



Branch Switching from Singular Points in higher-dimensional continuation

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Abstract

We explain here how to perform branch switching when a singular point is found during higher-dimensional continuation on a k -dimensional variety. This document is based on the information given in [1, 2, 3].

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1 Introduction

A system of equations

$$\mathbf{F}(\mathbf{u}) = \mathbf{0}, \quad (1)$$

with $\mathbf{u} \in \mathbb{R}^n$ and $\mathbf{F} : \mathbb{R}^n \rightarrow \mathbb{R}^{n-k}$, defines a k -dimensional variety \mathcal{M} . Points \mathbf{u}^* that satisfy (1) but at which the Jacobian of \mathbf{F} , $\mathbf{F}_{\mathbf{u}}$, is not full rank, i.e. $\text{rank}(\mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)) < n - k$, are singular points.

We will treat here the case where a higher-dimensional continuation is progressing on a branch Γ_0 of \mathcal{M} and a singular point is found [1, 2]. This can be detected, for instance, by a change on the sign of the determinant of the Jacobian of \mathbf{F} . The main idea for branch switching is that the tangent space to Γ_0 is known (or estimated) and we want to compute the tangent space to the new branch Γ_1 in order to allow the continuation process to jump, or switch, to the new branch Γ_1 . The advantage of computing this tangent is that a chart can be created on the new branch, and the continuation can go on on the new branch. By doing this, there will be two charts around the singular point, the one created on the original branch, tangent to Γ_0 , and another one tangent to the bifurcating branch Γ_1 .

The outline of this report is as follows. First, the geometry of the solution variety near a singular point is discussed. Next, a Lyapunov-Schmidt decomposition is applied, which allows to split the original equations into two sets of equations. Then, an application of the Implicit Function Theorem gives the Bifurcation Equation (*BE*), that must be satisfied around the singular point. The Taylor series of the *BE* define the Algebraic Bifurcation Equation (*ABE*) that must also be satisfied, and another application of the Implicit Function Theorem gives a parametrized set of curves that trace out the solution variety around the singular point. Finally, since we already know one set of solutions of the *ABE*, it is possible to obtain the tangent space to the singular boundary which, in turn, allows to find a tangent to the new bifurcating branch.

2 Preliminaires

The right null space of $\mathbf{F}_{\mathbf{u}}$ is called Φ , and satisfies

$$\left. \begin{aligned} \mathbf{F}_{\mathbf{u}}(\mathbf{u})\Phi &= \mathbf{0} \\ \Phi^T \Phi &= \mathbf{I} \end{aligned} \right\}.$$

At a regular point \mathbf{u} , a basis of the right null space is also a basis of the tangent space to the variety at that point. This tangent space is k -dimensional because $\text{rank}(\mathbf{F}_{\mathbf{u}}(\mathbf{u})) = n - k$. However, at a singular point \mathbf{u}^* , the right null space becomes of dimension higher than k . For now, it will be assumed that on the singular point $\text{rank}(\mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)) = n - k - 1$, so the null space becomes $(k + 1)$ -dimensional.

A singular point can be found, for instance, by dicotomy between two near regular points \mathbf{u}_a and \mathbf{u}_b , where the k -dimensional tangent spaces are known. Then, an orthonormal basis with k vectors, $\{\phi_0, \dots, \phi_{k-1}\}$, can be found at \mathbf{u}^* by interpolation of the two known tangent spaces. This basis satisfies

$$\left. \begin{aligned} \mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)\phi_i &= \mathbf{0} \\ \phi_i^T \phi_j &= \delta_{ij} \end{aligned} \right\}, \quad (2)$$

for $i, j = 0, \dots, k - 1$. This is a basis of the tangent space to the branch Γ_0 where \mathbf{u}_a and \mathbf{u}_b lie. But at the singular point the right null space is $(k + 1)$ -dimensional, so there will be an additional right null vector $\phi_k \in \mathbb{R}^n$ and a left null vector $\psi \in \mathbb{R}^{n-k}$ that satisfy

$$\left. \begin{aligned} \mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)\phi_k &= \mathbf{0} \\ \phi_i^T \phi_k &= 0 \\ \phi_k^T \phi_k &= 1 \end{aligned} \right\}, \quad (3)$$

for $i = 0, \dots, k-1$, and

$$\left. \begin{array}{l} \psi^\top \mathbf{F}\mathbf{u}(\mathbf{u}^*) = \mathbf{0} \\ \psi^\top \psi = 1 \end{array} \right\}.$$

