

Stabilised multidimensional root finding

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1 Introduction

In a generalised notation, the objective of any calibration procedure, is to find a solution to the multidimensional, non-linear root-finding problem

$$\mathbf{f}(\mathbf{x}) = 0 \tag{1}$$

for $f \in \mathbb{R}^m$ and $x \in \mathbb{R}^n$. Frequently, the problem is overdetermined, i.e. $m > n$, and only a best fit can be found that minimises $|\mathbf{f}(\mathbf{x})|$ where $|\cdot|$ is chosen to be a suitable vector norm. Examples for multidimensional fitting algorithms are straight forward Newton-Raphson, variable metric methods such as the Broyden-Fletcher-Goldfarb-Shanno algorithm, and nonlinear least squares procedures such as the Levenberg-Marquardt or the NL2SOL methods [PTVF92, DGW81].

On other occasions, though, the problem (1) can be underdetermined, i.e. $m < n$, due to the fact that, for instance, a model that is to be calibrated effectively allows for a much larger number of calibration parameters to be varied than there are calibration instruments. An example for this is the calibration of the Libor market model of interest rates.

Whenever $m < n$, the result of any algorithm used to solve (1) can be highly depend on the initial guess, and can be undesirably sensitive to small changes in any of the parameter that are part of the functional equation $\mathbf{f}(\mathbf{x}) = 0$ but are not subject to the fitting procedure. In this case, the solution is considered to be not sufficiently *robust* or *stable*. The consequence of this for the calibration of a derivatives pricing model is that hedge ratios, if computed via re-calibration of the model, have unacceptably large noise levels and become practically useless.

A remedy for the lack of stability of the numerical solution to (1) is to amend the main problem by the introduction of a (usually somewhat idealised) reference point, and certain preference conditions. Typically, the reference point is also given as the initial guess for \mathbf{x} in the subsequent numerical algorithm, and is denoted by $\mathbf{x}_{\text{reference}}$. The amendment of (1) is then given by the task to solve (1) whilst trying to minimise the preference norm

$$p(\mathbf{x}) := \frac{1}{2} \cdot \mathbf{x}^\top \cdot S \cdot \mathbf{x} + \frac{1}{2} \cdot (\mathbf{x} - \mathbf{x}_{\text{reference}})^\top \cdot (\mathbf{x} - \mathbf{x}_{\text{reference}}) \tag{2}$$

for some symmetric¹ preference structure matrix S .

¹This is no loss of generality since any matrix can be decomposed into the sum of a symmetric matrix S and an asymmetric matrix A , and for any \mathbf{x} we have $\mathbf{x}^\top \cdot (S + A) \cdot \mathbf{x} = \mathbf{x}^\top \cdot S \cdot \mathbf{x}$ since $\mathbf{x}^\top \cdot A \cdot \mathbf{x} = 0$.

2 Newton-Raphson subject to Lagrange multiplier conditions

Let us denote the Jacobian of \mathbf{f} as $J \in \mathbb{R}^{m \times n}$, i.e.

$$J(\mathbf{x}) := (\nabla_{\mathbf{x}} \cdot \mathbf{f}^\top)^\top, \quad (3)$$

which means that the (h, i) -element of J is given by the partial derivative of the h -th element of \mathbf{f} with respect to the i -th element of \mathbf{x} : $j_{hi} = \partial_{x_i} f_h$. The k -th step of a Newton-Raphson iteration that is to take us from $\mathbf{x}^{(k)}$ to $\mathbf{x}^{(k+1)}$ must satisfy the Newton-Raphson stepping equation

$$J_k \cdot (\mathbf{x}^{(k)} - \mathbf{x}^{(k+1)}) = \mathbf{f}_k \quad (4)$$

or, equivalently,

$$\boldsymbol{\epsilon}_k(\mathbf{x}^{(k+1)}) = 0 \quad (5)$$

with

$$J_k := J(\mathbf{x}^{(k)}) \quad (6)$$

$$\mathbf{f}_k := \mathbf{f}(\mathbf{x}^{(k)}) \quad (7)$$

$$\boldsymbol{\epsilon}_k(\mathbf{x}^{(k+1)}) := J_k \cdot \mathbf{x}^{(k+1)} - J_k \cdot \mathbf{x}^{(k)} + \mathbf{f}_k. \quad (8)$$

