1 Fixed point iteration

Theorem 1 (Fixed point iteration theorem [3]). If $g : [a,b] \to [a,b]$ is continuous then g(x) has a fixed point, x^* , such that $g(x^*) = x^*$. Furthermore, if |g'(x)| < 1 for all $x \in [a,b]$ then this fixed point is unique on [a,b] and the fixed point iteration $x_{n+1} = g(x_n)$ will converge to x^* for all choices of $x_0 \in [a,b]$.

Proof. Under the first assumption the fixed point exists by the Brouwer fixed point theorem [3]. It suffices to prove that g(x) is a contraction mapping [3] under the second assumption:

$$|g(x) - g(y)| \le |g'(z)| |x - y| < |x - y|$$

where $z \in [x, y] \subset [a, b]$. Thus the mapping contracts and by the contraction mapping theorem $x_n \to x^*$, the unique fixed point.

The plane \mathbb{R}^2 may be divided into four regions for some g(x) with respect to one of its fixed point x^* , depending on the behaviour g(x) takes while in a given region. Chiefly, one is concerned with when $|g(x) - x^*| < |x - x^*|$, so that g(x) is said to converge.

A region where g(x) converges is bounded by points satisfying $|g(x) - x^*| = |x - x^*|$. For such a boundary, either $g(x) - x^* = x - x^*$ or $g(x) - x^* = x^* - x$. The former indicates that the boundary consists of additional fixed points, g(x) = x. The latter gives the boundary $g(x) = 2x^* - x$. One may summarize that if g(x) lies between the lines x and $2x^* - x$ then g(x) will be closer to the fixed point x^* than x.

The second division of behaviour is whether $\operatorname{sign}(g(x) - x^*) = \operatorname{sign}(x - x^*)$. If this is true then g(x) converges (or diverges) monotonically towards (or away from) x^* in this region. If this is false then g(x) oscillates around x^* . The boundary between these two regions is where $\operatorname{sign}(g(x) - x^*) = 0$, or where $g(x) = x^*$.

We are now prepared to describe the four regions of a fixed point function in 1D, based on these behaviours (convergence/divergence, monotonic/oscillation):

- **Region 1:** if $g(x) < x < x^*$ or $g(x) > x > x^*$ then g(x) diverges monotonically from x^* ;
- **Region 2:** if $x < g(x) < x^*$ or $x > g(x) > x^*$ then g(x) converges monotonically towards x^* ;
- **Region 3:** if $x < x^* < g(x) < 2x^* x$ or $x > x^* > g(x) > 2x^* x$ then g(x) converges with oscillations towards x^* ;
- **Region 4:** if $x < x^* < 2x^* x < g(x)$ or $x > x^* > 2x^* x > g(x)$ then g(x) diverges with oscillations from x^* .

2 Newton-Raphson method

The Newton-Raphson method uses the following sequence:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

This method converges quadratically near the root x^* ($f(x^*) = 0$). The following theorem describes the conditions under which the convergence is quadratic.

Theorem 2 (Newton-Raphson [3]). Theorem on existence, uniqueness and convergence of Newton-Raphson. Let f be some function such that $f(x^*) = 0$ for some $x^* \in \mathbb{R}$ and $f'(x^*) \neq 0$. Let $I_{\delta} = [x^* - \delta, x^* + \delta]$ be some interval around x^* such that $f \in C^2(I_{\delta})$ and

$$\frac{|f''(x)|}{|f'(y)|} \le A$$

for all x and y in I_{δ} for some A > 0. Then there exists some neighbourhood of the root x^* within I_{δ} such that the sequence $x_n \to x^*$ quadratically.

The proof is omitted but may be found in many introductory numerical analysis textbooks. Of particular importance to the size of the neighbourhood on which convergence is quadratic is the magnitude of A.

Newton-Raphson may be viewed as a fixed point iteration:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = g_f(x_n).$$

The same geometry as expressed in section 1 applies to this function $g_f(x)$. As such, the Newton-Raphson method gives convergent iterations when $g_f(x)$ lies within regions 2 and 3, as defined in section 1.

To see where $(x, g_f(x))$ lies one may find for which functions f(x) does $g_f(x)$ intersect the lines y = x and $y = 2x^* - x$, where x^* is a root of f(x):

$$x = x - \frac{f(x)}{f'(x)} \implies f(x) = 0, \ f'(x) = \infty,$$
$$2x^* - x = x - \frac{f(x)}{f'(x)} \implies f'(x) = -\frac{f(x)}{2(x^* - x)}.$$

This second intersection, between $g_f(x)$ and $2x^* - x$, defines a first order ODE:

$$\begin{cases} f'_C(x) = -\frac{f_C(x)}{2(x^* - x)} \\ f_C(x^*) = 0. \end{cases}$$
(1)

The solution to this ODE is $f_C(x) = C\sqrt{x - x^*}$ for some constant $C \in \mathbb{C}$.

The lines $f_C(x)$ are transformed into the line $2x^* - x$ when Newton-Raphson is applied to them. For $x < x^* C$ is imaginary; to avoid this one may redefine $f_C(x)$ as

$$f_C(x) = C\sqrt{|x - x^*|}.$$
 (2)

If the function f(x) is tangential to $f_C(x)$ for some x for any C then $g_f(x)$ lies on the border of regions 3 and 4. Therefore, for $g_f(x)$ to lie within regions 2 and 3 (and thus always converge to the root x^*) the function f(x) must cross the lines $f_C(x)$ monotonically. That is, the function

$$C(x) = \frac{f(x)}{\sqrt{|x - x^*|}}$$

must be strictly monotonic.

C(x) cannot be known explicitly without knowledge of the root x^* . As such, the conditions presented above for guaranteed convergence of the Newton-Raphson method are not immediately useful. However, it gives some idea on the geometry of the problem. Also, it should be clear that if f''(x) has the same sign as -f(x) then we can guarantee convergence.

Branin suggests an adjustment to Newton-Raphson [1]:

$$x_{n+1} = x_n - \frac{f(x)}{|f'(x)|}.$$

This naturally assumes that f(x) > 0 when $x < x^*$ and f(x) < 0 when $x > x^*$. If the reverse is true, one may apply the method to -f(x). Using this method requires knowledge of the position of x^* with respect to x. However, if one has this knowledge then this method may overcome many of the pitfalls of Newton-Raphson. The lines $f_C(x)$ must also incorporate the sign change for this method:

$$f_C(x) = C \operatorname{sign}(x - x^*) \sqrt{|x - x^*|}$$

2.1 Higher dimensions

Newton's method may be generalized to higher dimensions by replacing the derivative term with the Jacobian or total derivative, denoted here by $J_f(x)$. For f(x) a vector field $(f : \mathbb{R}^n \to \mathbb{R}^n) J_f(x)$ is a matrix (of size $n \times n$).

$$x_{n+1} = x_n - J_f(x_n)^{-1} f(x_n)$$
(3)

Theorem 3 (Kantorovich (nb: citation needed)). Let $X \subset \mathbb{R}^n$ be open and $F : \mathbb{R}^n \to \mathbb{R}^n$ a differentiable function with J_F (the Jacobian of F) locally Lipschitz continuous (in some operator norm). Let $x_0 \in X$ and let $J_F(x_0)$ be invertible.