Here, the left null space is one-dimensional because we assumed $\text{rank}(\mathbf{F}\mathbf{u}(\mathbf{u}^*)) = n - k - 1$ and we only have one vector ψ . In general, on a singular point, it is $\text{rank}(\mathbf{F}\mathbf{u}(\mathbf{u}^*)) < n - k$ and there is a left null space Ψ that satisfies

$$\left. \begin{array}{l} \Psi^\top \mathbf{F}\mathbf{u}(\mathbf{u}^*) = \mathbf{0} \\ \Psi^\top \Psi = \mathbf{I} \end{array} \right\}.$$

3 Splitting of the equations

Imagine a regular point \mathbf{u} near a singular point \mathbf{u}^* . We can project the vector from \mathbf{u}^* to \mathbf{u} to the right null space Φ at \mathbf{u}^* and to a space orthogonal to this right null space. So we can write

$$\mathbf{u} = \mathbf{u}^* + \Phi \mathbf{s} + \mathbf{a}, \quad (4)$$

with

$$\Phi^\top \mathbf{a} = 0.$$

That is, the vector of point \mathbf{u} near \mathbf{u}^* can be seen as the sum of the vector of the singular point, a vector on the right null space (\mathbf{s} gives a linear combination of the basis of the null space) and a vector \mathbf{a} which is orthogonal to the right null space. In fact, this can be done using any point $\hat{\mathbf{u}}$ of the variety, even if it is not singular.

The Lyapunov-Schmidt decomposition consists on doing the same thing for both the range and the domain of \mathbf{F} . It is a natural splitting of the domain and the range that derives from the fundamental theorem of linear algebra.

Splitting of the range

The left null space of the Jacobian, $\ker(\mathbf{F}\mathbf{u}^\top)$ or Ψ , is the orthogonal complement of the column space (or range or image), $\text{im}(\mathbf{F}\mathbf{u})$, of the Jacobian [4]. We can write, thus,

$$\mathbf{F}(\mathbf{u}) = \psi\psi^\top \mathbf{F}(\mathbf{u}) + (\mathbf{I} - \psi\psi^\top) \mathbf{F}(\mathbf{u}). \quad (5)$$

It is clear that this is an identity. The first term is the projection of \mathbf{F} onto the left null space of the Jacobian, and the second term is the projection of \mathbf{F} onto the orthogonal complement of the left null space of the Jacobian. Or, in other words, the first term is the projection onto the orthogonal complement of the range of the Jacobian and the second term is the projection onto the range of the Jacobian.

Splitting of the domain

The right null space of the Jacobian, $\ker(\mathbf{F}\mathbf{u})$ or Φ , is the orthogonal complement of the row space (or coimage), $\text{im}(\mathbf{F}\mathbf{u}^\top)$, of the Jacobian [4]. We can then write

$$\mathbf{u} - \mathbf{u}^* = \Phi\Phi^\top(\mathbf{u} - \mathbf{u}^*) + (\mathbf{I} - \Phi\Phi^\top)(\mathbf{u} - \mathbf{u}^*). \quad (6)$$

Here the first term is the projection onto the right null space and the second term is the projection onto the row space.

Comparing (4) and (6) it can be seen that

$$\mathbf{s} = \Phi^\top(\mathbf{u} - \mathbf{u}^*)$$

and

$$\mathbf{a} = (\mathbf{I} - \Phi\Phi^\top)(\mathbf{u} - \mathbf{u}^*).$$

It is easy to check that the vector \mathbf{a} is in fact orthogonal to the right null space because $\Phi^\top(\mathbf{I} - \Phi\Phi^\top) = \mathbf{0}$.