The core idea of the stabilised Newton-Raphson algorithm is that each step, instead of being determined by the solution of (5), is to find the vector $\mathbf{x}^{(k+1)}$ that minimises the modified preference norm²

$$\tilde{p}(\mathbf{x}^{(k+1)}) := \frac{1}{2} \cdot \mathbf{x}^{(k+1)\top} \cdot M \cdot \mathbf{x}^{(k+1)} - \mathbf{x}^{(k+1)\top} \cdot \mathbf{x}_{\text{reference}} + \boldsymbol{\epsilon}_k^\top(\mathbf{x}^{(k+1)}) \cdot \boldsymbol{\lambda}_k \quad (9)$$

with $M := S + \mathbf{1}$ in a way that is locally independent on $\boldsymbol{\lambda}_k$, i.e. subject to

$$\nabla_{\boldsymbol{\lambda}_k} \cdot \tilde{p}(\mathbf{x}^{(k+1)}) = 0. \quad (10)$$

This approach is, of course, the method of Lagrange multipliers to incorporate affine constraints on the minimisation of a nonlinear objective function, and the constraint (10) is identical to the Newton-Raphson step condition (5). Minimising (9) subject to (10) is thus equivalent to the solution of the system

$$M \cdot \mathbf{x}^{(k+1)} = \mathbf{x}_{\text{reference}} - J_k^\top \cdot \boldsymbol{\lambda}_k \quad (11)$$

$$J_k \cdot \mathbf{x}^{(k+1)} = J_k \cdot \mathbf{x}^{(k)} - \mathbf{f}_k. \quad (12)$$

In the following, we require that the matrix M ought to be positive definite³, which is essentially equivalent to the assumption that the added preference structure conditions contained in the original matrix S are not mutually exclusive. We can thus solve (11) for the next guess:

$$\mathbf{x}^{(k+1)} = M^{-1} \cdot \mathbf{x}_{\text{reference}} - M^{-1} \cdot J_k^\top \cdot \boldsymbol{\lambda}_k \quad (13)$$

²We have subtracted the irrelevant constant term $\mathbf{x}_{\text{reference}}^\top \cdot \mathbf{x}_{\text{reference}}$.

³ It is possible to derive a stabilised multidimensional root finding algorithm without the requirement for M to be positive definite. In that case, however, a singular value decomposition of $J^\top J$ has to be performed which means that the method cannot be used in practice when the number of entries in the vector \mathbf{x} is very large.

In order to find $\boldsymbol{\lambda}_k$, we define $\boldsymbol{r} := M^{-1} \cdot \boldsymbol{x}_{\text{reference}}$ and substitute the above formal solution for $\boldsymbol{x}^{(k+1)}$ back into (12):

$$G_k \cdot \boldsymbol{\lambda}_k = J_k \cdot (\boldsymbol{r} - \boldsymbol{x}^{(k)}) + \boldsymbol{f}_k \quad (14)$$

with

$$G_k := J_k \cdot M^{-1} \cdot J_k^\top, \quad G_k \in \mathbb{R}^{m \times m} \quad (15)$$

Since m is typically much smaller than n , and since it is just possible that the set of calibration instruments is nearly singular, it is advisable to solve equation (14) by the aid of a singularity-safe method such as the Moore-Penrose method [Alb72]. Also, since n can potentially be a large number, direct calculation of M^{-1} is to be avoided. This is possible since M^{-1} only ever appears in combination with J_k^\top or $\boldsymbol{x}_{\text{reference}}$ in the above equations. We thus define H_k^\top as the solution of

$$M \cdot H_k^\top = J_k^\top \quad (16)$$

which means that

$$G_k := J_k \cdot M^{-1} \cdot J_k^\top. \quad (17)$$

The solution of the k -th iteration is now given by

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{r} - H_k^\top \cdot \boldsymbol{\lambda}_k. \quad (18)$$

Note that the k -th increment in \boldsymbol{x} , i.e. $\Delta \boldsymbol{x}^{(k)} := \boldsymbol{x}^{(k+1)} - \boldsymbol{x}^{(k)}$ is given by

$$\Delta \boldsymbol{x}^{(k)} = (\mathbf{1} - M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot J_k) \cdot (\boldsymbol{r} - \boldsymbol{x}^{(k)}) - M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot \boldsymbol{f}_k \quad (19)$$

and that the change in the objective function vector $\Delta \boldsymbol{f}_k := \boldsymbol{f}_{k+1} - \boldsymbol{f}_k$ is, to first order, given by

$$\begin{aligned} J_k \cdot \Delta \boldsymbol{x}^{(k)} &= J_k \cdot (\mathbf{1} - M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot J_k) \cdot (\boldsymbol{r} - \boldsymbol{x}^{(k)}) - J_k \cdot M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot \boldsymbol{f}_k \\ &= (\mathbf{1} - J_k \cdot M^{-1} \cdot J_k^\top \cdot G_k^{-1}) \cdot J_k \cdot (\boldsymbol{r} - \boldsymbol{x}^{(k)}) - J_k \cdot M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot \boldsymbol{f}_k \\ &= (\mathbf{1} - G_k \cdot G_k^{-1}) \cdot J_k \cdot (\boldsymbol{r} - \boldsymbol{x}^{(k)}) - G_k \cdot G_k^{-1} \cdot \boldsymbol{f}_k. \end{aligned} \quad (20)$$

