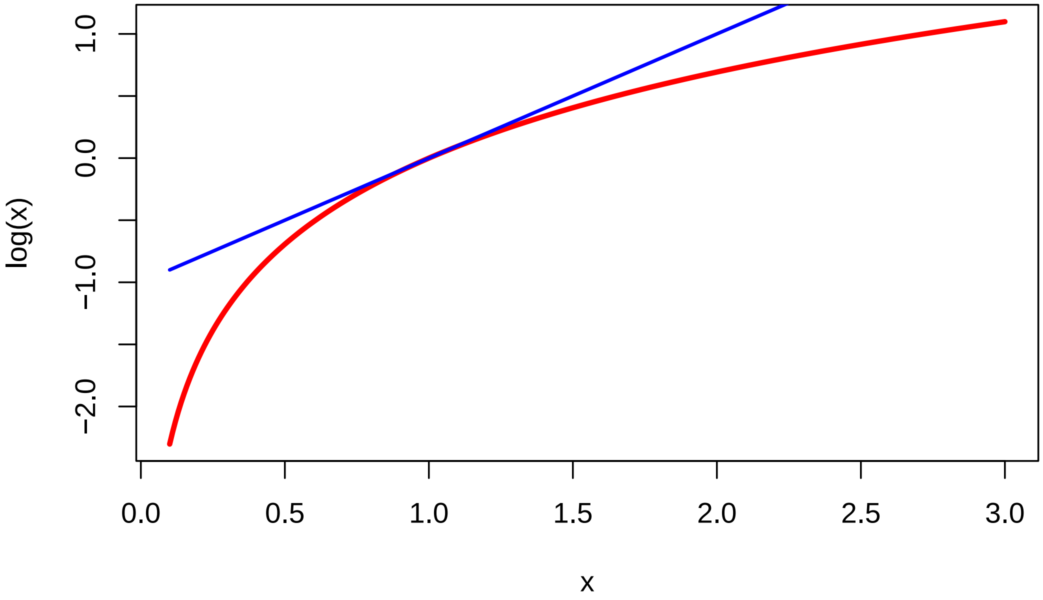


Figure 1: Linear Majorizer of the Log at +1

Note that the definition of majorization at a point always has to take the set $\mathcal{X}$ into account. If g majorizes f over $\mathcal{X}$ at y, then it may very well not majorize over a larger set. But, of course, it does majorize f at y over any subset of $\mathcal{X}$ containing y.

In most of our examples and applications $\mathcal{X}$ will be equal to $\mathbb{R}$, $\mathbb{R}^+$, or $\mathbb{R}^n$ but in some cases we consider majorization over an interval or, more generally, a convex subset of $\mathbb{R}^n$. If we do not explicitly mention the set on which g majorizes f, then we implicitly mean the whole domain of f. But we'll try to be as explicit as possible, because our treatment, unlike some earlier ones, does not just discuss majorization over the whole space where f is defined.

As an example, consider the cubic $f : x \rightarrow \frac{1}{3}x^3 - 4x$ which is majorized at $+1$ on the half-open interval $(-\infty, 4]$ by the quadratic $g : x \rightarrow \frac{4}{3} - 7x + 2x^2$. This particular quadratic is constructed, by the way, by solving the equations $f(1) = g(1), f'(1) = g'(1)$, and $f(4) = g(4)$. On the other hand it is easy to see that a non-trivial cubic f cannot be majorized at any y by a quadratic g on the whole real line, because $g - f$, which is again a non-trivial cubic, would have to be non-negative for all x, which is impossible.

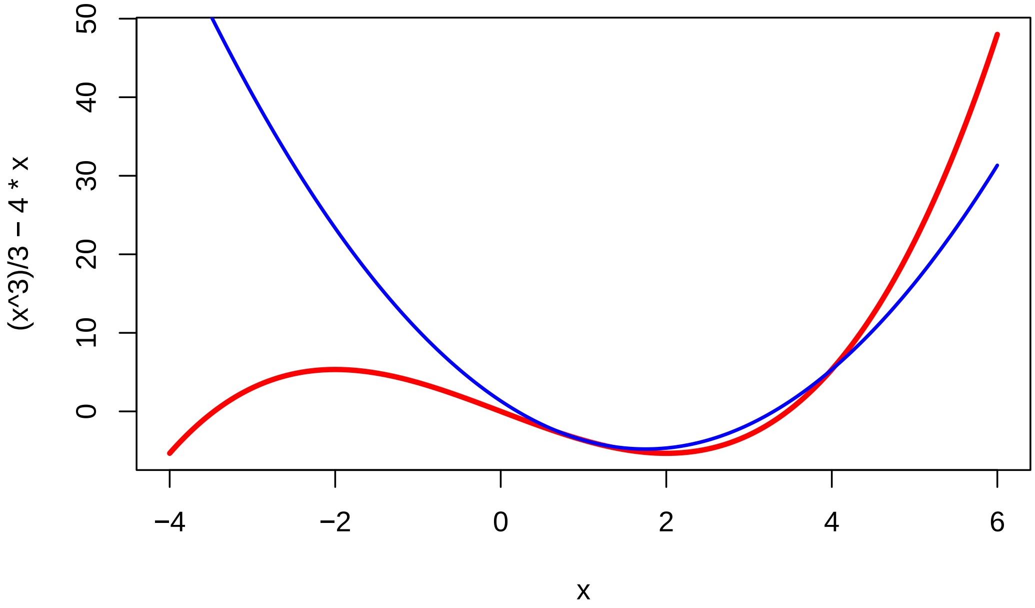


Figure 2: Quadratic Majorizer of a Cubic on an Interval

It follows directly from the definition that g majorizes f at y if and only if $g - f$ has a global minimum over $\mathcal{X}$, equal to zero, at y. And majorization is strict if this minimum is unique. Thus a necessary and sufficient condition for majorization at $y \in \mathcal{X}$ is

$$\min_{x \in \mathcal{X}} (g(x) - f(x)) = g(y) - f(y) = 0.$$

Since a global minimum is also a local minimum, it follows that if g majorizes f at $y \in \mathcal{X}$ then $g - f$ has a local minimum , equal to zero, over $\mathcal{X}$ at y. This is a convenient necessary condition for majorization. A sufficient condition for g to majorize f at y is that $g - f$ is a convex function with a minimum at y equal to zero. Because of convexity this minimum is then necessarily the global minimum.

If g majorizes f at $y \in \mathcal{X}$ then the points $y \in \mathcal{X}$ where $g(y) = f(y)$ are called *support points*. If majorization is strict there is only one support point. There can, however, be arbitrarily many.

Consider $f : x \rightarrow x^2 - 10\sin^2(x)$ and $g : x \rightarrow x^2$. Then g majorizes f on the real line, with support points at all integer multiples of π. This is illustrated in Figure 3.

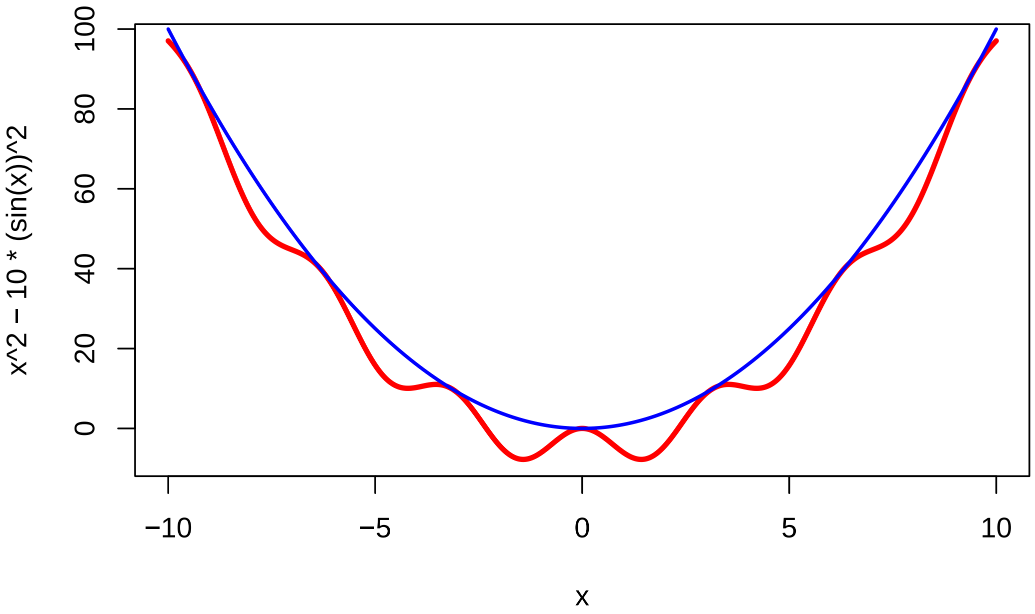


Figure 3: Quadratic Majorizer with an Infinite Number of Support Points

In fact if $f : x \rightarrow \max(x, 0)$ and $g : x \rightarrow |x|$ then g majorizes f at all $y \leq 0$, and thus there even is a continuum of support points. And actually f itself majorizes f at all $y \in \mathcal{X}$.

###Majorization on a Set

We can have different majorizations of f on $\mathcal{X}$ at different points $y_1, \cdots, y_n \in \mathcal{X}$. Now consider the situation in which we have a different majorization for each point $y \in \mathcal{X}$.

Suppose f is a real-valued function on $\mathcal{X}$ and g is a real-valued function on $\mathcal{X} \otimes \mathcal{X}$. We say that g is a *majorization scheme* for f *on* $\mathcal{X}$ if

- $g(x, y) \geq f(x)$ for all $x, y \in \mathcal{X}$,
- $g(y, y) = f(y)$ for all $y \in \mathcal{X}$.

Majorization is *strict* if the first condition can be replaced by

- $g(x, y) > f(x)$ for all $x, y \in \mathcal{X}$ with $x \neq y$.

Or, equivalently, if the second condition can be replaced by

- $g(x, y) = f(x)$ if and only if $x = y$.

We call g a *majorization scheme* for f on $\mathcal{X}$, because g automatically gives a majorization for f for every $y \in \mathcal{X}$. Thus a majorization of f on $\mathcal{X}$ at y is a real-valued function g on $\mathcal{X}$, a majorization scheme for f on $\mathcal{X}$ is a real-valued function on $\mathcal{X} \otimes \mathcal{X}$.

Because $g(x, y) \geq g(x, x) = f(x)$ for all $x, y \in \mathcal{X}$ we see that

$$f(x) = \min_{y \in \mathcal{X}} g(x, y)$$

for all $x \in \mathcal{X}$. Thus g majorizes f if and only if $f(x) = \min_{y \in \mathcal{X}} g(x, y)$ and the minimum is attained for $y = x$. Strict majorization means the minimum is unique. It follows that the majorization relation between functions is a special case of the augmentation relation.

As an example of a majorization scheme for $f : x \rightarrow -\log(1+\exp(-x))$ we use

$$g(x,y)=f(y)+f'(y)(x-y)+\frac{1}{8}(x-y)^2.$$

Also define the function h by $h(x,y)=f(x)$.

Function g is plotted in figure 2.5 in blue, function h is in red.

Note that the intersection of the graph of both g and h with the diagonal vertical plane $x=y$ is the set of (x,y,z) such that $x=y$ and $z=g(x,x)=h(x,x)=f(x)$. This is the white line in the plot.

Graphs of the intersection of the graphs of g and h with the vertical planes $y=c$ parallel to the x-axes at $y=-5,-2,0,2,5$ are in Ffigure @ref(fig.interplanes). The red lines are the intersections with h, i.e. the function f, the blue lines are the quadratics majorizing f at $y=-5,-2,0,2,5$.

Graphs of intersection of the graphs of g and h with the vertical planes $x=c$ parallel to the y-axes at $x=-5,-2,0,2,5$ are in figure @ref{fig.logitother}. They illustrate that $\min_y g(x,y)=f(x)$. The horizontal red lines are the intersections of the planes $x=c$ with the graph of h at $f(-5), f(-2), f(0), f(2)$, and $f(5)$.

The code to produce all three figures is in `logitcouple.R`.

Insert logitcouple.R Here

###Majorization Algorithm

The basic idea of a *majorization algorithm* is simple: it is the augmentation algorithm applied to the majorization function.

Suppose our current best approximation to the minimum of f is $x^{(k)}$, and we have a g that majorizes f on $\mathcal{X}$ in $x^{(k)}$. If $x^{(k)}$ already minimizes g we stop, otherwise we update $x^{(k)}$ to $x^{(k+1)}$ by minimizing g over $\mathcal{X}$.

If we do not stop, we have the *sandwich inequality*

$$f(x^{(k+1)})\leq g(x^{(k+1)})<g(x^{(k)})=f(x^{(k)}),$$

and in the case of strict majorization even

$$f(x^{(k+1)})<g(x^{(k+1)})<g(x^{(k)})=f(x^{(k)}).$$

We then select a new function g that majorizes f on $\mathcal{X}$ at $x^{(k+1)}$. Repeating these steps produces a decreasing sequence of function values, and the

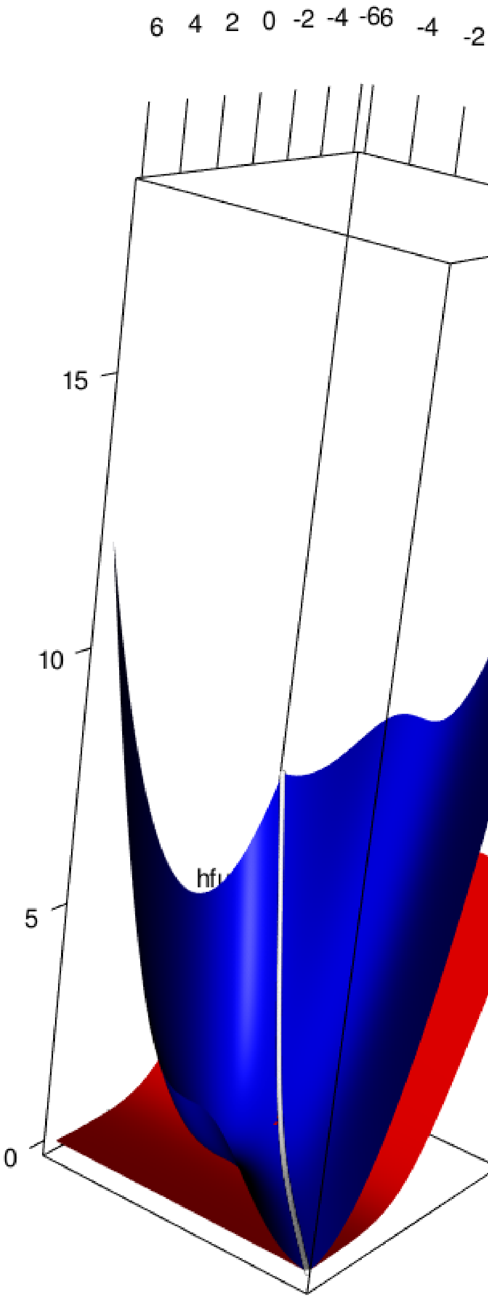


Figure 2.5: Majorization Scheme for log(1+exp(x))

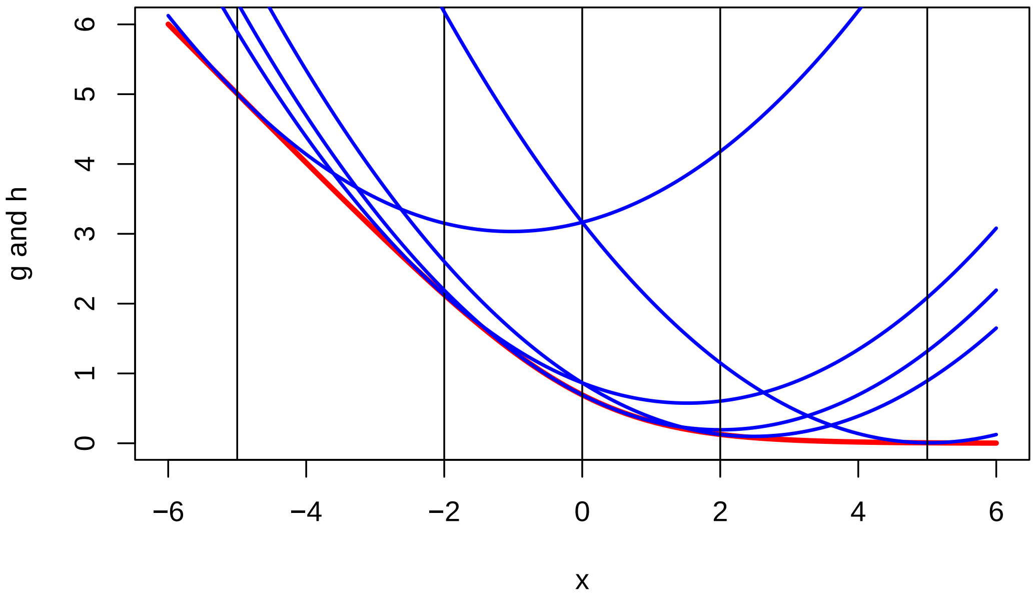


Figure 2.6: Intersections of g with $y = c$ planes

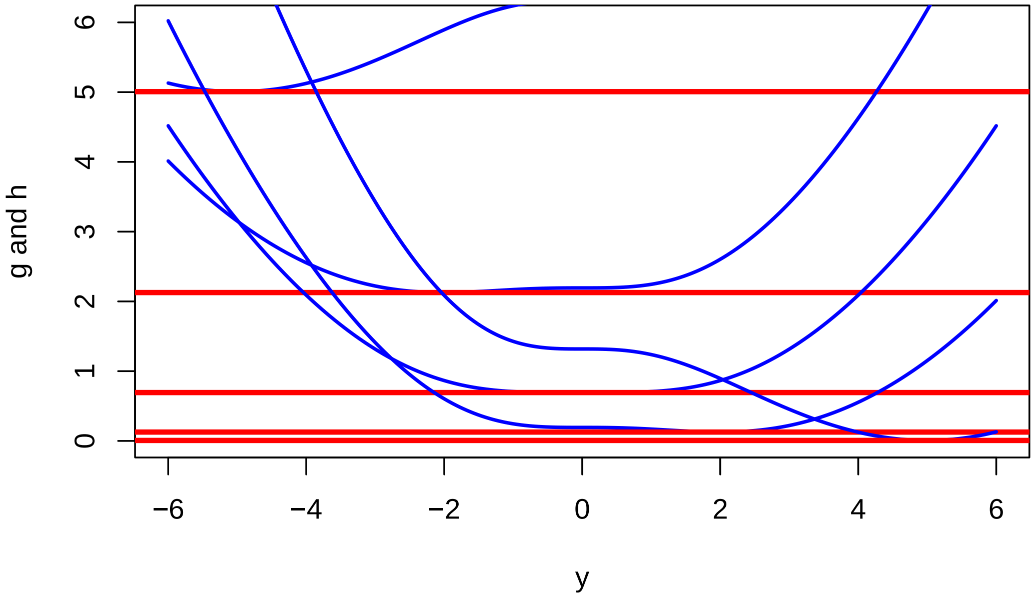


Figure 2.7: Intersections of g with $x = c$ planes

usual compactness and continuity conditions guarantee convergence of both sequences $x^{(k)}$ and $f(x^{(k)})$.

Here is an artificial example, chosen because of its simplicity. Consider $f(x) = x^4 - 10x^2$. Because $x^2 \geq y^2 + 2y(x-y) = 2yx - y^2$ we see that $g(x,y) = x^4 - 20yx + 10y^2$ is a suitable majorization function. The majorization algorithm is $x^{(k+1)} = \sqrt[3]{5x^{(k)}}$.

The first iterations of the algorithm are illustrated in Figure 1. We start with $x^{(0)} = 3$, where f is -9. Then $g(x,3)$ is the blue function. It is minimized at $x^{(1)} \approx 2.4662$, where $g(x^{(1)},3) \approx -20.9795$, and $f(x^{(1)}) \approx -23.8288$. We then majorize by using the green function $g(x,x^{(1)})$, which has its minimum at about 2.3103, equal to about -24.6430. The corresponding value of f at this point is about -24.8861. Thus we are rapidly getting close to the local minimum at $\sqrt{5} \approx 2.2361$, with value -25. The linear convergence rate at the stationary point is $\frac{1}{3}$.

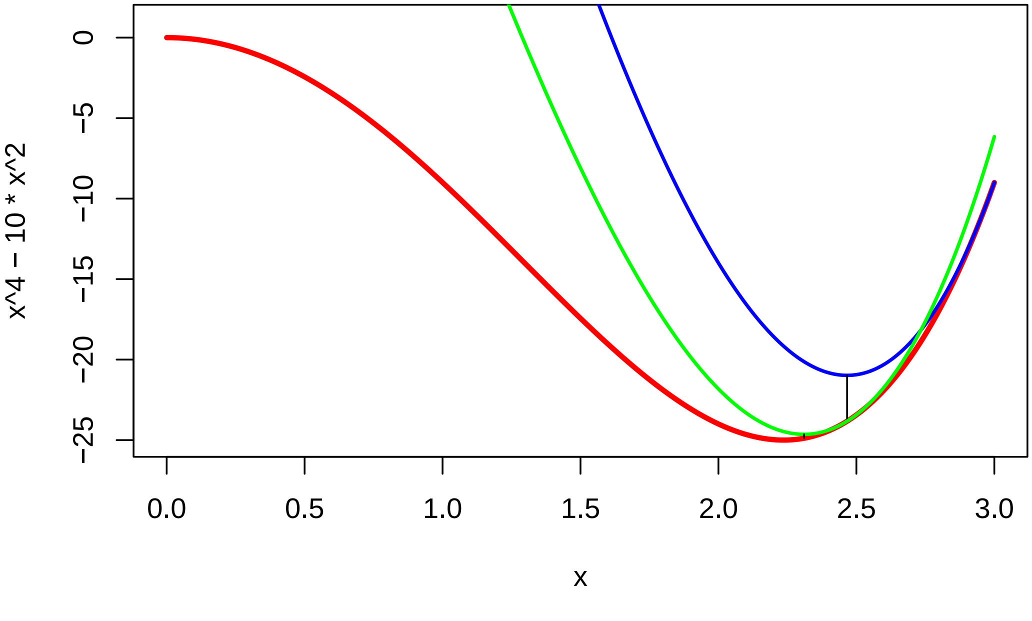


Figure 1: Toy example, first iterations

Table 1 show the iterations to convergence, with an estimate of the iteration radius in the last column.

```
## Iteration:    1 fold:   -9.00000000 fnew:  -23.82883884 xold:    3.00000000 xnew:
## Iteration:    2 fold:  -23.82883884 fnew:  -24.88612919 xold:    2.46621207 xnew:
## Iteration:    3 fold:  -24.88612919 fnew:  -24.98789057 xold:    2.31029165 xnew:
## Iteration:    4 fold:  -24.98789057 fnew:  -24.99867394 xold:    2.26054039 xnew:
## Iteration:    5 fold:  -24.99867394 fnew:  -24.99985337 xold:    2.24419587 xnew:
## Iteration:    6 fold:  -24.99985337 fnew:  -24.99998373 xold:    2.23877400 xnew:
## Iteration:    7 fold:  -24.99998373 fnew:  -24.99999819 xold:    2.23696962 xnew:
## Iteration:    8 fold:  -24.99999819 fnew:  -24.99999980 xold:    2.23636848 xnew:
## Iteration:    9 fold:  -24.99999980 fnew:  -24.99999998 xold:    2.23616814 xnew:
## Iteration:   10 fold:  -24.99999998 fnew:  -25.00000000 xold:    2.23610137 xnew:
## Iteration:   11 fold:  -25.00000000 fnew:  -25.00000000 xold:    2.23607911 xnew:
## Iteration:   12 fold:  -25.00000000 fnew:  -25.00000000 xold:    2.23607169 xnew:
## Iteration:   13 fold:  -25.00000000 fnew:  -25.00000000 xold:    2.23606921 xnew:
## Iteration:   14 fold:  -25.00000000 fnew:  -25.00000000 xold:    2.23606839 xnew:
## Iteration:   15 fold:  -25.00000000 fnew:  -25.00000000 xold:    2.23606811 xnew:
```

Table 1: Toy example, iterations to convergence

We also show the cobwebplot (see section 14.11.2) for the iterations, which illustrates the decrease of the difference between subsequent iterates.

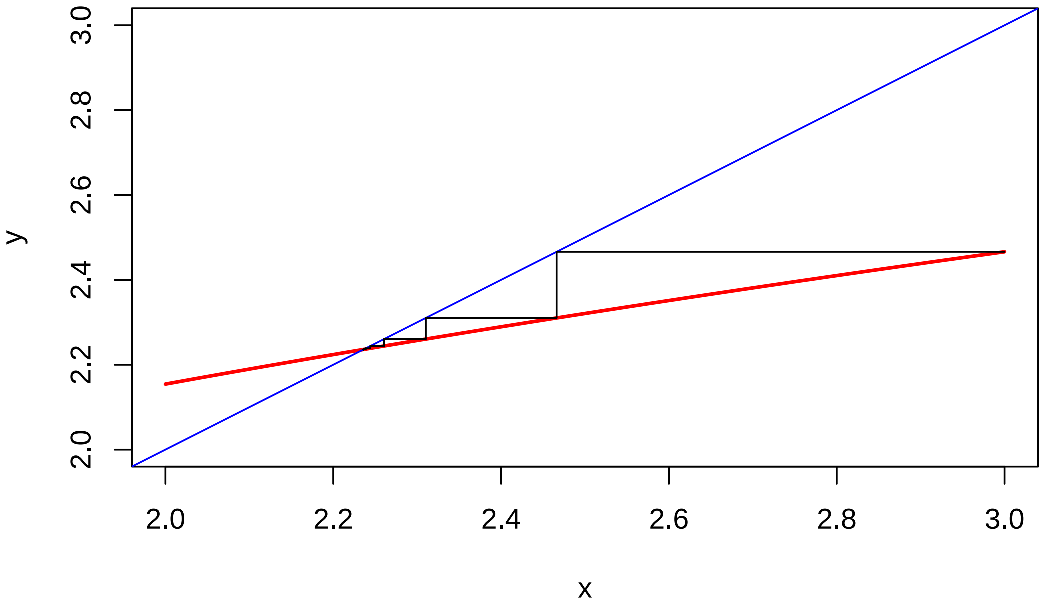


Figure 2

###Alternative Definitions

Suppose f and g are arbitrary real-valued functions on $\mathcal{X}$. Define

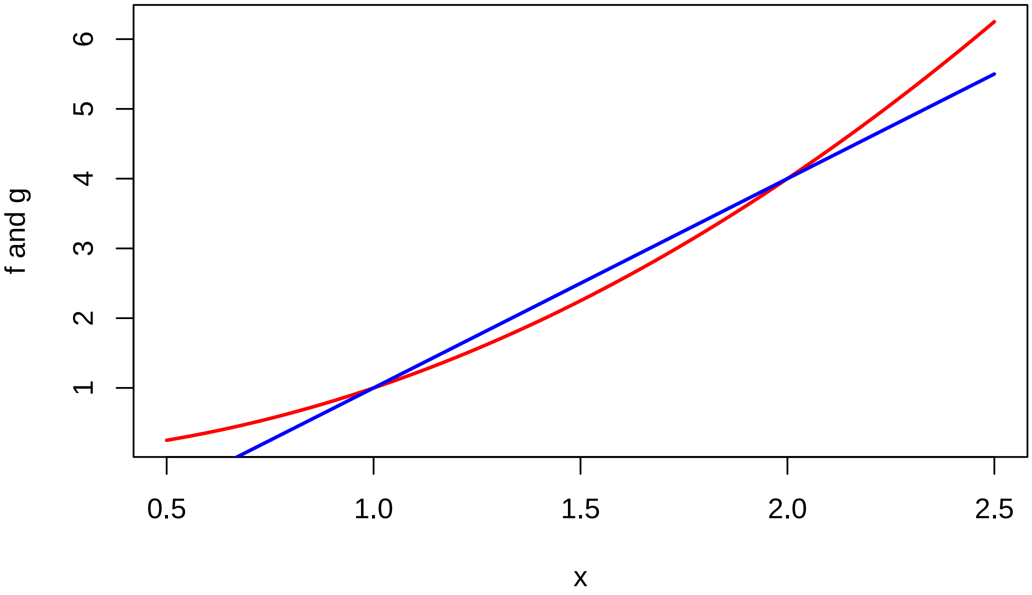
$$\begin{aligned}\mathcal{S}_-(f,g) &:=\{x\in\mathcal{X}\mid f(x)\leq g(x)\},\\ \mathcal{S}_0(f,g) &:=\{x\in\mathcal{X}\mid f(x)=g(x)\}.\end{aligned}$$

Thus $\mathcal{S}_0(f,g)\subseteq\mathcal{S}_-(f,g)$. Then if

$$\begin{aligned}&x\in\mathcal{S}_0(f,g),\\ &y\in\mathop{\mathbf{argmin}}_{x\in\mathcal{S}_-(f,g)} g(x),\end{aligned}$$

we have

$$f(y)\leq g(y)\leq g(x)=f(x).$$



##Relatives

###The Concave-Convex Procedure

The Concave-Convex Procedure (CCCP) was first proposed by Yuille and Rangarajan (2003). Its global convergence was studied using the Zangwill theory by Sriperumbudur and Lanckriet (2012), and its rate of convergence using block relaxation theory by Yen et al. (2012). The CCCP was discussed in a wider optimization context by Lipp and Boyd (2015).

The starting point of Yuille and Rangarajan, in the context of energy functions for discrete dynamical systems, is the decomposition of a function f with bounded Hessian into a sum of a convex and a concave function. As we shall show in section 9.2.1 on differences of convex functions any function on a compact set with continuous second derivatives can be decomposed in this way. If $f = u + v$ with u convex and v concave, then the CCCP is the algorithm

$$\mathcal{D}u(x^{(k+1)}) = -\mathcal{D}v(x^{(k)}).$$

Now, by tangential majorization, $f(x) \leq g(x, y)$ with

$$g(x, y) = u(x) + v(y) + (x - y)'\mathcal{D}v(y).$$

The function g is convex in x, and consequently the majorization algorithm in this case is exactly the CCCP.

###Generalized Weiszfeld Methods

We discuss Weiszfeld's algorithm for the single facility location problem, or equivalently for the spatial median problem, in section 7.3.2. But, in an important early article, Voss and Eckhardt (1980) pointed out that Weiszfeld's algorithm is a member of a much more general class of algorithms, whch they called *Generalized Weiszfeld Methods*.

The problem Voß and Eckhardt consider is to minimize a twice continuously differentiable f over a polyhedron $\mathcal{X} \subseteq \mathbb{R}^n$, defined by a number of linear inequalities. They assume that f is bounded from below on $\mathcal{X}$ and that the sublevel sets $\{x \mid f(x) \leq \gamma\}$ have a empty of bounded intersection with $\mathcal{X}$. They define the quadratic approximation

$$g(x, y) = f(y) + (x - y)'\mathcal{D}f(y) + \frac{1}{2}(x - y)'A(y)(x - y)$$

for which they assume that $g(x, y) \geq f(x)$ for all $x \in \mathcal{X}$. In addition the spectral norm $\|A(y)\|$ is must be bounded from above on $\mathcal{X}$ by A_∞, and the smallest eigenvalue of $A(y)$ must be bounded from below on $\mathcal{X}$ by a positive number γ_0. Their algorithm is

$$x^{(k+1)} = \mathop{\mathbf{argmin}}_{x \in \mathcal{X}} g(x, x^{(k)}).$$

This, of course, is a majorization algorithm. In fact, it is an example of the quadratic mjaorization algorithms we discuss in detail in chapter 10. Voß and Eckhardt proceed to prove global convergence, which actually follows directly from Zangwill's theory, and local linear convergence, which follows from Ostrowski's theorem.

###The EM Algorithm

###The Lower-Bound Principle

2.4.2 Dinkelbach Majorization

Suppose f is defined on X and g on $X \otimes X$. Then we say that g *G-majorizes* f at $y \in X$ if

$$\begin{aligned} f(x) &\leq g(x,y), \\ f(y) &= g(y,y), \end{aligned}$$

We say that g G-majorizes f on X if it majorizes f for each $y \in X$.

Suppose f is defined on X and h on $X \otimes X$. Then we say that h *H-majorizes* f at $y \in X$ if

$$\begin{aligned} f(x) - f(y) &\leq h(x,y), \\ h(y,y) &= 0. \end{aligned}$$

Theorem: If h H-majorizes f at y, then g defined by $g(x,y) = f(y) + h(x,y)$ G-majorizes f at y. Conversely, if g G-majorizes f at y, then h defined by $h(x,y) = g(x,y) - f(y)$ H-majorizes f at y.

Suppose f is defined on X and h on $X \otimes X$. Then we say that h *D-majorizes* f at $y \in X$ if

$$\begin{aligned} h(x,y) < 0 &\Rightarrow f(x) < f(y), \\ h(y,y) &= 0. \end{aligned}$$

Theorem If h H-majorizes f at y, then h D-majorizes f at y.

The difference between D-majorization and H-majorization is that if $h(x,y) > 0$ we can have $f(x) - f(y) > h(x,y)$.

Quick note: D-majorization is also

$$g(x,y) = f(y) + h(x,y) < f(y) = g(y,y) \Rightarrow f(x) < f(y)$$

If $f(x) = a(x)/b(x)$, with $b(x) > 0$ for all $x \in X$, then $h(x,y) = a(x) - f(y)b(x)$ D-majorizes $f(x)$ at y.

##Further Results

###Rate of Convergence

Majorization is a special case of our results for augmentation previous theory, because $\mathcal{X} = \mathcal{Y}$ and because $y(x) = x$.

This implies that $\mathcal{D}_2(x,x) = 0$ for all x, and consequently $\mathcal{D}_{12} = -\mathcal{D}_{22}$. Thus $\mathcal{M}(x) = -\mathcal{D}_{11}^{-1}\mathcal{D}_{12}$.

Again, to some extent, finding a majorization function is an art. Many of the classical inequalities can be used (Cauchy-Schwarz, Jensen, H"older, Young, AM-GM, and so on).

###Univariate and Separable Functions

Many of our examples are majorizations of a real-valued function f of a single real variable over the real line $\mathbb{R}$. This is partly for mathematical convenience, because many results are simpler in the univariate case. And partly for didactic reasons, because plots and tables are more easy to visualize and interpret.

As pointed out by J. De Leeuw and Lange (2009) looking at the univariate case is obviously restrictive, but not as restrictive as it seems. Many of the functions in optimization and statistics are *separable*, which means they are of the form

$$f(x) = \sum_{i=1}^n f_i(x_i),$$

and majorizing each of the univariate f_i gives a majorization of f. Note that if $f(x) = \prod_{i=1}^n f_i(x)$, where the f_i are positive, can be turned into a separable problem by taking logarithms.

In addition it is often possible to majorize a non-separable function by a separable one. Suppose, for example, that

$$f(x) = \frac{1}{2}\sum_{i=1}^n\sum_{j=1}^n w_{ij}f_i(x_i)f_j(x_j),$$

where $W=\{w_{ij}\}$ is positive semi-definite. Suppose we can find a diagonal D such that $W\lesssim D$ then for any two vectors u and v in $\mathbb{R}^n$

$$\begin{aligned}u'Wu=(v+(u-v))'W(v+(u-v))\leq\\ v'Wv+(u-v)'Wv+(u-v)'D(u-v)=\\ (u-z)'D(u-z)+v'(W-WD^{-1}W)v,\end{aligned}$$

where $z\overset{\Delta}{=}(I-D^{-1}W)v$. Thus

$$f(x)\leq\frac{1}{2}\sum_{i=1}^n d_i(f_i(x)-z_i(y))^2+\frac{1}{2}\sum_{i=1}^n\sum_{j=1}^n h_{ij}f_i(y)f_j(y),$$

with $H\overset{\Delta}{=}W-WD^{-1}W$. The majorizer we have constructed is separable.

###Differentiable Functions

We first show that differentiable majorizations of differentiable functions must have certain properties at the support point.

Theorem: Suppose f and g are differentiable at y. If g majorizes f at y, then

- $g(y)=f(y)$,
- $g'(y)=f'(y)$,

If f and g are twice differentiable at y, then in addition

- $g''(y)\geq f''(y)$,

and if g majorizes f strictly

- $g''(y)>f''(y)$.

Proof: If g majorizes f at y then $g-f$ has a minimum at y. Now use the familiar necessary conditions for the minimum of a differentiable function, which say the derivative at the minimum is zero and the second derivative is non-negative. **QED**

The conditions in the theorem are only necessary because they are local, they only say something about the value of g and its derivatives at y. But majorization is a global relation to make global statements we need conditions like convexity. We already know that if $g-f$ is convex with a minimum at y equal to zero, then g majorizes f at y. For differentiable f and g this means that if $f-g$ is convex then g majorizes f at y if and only if $f(y)=g(y)$ and $f'(y)=g'(y)$. And for twice-differentiable f and g with $f''(x)\geq 0$ for all x again g majorizes f at y if and only if $f(y)=g(y)$ and $f'(y)=g'(y)$.

In the case of majorization at a single y we have $f'(y)=g'(y)$ for differentiable functions. If g majorizes f on $\mathcal{Y}\subseteq\mathcal{X}$ then $g(x,y)-f(x)\geq 0$ for all $x\in\mathcal{X}$ and all $y\in\mathcal{Y}$. Thus

$$0=g(y,y)-f(y)=\min_{x\in\mathcal{X}} g(x,y)-f(x)$$

for each $y\in\mathcal{Y}$. In addition

$$f(x)=g(x,x)=\min_{y\in\mathcal{Y}} g(x,y).$$

In the case of majorization at a single y we had $f'(y)=g'(y)$ for differentiable functions. In general the function f defined by $f(x)=\min_{y\in\mathcal{Y}} g(x,y)$ is not differentiable. If the partials $\mathcal{D}_1 g$ are continuous then the derivative at x in the direction z satisfies

$$df_z(x)=\min_y\{z'D_1g(x,y)\mid f(x)=g(x,y)\}.$$

In the case of strict majorization this gives

$$\mathcal{D}f(x)=\mathcal{D}_1g(x,x).$$

Theorem **??** can be generalized in many directions if differentiability fails. If f has a left and right derivatives in y, for instance, and g is differentiable, then

$$f'_R(y)\leq g'(y)\leq f'_L(y).$$

If f is convex, then $f'_L(y)\leq f'_R(y)$, and $f'(y)$ must exist in order for a differentiable g to majorize f at y. In this case $g'(y)=f'(y)$.

For nonconvex f more general differential inclusions are possible using the four Dini derivatives of f at y [see, for example, McShane, 1944, Chapter V].

Locally Lipschitz functions, Proximinal and Frechet and Clarke subgradients, sandwich and squeeze theorems

One-sided Chebyshev. Find $g \in \mathcal{G}$ such that $g \geq f$, $g(y) = f(y)$ and $\sup_x |g(x) - f(x)|$ is minimized. For instance $\mathcal{G}$ can be the convex functions, or the polynomials of a certain degree, or piecewise linear functions or splines.

###Composition

Theorem: [**Sum of functions**] Suppose h is defined on $\mathcal{X} \otimes \mathcal{U}$ and $f(x) = \int_U h(x,u)dF(u)$. Suppose k is defined on $\mathcal{X} \otimes \mathcal{X} \otimes \mathcal{U}$ and satisfies

$$h(x,u) = k(x,x,u) = \min_{y\in\mathcal{X}} k(x,y,u)$$

for all $x \in \mathcal{X}$ and $u \in \mathcal{U}$. Then g defined by

$$g(x,y) = \int_U k(x,y,u)dF(u)$$

satisfies

$$f(x) = \min_{y\in\mathcal{X}} g(x,y)$$

Proof: $h(x,u) = k(x,x,u) \leq k(x,y,u)$. Integrate to get $f(x) = g(x,x) \leq g(x,y)$. **QED**

Theorem: [**Inf of functions**] Suppose $f = \inf_u v(\bullet,u)$ and let $X(u) = \{x | f(x) = v(x,u)\}$. Suppose $y \in X(u)$ and g majorizes $v(\bullet,u)$ at y. Then g majorizes f at y.

Proof: $g(x) \geq v(x,u) \geq \inf_u v(x,u) = f(x)$, and because $y \in X(u)$ also $g(y) = v(y,u) = f(y)$. **QED**

Observe the theorem is not true for *sup*, and also we cannot say that if $w(\bullet,u)$ majorizes $v(\bullet,u)$ for all u at y, then $g = \inf_u w(\bullet,u)$ majorizes f at y.

Theorem: [**Composition of functions**] If g majorizes f at y and $\gamma : \mathbb{R} \rightarrow \mathbb{R}$ is non-decreasing, then $\gamma \circ g$ majorizes $\gamma \circ f$ at y. If, in addition, γ majorizes the non-decreasing $\eta : \mathbb{R} \rightarrow \mathbb{R}$ at $g(y)$, then $\gamma \circ g$ majorizes $\eta \circ f$.

Proof: $g(x) \geq f(x)$ and thus $\gamma(g(x)) \geq \gamma(f(x))$. Also $g(y) = f(y)$ and thus $\gamma(g(y)) = \gamma(f(y))$. For the second part we have $\gamma(g(x)) \geq \eta(g(x)) \geq \eta(f(x))$ and $\gamma(g(y)) = \eta(g(y)) = \eta(f(y))$. **QED**

Theorem: Suppose $f = \min_k f_k$ and let S_i be the set where $f = f_i$. If $y \in S_i$ and g majorizes f_i at y, then g majorizes f at y.