So, looking at (5) and using (4), we can say that, near \mathbf{u}^* , $\mathbf{F}(\mathbf{u}) = \mathbf{0}$ if and only if

$$\psi^\top \mathbf{F}(\mathbf{u}^* + \Phi \mathbf{s} + \mathbf{a}) = 0 \quad (7)$$

and

$$(\mathbf{I} - \psi\psi^\top)\mathbf{F}(\mathbf{u}^* + \Phi \mathbf{s} + \mathbf{a}) = \mathbf{0}. \quad (8)$$

Thus, we can write

$$\mathbf{F}(\mathbf{u}) = \begin{cases} \psi^\top \mathbf{F}(\mathbf{u}^* + \Phi \mathbf{s} + \mathbf{a}) \\ (\mathbf{I} - \psi\psi^\top)\mathbf{F}(\mathbf{u}^* + \Phi \mathbf{s} + \mathbf{a}) \end{cases}.$$

4 Bifurcation Equation and Algebraic Bifurcation Equation

The Jacobian of (8) with respect to \mathbf{a} is non-singular (the inverse of the Jacobian with respect to \mathbf{a} is the Pseudoinverse of the Jacobian of \mathbf{F}), so the Implicit Function Theorem gives the existence of $\mathbf{a}(\mathbf{s})$ around $\mathbf{s} = \mathbf{0}$ with $\mathbf{a}(\mathbf{0}) = \mathbf{0}$ that satisfies (8). Using this function in (7) yields the Bifurcation Equation (BE):

$$BE(\mathbf{s}) = \psi^\top \mathbf{F}(\mathbf{u}^* + \Phi \mathbf{s} + \mathbf{a}(\mathbf{s})) = 0. \quad (9)$$

This is a system with one equation for each dimension of the left null space (in this text we assumed 1) and one unknown for each dimension of the right null space ($k+1$). In addition, the Jacobian is identically zero at the origin. To see that, take the first derivative of the BE with respect to \mathbf{s} ,

$$BE_{\mathbf{s}}(\mathbf{s}) = \psi^\top \mathbf{F}_{\mathbf{u}}(\mathbf{u}^* + \Phi \mathbf{s} + \mathbf{a}(\mathbf{s}))(\Phi + \mathbf{a}_{\mathbf{s}}(\mathbf{s})). \quad (10)$$

Now, differentiating (8) with respect to \mathbf{s} and evaluating at $\mathbf{s} = \mathbf{0}$ we have that it must be

$$\mathbf{a}_{\mathbf{s}}(\mathbf{0}) = \mathbf{0},$$

and introducing this into (10) for $\mathbf{s} = \mathbf{0}$ we have

$$BE_{\mathbf{s}}(\mathbf{0}) = \psi^\top \mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)\Phi = \mathbf{0}. \quad (11)$$

Every solution of the BE near $\mathbf{s} = \mathbf{0}$ corresponds to a solution of the original singular problem, and every solution of the singular problem near \mathbf{u}^* corresponds to a solution \mathbf{s} of the BE. That is because, in fact, vector \mathbf{s} gives a linear combination of the vectors of a basis of the right null space Φ . For example, if it is $k = 2$, the vector $\mathbf{s} = (s^0, s^1, s^2)$ gives a point in the $k+1 = 3$ dimensional null space of $\mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)$ in the basis $\{\phi_0, \phi_1, \phi_2\}$, columns of Φ . So, around $\mathbf{s} = \mathbf{0}$, each solution \mathbf{s} of the BE (9) gives a point in the null space Φ which can be projected to a point on the variety by using $\mathbf{a}(\mathbf{s})$ in (4). We do not actually have an expression for $\mathbf{a}(\mathbf{s})$, but the coefficients in a Taylor series expansion for \mathbf{a} can be found by repeated differentiation of (8) [3].

We just saw that the linearization of the BE is zero at $\mathbf{s} = \mathbf{0}$ (11), but we can avoid this in order to apply the Implicit Function Theorem by introducing a small number ϵ such that

$$BE(\epsilon, \mathbf{s}) = \frac{1}{\epsilon^2} BE(\epsilon \tilde{\mathbf{s}}).$$

We are just performing a change of variable by setting $\mathbf{s} = \epsilon \tilde{\mathbf{s}}$. The length of the vector \mathbf{s} can now be set using ϵ , so $\tilde{\mathbf{s}}$ is chosen to be a normalized vector, and since the BE is equal to zero, we can multiply it by $\frac{1}{\epsilon^2}$ without modifying its solutions. We are introducing one variable (ϵ) and one equation ($\tilde{\mathbf{s}}$ of norm one). By an abuse of language, we will write \mathbf{s} instead of $\tilde{\mathbf{s}}$.