Define $h_0 = -J_F(x_0)^{-1}F(x_0)$ and assume the ball $B(x_0 + h_0, ||h_0||)$ is contained in X and J_F has Lipschitz constant M inside this ball. Define the following sequences:

- $h_k = -J_F(x_k)F(x_k);$
- $\alpha_k = M \|J_F(x_k)^{-1}\| \|h_k\|;$
- $x_{k+1} = x_k + h_k$.

If $\alpha_0 \leq 1/2$ then there exists $x^* \in \overline{B}(x_1, ||h_0||)$ and $x_k \to x^*$ with at least linear order of convergence.

The proof is omitted (nb: for now?) but indicates three conditions that restrict the neighbourhood for which the method converges quadratically:

- the size of the Lipschitz constant M;
- the bound of $||J_F(x)^{-1}||$ in the neighbourhood $(||J_F(x)^{-1}|| \le L);$
- the size of the domain where F is appropriately smooth.

The size of the basin of attraction is then proportional to 1/ML, assuming the third condition is not violated anywhere within the basin.

One is concerned with when $||x_{n+1} - x^*|| < ||x_n - x^*||$, as this is where the method converges unconditionally. Divergence occurs when the reverse inequality is true. Equality is then the boundary between these regions, as in the 1D case. As was done there we search for an equation that governs when such an equality occurs.

Any vector with the same norm as $x_n - x^*$ is a rotation of $x_n - x^*$ around the origin. Thus, if R is a rotation matrix $(R^{\top}R = I)$ then

$$x_{n+1} - x^* = x_n - x^* - J_f(x_n)^{-1} f(x_n)$$

= $R(x_n - x^*).$

Simplifying and isolating for $f(x_n)$ we arrive at:

$$f(x_n) = J_f(x_n)(I - R)(x_n - x^*).$$
(4)

If f satisfies this equation for a point $x_n \in \mathbb{R}^n$ then that point is on the boundary between convergence and divergence. The existence of such a boundary permits (but does not guarantee) the existence of cycles. The closest boundary of this nature to the fixed point is necessarily unstable. A second boundary beyond the first may be either stable or unstable.

The equation is not readily solvable for general rotations. However, for R = -I (the antipodal rotation) one can extend the result from 1D to higher dimensions. That is, the vector field:

$$f(x) = \begin{bmatrix} \sqrt{|x_1|} \\ \vdots \\ \sqrt{|x_n|} \end{bmatrix}$$

is one possible solution for R = -I.

Note that any particular solution immediately defines a family of solutions. Let f(x) be a solution to the governing equation 4. Then Af(x) for any matrix $A \in \mathbb{R}^{n \times n}$ is also a solution:

$$J_{Af}(x_n) = AJ_f(x_n) \implies Af(x_n) = J_{Af}(x_n)(I - R)(x_n - x^*).$$



Figure 1: The lines $g_C(x)$ which represent the geometry in which g(x) is ideally monotonic.

3 Newton-Raphson on a fixed point function

A function with a fixed point may be posed as a function with a root by taking $f_q(x) = g(x) - x$. The iteration appears as

$$x_{n+1} = x_n - \frac{g(x_n) - x_n}{g'(x_n) - 1} = x_n - \frac{f_g(x_n)}{f'_g(x_n)}$$

All properties elaborated in section 2 apply to g(x) - x. In particular, the function C(x) should again be ideally strictly monotonic:

$$C(x) = \frac{g(x) - x}{\sqrt{|x - x^*|}}$$

As well, we have again the property that Newton-Raphson will converge if g''(x) has the same sign as x - g(x).

One may now ask for necessary and sufficient conditions for the convergence of Newton-Raphson if g(x) lies within any of the four regions described in section 1. To answer these questions, one may examine properties of the lines $g_C(x) = x + C\sqrt{|x-x^*|}$ when $g_C(x)$ lies within any of the four regions.

Region 1 $(g(x) < x < x^*$ or $g(x) > x > x^*$): Given that $\sqrt{|x - x^*|}$ is non-negative, $g_C(x) < x$ only if C < 0 and $g_C(x) > x$ only if C > 0. Thus, if $g_C(x)$ lies within region 1 then

- $\operatorname{sign}(C) = \operatorname{sign}(x x^*);$
- $g'_C(x) > 1$.

Region 2 $(x < g(x) < x^*$ or $x > g(x) > x^*$): The lower boundary is already defined by C = 0 by the above work. Likewise, by the above work $\operatorname{sign}(C) \neq \operatorname{sign}(x - x^*)$. Next, one examines where $g_C(x) < x^*$:

$$\begin{split} C < & \frac{x^* - x}{\sqrt{|x^* - x|}} \\ < & \mathrm{sign}(x^* - x)\sqrt{|x^* - x|} \\ \implies & C^2 \begin{cases} < |x^* - x| & x^* > x \\ > |x^* - x| & x^* < x. \end{cases} \end{split}$$

One can also show that $g'_C(x)$ is bounded within this region:

$$\begin{split} g_C'(x) &= 1 + \operatorname{sign}(x - x^*) \frac{C}{2\sqrt{|x - x^*|}} \\ &> 1 + \operatorname{sign}(x - x^*) \frac{C}{2|C|} \\ &= 1 + \frac{1}{2} \operatorname{sign}(x - x^*) \operatorname{sign}(C) \\ &= \frac{1}{2}, \\ g_C'(x) &< 1 + \operatorname{sign}(x - x^*) \lim_{x \to \pm \infty} \frac{C}{2\sqrt{|x - x^*|}} \\ &= 1 + 0 = 1, \\ \implies 1/2 < g_C'(x) < 1. \end{split}$$

Thus, if $g_C(x)$ is in region 2 then

- $\operatorname{sign}(C) \neq \operatorname{sign}(x x^*)$ and $|x^* x| > C^2$;
- $1/2 < g'_C(x) < 1.$

Region 3: As before, the lower boundary is defined by the previous work. For the upper boundary, one considers where $g_C(x) < 2x^* - x$:

$$\begin{aligned} x + C\sqrt{|x - x^*|} &< 2x^* - x \\ C &< \operatorname{sign}(x^* - x)2\sqrt{|x^* - x|} \\ \implies \frac{C^2}{4} \begin{cases} < |x^* - x| & x^* > x \\ > |x^* - x| & x^* < x. \end{cases} \end{aligned}$$