Proof: First $g(x) \geq f_i(x) \geq \min_k f_k(x) = f(x)$. Because $y \in S_i$ also $g(y) = f_i(y) = f(y)$. **QED**

This implies that if $f = \min_k f_k$ has a quadratic majorizer at each y, if each of the f_k has a quadratic majorizer at each y.

###Majorization Duality

Because $g(x,y) \geq g(x,x) = f(x)$ for all $x, y \in \mathcal{X}$ we have seen that

$$f(x) = \min_{y\in\mathcal{X}} g(x,y)$$

for all $x \in \mathcal{X}$. Thus

$$\min_{x\in\mathcal{X}} f(x) = \min_{x\in\mathcal{X}} \min_{y\in\mathcal{X}} g(x,y) = \min_{y\in\mathcal{X}} h(y).$$

where

$$h : y \rightarrow \min_{x\in\mathcal{X}} g(x,y).$$

Suppose, for example, that our majorization on $\mathcal{X}$ is of the form

$$g(x,y) = f(y) + (x-y)'\mathcal{D}f(y) + \frac{1}{2}(x-y)'A(y)(x-y),$$

with $A(y)$ positive definite for all y. This can be rewritten as

$$\begin{aligned} g(x,y) = f(y) - \frac{1}{2}(\mathcal{D}f(y))'A^{-1}(y)\mathcal{D}f(y)+ \\ + (x-z(y))'A(y)(x-z(y)), \end{aligned}$$

with $z(y) \overset{\Delta}{=} y - A^{-1}(y)\mathcal{D}f(y)$, and thus

$$\begin{aligned} h(y) = \min_{x\in\mathcal{X}} g(x,y) = f(y) - \frac{1}{2}(\mathcal{D}f(y))'(A(y))^{+}\mathcal{D}f(y)+ \\ + \min_{x\in\mathcal{X}}(x-z(y))'A(y)(x-z(y)). \end{aligned}$$

###Necessary Conditions by Majorization

Suppose g on $\mathcal{X}\otimes\mathcal{X}$ majorizes f on $\mathcal{X}$. We show that a necessary condition for $\hat{x}$ to be a minimizer of f on $\mathcal{X}$ is that $\hat{x}$ minimizes the majorization function $g(\bullet,\hat{x})$ on $\mathcal{X}$.

Theorem: If

$$\hat{x}\in\mathop{\mathbf{Arg\,min}}_{x\in\mathcal{X}} f(x),$$

then

$$\hat{x}\in\mathop{\mathbf{Arg\,min}}_{x\in\mathcal{X}} g(x,\hat{x}).$$

Proof: Suppose $\overline{x}\in\mathcal{X}$ is such that $g(\overline{x},\hat{x})<g(\hat{x},\hat{x})$. Then

$$f(\overline{x})\leq g(\overline{x},\hat{x})<g(\hat{x},\hat{x})=f(\hat{x}),$$

which contradicts that $\hat{x}$ minimizes f. **QED**

As an example, suppose that we have a quadratic majorization of the form

$$f(x)\leq f(y)+(x-y)'\mathcal{D}f(y)+\frac{1}{2}(x-y)'A(x-y),$$

with A positive definite. If $\hat{x}$ minimizes f over $\mathcal{X}$, then we must have

$$\hat{x}\in\mathop{\mathbf{Arg\,min}}_{x\in\mathcal{X}}\ (x-\hat{z})'A(x-\hat{z}),$$

with $\hat{z}\overset{\Delta}{=}\hat{x}-A^{-1}\mathcal{D}f(\hat{x})$. Thus $\hat{x}$ must be the weighted least squares projection of $\hat{z}$ on $\mathcal{X}$. If $\mathcal{X}$ is all of $\mathbb{R}^n$ then we must have $\hat{x}=\hat{z}$, which means $\mathcal{D}f(\hat{x})=0$.

For a concave function f on a bounded set we have $g(x,y)=f(y)+(x-y)'\mathcal{D}f(y)$, and thus the necessary condition for a minimum is

$$\hat{x}\in\mathop{\mathbf{Arg\,min}}_{x\in\mathcal{X}} x'\mathcal{D}f(\hat{x}).$$

###Majorizing Constraints

Consider the nonlinear programming problem of minimizing f_0 over $x\in\mathcal{X}$ under the *functional constraints* $f_i(x)\leq 0$ for $i=1,\cdots,n$.

Suppose g_i majorizes f_i on $\mathcal{X}$. Consider the algorithm

$$x^{(k+1)}\in\mathop{\mathbf{argmin}}_{x\in\mathcal{X}}\{g_0(x,x^{(k)})\mid g_i(x,x^{(k)})\leq 0\}.$$

Lipp and Boyd [2014] propose this algorthm for the case in which the f_i are DC (differences of convex functions), as a generalization of the Convex-Concave procedure of II.1.3.2. We show the algorithm is stable. Remember that $x \in \mathcal{X}$ is *feasible* if it satisfies the functional constraints.

Result: If $x^{(k)}$ is feasible, then $x^{(k+1)}$ is feasible and $f_0(x^{(k+1)}) \leq f_0(x^{(k)})$.

Proof: By majorization, for $i = 1, \cdots, n$ we have

$$f_i(x^{(k+1)}) \leq g_i(x^{(k+1)}, x^{(k)}) \leq 0.$$

Second, the sandwich inequality says

$$f_0(x^{(k+1)}) \leq g_0(x^{(k+1)}, x^{(k)}) \leq g_0(x^{(k)}, x^{(k)}) = f_0(x^{(k)}).$$

QED

Note that it may not be necessary to majorize all functions f_i. Or, in other words, for some we can choose the trivial majorization $g_i(x, y) = f_i(x)$.

###Majorizing Value Functions

Suppose $f(x) = \max_{y \in \mathcal{Y}} g(x, y)$ and $g(x, y) = \min_{z \in \mathcal{X}} h(x, y, z)$, i.e. $h(x, y, z) \geq g(x, y)$ for all $x, z \in \mathcal{X}$ and $y \in \mathcal{Y}$ and $h(x, y, x) = g(x, y)$ for all $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, by weak duality,

$$f(x) = \max_{y \in \mathcal{Y}} \min_{z \in \mathcal{X}} h(x, y, z) \leq \min_{z \in \mathcal{X}} \max_{y \in \mathcal{Y}} h(x, y, z) = \min_{z \in \mathcal{X}} k(x, z),$$

where

$$k(x, z) \overset{\Delta}{=} \max_{y \in \mathcal{Y}} h(x, y, z).$$

Note that

$$k(x, x) = \max_{y \in \mathcal{Y}} h(x, y, x) = \max_{y \in \mathcal{Y}} g(x, y) = f(x),$$

which means that actually

$$f(x) = \min_{z \in \mathcal{X}} k(x, z)$$

and thus k majorizes f in z.

Note: See how the following fits in 03/07/15. Or does it ?

Suppose the problem we want to solve is minimizing $g(x, y)$ over $x \in X$ and $y \in Y$. If both minimizing $g(x, y)$ over $x \in X$ for fixed $y \in Y$ and minimizing

$g(x, y)$ over $y \in Y$ for fixed $x \in X$ is easy, then we often use block-relaxation, alternating the two conditional minimization problems until convergence.

But now suppose only one of the two problems, say minimizing $g(x, y)$ over $y \in Y$ for fixed $x \in X$, is easy. Define

$$f(x) = \min_{y \in Y} g(x, y)$$

and let $y(x)$ be any $y \in Y$ such that $f(x) = g(x, y(x))$.

Suppose we have a majorizing function $h(x, z)$ for $f(x)$. Thus

$$\begin{aligned} f(x) &\leq h(x, z) \qquad &\forall x, z \in X, \\ f(x) &= h(x, x) \qquad &\forall x \in X. \end{aligned}$$

Suppose our current best solution for x is $\tilde{x}$, with corresponding $\tilde{y} = y(\tilde{x})$. Let x^+ be any minimizer of $h(x, \tilde{x})$ over $x \in X$. Now

$$g(x^+, y(x^+)) = f(x^+) \leq h(x^+, \tilde{x}) \leq h(\tilde{x}, \tilde{x}) = f(\tilde{x}) = g(\tilde{x}, y(\tilde{x}))$$

which means that $(x^+, y(x^+))$ gives a lower loss function value than $(\tilde{x}, y(\tilde{x}))$. Thus we have, under the usual conditions, a convergent algorithm.

Note: See how the following fits in 03/13/15. Or does it ?

Suppose $g(x) = \min_{y \in \mathcal{Y}} f(x, y)$ and $f(x, y) = \min_{z \in \mathcal{X}} h(x, z, y)$. Define $k(x, z) \overset{\Delta}{=} \min_{y \in \mathcal{Y}} h(x, z, y)$. Then

$$g(x) = \min_{y \in \mathcal{Y}} f(x, y) = \min_{y \in \mathcal{Y}} \min_{z \in \mathcal{X}} h(x, z, y) = \min_{z \in \mathcal{X}} \min_{y \in \mathcal{Y}} \min_{z \in \mathcal{X}} h(x, z, y) = \min_{z \in \mathcal{X}} k(x, z).$$

$$k(x, x) = \min_{y \in \mathcal{Y}} h(x, x, y) = \min_{y \in \mathcal{Y}} f(x, y) = g(x)$$

Not necessary that $\mathcal{Y} = \mathcal{X}$. Only h has to majorize f for k to majorize, f can be anything. This may be in the composition section.

##Some Examples

###The Reciprocal

Minimizing the function $f(x) = ax - \log(x)$, where $a > 0$ is a constant, over $x > 0$ is trivial. The first and second derivatives of f are

$$f'(x) = a - \frac{1}{x},$$

and

$$f''(x) = \frac{1}{x^2}.$$

We see from $f''(x) > 0$ that f is strictly convex on the positive reals. It has its unique minimum for $a - 1/x = 0$, i.e. for $x = 1/a$, and the minimum value is $1 + \log(a)$.

Thus iterative algorithms to minimize the function, which can also be thought of as iterative algorithms to compute the reciprocal of a positive number a, are of little interest in themselves. But it is of some interest to compare various algorithms, such as different majorization methods, in terms of robustness, speed of convergence, and so on.

Here are plots of the function f for $a = 1/3$ and for $a = 3/2$.

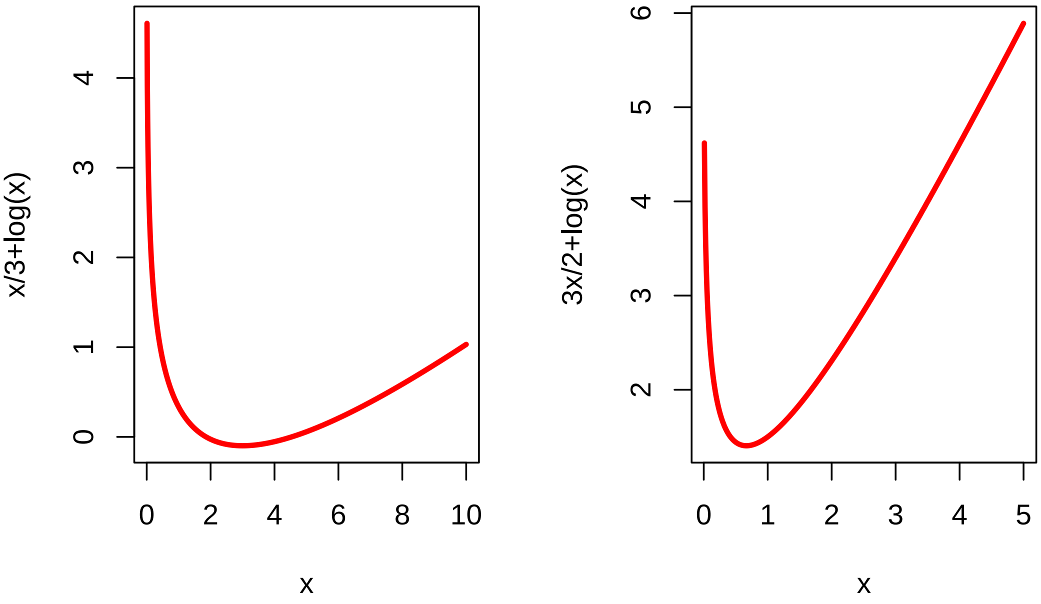


Figure 1: ax+log(x) for a = 1/3 (left) and a=3/2 (right)

Because $-\log(x) = \log(1/x)$ the concavity of the logarithm shows that

$$\log(\frac{1}{x}) \leq \log(\frac{1}{y}) + y\left(\frac{1}{x} - \frac{1}{y}\right),$$

or

$$-\log(x) \leq -\log(y) + \frac{y}{x} - 1.$$

Thus

$$g(x,y) = ax - \log(y) + \frac{y}{x} - 1$$

majorizes f, and minimizing the majorizer gives the very simple algorithm

$$x^{(k+1)} = \sqrt{\frac{x^{(k)}}{a}}.$$

The derivative of the update function $h(x) \overset{\Delta}{=} \sqrt{x/a}$ at $1/a$ is $1/2$. Thus our majorization iterations have linear convergence, with ratio $1/2$. If $x^{(0)} < 1/a$ the algorithm generates an increasing sequence converging to $1/a$. If $x^{(0)} > 1/a$ we have a decreasing sequence converging to $1/a$. Because $ax^{(k+1)} = \sqrt{ax^{(k)}}$ we have the explicit expression

$$x^{(k)} = a^{\left(\frac{1}{2^k}-1\right)}\left(x^{(0)}\right)^{\left(\frac{1}{2^k}\right)}.$$

Here we show the majorization for $a = 3/2$ and y equal to $1/10, 1$ and $3/2$.

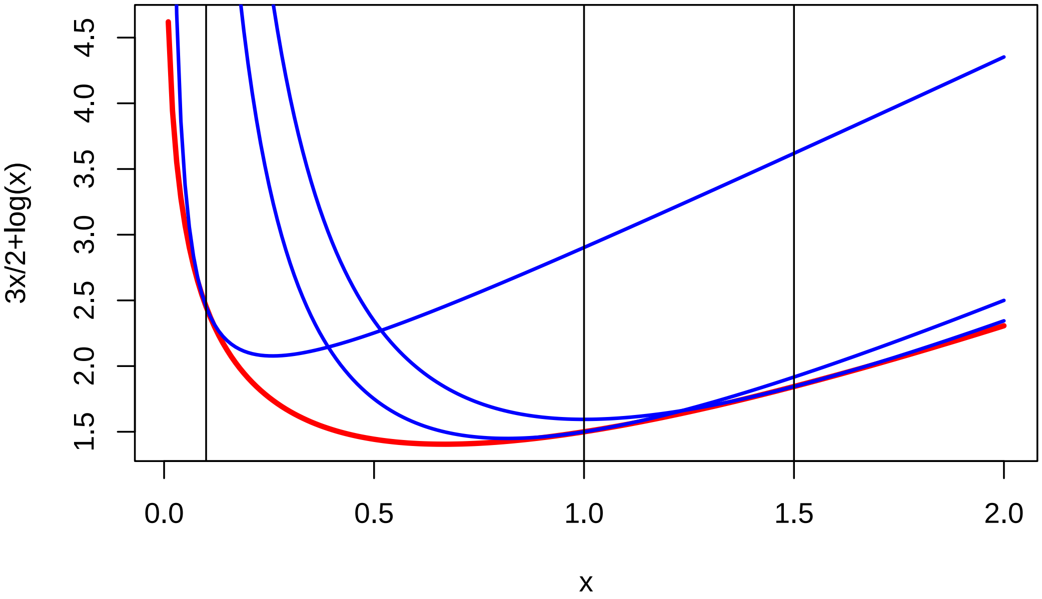


Figure 2: Majorization of 3x/2+log(x) at y=1/10,1, and 3/2

###Cubics and Quartics

Suppose f is a cubic, which is non-trivial in the sense that its third derivative is non-zero. Thus f has no minimum or maximum, because it is unbounded below and above. This immediately shows there can be no linear or quadratic majorizer g of f, because if there was then $g-f$ would be a non-trivial cubic, which does not have a minimum.

For a quadratic g to majorize a non-trivial quartic f at y we must have

$$f(y)+f'(y)(x-y)+\frac{1}{2}f''(y)(x-y)^2+\frac{1}{6}f'''(y)(x-y)^3+\frac{1}{24}f^{iv}(x-y)^4\leq \\ f(y)+f'(y)(x-y)+\frac{1}{2}c(x-y)^2,$$

for all x. Of course $f^{iv}(y)$ is a constant, independent of y, for a quartic. This can be written as $\frac{1}{2}(x-y)^2q(x)\leq 0$ for all x, where

$$q(x)\stackrel{\Delta}{=}(f''(y)-c)+\frac{1}{3}f'''(y)(x-y)+\frac{1}{12}f^{iv}(y)(x-y)^2.$$

If $f^{iv}>0$ no quadratic majorization exists. If $f^{iv}<0$ we complete the square to

$$q(x)=\frac{1}{12}f^{iv}\left(x-y+2\frac{f'''(y)}{f^{iv}}\right)^2+\left(f''(y)-\frac{1}{3}\frac{(f'''(y))^2}{f^{iv}}-c\right),$$

and see we must have

$$c\geq c(y)\stackrel{\Delta}{=}f''(y)-\frac{1}{3}\frac{(f'''(y))^2}{f^{iv}}.$$

Example 1: In our first example we use the polynomial $f(x)=1+5x+5x^2-5x^3-6x^4$, and we show quadratic majorizers using $c=c(y)$ for y equal to $-.75,-.25,+.25$, and $+.75$.

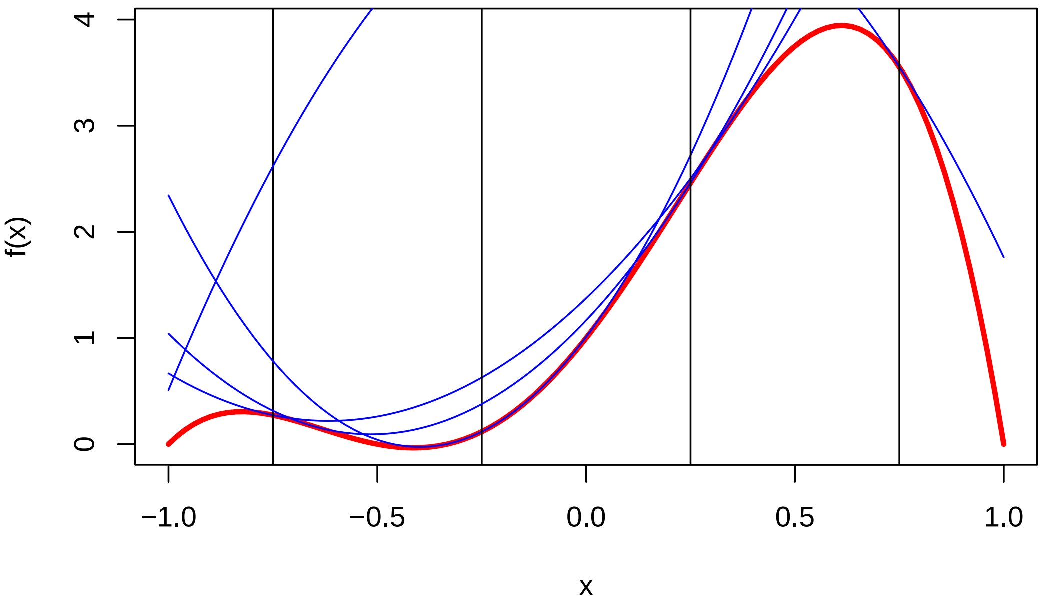


Figure 1: Quadratic Majorization of a Quartic

Note that the quadratic majorizer for $y = .75$ is concave, which means it does not have a minimum and we cannot carry out a majorization step. All four majorizers have two support points, one at y and the other at $y - 2\frac{f'''(y)}{f^{iv}(y)}$, which is the solution of $q(x) = 0$ if $c = c(y)$. The `R` code for drawing the figures is in `quarticCubicMe.R`. Note the function `quarticCubicMe` does not return anything, it is merely used for its graphical side effects.

Insert quarticCubicMe.R Here

The majorization algorithm corresponding to our quadratic majorization is

$$x^{(k+1)} = x^{(k)} - \frac{f'(x^{(k)})}{c(x^{(k)})}.$$

If it converges to a stationary point at x with $f'(x) = 0$ and $f''(x) \geq 0$ then the iteration radius is

$$\kappa(x) = 1 - \frac{f''(x)}{c(x)}.$$

Note that in the quartic case both f'' and c are quadratics, so the convergence rate λ is a ratio of two quadratics. If $f''(x) > 0$ and $f'''(x) \neq 0$ then $0 < \lambda(x) < 1$. If $f'''(x) = 0$ then $\lambda(x) = 0$ and we have superlinear convergence. If $f''(x) = 0$ and $f'''(x) \neq 0$ we have $\lambda(x) = 1$ and convergence is sublinear.

Example 2: We illustrate this with the quartic

$$f(x) = +\frac{5}{6}x + \frac{3}{4}x^2 + \frac{1}{6}x^3 - \frac{1}{24}x^4$$

which has both $f'(-1) = 0$ and $f''(-1) = 0$. Quadratic majorizers are shown in Figure 2.

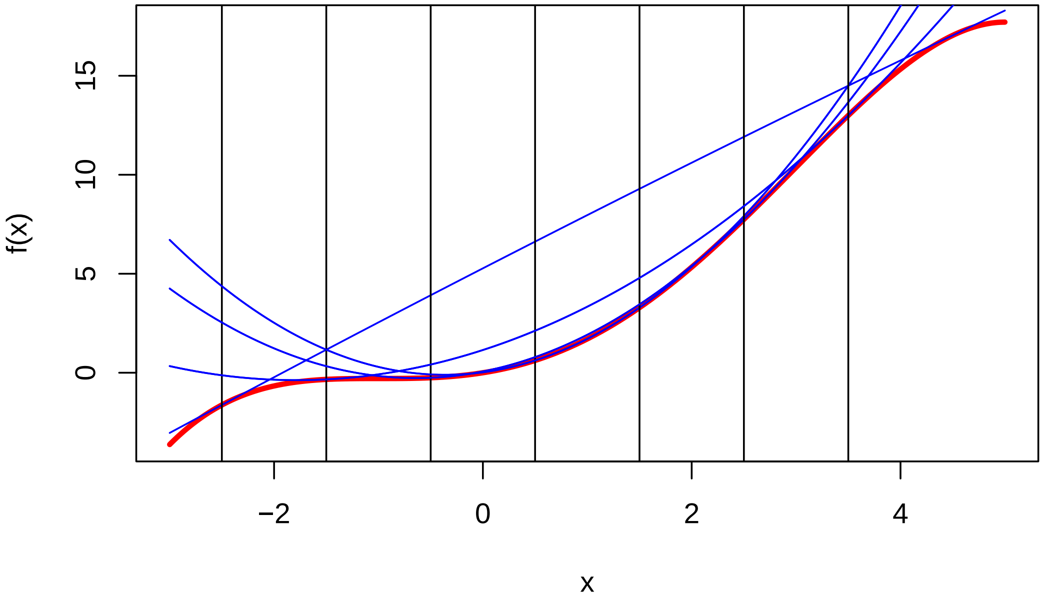


Figure 2: Quadratic Majorization of a Quartic at a Saddlepoint

The iterative majorization algorithm in `itQuartic.R`, which stops if we have reached a solution to within 1e-10, has not converged after 100,000 iterations.

```
Iteration:  100000 xold:   -0.99998667 xnew:   -0.99998667 fold:   -0.29166667 fnew:
$x
[1] -0.9999867

$lbd
[1] 0.99998
```

Insert itQuartic.R Here

Example 3: The next quartic has $f'(1) = 0$ and $f'''(1) = 0$. This implies that $f(1 + x) = f(1 - x)$ for all x, which in turn implies that quadratic majorizers using $c = c(y)$ have their minima or maxima at 1. We identify the polynomial by requiring $f(0) = 0$, $f''(1) = 1$ and $f^{iv}(1) = 1$. This gives

$$f(x) = -\frac{5}{6}x + \frac{1}{4}x^2 + \frac{1}{6}x^3 - \frac{1}{24}x^4.$$

Quadratic majorizers are in Figure 3.

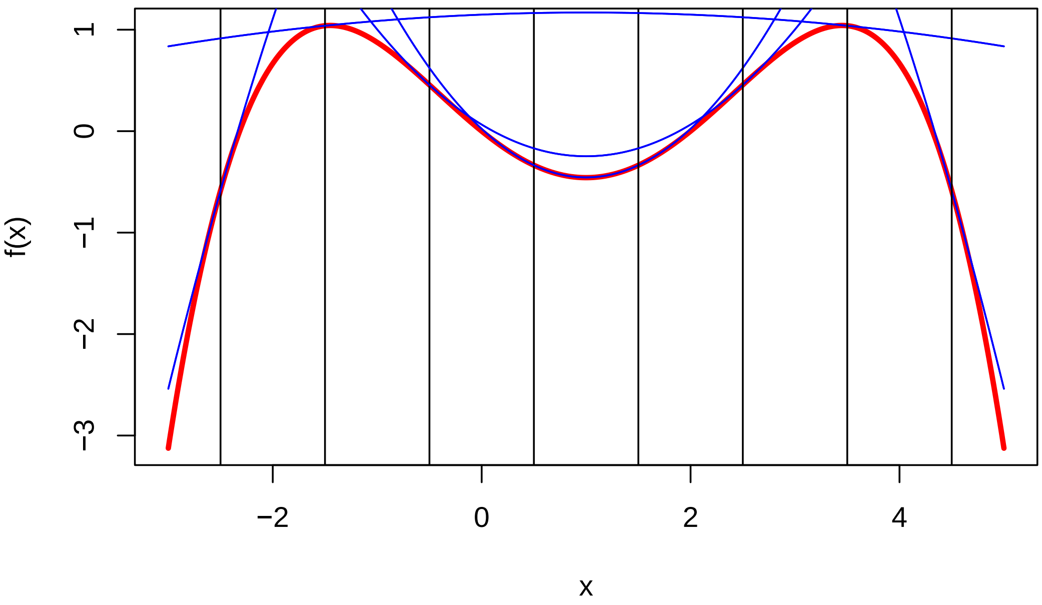


Figure 3: Quadratic Majorization of a Symmetric Quartic

In this case the majorization algorithm converges to the solution $x = 1$ in a single iteration, no matter where we start. This is true even if the quadratic is concave, because then the update actually goes to the *maximum* of the majorizing quadratic (which means that, strictly speaking, we do not make a majorization step).

If we want to majorize a quartic f by a cubic

$$g(x) = f(y) + f'(y)(x - y) + \frac{1}{2}c(x - y)^2 + \frac{1}{6}d(x - y)^3,$$

then we can use the same reasoning as before to come up with

$$c \geq c_d(y) \triangleq f''(y) - \frac{1}{3}\frac{(f'''(y)-d)^2}{f^{iv}}.$$

In each iteration we have to minimize the cubic g over x. This needs to be qualified, of course, because the cubic does not have a minimum. So we modify the rule to choosing the local minimum of the cubic, if there is one. Differentiating the implicit function for the update x^+ gives

$$\mathcal{D}x^+(y) = 1 - \frac{f''(y)}{c + d(x^+(y) - y)},$$

and thus at a fixed point x the iteration radius, using $c = c_d(y)$, it is

$$\lambda(x) = 1 - \frac{f''(x)}{c_d(x)}.$$

We have fast convergence if d is close to $f'''(x)$, and superlinear convergence if $d = f'''(x)$.

Example 4: In Figure 4 we use the quartic $1+5x+5x^2-5x^3-6x^4$ again to illustrate cubic majorization with d cleverly chosen to be $f'''(x_\infty)$. The cubic majorization functions are much closer than the quadratic ones in Figure 1.

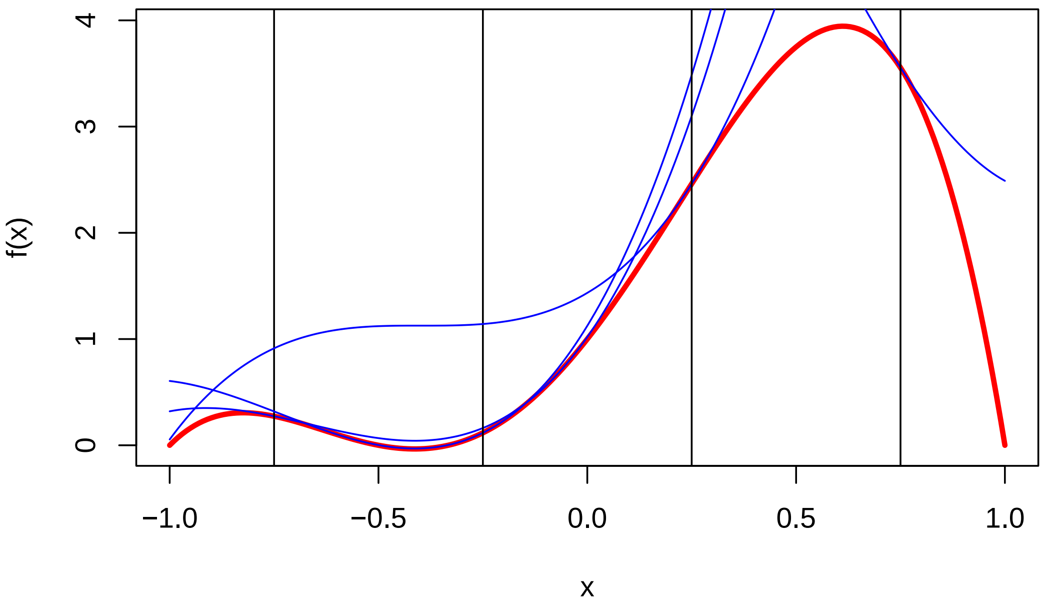


Figure 4: Cubic Majorization of a Quartic

Table 1 shows different iteration counts for different values of d. In this case we have $f'''(x) = 29.50256$, where $x = -0.4132122$.

d	*iterations*	*rate*
0	11	0.16627
5	11	0.12093
10	10	0.08016
15	09	0.04598
20	08	0.02027
25	06	0.00462
30	04	0.00005

Table 1: Cubic Majorization of a Quartic

###Normal PDF and CDF

For a nice regular example we use the celebrated functions

$$\begin{aligned}\phi(x) &= \frac{1}{\sqrt{2\pi}}e^{-z^2/2},\\ \Phi(x) &= \int_{-\infty}^{x}\phi(z)\,dz.\end{aligned}$$

Of course $\Phi'(x) = \phi(x)$. And consequently

$$\begin{aligned}\Phi''(x) &= \phi'(x) = -x\phi(x),\\ \Phi'''(x) &= \phi''(x) = -(1-x^2)\phi(x),\\ \Phi^{iv}(x) &= \phi'''(x) = -x(x^2-3)\phi(x).\end{aligned}$$

To obtain quadratic majorizers we must bound the second derivatives. We can bound $\Phi''(x)$ by setting its derivative equal to zero. We have $\Phi'''(x) = 0$ for $x = \pm 1$, and thus $|\Phi''(x)| \leq \phi(1)$. In the same way $\phi'''(x) = 0$ for $x = 0$ and $x = \pm\sqrt{3}$. At those values $|\phi''(x)| \leq 2\phi(\sqrt{3})$. More precisely, it follows that

$$\begin{aligned}0 \leq \Phi'(x) = \phi(x) &\leq \phi(0),\\ -\phi(1) \leq \Phi''(x) = \phi'(x) &\leq \phi(1),\\ -\phi(0) \leq \Phi'''(x) = \phi''(x) &\leq 2\phi(\sqrt{3}).\end{aligned}$$

Thus we have the quadratic majorizers

$$\Phi(x) \leq \Phi(y) + \phi(y)(x-y) + \frac{1}{2}\phi(1)(x-y)^2,$$

and

$$\phi(x) \leq \phi(y) - y\phi(y)(x-y) + \phi(\sqrt{3})(x-y)^2.$$

The majorizers are illustrated for both Φ and ϕ at the points $y = 0$ and $y = -3$ in Figure 1.

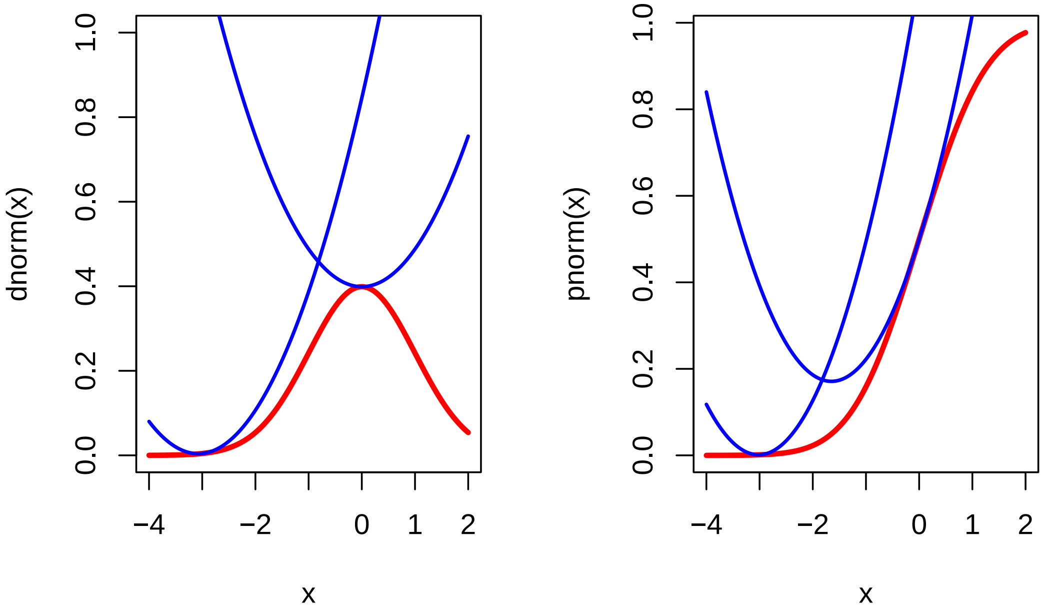


Figure 1: Quadratic Majorization of Normal PDF and CDF

The inequalities in this section may be useful in majorizing multivariate functions involving ϕ and Φ. They are mainly intended, however, to illustrate construction of quadratic majorizers in the smooth case.

###Logistic PDF and CDF

#Majorization Inequalities

##Introduction

2.5 The AM/GM Inequality

###Absolute Values

###Absolute Values

Suppose the problem we have to solve is to minimize

$$f(x)=\sum_{i=1}^n w_i|h_i(x)|$$

over $x\in\mathcal{X}$. Here $h_i(x)$ is supposed to be differentiable. In statistics it typically is a residual, for instance $h_i(x)=y_i-z_i'x$. Suppose, for the time being, that $h_i(x)\neq 0$. Then we have the majorization

$$\sum_{i=1}^n w_i|h_i(x)|\leq\frac{1}{2}\sum_{i=1}^n\frac{w_i}{|h_i(y)|}(h_i^2(x)+h_i^2(y)),$$

and we must minimize

$$g(x,y):=\sum_{i=1}^n\frac{w_i}{|h_i(y)|}h_i^2(x),$$

which is a weighted least squares problem.

The simplest case of this is the one-dimensional example is $h_i(x)=y_i-x$, which means we want to compute the weighted median. The algorithm is simply

$$x^{(k+1)}=\frac{\sum_{i=1}^n u_i(x^{(k)})y_i}{\sum_{i=1}^n u_i(x^{(k)})},$$

where

$$u_i(x)=\frac{w_i}{\mid y_i-x\mid}.$$

We have assumed, so far, in this example that $h_i(y)\neq 0$. If $h_i(y)=0$ at some point in the iterative process then the majorization function does not exist, and we cannot compute the upgrade. One easy way out of this problem is to minimize

$$f_\epsilon(x)=\sum_{i=1}^n w_i\sqrt{h_i^2(x)+\epsilon^2}$$

for small values of ϵ. Clearly if $\epsilon_1 > \epsilon_2$ then

$$\min_x f_{\epsilon_1}(x) = f_{\epsilon_1}(x_1) > f_{\epsilon_2}(x_1) \geq \min_x f_{\epsilon_2}(x).$$

It follows that

The function f_ϵ is differentiable. We find

$$\mathcal{D}f_\epsilon(x) = \sum_{i=1}^n w_i \frac{h_i(x)}{\sqrt{h_i^2(x)+\epsilon^2}} \mathcal{D}h_i(x),$$

and

$$\mathcal{D}^2 f_\epsilon(x) = \sum_{i=1}^n w_i \frac{1}{\sqrt{h_i^2(x)+\epsilon^2}} \left\{ \frac{\epsilon^2}{h_i^2(x)+\epsilon^2} \left(\mathcal{D}h_i(x)\right)^2 + h_i(x)\mathcal{D}^2 h_i(x) \right\}.$$

With obvious modifications the same formulas apply if x is a vector of unknowns, for instance if $h(x) = y - Zx$.

By the implicit function theorem the function $x(\epsilon)$ defined by $\mathcal{D}f_\epsilon(x(\epsilon)) = 0$ is differentiable, with derivative

$$\mathcal{D}x(\epsilon) = \epsilon \frac{\sum_{i=1}^n w_i \left[h_i^2(x(\epsilon))^2 + \epsilon^2\right]^{-\frac{3}{2}} h_i(x(\epsilon))\mathcal{D}h_i(x(\epsilon))}{\mathcal{D}^2 f_\epsilon(x(\epsilon))}$$

For the weighted median the iterates are still the same weighted averages, but now with weights

$$u_i(x,\epsilon) = \frac{w_i}{\sqrt{(y_i - x)^2 + \epsilon^2}}.$$

Differentiating the algorithmic map gives the convergence ratio

$$\kappa_\epsilon(x) \triangleq \frac{\sum_{i=1}^n u_i(x,\epsilon) \frac{(y_i-x)^2}{(y_i-x)^2+\epsilon^2}}{\sum_{i=1}^n u_i(x,\epsilon)}.$$

Clearly

$$\min_i \frac{(y_i-x)^2}{(y_i-x)^2+\epsilon^2} \leq \kappa_\epsilon(x) \leq \max_i \frac{(y_i-x)^2}{(y_i-x)^2+\epsilon^2},$$

which implies $\kappa_\epsilon(x) < 1$. If $y_i \neq x$ for all i, then $\lim_{\epsilon\rightarrow 0} \kappa_\epsilon(x) = 1$ and convergence is asymptotically sublinear.

Insert mediJan.R Here

2.5.1 Gini Mean Difference

Alternatively, we can minimize the Gini Mean Difference of the $f_i(\theta)$. Now

$$\sum_{i=1}^n\sum_{j=1}^n \mid f_i(\theta)-f_j(\theta)\mid\leq$$

$$\sum_{i=1}^n\sum_{j=1}^n\frac{1}{\mid f_i(\xi)-f_j(\xi)\mid}(f_i(\theta)-f_j(\theta))^2+\text{terms},$$

which can be rewritten as

$$\cdots=\sum_{i=1}^n\sum_{j=1}^n w_{ij}(\xi)f_i(\theta)f_j(\theta)+\text{terms},$$

minimization of which is a weighted least squares problem.

###Location Problems

The *Fermat-Weber problem* is to find a point $x\in\mathbb{R}^m$ such that the sum of the Euclidean distances to m given points $y_1,\cdots,y_m$ is minimized. Thus our loss function is

$$f(x)=\sum_{j=1}^m w_jd(x,y_j),$$

where the w_j are positive weights. Other names are the *single facility location problem* or the *spatial median* problem.

An early iterative algorithm to solve the Fermat-Weber problem was proposed by Weiszfeld (1937). For a translation see Weiszfeld and Plastria (2009).

Here we show how to use the arithmetic mean-geometric mean inequality for majorization. Suppose our problem is to minimize

$$f(X)=\sum_{i=1}^n\sum_{j=1}^n w_{ij}d_{ij}(X),$$

where the w_{ij} are non-negative weights, and the $d_{ij}(X)$ are again Euclidean distances. This is a *location problem.* To make it interesting, we suppose that some of the points (facilities) are fixed, others are the variables we have to minimize over. Observe that this is a convex, but non-differentiable, optimization problem.

We use the AM-GM inequality in the form

$$d_{ij}(X)d_{ij}(Y) \leq \frac{1}{2}(d_{ij}^2(X) + d_{ij}^2(Y)).$$

If $d_{ij}(Y) > 0$ then

$$d_{ij}(X) \leq \frac{1}{2}\frac{d_{ij}^2(X) + d_{ij}^2(Y)}{d_{ij}(Y)}.$$

Using the notation from Example a.a we now find

$$\phi(X) \leq \frac{1}{2}(\text{tr } X'B(Y)X + \text{tr } Y'B(Y)Y),$$

which gives us a quadratic majorization.

If X is partitioned into X_1 and X_2, with rows which are fixed and rows which are to be determined (facilities which have to be located), and B is partitioned correspondingly, then the algorithm we find is

$$X_2^{(k+1)} = B_{22}(X^{(k)})^{-1}B_{21}(X^{(k)})X_1.$$

2.5.2 The Lasso and the Bridge

##Polar Norms and the Cauchy-Schwarz Inequality

2.5.3 Rayleigh Quotient

Rewrite for minimizing 02/22/15, by maximizing x'Bx over x'Ax=1.