The BE can be written in indicial notation as

$$\psi^\top \mathbf{F}(\mathbf{u}^* + \sum_{i=0}^k \phi_i s^i + \mathbf{a}(s^0, \dots, s^k)) = 0, \quad (12)$$

and after the change of variable and the scale by $\frac{1}{\epsilon^2}$ it becomes

$$\frac{1}{\epsilon^2} \psi^\top \mathbf{F}(\mathbf{u}^* + \epsilon \sum_{i=0}^k \phi_i s^i + \mathbf{a}(\epsilon s^0, \dots, \epsilon s^k)) = 0, \quad (13)$$

with

$$\sum_i s^i s^i = 1. \quad (14)$$

Note that the same change of variable can be applied in (4),

$$\mathbf{u}(\epsilon) = \mathbf{u}^* + \epsilon \sum_{i=0}^k \phi_i s^i + \mathbf{a}(\epsilon s^0, \dots, \epsilon s^k). \quad (15)$$

A Taylor series in ϵ around 0 of (13) is

$$\frac{1}{\epsilon^2} \psi^\top \mathbf{F} = \sum_{i,j} \psi^\top \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_i \phi_j s^i s^j + \epsilon \sum_{i,j,l} (\psi^\top \mathbf{F}_{\mathbf{u}\mathbf{u}\mathbf{u}} \phi_i \phi_j \phi_l s^i s^j s^l + \psi^\top \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_l \mathbf{a}_{,s^i,s^j} s^l) + \dots \quad (16)$$

This can be obtained by differentiating (13) with respect to ϵ or by first differentiating (12) with respect to \mathbf{s} and then performing the change of variables.

The first term of the Taylor series is the Algebraic Bifurcation Equation (ABE):

$$\sum_{i,j} \psi^\top \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_i \phi_j s^i s^j = 0.$$

The ABE has to be zero around the singular point ($\epsilon = 0$) because of (13) and because the other terms of the expansion are already zero for $\epsilon = 0$.

Now, if the ABE is satisfied and the first order term of the expansion (16) is non-zero, i.e.

$$\sum_{i,j,l} (\psi^\top \mathbf{F}_{\mathbf{u}\mathbf{u}\mathbf{u}} \phi_i \phi_j \phi_l s^i s^j s^l + \psi^\top \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_l \mathbf{a}_{,s^i,s^j} s^l) \neq 0,$$

we can apply the Implicit Function Theorem on (13) to say that a set of functions $s^i(\epsilon)$ with $s^i(0) = s_{ABE}^i$ exists in a neighborhood of $\epsilon = 0$. The solution of the ABE with (14) corresponds to a $(k-1)$ -manifold on \mathcal{M} that passes through \mathbf{u}^* . And all the solutions of the ABE alone can be parametrized by ϵ . Varying s^i subject to the ABE traces out the variety on the neighbourhood of the singular point.

To see that, remember that \mathbf{s} gives a linear combination of the vectors of a basis of the right null space Φ . We can think of \mathbf{s} (which is now of norm 1) as giving a direction in the null space, and ϵ gives how far we move from the singular point in that direction. Then, we can obtain a point on the variety using (15). The ABE is just one equation, and together with (14) we have 2 equations that \mathbf{s} must satisfy. The vector \mathbf{s} has $k+1$ components (dimension of the right null