As in region 2, one can show that $g'_C(x)$ is bounded in region 3:

$$g'_C(x) > 1 + \operatorname{sign}(x - x^*) \frac{C}{|C|} = 0.$$

Thus, if $g_C(x)$ is in region 3 then

- $\operatorname{sign}(C) \neq \operatorname{sign}(x x^*)$ and $C^2/4 < |x^* x| < C^2$;
- $0 < g'_C(x) < 1/2.$

Region 4: No extra work is required for this region. If $g_C(x)$ is in region 4 then

- $\operatorname{sign}(C) \neq \operatorname{sign}(x x^*)$ and $|x^* x| < C^2/4$;
- $g'_C(x) < 0.$

From the conditions on $g'_C(x)$ one may extract conditions on any given function g(x) that lies within one of the given regions for Newton's method to converge:

- g(x) lies in region 1 then g'(x) > 1 is a necessary condition for convergence;
- g(x) lies in region 2 then g'(x) < 1 is a necessary condition and g'(x) < 1/2 is a sufficient condition;
- g(x) lies in region 3 then g'(x) < 1/2 is a necessary condition and g'(x) < 0 is a sufficient condition;
- g(x) lies in region 4 then g'(x) < 0 is a necessary condition.

4 Application to alternating Schwarz

Consider the alternating Schwarz method for a general second order nonlinear differential equation:

$$\begin{cases} F(x, u_1^n, (u_1^n)', (u_1^n)'') = 0 & x \in [a, \beta] \\ u_1^n(a) = A \\ u_1^n(\beta) = u_2^{n-1}(\beta) \end{cases} \begin{cases} F(x, u_2^n, (u_2^n)', (u_2^n)'') = 0 & x \in [\alpha, b] \\ u_2^n(\alpha) = u_1^n(\alpha) \\ u_2^n(b) = B. \end{cases}$$
(5)

We can think of the operation to solve for u_1^n as a function $G_1 : \mathbb{R} \to \mathbb{R}$ such that $G_1(u_2^{n-1}(\beta)) = u_1^n(\alpha)$. Likewise, $G_2(u_1^n(\alpha)) = u_2^n(\beta)$ and $G_2(G_1(\gamma)) = \gamma$ is a fixed point iteration.

Let $G(\gamma) = G_2 \circ G_1(\gamma)$, where γ replaces $u_2^{n-1}(\beta)$ in equation (5). We will consider a single iteration and therefore drop the superscripts in the notation. To establish how the solution of an ODE at a given point depends on the value of its endpoint, one can differentiate the ODE with respect to the endpoint:

$$\begin{cases} \frac{\partial F}{\partial u} \frac{du_1}{d\gamma} + \frac{\partial F}{\partial u'} \frac{du'_1}{d\gamma} + \frac{\partial F}{\partial u''} \frac{du''_1}{d\gamma} = 0 & x \in [a, \beta] \\ \frac{du_1(a)}{d\gamma} = 0 \\ \frac{du_1(\beta)}{d\gamma} = 1. \end{cases}$$

Let $g_1(x) = \frac{du_1}{d\gamma}$, then the ODE above may be written as:

$$\begin{cases} J(u_1, u_1', u_1'') \cdot (g_1, g_1', g_1'') = 0 & x \in [a, \beta] \\ g_1(a) = 0 \\ g_1(\beta) = 1, \end{cases}$$

where J(u, u', u'') is the Jacobian of F(x, u, u', u''):

$$J(u, u', u'') = \left(\frac{\partial F}{\partial u}, \frac{\partial F}{\partial u'}, \frac{\partial F}{\partial u''}\right).$$
(6)

Then $\frac{du_1(\alpha)}{d\gamma} = g_1(\alpha)$. Likewise, if $g_2(x) = \frac{du_2}{d\gamma}$ then

$$\begin{cases} J(u_2, u'_2, u''_2) \cdot (g_2, g'_2, g''_2) = 0 & x \in [\alpha, b] \\ g_2(\alpha) = \frac{du_1(\alpha)}{d\gamma} = g_1(\alpha) \\ g_2(b) = 0. \end{cases}$$

Therefore, $G'(\gamma) = G'_2(G_1(\gamma))G'_1(\gamma) = g_2(\beta).$

$$G'(\gamma) = \frac{du_2(\beta)}{d\gamma} = \frac{\partial u_2(\beta)}{\partial u_1(\alpha)} \frac{du_1(\alpha)}{d\gamma}.$$

There is an implicit assumption here that $G(\gamma)$ is differentiable. If the problem is continuous with respect to the boundary data then $G(\gamma) \in C(\mathbb{R})$. If, instead, a small perturbation in the boundary data leads to large change in the solution then we will lose the continuity of $G(\gamma)$ and most likely its differentiability. One must then be careful when applying these methods to such problems. Throughout this paper we will assume $G(\gamma) \in C(\mathbb{R})$. We will also assume the problem is nonsingular and therefore the fixed point is unique.

Note if F(x, u, u', u'') is linear in u, u' and u'' then u depends linearly on the boundary conditions. This is reflected in g_1 and g_2 as neither depend on γ so long as J(u, u', u'') is not explicit in its inputs. Thus, $G''(\gamma) = 0$ for linear problems and Newton-Raphson performed on $G(\gamma)$ converges in a single step.

Applying Newton's method to $G(\gamma)$ gives the following algorithm:

$$(1) \begin{cases} F(x, u_1, u_1', u_1'') = 0\\ u_1(a) = A\\ u_1(\beta) = \gamma_n \end{cases}$$

$$(2) \begin{cases} F(x, u_2, u_2', u_2'') = 0\\ u_2(\alpha) = u_1(\alpha)\\ u_2(b) = B \end{cases}$$

$$(3) \begin{cases} J(u_1, u_1', u_1'') \cdot (g_1, g_1', g_1'') = 0\\ g_1(a) = 0\\ g_1(\beta) = 1 \end{cases}$$

$$(4) \begin{cases} J(u_2, u_2', u_2'') \cdot (g_2, g_2', g_2'') = 0\\ g_2(\alpha) = g_1(\alpha)\\ g_2(b) = 0 \end{cases}$$

$$(5)\gamma_{n+1} = \gamma_n - \frac{u_2(\beta) - \gamma_n}{g_2(\beta) - 1}.$$

$$(7)$$

Steps (2) and (3) can be performed simultaneously. Since step (4) is a linear ODE it does not necessarily require step (3) as one can solve instead

(4*)
$$\begin{cases} J(u_2, u'_2, u''_2) \cdot (g_3, g'_3, g''_3) = 0\\ g_3(\alpha) = 1\\ g_3(b) = 0 \end{cases}$$

and use $G'(\gamma) = g_1(\alpha)g_3(\beta)$ in place of $g_2(\beta)$ in step (5).