We go back to maximizing the Rayleigh quotient

$$\lambda(x) = \frac{x'Ax}{x'Bx},$$

where we now assume that both A and B are positive definite. Maximizing λ is equivalent to maximizing $\sqrt{x'Ax}$ on the condition that $\sqrt{x'Bx} = 1$. By Cauchy-Schwartz

$$\sqrt{x'Ax} \geq \frac{1}{\sqrt{y'Ay}}x'Ay,$$

and thus for the majorization we maximize $x'Ax$ over $x'Bx = 1$. This defines an algorithmic map which sets the update of x proportional to $B^{-1}Ax$, i.e. we have a shown global convergence of the power method to compute the largest generalized eigenvalue.

We can also establish the linear convergence rate quite easily, using Ostrowski (1966). For definiteness we normalize in each iteration, and set

$$\mathcal{A}(\omega) = \frac{B^{-1}A\omega}{\|B^{-1}A\omega\|}.$$

At a point ω which has $B^{-1}A\omega = \lambda_1\omega$, and $\omega'\omega = 1$ we have

$$\mathcal{M}(\omega) = \frac{1}{\lambda_1}(I - \omega\omega')B^{-1}A.$$

It follows that $\mathcal{M}$ has eigenvalues 0 and $\frac{\lambda_s}{\lambda_1}$, with λ_s the "remaining'' eigenvalues of $B^{-1}A$. Thus if λ_1 is the largest eigenvalue, we find a linear rate of $\rho = \frac{\lambda_1}{\lambda_2}$.

There are several things in this analysis which may go wrong, and they are all quite instructive.

2.5.4 The Majorization Method for MDS

The first is an algorithm for multidimensional scaling, developed by J. De Leeuw (1977). We want to minimize

$$\sigma(X) = \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} w_{ij}(\delta_{ij} - d_{ij}(X))^2,$$

with $d_{ij}(X)$ again Euclidean distance, i.e.

$$d_{ij}(X) = \sqrt{(x_i - x_j)'(x_i - x_j)}.\check{\text{N}}$$

We suppose weights w_{ij} and dissimilarities δ_{ij} are symmetric and hollow (zero diagonal), and satisfy

$$\frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} w_{ij}\delta_{ij}^2 = 1.$$

We now define the following objects

$$\eta^2(X) \triangleq \sum_{i=1}^{m}\sum_{j=1}^{m} w_{ij}d_{ij}(X)^2, \tag{2.6}$$

$$\rho(X) \triangleq \sum_{i=1}^{m}\sum_{j=1}^{m} w_{ij}\delta_{ij}d_{ij}(X). \tag{2.7}$$

Thus

$$\sigma(X) = 1 - 2\rho(X) + \frac{1}{2}\eta^2(X).$$

The next step is to use matrices. Let

$$v_{ij} = \begin{cases} -w_{ij} & \text{if } i \neq j, \\ \sum_{k\neq i}^{m} w_{ik} & \text{if } i = j, \end{cases} \tag{2.8}$$

$$b_{ij}(X) = \begin{cases} -\frac{w_{ij}\delta_{ij}}{d_{ij}(X)} & \text{if } i \neq j, \\ \sum_{k\neq i}^{m} \frac{w_{ik}\delta_{ik}}{d_{ik}(X)} & \text{if } i = j. \end{cases} \tag{2.9}$$

Now

$$\sigma(X) = 1 - \text{tr}X'B(X)X + \frac{1}{2}\text{tr}X'VX.$$

By Cauchy-Schwarz,

$$d_{ij}(X) \geq \frac{(x_i - x_j)'(y_i - y_j)}{d_{ij}(Y)},$$

which implies

$$\text{tr}X'B(X)X \geq \text{tr}X'B(Y)Y.$$

Now let

$$\overline{X} = V^+B(X)X.$$

This is called the *Guttman-transform* of a matrix X. Using this transform we see that for all pairs of configurations (X, Y)

$$\sigma(X) \leq 1 - \text{tr } X'B(Y)Y + \frac{1}{2}\text{tr } X'VX = \tag{2.10}$$

$$= 1 - \text{tr } XV\overline{Y} + \frac{1}{2}\text{tr } X'VX = \tag{2.11}$$

$$= 1 - \frac{1}{2}\text{tr } \overline{Y}'V\overline{Y} + \frac{1}{2}\text{tr } (X - \overline{Y})'V(X - \overline{Y}), \tag{2.12}$$

while for all configurations

$$X$$

we have

$$\sigma(X)=1-\frac{1}{2}\mathrm{tr}\ \overline{X}'V\overline{X}+\frac{1}{2}\mathrm{tr}\ (X-\overline{X})'V(X-\overline{X}).$$

##Conjugates and Young’s Inequality

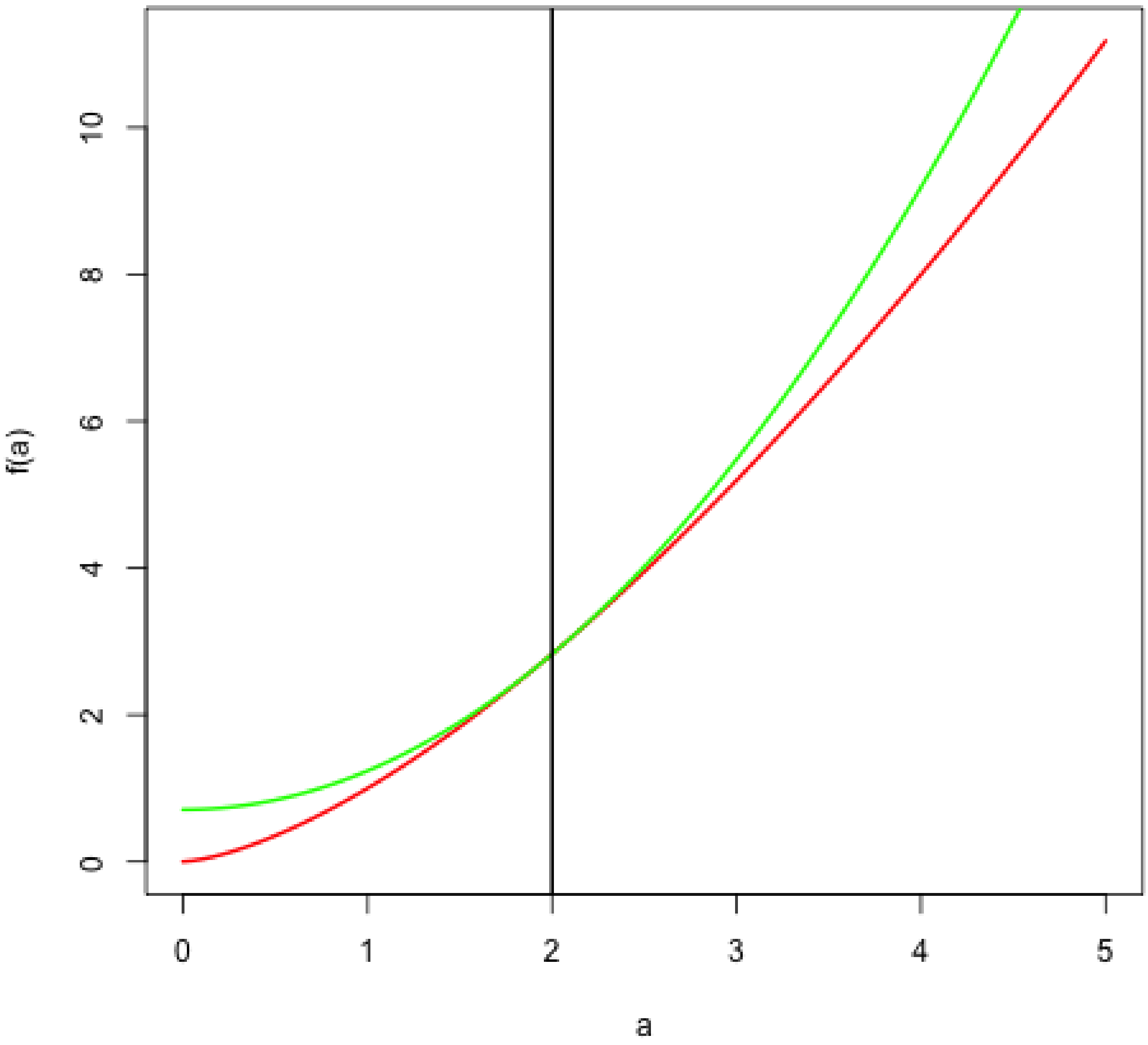
Example: Let $0<r<2$, $p=\frac{2}{r}$, and $q=\frac{2}{2-r}$. Then the previous result, applied to x^r and y^{2-r}, becomes

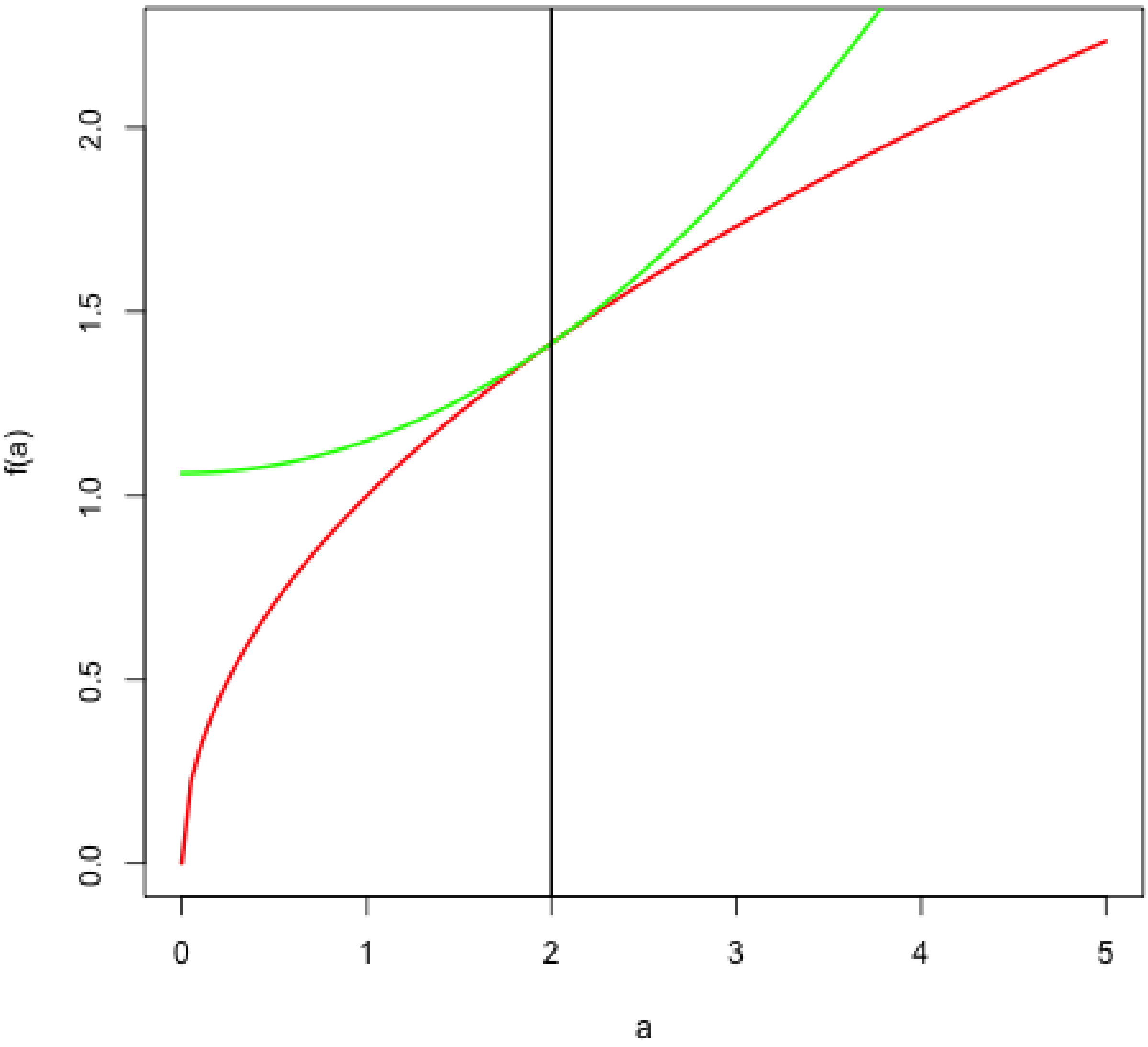
$$x^ry^{2-r}\leq\frac{r}{2}x^2+\frac{2-r}{2}y^2,$$

which provides us with a quadratic majorization for x^r for all $0<r<2$. We have equality if and only if $x=y$.

```
showMe <- function (b, r, up = 5) {
    a <- seq (0, up, length = 100)
    ar <- a ^ r
    plot (a, ar, type = "l", col = "RED",
          ylab="f(a)", lwd = 2)
    br <- (r * (a ^ 2)) / 2 + (((2 - r)  * (b ^ 2))/ 2)
    br <- br / (b ^ (2 - r))
    lines (a, br, col = "GREEN", lwd = 2)
    abline (v = b, lwd = 2)
}
```

Here is an example with $y=2$ and $r=1.5$.


f(a)
0
2
4
6
8
10
0
1
2
3
4
5
a



One important application of these results is majorization of powers of Euclidean distances $(\sqrt{x'Ax})^r$ by quadratic forms. We find, for $0 < r < 2$,

$$(\sqrt{x'Ax})^r \leq \frac{1}{(\sqrt{y'Ay})^{(2-r)}}\left\{\frac{r}{2}x'Ax+\frac{2-r}{2}y'Ay\right\}$$

###Support Vector Machines

Chapter 3

Using Convexity

3.1 Using Convexity

There are two major ways in which we use convexity in majorization.

First, we can use the definition of convex functions directly. Thus we rely on the inequality

$$f(\sum_{i=1}^n w_i x_i) \geq \sum_{i=1}^n w_i f(x_i),$$

where the w_i are non-negative weights adding up to one. This inequality separates the variables, in the sense that it allows us to substitute a sum of univariate functions for a multivariate one.

Second, we can use the results on the derivatives of convex functions. If f is convex, then

$$f(x) \geq f(y) + z'(x - y),$$

with $z \in \partial f(y)$, the subgradient of f at y. Thus convex functions have a linear minorizer. In the same way concave functions have a linear majorizer.

##Jensen's Inequality

Jensen's inequality is often formulated in probabilistic terms, using expected values. It is a direct reformulation of the definition of a concave function.

Theorem: Suppose g is a concave function on $\mathcal{S} \subset \mathbb{R}^n$, and suppose π is a weight function such that $\int_{\mathcal{S}} \pi(x)dx = 1$, and $\mu \overset{\Delta}{=} \int_{\mathcal{S}} x\pi(x)dx$ is finite. Then

$\int_{\mathcal{S}}\pi(x)g(x)dx \leq g(\mu)$, with equality if and only if

$$g$$

is linear a.e.

Proof: If g is concave, then $g(x) \leq g(\mu) + (x-\mu)'\eta(\mu)$, where $\eta(\mu)$ is an arbitrary element of the subgradient of g at μ. Multiplying both sides by $\pi(x)$, and integrating gives the required result. **QED**

3.1.1 Tomography

Suppose the function f we must minimize is defined by

$$f(x) = h(\sum_{i=1}^n w_i x_i),$$

where h is a convex function of a single variable, and w is a vector of positive numbers.

If y is another vector of n positive numbers we can write

$$f(x) = h\left(\sum_{i=1}^n \left(\frac{w_i y_i}{w'y}\right)\left(\frac{w'y}{y_i}x_i\right)\right),$$

and if g is defined as

$$g(x,y) = \sum_{i=1}^n \left(\frac{w_i y_i}{w'y}\right) h\left(\frac{w'y}{y_i}x_i\right)$$

then, by the defintion of convexity, $f(x) \leq g(x,y)$. Also, clearly, $f(x) = g(x,x)$ and thus we have a majorization on $(\mathbb{R}^+)^n$.

Alternatively, for any positive vector π with elements adding up to one,

$$f(x) = h\left(\sum_{i=1}^n \pi_i\left(\frac{w_i}{\pi_i}(x_i - y_i) - w'y\right)\right),$$

and the majorization is g defined by

$$g(x,y) = \sum_{i=1}^n \pi_i h\left(\frac{w_i}{\pi_i}(x_i - y_i) - w'y\right).$$

###Logs of Sums and Integrals

Suppose we want to minimize

$$f(x) = -\log \int_{\mathcal{Z}} p(x,z)dz$$

where $p : \mathcal{X} \otimes \mathcal{Z} \rightarrow \mathbb{R}^+$.

It is convenient to define

$$\begin{aligned} p(z \mid x) &\triangleq \frac{p(x,z)}{\int_{\mathcal{Z}} p(x,z)dz}, \\ q(x,y) &\triangleq \int_{\mathcal{Z}} p(z \mid y)\log p(x,z)dz, \end{aligned}$$

and

$$g(x,y) = f(y) + q(y,y) - q(x,y).$$

Theorem: For all $x, y \in \mathcal{X}$ we have $f(x) \leq g(x,y)$ with equality if and only if $p(x,z) = p(y,z)$ a.e. Consequently g majorizes f on $\mathcal{X}$.

Proof: By Jensen's inequality

$$\begin{aligned} \log \frac{\int_{\mathcal{Z}} p(x,z)dz}{\int_{\mathcal{Z}} p(y,z)dz} &= \log \int_{\mathcal{Z}} p(z \mid y)\frac{p(x,z)}{p(y,z)}dz \geq \\ &\geq \int_{\mathcal{Z}} p(z \mid y)\log \frac{p(x,z)}{p(y,z)}dz = \\ &= \int_{\mathcal{Z}} p(z \mid y)\log p(x,z)dz - \int_{\mathcal{Z}} p(z \mid y)\log p(y,z)dz. \end{aligned}$$

Thus

$$-f(x) + f(y) \geq q(x,y) - q(y,y)$$

But this exactly the statement of the theorem. **QED**

Maximizing the right-hand-side by block relaxation is the EM algorithm (Dempster, Laird, and Rubin (1977)). Usually, of course, the EM algorithm is presented in probabilistic terms using the concept of likelihood and expectation. This has considerable heuristic value, but it detracts somewhat from seeing the essential engine of the algorithm, which is the majorization.

##The EM Algorithm

The E-step of the EM algorithm, in our terminology, is the construction of a new majorization function. We prefer a nonstochastic description of EM, because maximizing integrals is obviously a more general problem.

#Tangential Majorization

##Using the Tangent

3.1.2 Majorizing and Minorizing the Logarithm

The logarithm is concave. Consequently, for all positive x and y, we have the linear majorizer

$$\log x \leq \log y + \frac{1}{y}(x - y) = \log y + \frac{x}{y} - 1.$$

We can apply the same concavity to get a minorizer

$$\log \frac{1}{x} \leq \log \frac{1}{y} + y(\frac{1}{x} - \frac{1}{y}),$$

which is

$$\log x \geq \log y - \frac{y}{x} + 1.$$

These majorizers and minorizers of the logarithm are illustrated in Figure 1 for $y = 1$ and $y = 5$.

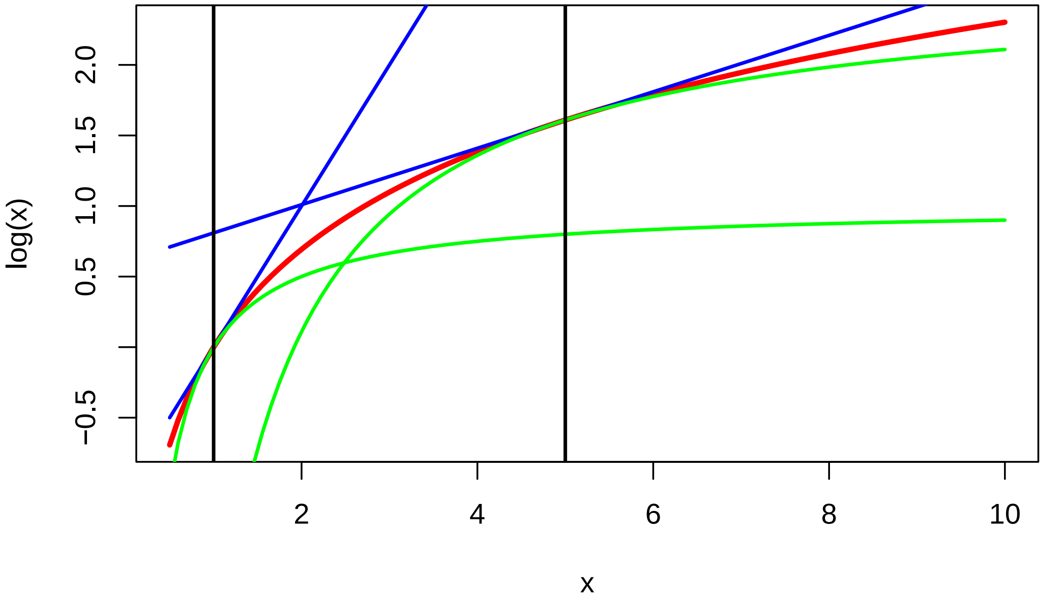


Figure 1: Majorization and Minorization of Logarithm

More generally, we have

$$\log x \leq \log y + \frac{1}{p}\left\{\left(\frac{x}{y}\right)^{p} - 1\right\}$$

for all $p > 0$ and

$$\log x \geq \log y + \frac{1}{p}\left\{\left(\frac{x}{y}\right)^{p} - 1\right\}$$

for all $p < 0$. See Figure 2, where $y = 5$ and $p = \{-2, -1, 1, 2\}$.

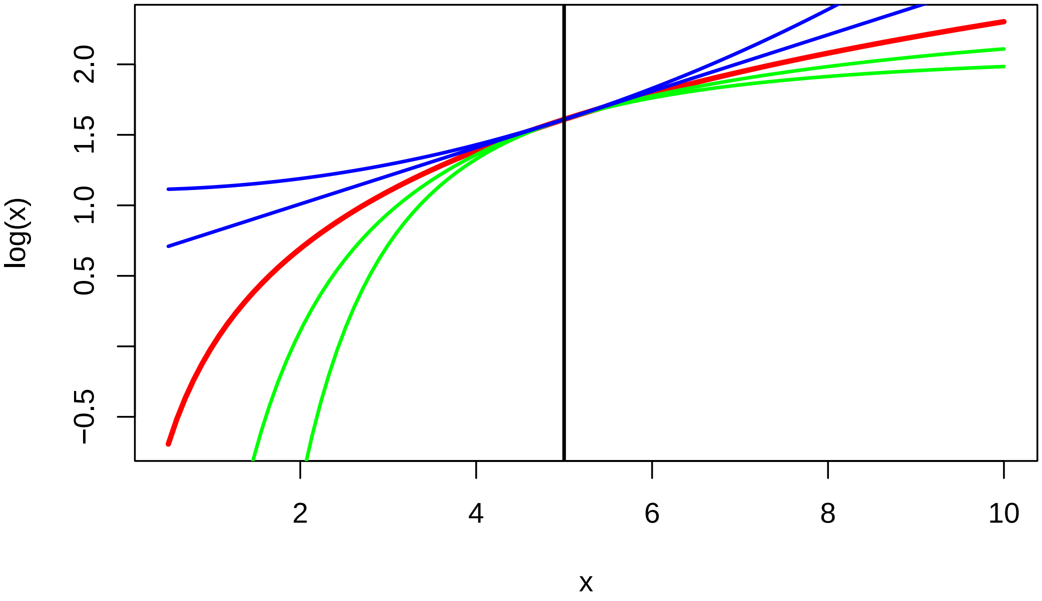


Figure 2: Majorization and Minorization of Logarithm

3.1.3 Aspects of Correlation Matrices

Suppose $\underline{x}_j, \cdots, \underline{x}_m$ are random variables, and $\mathcal{K}_j$ are convex cones of Borel-measurable real-valued functions of $\underline{x}_j$ with finite variance. The elements of $\mathcal{K}_j$ are called *transformations* of the variable $\underline{x}_j$.

For instance, $\mathcal{K}_j$ can be the cone of monotone transformations, or the subspace of splines with given knots, or the subspace of quantifications of a categorical variable

A transformation $\kappa \in \mathcal{K}$ is standardized if $\mathbf{E}(\kappa(\underline{x})) = 0$ and $\mathbf{E}(\kappa^2(\underline{x})) = 1$. Standardized transformations define a sphere $\mathcal{S}_j$.

Now suppose f is a concave and differentiable function defined on the space of all correlation matrices R between m random variables. Suppose we want to minimize

$$g(\kappa_1, \cdots, \kappa_m) \triangleq f(R(\kappa_1(\underline{x}_1), \cdots, \kappa_m(\underline{x}_m)))$$

over all transformations $\kappa_j \in \mathcal{K}_j \cap \mathcal{S}_j$.

Because f is concave

$$f(R) \leq f(S) + \text{ tr } \nabla f(S)(R - S).$$

Collect the partials in the matrix G. A majorization algorithm can minimize

$$\sum_{i=1}^{m}\sum_{j=1}^{m} g_{ij}(S)\mathbf{E}(\kappa_i\kappa_j),$$

over all standardized transformations, which we do with block relaxation using m blocks. In each block we must maximize a linear function on a cone, under a quadratic constraint, which is usually not hard to do.

This algorithm generalizes ACE, CA, and many other forms of MVA with OS. It was proposed first by De Leeuw [1988a], with additional theretical results in De Leeuw [1988b]. The function f can be based on multiple correlations, eigenvalues, determinants, and so on.

3.1.4 Partially Observed Linear Systems

J. De Leeuw (2004) discusses the problem of finding an approximate solution to the homogeneous linear system $AB = 0$ when there are cone and orthonormality restrictions on the columns of A and when some elements of B are restricted to known values, most commonly to zero. Think of the columns of A as variables or sets of variables, and think of B as regression coefficients or weights.

The loss function used by J. De Leeuw (2004) is

$$f(R) \stackrel{\Delta}{=} \min_{B \in \mathcal{B}} \mathbf{tr} B'RB, \tag{1}$$

with $R \stackrel{\Delta}{=} A'A$ and with $\mathcal{B}$ coding the constraints on B. Note that the computation of the optimal B in (1) is a least squares problem, and even with linear inequality constraints on B it is still a straightforward quadratic programming problem.

The function f in (1) is the pointwise minimum of linear functions in R, and thus it is a concave function of R. This means we are in the "aspects of correlation matrices" framework discussed in the previous section.

In particular we define

$$B(R) \overset{\Delta}{=} i\{\hat{B} \mid \mathbf{tr}\ \hat{B}'R\hat{B} = \min_{B\in\mathcal{B}} \mathbf{tr}\ B'RB\},$$

then the subgradient of f at R is

$$\partial f(R) = \mathbf{conv}(BB' \mid B \in B(R)).$$

The subgradient inequality now says that for all correlation matrices R and S we have $f(R) \leq \mathbf{tr}\ \nabla R$ for all $\nabla \in \partial f(S)$.

The constraints on A discussed in J. De Leeuw (2004) make it possible to fit a wide variety of multivariate analysis techniques. Columns of A, or variables, are partitioned into blocks. Some blocks contain only a single variable, such variables are called *single.* Some blocks are constrained to be orthoblocks, which means that the variabes in the block are required to be orthonormal. Single variables may be cone-constrained, which means the corresponding column of A is constrained to be in a cone in $\mathbb{R}^n$. And orthoblocks may be subspace-constrained, which means all columns must be in the same subspace.

We mention some illustrative special cases here. Common factor analysis of a data matrix Y means finding an approximate solution to the system

$$\begin{bmatrix} Y & \mid & U & \mid & E \end{bmatrix} \begin{bmatrix} I \\ -\Gamma \\ -\Delta \end{bmatrix} = 0$$

with $U'U = I$, $E'E = I$, $U'E = 0$, and Δ diagonal. The *common factor scores* are in U, the *unique factor scores* in E, the *factor loadings* in Γ and the *uniquenesses* in Δ. This example can be generalized to cover structural equation models

Homeogeneity analysis Gifi (1990) is the linear system

$$\begin{bmatrix} X & \mid & Q_1 & \mid & \cdots & \mid & Q_m \end{bmatrix} \begin{bmatrix} I & I & I & \cdots & I \\ -\Gamma_1 & 0 & 0 & \cdots & 0 \\ 0 & -\Gamma_2 & 0 & \cdots & 0 \\ 0 & 0 & -\Gamma_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -\Gamma_m \end{bmatrix} = 0$$

where X is and orthoblock of object scores, while the Q_j are orthoblocks in the subspaces defined by the indicator matrices (or B-spline bases) of variable j. For single variables Q_j only has a single column, which can be cone-constrained. For *multiple correspondence analysis* X and all Q_j have the same number of columns. For *nonlinear principal component analysis* all variables are single and the Γ_j are $1 \times p$.

In both examples the majorization algorithm is actually an alternating least squares algorithm. In the factor analysis example the loss functon is

$$\sigma(Y, U, \Gamma, E, \Delta) = \|Y - U\Gamma - E\Delta\|^2,$$

and in homogeneity analysis it is

$$\sigma(X, Q_1 \cdots, Q_m, \Gamma_1, \cdots, \Gamma_j) = \sum_{j=1}^m \|X - Q_j\Gamma_j\|^2.$$

3.1.5 Gpower

** Rewrite for minimizing a concave function 02/21/15 **

Consider the problem of maximizing a convex function f on a compact set $\mathbf{X}$. The function is not necessarily differentiable, the constraint set is not necessarily convex. Define

$$f^\star \overset{\Delta}{=} \max_{x \in \mathcal{X}} f(x).$$

For all x, y and $z \in \partial f(y)$ we have the subgradient inequality

$$f(x) \geq f(y) + z'(x - y).$$

Thus the majorization algorithm is

$$x^{(k+1)} \in \mathop{\mathbf{Arg\,max}}_{x \in \mathcal{X}} z'x,$$

where z is any element of $\partial f(x^{(k)})$.

Define

$$\delta(y) \overset{\Delta}{=} \max_{x \in \mathcal{X}} z'(x - y)$$

where $z \in \partial f(y)$. Then $\delta(y) \geq 0$ and $\delta(y)$ vanishes only when z is in the normal cone to $\mathbf{conv}(\mathcal{X})$ at y.

$$f(x^{(k+1)}) \geq f(x^{(k)}) + \delta(x^{(k)}).$$

It follows that

$$f(x^{(k+1)}) - f(x^{(0)}) = \sum_{i=0}^{k}(f(x^{(i+1)}) - f(x^{(i)})) \geq \sum_{i=0}^{k} \delta(x^{(i)}),$$

and

$$S_k \overset{\Delta}{=} \sum_{i=0}^{k} \delta(x^{(i)}) \leq f^\star - f(x^{(0)}). \tag{1}$$

Thus the partial sums S_k define an increasing sequence, which is bounded above and consequently converges. This implies its terms converge to zero. i.e.

$$\lim_{k\to\infty} \delta(x^{(k)}) = 0.$$

If

$$\delta_k \overset{\Delta}{=} \min_{0\leq i\leq k} \delta(x^{(i)}),$$

then, from (1),

$$\delta_k \leq \frac{f^* - f(x^{(0)})}{k+1}.$$

3.2 Broadening the Scope

3.2.1 Differences of Convex Functions

For d.c. functions (differences of convex functions) such as $\phi = \alpha - \beta$ we can write $\phi(\omega) \leq \alpha(\omega) - \beta(\xi) - \eta'(\omega - \xi)$, with $\eta \in \partial\beta(\xi)$. This gives a convex majorizer. Interesting, because basically all twice differentiable functions are d.c.

** Add: convexification 02/21/15 **

Suppose $f(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$. If we look for a majorization then our first thought is to majorize the first term, because the second is already nicely quadratic. But in this case we proceed the other way around.

In fact, let's consider the more general case $f(x) = \frac{1}{4}x^4 - h(x)$, where h is convex and differentiable. Note f is indeed the difference of two convex functions. We see that $f'(x) = x^3 - h'(x)$ and $f''(x) = 3x^2 - h''(x)$.

Using tangential majorization for h gives

$$g(x,y) = \frac{1}{4}x^4 - h(y) - h'(y)(x-y).$$

Clearly g is convex in x for every y, and since $\mathcal{D}_1 g(x,y) = x^3 - h'(y)$ we have

$$x^{(k+1)} = \sqrt[3]{h'(x^{(k)})}.$$

The iteration radius at a fixed point turns out to be

$$\kappa(x) = \frac{h''(x)}{f''(x) + h''(x)} = \frac{1}{3}\frac{h''(x)}{x^2}.$$

For $h(x) = \frac{1}{2}x^2$ we have $h'(x) = x$. Convergence is to ±1, and thus, using l'Hôpital's rule,

$$\kappa(1) = \lim_{x \rightarrow 1} \frac{\sqrt[3]{x} - 1}{x - 1} = \frac{1}{3}.$$

For $h(x) = |x|$ we have $h'(x) = \pm 1$ if $x \neq 0$, and thus $x^{(k+1)} = \pm 1$. The algorithm finishes in a single step, with the correct solution.

3.2.2 Convexifiable Functions

3.2.3 Piecewise Linear Majorization

Chapter 4

Quadratic Majorization

4.1 Introduction

As we said, it is desirable that the subproblems in which we minimize the majorization function are simple. One way to guarantee this is to try to find a *convex quadratic majorizer*. We mostly limit ourselves to convex quadratic majorizers because on $\mathbb{R}^n$ concave ones have no minima and are of little use for algorithmic purposes. Of course on compact sets minimizers of concave quadratics do exist, and may be useful in some circumstances.

A quadratic g majorizes f at y on $\mathbb{R}^n$ if $g(y) = f(y)$ and $g(x) \geq f(x)$ for all x. If we write it in the form

$$g(x) = f(y) + (x-y)'b + \frac{1}{2}(x-y)'A(x-y)$$

then $g(y) = f(y)$. For differentiable f we have in addition $b = \mathcal{D}f(y)$ and for twice-differentiable f we have $A \gtrsim \mathcal{D}f^2(y)$. If we limit ourselves to convex quadratic majorizers, we must also have $A \gtrsim 0$.

We mention some simple properties of quadratic majorizers on $\mathbb{R}^n$.

1. If a quadratic g majorizes a twice-differentiable convex function f at y, then g is a convex quadratic. This follows from $g''(y) \geq f''(y) \geq 0$.

2. If a concave quadratic g majorizes a twice-differentiable function f at y, then f is concave at y. This follows from $0 \geq g''(y) \geq f''(y)$.

3. Quadratic majorizers are not necessarily convex. In fact, they can even be concave. Take $f(x)=-x^2$ and $g(x)=-x^2+\frac{1}{2}(x-y)^2$.

4. For some functions quadratic majorizers may not exist. Suppose, for example, that f is a cubic. If g is quadratic and majorizes f, then we must have $d=g-f\geq 0$. But $d=g-f$ is a cubic, and thus $d<0$ for at least one value of x.

5. Quadratic majorizers may exist almost everywhere, but not everywhere. Suppose, for example, that $f(x)=|x|$. Then f has a quadratic majorizer at each y except for $y=0$. If $y\neq 0$ we can use, following Heiser (1986), the arithmetic mean-geometric mean inequality in the form
$$\sqrt{x^2y^2}\leq\frac{1}{2}(x^2+y^2),$$
and find
$$|x|\leq\frac{1}{2|y|}x^2+\frac{1}{2}|y|.$$
If g majorizes $|x|$ at 0, then we must have $ax^2+bx\geq|x|$ for all $x\neq 0$, and thus $a|x|+b\mathbf{sign}(x)\geq 1$ for all $x\neq 0$. But for $|x|<\frac{1+|b|}{a}$ and $\mathbf{sign}(x)=-\mathbf{sign}(b)$, we have $a|x|+b\,\mathbf{sign}(x)<1$.

##Existence of Quadratic Majorizers

We first study the univariate case, following J. De Leeuw and Lange (2009). If a quadratic g majorizes a differentiable f over $\mathcal{X}$ at y then we must have
$$g(x,y)=f(y)+f'(y)(x-y)+\frac{1}{2}a(y)(x-y)^2\geq f(x)$$
for all $x\in\mathcal{X}$. Define
$$\delta(x,y):=\frac{f(x)-f(y)-f'(y)(x-y)}{\frac{1}{2}(x-y)^2}$$
with, for continuity, $\delta(y,y)=f''(y)$. Then we must have
$$a(y)\geq\sup_{x\in\mathcal{X}}\delta(x,y),$$
and consequently a quadratic majorizer exists if and only if
$$a^\star(y):=\sup_{x\in\mathcal{X}}\delta(x,y)<\infty.$$

By the mean value theorem there is some z between x and y such that $\delta(x,y) = f''(z)$. Thus if f'' is bounded on $\mathcal{X}$ a quadratic majorizer exists. And if f'' is unbounded on $\mathcal{X}$ a quadratic majorizer does not exist.

From Taylor's theorem with integral form of the remainder

$$\delta(x,y) = 2\int_0^1 \lambda f''(\lambda y + (1-\lambda)x)d\lambda,$$

which gives, by differentiating under the integral sign,

$$\mathcal{D}_1\delta(x,y) = 2\int_0^1 \lambda(1-\lambda)f'''(\lambda y + (1-\lambda)x)d\lambda.$$

We now generalize some of these results to the multivariate case. If a quadratic g majorizes a differentiable f at y then we must have

$$g(x,y) = f(y) + (x-y)'\mathcal{D}f(y) + \frac{1}{2}(x-y)'A(x-y) \geq f(x)$$

for all x. This can be rewritten as the infinite system of linear inequalities in the elements of A

$$(x-y)'A(x-y) \geq 2b(x,y), \tag{4.1}$$

with

$$b(x,y) := f(x) - f(y) - (x-y)'\mathcal{D}f(y).$$

If A satisfies the inequalities (1), then clearly any $B \gtrsim A$ also satifies them, and the set of all matrices satisfying (4.1) is a closed convex set $\mathcal{A}(y)$. Quadratic majorizers at y exist if and only if $\mathcal{A}(y)$ is non-empty. Moreover if $B \gtrsim \mathcal{D}^2 f(x)$ for all x then $B \in \mathcal{A}(y)$ for all y. Thus uniform boundedness of the second derivatives is sufficient for quadratic majorizers to exist. Note that if f is concave then $b(x,y) \leq 0$ for all x, and thus any $A \gtrsim 0$, including $A = 0$, satisfies (4.1).

Although $\mathcal{A}(y)$ is convex and closed, it is generally not a simple object. We can give a simple necessary and sufficient condition for it to be non-empty. Choose an arbitrary positive definite V. Define

$$\delta_V(x,y) := \frac{b(x,y)}{\frac{1}{2}(x-y)'V(x-y)},$$

and

$$\beta_V(y) := \sup_x \delta_V(x,y).$$

Suppose $\beta_V(y) < \infty$. Take $A = \beta_V(y)V$. Then for all x we have

$$(x-y)'A(x-y) = \beta_V(y)(x-y)'V(x-y) \geq 2b(x,y)$$

and thus A is a solution of (4.1). In fact, any $A \gtrsim \beta_V(y)V$ is a solution. Conversely suppose $\beta_V(y) = \infty$ and A is a solution to (4.1), with largest eigenvalue $\lambda_{\max}$. Then there is a x such that $\delta_V(x,y) > \lambda_{\max}$, and thus $2b(x,y) > \lambda_{\max}(x-y)'V(x-y)$, and $(x-y)'A(x-y) > \lambda_{\max}(x-y)'V(x-y)$, a contradiction. It follows that $\beta_V(y) < \infty$ is necessary and sufficient for (4.1) to be solvable and for f to have a quadratic majorization at y.

Nothing in this argument assumes that A is positive semidefinite or that $\beta_V(y) \geq 0$. In fact, for concave f we have $\beta_V(y) \leq 0$. Also, of course, there is nothing that implies that the sup is actually attained at some z. Note that the condition $\beta_V(y) < \infty$ is independent of V, although the value $\beta_V(y)$, if finite, depends on both V and y.

We do know, from Taylor's Theorem (see section III.14.2.3), that if f is twice continuously differentiable at y then

$$\delta_V(x,y) = 2\frac{(x-y)'\left\{\int_0^1 (1-\tau)\mathcal{D}^2 f(x+\tau(y-x))d\tau\right\}(x-y)}{(x-y)'V(x-y)}.$$

It follows that

$$\beta_V(y) \geq \limsup_{x\rightarrow y} \delta_V(x,y) = \lambda_{\max}(V^{-1}\mathcal{D}^2 f(y)).$$

Also, because of the concavity of the minimum eigenvalue,

$$\delta_V(x,y) \geq \lambda_{\min}\left(2\int_0^1 (1-\tau)\mathcal{D}^2 f(x+\tau(y-x))d\tau\right) \geq \min_{0\leq\tau\leq 1} \lambda_{\min}\left(\mathcal{D}^2 f(x+\tau(y-x))\right),$$

and thus quadratic majorizations do not exist for any y if $\lambda_{\min}\left(\mathcal{D}^2 f(x)\right)$ is unbounded.

Example: As an example, consider f defined by $f(x) = \sum_{i=1}^n \log(1 + \exp(r_i'x))$. The function is convex, and as we have shown $\mathcal{D}^2 f(x) \leq \frac{1}{4}R'R$. Let's look at the case in which x has only two elements (as in simple logistic regression). We first study a simple subset of $\mathcal{A}(y)$, those matrices which are positive definite and have equal diagonal elements. Thus

$$A = \beta\begin{bmatrix}1 & \rho\\ \rho & 1\end{bmatrix},$$

with $\beta > 0$ and $-1 < \rho < +1$. Simply choose a ρ and then numerically compute the corresponding $\beta_\rho(y)$. This will give a convex region that is within $\mathcal{A}(y)$.