space), so we have 2 equations and $k + 1$ variables. Hence, the solution of the ABE with (14) is a $k + 1 - 2 = k - 1$ dimensional variety. For ease of interpretation, think of the case $k = 2$. We call the solution curve of the ABE with (14) as \mathbf{s}_{ABE} . Each point of this curve gives a possible value of \mathbf{s} , which represents a possible direction in the null space. Since all the \mathbf{s} on this curve are of norm one, ϵ allows to choose how far to move from the singular point for a given direction. When $\epsilon = 0$ the direction is still given, but since we do not move far away, we are exactly on the singular point. Now, take a point of the solution curve \mathbf{s}_{ABE} . This is a specific value of \mathbf{s} , which gives a specific direction on the null space. Keeping this direction and modifying ϵ we trace a curve that can be projected on the solution variety \mathcal{M} . Doing the same for another value of \mathbf{s} (another point of the curve \mathbf{s}_{ABE} , another direction on the null space), we trace a different curve on the solution variety. So, by modifying \mathbf{s} subject to the ABE , i.e. taking all points of the curve, we trace out the solution variety \mathcal{M} on a neighborhood of the singular point \mathbf{u}^* .

5 Tangents

We already know one set of solution of the ABE : any vector \mathbf{s} with $s^k = 0$. This is because we chose the first k null vectors to be a basis of the tangent space to Γ_0 in (2) and (3). The ABE can therefore be written as

$$s^k \left(\sum_{i=0}^k N_i s^i \right) = 0,$$

with $N_i = \psi^\top \mathbf{F} \mathbf{u} \mathbf{u} \phi_i \phi_k$ for $i = 0, \dots, k$. Here, the N_i can be seen as the components of a vector $\mathbf{N} \in \mathbb{R}^{k+1}$ in s -space orthogonal to the bifurcating branch Γ_1 (fig.). The vectors on the tangent space of the singular boundary shared by Γ_0 and Γ_1 must be on the tangent space to Γ_0 and on the tangent space to Γ_1 . Thus, they can be determined by

$$\left. \begin{array}{l} s^k = 0 \\ \sum_{i=0}^k N_i s^i = 0 \end{array} \right\}. \quad (17)$$

Let $\{\sigma_0, \dots, \sigma_{k-2}\}$ be an orthonormal basis of the $(k-1)$ -dimensional tangent space defined by (17). A basis of the tangent space to the bifurcating branch Γ_1 is made of these vectors σ_i with an additional vector

$$\sigma_{k-1} = (N_k N_0, \dots, N_k N_{k-1}, -\sum_{i=0}^{k-1} N_i N_i).$$

This vector is orthogonal to the other σ_i (to form a basis) and to \mathbf{N} (it is a vector on the tangent space to Γ_1), but it is not normalized. Note that the vectors σ are in s -space, so $\sigma = (\sigma^0, \sigma^1, \sigma^2)$ is the vector $\sigma^0 \phi_0 + \sigma^1 \phi_1 + \sigma^2 \phi_2$ in \mathbb{R}^n .

Indeed, the curve \mathbf{s}_{ABE} must contain points that give vectors on the null space that lie on the tangent space to Γ_0 , but must also contain points that give vectors that lie on the tangent space to the bifurcating branch Γ_1 , since all the solution variety is traced out around the singular point. In fact, the first k vectors of the basis of the null space lie on the tangent space to Γ_0 , and the $k+1$ -th vector is orthogonal to the previous ones. So, among all the points of the curve \mathbf{s}_{ABE} , those with $s^k = 0$ are the ones giving the branch Γ_0 of the variety. All the other points of \mathbf{s}_{ABE} trace out the bifurcating branch Γ_1 . In addition, it can be seen that these other values of \mathbf{s}_{ABE} are orthogonal to a vector \mathbf{N} that can be computed. Those points in \mathbf{s}_{ABE} that satisfy both conditions (17) are the ones giving the tangent space to the singular boundary, which can be seen as the intersection of the tangent spaces of Γ_0 and Γ_1 . If vectors σ_i give a basis of this tangent space, a basis of the tangent spaces to Γ_0 and Γ_1 can be expressed using this vectors with and additional one. In the case of Γ_1 , this additional vector must be orthogonal to \mathbf{N} .