We have examined in detail the desired properties of $G(\gamma)$ when solving a fixed point problem with Newton-Raphson (see section 3). We focus on the necessary property that $G'(\gamma) \neq 1$. The following theorem makes sure a reasonable $G(\gamma)$ satisfies this near γ^* .

Theorem 4. Let u(x) solve the second order ODE

$$\begin{cases} F(u, u', u'') = 0 & x \in [a, b] \\ u(a) = A \\ u(b) = B. \end{cases}$$

Let $u_1(x)$, $u_2(x)$, $g_1(x)$, $g_2(x)$ be defined as in equation (7) with $\gamma_n = \gamma$. Let $G(\gamma) = u_2(\beta)$. Let J(x, y, z) be defined as in equation (6).

If $G(\gamma) \in C^1(\mathbb{R})$ and J(u, u', u'') is nonsingular on both [a, b] and $[\alpha, \beta]$, in the sense that the solution v(x) to the ODE

$$\begin{cases} J(u, u', u'') \cdot (v, v', v'') = 0 & x \in \Omega \\ v(x) = 0 & x \in \partial \Omega \end{cases}$$

is unique (and equal to the zero function), then $G'(\gamma) \neq 1$ in an interval around $u(\beta)$. As a corollary, the function $G(\gamma) - \gamma$ is monotonic in this interval.

Proof. It suffices to show $G'(u(\beta)) \neq 1$. As has been shown earlier, $G'(\gamma) = g_2(\beta)$. Consider the difference between $g_1(x)$ and $g_2(x)$ in the region of overlap, $g(x) = g_2(x) - g_1(x)$. This function satisfies:

$$\begin{cases} J(u_2, u'_2, u''_2) \cdot (g, g', g'') = (J(u_2, u'_2, u''_2) - J(u_1, u'_1, u''_1)) \cdot (g_1, g'_1, g''_1) & x \in [\alpha, \beta] \\ g(\alpha) = 0 \\ g(\beta) = G'(\gamma) - 1. \end{cases}$$

For $\gamma = u(\beta)$, $u_1 = u_2 = u$ in the region of overlap and the right hand side is zero. If $G'(u(\beta)) = 1$ then g(x) = 0 by the assumption that J(u, u', u'') is nonsingular on $[\alpha, \beta]$. Define the function $\hat{g}(x)$:

$$\hat{g}(x) = \begin{cases} g_1(x) & x \in [a, \alpha] \\ g_2(x) & x \in (\alpha, b]. \end{cases}$$

This function satisfies:

$$\begin{cases} J(u, u', u'') \cdot (\hat{g}, \hat{g}', \hat{g}'') = 0\\ \hat{g}(a) = \hat{g}(b) = 0. \end{cases}$$

By the assumption that J(u, u', u'') is nonsingular on [a, b] it must be that $\hat{g}(x) = 0$. This contradicts $G'(u(\beta)) = 1$. Therefore, $G'(u(\beta)) \neq 1$. Since $G(\gamma) \in C^1(\mathbb{R})$ there is a neighbourhood of $u(\beta)$ for which $G'(\gamma) \neq 1$.

If we consider instead $u_1 \neq u_2$ in the overlap region then the problem presented in the above theorem has a nonzero right hand side. Because of this it is no longer necessary that g(x) = 0. However, if u_1 and u_2 continue to converge to the same limit then the right hand side converges to zero. The function g(x)then has a magnitude related to the difference between u_1 and u_2 .

One can use similar strategies to prove that $G(\gamma)$ is monotonic under certain conditions. For α in some neighbourhood of β this implies $G'(\gamma) > 0$, as an increasing boundary condition should cause the solution nearby to likewise increase. The theorem presents this exclusively for Dirichlet transmission conditions, but the theorem applies more broadly.

Theorem 5. If the problem

$$\begin{cases} F(u, u', u'') = 0 & x \in \Omega\\ u(x) = h(x) & x \in \partial \Omega \end{cases}$$

is nonsingular on $[a, \alpha]$ and $[\beta, b]$, in the sense that there exists a unique solution to the problem on those domains and that the continuations of these solutions are also unique, then the function $G(\gamma)$ is strictly monotonic.

Proof. It suffices to show that $G(\gamma_1) = G(\gamma_2)$ implies $\gamma_1 = \gamma_2$.

Let u_1^j solve the problem on $[a, \beta]$ with $u_1^j(\beta) = \gamma_j$. Likewise, u_2^j solves the problem on $[\alpha, b]$ with $u_2^j(\alpha) = u_1^j(\alpha)$. Suppose $u_2^1(\beta) = u_2^2(\beta)$. Then both u_2^1 and u_2^2 solve the same problem on $[\beta, b]$. By assumption, this must mean $u_2^1 = u_2^2$ and $u_1^1(\alpha) = u_1^2(\alpha)$. By a similar argument, this implies u_1^1 and u_1^2 solve the same problem on $[a, \alpha]$. Again by assumption $u_1^1 = u_1^2$ and $\gamma_1 = \gamma_2$.

While we are now confident that many of the problems we encounter will have $G'(\gamma) \neq 0$ we are more interested in if $G(\gamma) - \gamma$ is monotonic. To that end, we present the following lemma, which acts as a converse to the mean value theorem for certain functions, and a corollary to this lemma giving sufficient conditions for $G'(\gamma) \neq 1$.

Lemma 1. If $f \in C^2([a,b])$, $f''(x) \neq 0$ for all $x \in (a,b)$ and f'(c) = 0 for some $c \in (a,b)$ then there exists $x_0 \in (a,b)$ such that $f(x_0)$ is equal to either f(a) or f(b). Moreover, there is only one local extrema on this interval.

Proof. We begin by showing that if $f'(c_1) = f'(c_2) = 0$ then $c_1 = c_2$. Consider the region $[c_1, c_2]$. By the mean value theorem there must exist a point $c_3 \in (c_1, c_2)$ such that $f''(c_3) = 0$. This contradicts the assumption that $f''(x) \neq 0$ for all $x \in (a, b)$, unless (c_1, c_2) is the empty set. Therefore, $c_1 = c_2$.

Suppose the statement is not true, that is for all $x_0 \in (a, b)$ $f(x_0) \neq f(a)$ and $f(x_0) \neq f(b)$. Then it must be that either $f(a) < f(x_0) < f(b)$ for all $x_0 \in (a, b)$ or $f(a) > f(x_0) > f(b)$. Then f(x) is monotonic on $[a, c_1]$ and $[c_2, b]$ where $f'(c_1) = f'(c_2) = 0$. We have already shown that $c_1 = c_2 = c$. Thus f(x) is monotonic on [a, b], and $f'(x) \ge 0$ or $f'(x) \le 0$. WLOG we consider the former.