More generally we can parametrize A by using

$$A = \beta \begin{bmatrix} \alpha & \gamma \\ \gamma & 1-\alpha \end{bmatrix},$$

with $\beta > 0$, $0 < \alpha < 1$, and $\gamma^2 < \alpha(1-\alpha)$. The constraints on α and γ define the interior of a circle in the plane with center $(\frac{1}{2}, 0)$ and radius $\frac{1}{2}$. For each element in the circle we can compute the corresponding $\beta_V(y)$, which will give a complete description of $\mathcal{A}(y)$.

##Convergence

Suppose a is such that

$$g(x,y) = f(y) + f'(y)(x-y) + \frac{1}{2}a(x-y)^2 \tag{4.2}$$

majorizes $f(x)$ for all y. The majorization algorithm is simply

$$x^{(k+1)} = x^{(k)} - \frac{1}{a}f'(x^{(k)}),$$

i.e. it is a gradient algorithm with constant step size. From Ostrowski's Theorem the linear convergence rate is

$$\kappa(x_\infty) = 1 - \frac{f''(x_\infty)}{a}. \tag{4.3}$$

Note that if g in (4.2) majorizes f, then any g of the same form with a larger a also majorizes f. But (4.3) shows a smaller a will generally lead to faster convergence.

For all k we have

$$f(x^{(k+1)}) \leq g(x^{(k+1)}, x^{(k)}) = f(x^{(k)}) - \frac{1}{2}\frac{(f'(x^{(k)}))^2}{a}.$$

Adding these inequalities gives

$$f(x^{(k+1)}) - f(x^{(0)}) = \sum_{i=0}^{k}(f(x^{(i+1)}) - f(x^{(i)}) \leq -\frac{1}{2a}\sum_{i=0}^{k}(f'(x^{(i)}))^2,$$

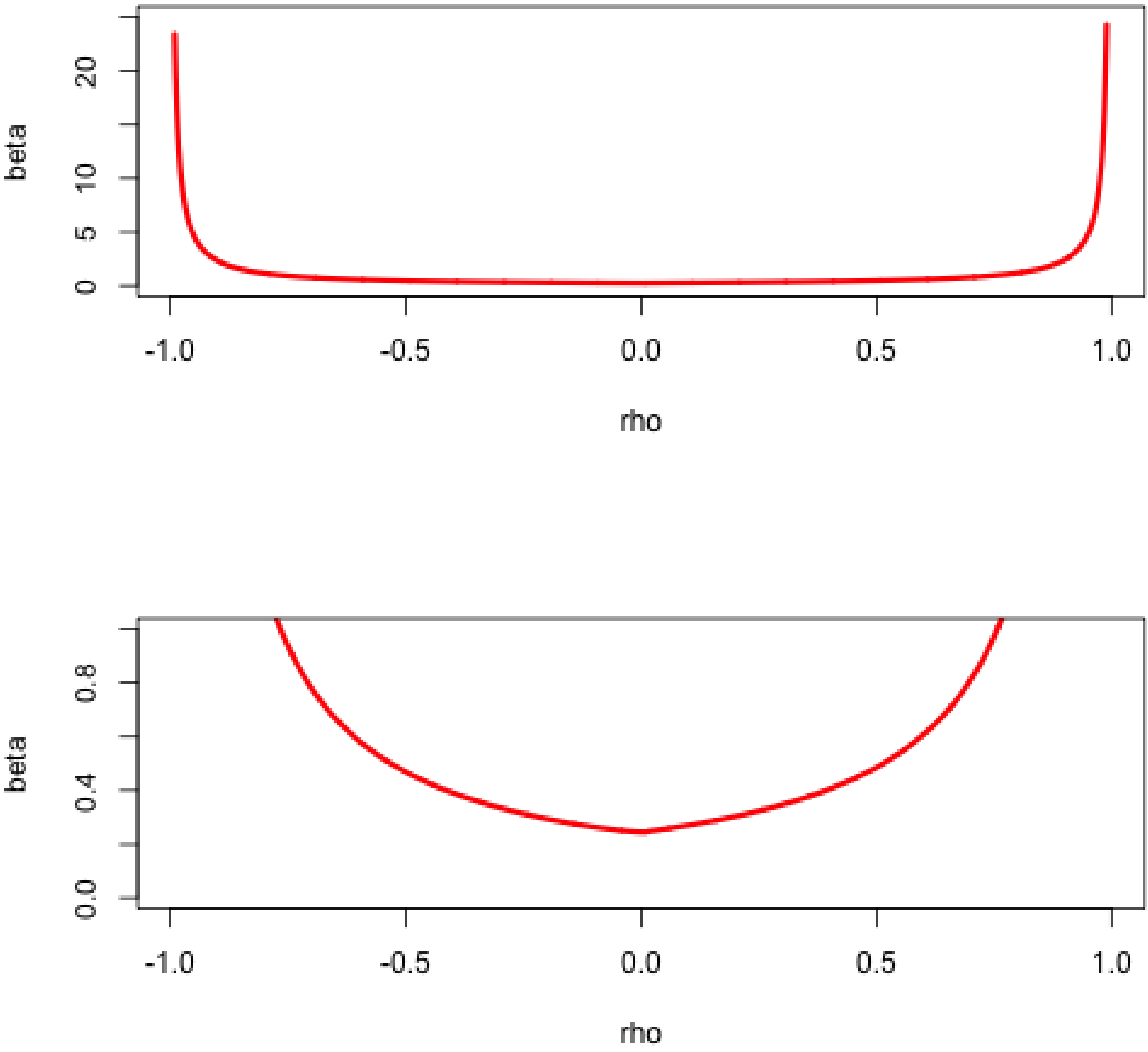


Figure 4.1: Set A(y) for logistic example

and thus, with $f_\star = \min f(x)$,

$$\frac{1}{2a}\sum_{i=0}^{k}(f'(x^{(i)}))^2 \leq f(x^{(0)}) - f_\star. \tag{4.4}$$

The left hand side of (4.4) is an increasing sequence which is bounded above, and consequently converges. This implies

$$\lim_{k\rightarrow\infty} f'(x^{(k)}) = 0$$

Generalize to more variables, generalize to constraints.

##Bounding Second Derivatives

The first result, which has been widely applied, applies to functions with a continuous and uniformly bounded second derivative Böhning and Lindsay (1988).

Theorem: If f is twice differentiable and there is an $a > 0$ such that $f''(x) \leq a$ for all x, then for each y the convex quadratic function

$$g(x) = f(y) + f'(y)(x-y) + \frac{1}{2}a(x-y)^2.$$

majorizes f at y.

Proof: Use Taylor's theorem in the form

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

with ξ on the line connecting x and y. Because $f''(\xi) \leq a$, this implies $f(x) \leq g(x)$, where g is defined above. **QED**

This result is very useful, but it has some limitations. In the first place we would like a similar result for functions that are not everywhere twice differentiable, or even those that are not everywhere differentiable. Second, the bound does take into account that we only need to bound the second derivative on the interval between x and y and not on the whole line. This may result in a bound which is not sharp. In particular we shall see below that substantial improvements can result from a non-uniform bound $a(y)$ that depends on the support point y.

If $\mathcal{D}^2f(x) \lesssim D$ for all $x \in \mathcal{X}$, then

$$\phi(\omega) \leq \phi(\xi) + (\omega-\xi)'\nabla\phi(\xi) + \frac{1}{2}(\omega-\xi)'D(\omega-\xi).$$

Let $\eta(\xi) = \xi - D^{-1}\nabla\phi(\xi)$, then

$$\phi(\omega) \leq \phi(\xi) - \frac{1}{2}\nabla\phi(\xi)'D^{-1}\nabla\phi(\xi) + \frac{1}{2}(\omega-\eta(\xi))'D(\omega-\eta(\xi)).$$

Thus here we have quadratic majorizers.

###Normal Density and Distribution

For a nice regular example we use the celebrated functions

$$\begin{aligned}\phi(x) &= \frac{1}{\sqrt{2\pi}}e^{-z^2/2},\\ \Phi(x) &= \int_{-\infty}^{x}\phi(z)\,dz.\end{aligned}$$

Then

$$\begin{aligned}\Phi'(x) = \phi(x),&&\\ \Phi''(x) = \phi'(x) &=& -x\phi(x),\\ \Phi'''(x) = \phi''(x) &=& -(1-x^2)\phi(x),\\ \Phi''''(x) = \phi'''(x) &=& -x(x^2-3)\phi(x).\end{aligned}$$

To obtain quadratic majorizers we must bound the second derivatives. We can bound $\Phi''(x)$ by setting its derivative equal to zero. We have $\Phi'''(x) = 0$ for $x = \pm 1$, and thus $|\Phi''(x)| \leq \phi(1)$. In the same way $\phi'''(x) = 0$ for $x = 0$ and $x = \pm\sqrt{3}$. At those values $|\phi''(x)| \leq 2\phi(\sqrt{3})$. More precisely, it follows that

$$\begin{aligned}0 \leq \Phi'(x) &=& \phi(x) &\leq& \phi(0),\\ -\phi(1) \leq \Phi''(x) &=& \phi'(x) &\leq& \phi(1),\\ -\phi(0) \leq \Phi'''(x) &=& \phi''(x) &\leq& 2\phi(\sqrt{3}).\end{aligned}$$

Thus we have the quadratic majorizers

$$\Phi(x) \leq \Phi(y) + \phi(y)(x-y) + \frac{1}{2}\phi(1)(x-y)^2,$$

and

$$\phi(x) \leq \phi(y) - y\phi(y)(x-y) + \phi(\sqrt{3})(x-y)^2.$$

The majorizers are illustrated for both Φ and ϕ at the points $y = 0$ and $y = -3$ in Figures 1 and 2. The inequalities in this section may be useful in majorizing multivariate functions involving ϕ and Φ. They are mainly intended, however, to illustrate construction of quadratic majorizers in the smooth case.}

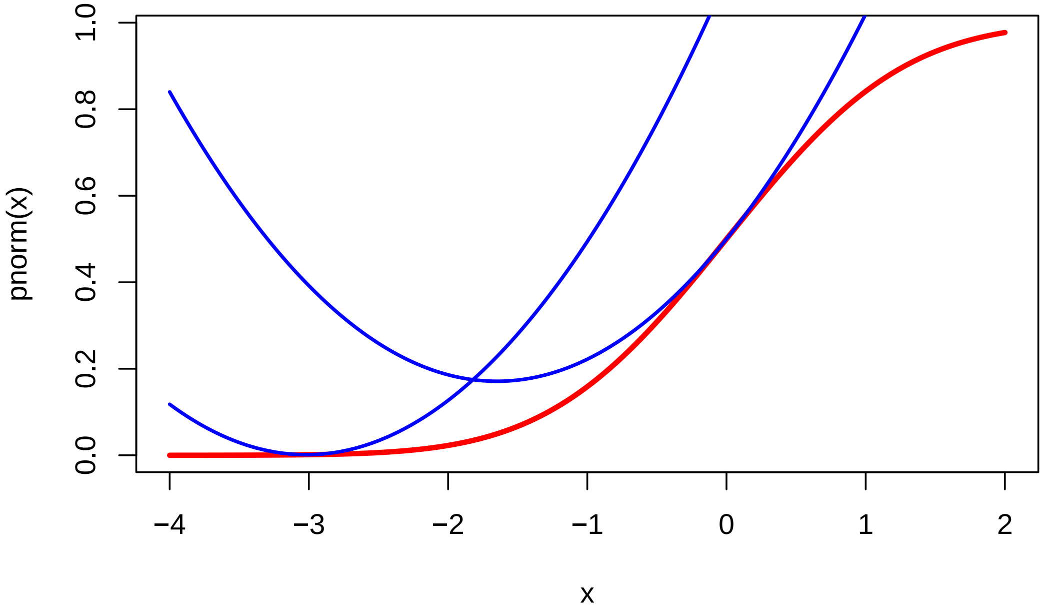


Figure 1: Quadratic Majorization of Normal Distribution

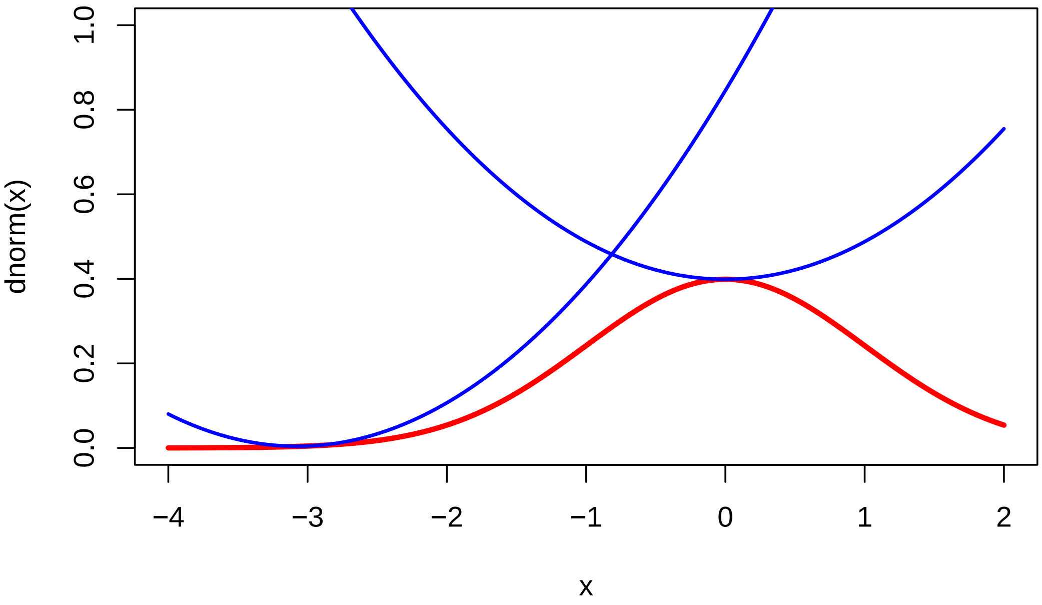


Figure 2: Quadratic Majorization of Normal Density

The drawings are made by the code in `normal.R`.

Insert normal.R here

4.1.1 Nondiagonal Weights in Least Squares

An even simpler example of quadratic majorization of a quadratic function is the following. Suppose we want to solve the problem of minimizing

$$\phi(\omega) = (y-\omega)'W(y-\omega),$$

over $\omega \in \Omega$, where Ω is the cone of isotonic vectors. This problem can be solved by general quadratic programming techniques (compare, for example, Lawson and Hanson (1974)), but it is easier in many respects to use iterated monotone regression.

Suppose we can find a diagonal D such that $W \lesssim D$. A simple choice would be $D = \lambda_+ I$, with λ_+ the largest eigenvalue of W, but sometimes other choices may be more appropriate.

This idea can be generalized. Suppose we want to minimize

$$f(x)=\sum_{i=1}^n\sum_{j=1}^m w_{ij}(y_{ij}-h_{ij}(x))^2$$

Then, using

$$y_{ij}-h_{ij}(x)=(y_{ij}-h_{ij}(\tilde{x}))+(h_{ij}(\tilde{x})-h_{ij}(x))$$

we find

$$f(x)=f(\tilde{x})+2\sum_{i=1}^n\sum_{j=1}^m w_{ij}(y_{ij}-h_{ij}(\tilde{x}))(h_{ij}(\tilde{x})-h_{ij}(x))+\sum_{i=1}^n\sum_{j=1}^m w_{ij}(h_{ij}(\tilde{x})-h_{ij}(x))^2.$$

Now suppose we can find $a_i\geq 0$ and $b_j\geq 0$ such that $w_{ij}\leq a_ib_j$ for all i,j. Then

$$\sum_{i=1}^n\sum_{j=1}^m w_{ij}(h_{ij}(\tilde{x})-h_{ij}(x))^2\leq\sum_{i=1}^n\sum_{j=1}^m a_ib_j(h_{ij}(\tilde{x})-h_{ij}(x))^2,$$

and

$$f(x)\leq f(\tilde{x})+\sum_{i=1}^n\sum_{j=1}^m a_ib_j(\tilde{y}_{ij}-h_{ij}(x))^2-$$

$$\tilde{y}_{ij}=\frac{w_{ij}}{a_ib_j}y_{ij}+(1-\frac{w_{ij}}{a_ib_j})h_{ij}(\tilde{x})$$

###Quadratic on a Sphere

Suppose we want to minimize

$$f(x)=x'Ax+2b'x+c$$

over x satisfying $x'Dx=1$, with D positive definite. In addition, we require $x\in\mathcal{K}$, with $\mathcal{K}$ a convex cone. This problem is important in several optimal scaling problems. It can be solved by using the modified eigenvalue methods of section III.1.9.7, or by the decomposition method of I.6.5.1, but here we give a simple majorization method.

Find λ such that $D^{-\frac12}AD^{-\frac12}\lesssim\lambda I$. Then

$$x'Ax\leq y'Ay+2(x-y)'Ay+\lambda(x-y)'D(x-y)$$

and thus

$$g(x,y) := c + y'Ay + 2(x-y)'Ay + 2b'x + \lambda(x-y)'D(x-y)$$

majorizes f.

Minimizing g over $x'Dx = 1$ and $x \in \mathcal{K}$ amounts to minimizing

$$h(x) := (x-z)'D(x-z)$$

with

$$z := -D^{-1}((A-\lambda D)y + b)$$

over $x \in \mathcal{K}$ and then normalizing the solution such that $x'Dx = 1$.

The function `quadSphere` solves the problem from this section. Note that the cone can be the whole space, in which case we minimize the quadratic on the ellipsoid $x'Dx = 1$, and we can have $b = 0$, in which case we compute the generalized eigenvector corresponding with the smallest generalized eigenvalue of the pair (A, D). Also note that A can be indefinite.

Insert quadSphere.R Here

4.1.2 Gifi Goes Logistic

4.1.3 A Matrix Example

Kiers (1990) considers the problem of minimizing a function of the form

$$\phi(X) = c + \text{tr } AX + \sum_{j=1}^{m} \text{tr } B_jXC_jX',$$

over all $n \times p$ matrices X, possibly with restrictions. He shows that this covers a large number of matrix problems commonly considered in psychometrics.

4.1.4 Gauss-Newton Majorization

The least squares loss function was defined here. It has the form

$$f(x) = \frac{1}{2}\sum_{j=1}^{m}\sum_{\ell=1}^{m} w_{j\ell}\, g_j(x) g_\ell(x),$$

where W is an $m \times m$ positive semi-definite matrix of *weights*, and we minimize f over $x \in \mathcal{X}$.

Now

$$\mathcal{D}f(x) = \sum_{j=1}^m \sum_{\ell=1}^m w_{j\ell} g_j(x) \mathcal{D}g_\ell(x),$$

and

$$\mathcal{D}^2 f(x) = \sum_{j=1}^m \sum_{\ell=1}^m w_{j\ell} \left\{ g_j(x)\mathcal{D}^2 g_\ell(x) + \mathcal{D}g_j(x)(\mathcal{D}g_\ell(x))' \right\}.$$

The structure of the Hessian suggest to define

$$A(x) \triangleq \sum_{j=1}^m \sum_{\ell=1}^m w_{j\ell} g_j(x)\mathcal{D}^2 g_\ell(x),$$
$$B(x) \triangleq \sum_{j=1}^m \sum_{\ell=1}^m w_{j\ell} \mathcal{D}g_j(x)(\mathcal{D}g_\ell(x))'.$$

We have $\mathcal{D}^2 f(x) = A(x) + B(x)$. Note that $B(x)$ is positive semi-definite for all x.

In the classical Gauss-Newton method we make the approximation

$$f(x) \approx f(y) + (x-y)'\mathcal{D}f(y) + \frac{1}{2}(x-y)'B(y)(x-y),$$

and the corresponding iterative algorithm is

$$x^{(k+1)} = x^{(k)} - B^{-1}(x^{(k)})\mathcal{D}f(x^{(k)}).$$

If the algorithm converges to x, and the $g_j(x)$ are small, then the least squares loss function will be small, and $A(x)$ will be small as well. Since the iteration matrix is

$$\mathcal{M}(x) = I - B^{-1}(x)\mathcal{D}^2 f(x) = -B^{-1}(x)A(x),$$

we can expect rapid convergence. But convergence is not guaranteed, and consequently we need safeguards. Majorization provides one such safeguard.

If we can find $\gamma(y)$ such that

$$\sup_{0 \leq \lambda \leq 1} z'A(y+\lambda z)z \leq \gamma(y)z'z$$

Note: Use Nesterov's Gauss-Newton paper 03/13/15

###Marginal Functions

Chapter 5

Using Higher Derivatives

##Introduction

##Mean Value Majorization

Suppose f is differentiable in an open set $\mathcal{X}$ containing both x and y and the line connecting them. We can use the mean value theorem in the inequality form

$$f(x) \leq f(y) + \sup_{0 \leq \lambda \leq 1} (x-y)'\mathcal{D}f(y+\lambda(x-y))$$

Define, for fixed x, y

$$h(\lambda) \stackrel{\Delta}{=} (x-y)'\mathcal{D}f(y+\lambda(x-y))$$

The maximum of h is attained at either $\lambda = 0$, or $\lambda = 1$, or at a point in the interior of the unit interval where the derivative with respect to λ vanishes. Now

$$\mathcal{D}h(\lambda) = (x-y)'\mathcal{D}^2f(y+\lambda(x-y))(x-y).$$

Thus for concave f we see that h is decreasing, and we recover our previous result

$$f(x) \leq f(y) + (x-y)'\mathcal{D}f(y).$$

For convex f, for which h is increasing, we find

$$f(x) \leq f(y) + (x-y)'\mathcal{D}f(x).$$

For the univariate cubic $f(x)=a+bx+\frac{1}{2}cx^2+\frac{1}{6}dx^3$ we have

$$\mathcal{D}f(x)=b+cx+\frac{1}{2}dx^2,$$

and thus we must compute $\sup_{0\leq\lambda\leq 1}h(\lambda)$ where

$$h(\lambda)\overset{\Delta}{=}z(b+c(y+\lambda z)+\frac{1}{2}d(y+\lambda z)^2),$$

where $z\overset{\Delta}{=}x-y$. If $dz^3>0$ the quadratic h is convex, and the maximum is attained at one of the endpoints, i.e.

$$\sup_{0\leq\lambda\leq 1}h(\lambda)=\max\{z(b+cy+\frac{1}{2}dy^2),z(b+cx+\frac{1}{2}dx^2)\}$$

$$cz+\frac{1}{2}dz(x+y)>0$$

5.1 Taylor Majorization

5.1.1 Second Order

We can take this one step further. Obviously

$$f(x)\leq f(y)+(x-y)'\nabla f(y)+\frac{1}{2}\sup_{0\leq\lambda\leq 1}(x-y)'\nabla^2f(y+\lambda(x-y))(x-y).$$

The main problem with these approaches based on the mean value theorem is that the majorizing function may not be simple. Nevertheless the approach can also be used to arrive at bounds which are computationally convenient.

For a univariate cubic $f(x)=a+bx+\frac{1}{2}cx^2+\frac{1}{6}dx^3$ we find the majorization

$$\begin{aligned}f(x)\leq f(y)+f'(y)(x-y)+\frac{1}{2}(x-y)^2\max_{0\leq\lambda\leq 1}(c+d(x+\lambda(y-x)))=\\=f(y)+f'(y)(x-y)+\frac{1}{2}(x-y)^2\begin{cases}c+d\max(x,y)&\text{if }d\geq 0,\\c+d\min(x,y)&\text{if }d\leq 0,\end{cases}\end{aligned}$$

For the exponent

$$\exp(x) \leq \exp(y) + \exp(y)(x-y) + \frac{1}{2}(x-y)^2 \sup_{0\leq\lambda\leq 1} \exp(y+\lambda(x-y)) =$$
$$= \exp(y) + \exp(y)(x-y) + \frac{1}{2}(x-y)^2 \exp(\max(x,y))$$

For the folium with $f(x) = x_1^3 + x_2^3 - 3x_1x_2$ we have

$$\mathcal{D}^2 f(x) = \begin{bmatrix} 6x_1 & -3 \\ -3 & 6x_2 \end{bmatrix}.$$

Thus a simple majorizer is given by *(incorrect 03/03/15)*

$$g(x,y) = f(y) + (x-y)'\mathcal{D}f(y) + \max(x_1,x_2)(x-y)'V(x-y),$$

with

$$V = \begin{bmatrix} 6 & -3 \\ -3 & 6 \end{bmatrix}.$$

NB: see probit section for $f''(x)$ decreasing. 03/03/15

5.1.2 Higher Order

From Taylor's theorem with Lagrange form of the remainder discussed in [A:Taylor] it follows that

$$f(x) \leq g_p(x,y) + \frac{1}{(p+1)!} \sup_{0\leq\lambda\leq 1} < \mathcal{D}^{p+1} f(x+\lambda(y-x)), (x-y)^{p+1} >,$$

where g_p is the $p-$degree Taylor polynomial at y.

If all elements of the array in $\frac{1}{(p+1)!}\mathcal{D}^{p+1}f(x+\lambda(y-x))$ are less than κ in absolute value for all x, y and λ, then this implies

$$f(x) \leq g_p(x,y) + \kappa \left\{ \sum_{i=1}^n |x_i - y_i| \right\}^{p+1}$$

We can also use the Frobenius norm and Cauchy-Schwartz to obtain

$$f(x) \leq g_p(x,y) + \kappa(x,y)\|x-y\|^{p+1},$$

where

$$\kappa(x,y) \triangleq \frac{1}{(p+1)!}\sup_{0\leq\lambda\leq 1}\|\mathcal{D}^{p+1}f(x+\lambda(y-x))\|.$$

Of course it remains to be seen if these formulas actually lead to useful majorization algorithms. For higher p they will undoubtedly have fast convergence, but the optimizations in each iteration involve higher order multivariate polynomials and look pretty daunting.

5.2 Nesterov Majorization

Suppose f is a function with third derivatives that are bounded in the sense that

$$\langle\mathcal{D}^3f(x),(x-y)^3\rangle \leq K_3\|x-y\|^3. \tag{1}$$

It is sufficient for this that the Hessian is Lipschitz continuous with Lipschitz constant K_3. Majorization based on (1) was first discussed in an important article by Nesterov and Polyak (2006)

Under these conditions we have the majorizer

$$g(x,y) = f(y) + (x-y)'\mathcal{D}f(y) + \frac{1}{2}(x-y)'\mathcal{D}^2f(y)(x-y) + \frac{1}{6}K_3\|x-y\|^3.$$

The term $\|x-y\|^3$ is convex in x, but the majorizer g itself is generally not convex, although it is convex whenever f is. Majorizer g has continuous first derivatives

$$\mathcal{D}_1g(x,y) = \mathcal{D}f(y) + \mathcal{D}^2f(y)(x-y) + \frac{1}{2}K_3\|x-y\|(x-y),$$

and for $x \neq y$ the second derivative is

$$\mathcal{D}_{11}g(x,y) = \mathcal{D}^2f(y) + \frac{1}{2}K_3\|x-y\|\left(I + \frac{(x-y)(x-y)'}{(x-y)'(x-y)}\right).$$

It follows that

$$\mathcal{D}^2f(y) + \frac{1}{2}K_3\|x-y\| \lesssim \mathcal{D}_{11}g(x,y) \lesssim \mathcal{D}^2f(y) + K_3\|x-y\|,$$

and thus, by the squeeze theorem,

$$\lim_{x\rightarrow y}\mathcal{D}_{11}g(x,y)=\mathcal{D}^2 f(y).$$

The majorization algorithm is, as usual,

$$x^{(k+1)}=\mathop{\mathbf{argmin}}_{x} g(x,x^{(k)}),$$

and the majorizer is minimized at a point where $\mathcal{D}_1 g(x,x^{(k)})=0$. We write the stationary equation as

$$\left(\mathcal{D}^2 f(y)+\frac{1}{2}K_3\|x-y\|I\right)(x-y)=-\mathcal{D}f(y).$$

We write this as two equations, using what is effectively a form of decomposition.

$$\left(\mathcal{D}^2 f(y)+\frac{1}{2}K_3\delta I\right)(x-y)=-\mathcal{D}f(y), \tag{2a}$$

$$\delta=\|x-y\|. \tag{2b}$$

Let $\mathcal{D}^2 f(y)=K\Lambda K'$ be an eigen decomposition, and define $g\overset{\Delta}{=}-K'\mathcal{D}f(y)$ and $z=K'(x-y)$. Then solving

$$\left(\Lambda+\frac{1}{2}K_3\delta I\right)z=g$$

for z and using $(2b)$ gives the *secular equation* in δ

$$\delta^2=\sum_{i=1}^n\frac{g_i^2}{(\lambda_i+\frac{1}{2}K_3\delta)^2}$$

The Cartesian folium is

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

Thus

$$f(x+u,y+v)=f(x,y)+3au+3bv+3xu^2-3uv+3yv^2+u^3+v^3.$$

with

$$
\begin{aligned}
a &\overset{\Delta}{=} x^2 - y,\\
b &\overset{\Delta}{=} y^2 - x.
\end{aligned}
$$

If

$$h(u,v) \overset{\Delta}{=} \frac{(u^3+v^3)^{\frac{2}{3}}}{u^2+v^2}$$

then

$$\max_{u,v} h(u,v) = \max_{u^2+v^2=1} (u^3+v^3)^{\frac{2}{3}} = \max_{\theta}\ (\sin^3(\theta)+\cos^3(\theta))^{\frac{2}{3}} = 1,$$

and thus

$$u^3+v^3 \leq (u^2+v^2)^{\frac{3}{2}}.$$

This gives the majorization we are looking for

$$g(x+u,y+v) = f(x,y) + 3au + 3bv + 3xu^2 - 3uv + 3yv^2 + (u^2+v^2)^{\frac{3}{2}}$$

The derivatives are

$$
\begin{aligned}
\mathcal{D}_1 g(u,v) &= 3a + 6xu - 3v + 3\lambda u,\\
\mathcal{D}_2 g(u,v) &= 3b + 6yv - 3v + 3\lambda v.
\end{aligned}
$$

with $\lambda \overset{\Delta}{=} \sqrt{u^2+v^2}$. Thus

$$\begin{bmatrix} 2x+\lambda & -1 \\ -1 & 2y+\lambda \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} -a \\ -b \end{bmatrix},$$

or

$$\begin{bmatrix} u \\ v \end{bmatrix} = -\frac{1}{(2x+\lambda)(2y+\lambda)-1} \begin{bmatrix} 2y+\lambda & 1 \\ 1 & 2x+\lambda \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}.$$

Thus we must have

$$\lambda^2 = u^2+v^2 = \frac{((2y+\lambda)a+b)^2 + ((2x+\lambda)b+a)^2}{((2x+\lambda)(2y+\lambda)-1)^2}$$

$$f(x) = \frac{1}{6}\sum_{i=1}^n x_i^3 + \frac{1}{2}x'Ax$$

$$f(x)=f(y)+(x-y)'\mathcal{D}f(y)+\frac{1}{2}(x-y)'\mathcal{D}^2f(y)(x-y)+\frac{1}{6}\sum_{i=1}^n(x_i-y_i)^3.$$

$$h(z)\triangleq\frac{\sum_{i=1}^n z_i^3}{(z'z)^{\frac{3}{2}}}$$

$$\max_z h(z)=\max_{z'z=1}\sum_{i=1}^n z_i^3=1.$$

Thus

$$g(x)=f(y)+(x-y)'\mathcal{D}f(y)+\frac{1}{2}(x-y)'\mathcal{D}^2f(y)(x-y)+\frac{1}{6}\{(x-y)'(x-y)\}^{\frac{3}{2}}$$

majorizes f at y. Now

$$\mathcal{D}g(x)=\mathcal{D}f(y)+\mathcal{D}^2f(y)(x-y)+\frac{1}{2}\lambda(x)(x-y)$$

and

$$\mathcal{D}^2g(x)=\mathcal{D}^2f(y)+\frac{1}{2}\lambda(x)I+\frac{1}{2}\frac{1}{\lambda(x)}(x-y)(x-y)'$$

where $\lambda(x)=\sqrt{(x-y)'(x-y)}$.

Suppose f is a multivariate quartic with bounds on the third and fourth derivatives. Thus

$$g(x,y)=f(y)+(x-y)'\mathcal{D}f(y)+\frac{1}{2}(x-y)'\mathcal{D}^2f(y)(x-y)+\\+\frac{1}{6}K_3\|x-y\|^3+\frac{1}{24}K_4\|x-y\|^4 \quad (5.1)$$

We minimize g over x, as usual. Thus we must solve

$$\left[\mathcal{D}^2f(y)+\frac{1}{2}K_3\|x-y\|I+\frac{1}{6}K_4\|x-y\|^2I\right](x-y)=-\mathcal{D}f(y).$$

Expand this to the two equations

$$\left[\mathcal{D}^2f(y)+\frac{1}{2}K_3\delta I+\frac{1}{6}K_4\delta^2I\right](x-y)=-\mathcal{D}f(y),\\ \|x-y\|=\delta.$$

##Examples

5.2.1 Revisiting the Reciprocal

Here we come back to the function $f : x \rightarrow ax - \log x$.

We start with a new majorization of the logarithm. In other contexts the logarithm, which is concave, has been majorized by a linear function. Since our f uses the negative logarithm, which is convex, that will not work in our case. By Taylor

$$\log(x) = \log(y) + \frac{1}{y}(x-y) - \frac{1}{2}\frac{1}{z^2}(x-y)^2,$$

where z is between x and y. Thus if we define

$$h(x,y) \triangleq \log(y) + \frac{1}{y}(x-y) - \frac{1}{2}\begin{cases}\frac{(x-y)^2}{x^2} & \text{if } x \leq y,\\ \frac{(x-y)^2}{y^2} & \text{otherwise.}\end{cases}$$

then, for all $x > 0$ and $y > 0$,

$$\log(x) \geq h(x,y),$$

and thus, with $g(x,y) = ax - h(x,y)$, we have $f(x) \leq g(x,y)$. with equality if and only if $x = y$.

Now g, as a function of x, is differentiable on the positive reals for all y. In fact

$$\mathcal{D}_1 g(x,y) = a - \frac{1}{y} + \begin{cases}\frac{y}{x^3}(x-y) & \text{if } x \leq y,\\ \frac{1}{y^2}(x-y) & \text{otherwise.}\end{cases}$$

Let us find the solutions of $\mathcal{D}_1 g(x,y) = 0$. First check if

$$a - \frac{1}{y} + \frac{1}{y^2}(x-y) = 0$$

has a root $x \geq y$. The unique root is $x = 2y - ay^2$. Thus if $2y - ay^2 \geq y$, i.e. if $y \leq \frac{1}{a}$, this gives a solution to $\mathcal{D}_1 g(x,y) = 0$. Note that the update in this case is the same update as Newton's update for the reciprocal.

Matters are a bit more complicated for finding a solution of

$$a - \frac{1}{y} + \frac{y}{x^3}(x-y) = 0.$$

with $x \leq y$. The equation can be written as the cubic equation in x

$$(a - \frac{1}{y})x^3 + yx - y^2 = 0.$$

If $y > \frac{1}{a}$ then the cubic has only one real root. Because if there are two, then by Rolle the derivative should vanish somewhere on the interval between them, but the derivative is always positive. Since the cubic is negative for $x = 0$ and positive for $x = y$, the unique root is between zero and y, and thus satisfies $\mathcal{D}_1 g(x, y) = 0$.

5.2.2 Logit

The logistic distribution

$$\Psi(x) = \frac{1}{1 + \exp(-x)}$$

increases from zero to one on the real line. As we have seen before, the function

$$f(x) = x - \log \Psi(x) = \log(1 + \exp(x))$$

is strictly convex. This follows directly from

$$\begin{aligned} f'(x) &= \Psi(x), \\ f''(x) &= \Psi(x)(1 - \Psi(x)), \end{aligned}$$

because the first derivative is increasing and the second derivative is positive.

Theorem: The r-th derivative $f^{(r)}(x)$ is a polynomial in $\Psi(x)$ of degree r. Consequently for all r there are two finite real numbers $m_r < M_r$ such that $m_r \leq f^{(r)}(x) \leq M_r$ for all x.

Proof: We know that $f'(x) = \Psi(x)$, and thus the result is true for $r = 1$. Now proceed by induction. If $f^{(r)}(x) = P_r(\Psi(x))$ for some polynomial P_r of degree r, then

$$f^{(r+1)}(x) = P_r'(\Psi(x))\Psi(x)(1 - \Psi(x)),$$

which is indeed a polynomial in $\Psi(x)$ of degree $r + 1$. In addition

$$\begin{aligned} \sup_x f^{(r)}(x) &= \max_{0 \leq s \leq 1} P_r(s), \\ \inf_x f^{(r)}(x) &= \min_{0 \leq s \leq 1} P_r(s), \end{aligned}$$

and the quantities on the right-hand side are clearly finite. **QED**

We illustrate the theorem by computing some higher derivatives

$$f^{(3)}(x) = \Psi(x)(1-\Psi(x))(1-2\Psi(x)),$$

$$f^{(4)}(x) = \Psi(x)(1-\Psi(x))(1-6\Psi(x)+6\Psi^2(x)),$$

$$f^{(5)}(x) = \Psi(x)(1-\Psi(x))(1-2\Psi(x))(1-12\Psi(x)+12\Psi^2(x))$$

which implies

$$-\frac{1}{18}\sqrt{3} \leq f^{(3)}(x) \leq +\frac{1}{18}\sqrt{3},$$

$$-\frac{1}{8} \leq f^{(4)}(x) \leq \frac{1}{24}$$

The derivatives of orders 2 to 5 are in Figure 1.

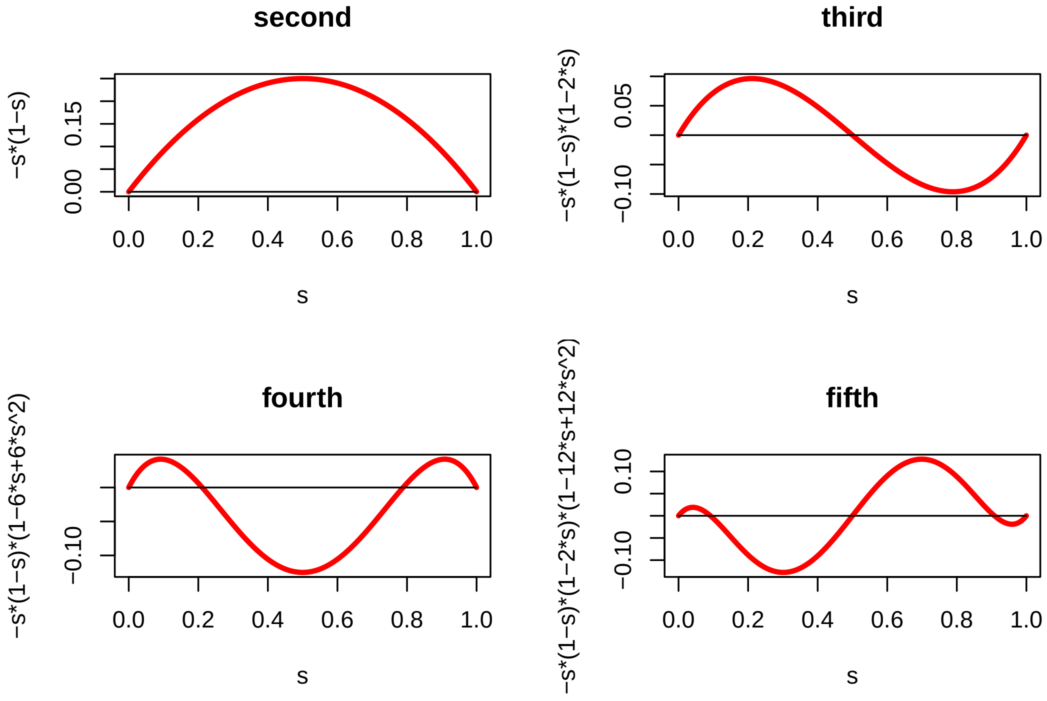


Figure 1: Derivatives of the Log-logistic

And here is some `R` code for drawing the figure.

Insert logDers.R Here

We now look more closely at the polynomials P_r. From the proof of the we see that for $r > 1$ we have $P_r(0) = P_r(1) = 0$. Because $P_2(s) = P_2(1-s)$ we see that actually $P_r(s) = P_r(1-s)$ for all even r and $P_r(s) = -P_r(1-s)$ for all odd $r > 1$. This implies that $P_r(\frac{1}{2}) = 0$ for all odd $r > 1$.

We can go further than this and derive an explicit formula for the polynomials. The difference/differential equation we have to solve is $P_{r+1}(x) = x(1-x)P_r'(x)$, where $P_1(x) = 1-x$. Its general solution is

$$P_r(x) = \sum_{j=1}^{r}(-1)^{j-1}(j-1)!S(j,r)x^j$$

where the $S(j,r)$ are the Stirling numbers of the second kind (the number of ways of partitioning r elements into j non-empty subsets).

The code in `logitPom.R` computes the polynomials P_r. With `logitPomRecursive(n)` we compute all polynomials up to order n, their roots, and their maximum and minimum values. With `logitPomDirect(n)` we do the same, using the formula with Stirling numbers.

Insert logitPom.R Here

Maybe useful 03/02/15

$$-\log(1-\Psi(x)) = -\log(1-\frac{1}{1+\exp(-x)}) = x+\log(1+\exp(-x))$$

$$x+\log(1+\exp(-x)) = \sum_{s=1}^{\infty}\frac{(\Psi(x))^s}{s}$$

###Probit

Chapter 6

Sharp Majorization

##Introduction

6.1 Comparing Majorizations

The set of all real-valued functions $\mathcal{M}_Y(f)$ that majorize f on $\mathcal{Y}$ is convex.