The notation G_k^{-1} hereby stands for the Moore-Penrose inverse of G_k which is defined even when the symmetric matrix G_k has zero eigenvalues. The interpretation of the decomposition (19) is as follows: First, in order to obtain the increment $\Delta \boldsymbol{x}^{(k)}$ that will take us from $\boldsymbol{x}^{(k)}$ to $\boldsymbol{x}^{(k+1)}$, compute *minimum reference bias step*

$$\Delta \boldsymbol{x}_{\text{minimum bias}}^{(k)} = M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot \boldsymbol{f}_k. \quad (21)$$

Then, take the difference vector between the preference-corrected reference \boldsymbol{r} and $\boldsymbol{x}^{(k)}$, and project it such that the remaining projection represents a move as closely as possible to the preference-corrected reference \boldsymbol{r} whilst not violating the Newton-Raphson condition (5) by means of projection onto the kernel of the Newton-Raphson step operator ($M^{-1} \cdot J_k^\top \cdot G_k^{-1}$)

applied to the *range* of $(\mathbf{r} - \mathbf{x}^{(k)})$ under J_k . In other words, imagine we were to simply add $(\mathbf{r} - \mathbf{x}^{(k)})$ to the minimum bias step $\Delta \mathbf{x}_{\text{minimum bias}}^{(k)}$. If the minimum bias step moves us to an updated guess for which the objective vector is identically zero, i.e. if $\Delta \mathbf{x}_{\text{minimum bias}}^{(k)}$ moves us to a solution of the calibration problem, then, to first order, the addition of $(\mathbf{r} - \mathbf{x}^{(k)})$ would mean that $\mathbf{f}_{k+1} \simeq J_k \cdot (\mathbf{r} - \mathbf{x}^{(k)})$ which in turn would mean that, thereafter, we have to take another step to compensate. This subsequent step, though, to first order, would start with the minimum bias component $M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot \mathbf{f}_{k+1}$ which in turn would be, to first order $M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot J_k \cdot (\mathbf{r} - \mathbf{x}^{(k)})$. Thus, instead of adding $(\mathbf{r} - \mathbf{x}^{(k)})$ to the minimum bias step in the k -th iteration, we only add the projection of $(\mathbf{r} - \mathbf{x}^{(k)})$ that will not⁴ give rise to the need of additional corrections in the next step, i.e. $(\mathbf{1} - M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot J_k) \cdot (\mathbf{r} - \mathbf{x}^{(k)})$. It is, incidentally, easy enough to see that $P_k := M^{-1} \cdot J_k^\top \cdot G_k^{-1} \cdot J_k$ is a projection operator, i.e. satisfies $P_k^l = P_k$ for any positive integer l , and thus $(\mathbf{1} - P_k)$ is also a projection operator, whence one may say: *a stabilised Newton-Raphson step consists of the minimum bias increment that moves the current iteration point towards a solution of the nonlinear problem satisfying the given preference structure conditions as closely as possible, plus the projection of the current distance to the preference-structure corrected reference point onto the kernel of the Newton-Raphson step operator.*

In practice, the complete step (19) may easily move the current point outside the range within which the linear approximation that is at the heart of the Newton-Raphson method is valid. This may happen for two reasons. Firstly, the projection of $(\mathbf{r} - \mathbf{x}^{(k)})$ onto $(\mathbf{1} - P_k)$ may be very large due to the fact that the current point is a long way away from the preference-structure corrected reference point \mathbf{r} . This happens when calibration can only be achieved at a considerable distance from \mathbf{r} . In this case, it is advisable, if the iteration $\mathbf{x}^{(k)}$ to $\mathbf{x}^{(k+1)}$ did not succeed in an improvement of the chosen error norm for $\mathbf{f}(\mathbf{x}^{(k+1)})$, to reduce the size of the contribution in the direction towards \mathbf{r} in a binary nesting loop until either an improvement of $\mathbf{f}(\mathbf{x}^{(k+1)})$ over $\mathbf{f}(\mathbf{x}^{(k)})$ has been achieved, or until the binary nesting size is below machine precision. Secondly, the minimum bias increment itself may be too large due to the Newton-Raphson step operator being nearly singular or due to the fact that the current point is a long way from calibration. Thus, if the minimum bias step alone still does not lead to an improvement of $|\mathbf{f}|$, it may be necessary to carry out a secondary binary nesting to scale down the step size along $\Delta \mathbf{x}_{\text{minimum bias}}^{(k)}$ until an improvement in the objective function can be found. Naturally, if this also fails, the fitting procedure must terminate and return the current point $\mathbf{x}^{(k)}$.

References

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⁴to first order