Let $S_1 = [a, c)$ and $S_2 = (c, b]$, and let $s_1 = \max_{x \in S_1} f'(x) > 0$ and $s_2 = \max_{x \in S_2} f'(x) > 0$. WLOG, $s_1 > s_2$. Since f'(x) is continuous, there exists $x_1 \in S_1$ such that $f'(x_1) = s_2 = f'(x_2)$ for some $x_2 \in S_2$. Therefore, again by the mean value theorem, $f''(x_3) = 0$ for some $x_3 \in (x_1, x_2)$. This contradicts the assumption that $f''(x) \neq 0$ on the interval. Thus, it must be that the statement is true.

Corollary 1. If $G(\gamma) \in C^2(\mathbb{R})$ and $G''(\gamma^*) = 0$ implies $G(\gamma^*) = \gamma^*$ then either $G'(\gamma) \neq 1$ for all γ or the problem is singular.

Proof. Consider $f(\gamma) = G(\gamma) - \gamma$ and the domains $(-\infty, \gamma^*]$ and $[\gamma^*, \infty)$. Apply the previous lemma to $f(\gamma)$, noting that $f(\gamma^*) = 0$ and $\lim_{\pm \gamma \to \infty} f(\gamma) = \pm \infty$. Therefore, if $f'(\gamma_1) = 0$ for some $\gamma_1 \neq \gamma^*$ then $f(\gamma_2) = 0$ for some $\gamma_2 \neq \gamma^*$. This implies $G(\gamma)$ has two fixed points, and therefore the problem has two solutions.

We examine the problem

$$\begin{cases} u_{xx} = 0 & x \in [a, b] \\ u(a) = u(b) = 0 \end{cases}$$

with exact solution u = 0 and Robin transmission conditions:

$$u_1'^n(\beta) + C_1 u_1^n(\beta) = \gamma, \quad u_2'^n(\alpha) + C_2 u_2^n(\alpha) = u_1'^n(\alpha) + C_2 u_1^n(\alpha).$$

The solutions at each step are linear functions, and so the fixed point function $G(\gamma)$ is straightforward to find:

$$G(\gamma) = \gamma \frac{1 - C_1(b - \beta)}{1 + C_1(\beta - a)} \frac{1 + C_2(\alpha - a)}{1 - C_2(b - \alpha)}$$

Since $G(\gamma)$ is linear, the Newton-Raphson iteration converges in a single iteration. More interestingly, the slope $G'(\gamma)$ may take on any real value depending on the choices of C_1 and C_2 . Fixing α and β and considering $G'(\gamma)$ as a function on \mathbb{R}^2 , we have that $G' : \mathbb{R}^2 \to \mathbb{R}$.

Such a function is not continuous: there are singularities along the lines $C_1 = \frac{-1}{\beta - a}$ and $C_2 = \frac{1}{b - \alpha}$. There are also roots along the lines $C_1 = \frac{1}{b - \beta}$ and $C_2 = \frac{-1}{\alpha - a}$. These lines also divide the boundaries between which of the four regions the fixed point iteration lies within. While near the singularities, $G(\gamma)$ is in either region 1 or 4; while away, regions 2 or 3. When one of the two constants is between these lines while the other is not, $G(\gamma)$ is in either region 3 or 4; if both or neither are between the lines then $G(\gamma)$ is in region 1 or 2.

While this only applies to this particular problem, it shows that the fixed point iteration $G(\gamma)$ may appear in any of the four regions with any slope.



Figure 2: $G'(\gamma)$ as a function of C_1 and C_2 for a = -b = -1 and $\alpha = -\beta = -0.2$. The regions yellow, green, blue and white correspond to the regions 1, 2, 3 and 4, respectively.

Consider a second example for which we may write out explicitly $G'(\gamma^*)$:

$$\begin{cases} u_{xx} - C\sin(u) = 0 & x \in [-1, 1] \\ u(-1) = u(1) = 0 \end{cases}$$

with $\alpha = -\beta = -0.2$ and C > 0. The solution to the problem is u = 0. Using the same Robin transmission conditions as earlier, we have the following equation for $G'(\gamma^*)$:

$$G'(\gamma^*) = \frac{\sqrt{C}\cosh(0.8\sqrt{C}) + C_2\sinh(0.8\sqrt{C})}{\sqrt{C}\cosh(1.2\sqrt{C}) + C_1\sinh(1.2\sqrt{C})} \frac{\sqrt{C}\cosh((-0.8)\sqrt{C}) + C_1\sinh((-0.8)\sqrt{C})}{\sqrt{C}\cosh((-1.2)\sqrt{C}) + C_2\sinh((-1.2)\sqrt{C})}$$

The regions that $G(\gamma)$ lies in are determined by the value of $G'(\gamma^*)$ and certain conditions. For example, if the problem is nonsingular then $G(\gamma)$ cannot cross between regions 1 and 2. If $G(\gamma)$ is known to be monotonic then it cannot cross between regions 2 and 3. The example problem presented here is known to be nonsingular and the corresponding $G(\gamma)$ is monotonic for all C_1 and C_2 (nb: prove?), and so $G'(\gamma^*)$ informs us whether the fixed point iteration lies within regions 1, 2 or the combination of 3 and 4 for every choice of γ .

For C = 1 and $p = C_1 = -C_2 = -2$ we have that $G(\gamma)$ is in region 1. As such, the fixed point iteration diverges away from the root. The Newton-Raphson iteration, on the other hand, will converge. This may be seen in figure 5. The choice p > 0 is apparently natural and for most problems examined will place $G(\gamma)$ in region 2.

For C < 0 the problem in u is possibly singular, especially with Robin boundary conditions and certain subintervals.



Figure 3: $G'(\gamma^*)$ as a function of C_1 and C_2 for the second example problem with C = 1. The regions yellow, green, blue and white correspond to the regions 1, 2, 3 and 4, respectively.



Figure 4: $G'(\gamma^*)$ as a function of $p = C_1 = -C_2$ and C. The region blue corresponds to region 2 and the region yellow to region 3.



Figure 5: The fixed point function $G(\gamma)$ and the corresponding Newton-Raphson iteration for the second example problem with C = 1 and $p = C_1 = -C_2 = -2$.

Under certain conditions one may be able to show that $G(\gamma)$ is restricted to specific regions. As an example, we reprove a result from Lui [2].