If we order $\mathcal{M}_Y(f)$ by $g \leq_Y h$ if $g(y) \leq h(y)$ for all $y \in \mathcal{Y}$, then $\langle \mathcal{M}_Y(f), \leq_Y \rangle$ is a lattice, because if g and h majorize f on $\mathcal{Y}$, then so do the pointwise maximum and minimum of g and h.

In fact the lattice $\langle \mathcal{M}_Y(f), \leq_Y \rangle$ is inf-complete, because the pointwise infimum of a set of majorizing functions again majorizes. Clearly f itself is the minimal element of the lattice. The lattice is not sup-complete, although it is if we consider the set of extended real valued functions which can take the value $+\infty$.

** The following needs to be repaired – only true for majorization at a point 03/28/15 **

Note, however, that the pointwise maximum of a finite number of majorizing functions does majorize. If $f(x) \leq g_i(x,y)$ and $f(x) = g_i(x,x)$ for all $i = 1, \cdots, n$ then $f(x) = \max_{i=1}^n g_i(x,x)$ and $f(x) \leq \max_{i=1}^n g_i(x,y)$. But if $\mathcal{I}$ is infinite, then $\sup_{i\in\mathcal{I}} g_i(x,y)$ can be infinite as well, and in that case it is not a majorization function. In contrast it is always true that $f(x) \leq \inf_{i\in I} g_i(x,y)$.

We can actually give an even stronger result than inf-completeness. Suppose $g_i(x,y_i) - f(x) \geq 0$ for all $i = 1,\cdots,n$ and for all $x \in \mathcal{X}$, and $g_i(y_i,y_i) - f(y_i) = 0$ for all $i = 1,\cdots,n$. Thus g_i majorizes f at y_i. Now let

$$h(x) = \min_{i=1}^{n} \, (g_i(x,y_i) - f(x))$$

then $h(x) \geq 0$ for all $x \in \mathcal{X}$ and $h(y_i) = 0$ for all $i = 1,\cdots,n$. Thus $f(x) + h(x) = \min_{i=1}^n g_i(x,y_i)$ majorizes f at $y_1,\cdots,y_n$.

As an example, consider the function $f : x \rightarrow x^4$ on $[-1,+1]$. On that interval we have $f''(x) \leq 12$ and thus if $-1 \leq y \leq +1$ we have the quadratic majorizer

$$g(x,y) = y^4 + 4y^3(x-y) + 6(x-y)^2.$$

Now take the y_i to be the 11 points $-1.0, -0.8, \cdots, 0.8, 1.0$ and take $h(x)$ to be the minimum of the $g(x,y_i)$.

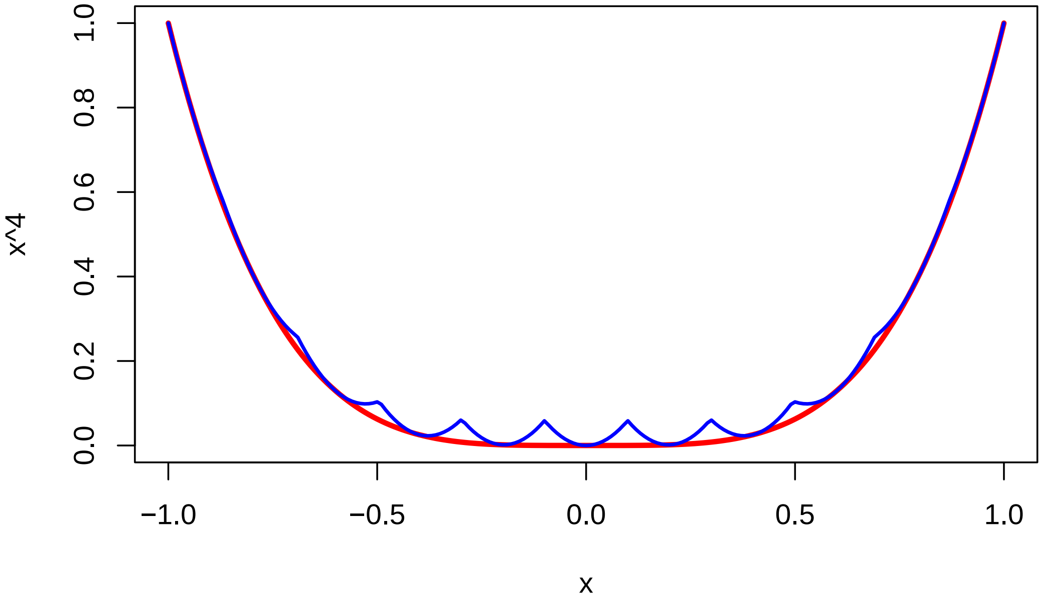


Figure 1: Piecewise Quadratic Majorization at Multiple Points of a Quartic

Of course $\min_{-1\leq y\leq +1} g(x,y) = f(x)$ which means we can make the majorization as sharp as we want by increasing the number of support points.

6.2 Sharp Quadratic Majorization

A quadratic function

$$g(x) = c + b(x - y) + \frac{1}{2}a(x - y)^2$$

majorizes f in y if and only if $c = f(y)$, $b = f'(y)$, and

$$a \geq A(y) \overset{\Delta}{=} \sup_{x \neq y} \delta(x|y),$$

where

$$\delta(x|y) \overset{\Delta}{=} \frac{f(x) - f(y) - f'(y)(x - y)}{\frac{1}{2}(x - y)^2}.$$

We find the *best quadratic majorization* of f in y by choosing $a = A(y)$.

To study the relation between f and its quadratic majorizers more in depth, we define $\phi : \mathbb{R}^3 \Rightarrow \mathbb{R}$ and $\delta : \mathbb{R}^3 \Rightarrow \mathbb{R}$ by

$$\phi(x, y, a) \overset{\Delta}{=} f(y) + f'(y)(x - y) + \frac{1}{2}a(x - y)^2$$

and $\delta(x, y, a) \overset{\Delta}{=} f(x) - \phi(x, y, a)$. We also define slices of these functions, using bullets. Thus, for example, $\phi(\bullet, y, a)$ is a function of a single variable, with y and a fixed at unique values.

Now $\phi(\bullet, y, a) \gtrsim f(x)$ if and only if $\delta(x, y, a) \leq 0$ for all x, which is true if and only if $\delta^\star(y, a) = 0$, where

$$\delta^\star(y, a) \overset{\Delta}{=} \sup_x \delta(x, y, a).$$

Note that $\delta(y, y, a) = 0$, and thus generally $\delta^\star(y, a) \geq 0$.

Because $\delta(x, y, \bullet)$ is linear in a, we see that $\delta^\star(y, \bullet)$ is convex. In other words,

$$\mathcal{A}(y) \overset{\Delta}{=} \{a \mid \delta^\star(y, a) \leq 0\}$$

is an interval, which may be empty. Now $\phi(\bullet, y, a) \gtrsim_y f(x)$ if and only if $a \in \mathcal{A}(y)$. If $\mathcal{A}(y) = \emptyset$ then no quadratic majorization exists.

Since $a \in \mathcal{A}(y)$ implies $b \in \mathcal{A}(y)$ for all $b \geq a$, we see that $\mathcal{A}(y)$ is either empty, or an interval of the form $[a_\star(y), +\infty)$ or $(a_\star(y), +\infty)$, with

$$a_\star(y) \overset{\Delta}{=} \inf_a \mathcal{A}(y).$$

If $\mathcal{A}(y) = \emptyset$ we set $a_\star(y) = +\infty$. The majorization function $\phi(\bullet, y, a_\star(y))$ is called the *sharpest quadratic majorization* of f at y (J. De Leeuw and Lange 2009).

Now

$$\delta'(x) = f'(x) - f'(y) - a(x - y),$$

and

$$\delta''(x) = f''(x) - a.$$

We see that δ is concave if $a \geq \sup_x f''(x)$. Moreover δ is increasing if $\delta' \geq 0$, i.e. if

$$\frac{f'(x) - f'(y)}{x - y}\begin{cases}\geq a & \text{if } x > y\\ \leq a & \text{if } x < y\end{cases}$$

for all x.

Thus if δ has a maximum at $\hat{x}$ we must have

$$a = \frac{f'(\hat{x}) - f'(y)}{\hat{x} - y},$$

as well as

$$a \geq f''(\hat{x}).$$

At the maximum

$$\delta(\hat{x}) = f(\hat{x}) - f(y) - \frac{1}{2}(f'(\hat{x}) + f'(y)).$$

###Existence

As we have seen in section II.5.5.2 quadratic majorizers exist if $\beta_V(y) < \infty$. Although $\beta_V(y) < \infty$ is independent of V, the numerical value of $\beta_V(y)$ does depend on V, and of course on y.

We say that a *sharp quadratic majorizer* exists if $\beta_V(y) = \max_x \delta_V(x, y)$, i.e. if the supremum is attained. We the define the sharp quadratic majorizer of f at y as g with

$$g(x, y) = f(y) + (x - y)'\mathcal{D}f(y) + \frac{1}{2}\beta_V(y)(x - y)'V(x - y)$$

The corresponding majorization algorithm is

$$x^{(k+1)} = x^{(k)} - \frac{1}{\beta_V(x^{(k)})} V^{-1} \mathcal{D}f(x^k).$$

If f is convex we can generalize the tangential majorization algorithm of J. De Leeuw and Lange (2009), section 6, to compute β. For convex f

$$b(x) \geq f(z) + (x-z)'\mathcal{D}f(z) - f(y) - (x-y)'\mathcal{D}f(y),$$

and thus

$$b(x) \geq \frac{u'd + c}{\frac{1}{2}u'u}, \tag{3}$$

with

$$\begin{aligned} u &:= x - y, \\ d &:= \mathcal{D}f(z) - \mathcal{D}f(y), \\ c &:= f(z) - f(y) + (y-z)'\mathcal{D}f(z). \end{aligned}$$

If the derivative of the minorizer on the right hand side of (3) vanishes we have u proportional to d, say $u = \lambda d$. It remains to maximize over λ. The maximum exists because convexity implies $c \leq 0$ and it is attained for $\lambda = -2\frac{c}{d'd}$. Thus tangential majorization gives the algorithm

$$x^{(k+1)} = y - 2\frac{f(x^{(k)}) - f(y) + (y - x^{(k)})'\mathcal{D}f(x^{(k)})}{(\mathcal{D}f(x^{(k)}) - \mathcal{D}f(y))'(\mathcal{D}f(x^{(k)}) - \mathcal{D}f(y))}(\mathcal{D}f(x^{(k)}) - \mathcal{D}f(y))$$

Insert exist.R Here

We can compute the generalization β_V with basically the same tangential majorization algorithm.

$$x^{(k+1)} = y - 2\frac{f(x^{(k)}) - f(y) + (y - x^{(k)})'\mathcal{D}f(x^{(k)})}{(\mathcal{D}f(x^{(k)}) - \mathcal{D}f(y))'V^{-1}(\mathcal{D}f(x^{(k)}) - \mathcal{D}f(y))}V^{-1}(\mathcal{D}f(x^{(k)}) - \mathcal{D}f(y))$$

Quadratic majorization with $A = \beta_V V$ updates x with

$$x^{(k+1)} = x^{(k)} - \frac{1}{\beta_V(x^{(k)})} V^{-1} \mathcal{D}f(x^k),$$

which has an iteration matrix at a solution x equal to

$$\mathcal{M}(x)=I-\frac{1}{\lambda_+(V^{-1}\mathcal{D}^2f(x))}V^{-1}\mathcal{D}^2f(x),$$

and an iteration radius

$$\kappa(x)=1-\frac{\lambda_2(V^{-1}\mathcal{D}^2f(x))}{\lambda_1(V^{-1}\mathcal{D}^2f(x))},$$

where $\lambda_1\geq\lambda_2$ are the two largest eigenvalues of $V^{-1}\mathcal{D}^2f(x)$.

As an example, consider f defined by $f(x)=\sum_{i=1}^n\log(1+\exp(r_i'x))$. The function is convex, and as we have shown $\mathcal{D}^2f(x)\leq\frac{1}{4}R'R$.

###Optimality with Two Support Points

Building on earlier work by Groenen, Giaquinto, and Kiers (2003), Van Ruitenburg (2005) proves that a quadratic function g majorizing a differentiable function f at two points must be a sharp quadratic majorizer. We summarize his argument here.

Lemma 1: Suppose two quadratic functions $g_1\neq g_2$ both majorize the differentiable function f at y. Then either g_1 strictly majorizes g_2 at y or g_1 strictly majorizes g_2 at y.

Proof: We have

$$g_1(x)=f(y)+f'(y)(x-y)+\frac{1}{2}a_1(x-y)^2, \tag{1a}$$

$$g_2(x)=f(y)+f'(y)(x-y)+\frac{1}{2}a_2(x-y)^2, \tag{1b}$$

with $a_1\neq a_2$. Subtracting $(1a)$ and $(1b)$ proves the lemma. **QED**

Lemma 2: Suppose the quadratic function g_1 majorizes a differentiable function f at y and $z_1\neq y$ and that the quadratic function g_2 majorizes f at y and $z_2\neq y$. Then $g_1=g_2$.

Proof: Suppose $g_1\neq g_2$. Since both g_1 and g_2 majorize f at y, Lemma 1 applies. If g_2 strictly majorizes g_1 at y, then $g_1(z_2)<g_2(z_2)=f(z_2)$, and g_1 does not majorize f. If g_1 strictly majorizes g_2 at y, then similarly $g_2(z_1)<g_1(z_1)=f(z_1)$, and g_2 does not majorize f. Unless $g_1=g_2$, we reach a contradiction. **QED**

We now come to Van Ruitenburg's main result.

Theorem 1: Suppose a quadratic function g_1 majorizes a differentiable function f at y and at $z \neq y$, and suppose $g_2 \neq g_1$ majorizes f at y. Then g_2 strictly majorizes g_1 at y.

Proof: Suppose g_1 strictly majorizes g_2. Then $g_2(z) < g_1(z) = f(z)$ and thus g_2 does not majorize f. The result now follows from Lemma 1. **QED**

6.2.1 Even and Odd Functions

If f is even then

$$\begin{aligned}\delta(-y,y,a) &= +2yf'(y) - 2ay^2,\\ \mathcal{D}_1\delta(-y,y,a) &= -2f'(y) + 2ay,\\ \mathcal{D}_{11}\delta(-y,y,a) &= f''(y) - a.\end{aligned}$$

If $a = f'(y)/y$ then both $\delta(-y,y,a) = 0$ and $\mathcal{D}_1\delta(-y,y,a) = 0$.

$$f(x) - f(y) - f'(y)(x-y) - \frac{1}{2}\frac{f'(y)}{y}(x-y)^2 \leq 0 \qquad \forall x$$

If f satisfies the differential inequality

$$f''(x) \leq \frac{f'(x)}{x} \qquad \forall x$$

then $\delta(x,y,f'(y)/y)$ is

Assuming that $f(x)$ is even, i.e. $f(x) = f(-x)$ for all x, simplifies the construction of quadratic majorizers. If an even quadratic g satisfies $g(y) = f(y)$ and $g'(y) = f'(y)$, then it also satisfies $g(-y) = f(-y)$ and $g'(-y) = f'(-y)$. If in addition g majorizes f at either y or $-y$, then it majorizes f at both y and $-y$, and Theorem **??** implies that it is the best possible majorization at both points. This means we only need an extra condition to guarantee that g majorizes f. The next theorem, essentially proved in the references Groenen, Giaquinto, and Kiers (2003), Jaakkola and Jordan (2000), Hunter and Li (2005), by other techniques, highlights an important sufficient condition.

Theorem: Suppose $f(x)$ is an even, differentiable function on $\mathbb{R}$ such that the ratio $f'(x)/x$ is decreasing on $(0, \infty)$. Then the even quadratic

$$g(x) \quad = \quad \frac{f'(y)}{2y}(x^2 - y^2) + f(y)$$

is the best majorizer of $f(x)$ at the point y.

Proof: It is obvious that $g(x)$ is even and satisfies the tangency conditions $g(y) = f(y)$ and $g'(y) = f'(y)$. For the case $0 \leq x \leq y$, we have

$$\begin{aligned} f(y) - f(x) &= \int_x^y f'(z)\,dz \\ &= \int_x^y \frac{f'(z)}{z} z\,dz \\ &\geq \frac{f'(y)}{y} \int_x^y z\,dz \\ &= \frac{f'(y)}{y} \frac{1}{2}(y^2 - x^2) \\ &= f(y) - g(x), \end{aligned}$$

where the inequality comes from the assumption that $f'(x)/x$ is decreasing. It follows that $g(x) \geq f(x)$. The case $0 \leq y \leq x$ is proved in similar fashion, and all other cases reduce to these two cases given that $f(x)$ and $g(x)$ are even. **QED**

There is an condition equivalent to the sufficient condition of Theorem **??** that is sometimes easier to check.

Theorem: The ratio $f'(x)/x$ is decreasing on $(0, \infty)$ if and only $f(\sqrt{x})$ is concave. The set of functions satisfying this condition is a closed under the formation of (a) positive multiples, (b) convex combinations, (c) limits, and (d) composition with a concave increasing function $g(x)$.

Proof: Suppose $f(\sqrt{x})$ is concave in x and $x > y$. Then the two inequalities

$$\begin{aligned} f(\sqrt{x}) &\leq f(\sqrt{y}) + \frac{f'(\sqrt{y})}{2\sqrt{y}}(x - y) \\ f(\sqrt{y}) &\leq f(\sqrt{x}) + \frac{f'(\sqrt{x})}{2\sqrt{x}}(y - x) \end{aligned}$$

are valid. Adding these, subtracting the common sum $f(\sqrt{x})+f(\sqrt{y})$ from both sides, and rearranging give

$$\frac{f'(\sqrt{x})}{2\sqrt{x}}(x-y) \quad \leq \quad \frac{f'(\sqrt{y})}{2\sqrt{y}}(x-y).$$

Dividing by $(x-y)/2$ yields the desired result

$$\frac{f'(\sqrt{x})}{\sqrt{x}} \quad \leq \quad \frac{f'(\sqrt{y})}{\sqrt{y}}.$$

Conversely, suppose the ratio is decreasing and $x > y$. Then the mean value expansion

$$f(\sqrt{x}) \quad = \quad f(\sqrt{y}) + \frac{f'(\sqrt{z})}{2\sqrt{z}}(x-y)$$

for $z \in (y, x)$ leads to the concavity inequality.

$$f(\sqrt{x}) \quad \leq \quad f(\sqrt{y}) + \frac{f'(\sqrt{y})}{2\sqrt{y}}(x-y).$$

The asserted closure properties are all easy to check. **QED**

As examples of property (d) of Theorem **??**, note that the functions $g(x) = \ln x$ and $g(x) = \sqrt{x}$ are concave and increasing. Hence, if $f(\sqrt{x})$ is concave, then $\ln f(\sqrt{x})$ and $f(\sqrt{x})^{1/2}$ are concave as well.

6.3 Sharp Piecewise Linear

Suppose f is a real function of a real variable. For each $x \neq y$ define

$$\delta_f(x,y) := \frac{f(x)-f(y)}{x-y}.$$

If f is differentiable at y we set $\delta_f(y,y) = f'(y)$. Also define

$$\underline{\delta}_f(y) := \inf_{x>y} \delta_f(x,y),$$
$$\overline{\delta}_f(y) := \sup_{x<y} \delta_f(x,y).$$

Of course $\underline{\delta}_f(y)$ could be $-\infty$ and/or $\overline{\delta}_f(y)$ could be $+\infty$, and we will take these possibilities into account.

Note that if f is differentiable at y and $\delta_f(x,y)$ is increasing in x then $\underline{\delta}_f(y) = \overline{\delta}_f(y) = f'(y)$. If $\delta_f(x,y)$ is decreasing in x then $\underline{\delta}_f(y) = \lim_{x\rightarrow+\infty}\delta_f(x,y)$ and $\overline{\delta}_f(y) = \lim_{x\rightarrow-\infty}\delta_f(x,y)$.

If $x > y$ then $\delta_f(x,y) \geq \underline{\delta}_f(y)$ and thus

$$f(x) \geq f(y) + \underline{\delta}_f(y)(x-y).$$

If $x < y$ then $\delta_f(x,y) \leq \overline{\delta}_f(y)$ and thus also

$$f(x) \geq f(y) + \overline{\delta}_f(y)(x-y).$$

This means that if we define the extended real valued function

$$h(x,y) := \begin{cases} f(y) + \overline{\delta}_f(y)(x-y) & \text{if } x < y, \\ f(y) + \underline{\delta}_f(y)(x-y) & \text{if } x > y, \\ f(y) & \text{if } x = y, \end{cases}$$

then $f(x) \geq h(x,y)$ for all x and y and we have a minorization function consisting of two line segments.

If $f(x) = |x|$ then $\delta_f(x,0) = \mathbf{sign}(x)$. Thus $\underline{\delta}_f(0) = 1$ and $\overline{\delta}_f(0) = -1$. It follows that $h(x,0) = |x|$, as expected.

If $f(x) = ax^2 + bx + c$ then $\delta_f(x,y) = a(x+y) + b$. Thus if $a > 0$ we have $\underline{\delta}_f(y) = \overline{\delta}_f(y) = a$ and $h(x,y) = f(y) + a(x-y)$. If $a < 0$ we have $\underline{\delta}_f(y) = -\infty$ and $\overline{\delta}_f(y) = +\infty$.

If $f(x) = ax^3 + bx^2 + cx + d$, with $a \neq 0$, then $\delta_f(x,y) = ax^2 + (ay+b)x + (ay^2 + by + c)$. Suppose $a > 0$. Then $\overline{\delta}_f(y) = +\infty$. The minimum of $\delta_f(x,y)$ over x is attained at $-(ay+b)/2a$, and thus

$$\underline{\delta}_f(y) = \begin{cases} f'(y) & \text{if } y \geq -\frac{b}{3a}, \\ \min_x \delta_f(x,y) & \text{if } y < -\frac{b}{3a}. \end{cases}$$

If $a < 0$ we find, in the same way, that $\underline{\delta}_f(y) = -\infty$ and that

$$\overline{\delta}_f(y) = \begin{cases} f'(y) & \text{if } y \leq -\frac{b}{3a}, \\ \max_x \delta_f(x,y) & \text{if } y > -\frac{b}{3a}. \end{cases}$$

Consider the quartic $f(x) = ax^4 + bx^3 + cx^2 + dx + e$, with $a \neq 0$. We have

$$\delta_f(x, y) = ax^3 + (ay + b)x^2 + (ay^2 + by + c)x + (ay^3 + by^2 + cy + d).$$

Also the derivative of δ_f with respect to x is is the quadratic

$$\delta'_f(x, y) = 3ax^2 + 2(ay + b)x + (ay^2 + by + c).$$

First suppose $a < 0$. This case turns out to be uninteresting, because $\underline{\delta}_f(y) = -\infty$ and $\overline{\delta}_f(y) = +\infty$. So assume $a > 0$. If $\delta'_f(x, y)$ has no real roots (or two equal real roots), as a function of x for fixed y, then $\delta'_f(x, y) \geq 0$ for all x and $\delta_f(x, y)$ is increasing in x, and $\underline{\delta}_f(y) = \overline{\delta}_f(y) = f'(y)$.

If $\delta'_f(x, y)$ has two real roots, then $\delta_f(x, y)$ has a local maximum at the smallest root, say x_1, and a local minimum at the largest root, say x_2. There is also a $x_0 < x_1$ with $\delta_f(x_0, y) = \delta_f(x_2, y)$ and an $x_3 > x_2$ such that $\delta_f(x_3, y) = \delta_f(x_1, y)$. Now

$$\underline{\delta}_f(y) = \begin{cases} f'(y) & \text{if } y \geq x_0, \\ \delta_f(x_2, y) & \text{if } x_0 \leq y \leq x_2, \\ f'(y) & \text{if } y \geq x_2. \end{cases}$$

Of course in the same way

$$\overline{\delta}_f(y) = \begin{cases} f'(y) & \text{if } y \leq x_1, \\ \delta_f(x_1, y) & \text{if } x_1 \leq y \leq x_3, \\ f'(y) & \text{if } y \geq x_3. \end{cases}$$

A simple numerical example sets $a = 1$, $c = -4$, and $b = d = e = 0$. Thus $f(x) = x^4 - 4x^2$. Moreover $\delta_f(x, 0) = x^3 - 4x$, and $\delta'_f(x, 0) = 3x^2 - 4$. The roots of the quadratic are $x_1 = -\frac{2}{3}\sqrt{3}$ and $x_2 = +\frac{2}{3}\sqrt{3}$. Also $x_0 = -\frac{4}{3}\sqrt{3}$ and $x_2 = +\frac{4}{3}\sqrt{3}$. Thus $\underline{\delta}_f(0) = -3.079201$ and $\overline{\delta}_f(0) = +3.079201$. Using these values we can plot the broken-line minorization of $f(x) = x^4 - 4x^2$ at $y = 0$. Compare this with the sharp quadratic minorization at $y = 0$, which is the function $g(x) = -4x^2$.

6.4 Examples

6.4.1 The cosine

The function $f : x \rightarrow \cos(x)$ provides a simple example of majorization, also used by Lange (2016 (in press)). We work out some additional details. Start with

$$\cos(x) = \cos(y) - \sin(y)(x-y) - \frac{1}{2}\cos(y)(x-y)^2 + \frac{1}{6}\sin(y)(x-y)^3 + \frac{1}{24}\cos(y)(x-y)^4 + \ldots \tag{1}$$

Since $f''(x) = \cos(x) \leq 1$ we see that

$$g(x,y) := \cos(y) - \sin(y)(x-y) + \frac{1}{2}(x-y)^2$$

provides a uniform quadratic majorizer. Thus the iteration map

$$A(x) = x + \sin(x)$$

provides a uniform quadratic majorization algorithm.

Now

$$\frac{A(x) - \pi}{x - \pi} = 1 - \frac{\sin(x-\pi)}{x-\pi},$$

and for $0 < x < 2\pi$ we have $0 < 1 - \frac{\sin(x-\pi)}{x-\pi} < 1$, and thus the algorithm converges to π. As Lange (2016 (in press)) points out the algorithm has a cubic rate of convergence, because

$$A(\pi + x) - \pi = x + \sin(\pi + x) = \frac{1}{6}x^3 + o(x^3),$$

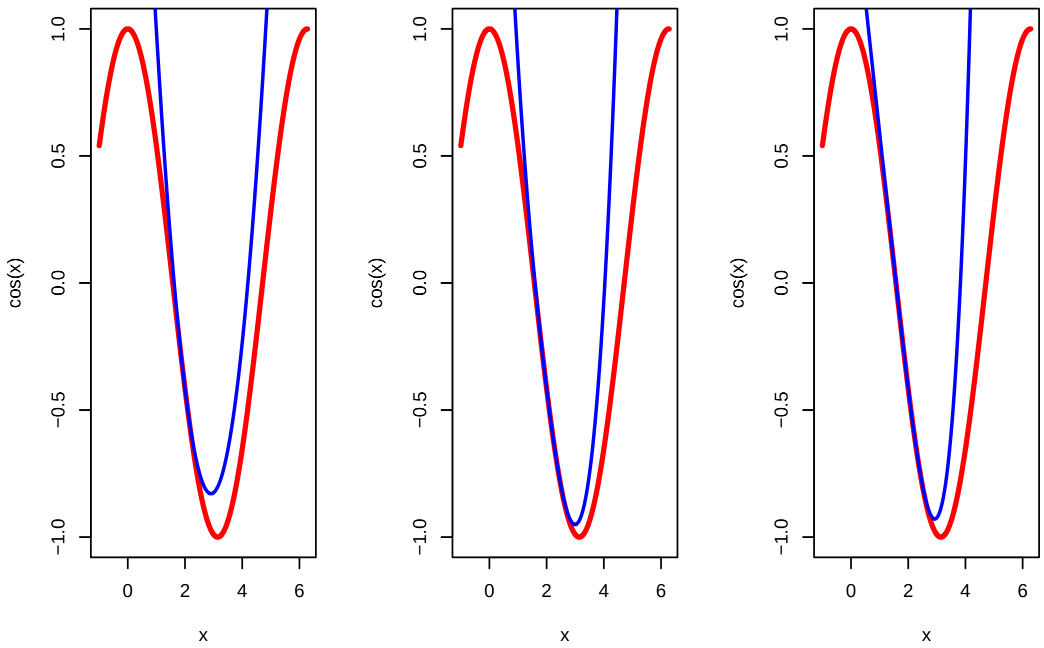
and thus

$$\lim_{x \rightarrow 0} \frac{A(\pi + x) - \pi}{x^3} = \frac{1}{6}.$$

As a consequence of cubic convergence, there is not much that can be done to improve the algorithm (which is of very limited practical usefulness anyway). Of course we could use the more precise majorizations

$$\cos(x) \leq \cos(y) - \sin(y)(x-y) - \frac{1}{2}\cos(y)(x-y)^2 + \frac{1}{6}|x-y|^3,$$
$$\cos(x) \leq \cos(y) - \sin(y)(x-y) - \frac{1}{2}\cos(y)(x-y)^2 + \frac{1}{6}\sin(y)(x-y)^3 + \frac{1}{24}(x-y)^4,$$

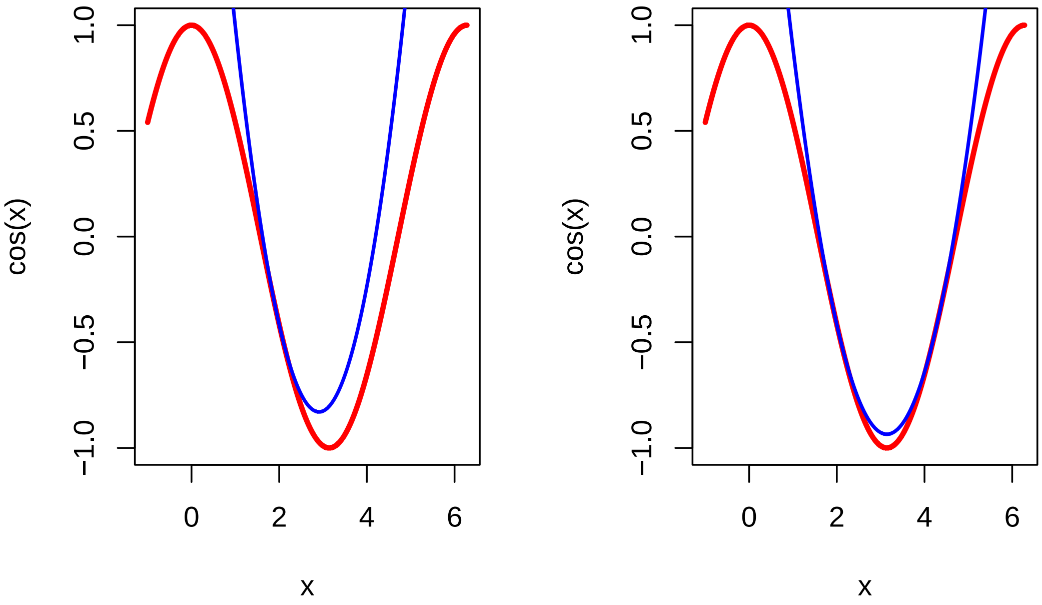
but they mostly increase the amount of computation in an iteration and do not improve much. The quadratic majorization at $y = 2$ has its minimum at 2.1974, the cubic majorization at 2.9952, and the quartic majorization at 2.9270. The three majorizations at $y = 2$ are shown in Figure 1.



As a curiosity, we could also consider the sharp quadratic majorization

$$g(x,y)=\cos(y)-\sin(y)(x-y)+\frac{1}{2}\frac{\sin(y)}{\pi-y}(x-y)^2$$

which has support points at $x=y$ and $x=2\pi-y$. Because of symmetry the correspondng majorization algorithm converges to $x=\pi$ in a single step in this case. In Figure 2 we show the uniform and sharp quadratic majorizations for $y=2$.



6.4.2 The Rasch Model

The Rasch model for item analysis says that that the probability that person i gives a correct response to item j is

$$\pi_{ij}=\frac{\exp(\theta_i+\epsilon_j)}{1+\exp(\theta_i+\epsilon_j)}.$$

The likelihood is

$$L=\prod_{i=1}^n\prod_{j=1}^m\pi_{ij}^{y_{ij}}(1-\pi_{ij})^{1-y_{ij}},$$

which means that the negative log-likelihood has the form

$$\mathcal{L}=\sum_{i=1}^n\sum_{j=1}^m\log[1+\exp(\theta_i+\epsilon_j)]-\sum_{i=1}^n y_{i\star}\theta_i+\sum_{j=1}^m y_{\star j}\epsilon_j.$$

Now consider $g(x)=\log(1+e^x)$, which we can write as $g(x)=\log(1-\pi(x))$. We find

$$g'(x)=\frac{e^x}{1+e^x}=\pi(x),$$
$$g''(x)=\frac{e^x}{(1+e^x)^2}=\pi(x)(1-\pi(x)),$$

thus $0 \leq g''(x) \leq \frac{1}{4}$, which shows we can apply quadratic majorization in this case.

We leave the details of the majorization, which are just "completing the square' ' as usual, to the reader. The algorithm forms the matrix H with elements

$$h_{ij} = (\theta_i + \epsilon_j) - 2(\pi_{ij} + y_{ij}),$$

and it updates the parameter estimates by computing row and column averages of this matrix.

###Logits

6.4.3 Probits

We define the *normal density*

$$\phi(x) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}x^2),$$

and the *normal distribution function*

$$\Phi(x) = \int_{-\infty}^{x} \phi(z)dz$$

in the usual way. In addition we define

$$f(x) = -\log \Phi(x).$$

Clearly

$$f'(x) = -\frac{\phi(x)}{\Phi(x)}$$

$$f''(x) = \frac{x\phi(x)}{\Phi(x)} + \left[\frac{\phi(x)}{\Phi(x)}\right]^2.$$

We can get more insight into these derivatives by rewriting them as conditional expectations. If $u = \phi(z)$ then $du = -z\phi(z)dz$ and thus

$$\int_{-\infty}^{x} z\phi(z)dz = -\int_{0}^{\phi(x)} du = -\phi(x),$$

which implies

$$f'(x) = \frac{\int_{-\infty}^{x} z\phi(z)dz}{\int_{-\infty}^{x} \phi(z)dz} = \mathbf{E}(z|z < x).$$

This shows that $f'(x) < 0$ and thus f is decreasing.

Now in the same way we can define $u = z\phi(z)$ and use $du = (1 - z^2)\phi(z)$ to derive

$$\int_{-\infty}^{x} (1 - z^2)\phi(z)dz = \int_{0}^{x\phi(x)} du = x\phi(x),$$

which implies

$$1 - \mathbf{E}(z^2|z < x) = \frac{x\phi(x)}{\Phi(x)},$$

and thus

$$f''(x) = 1 - [\mathbf{E}(z^2|z < x) + \mathbf{E}(z|z < x)] = 1 - \mathbf{V}(z|z < x).$$

This shows that $0 < f''(x) < 1$, and thus f is convex and has a bounded second derivative. Moreover $f''(x)$ is decreasing, which implies that f' is concave. Also

$$\begin{aligned} \lim_{x \to -\infty} f''(x) &= 1, \\ \lim_{x \to +\infty} f''(x) &= 0. \end{aligned}$$

A function g majorizes our function f in a point y if $g(x) \geq f(x)$ for all x and $g(y) = f(y)$. A quadratic function

$$g(x) = c + b(x - y) + \frac{1}{2}a(x - y)^2$$

majorizes f in y if and only if $c = f(y)$, $b = f'(y)$, and

$$a \geq A(y) = \sup_{x \neq y} \delta(x|y),$$

where

$$\delta(x|y) = \frac{f(x) - f(y) - f'(y)(x - y)}{\frac{1}{2}(x - y)^2}.$$

We find the *best quadratic majorization* of f in y by choosing $a = A(y)$.

Since $\delta(x|y = f''(z)$ for some z between x and y, we see that $\delta(x|y) < 1$ for all x. On the other hand

$$\lim_{x\rightarrow -\infty}\delta(x,y)=1,$$

and consequently $A(y) = 1$ for all y. Thus the best quadratic majorization is actually the *uniform quadratic majorization*

$$g(x)=f(y)+f'(y)(x-y)+\frac{1}{2}(x-y)^2.$$

Chapter 7

Local and Localized Majorization

##Introduction

7.0.1 Majorization in a Neighborhood

Consider the cubic $f(x) = 2x - x^2 + \frac{1}{6}x^3$. It is an increasing function on the real line, with a root at $x = 0$, and a saddle point at $x = 2$.

We know that cubics do not have quadratic majorizers, but we can try to find a quadratic

$$g(x, y) = f(y) + f'(y)(x - y) + \frac{1}{2}a(x - y)^2$$

such that $g(x, y) \geq f(x)$ for all $x \geq 2$ and such that

$$y - \frac{f'(y)}{a} \geq 2$$

if $y \geq 2$.

The condition $g(x, y) \geq f(x)$ for all $x \geq 2$ is

$$a \geq f''(y) + \frac{1}{3}f'''(y)(2 - y),$$

which is in our case

$$a \geq \frac{2}{3}(y-2).$$

We have

$$y - \frac{f'(y)}{a} \geq 2$$

for

$$a \geq \frac{1}{2}(y-2).$$

If $|\mathcal{D}_{ij}f(x)| \leq K$ for all i,j and x then

$$z'\mathcal{D}^2 f(x)z \leq \sum_{i=1}^n \sum_{i=1}^n K|z_i||z_j] = K(\sum_{i=1}^n |z_i|)^2 \leq n^2 K z'z$$

This can be extended easily to higher order partials

$$< \mathcal{D}^p(x), z \otimes \cdots \otimes z > \leq K(\sum_{i=1}^n |z_i|)^p \leq n^p (z'z)^p$$

Minimize $f : x \rightarrow x^4$ on $[-1,+1]$, where $f''(x) \leq 12$, and thus if $-1 \leq x \leq +1$ and $-1 \leq y \leq +1$

$$f(x) \leq g(x,y) = y^4 + 4y^3(x-y) + 6(x-y)^2.$$

The majorizer is minimized at $x = y - \frac{1}{3}y^3$. Thus the majorization algorithm is

$$x^{(k+1)} = x^{(k)} - \frac{1}{3}(x^{(k)})^3,$$

which converges monotonically to zero if started with $-1 \leq x^{(0)} \leq +1$. Because

$$\lim_{k\rightarrow\infty} \frac{x^{(k+1)}}{x^{(k)}} = 1$$

convergence is sublinear.

7.0.2 Cartesian Folium

If we minimize

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

on the rectangle defined by $0 \leq x \leq K$ and $0 \leq y \leq K$ then we can apply quadratic majorization

$$\begin{aligned} x^3 &\leq x_0^3 + 3x_0^2(x - x_0) + 3K(x - x_0)^2, \\ y^3 &\leq y_0^3 + 3y_0^2(y - y_0) + 3K(y - y_0)^2, \end{aligned}$$

and thus the algorithmic map is

$$\mathcal{A}(x, y) = \frac{1}{2K}\begin{bmatrix} -x^2 + 2Kx + y \\ -y^2 + 2Ky + x \end{bmatrix}.$$

The linear convergence rate is $1 - \frac{1}{2K}$.

7.0.3 Univariate Cubics

Suppose the problem is to minimize the cubic

$$f(x) = \alpha + \beta x + \frac{1}{2}\gamma x^2 + \frac{1}{6}\delta x^3$$

with $\delta \neq 0$. Since the cubic has no majorizers, we will find a local majorizer on the interval $[A, B]$.

From $f''(x) = \gamma + \delta x$ we see that

$$K(A, B) \overset{\Delta}{=} \max_{A \leq z \leq B} f''(z) = \gamma + \begin{cases} \delta B & \text{if } \delta > 0, \\ \delta A & \text{if } \delta < 0. \end{cases}$$

and thus, if $y \in [A, B]$,

$$f(x) \leq f(y) + f'(y)(x - y) + \frac{1}{2}K(A, B)(x - y)^2$$

over $A \leq x \leq B$.

If $K(A, B) > 0$ the majorizing quadratic has a minimum at

$$x = y - \frac{\beta + \gamma y + \frac{1}{2}\delta y^2}{K(A, B)}$$

This minimum can, of course, be outside the interval $[A, B]$, in which case the minimum of the quadratic is attained at one of the end-points. The minimum of the quadratic can be in the interval, but the function value at the minimum of the quadratic can be larger than the function value at one of the end-points. In that case, again, the majorization algorithm chooses one of the end-points. If $K(A, B) \leq 0$ the majorizer does not have a minimum and thus the minimum on the interval is attained at either A or B. Code in `R` is in the file `cubicBound.R`.