Example

For $k = 2$, the vector $\mathbf{s} = (s^0, s^1, s^2)$ gives a point in the $k + 1 = 3$ dimensional null space of $\mathbf{F}\mathbf{u}(\mathbf{u}^*)$ in the basis $\{\phi_0, \phi_1, \phi_2\}$. We have also

$$\mathbf{N} = (N_0, N_1, N_2) = (\psi^\top \mathbf{F}\mathbf{u}\mathbf{u}\phi_0\phi_2, \psi^\top \mathbf{F}\mathbf{u}\mathbf{u}\phi_1\phi_2, \psi^\top \mathbf{F}\mathbf{u}\mathbf{u}\phi_2\phi_2)$$

The branch corresponding to Γ_0 is $s^2 = 0$:

$$\mathbf{u} = \mathbf{u}^* + \epsilon(\phi_0 s^0 + \phi_1 s^1) + \mathbf{a}(\epsilon s^0, \epsilon s^1, 0) \left. \vphantom{\begin{matrix} \mathbf{u} = \mathbf{u}^* + \epsilon(\phi_0 s^0 + \phi_1 s^1) + \mathbf{a}(\epsilon s^0, \epsilon s^1, 0) \\ s^0 s^0 + s^1 s^1 = 1 \end{matrix}} \right\}.$$

And the bifurcating branch Γ_1 is:

$$\mathbf{u} = \mathbf{u}^* + \epsilon(\phi_0 s^0 + \phi_1 s^1 + \phi_2 s^2) + \mathbf{a}(\epsilon s^0, \epsilon s^1, \epsilon s^2) \left. \vphantom{\begin{matrix} \mathbf{u} = \mathbf{u}^* + \epsilon(\phi_0 s^0 + \phi_1 s^1 + \phi_2 s^2) + \mathbf{a}(\epsilon s^0, \epsilon s^1, \epsilon s^2) \\ N_0 s^0 + N_1 s^1 + N_2 s^2 = 0 \\ s^0 s^0 + s^1 s^1 + s^2 s^2 = 1 \end{matrix}} \right\}.$$

In this case, the singular set is a curve, so the tangent to this singular set (basis of the solution of (17)) is $\boldsymbol{\sigma}_0 = (-N_1, N_0, 0)$, which is a vector orthogonal to \mathbf{N} with $s^2 = 0$. This gives the vector $-N_1\phi_0 + N_0\phi_1$ in \mathbb{R}^n . The tangent vector to the bifurcating branch Γ_1 orthogonal to $\boldsymbol{\sigma}_0$ is then $\boldsymbol{\sigma}_1 = (N_0N_2, N_1N_2, -N_0N_0 - N_1N_1)$ in s -space, which is the vector $N_0N_2\phi_0 + N_1N_2\phi_1 + (-N_0N_0 - N_1N_1)\phi_2$ in \mathbb{R}^n , not normalized.

6 Conclusions

When a singular point is found in the current branch Γ_0 that is being continued, its k -dimensional tangent space is estimated using \mathbf{u}_a and \mathbf{u}_b , and the left null vector $\boldsymbol{\psi}$ computed. The tangent to the bifurcating branch Γ_1 can then be obtained by computing vector \mathbf{N} . Since the Hessian is a tensor, each of the components N_i of \mathbf{N} can be computed as

$$N_i = \sum_{p=0}^{n-k-1} \sum_{a=0}^{n-1} \sum_{b=0}^{n-1} \psi^p \mathbf{F}_{a,b}^p \phi_i^a \phi_k^b$$

for $i = 0, \dots, k$. Here, ϕ_i^a is the a -th component of the i -th column vector of $\boldsymbol{\Phi}$, ψ^p is the p -th component of the row vector $\boldsymbol{\psi}^\top$ and $\mathbf{F}_{a,b}^p$ is $\frac{\partial f^p}{\partial u_a \partial u_b}$, where f^p is the p -th equation of \mathbf{F} and u_a and u_b are the a -th and b -th variables inside \mathbf{u} . Once \mathbf{N} is obtained, the tangent (not normalized) to the bifurcating branch Γ_1 is

$$N_k N_0 \phi_0 + \dots + N_k N_{k-1} \phi_{k-1} - \left(\sum_{i=0}^{k-1} N_i N_i \right) \phi_k$$

in \mathbb{R}^n .

This could be specially useful if a quadratic formulation of (1) is assumed. In such case, the Hessian of the equations, $\mathbf{F}\mathbf{u}\mathbf{u}$, is constant and, thus, always available. If the Hessian is not always available, an approximation of the vectors can also be found in principle [2].

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