Theorem 6 (Theorem 2 from [2]). Consider the equation

$$\begin{cases} u''(x) + f(x, u, u') = 0 & x \in [a, b] \\ u(a) = u(b) = 0 \end{cases}$$

under the assumptions that

- $f \in C^1([a,b] \times \mathbb{R} \times \mathbb{R})$,
- $\frac{\partial f(x,v,v')}{\partial u} \leq 0$ for all $x \in [a,b]$ and $v \in H^1_0([a,b])$,
- $|f(x,v,v')| \leq C(1+|v'|^{\eta})$ for all $x \in [a,b]$ and $v \in H_0^1([a,b])$ and some $C > 0, \ 0 < \eta < 1$.

The problem is solved using alternating Schwarz with two subdomains and Dirichlet transmission conditions. Then $G(\gamma)$ for this problem lies within region 2.

Proof. It suffices to prove that the problem is nonsingular and $0 < G'(\gamma) < 1$ for all $\gamma \in \mathbb{R}$. The nonsingularity of the problem is guaranteed by proposition 2 from [2]. As Lui points out, this also means the problem is nonsingular on any subdomain. Using theorem 5 this gives monotonicity of $G(\gamma)$. Moreover, if

u(x) = 0 for any $x \in (a, b)$ then the problem would be singular on the domains [a, x] and [x, b]. As such, u(x) has the same sign as γ and $G'(\gamma) > 0$.

Consider the problem in g_1 :

$$\begin{cases} g_1''(x) + \frac{\partial f}{\partial u}g_1 + \frac{\partial f}{\partial u'}g_1' = 0 & x \in [a, \beta] \\ g_1(a) = 0 \\ g_1(\beta) = 1. \end{cases}$$

From the second assumption on f the operator on g_1 satisfies a maximum principle (see, for example, [2]). Therefore, $g_1(x) < 1$ for all $x \in (a, \beta)$. By the same reasoning, $g_2(x) < g_1(\alpha) < 1$ for all $x \in (\alpha, b)$ and $G'(\gamma) < 1$. Incidentally, the same maximum principle applies for the operator on $-g_1$ and $-g_2$, and so $G'(\gamma) > 0$ as we had before.

Recall from section 3 the function C(x). In the context of domain decomposition, this function becomes:

$$C(\gamma) = \frac{G(\gamma) - \gamma}{\sqrt{|\gamma - \gamma^*|}}.$$

While it is ideal that this function is strictly monotonic, this cannot be guaranteed.

4.1 Higher dimensions

Now consider a more general alternating Schwarz, again for a second order nonlinear differential equation but on a domain $\Omega \in \mathbb{R}^d$:

$$\begin{cases} F(x, u_1^n, Du_1^n, D^2u_1^n) = 0 & x \in \Omega_1 \\ u_1^n(x) = h(x) & x \in \partial\Omega \\ u_1^n(x) = u_2^{n-1}(x) & x \in \Gamma_1 \end{cases} \begin{cases} F(x, u_2^n, Du_2^n, D^2u_2^n) = 0 & x \in \Omega_2 \\ u_2^n(x) = h(x) & x \in \partial\Omega \\ u_2^n(x) = u_1^n(x) & x \in \Gamma_2, \end{cases}$$

where $\Gamma_1 = \partial \Omega_1 \setminus \partial \Omega$ and $\Gamma_2 = \partial \Omega_2 \setminus \partial \Omega$. Note that Du (and D^2u) represents the collection of the partial derivatives (and second partial derivatives, including mixed derivatives) of the function u(x).

As in the 1D case, one can construct the implicit function $G: L_2(\Gamma_1) \to L_2(\Gamma_1)$ using the following two steps:

$$(1) \begin{cases} F(x, u_1, Du_1, D^2u_1) = 0 \\ u_1(\partial\Omega) = h \\ u_1(\Gamma_1) = \gamma \end{cases} (2) \begin{cases} F(x, u_2, Du_2, D^2u_2) = 0 \\ u_2(\partial\Omega) = h \\ u_2(\Gamma_2) = u_1(\Gamma_2) \end{cases}$$

so that $G(\gamma) = u_2(\Gamma_1)$.

We are now interested in modifying the third and fourth steps of the algorithm presented for 1D so that they may be applied to higher dimensions. Let us focus on the discrete case, where $\gamma \in \mathbb{R}^N$ for some N. Then $G(\gamma)$ is a vector field and $G'(\gamma) \in \mathbb{R}^{N \times N}$ for each γ . As well, the derivative of u_1 with respect to γ is now a Jacobian. Let $g_1: \Omega_1 \to \mathbb{R}^N$ represent $\frac{\partial u_1}{\partial \gamma}$. Then the third step may be written as:

(3)
$$\begin{cases} J(u_1) \cdot g_1 = 0\\ g_1(\partial \Omega) = 0\\ g_1(\Gamma_1) = I \end{cases}$$

where the last line signifies that the *i*-th entry of $g_1(x_j)$ is equal to $\delta_{i,j}$ (the Kronecker delta) for all $x_i \in \Gamma_1$.

Using the same representation for the other domain, one may write the fourth step as:

(4)
$$\begin{cases} J(u_2) \cdot g_2 = 0\\ g_2(\partial \Omega) = 0\\ g_2(\Gamma_2) = I \end{cases}$$

so that $G'(\gamma) = g_1(\Gamma_2)g_2(\Gamma_1) = g_2(\Gamma_1)g_1(\Gamma_2).$

The fifth step is then standard high dimension Newton-Raphson:

(5)
$$\gamma_{n+1} = \gamma_n - (G'(\gamma_n) - I)^{-1} (G(\gamma_n) - \gamma_n)$$

= $\gamma_n - (g_1(\Gamma_2)g_2(\Gamma_1) - I)^{-1} (u_2(\Gamma_1) - \gamma_n).$

Theorem 5 can be generalized to higher dimensions.

Theorem 7. If the problem

$$\begin{cases} F(u, Du, D^2u) = 0 & x \in \Omega\\ u(x) = h(x) & x \in \partial \Omega \end{cases}$$

is nonsingular on $\Omega \setminus \Omega_1$ and $\Omega \setminus \Omega_2$ in the sense that there exists a unique solution to the problem on those domains and the continuations of these solutions are also unique, then $G(\gamma)$ is injective.

Proof. The proof is identical to that for theorem 5 with all objects replaced by their higher dimension counterparts.

If $G(\gamma)$ is also continuous (we require differentiable to use Newton's method) and it can be proven that alternating Schwarz converges unconditionally to a unique solution (ex. theorem 2 from [2]) then any starting point defines a path leading to the fixed point. These paths do not intersect and $G(\gamma)$ is monotonic along each path, in the sense that if the path were parametrized by a variable s then $\gamma(s_2) = G(\gamma(s_1))$ implies $s_2 > s_1$.