Insert cubicBound.R Here

If the iterations stay in the interior of the interval they converge to a local minimum at $\hat{x}$ with rate

$$\kappa = 1 - \frac{\gamma + \delta\hat{x}}{K(A, B)}$$

Consider, for example, the cubic $f(x) = \frac{1}{3}x^3 - \frac{1}{2}x^2 + cx$, where $0 \leq c \leq \frac{1}{4}$. The function has a local maximum at $\frac{1}{2} - \frac{1}{2}\sqrt{1-4c}$ and a local minimum at $\frac{1}{2} + \frac{1}{2}\sqrt{1-4c}$. Both are in the unit interval. The majorization algorithm, using $K(0, 1) = 1$, has the update rule

$$x^{(k+1)} = -(x^{(k)})^2 + 2x^{(k)} - c.$$

If started in the interval $(\frac{1}{2} - \frac{1}{2}\sqrt{1-4c}, \frac{1}{2} + \frac{1}{2}\sqrt{1-4c})$ the algorithm converges monotonically to the local minimum at $\frac{1}{2} + \frac{1}{2}\sqrt{1-4c}$ with rate $\kappa = 1 - \sqrt{1-4c}$, which is close to zero if c is close to zero and close to one if c is close to $\frac{1}{4}$. Here are two runs, the first one is fast, with $c = .001$, the second one is slow, with $c = .249$.

```
> cubicBound(c(0,.001,-.5,1/3),0,1)
Iteration:    1 fold:   -0.08283333 fnew:   -0.13968825 xold:    0.50000000 xn
Iteration:    2 fold:   -0.13968825 fnew:   -0.16376999 xold:    0.74900000 xn
Iteration:    3 fold:   -0.16376999 fnew:   -0.16565882 xold:    0.93599900 xn
Iteration:    4 fold:   -0.16565882 fnew:   -0.16566717 xold:    0.99490387 xn
Iteration:    5 fold:   -0.16566717 fnew:   -0.16566717 xold:    0.99897403 xn
Iteration:    6 fold:   -0.16566717 fnew:   -0.16566717 xold:    0.99899895 xn
$itel
[1] 6

$f
[1] -0.1656672
```

```
$x
[1] 0.998999

> cubicBound(c(0,.249,-.5,1/3),0,1)
Iteration:    1 fold:    0.04116667 fnew:    0.04116567 xold:    0.50000000 xnew:
Iteration:    2 fold:    0.04116567 fnew:    0.04116467 xold:    0.50100000 xnew:
Iteration:    3 fold:    0.04116467 fnew:    0.04116368 xold:    0.50199900 xnew:
Iteration:    4 fold:    0.04116368 fnew:    0.04116270 xold:    0.50299500 xnew:
Iteration:    5 fold:    0.04116270 fnew:    0.04116174 xold:    0.50398603 xnew:
...
...
Iteration:   89 fold:    0.04114559 fnew:    0.04114559 xold:    0.53141255 xnew:
Iteration:   90 fold:    0.04114559 fnew:    0.04114559 xold:    0.53142580 xnew:
Iteration:   91 fold:    0.04114559 fnew:    0.04114559 xold:    0.53143822 xnew:
Iteration:   92 fold:    0.04114559 fnew:    0.04114559 xold:    0.53144986 xnew:
Iteration:   93 fold:    0.04114559 fnew:    0.04114559 xold:    0.53146077 xnew:
Iteration:   94 fold:    0.04114559 fnew:    0.04114559 xold:    0.53147099 xnew:
$itel
[1] 94

$f
[1] 0.04114559

$x
[1] 0.5314806
```

We can also make cobweb plots for these two runs. They are in the figures below.

7.0.4 Majorization on the Sphere

The problem of minimizing f over a closed set $\mathcal{X}$ can be formulated as

$$\inf_{r\geq 0}\min_{x\in\mathcal{X}\cap\mathcal{S}_r} f(x),$$

where $\mathcal{S}_r \overset{\Delta}{=} \{x \mid x'x = r\}$. The set $\mathcal{X}\cap\mathcal{S}_r$ is compact so the inner minimum $f_r = \min_{x\in\mathcal{X}\cap\mathcal{S}_r} f(x)$ is attained for continuous f.

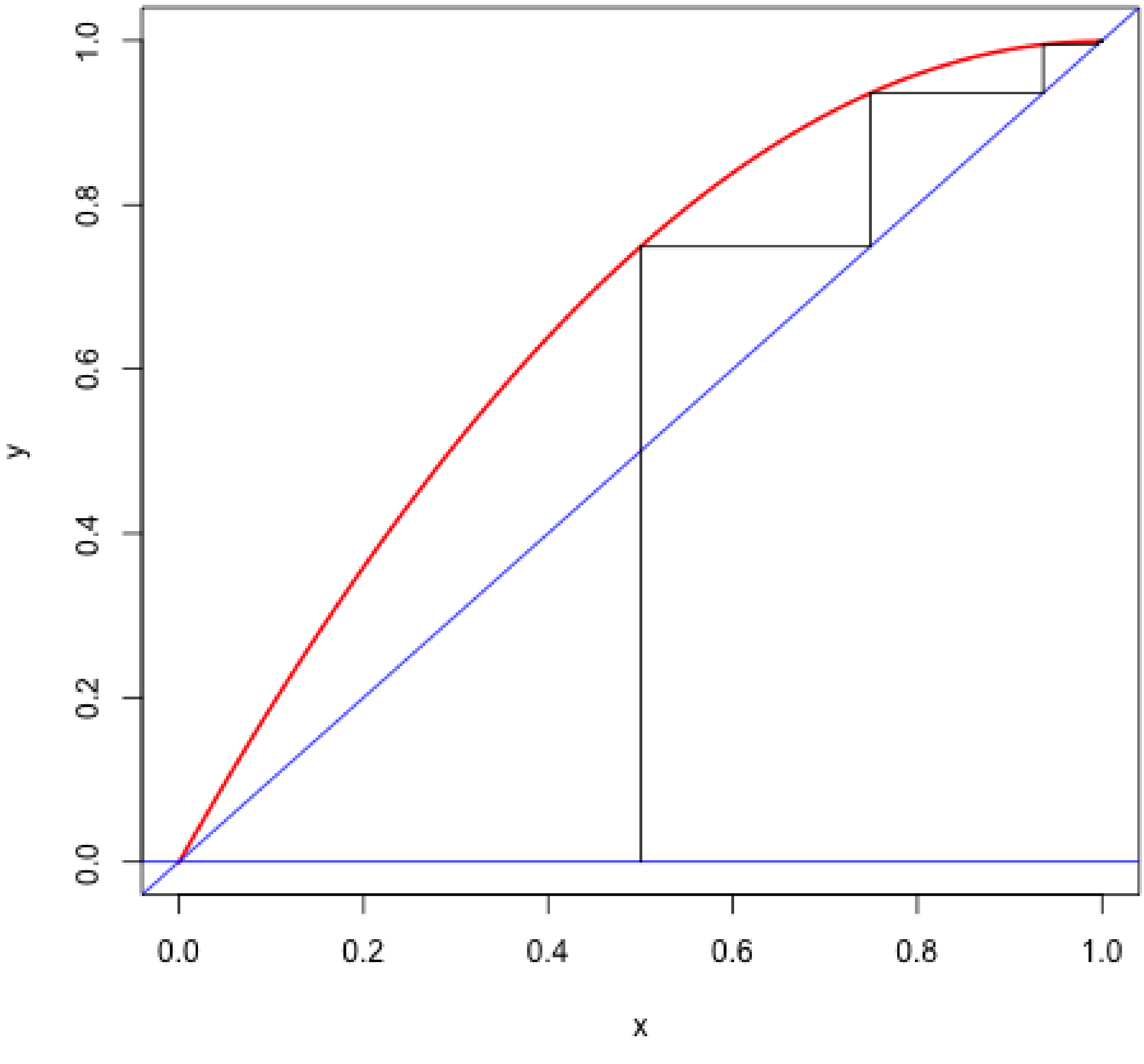


Figure 7.1: Cobweb Plot for c=0.001

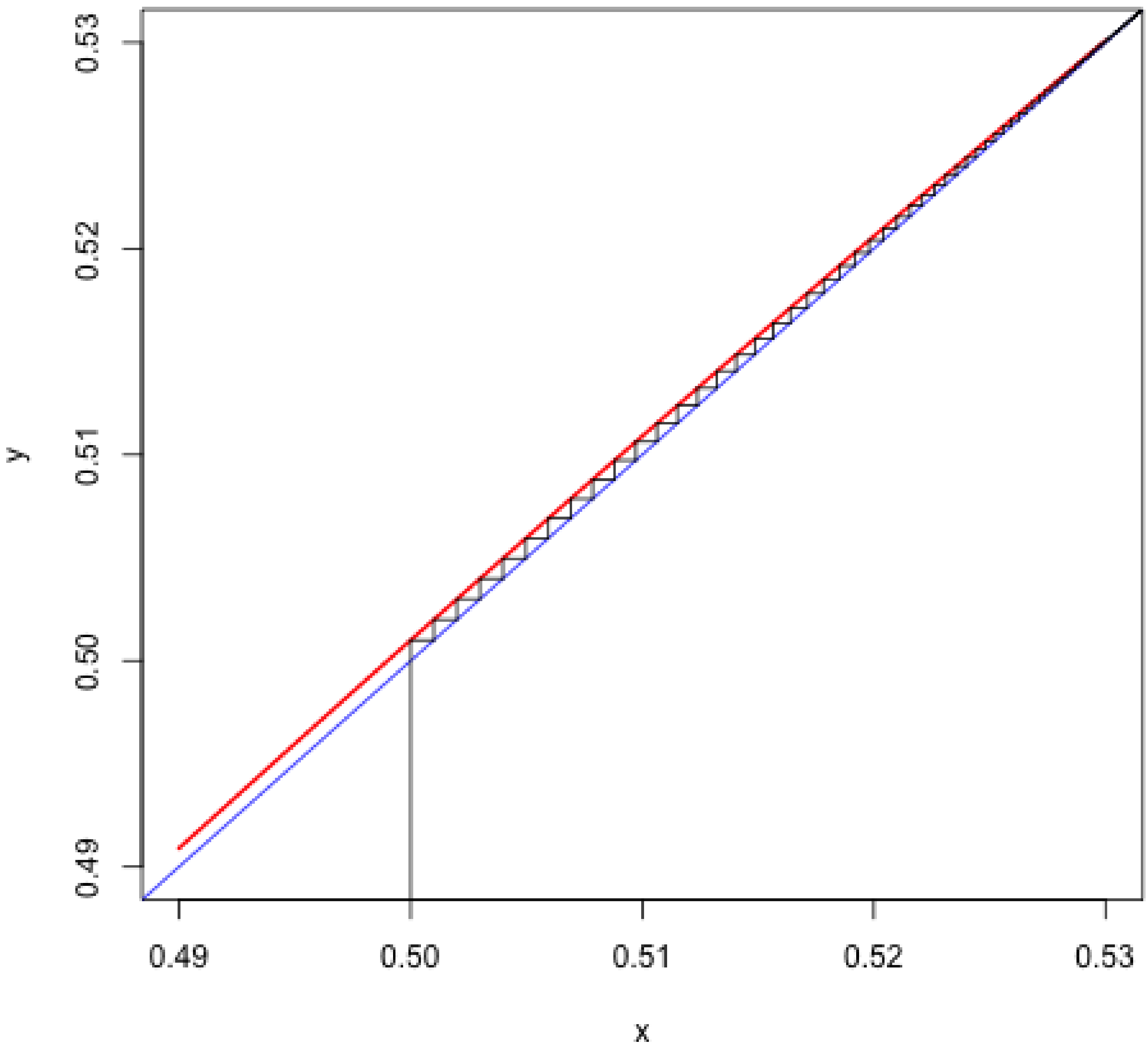


Figure 7.2: Cobweb Plot for c=0.249

If f is continuously differentiable on the ball $\mathcal{T}_r \overset{\Delta}{=} \{x \mid x'x \leq r\}$ then

$$h_r(y) \overset{\Delta}{=} \max_{z\in\mathcal{T}_r} \max_{0\leq\lambda\leq 1} z'\mathcal{D}^2 f(y+\lambda z))z$$

is well-defined. If $x, y \in \mathcal{S}_r$ then $y + \lambda(x-y) \in \mathcal{T}_r$ for all $0 \leq \lambda \leq 1$. So

$$f(x) \leq f(y) + (x-y)'\mathcal{D}f(y) + h_r(y)(r - x'y),$$

and we have a linear majorization on $\mathcal{S}_r$. The corresponding majorization algorithm is

$$x^{(k+1)} = \mathcal{P}_r(x^{(k)} - \frac{1}{h_r(x^{(k)})}\mathcal{D}f(x^{(k)})),$$

with $\mathcal{P}_r$ projection on the sphere $\mathcal{S}_r$.

S-majorization by a quadratic. The sublevel set for

$$g(x,y) = f(y) + (x-y)'b + \frac{1}{2}(x-y)'A(x-y)$$

with A positive definite is the ellipse

$$\mathcal{L}(y) = \{x \mid (x - z(y))'A(x - z(y)) \leq b'A^{-1}b\},$$

with $z \overset{\Delta}{=} y - A^{-1}b$. Thus for S-majorization we need to choosed A and b in such a way that g majorizes f on $\mathcal{L}(y)$. The problem is simplified, of course, if we choose $b = \mathcal{D}f(y)$.

7.0.5 Majorization on a Hyperrectangle

Here we discuss the work of Mönnigmann (2011) and others.

7.1 Proximal Point Majorization

We usually write $f(x) \leq g(x,y)$ for the key property of the majorizing function. One can also write $f(x) \leq f(x) + d(x,y)$ with $d(x,y) := g(x,y) - f(x)$ Thus $d(x,y)$ is non-negative, and $d(x,x) = 0$, i.e. $d(x,y)$ is distance-like.

Bregman

$$f(x) \leq f(x) + \lambda\|x - y\|^2$$

$$x^{(k+1)} = \mathop{\mathbf{argmin}}_{x} f(x) + \lambda_k \|x - x^{(k)}\|^2$$

The majorization algorithm updates by the rule

$$x^{(k+1)} \in \mathop{\mathbf{argmax}}_{x} f(x) + d(x, x^{(k)})$$

This shows majorization algorithms are generalized proximal point algorithms (for which there is a lot of theory). In the EM context this is used by Stephane Chretien, Alfred Hero, Paul Tseng and others to study algorithms. In fact, they often study

$$x^{(k+1)} \in \mathop{\mathbf{argmax}}_{x} f(x) + \lambda_k d(x, x^{(k)})$$

with λ_k a sequence of non-negative numbers.

7.2 Sub-level Majorization

Stability of the majorization algorithm is guaranteed by the sandwich inequality, which says that

$$f(x^{(k+1)}) \leq g(x^{(k+1)}, x^{(k)}) \leq g(x^{(k)}, x^{(k)}) = f(x^{(k)}).$$

The first inequality in the chain comes from the majorization condition $f(x) \leq g(x, y)$ for all $x, y \in X$. There is, however, a weaker condition which still implies the same inequality.

Suppose that we merely require that the majorization function g satisfies

$$g(x, y) \leq g(y, y) \Rightarrow f(x) \leq g(x, y).$$

Then we still have $g(x^{(k+1)}, x^{(k)}) \leq g(x^{(k)}, x^{(k)}) = f(x^{(k)})$, and as a consequence also $f(x^{(k+1)}) \leq g(x^{(k+1)}, x^{(k)})$. The sandwich inequality still applies.

The weaker localized majorization condition, which we will call *sublevel majorization* (or simply *S-majorization*) from now on, says that g majorizes f on the *sublevel set*

$$\mathcal{L}(y) \overset{\Delta}{=} \{x \in X \mid g(x,y) \leq g(y,y) = f(y)\},$$

while for $x \notin \mathcal{L}(y)$ we can have $f(x) > g(x,y)$. In other words, $g(x,y) - f(x)$ must have a global minimum equal to zero on $\mathcal{L}(y)$ at y.

S-majorization is easy to visualize for a univariate quadratic majorizer

$$g(x,y) = f(y) + f'(y)(x-y) + \frac{1}{2}a(x-y)^2,$$

which has $g(x,y) \leq f(y)$ if x is in the interval with end-points y and $y - \frac{2f'(y)}{a}$. For quadratic S-majorization of a cubic f, for example, we must have

$$a \geq f''(y) + \frac{1}{3}f'''(y)(x-y)$$

at both end-points of the interval $I(y)$, which means we must have both $a \geq f''(y)$ and

$$a^2 - af''(y) + \frac{2}{3}f'''(y)f'(y) \geq 0. \tag{1}$$

If the quadratic (1) has no real roots, or two equal real roots, then it is always non-negative, and we have sub-level majorization of the cubic at y if $a \geq f''(y)$. Now suppose the quadratic (1) has two different real roots, say $p(y) < q(y)$. We have $p(y) + q(y) = f''(y)$. Thus if $p(y)$ and $q(y)$ are non-negative, then $0 \leq p(y) \leq q(y) \leq f''(y)$, and we have sub-level majorization for $a \geq f''(y)$. If $p \leq 0$ and $q \geq 0$ then $q = f''(y) - p \geq f''(y)$ and thus $a \geq q(y)$. If both $p(y) \leq 0$ and $q(y) \leq 0$ then $f''(y) \leq p(y) < q(y) \leq 0$, and thus $\overline{a}(y) = 0$ and sub-level majorization is linear.

Near a local minimum, where $f''(y) \geq 0$ and $f'(y)$ is close to zero, the two roots of the quadratic are approximately $q = f''(y) - \frac{2}{3}f'(y)$ and $p = \frac{2}{3}f'(y)$.

note: 030615 Add the example from the paper and the reference

Quadratic sub-level majorization in the multivariate case. We have

$$g(x,y) = f(y) + (x-y)'\mathcal{D}f(y) + \frac{1}{2}(x-y)'A(x-y)$$

for some A which we assume to be positive definite for now. Then $g(x,y)\leq f(y)$ if and only if

$$(x-z)'A(x-z)\leq(\mathcal{D}f(y))'A^{-1}\mathcal{D}f(y),$$

with $z=y-A^{-1}\mathcal{D}f(y)$. For given y and A this means x must be in an ellipse centered at z, but note that if A changes then shape, radius, and center of the ellipse change.

If $A=aH$ with H fixed, then we have the more manageable inequality

$$\frac{1}{a^2}\geq\frac{(x-z)'H(x-z)}{(\mathcal{D}f(y))'H\mathcal{D}f(y)}$$

7.3 Dinkelbach Majorization

In S-majorization we make sure the sandwich inequality remains true by requiring that

$$g(x,y)\leq g(y,y)=f(y)\Rightarrow f(x)\leq g(x,y).$$

An alternative requirement, that also leads to a sandwich inequality, is

$$g(x,y)\leq g(y,y)=f(y)\Rightarrow f(x)\leq f(y),$$

or, in iteration terms, If $g(x^{(k+1)},x^{(k)})\leq g(x^{(k)},x^{(k)})$ then $f(x^{(k+1)})\leq f(x^{(k)})$.

Suppose f is a real-valued function on $\mathcal{X}$ and g is a real-valued function on $\mathcal{X}\otimes\mathcal{X}$. We say that *$g$ Dinkelbach majorizes f on $\mathcal{X}$* if * if $g(x,y)\leq g(y,y)$ then $f(x)\leq f(y)$ for all $x,y\in\mathcal{X}$, * $g(y,y)=f(y)$ for all $y\in\mathcal{X}$.

Dinkelbach Majorization is *strict* if the first condition can be replaced by * if $g(x,y)<g(y,y)$ then $f(x)<f(y)$ for all $x,y\in\mathcal{X}$.

The D here stands for Dinkelbach, who proposed a forerunner of D majorization in a classic fractional programming article Dinkelbach (1967). In S-majorization we require that g majorizes f on the sublevel set

$$\mathcal{L}(y)=\{x\in\mathcal{X}\mid g(x,y)\leq g(y,y)\}.$$

In D-majorization we require that f attains its maximum on the sublevel set $\mathcal{L}(y)$ at y.

Suppose f is a fractional function of the form

$$f(x)=\frac{a(x)}{b(x)},$$

with $b(x)>0$ for $x\in\mathcal{X}$. Then

$$g(x,y)=f(y)+a(x)-f(y)b(x)$$

D-majorizes f on $\mathcal{X}$.

Clearly

$$g(y,y)=f(y)+a(y)-\frac{a(y)}{b(y)}b(y)=f(y).$$

Moreover $g(x,y)\leq g(y,y)$ can be written as

$$f(y)+a(x)-f(y)b(x)\leq f(y)$$

which implies $f(x)\leq f(y)$.

Suppose

$$g(x,y)=f(y)+f'(y)(x-y)+\frac{1}{2}a(x-y)^2,$$

with $a>0$. Now $g(x,y)\leq f(y)$ if and only if

$$(x-y)(f'(y)+\frac{1}{2}a(x-y))\leq 0,$$

Or x must be in the interval between y and $y-\frac{2f'(y)}{a}$. For a cubic

$$f(x)=f(y)+f'(y)(x-y)+\frac{1}{2}f''(y)(x-y)^2+\frac{1}{6}f'''(x-y)^3$$

we require that

$$(x-y)(f'(y)+\frac{1}{2}f''(y)(x-y)+\frac{1}{6}f'''(x-y)^2)\leq 0$$

for all x in the interval between y and $y-\frac{2f'(y)}{a}$.

Suppose f is increasing and differentiable. We have $f'(y)\geq 0$ for all y. Thus for any

$$x\in[y-\frac{2f'(y)}{a},y]$$

we have $x \leq y$ and consequently $f(x) \leq f(y)$. In other words: an increasing function is Dinkelbach majorized by any convex quadratic.

Consider f with $f(x) = \frac{1}{4}x^4$ and let us majorize at $y = 1$ by a convex quadratic g which has both $g(1) = f(1) = \frac{1}{4}$ and $g'(1) = f'(1) = 1$. It follows that

$$g(x) = ax^2 + (1-2a)x + (a - \frac{3}{4})$$

for some $a \geq 0$. Note that if we would also require that $g''(1) \geq h''(1)$ then we need $a \geq \frac{3}{2}$.

If we compute $h = g - f$ we find

$$h(x) = -\frac{1}{4}(x-1)^2(x^2 + 2x + (3-4a)).$$

Majorization at y would mean $h(x) \geq 0$ for all x, which is clearly impossible because $h(x)$ will be negative for x very large and x very small.

We have $h(x) \geq 0$ if and only if $q(x) \overset{\Delta}{=} x^2 + 2x + (3-4a) \leq 0$.The quadratic q can only be non-positive if it has two real roots, which happens if $a \geq \frac{1}{2}$, and then q is non-positive between its two real roots, which are $-1 - \sqrt{4a-2}$ and $-1 + \sqrt{4a-2}$.

The sublevel set $\mathcal{L}(1) = \{x \mid g(x) \leq \frac{1}{4}\}$ is the interval $[\frac{a-1}{a}, 1]$. For S-majorization we need $h(x) \geq 0$ for all $x \in \mathcal{L}(1)$, which means that interval $[\frac{a-1}{a}, 1]$ must be a subset of interval $[-1-\sqrt{4a-2}, -1+\sqrt{4a-2}]$. Thus we must have $1 \leq -1 + \sqrt{4a-2}$ as well as $\frac{a-1}{a} \geq -1 - \sqrt{4a-2}$. The first inequality gives $a \geq \frac{3}{2}$, the second one $a \geq \frac{1}{2}$. Thus we have S-majorization at $y = 1$ if and only if $a \geq \frac{3}{2}$. Figure 1 shows the S-majorization with $a = 3/2$, first globally, and then in closeup with $\mathcal{L}(1) = [\frac{1}{3}, 1]$ on the horizontal axis. Note that the S-majorizer is certainly not a majorizer. Also note that $a = 3/2$ actually makes $g''(1) = f''(1)$, which means the quadratic S-majorizer is the quadratic approximation used in Newton's method.

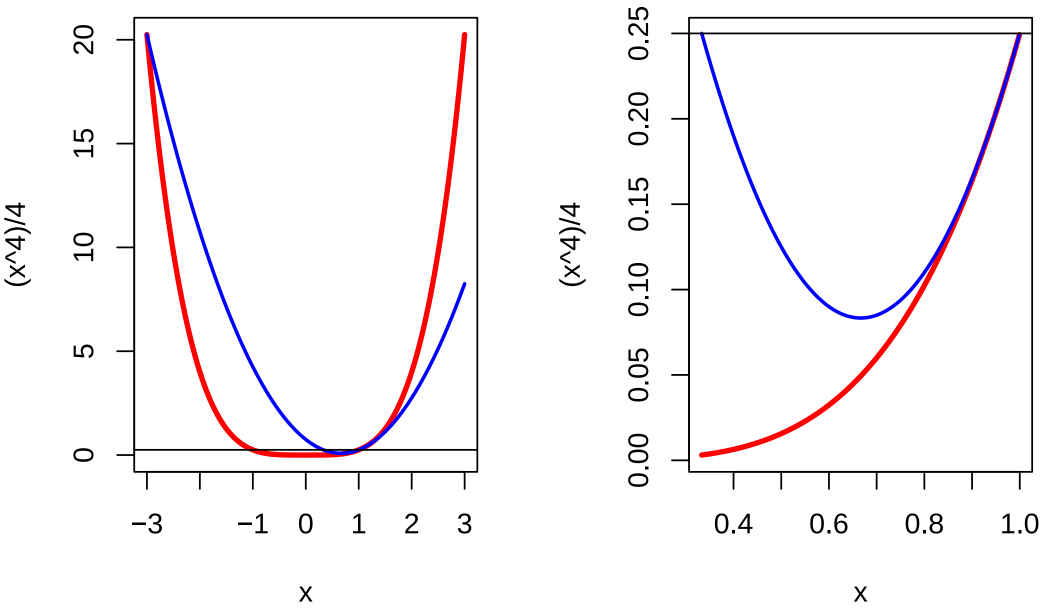


Figure 1: S-majorization at y = 1 for a = 1.5.

For D-majorization we need $f(x) \leq f(1) = \frac{1}{4}$ for all $x \in \mathcal{L}(1)$ which is the case if $\frac{a-1}{a} \geq -1$, i.e. g D-majorizes f at $y = 1$ if and only if $a \geq \frac{1}{2}$. In figure 2 we see that a D-majorizer can actually be a minorizer ! Of course the S-majorization in figure 1 is also a D-majorization.

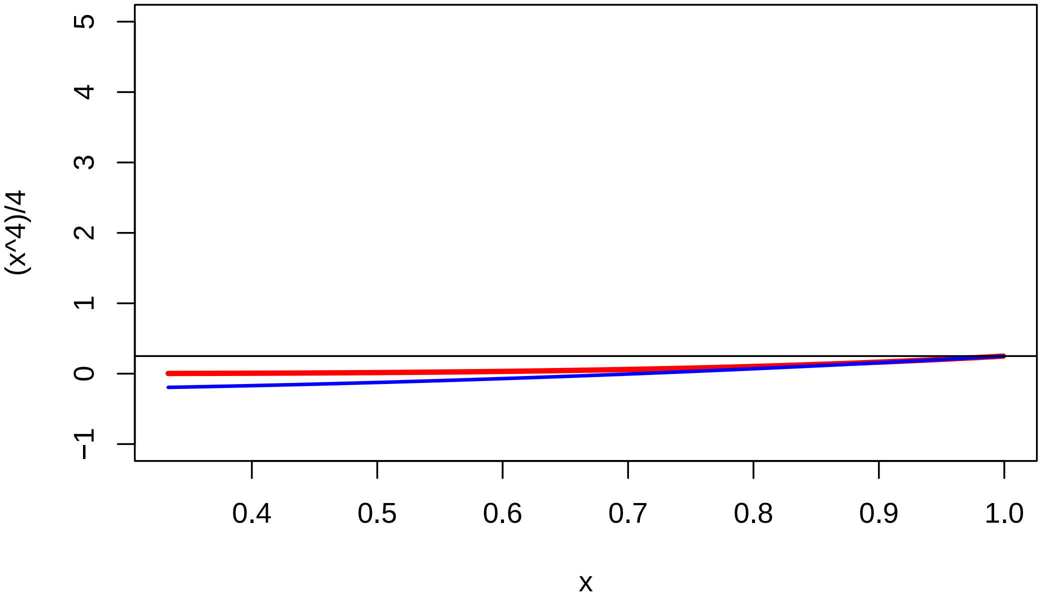


Figure 2: D-majorization at y = 1 for a = 0.5.

Chapter 8

Background

8.1 Introduction

8.2 Analysis

###SemiContinuities

The *lower limit* or *limit inferior* of a sequence $\{x_i\}$ is defined as

$$\liminf_{i\rightarrow\infty} x_i = \lim_{i\rightarrow\infty}\left[\inf_{k\geq i} x_k\right] = \sup_{i\geq 0}\left[\inf_{k\geq i} x_k\right].$$

Alternatively, the limit inferior is the smallest cluster point or subsequential limit

$$\liminf_{i\rightarrow\infty} x_i = \min\{y \mid x_{i_\nu} \rightarrow y\}.$$

In the same way

$$\limsup_{i\rightarrow\infty} x_i = \lim_{i\rightarrow\infty}\left[\sup_{k\geq i} x_k\right] = \inf_{i\geq 0}\left[\sup_{k\geq i} x_k\right].$$

We always have

$$\inf_i x_i \leq \liminf_{i\rightarrow\infty} x_i \leq \limsup_{i\rightarrow\infty} x_i \leq \sup_i x_i.$$

Also if $\liminf_{i\rightarrow\infty} x_i = \limsup_{i\rightarrow\infty} x_i$ then

$$\lim_{i\rightarrow\infty} x_i = \liminf_{i\rightarrow\infty} x_i = \limsup_{i\rightarrow\infty} x_i.$$

The *lower limit* or *limit inferior* of a function at a point $\overline{x}$ is defined as

$$\liminf_{x\rightarrow\overline{x}} f(x) = \sup_{\delta>0}\left[\inf_{x\in\mathcal{B}(\overline{x},\delta)} f(x)\right],$$

where

$$\mathcal{B}(\overline{x},\delta) \overset{\Delta}{=} \{x \mid \|x-\overline{x}\| \leq \delta\}.$$

Alternatively

$$\lim_{i\rightarrow\infty} x_i = \liminf_{x\rightarrow\overline{x}} f(x) = \min\{y \mid x_i \rightarrow \overline{x} \text{ and } f(x_i) \rightarrow y\}.$$

In the same way

$$\limsup_{x\rightarrow\overline{x}} f(x) = \inf_{\delta>0}\left[\sup_{x\in\mathcal{B}(\overline{x},\delta)} f(x)\right],$$

A function is *lower semi-continuous* at $\overline{x}$ if

$$\liminf_{x\rightarrow\overline{x}} f(x) \geq f(\overline{x})$$

Since we always have $\liminf_{x\rightarrow\overline{x}} f(x) \leq f(\overline{x})$ we can also define lower semi-continuity as

$$\liminf_{x\rightarrow\overline{x}} f(x) = f(\overline{x}).$$

A function is *upper semi-continuous* at $\overline{x}$ if

$$\limsup_{x\rightarrow\overline{x}} f(x) = f(\overline{x}).$$

We have

$$\liminf_{x\rightarrow\overline{x}} f(x) \leq \limsup_{x\rightarrow\overline{x}} f(x).$$

A function is *continuous* at $\overline{x}$ if and only if it is both lower semicontinuous and upper semicontinous, i.e. if

$$f(\overline{x}) = \lim_{x\rightarrow\overline{x}} f(x) = \liminf_{x\rightarrow\overline{x}} f(x) = \limsup_{x\rightarrow\overline{x}} f(x).$$

###Directional Derivatives

The notation and terminology are by no means standard. We generally follow Demyanov (2010).

The *lower Dini directional derivative* of f at x in the direction z is

$$\delta^-f(x,z)\triangleq\liminf_{\alpha\downarrow 0}\frac{f(x+\alpha z)-f(x)}{\alpha}=\sup_{\delta>0}\inf_{0<\alpha<\delta}\frac{f(x+\alpha z)-f(x)}{\alpha}.$$

and the corresponding *upper Dini directional derivative* is

$$\delta^+f(x,z)\triangleq\limsup_{\alpha\downarrow 0}\frac{f(x+\alpha z)-f(x)}{\alpha}=\inf_{\delta>0}\sup_{0<\alpha<\delta}\frac{f(x+\alpha z)-f(x)}{\alpha},$$

If

$$\delta f(x,z)=\lim_{\alpha\downarrow 0}\frac{f(x+\alpha z)-f(x)}{\alpha}$$

exists, i.e. if $\delta^+f(x,z)=\delta^-f(x,z)$, then it we simply write $\delta f(x,z)$ for the Dini directional derivative of f at x in the direction z.@penot_13 calls this the *radial derivative* and Schirotzek (2007) calls it the *directional Gateaux derivative.* If $\delta f(x,z)$ exists f is *Dini directionally differentiable* at x in the direction z, and if $\delta f(x,z)$ exists at x for all z we say that f is *Dini directionally differentiable* at x. Delfour (2012) calls f *semidifferentiable* at x.

In a similar way we can define the *Hadamard lower and upper directional derivatives.* They are

$$d^-f(x,z)\triangleq\liminf_{\substack{\alpha\downarrow 0\\ u\rightarrow z}}\frac{f(x+\alpha u)-f(x)}{\alpha}=\sup_{\delta>0}\inf_{\substack{u\in\mathcal{B}(z,\delta)\\ \alpha\in(0,\delta)}}\frac{f(x+\alpha u)-f(x)}{\alpha},$$

and

$$d^+f(x,z)\triangleq\limsup_{\substack{\alpha\downarrow 0\\ u\rightarrow z}}\frac{f(x+\alpha u)-f(x)}{\alpha}=\inf_{\delta>0}\sup_{\substack{u\in\mathcal{B}(z,\delta)\\ \alpha\in(0,\delta)}}\frac{f(x+\alpha u)-f(x)}{\alpha},$$

The Hadamard directional derivative $df(x,z)$ exists if both $d^+f(x,z)$ and $d^-f(x,z)$ exist and are equal. In that case f is *Hadamard directionally differentiable* at x in the direction z, and if $df(x,z)$ exists at x for all z we say that f is Hadamard directionally differentiable at x.

Generally we have

$$d^- f(x,z) \leq \delta^- f(x,z) \leq \delta^+ f(x,z) \leq d^+ f(x,z)$$

The *classical directional derivative* of f at x in the direction g is

$$\Delta f(x,z) \triangleq \lim_{\alpha \rightarrow 0} \frac{f(x+\alpha z) - f(x)}{\alpha}.$$

Note that for the absolute value function at zero we have $\delta f(0,1) = df(0,1) = 1$, while $\Delta f(0,1) = \lim_{\alpha \rightarrow 0} \mathbf{sign}(\alpha)$ does not exist. The classical directional derivative is not particularly useful in the context of optimization problems.

8.2.1 Differentiability and Derivatives

The function f is *Gateaux differentiable* at x if and only if the Dini directional derivative $\delta f(x,z)$ exists for all z and is linear in z. Thus $\delta f(x,z) = G(x)z$

The function f is *Hadamard differentiable* at x if the Hadamard directional derivative $df(x,z)$ exists for all z and is linear in z.

Function f is *locally Lipschitz* at z if there is a ball $\mathcal{B}(z,\delta)$ and a $\gamma > 0$ such that $\|f(x) - f(y)| \leq \gamma \|x - y\|$ for all $x, y \in \mathcal{B}(z,\delta)$.

If f is locally Lipschitz and Gateaux differentiable then it is Hadamard differentiable.

If the Gateaux derivative of f is continuous then f is Frechet differentiable.

Define Frechet differentiable

The function f is Hadamard differentiable if and only if it is Frechet differentiable.

Gradient, Jacobian

###Taylor's Theorem

Suppose $f : \mathcal{X} \rightarrow \mathbb{R}$ is $p+1$ times continuously differentiable in the open set $\mathcal{X} \subseteq \mathbb{R}^n$. Define, for all $0 \leq s \leq p$,

$$h_s(x,y) \triangleq \frac{1}{s!} \langle \mathcal{D}^s f(y), (x-y)^s \rangle,$$

as the inner product of the s-dimensional array of partial derivatives $\mathcal{D}^s f(y)$ and the s-dimensional outer power of $x-y$. Both arrays are super-symmetric, and have dimension n^s. By convention $h_0(x,y)=f(y)$.

Also define the *Taylor Polynomials*

$$g_p(x,y)\overset{\Delta}{=}\sum_{s=0}^p h_s(x,y)$$

and the *remainder*

$$r_p(x,y)\overset{\Delta}{=}f(x)-g_p(x,y).$$

Assume $\mathcal{X}$ contains the line segment with endpoints x and y. Then *Lagrange's form of the remainder* says there is a $0\leq\lambda\leq 1$ such that

$$r_p(x,y)=\frac{1}{(p+1)!}\langle\mathcal{D}^{p+1}f(x+\lambda(y-x)),(x-y)^{p+1}\rangle,$$

and the *integral form of the remainder* says

$$r_p(x,y)=\frac{1}{p!}\int_0^1(1-\lambda)^p\langle\mathcal{D}^{p+1}f(x+\lambda(y-x)),(x-y)^p\rangle d\lambda.$$

8.2.2 Implicit Functions

The classical implicit function theorem is discussed in all analysis books. I am particularly fond of Spivak (1965). The history of the theorem, and many of its variations, is discussed in Krantz and Parks (2003) and a comprenhensive modern treatment, using the tools of convex and variational analysis, is in Dontchev and Rockafellar (2014).

Suppose $f:\mathbb{R}^n\otimes\mathbb{R}^m\mapsto\mathbb{R}^m$ is continuously differentiable in an open set containing (x,y) where $f(x,y)=0$. Define the $m\times m$ matrix

$$A(x,y)\overset{\Delta}{=}\mathcal{D}_2f(x,y)$$

and suppose that $A(x,y)$ is non-singular. Then there is an open set $\mathcal{X}$ containing x and an open set $\mathcal{Y}$ containing y such that for every $x\in\mathcal{X}$ there is a unique $y(x)\in\mathcal{Y}$ with $f(x,y(x))=0$.

The function $y:\mathbb{R}^n\mapsto\mathbb{R}^m$ is differentiable. If we differentiate $f(x,y(x))=0$ we find

$$\mathcal{D}_1f(x,y(x))+\mathcal{D}_2(x,f(x))\mathcal{D}y(x),$$

and thus

$$\mathcal{D}y(x) = -[\mathcal{D}_2 f(x,y(x))]^{-1}\mathcal{D}_1 f(x,y(x)).$$

As an example consider the eigenvalue problem

$$\begin{aligned} A(x)y &= \lambda y, \\ y'y &= 1 \end{aligned}$$

where A is a function of a real parameter x. Then

$$\begin{bmatrix} A(x)-\lambda I & -x \\ x' & 0 \end{bmatrix} \begin{bmatrix} \mathcal{D}y(x) \\ \mathcal{D}\lambda(x) \end{bmatrix} = \begin{bmatrix} -\mathcal{D}A(x)x \\ 0 \end{bmatrix},$$

which works out to

$$\begin{aligned} &\mathcal{D}\lambda(x) = y(x)'\mathcal{D}A(x)y(x), \\ &\mathcal{D}y(x) = -(A(x)-\lambda(x)I)^{+}\mathcal{D}A(x)y(x). \end{aligned}$$

8.2.3 Necessary and Sufficient Conditions for a Minimum

Directional derivatives can be used to provide simple necessary or sufficient conditions for a minimum (Floudas (2009), propositions 8 and 9).

Result: If x is a local minimizer of f then $\delta^{-}f(x,z) \geq 0$ and $d^{-}f(x,z) \geq 0$ for all directions z. If $d^{-}f(x,z) > 0$ for all $z \neq 0$ then f has a strict local minimum at x.

The special case of a quadratic deserves some separate study, because the quadratic model is so prevalent in optimization. So let us look at $f(x) = c + b'x + \frac{1}{2}x'Ax$, with A symmetric. Use the eigen-decomposition $A = K\Lambda K'$ to change variables to $\tilde{x} \overset{\Delta}{=} K'x$, also using $\tilde{b} \overset{\Delta}{=} K'b$. Then $f(\tilde{x}) = c + \tilde{b}'\tilde{x} + \frac{1}{2}\tilde{x}'\Lambda\tilde{x}$, which we can write as

$$\begin{aligned} f(\tilde{x}) = c &- \frac{1}{2}\sum_{i\in I_+\cup I_-}\frac{\tilde{b}_i^2}{\lambda_i} \\ &+\frac{1}{2}\sum_{i\in I_+}|\lambda_i|(\tilde{x}_i+\frac{\tilde{b}_i}{\lambda_i})^2+ \\ &-\frac{1}{2}\sum_{i\in I_-}|\lambda_i|(\tilde{x}_i+\frac{\tilde{b}_i}{\lambda_i})^2+ \\ &+\sum_{i\in I_0}\tilde{b}_i\tilde{x}_i. \end{aligned}$$

Here

$$\begin{aligned} I_+&\overset{\Delta}{=}\{i\mid\lambda_i>0\}, \\ I_-&\overset{\Delta}{=}\{i\mid\lambda_i<0\}, \\ I_0&\overset{\Delta}{=}\{i\mid\lambda_i=0\}. \end{aligned}$$

* If I_- is non-empty we have $\inf_x f(x)=-\infty$. * If I_- is empty, then f attains its minimum if and only if $\tilde{b}_i=0$ for all $i\in I_0$. Otherwise again $\inf_x f(x)=-\infty$.

If the minimum is attained, then

$$\min_x f(x)=c-\frac{1}{2}b'A^+b,$$

with A^+ the Moore-Penrose inverse. And the minimum is attained if and only if A is positive semi-definite and $(I-A^+A)b=0$.

8.3 Point-to-set Maps

###Continuities

8.3.1 Marginal Functions and Solution Maps

Suppose $f:\mathbb{R}^n\otimes\mathbb{R}^n\rightarrow\mathbb{R}$ and $g(x)=\min_y f(x,y)$. Suppose the minimum is attained at a unique $y(x)$, where $\mathcal{D}_2f(x,y(x))=0$. Then obviously $g(x)=$

$f(x, y(x))$. Differentiating g gives

$$\mathcal{D}g(x) = \mathcal{D}_1 f(x, y(x)) + \mathcal{D}_2 f(x, y(x))\mathcal{D}y(x) = \mathcal{D}_1 f(x, y(x)). \qquad (1)$$

To differentiate the solution map we need second derivatives of f. Differentiating the implicit definition $\mathcal{D}_2 f(x, y(x)) = 0$ gives

$$\mathcal{D}_{21} f(x, y(x)) + \mathcal{D}_{22} f(x, y(x))\mathcal{D}y(x) = 0,$$

or

$$\mathcal{D}y(x) = -[\mathcal{D}_{22} f(x, y(x))]^{-1}\mathcal{D}_{21} f(x, y(x)). \qquad (2)$$

Now combine both (1) and (2) to obtain

$$\mathcal{D}^2 g(x) = \mathcal{D}_{11} f(x, y(x)) - \mathcal{D}_{12} f(x, y(x))[\mathcal{D}_{22} f(x, y(x))]^{-1}\mathcal{D}_{21} f(x, y(x)). \quad (3)$$

We see that if $\mathcal{D}^2 f(x, y(x)) \gtrsim 0$ then $0 \lesssim \mathcal{D}^2 g(x) \lesssim \mathcal{D}_{11} f(x, y(x))$.

Now consider minimization problem with constraints. Suppose $h_1, \cdots, h_p$ are twice continuously differentiable functions on $\mathbb{R}^m$, and suppose

$$\mathcal{Y} = \{y \in \mathbb{R}^m \mid h_1(y) = \cdots = h_p(y) = 0\}.$$

Define

$$g(x) \stackrel{\Delta}{=} \min_{y \in \mathcal{Y}} f(x, y),$$

and

$$y(x) \stackrel{\Delta}{=} \mathop{\mathbf{argmin}}_{y \in \mathcal{Y}} f(x, y),$$

where again we assume the minimizer is unique and satisfies

$$\begin{aligned} \mathcal{D}_2 f(x, y(x)) - \sum_{s=1}^{p} \lambda_s(x)\mathcal{D}h_s(y(x)) &= 0, \\ h_s(y(x)) &= 0. \end{aligned}$$

Differentiate again, and define

$$\begin{aligned} A(x) &\stackrel{\Delta}{=} \mathcal{D}_{22} f(x, y(x)), \\ H_s(x) &\stackrel{\Delta}{=} \mathcal{D}^2 h_s(y(x)), \\ E(x) &\stackrel{\Delta}{=} -\mathcal{D}_{21} f(x, y(x)), \\ B(x) &\stackrel{\Delta}{=} \mathcal{D}H(y(x)), \end{aligned}$$

and

$$C(x) \overset{\Delta}{=} A(x) - \sum_{s=1}^{p} \lambda_s H_s(x).$$

Then

$$\begin{bmatrix} C(x) & -B(x) \\ B'(x) & 0 \end{bmatrix} \begin{bmatrix} \mathcal{D}y(x) \\ \mathcal{D}\lambda(x) \end{bmatrix} = \begin{bmatrix} E(x) \\ 0 \end{bmatrix},$$

which leads to

$$\begin{aligned} \mathcal{D}y(x) &= \left\{ I - B(x) \left[B'(x) C^{-1}(x) B(x) \right]^{-1} B'(x) \right\} C^{-1}(x) E(x), \\ \mathcal{D}\lambda(x) &= \left[B'(x) C^{-1}(x) B(x) \right]^{-1} B'(x) C^{-1}(x) E(x). \end{aligned}$$

There is an alternative way of arriving at basically the same result. Suppose the manifold $G(x) = 0$ is parametrized locally as $x = F(w)$. Then

$$y(z) = \mathop{\mathbf{Arg}\,\mathbf{min}}_{w} f(F(w), z),$$

and $G(F(w)) = 0$, i.e. $\mathcal{D}G(F(w))\mathcal{D}F(w) = 0$. Let $h(w, z) = f(F(w), z)$. Then

$$\mathcal{D}y(z) = -[\mathcal{D}_{11} f(F(w(z)), z)]^{-1} \mathcal{D}_{12} h(F(w(z)), z).$$

$$\mathcal{D}_{11} f(F(w(z)), z) = \mathcal{D}_1 f \mathcal{D}^2 F_i + (\mathcal{D}F)' \mathcal{D}_{11} \mathcal{D}F$$

###Solution Maps

##Basic Inequalities

8.3.2 Jensen's Inequality

8.3.3 The AM-GM Inequality

The Arithmetic-Geometric Mean Inequality is simple, but quite useful for majorization. For completeness, we give the statement and proof here.

Theorem: If $x \geq 0$ and $y \geq 0$ then $\sqrt{xy} \leq \frac{1}{2}(x + y)$, with equality if and only if $x = y$.

Proof: Expand $(\sqrt{x} - \sqrt{y})^2 \geq 0$, and collect terms. **QED**

Corollary: $\mid xy \mid \leq \frac{1}{2}(x^2 + y^2)$

Proof: Just a simple rewrite of the theorem. **QED**

###Polar Norms and the Cauchy-Schwarz Inequality

Theorem: Suppose $x, y \in \mathbb{R}^n$. Then $(x'y)^2 \leq x'x.y'y$, with equality if and only if x and y are proportional.

Proof: The result is trivially true if either x or y is zero. Thus we suppose both are non-zero. We have $h(\lambda) \stackrel{\Delta}{=} (x - \lambda y)'(x - \lambda y) \geq 0$ for all λ. Thus

$$\min_{\lambda} h(\lambda) = x'x - \frac{(x'y)^2}{y'y} \geq 0,$$

which is the required result. **QED**

8.3.4 Young's Inequality

The AM-GM inequality is a very special cases of Young's inequality. We derive it in a general form, using the coupling functions introduced by Moreau. Suppose f is a real-valued function on $\mathcal{X}$ and g is a real-valued function on $\mathcal{X} \times \mathcal{Y}$, called the *coupling* function. Here $\mathcal{X}$ and $\mathcal{Y}$ are arbitrary. Define the g*-conjugate* of f by

$$f_g^\circ(y) \stackrel{\Delta}{=} \sup_{x \in \mathcal{X}} \{g(x, y) - f(x)\}$$

Then $g(x, y) - f(x) \leq f_g^\circ(y)$ and thus $g(x, y) \leq f(x) + f_g^\circ(y)$, which is the generalized Young's inequality. We can also write this in the form that directly suggests minorization

$$f(x) \geq f_g^\circ(y) + g(x, y).$$

The classical coupling function is $g(x, y) = xy$ with both x and y in the positive reals. If we take $f(x) = \frac{1}{p}x^p$, with $p > 1$, then

$$f_g^\circ(y) = \sup_{x} \{xy - \frac{1}{p}x^p\}.$$

The sup is attained for $x = y^{\frac{1}{p-1}}$, from which we find $f_g^\circ(y) = \frac{1}{q}y^q$, with $q \stackrel{\Delta}{=} \frac{p}{p-1}$.

Thus if $p, q > 1$ such that

$$\frac{1}{p} + \frac{1}{q} = 1.$$

Then for all $x, y > 0$ we have

$$xy \leq \frac{x^p}{p} + \frac{y^q}{q},$$

with equality if and only if $y = x^{p-1}$.

8.4 Fixed Point Problems and Methods

As we have emphasized before, the algorithms discussed in this books are all special cases of block relation methods. But block relation methods are often appropriately analyzed as *fixed point methods*, which define an even wider class of iterative methods. Thus we will not discuss actual fixed point algorithms that are not block relation methods, but we will use general results on fixed point methods to analyze block relaxation methods.

A (stationary, one-step) fixed point method on $\mathcal{X} \subseteq \mathbb{R}^n$ is defined as a map $A : \mathcal{X} \rightarrow \mathcal{X}$. Depending on the context we refer to A as the *update map* or *algorithmic map*. Iterative sequences are generated by starting with $x^{(0)} \in \mathcal{X}$ and then setting

$$x^{(k)} = A(x^{(k-1)}) = A^k(x^{(0)}).$$

for $k = 1, 2, \cdots$. Such a sequence is also called the *Picard sequence* generated by the map.

If the sequence $x^{(k)}$ converges to, say, x_∞, and if A is continuous, then $x_\infty = A(x_\infty)$, and thus x_∞ is a *fixed point* of A on $\mathcal{X}$. The set of all $x \in \mathcal{X}$ such that $x = A(x)$ is called the *fixed point set* of A on $\mathcal{X}$, and is written as $\mathcal{F}_{\mathcal{X}}$.

The literature on fixed point methods is truly gigantic. There are textbooks, conferences, and dedicated journals. A nice and compact treatment, mostly on existence theorems for fixed points, is Smart (1974). An excellent modern overview, concentrating on metrical fixed point theory and iterative computation, is Berinde (2007).

The first key result in fixed point theory is the *Brouwer Fixed Point Theorem*, which says that for compact convex $\mathcal{X}$ and continuous A there is at least one

$x \in \mathcal{F}_{\mathcal{X}}(A)$. The second is the *Banach Fixed Point Theorem*, which says that if $\mathcal{X}$ is a non-empty complete metric space and A is a *contraction*, i.e. $d(A(x), A(y)) < \kappa\ d(x, y)$ for some $0 \leq \kappa < 1$, then the Picard sequence $x^{(k)}$ converges from any starting point $x^{(0)}$ to the unique fixed point of A in $\mathcal{X}$.

Much of the fixed point literature is concerned with relaxing the contraction assumption and choosing more general spaces on which the various mappings are defined. I shall discuss some of the generalizations that we will use later in this book.

First, we can generalize to point-to-set maps $A : \mathcal{X} \rightarrow 2^{\mathcal{X}}$, where $2^{\mathcal{X}}$ is the *power set* of $\mathcal{X}$, i.e. the set of all subsets. Point-to-set maps are also called *correspondences* or *multivalued maps.* The Picard sequence is now defined by $x^{(k)} \in A(x^{(k-1)})$ and we have a fixed point $x \in \mathcal{F}_{\mathcal{X}}(A)$ if and only if $x \in A(x)$. The generalization of the Brouwer Fixed Point Theorem is the *Kakutani Fixed Point Theorem.* It assumes that $\mathcal{X}$ is non-empty, compact and convex and that $A(x)$ is non-empty and convex for each $x \in \mathcal{X}$. In addition, the map A must be *closed* or *upper semi-continuous* on $\mathcal{X}$, i.e. whenever $x_n \rightarrow x_\infty$ and $y_n \in A(x_n)$ and $y_n \rightarrow y_\infty$ we have $y_\infty \in A(x_\infty)$. Under these conditions Kakutani's Theorem asserts the existence of a fixed point.

Our discussion of the global convergence of block relaxation algorithms, in a later chapter, will be framed using fixed points of point-to-set maps, assuming the closedness of maps.

In another generalization of iterative algorithms we get rid of the one-step and the stationary assumptions. The iterative sequence is

$$x^{(k)} \in A_k(x^{(0)}, x^{(1)}, \cdots, x^{(k-1)}).$$

Thus the iterations have perfect memory, and the update map can change in each iteration. In an ℓ-step method, memory is less than perfect, because the update is a function of only the previous ℓ elements in the sequence. Formally, for $k \geq \ell$,

$$x^{(k)} \in A_k(x^{(k-l)}, \cdots, x^{(k-1)}),$$

with some special provisions for $k < \ell$.

Any ℓ-step method on $\mathcal{X}$ can be rewritten as a one-step method on

$$\underbrace{\mathcal{X} \otimes \mathcal{X} \otimes \cdots \otimes \mathcal{X}}_{\ell \text{ times}}.$$

This makes it possible to limit our discussion to one-step methods. In fact, we will mostly discuss block-relaxation methods which are stationary one-step fixed point methods.

For non-stationary methods it is somewhat more complicated to define fixed points. In that case it is natural to define a set $\mathcal{S}\subseteq\mathcal{X}$ of *desirable points* or *targets*, which for stationary algorithms will generally, but not necessarily, coincide with the fixed points of A. The questions we will then have to answer are if and under what conditions our algorithms converge to desirable points, and if they converge how fast the convergence will take place.

8.4.1 Subsequential Limits

##Convex Functions

##Composition

8.4.2 Differentiable Convex Functions

If a function f attains its minimum on a convex set $\mathcal{X}$ at x, and f is differentiable at x, then $(x-y)'\mathcal{D}f(x)\geq 0$ for all $y\in\mathcal{X}$.

If f attains its minimum on $[a,b]$ at a, and f is differentiable at a, then $f'(a)\geq 0$. Or, more precisely, if f is differentiable from the right at a and $f'_R(a)\geq 0$.

Suppose $\mathcal{X}=\{x\mid x'x\leq 1\}$ is the unit ball and a differentiable f attains its a minimum at x with $x'x=1$. Then $(x-y)'\mathcal{D}f(x)\geq 0$ for all $y\in\mathcal{X}$. This is true if and only if

$$\begin{aligned}\min_{y\in\mathcal{X}}(x-y)'\mathcal{D}f(x)=x'\mathcal{D}f(x)-\max_{y\in\mathcal{X}}y'\mathcal{D}F(x)&=\\=x'\mathcal{D}f(x)-\|\mathcal{D}f(x)\|=0.\end{aligned}$$

By Cauchy-Schwartz this means that $\mathcal{D}f(x)=\lambda x$, with $\lambda=x'\mathcal{D}f(x)=\|\mathcal{D}f(x)\|$.

As an aside, if a differentiable function f attains its minimum on the unit sphere $\{x\mid x'x=1\}$ at x then $f(x/\|x\|\|)$ attains is minimum over $\mathbb{R}^n$ at x.

Setting the derivative equal to zero shows that we must have $\mathcal{D}f(x)(I-xx')=0$, which again translates to $\mathcal{D}f(x)=\lambda x$, with $\lambda=x'\mathcal{D}f(x)=\|\mathcal{D}f(x)\|$.

##Zangwill Theory

8.4.3 Algorithms as Point-to-set Maps

The theory studies iterative algorithms with the following properties. An algorithm works in a space Ω. It consists of a triple $(\mathcal{A},\psi,\mathcal{P})$, with $\mathcal{A}$ a mapping of Ω into the set of nonempty subsets of Ω, with ψ a real-valued function on Ω, and with $\mathcal{P}$ a subset of Ω. We call $\mathcal{A}$ the *algorithmic map* or the *update*, ψ the *evaluation function* and $\mathcal{P}$ the *desirable points.*

The algorithm works as follows.

1. start at an arbitrary $\omega^{(0)}\in\Omega$,
2. if $\omega^{(k)}\in\mathcal{P}$, then we stop,
3. otherwise we construct the *successor* by the rule $\omega^{(k+1)}\in\mathcal{A}(\omega^k)$.

We study properties of the sequences $\omega^{(k)}$ generated by the algorithm, in particular their convergence.

8.4.4 Convergence of Function Values

For this method we have our first (rather trivial) convergence theorem.

Theorem: If * Ω is compact, * ψ is jointly continuous on Ω,

then

- The sequence $\{\psi^{(k)}\}$ converges to, say, ψ^∞,
- the sequence $\{\omega^{(k)}\}$ has at least one convergent subsequence,
- if ω^∞ is an accumulation point of $\{\omega^{(k)}\}$, then $\psi(\omega^\infty)=\psi^\infty$.

Proof: Compactness and continuity imply that ψ is bounded below on Ω, and the minima in each of the substeps exist. This means that $\{\psi^{(k)}\}$ is nonincreasing and bounded below, and thus convergent. Existence of convergent subsequences is guaranteed by Bolzano-Weierstrass, and if we have a subsequence $\{\omega^{(k)}\}_{k\in\mathcal{K}}$ converging to ω^∞ then by continuity $\{\psi(\omega^{(k)})\}_{k\in\mathcal{K}}$ converges to $\psi(\omega^\infty)$. But all subsequences of a convergent sequence converge to the same point, and thus $\psi(\omega^\infty)=\psi^\infty$. **QED**

Remark: The assumptions in the theorem can be relaxed. Continuity is not necessary. Think of the function $\psi(x)=\sum_{s=1}^p \mathrm{sign}(x_s)$, which clearly is minimized in a single cycle. Typically, however, statistical problems exhibit continuity, so it may not be worthwhile to actually relax the assumption.

Compactness is more interesting. If we define the level sets

$$\Omega_0 \overset{\Delta}{=} \{\omega\in\Omega \mid \psi(\omega)\leq\psi^{(0)}\},$$

then obviously it is sufficient to assume that Ω_0 is compact. The same thing is true for the even weaker assumption that the iterates $\omega^{(k)}$ are in a compact set.

We do not assume the sets Ω_s are connected, i.e. they could be discrete. For instance, we could minimize $\|X\beta-y-\delta\|^2$ over β and δ, under the constraint that the elements of δ take only two different unspecified values. This is not difficult to do with block-relaxation, but generally problems with discrete characteristics present us with special problems and complications. Thus, in most instances, we have connected sets in mind. For discrete components, the usual topology of $\mathbb{R}^s$ may not be the most natural one to study convergence.

In several problems in statistics the sets Ω_s can be infinite-dimensional. This is true, for instance, in much of semi-parametric and non-parametric statistics. We mostly ignore the complications arising from infinite dimensionality (again, of a topological nature), because in actual computations we work with finite-dimensional approximations anyway.

Theorem **??** is very general, but the conclusions are quite weak. We have convergence of the function values, but about the sequence $\{\omega^{(k)}\}$ we only know that it has one or more accumulation points, and that all accumulation points have the same function value. We have not established other desirable properties of these accumulation points.

In order to prove global convergence (i.e. convergence from any initial point) we use the general theory developed initially by Zangwill (1969) (and later by Polak (1969), R. R. Meyer (1976), G. G. L. Meyer (1975), and others). The best introduction and overview is perhaps the volume edited by Huard ((Ed) (1979)).

8.4.5 Convergence of Solutions

Theorem: [Zangwill]

- If $\mathcal{A}$ is *uniformly compact* on Ω, i.e. there is a compact $\Omega_0 \subseteq \Omega$ such that $\mathcal{A}(\omega) \subseteq \Omega_0$ for all $\omega \in \Omega$,
- If $\mathcal{A}$ is *upper-semicontinuous* or *closed* on $\Omega - \mathcal{P}$, i.e. if $\xi_i \in \mathcal{A}(\omega_i)$ and $\xi_i \rightarrow \xi$ and $\omega_i \rightarrow \omega$ then $\xi \in \mathcal{A}(\omega)$,
- If $\mathcal{A}$ is *strictly monotonic* on $\Omega - \mathcal{P}$, i.e. $\xi \in \mathcal{A}(\omega)$ implies $\psi(\xi) < \psi(\omega)$ if ω is not a *desirable point.* then all accumulation points of the sequence $\{\omega^{(k)}\}$ generated by the algorithm are desirable points.

Proof: Compactness implies that $\{\omega^{(k)}\}$ has a convergent subsequence. Suppose its index-set is $\mathcal{K} = \{k_1, k_2, \cdots\}$ and that it converges to $\omega_{\mathcal{K}}$. Since $\{\psi(\omega^{(k)})\}$ converges to, say ψ_∞, we see that also

$$\{\psi(\omega^{(k_1)}), \psi(\omega^{(k_2)}), \cdots\} \rightarrow \psi_\infty.$$

Now consider $\{\omega^{(k_1+1)}, \omega^{(k_2+1)}, \cdots\}$, which must again have a convergent subsequence. Suppose its index-set is $\mathcal{L} = \{\ell_1 + 1, \ell_2 + 1, \cdots\}$ and that it converges to $\omega_{\mathcal{L}}$. Then $\psi(\omega_{\mathcal{K}}) = \psi_(\omega_{\mathcal{L}}) = \psi_\infty$.

Assume $\omega_{\mathcal{K}}$ is not a fixed point. Now

$$\{\omega^{(\ell_1)}, \omega^{(\ell_2)}, \cdots\} \rightarrow \omega_{\mathcal{K}}$$

and

$$\{\omega^{(\ell_1+1)}, \omega^{(\ell_2+1)}, \cdots\} \rightarrow \omega_{\mathcal{L}},$$

with $\omega^{(\ell_j+1)} \in \mathcal{A}(\omega^{(\ell_j+1)}$. Thus, by usc, $\omega_{\mathcal{L}} \in \mathcal{A}(\omega_{\mathcal{K}})$. If $\omega_{\mathcal{K}}$ is not a fixed point, then strict monotonicity gives gives $\psi(\omega_{\mathcal{L}}) < \psi(\omega_{\mathcal{K}})$, which contradicts our earlier $\psi(\omega_{\mathcal{K}}) = \psi_(\omega_{\mathcal{L}})$. **QED**

The concept of closedness of a map can be illustrated with the following picture, showing a map which is not closed at at least one point.

We have already seen another example: Powell's coordinate descent example shows that the algorithm map is not closed at six of the edges of the cube $\{\pm 1, \pm 1, \pm 1\}$.

It is easy to see that desirable points are generalized fixed points, in the sense that $\omega \in \mathcal{P}$ is equivalent to that $\omega \in \mathcal{A}(\omega)$. According to Zangwill's theorem

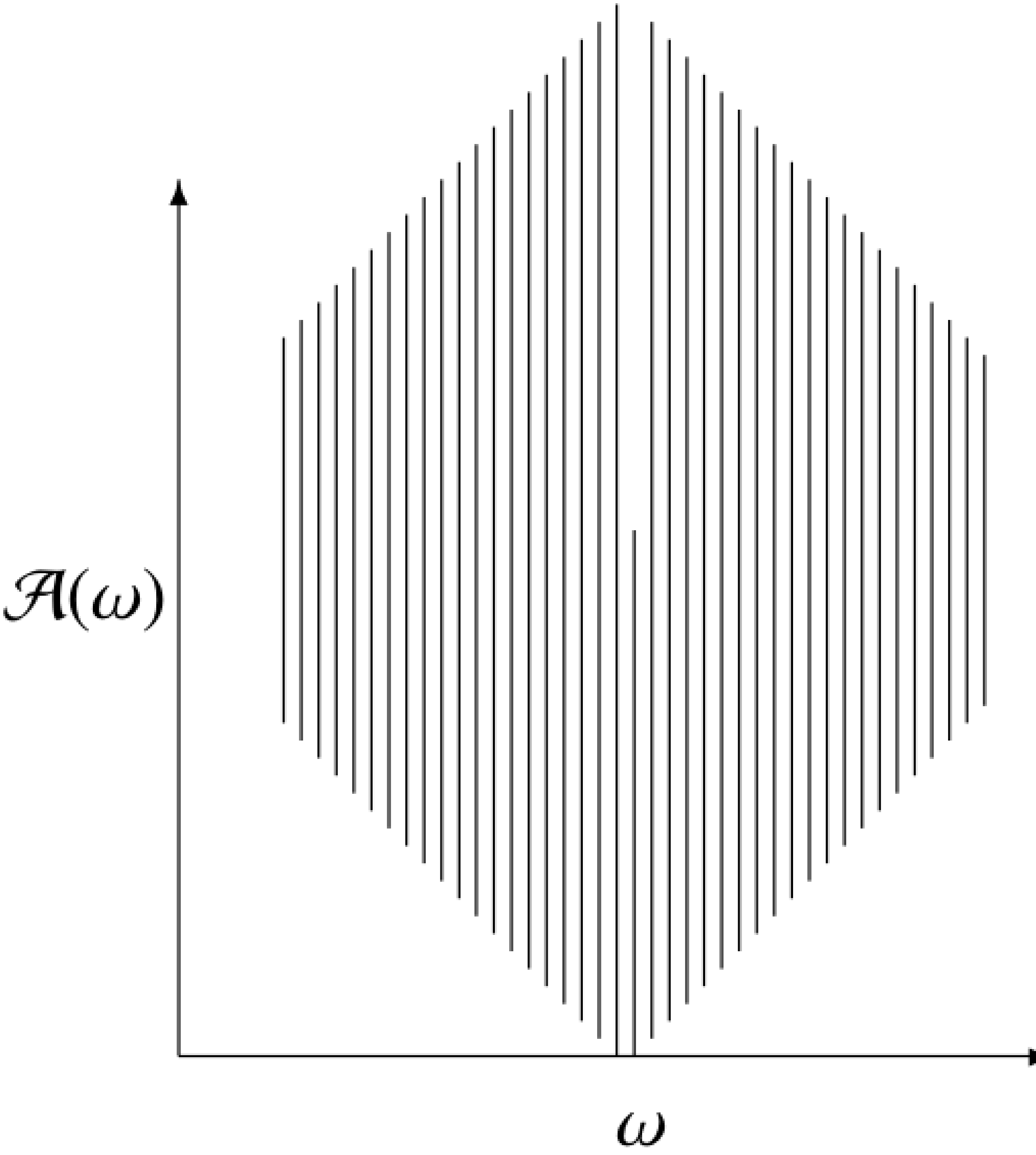


Figure 8.1: The map is not closed

each accumulation point is a generalized fixed point. This, however, does not prove convergence, because there can be many accumulation points. If we redefine fixed points as points such that $\mathcal{A}(\omega) = \{\omega\}$, then we can strengthen the theorem [Meyer, 1976].

Theorem: [Meyer] Suppose the conditions of Zangwill's theorem are satisfied for the stronger definition of a fixed point, i.e. $\xi \in \mathcal{A}(\omega)$ implies $\psi(\xi) < \psi(\omega)$ if ω is not a fixed point, then in addition to what we had before $\{\omega^{(k)}\}$ is *asymptotically regular*, i.e. $\|\omega^{(k)} - \omega^{(k+1)}\| \rightarrow 0$.

Proof: Use the notation in the proof of Zangwill's theorem. Suppose $\|\omega^{(\ell_i+1)} - \omega^{(\ell_i)}\| > \delta > 0$. Then $\|\omega_{\mathcal{L}} - \omega_{\mathcal{K}}\| \geq \delta$. But $\omega_{\mathcal{K}}$ is a fixed point (in the strong sense) and thus $\omega_{\mathcal{L}} \in \mathcal{A}(\omega_{\mathcal{K}}) = \{\omega_{\mathcal{K}}\}$, a contradiction. **QED**

Theorem: [Ostrowski] If the bounded sequence $\Omega = \{\omega^{(k)}\}$ satisfies $\|\omega^{(k)} - \omega^{(k+1)}\| \rightarrow 0$, then the derived set Ω' is either a point or a continuum.

Proof: We follow Ostrowski [1966, pages 203–204]. A *continuum* is a closed set, which is not the union of two or more disjoint closed sets. Of course the derived set is closed. Suppose it is the union of the disjoint closed sets C_1 and C_2, which are a distance of at least p apart. We can choose k_0 such that $\|\omega^{(k)} - \omega^{(k+1)}\| \leq \frac{p}{3}$ for all $k \geq k_0$. **QED**

Only if the derived set is a single point, we have actual convergence. Thus Meyer's theorem still does not prove actual convergence, but it is close enough for all practical purposes. Observe boundedness is essential in Theorem **??**, otherwise the derived set may be empty, think of the series $\sum \frac{1}{k}$.

8.5 Rates of Convergence

The basic result we use is due to Perron and Ostrowski (1966).

Theorem: * If the iterative algorithm $x^{(k+1)} = \mathcal{A}(x^{(k)})$, converges to x_∞, * and $\mathcal{A}$ is differentiable at x_∞, * and $0 < \rho = \|\mathcal{DA}(\omega_\infty)\| < 1$,

then the algorithm is linearly convergent with rate ρ.

Proof:

QED

The norm in the theorem is the spectral norm, i.e. the modulus of the maximum eigenvalue. Let us call the derivative of A the *iteration matrix* and write it as $\mathcal{M}$. In general block relaxation methods have linear convergence, and the linear convergence can be quite slow. In cases where the accumulation points are a continuum we have sublinear rates. The same things can be true if the local minimum is not strict, or if we are converging to a saddle point.

Generalization to non-differentiable maps.

Points of attraction and repulsion.

Superlinear etc

8.5.1 Over- and Under-Relaxation

8.5.2 Acceleration of Convergence of Fixed Point Methods

8.6 Matrix Algebra

8.6.1 Eigenvalues and Eigenvectors of Symmetric Matrices

In this section we give a fairly complete introduction to eigenvalue problems and generalized eigenvalue problems. We use a constructive variational approach, basically using the Rayleigh quotient and deflation. This works best for positive semi-definite matrices, but after dealing with those we discuss several generalizations.

Suppose A is a positive semi-definite matrix of order n. Consider the problem of maximizing the quadratic form $f(x) = x'Ax$ on the sphere $x'x = 1$. At the maximum, which is always attained, we have $Ax = \lambda x$, with λ a Lagrange multiplier, as well as $x'x = 1$. It follows that $\lambda = f(x)$. Note that the maximum is not necessarily attained at a unique value. Also the maximum is zero if and only if A is zero.

Any pair (x, λ) such that $Ax = \lambda x$ and $x'x = 1$ is called an *eigen-pair* of A. The members of pair are the *eigenvector* x and the corresponding *eigenvalue* λ.

Result 1: Suppose (x_1, λ_1) and (x_2, λ_2) are two eigen-pairs, with $\lambda_1 \neq \lambda_2$. Then premultiplying both sides of $Ax_2 = \lambda_2 x_2$ by x_1' gives $\lambda_1 x_1' x_2 = \lambda_2 x_1' x_2$, and thus $x_1' x_2 = 0$. This shows that A cannot have more than n distinct eigenvalues. If there were $p > n$ distinct eigenvalues, then the $n \times p$ matrix X, which has the corresponding eigenvectors as columns, would have column-rank p and row-rank n, which is impossible. In words: one cannot have more than n orthonormal vectors in $n-$dimensional space. Suppose the distinct values are $\tilde{\lambda}_1 > \cdots > \tilde{\lambda}_s$, with $s = 1, \cdots, p$. Thus each of the eigenvalues λ_i is equal to one of the $\tilde{\lambda}_s$.

Result 2: If (x_1, λ) and (x_2, λ) are two eigen-pairs with the same eigenvalue λ then any linear combination $\alpha x_1 + \beta x_2$, suitably normalized, is also an eigenvector with eigenvalue λ. Thus the eigenvectors corresponding with an eigenvalue λ form a linear subspace of $\mathbb{R}^n$, with dimension, say, $1 \leq n_s \leq n$. This subspace can be given an orthonormal basis in an $n \times n_s$ matrix X_s. The number n_s is the *multiplicity* of $\tilde{\lambda}_s$, and by implication of the eigenvalue λ_i equal to $\tilde{\lambda}_s$.

Of course these results are only useful if eigen-pairs exist. We have shown that at least one eigen-pair exists, the one corresponding to the maximum of f on the sphere. We now give a procedure to compute additonal eigen-pairs.

Consider the following algorithm for generating a sequence $A^{(k)}$ of matrices. We start with $k = 1$ and $A^{(1)} = A$. 1. **Test:** If $A^{(k)} = 0$ stop. 2. **Maximize:** Computes the maximum of $x' A^{(k)} x$ over $x'x = 1$. Suppose this is attained at an eigen-pair $(x^{(k)}, \lambda^{(k)})$. If the maximizer is not unique, select an arbitrary one. 3. **Orthogonalize:** Replace $x^{(k)}$ by $x^{(k)} - \sum_{\ell=1}^{k-1}((x^{(\ell)})' x^{(k)}) x^{(\ell)}$. 4. **Deflate:** Set $A^{(k+1)} = A^{(k)} - \lambda^{(k)} x^{(k)} (x^{(k)})'$, 5. **Update:** Go back to step 1 with k replaced by $k + 1$.

If $k = 1$ then in step (2) we compute the largest eigenvalue of A and a corresponding eigenvector. In that case there is no step (3). Step (4) constructs $A^{(2)}$ by *deflation*, which basically removes the contribution of the largest eigenvalue and corresponding eigenvector. If x is an eigenvector of A with eigenvalue $\lambda < \lambda^{(1)}$, then

$$A^{(2)} x = Ax - \lambda^{(1)} x^{(1)} (x^{(1)})' x = Ax = \lambda x$$

by result (1) above. Also, of course, $A^{(2)} x^{(1)} = 0$, so $x^{(1)}$ is an eigenvector of $A^{(2)}$ with eigenvalue 0. If $x \neq x^{(1)}$ is an eigenvector of A with eigenvalue

$\lambda = \lambda^{(1)}$, then by result (2) we can choose x such that $x'x^{(1)} = 0$, and thus

$$A^{(2)}x = Ax - \lambda x^{(1)}(x^{(1)})'x = \lambda(I - x^{(1)}(x^{(1)})')x = \lambda x.$$

We see that $A^{(2)}$ has the same eigenvectors as A, with the same multiplicities, except for $\lambda^{(1)}$, which now has its old multiplicity -1, and zero, which now has its old multiplicity $+1$. Now if $x^{(2)}$ is the eigenvector corresponding with $\lambda^{(2)}$, the largest eigenvalue of $A^{(2)}$, then by result (1) $x^{(2)}$ is automatically orthogonal to $x^{(1)}$, which is an eigenvalue of $A^{(2)}$ with eigenvalue zero. Thus step (3) is not ever necessary, although it will lead to more precise numerical computation.

Following the steps of the algorithm we see thatit defines p orthonormal matrices X_s, which moreover satisfy $X_s'X_t = 0$ for $s \neq t$, and with $\sum_{s=1}^{p} n_s =$ **rank**(A). Also

$$A = \sum_{s=1}^{p} \tilde{\lambda}_s P_s, \tag{1a}$$

where P_s is the projector X_sX_s'. This is the *eigen decomposition* or the *spectral decomposition* of a positive semi-definite A.

Our algorithm stops when $A^{(k)} = 0$, which is the same as $\sum_{s=1}^{p} n_s =$ **rank**(A). If **rank**$(A) < n$ then the minimum eigenvalue is zero, and has multiplicity $n -$ **rank**(A). $P_s = I - P_1 - \cdots - P_{s-1} = X_sX_s'$ is the orthogonal projector of the null-space of A, with **rank**$(Q) =$ **tr**$(Q) = n -$ **rank**(A). Using the square orthonormal

$$X = \begin{bmatrix} X_1 & \cdots & X_s \end{bmatrix}$$

we can write the eigen decomposition in the form

$$A = X\Lambda X', \tag{1b}$$

where the last $n -$ **rank**(A) diagonal elements of Λ are zero. Equation $(1b)$ can also be written as

$$X'AX = \Lambda, \tag{1c}$$

which says that the eigenvectors diagonalize A and that A is orthonormally similar to the diagonal matrix of eigenvalues,

We have shown that the largest eigenvalue and corresponding eigenvector exist, but we have not indicated , at least in this section, how to compute them. Conceptually the power method is the most obvious way. It is a tangential minorization method, using the inquality $x'Ax \geq y'Ay + 2y'A(x - y)$, which means that the iteration function is

$$x^{(k+1)} = \frac{Ax^{(k)}}{\|Ax^{(k)}\|}.$$

See the Rayleigh Quotient section for further details.

We now discuss a first easy generalization. If A is real and symmetric but not necessarily positive semi-definite then we can apply our previous results to the matrix $A + kI$, with $k \geq \min_i \lambda_i$. Or we can apply it to $A^2 = X\Lambda^2X'$. Or we can modify the algorithm if we run into an $A^{(k)} \neq 0$ with maximum eigenvalue equal to zero. If this happens we switch to finding the smallest eigenvalues, which will be negative. No matter how we modify the constructive procedure, we will still find an eigen decomposition of the same form ($1a$) and ($1b$) as in the positive semi-definite case.

The second generalization, also easy, are *generalized eigenvalues* of a pair of real symmetric matrices (A, B). We now maximize $f(x) = x'Ax$ over x satisfying $x'Bx = 1$. In data analysis, and the optimization problems associated with it, we almost invariably assume that B is positive definite. In fact we might as well make the weaker assumption that B is positive semi-definite, and $Ax = 0$ for all x such that $Bx = 0$. Suppose

$$B = \begin{bmatrix} K & K_\perp \end{bmatrix} \begin{bmatrix} \Lambda^2 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} K' \\ K_\perp' \end{bmatrix}$$

is an eigen decomposition of B. Change variables by writing X as $x = K\Lambda^{-1}u + K_\perp v$. Then $x'Bx = u'u$ and $x'Ax = u'\Lambda^{-1}K'AK\Lambda^{-1}u$. We can find the generalized eigenvalues and eigenvectors from the ordinary eigen decomposition of $\Lambda^{-1}K'AK\Lambda^{-1}$. This defines the $u^{(s)}$ in $x^{(s)} = K\Lambda^{-1}u^{(s)} + K_\perp v$, and the choice of v is completely arbitrary.

Now suppose L is the square orthonormal matrix of eigenvectors diagonalizing $\Lambda^{-1}K'AK\Lambda^{-1}$, with Γ the corresponding eigenvalues, and $S \triangleq K\Lambda^{-1}L$. Then $S'AS = \Gamma$ and $S'BS = I$. Thus S diagonalizes both A and B. For the more general case, in which we do not assume that $Ax = 0$ for all x with $Bx = 0$, we refer to J. De Leeuw (1982).

8.6.2 Singular Values and Singular Vectors

Suppose A_{12} is an $n_1 \times n_2$ matrix, A_{11} is an $n_1 \times n_1$ symmetric matrix, and A_{22} is an $n_2 \times n_2$ symmetric matrix. Define

$$f(x_1, x_2) = \frac{x_1' A_{12} x_2}{\sqrt{x_1' A_{11} x_1}\sqrt{x_2' A_{22} x_2}}.$$

Consider the problem of finding the maximum, the minimum, and other stationary values of f.

In order to make the problem well-defined and interesting we suppose that the symmetric partitioned matrix

$$A \stackrel{\Delta}{=} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

is positive semi-definite. This has some desirable consequences.

Proposition: Suppose the symmetric partitioned matrix

$$A \stackrel{\Delta}{=} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

is positive semi-definite. Then * both A_{11} and A_{22} are positive semi-definite, * for all x_1 with $A_{11}x_1 = 0$ we have $A_{21}x_1 = 0$, * for all x_2 with $A_{22}x_2 = 0$ we have $A_{12}x_2 = 0$.

Proof: The first assertion is trivial. To prove the last two, consider the convex quadratic form

$$q(x_2) = x_1' A_{11} x_1 + 2x_1' A_{12} x_2 + x_2' A_{22} x_2$$

as a function of x_2 for fixed x_1. It is bounded below by zero, and thus attains its minimum. At this minimum, which is attained at some $\hat{x}_2$, the derivative vanishes and we have $A_{22}\hat{x}_2 = -A_{21}x_1$ and thus $q(\hat{x}_2) = x_1' A_{11} x_1 - \hat{x}_2' A_{22} \hat{x}_2$. If $A_{11}x_1 = 0$ then $q(\hat{x}_2) \leq 0$. But $q(\hat{x}_2) \geq 0$ because the quadratic form is positive semi-definite. Thus if $A_{11}x_1 = 0$ we must have $q(\hat{x}_2) = 0$, which is true if and only if $A_{22}\hat{x}_2 = -A_{21}x_1 = 0$. **QED**

Now suppose

$$A_{11} = \begin{bmatrix} K_1 & \overline{K}_1 \end{bmatrix} \begin{bmatrix} \Lambda_1^2 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} K_1' \\ \overline{K}_1' \end{bmatrix},$$

and

$$A_{22} = \begin{bmatrix} K_2 & \overline{K}_2 \end{bmatrix} \begin{bmatrix} \Lambda_2^2 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} K_2' \\ \overline{K}_2' \end{bmatrix}$$

are the eigen-decompositions of A_{11} and A_{22}. The $r_1 \times r_1$ matrix Λ_1^2 and the $r_2 \times r_2$ matrix Λ_2^2 have positive diagonal elements, and r_1 and r_2 are the ranks of A_{11} and A_{22}.

Define new variables

$$x_1 = K_1 \Lambda_1^{-1} u_1 + \overline{K}_1 v_1, \tag{1a}$$

$$x_2 = K_2 \Lambda_2^{-1} u_2 + \overline{K}_2 v_2. \tag{1b}$$

Then

$$f(x_1, x_2) = \frac{u_1' \Lambda_1^{-1} K_1' A_{12} K_2 \Lambda_2^{-1} u_2}{\sqrt{u_1' u_1}\sqrt{u_2' u_2}},$$

which does not depend on v_1 and v_2 at all. Thus we can just consider f as a function of u_1 and u_2, study its stationary values, and then translate back to x_1 and x_2 using ($1a$) and ($1b$), choosing v_1 and v_2 completely arbitrary.

Define $H \triangleq \Lambda_1^{-1} K_1' A_{12} K_2 \Lambda_2^{-1}$. The stationary equations we have to solve are

$$Hu_2 = \rho u_1,$$
$$H' u_1 = \rho u_2,$$

where ρ is a Lagrange multiplier, and we identify u_1 and u_2 by $u_1' u_1 = u_2' u_2 = 1$. It follows that

$$HH' u_1 = \rho^2 u_1,$$
$$H' H u_2 = \rho^2 u_2,$$

and also $\rho = f(u_1, u_2)$.

8.6.3 Canonical Correlation

Suppose A_1 is an $n \times m_1$ matrix and A_2 is an $n \times m_2$ matrix. The cosine of the angle between two linear combinations $A_1 x_1$ and $A_2 x_2$ is

$$f(x_1, x_2) = \frac{x_1' A_1' A_2 x_2}{\sqrt{x_1' A_1' A_1 x_1}\sqrt{x_2' A_2' A_2 x_2}}.$$

Consider the problem of finding the maximum, the minimum, and possible other stationary values of f.

are two matrices of dimensions, respectiSpecifically there exists a non-singular K of order n_1 and a non-singular L of order n_2 such that

$$\begin{aligned} K'A_1'A_1K &= I_1, \\ L'A_2'A_2L &= I_2, \\ K'A_1'A_2L &= D. \end{aligned}$$

Here I_1 and I_2 are diagonal, with the n_1 and n_2 leading diagonal elements equal to one and all other elements zero. D is a matrix with the non-zero canonical correlations in non-increasing order along the diagonal and zeroes everywhere else.

http://en.wikipedia.org/wiki/Principal_angles http://meyer.math.ncsu.edu/Meyer/PS_Files/AnglesBetweenCompSubspaces.pdf

###Eigenvalues and Eigenvectors of Asymmetric Matrices

If A is a square but asymmetric real matrix the eigenvector-eigenvalue situation becomes quite different from the symmetric case. We gave a variational treatment of the symmetric case, using the connection between eigenvalue problems and quadratic forms (or ellipses and other conic sections, if you have a geometric mind).That connection, howver, is lost in the asymmetric case, and there is no obvious variational problem associated with eigenvalues and eigenvectors.