Figure 6: The function $G(\gamma)$. On the left, the corresponding Newton-Raphson iteration is plotted along with the lines $y = \gamma$ and $y = 2\gamma^* - \gamma$. On the right, the lines $g_C(\gamma)$ show the function $C(\gamma)$ is not monotonic for this problem.

5 Period doubling in RASPEN (or RASPENlike methods)

Take as a counterexample the following differential equation:

$$u''(x) - \sin(3.6u(x)) = 0.$$

With homogeneous Dirichlet boundary conditions the solution to this problem is the zero function. Using Dirichlet transmission conditions one arrives at the function $G(\gamma)$ depicted in figure 6.

As seen in the figure, where $G(\gamma)$ is not monotonic with respect to the geometry of the lines $g_C(\gamma)$ (equivalent to $C(\gamma)$ no longer monotonic) the Newton-Raphson iteration enters into region 4. Due to the symmetry of the function $G(\gamma)$, this creates at least two 2-cycles where $G(\gamma)$ meets the line $y = 2\gamma^* - \gamma$. One of these 2-cycles is stable, and taking $\gamma_0 = 1.6$ (or somewhere nearby) the Newton-Raphson preconditioning will cause the iterations to converge to this cycle.

Indeed, the differential equation

$$u''(x) - \sin(au(x)) = 0$$
(8)

admits a period doubling set of cycles in the parameter *a* for the domain [-1, 1], $\alpha = -\beta = -0.2$ and $\gamma_0 = \pm 1.6$. The bifurcation diagram is shown in figure 7. The red points displayed result from choosing $\gamma_0 = -1.6$, while the black points from choosing $\gamma_0 = 1.6$. The first bifurcation is the separation of the 2-cycle



Figure 7: The bifurcation diagram for the sinusoid counterexample in the parameter *a*. The first bifurcation point is the separation of the 2-cycle into two separate 2-cycles, rather than one 4-cycle. After this, the bifurcation proceeds normally.

into two separate 2-cycles instead of the usual 4-cycle. Once this is done, period doubling sets in for each of these 2-cycles until the onset of chaos.

The chaos of this system collapses once it spreads out sufficiently to include the region where Newton-Raphson is convergent. That is, when the slope moves close enough to 1 the range of the cycles is so wide that it intersects with areas near enough to the fixed point such that Newton-Raphson converges quadratically. This collapse occurs between a = 3.812 and a = 3.813, after which these values of γ_0 (and possibly all values) lead to quadratically convergent sequences.

5.1 Wellposedness

Lemma 2 (Wellposedness). Equation 8 with homogeneous boundary conditions on the domain [-1, 1] is well-posed for $u \in C^2[-1, 1]$ and real-valued.

Proof. Firstly we prove that any solution u(x) to the equation lies between 1 and -1. First note that $|u''(x)| \leq 1$ since $u''(x) = \sin(au(x))$. Suppose there is a point \hat{x} such that $u(\hat{x}) = 1$. Then by the mean value theorem there exist $c_1 \in [-1, \hat{x})$ and $c_2 \in (\hat{x}, 1]$ such that $u'(c_1) = 1/(\hat{x}+1)$ and $u'(c_2) = -1/(1-\hat{x})$. By the same theorem there exists $c_3 \in (c_1, c_2)$ such that $u''(c_3) = (u'(c_2) - 1)$ $u'(c_1))/(c_2-c_1)$. That is

$$u''(c_3) = \frac{-\frac{1}{1-\hat{x}} - \frac{1}{\hat{x}+1}}{c_2 - c_1} = \frac{-\frac{\hat{x}-1+\hat{x}-1}{(1+\hat{x})(1-\hat{x})}}{c_2 - c_1} = \frac{-\frac{2}{1-\hat{x}^2}}{c_2 - c_1}$$
$$\leq \frac{-\frac{2}{1-\hat{x}^2}}{2} = \frac{-1}{1-\hat{x}^2} \leq -1$$

which contradicts $|u''(x)| \leq 1$ and so u(x) < 1. Similarly, u(x) > -1.

Secondly we prove that u(x) = 0 is the only solution lying between 1 and -1. Since the value of u(x) is less than one in magnitude for all values of $x \in [-1, 1]$ we may write

$$u(x) = \epsilon u_1(x) + \epsilon^2 u_2(x) + \epsilon^3 u_3(x) + \dots$$

for some $0 < \epsilon < 1$ such that $-1 \le u_i(x) \le 1$ for all $x \in [-1, 1]$. Then one may expand $\sin(au(x))$ into a Taylor series:

$$\sin(au(x)) = au(x) - a^3 u^3(x)/6 + \dots$$

= $\epsilon au_1(x) + \epsilon^2 au_2(x) + \epsilon^3 au_3(x) - \epsilon^3 a^3 u_1^3(x)/6 + \dots$

The equation in $\mathcal{O}(\epsilon)$ is:

$$u_1''(x) - au_1(x) = 0$$

which, combined with the homogeneous boundary conditions, has the unique solution $u_1(x) = 0$. The same is true of $u_2(x)$ in solving the equation in $\mathcal{O}(\epsilon^2)$. For $\mathcal{O}(\epsilon^3)$, given that $u_1(x) = 0$ we have the same equation for $u_3(x)$, so that $u_3(x) = 0$ as well. One may continue this for all orders of ϵ . Therefore, u(x) = 0.

5.2 Changing overlap

The overlap affects the position and length of the interval in a where the bifurcation occurs. For $\alpha = -\beta = -0.1$, the interval is roughly [2.25, 2.4] with $\gamma_0 = \pm 2$. For $\alpha = -\beta = -0.4$, the interval is roughly [9.10, 9.155] with $\gamma_0 = \pm 1.45$.

The bifurcation becomes smaller the larger the overlap, as may be seen when comparing figures 8 and 9. Note that we may not have chosen γ_0 such that we land within a cycle for all values of a, α and β . As such, the exact length of each bifurcation diagram here is only an estimate, though the distance between each bifurcation should be indicative of their sizes.

For example, for $\alpha = -\beta = -0.1$ we estimate the distance between the 4cycle and the 8-cycle as approximately 0.03. For $\alpha = -\beta = -0.2$ this value is roughly 0.07 and for $\alpha = -\beta = -0.4$ it is roughly 0.018. The dependence of these distances on the size of the overlap is then nonlinear.

5.3 Robin transmission conditions

We may change to Robin transmission conditions and find the same period doubling bifurcation pattern, albeit on a smaller scale. Replace the Dirichlet



Figure 8: Bifurcation diagram with $\alpha = -\beta = -0.1$ and $\gamma_0 = \pm 2$.



Figure 9: Bifurcation diagram with $\alpha = -\beta = -0.4$ and $\gamma_0 = \pm 1.45$.