Let us first define eigenvalues and eigenvectors in the asymmetric case. As before, an eigen-pair (x, λ) is a solution to the equation $Ax = \lambda x$ with $x \neq 0$. This can also be written as $(A - \lambda I)x = 0$, which shows that the eigenvalues are the solutions of the equation $\pi_A(\lambda) = \mathbf{det}(A - \lambda I) = 0$. Now the function π_A is the *characteristic polynomial* of A. It is a polynomial of degree n, and by the fundamental theorem of algebra there are n real and complex roots, counting multiplicities. Thus A has n eigenvalues, as before, although some of them can be complex

A first indication that something may be wrong, or least fundamentally different, is the matrix

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

The *characteristic equation* $\pi_A(\lambda) = \lambda^2 = 0$ has the root $\lambda = 0$, with multiplicity 2. Thus an eigenvector should satisfy

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

which merely says $x_2 = 0$. Thus A does not have two linearly independent, let alone orthogonal, eigenvectors.

A second problem is illustrated by the anti-symmetric matrix

$$A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

for which the characteristic polynomial is $\pi_A(\lambda) = \lambda^2 + 1$. The characteristic equations has the two complex roots $+\sqrt{-1}$ and $-\sqrt{-1}$. The corresponding eigenvectors are the columns of

$$\begin{bmatrix} 1 & 1 \\ \sqrt{-1} & -\sqrt{-1} \end{bmatrix}.$$

Thus both eigenvalues and eigenvectors may be complex. In fact if we take complex conjugates on both sides of $Ax = \lambda x$, and remember that A is real, we see that $\overline{Ax} = A\overline{x} = \overline{\lambda}\overline{x}$. Thus (x, λ) is an eigen-pair if and only if $(\overline{x}, \overline{\lambda})$ is. If A is real and of odd order it always has at least one real eigenvalue. If an eigenvalue λ is real and of multiplicity m, then there are m corresponding real and linearly independent eigenvectors. They are simply a basis for the null space of $A - \lambda I$.

A third problem, which by definition did not come up in the symmetric case, is that we now have an eigen problem for both A and its transpose A'. Since for all λ we have $\mathbf{det}(A - \lambda I) = \mathbf{det}(A' - \lambda I)$ it follows that A and A' have the same eigenvalues. We say that (x, λ) is a *right eigen-pair* of A if $Ax = \lambda x$, and (y, λ) is a *left eigen-pair* of A if $y'A = \lambda y'$, which is of course the same as $A'y = \lambda y$.

A matrix A is *diagonalizable* if there exists a non-singular X such that $X^{-1}AX = \Lambda$, with Λ diagonal. Instead of the spectral decomposition of symmetric matrices we have the decomposition $A = X\Lambda X^{-1}$ or $X^{-1}AX = \Lambda$. A matrix that is not diagonalizable is called *defective*.

Result: A matrix A is *diagonalizable* if and only if it has n linearly independent right eigenvectors if and only if it has n linearly independent left eigenvectors. We show this for right eigenvectors. Collect them in the columns of a matrix X. Thus $AX = X\Lambda$, with X non-singular. This implies $X^{-1}A = \Lambda X^{-1}$, and thus the rows of $Y = X^{-1}$ are n linearly independent left eigenvalues. Also $X^{-1}AX = \Lambda$. Conversely if $X^{-1}AX = \Lambda$ then $AX = X\Lambda$ and $A'X^{-1} = X^{-1}\Lambda$, so we have linearly independent left and right eigenvectors.

Result: If the n eigenvalues λ_j of A are all diferent then the eigenvectors x_j are linearly independent. We show this by contradiction. Select a maximally linearly independent subset from the x_j. Suppose there are $p < m$, so the eigenvectors are linearly dependent. Without loss of generality the maximally linearly independent subset can be taken as the first p. Then for all $j > p$ there exist α_{js} such that

$$x_j = \sum_{s=1}^{p} \alpha_{js} x_s. \tag{1}$$

Premultiply (1) with λ_j to get

$$\lambda_j x_j = \sum_{s=1}^{p} \alpha_{js} \lambda_j x_s. \tag{2}$$

Premultiply (1) by A to get

$$\lambda_j x_j = \sum_{s=1}^{p} \alpha_{js} \lambda_s x_s. \tag{3}$$

Subtract (2) from (3) to get

$$\sum_{s=1}^{p} \alpha_{js}(\lambda_s - \lambda_j) x_s = 0,$$

which implies that $\alpha_{js}(\lambda_s - \lambda_j) = 0$, because the x_s are linearly independent. Since the eigenvalues are unequal, this implies $a_{js} = 0$ and thus $x_j = 0$ for all $j > p$, contradicting that the x_j are eigenvectors. Thus $p = m$ and the x_j are linearly independent.

Note 030615 Add small amount on defective matrices. Add stuff on characteristic and minimal polynomials. Take about using the SVD instead.

8.6.4 Modified Eigenvalue Problems

Suppose we know an eigen decomposition $B = K\Phi K'$ of a real symmetric matrix B of order n, and we want to find an eigen decomposition of the rank-one modification $A = B + \gamma cc'$, where $\gamma \neq 0$. The problem was first discussed systematically by Golub (1973). Also see Bunch, Nielsen, and Sorensen (1978) for a more detailed treatment and implmentation.

Eigen-pairs of A must satisfy

$$(B + \gamma cc')x = \lambda x.$$

Change variables to $y = K'x$ and define $d \overset{\Delta}{=} K'c$. For the time being suppose all elements of d are non-zero and all elements of Φ are different, with $\phi_1 > \cdots > \phi_n$.

We must solve

$$(\Phi + \gamma dd')y = \lambda y,$$

which we can also write as

$$(\Phi - \lambda I)y = -\gamma(d'y)d.$$

Suppose (y, λ) is a solution with $d'y = 0$. Then $(\Phi - \lambda I)y = 0$ and because all ϕ_k are different y must be a vector with a single element, say y_k, not equal to zero. But then $d'y = y_k d_k$, which is non-zero. Thus $d'y$ is non-zero at a solution, and because eigenvectors are determined up to a scalar factor we may as well require $e'y = 1$.

Now solve

$$\begin{aligned}(\Phi - \lambda I)y &= -\gamma d,\\ d'y &= 1.\end{aligned}$$

At a solution we must have $\lambda \neq \phi_i$, because otherwise d_i would be zero. Thus

$$y_i = -\gamma\frac{d_i}{\phi_i - \lambda},$$

and we can find λ by solving

$$1 + \gamma\sum_{i=1}^{n}\frac{d_i^2}{\phi_i - \lambda} = 0.$$

If we define

$$f(\lambda)=\sum_{i=1}^{n}\frac{d_i^2}{\phi_i-\lambda},$$

then we must solve $f(\lambda)=-\frac{1}{\gamma}$. Let's first look at a particular f.

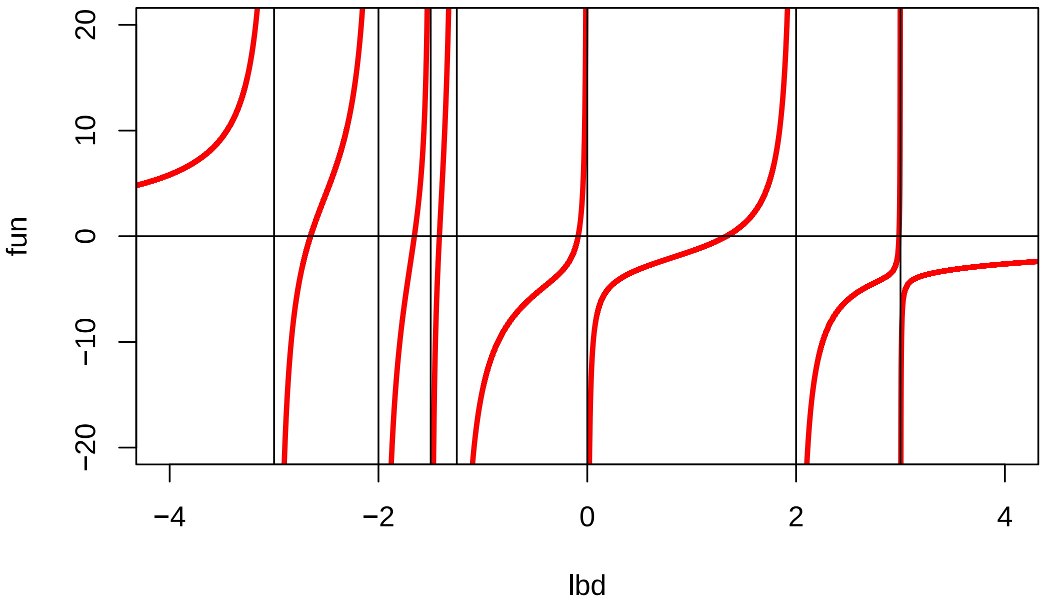


Figure 1: Linear Secular Equation

We have $f'(\lambda)>0$ for all λ, and

$$\lim_{\lambda\rightarrow-\infty}f(\lambda)=\lim_{\lambda\rightarrow+\infty}f(\lambda)=0.$$

There are vertical asymptotes at all ϕ_i, and between ϕ_i and ϕ_{i+1} the function increases from $-\infty$ to $+\infty$. For $\lambda<\phi_n$ the function increases from 0 to $+\infty$ and for $\lambda>\phi_1$ it increases from $-\infty$ to 0. Thus the equation $f(\lambda)=-1/\gamma$ has one solution in each of the $n-1$ open intervals between the ϕ_i. If $\gamma<0$ it has an additional solution smaller than ϕ_n and if $\gamma>0$ it has a solution larger than ϕ_1. If $\gamma<0$ then

$$\lambda_n<\phi_n<\lambda_{n-1}<\cdots<\phi_2<\lambda_1<\phi_1,$$

and if $\gamma>0$ then

$$\phi_n<\lambda_n<\phi_{n-1}\cdots<\phi_2<\lambda_2<\phi_1<\lambda_1.$$

Finding the actual eigenvalues in their intervals can be done with any root-finding method. Of course some will be better than other for solving this particular problem. See Melman Melman (1995), Melman (1997), and Melman (1998) for suggestions and comparisons.

We still have to deal with the assumptions that the elements of d are non-zero and that all ϕ_i are different. Suppose p elements of d_i are zero, without loss of generality it can be the last p. Partition Φ and d accordingly. Then we need to solve the modified eigen-problem for

$$\begin{bmatrix}\Phi_1+\gamma d_1d_1' & 0\\ 0 & \Phi_2\end{bmatrix}.$$

But this is a direct sum of smaller matrices and the eigenvalues problems for Φ_2 and $\Phi_1+\gamma d_1d_1'$ can be solved separately.

If not all ϕ_i are different we can partitioning the matrix into blocks corresponding with the, say, p different eigenvalues.

$$\begin{bmatrix}\phi_1I+\gamma d_1d_1' & \gamma d_1d_2' & \cdots & \gamma d_1d_p'\\ \gamma d_2d_1' & \phi_2I+\gamma d_2d_2' & \cdots & \gamma d_2d_p'\\ \vdots & \vdots & \ddots & \vdots\\ \gamma d_pd_1' & \gamma d_pd_2' & \cdots & \phi_pI+d_pd_p'\end{bmatrix}.$$

Now use the p matrices L_s which are square orthonormal of order n_s, and have their first column equal to $d_s/\|d_s\|$. Form the direct sum of the L_s and compute $L_s'(\Phi+\gamma dd')L_s$. This gives

$$\begin{bmatrix}\phi_1I+\gamma\|d_1\|^2e_1e_1' & \gamma\|d_1\|\|d_2\|e_1e_2' & \cdots & \gamma\|d_1\|\|d_p\|e_1e_p'\\ \gamma\|d_2\|\|d_1\|e_2e_1' & \phi_2I+\gamma\|d_2\|^2e_2e_2' & \cdots & \gamma\|d_2\|\|d_p\|e_2e_p'\\ \vdots & \vdots & \ddots & \vdots\\ \gamma\|d_p\|\|d_1\|e_pe_1' & \gamma\|d_p\|\|d_2\|e_pe_2' & \cdots & \phi_pI+\gamma\|d_p\|^2e_pe_p'\end{bmatrix}$$

with the e_s unit vectors, i.e. vectors that are zero except for element s that is one.

A row and column permutation makes the matrix a direct sum of the p diagonal matrices ϕ_sI of order n_s-1 and the $p\times p$ matrix

$$\begin{bmatrix}\phi_1+\gamma\|d_1\|^2 & \gamma\|d_1\|\|d_2\| & \cdots & \gamma\|d_1\|\|d_p\|\\ \gamma\|d_2\|\|d_1\|e_2e_1' & \phi_2+\gamma\|d_2\|^2 & \cdots & \gamma\|d_2\|\|d_p\|\\ \vdots & \vdots & \ddots & \vdots\\ \gamma\|d_p\|\|d_1\|e_pe_1' & \gamma\|d_p\|\|d_2\| & \cdots & \phi_p+\gamma\|d_p\|^2\end{bmatrix}$$

This last matrix satisfies our assumptions of different diagonal elements and nonzero off-diagonal elements, and consequently can be analyzed by using our previous results.

A very similar analysis is possible for modfied singular value decomposition, for which we refer to Bunch and Nielsen (1978)).

8.6.5 Quadratic on a Sphere

Another problem naturally leading to a different secular equation is finding stationary values of a quadratic function f defined by

$$f(x)=\frac{1}{2}x'Ax-b'x+c$$

on the unit sphere $\{x\mid x'x=1\}$. This was first studied by Forsythe and Golub (1965). Their treatment was subsequently simplified and extended by Spjøtvoll (1972) and Gander (1981). The problem has recently received some attention because of the development of trust region methods for optimization, and, indeed, because of Nesterov majorization.

The stationary equations are

$$\begin{aligned}(A-\lambda I)x&=b,\\ x'x&=1.\end{aligned}$$

Suppose $A=K\Phi K'$ with the $\phi_1\geq\cdots\geq\phi_n$, change variables to $y=K'x$, and define $d\overset{\Delta}{=}K'b$. Then we must solve

$$\begin{aligned}(\Phi-\lambda I)y&=d,\\ y'y&=1.\end{aligned}$$

Assume for now that the elements of d are non-zero. Then λ cannot be equal to one of the ϕ_i. Thus

$$y_i=\frac{d_i}{\phi_i-\lambda}$$

and we must have $h(\lambda)=1$, where

$$h(\lambda)\overset{\Delta}{=}\sum_{i=1}^n\frac{d_i^2}{(\phi_i-\lambda)^2}.$$

Again, let's look at an example of a particular h. The plots in Figure 1 show both f ad h. We see that $h(\lambda) = 1$ has 12 solutions, so the remaining question is which one corresponds with the minimum of f.

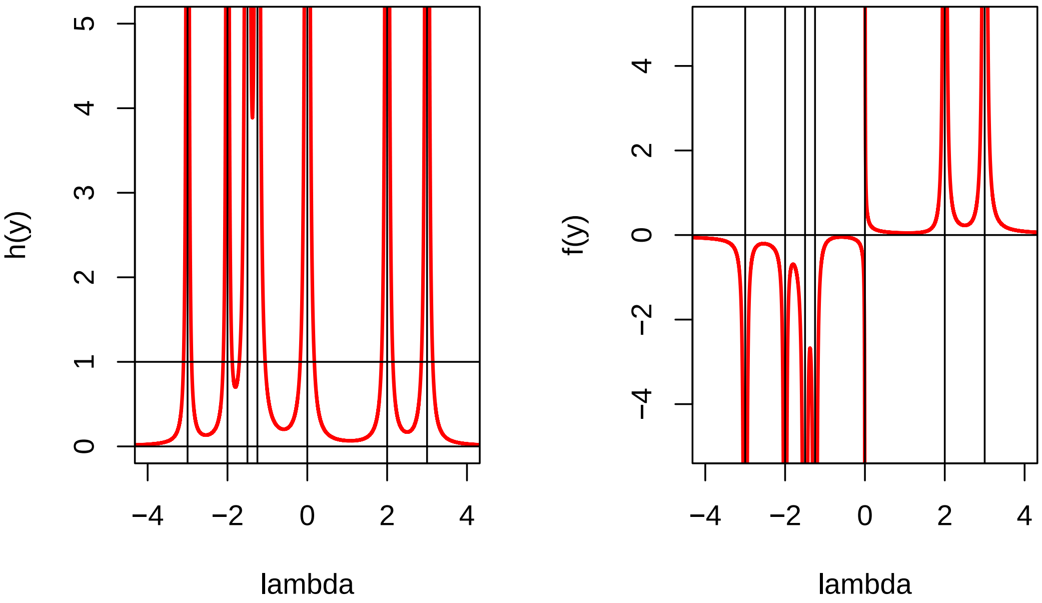


Figure 1: Quadratic Secular Equation

Again h has vertical asympotes at the ϕ_i. Beween two asymptotes h decreases from $+\infty$ to a minimum, and then increases again to $+\infty$. Note that

$$h'(\lambda) = 2\sum_{i=1}^{n} \frac{d_i^2}{(\phi_i - \lambda)^3},$$

and

$$h''(\lambda) = 6\sum_{i=1}^{n} \frac{d_i^2}{(\phi_i - \lambda)^4},$$

and thus h is convex in each of the intervals between asymptotes. Also h is convex and increasing from zero to $+\infty$ on $(-\infty, \phi_n)$ and convex and decreasing from $+\infty$ to zero on $(\phi_1, +\infty)$.

8.6.6 Generalized Inverses

8.6.7 Partitioned Matrices

8.7 Matrix Differential Calculus

8.7.1 Matrix Derivatives

A matrix, of course, is just an element of a finite dimensional linear vector space. We write $X \in \mathbb{R}^{n\times m}$, and we use the inner product $\langle X, Y\rangle = \mathbf{tr}X'Y$, and corresponding norm $\|X\| = \sqrt{\mathbf{tr}\ X'X}$. Thus derivatives of real-valued function of matrices, or derivatives of matrix-valued functions of matrices, are covered by the usual definitions and formulas. Nevertheless there is a surprisingly huge literature on differential calculus for real-valued functions of matrices, and matrix-valued functions of matrices.

One of the reason for the proliferation of publications is that a matrix-valued function of matrices can be thought of a function of for matrix space $\mathbb{R}^{n\times m}$ to matrix-space $\mathbb{R}^{p\times q}$, but also as a function of vector space $\mathbb{R}^{nm}$ to vector space $\mathbb{R}^{pq}$. There are obvious isomorphisms between the two representations, but they naturally lead to different notations. We will consistently choose the matrix-space formulation, and consequently minimize the role of the **vec**() operator and the special constructs such as the commutation and duplication matrix.

The other choice

Nevertheless having a compendium of the standard real-valued and matrix-valued functions available is of some interest. The main reference is the book by Magnus and Neudecker (1999). We will avoid using differentials and the **vec**() operator.

Suppose F is a matrix valued function of a single variable x. In other words $F : \mathbb{R} \rightarrow \mathbb{R}^{n\times m}$ is a matrix of functions, as in

$$F(x) = \begin{bmatrix} f_{11}(x) & f_{12}(x) & \cdots & f_{1m}(x) \\ f_{21}(x) & f_{22}(x) & \cdots & f_{2m}(x) \\ \vdots & \vdots & \ddots & \vdots \\ f_{n1}(x) & f_{n2}(x) & \cdots & f_{nm}(x) \end{bmatrix}.$$

Now the derivatives of any order of F, if they exist, are also matrix valued functions

$$\mathcal{D}^sF(x)=\begin{bmatrix}\mathcal{D}^sf_{11}(x)&\mathcal{D}^sf_{12}(x)&\cdots&\mathcal{D}^sf_{1m}(x)\\\mathcal{D}^sf_{21}(x)&\mathcal{D}^sf_{22}(x)&\cdots&\mathcal{D}^sf_{2m}(x)\\\vdots&\vdots&\ddots&\vdots\\\mathcal{D}^sf_{n1}(x)&\mathcal{D}^sf_{n2}(x)&\cdots&\mathcal{D}^sf_{nm}(x)\end{bmatrix}.$$

If F is a function of a vector $x\in\mathbb{R}^p$ then partial derivatives are defined similarly, as in

$$\mathcal{D}_{i_1\cdots i_s}F(x)=\begin{bmatrix}\mathcal{D}_{i_1\cdots i_s}f_{11}(x)&\mathcal{D}_{i_1\cdots i_s}f_{12}(x)&\cdots&\mathcal{D}_{i_1\cdots i_s}f_{1m}(x)\\\mathcal{D}_{i_1\cdots i_s}f_{21}(x)&\mathcal{D}_{i_1\cdots i_s}f_{22}(x)&\cdots&\mathcal{D}_{i_1\cdots i_s}f_{2m}(x)\\\vdots&\vdots&\ddots&\vdots\\\mathcal{D}_{i_1\cdots i_s}f_{n1}(x)&\mathcal{D}_{i_1\cdots i_s}f_{n2}(x)&\cdots&\mathcal{D}_{i_1\cdots i_s}f_{nm}(x)\end{bmatrix},$$

with $1\leq i_s\leq p$. The notation becomes slightly more complicated if F is a function of a $p\times q$ matrix X, i.e. an element of $\mathbb{R}^{p\times q}$. It then makes sense to write the partials as $\mathcal{D}_{(i_1,j_1)\cdots(i_s,j_s)}F(X)$ where $1\leq i_s\leq p$ and $1\leq j_s\leq q$.

8.7.2 Derivatives of Eigenvalues and Eigenvectors

This appendix summarizes some of the results in J. De Leeuw (2007a), J. De Leeuw (2008), and J. De Leeuw and Sorenson (2012). We refer to those reports for more extensive calculations and applications.

Suppose A and B are two real symmetric matrices depending smoothly on a real parameter θ. The notation below suppresses the dependence on θ of the various quantities we talk about, but it is important to remember that all eigenvalues and eigenvectors we talk about are functions of θ.

The *generalized eigenvalue* λ_s and the corresponding *generalized eigenvector* x_s are defined implicitly by $Ax_s=\lambda_sBx_s$. Moreover the eigenvector is identified by $x_s'Bx_s=1$. We suppose that in a neighborhood of θ the eigenvalue λ_s is unique and B is positive definite. A precise discussion of the required assumptions is, for example, in Wilkinson (1965) or Kato (1976).

Differentiating $Ax_s=\lambda_sBx_s$ gives the equation

$$(A-\lambda_sB)(\mathcal{D}x_s)=-((\mathcal{D}A)-\lambda_s(\mathcal{D}B))x_s+(\mathcal{D}\lambda_s)Bx_s,\tag{1}$$

while $x_s'Bx_s = 1$ gives

$$x_s'B(\mathcal{D}x_s) = -\frac{1}{2}x_s'(\mathcal{D}B)x_s. \tag{2}$$

Premultiplying (**1**) by x_s' gives

$$\mathcal{D}\lambda_s = x_s'((\mathcal{D}A) - \lambda_s(\mathcal{D}B))x_s$$

Now suppose $AX = BX\Lambda$ with $X'BX = I$. Then from (**1**), for $t \neq s$, premultiplying by x_t' gives

$$(\lambda_t - \lambda_s)x_t'B(Dx_s) = -x_t'((\mathcal{D}A) - \lambda_s(\mathcal{D}B))x_s.$$

If we define g by

$$g_t \triangleq \begin{cases} \frac{1}{\lambda_t - \lambda_s}x_t'((\mathcal{D}A) - \lambda_s(\mathcal{D}B))x_s & \text{for } t \neq s, \\ \frac{1}{2}x_t'(\mathcal{D}B)x_t & \text{for } t = s, \end{cases}$$

then $X'B(\mathcal{D}x_s) = -g$ and thus $\mathcal{D}x_s = -Xg$.

A first important special case is the *ordinary eigenvalue problem*, in which $B = I$, which obviously does not depend on θ, and consequently has $\mathcal{D}B = 0$. Then

$$\mathcal{D}\lambda_s = x_s'(\mathcal{D}A)x_s,$$

while

$$g_t \triangleq \begin{cases} \frac{1}{\lambda_t - \lambda_s}x_t'(\mathcal{D}A)x_s & \text{for } t \neq s, \\ 0 & \text{for } t = s. \end{cases}$$

If we use the Moore_Penrose inverse the derivatives of the eigenvector can be written as

$$\mathcal{D}x_s = -(A - \lambda_s I)^+(\mathcal{D}A)x_s.$$

Written in a different way this expression is

$$\mathcal{D}x_s = \sum_{t \neq s} \frac{u_{st}}{\lambda_s - \lambda_t}x_t,$$

with $U \triangleq X'(\mathcal{D}A)X$, so that $\mathcal{D}\lambda_s = u_{ss}$.

In the next important special case is the *singular value problem* The singular values and vectors of an $n \times m$ rectangular Z, with $n \geq m$, solve the equations

$Zy_s = \lambda_s x_s$ and $Z'x_s = \lambda_s y_s$. It follows that $Z'Zy_s = \lambda_s^2 y_s$, i.e. the right singular vectors are the eigenvectors and the singular values are the square roots of the eigenvalues of $A = Z'Z$.

Now we can apply our previous results on eigenvalues and eigenvectors. If $A = Z'Z$ then $\mathcal{D}A = Z'(\mathcal{D}Z) + (\mathcal{D}Z)'Z$. We have, at an isolated singular value λ_s,

$$\mathcal{D}\lambda_s^2 = y_s'(Z'(\mathcal{D}Z) + (\mathcal{D}Z)'Z)y_s = 2\lambda_s x_s'(\mathcal{D}Z)y_s,$$

and thus

$$\mathcal{D}\lambda_s = x_s'(\mathcal{D}Z)y_s.$$

For the singular vectors our previous results on eigenvectors give

$$\mathcal{D}y_s = -(Z'Z - \lambda_s^2 I)^+(Z'(\mathcal{D}Z) + (\mathcal{D}Z)'Z)y_s,$$

and in the same way

$$\mathcal{D}x_s = -(ZZ' - \lambda_s^2 I)^+(Z(\mathcal{D}Z)' + (\mathcal{D}Z)Z')x_s.$$

Now let $Z = X\Lambda Y'$, with X and Y square orthonormal, and with Λ and $n\times m$ diagonal matrix (with $\nabla\dashv\backslash\|(Z)$ positive diagonal entries in non-increasing order along the diagonal).

Also define $U \triangleq X'(DZ)Y$. Then $\mathcal{D}\lambda_s = u_{ss}$, and

$$\mathcal{D}y_s = \sum_{t\neq s} \frac{\lambda_s u_{st} + \lambda_t u_{ts}}{\lambda_s^2 - \lambda_t^2} y_t,$$

and

$$\mathcal{D}x_s = \sum_{t\neq s} \frac{\lambda_t u_{st} + \lambda_s u_{ts}}{\lambda_s^2 - \lambda_t^2} x_t.$$

Note that if Z is symmetric we have $X = Y$ and U is symmetric, so we recover our previous result for eigenvectors. Also note that if the parameter θ is actually element (i, j) of Z, i.e. if we are computing partial derivatives, then $u_{st} = x_{is}y_{jt}$.

The results on eigen and singular value decomposition can be applied in many different ways. mostly by simply using the product rule for derivatives, For a square symmetric A or order n, for example, we have

$$f(A) \triangleq \sum_{s=1}^{n} f(\lambda_s)x_s x_s'.$$

and thus

$$\mathcal{D}f(A)=\sum_{s=1}^{n}Df(\lambda_s)(\mathcal{D}\lambda_s)x_sx_s'+f(\lambda_s)(x_s(\mathcal{D}x_s)'+(\mathcal{D}x_s)x_s').$$

The generalized inverse of a rectangular Z is

$$Z^+\triangleq\sum_{s=1}^{r}\frac{1}{\lambda_s}y_sx_s',$$

where $r=\mathbf{rank}(Z)$. Summation is over the positive singular values, and for differentiability we must assume that the rank of Z is constant in a neighborhood of θ.

The Procrustus transformation of a rectangular Z, which is the projection of Z on the Stiefel manifold of orthonormal matrices, is

$$\mathbf{proc}(Z)\triangleq Z(Z'Z)^{-\frac{1}{2}}=\sum_{s=1}^{m}x_sy_s',$$

where we assume for differentiability that Z is of full column rank.

The projection of Z on the set of all matrices of rank less than or equal to r, which is of key importance in PCA and MDS, is

$$\Pi_r(Z)\triangleq\sum_{s=1}^{r}\lambda_sx_sy_s'=Z\sum_{s=1}^{r}y_sy_s',$$

where summation is over the r largest singular values.

8.8 Graphics and Code

8.8.1 Multidimensional Scaling

Many of the examples in the book are taken from the area of *multidimensional scaling (MDS)*. In this appendix we describe the basic MDS notation and terminology. Our approach to MDS is based on Kruskal [1964ab], using terminology and notation of De Leeuw [1977] and De Leeuw and Heiser [1982]. For a more recent and more extensive discussion of MDS see Borg and Groenen [2005].

The data in an MDS problem consist of information about the *dissimilarities* between pairs of *n objects*. Dissimilarities are like distances, in the sense that they give some information about physical or psychological closeness, but they need not satisfy any of the distance axioms. In metric MDS the dissimilarity between objects i and j is a given number δ_{ij}, usually positive and symmetric, with possibly some of the dissimilarities missing. In non-metric MDS we only have a partial order on some or all of the n^2 dissimilarities. We want to represent the n objects as n points in a *metric space* in such a way that the *distances* between the points approximate the dissimilarities between the objects.

An MDS loss function is typically of the form $\sigma(X,\Delta) = \|\Delta - D(X)\|$ for some norm, or pseudo-norm, on the space of $n \times n$ matrices. Here X are the n points in the metric space, with $D(X)$ the symmetric, non-negative, and hollow matrix of distances. The MDS problem is to minimize loss over all mappings X and all feasible Δ. In the metric MDS problems Δ is fixed at the observed data, in non-metric MDS any monotone transformation of Δ is feasible.

The definition of MDS we have given leaves room for all kinds of metric spaces and all kinds of norms to measure loss. In almost all applications both in this book and elsewhere, we are interested in *Euclidean MDS*, where the metric space is $\mathbb{R}^p$, and in loss functions that use the (weighted) sum of squares of residuals $r_{ij}(X,\Delta)$. Thus the loss function has the general form

$$\sigma(X,\Delta) = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij} r_{ij}^2(X,\Delta),$$

where X is an $n \times p$ matrix called the *configuration*.

The most popular choices for the residuals are

$$\begin{aligned}
R_1(X,\Delta) &= \Delta - D(X),\\
R_2(X,\Delta) &= \Delta^2 - D^2(X),\\
R_0(X,\Delta) &= \log\Delta - \log D(X),\\
R_S(X,\Delta) &= -\frac{1}{2}J_n(\Delta^2 - D^2(X))J_n.
\end{aligned}$$

Here Δ^2 and $\log\Delta$ are *elementwise* transformations of the dissimilarities, with corresponding transformations D^2 and $\log D$ of the distances. In R_S

we use the centering operator $J_n = I - \frac{1}{n}ee'$. For Euclidean distances, and centered X,

$$R_S(X, \Delta) = \Gamma(\Delta) - XX',$$

with $\Gamma(\Delta) \stackrel{\Delta}{=} -\frac{1}{2}J_n\Delta^2 J_n$. Metric Euclidean MDS, using R_S with unit weights, means finding the best rank p approximation to $\Gamma(\Delta)$, which can be done finding the p dominant eigenvalues and corresponding eigenvectors. This is also known as *Classical MDS* [Torgerson, 1958].

The loss function σ_1 that uses R_1 is called *stress* [Kruskal, 1964ab], the function σ_2 that uses R_2 is *sstress* [Takane et al, 1977], and loss σ_S that uses R_S is *strain* [De Leeuw and Heiser, 1982]. R_0 has been nameless so far, but it has been proposed by Ramsay [1977]. Because of its limiting properties (see below), we will call it *strull*.

Both R_1 ant R_2 are obviously special cases of

$$R_r(X, \Delta) = \Delta^r - D^r(X),$$

for which the corresponding loss function σ_r is called *r-stress*. Because

$$\lim_{r \to 0} \frac{R_r(X, \Delta)}{r} = \log \Delta - \log D(X)$$

we see that σ_0 is a limiting case of $\frac{1}{r^2}\sigma_r$.

There is some matrix notation that is useful in dealing with Euclidean MDS. Suppose e_i and e_j are unit vectors, with all elements equal to zero, except one element which is equal to one. Then

$$d_{ij}^2(X) = (e_i - e_j)'XX'(e_i - e_j) = \mathbf{tr}\ X'A_{ij}X = \mathbf{tr}\ A_{ij}C(X),$$

where $A_{ij} \stackrel{\Delta}{=} (e_i - e_j)(e_i - e_j)'$ and $C(X) \stackrel{\Delta}{=} XX'$. If we define

$$A_{ij}^{*p} \stackrel{\Delta}{=} \underbrace{A_{ij} \oplus \cdots \oplus A_{ij}}_{p \text{ times}},$$

and $\overline{x} = \mathbf{vec}(X)$ then $d_{ij}^2(X) = \overline{x}'A_{ij}^{*p}\overline{x}$, which allows us to work with vectors in $\mathbb{R}^{np}$ instead of matrices in $\mathbb{R}^{n \times p}$.

8.8.2 Cobweb Plots

Suppose we have a one-dimensional Picard sequence which starts at $x^{(0)}$, and then is defined by

$$x^{(k+1)} = f(x^{(k)}).$$

The cobweb plot draws the line $y = x$ and the function $y = f(x)$. A fixed point is a point where the line and the function intersect. We visualize the iteration by starting at $(x^{(0)}, f(x^{(0)})) = (x^{(0)}, x^{(1)})$, then draw a horizontal line to $(f(x^{(0)}), f(x^{(0)})) = (x^{(1)}, x^{(1)})$, then draw a vertical line to $(x^{(1)}, f(x^{(1)})) = (x^{(1)}, x^{(2)})$, and so on. For a convergent sequence we will see zig-zagging parallel to the axes in smaller and smaller steps to a point where the function and the line intersect.

An illustration will make this clear. The Newton iteration for the square root of a is

$$x^{(k+1)} = \frac{1}{2}\left(x^{(k)} + \frac{a}{x^{(k)}}\right).$$

The iterations for $a = .5$ starting with $x^{(0)} = .1$ are in the cobweb plot in figure 8.2.

In the code section there is `R` code for a general cobweb plotter with a variable number of parameters.

#Code

```
blockRelax <-
  function (f,
            x,
            g,
            itmax = 100,
            eps = 1e-8,
            verbose = TRUE) {
    k <- split (1:length (x), g)
    m <- length (k)
    fold <- f (x)
    itel <- 1
    blockFun <- function (z,  g,  y, i) {
      y[i] <- z
      return (g (y))
```

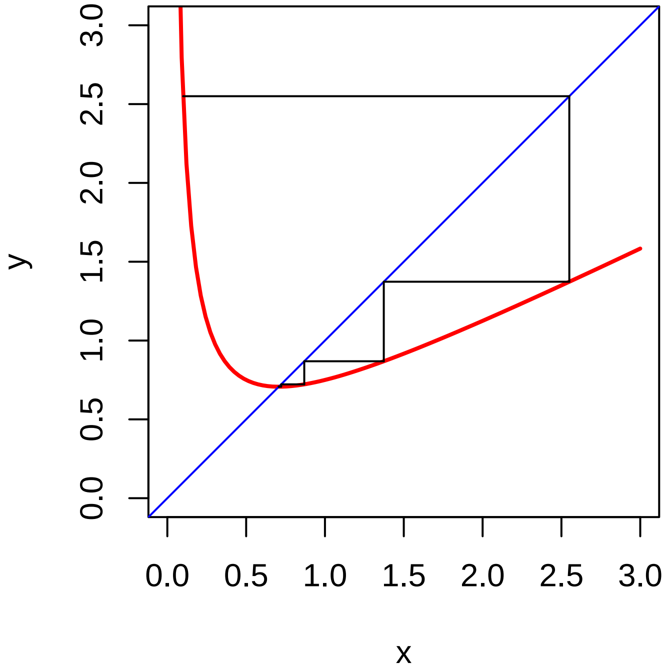


Figure 8.2: Cobweb plot for Newton Square Root Iteration

```
    }
    repeat {
      for (i in 1:m) {
        kk <- k[[i]]
        o <-
          optim (
            x[kk],
            blockFun,
            gr = NULL,
            g = f,
            y = x,
            i = kk,
            method = "BFGS"
          )
        x[kk] <- o$par
        fnew <- o$value
      }
      if (verbose)
        cat(
          "Iteration: ",
          formatC (itel, width = 3, format = "d"),
          "fold: ",
          formatC (
            fold,
            digits = 8,
            width = 12,
            format = "f"
          ),
          "fnew: ",
          formatC (
            fnew,
            digits = 8,
            width = 12,
            format = "f"
          ),
          "\n"
        )
      if ((itel == itmax) || ((fold - fnew) < eps))
        break
      itel <- itel + 1
      fold <- fnew
    }
    return (list (x = x, f = fnew))
  }
```

Code Segment 1: Block Relaxation

```
bls <-
  function (z,
            y,
            xold = rep(0, ncol(y)),
            blocks = as.list(1:ncol(y)),
            itmax = 100,
            eps = 1e-10,
            verbose = TRUE) {
    nblocks <- length (blocks)
    fold <- sum((z - y %*% xold) ^ 2)
    xopt <- qr.solve(y, z)
    eold <- sqrt (sum ((xold - xopt) ^ 2))
    itel <- 1
    repeat {
      xwork <- xold
      for (i in 1:nblocks) {
        u <- drop (y %*% xwork)
        yact <- y[, blocks[[i]], drop = FALSE]
        xact <- xwork[blocks[[i]]]
        yres <- z - (u - yact %*% xact)
        xwork[blocks[[i]]] <- qr.solve (yact, yres)
      }
      xnew <- xwork
      fnew <- sum((z - y %*% xnew) ^ 2)
      enew <- sqrt (sum ((xold - xnew) ^ 2))
      if (verbose) {
        cat(
        "itel: ",
        formatC(itel, digits = 3, width = 3),
        "fold: ",
        formatC(
          fold,
          digits = 6,
          width = 10,
          format = "f"
        ),
        "fnew: ",
        formatC(
          fnew,
          digits = 6,
          width = 10,
          format = "f"
        ),
        "ratio: ",
        formatC(
          enew / eold,
          digits = 6,
          width = 10,
          format = "f"
        ),
        "\n"
      )
    }
    if ((abs(fold - fnew) < eps) || (itel == itmax))
      break()
    fold <- fnew
    eold <- enew
    xold <- xnew
    itel <- itel + 1
  }
  return (x)
}
```

Code Segment 2: Block Least Squares

```
blockRate <-
  function (f,
            x,
            blocks = as.list (1:length(x)),
            numerical = FALSE,
            product_form = FALSE) {
    if (numerical) {
      h <- hessian (f, x)
    } else {
      h <- f (x)
    }
    nvar <- length (x)
    nblocks <- length (blocks)
    nb <- 1:nblocks
    nn <- 1:nvar
    g <-
      sapply (nn, function (i)
        which (sapply (blocks, function (x)
          any (i == x))))
    if (product_form) {
      sder <- diag (nvar)
      for (i in nb) {
        bi <- blocks [[i]]
        ei <- ifelse (outer(nn, bi, "=="), 1, 0)
        sder <-
          (diag(nvar) - ei %*% solve (h[bi, bi], h[bi, , drop = FALSE])) %*% sder
      }
    } else {
      alow <- h * ifelse (outer (g, g, ">="), 1, 0)
      sder <- -solve (alow, h - alow)
    }
    return (sder)
  }
```

Code Segment 3: Block Rate

```
cobwebPlotter <-
  function (xold,
            func,
            lowx = 0,
            hghx = 1,
            lowy = lowx,
            hghy = hghx,
            eps = 1e-10,
            itmax = 25,
            ...) {
    x <- seq (lowx, hghx, length = 100)
    y <- sapply (x, function (x)
      func (x, ...))
    plot (
      x,
      y,
      xlim = c(lowx , hghx),
      ylim = c(lowy, hghy),
      type = "l",
      col = "RED",
      lwd = 2
    )
    abline (0, 1, col = "BLUE")
    base <- 0
    itel <- 1
    repeat {
      xnew <- func (xold, ...)
      if (itel > 1) {
        lines (matrix(c(xold, xold, base, xnew), 2, 2))
      }
      lines (matrix(c(xold, xnew, xnew, xnew), 2, 2))
      if ((abs (xnew - xold) < eps) || (itel == itmax)) {
        break ()
      }
      base <- xnew
      xold <- xnew
      itel <- itel + 1
    }
  }
```

Code Segment 4: Cobweb Plotter

#NEWS

001 03/10/16

- First translation from gitbook

002 03/16/16

- Now generates legal tex
- crossrefs sorted out

003 03/17/16

- bibtex file completed

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