Figure 10: Bifurcation diagram using Robin transmission conditions with p = 1, $\alpha = -\beta = -0.2$ and $\gamma_0 = \pm 3.1$.

transmission conditions $(u_1(\beta) = \gamma_n, u_2(\alpha) = u_1(\alpha))$ with the optimal Robin transmission conditions $(u'_1(\beta) + pu_1(\beta) = \gamma_n, u'_2(\alpha) - pu_2(\alpha) = u'_1(\alpha) - pu'_1(\alpha))$. The bifurcation for p = 1 and $\alpha = -\beta = -0.2$ may be seen in figure 10. The initial guesses are $\gamma_0 = \pm 3.1$.

5.4 2D version

We set up the following problem in 2D:

$$\Delta u - \sin(au) = 0$$

on the square $[-1,1] \times [-1,1]$ with homogeneous Dirichlet boundary conditions on all sides. The function $G(\gamma)$ is now a function acting on the space of functions over [-1,1] and returns an element of the same. In the discrete version, $G(\gamma)$ takes a vector and returns a vector of the same size. Its derivative is therefore a Jacobian. We are now concerned with where $||G(\gamma) - \gamma^*|| \leq ||\gamma - \gamma^*||$.

Using a = 3.6, which gave 2-cycles in the 1D case, and γ_0 equal to a constant function we arrive at figure 11. The norm of both $G(\gamma)$ and $N(\gamma)$ do not approach the lines representing divergence of the method, meaning there are no cycles to be found for this value of a or these choices of the γ_0 function.

We note that there are two ways one may retrieve the 1D period doubling from this example. Firstly, one can dampen diffusivity in the y-direction:

$$u_{xx} + \epsilon u_{yy} - \sin(au) = 0$$

Secondly, one may exchange the homogeneous Dirichlet boundary conditions in



Figure 11

the *y*-direction for homogeneous or small-valued Neumann boundary conditions:

$$u_u(x,\pm 1) = \mu$$

For either $\epsilon = 0$ or $\mu = 0$ one retrieves exactly the period doubling of the 1D case. However, small values of ϵ and μ will also have period doubling. Figures 12 and 13 show results for nonzero ϵ and μ that produce period doubling.

It may be useful to prove that the undamped problem does not have any period doubling. That is, one needs to show that either the convergence region is all of the space or if there is a part that does not converge then it maps into a part that does converge.

The 1D eigenvalue problem that results from a Fourier transform in the y-direction, ie.

$$u_{xx} - \eta u - \sin(au) = 0$$

ι

with homogeneous Dirichlet BCs, changes the behaviour of the period doubling. Keeping *a* fixed, one finds that the maximum of the NR iteration (in absolute value) is proportional to η . That is, the larger η , the larger the jump of the iteration over the line $2\gamma^* - \gamma$. For η negative, this jump does not occur.

For sufficiently large η , the jump creates a singularity, i.e. $G'(\gamma) = 1$ for some γ , and the iteration enters into region 1. This usually means guaranteed convergence for the method, as it shoots out the iteration to a point where convergence is guaranteed. That is, the cycle is not stable/attractive.

Which values of η provide which behaviour depends on a. A larger a means stable cycles occur for smaller (more negative, not less magnitude) η . Ultimately this suggests that all values of a have stable cycles for some waves but very few.

Reducing the number of points in the y-direction to 4 (with two of these points on the boundary) allows us to visualize the vector field $G(\gamma)$. Figure 15



Figure 12: $\epsilon = 1e - 5$; the behaviour of the period doubling appears to have changed, though still appears between a = 3.5 and 3.8.



Figure 13: $\mu = 0.1$; no major changes in the period doubling are observed. Note that the exact solution is no longer zero and so $\|\gamma\|$ converges to a nonzero value outside of the period doubling region.



Figure 14: White represents area where divergence is occurring, with parameters: $\alpha = -\beta = -0.2$, 21 points in each direction, a = 5.



Figure 15: Contour plot of $||G(\gamma) - \gamma^*|| / ||\gamma - \gamma^*||$ overlaid with the vector field $G(\gamma)$. The vector field points towards the origin everywhere, though nonuniformly. A series of peaks extend along two symmetric (reflection over the line $\gamma_2 = -\gamma_1$) ridges. Two additional peaks may be seen in the upper right and lower left corners of the figure, aligned with the line $\gamma_2 = \gamma_1$. $\alpha = -\beta = -0.2$, a = 7.703, homogeneous Dirichlet boundary conditions, unperturbed Laplacian.

shows this vector field plotted on a contour plot of the ratio between $|G(\gamma) - \gamma^*|$ and $|\gamma - \gamma^*|$. Two peaks (values greater than or equal to 1) along the line $\gamma_1 = \gamma_2$ suggest the possibility of a cycle.

Indeed, figure 16 shows a period doubling example in this setup. Note the incredibly small region in both $\|\gamma\|$ and *a* that this period doubling resides. The basin of attraction of these cycles is also small, as indicated by the width of the chaos.

6 Proposed algorithm

We have seen in sections 4 and 5 that we cannot guarantee the monotonicity of $C(\gamma)$, nor the region of $G(\gamma)$ with general transmission conditions. However, we have also shown that under certain assumptions we can ensure $G(\gamma)$ lies within region 2. With this in mind, one may construct an algorithm to take advantage of the many properties discussed. This incorporates Branin's corrections to the Newton-Raphson method as well as checks on various conditions on G and G'.



Figure 16: $\alpha = -\beta = -0.2$, $\gamma_0 = -16.6382 * [1, 1]$, homogeneous Dirichlet boundary conditions, unperturbed Laplacian.

6.1 Notation and assumptions

Steps (1) through (3) from equation (7) remain unchanged. We will replace step (4) with (4^*) , and step (5) by

(5*)
$$\tilde{\gamma}_n = \gamma_n - \frac{u_2(\beta) - \gamma_n}{|g_1(\alpha)g_3(\beta) - 1|}$$

All affiliated functions and variables, including F, J and $G(\gamma)$, are as described in section 4.

Regions 1 through 4 are defined in section 1. The function $C(\gamma)$ is defined in section 4 but explained in greater detail in sections 2 and 3. The corresponding lines $g_C(\gamma)$ may be found in section 3.

It is assumed that $G(\gamma)$ lies within region 2. See theorem 6 for an example of conditions that will guarantee this.

6.2 Algorithm steps

- **1.** Select some $\gamma_0 \in \mathbb{R}$. Set n = 0.
- **2.** Calculate $G(\gamma_n)$ using steps (1) and (2) from equation (7) and $G'(\gamma_n)$ using steps (3) and (4*). If $G'(\gamma_n) = 1$ then set $\gamma_{n+1} = G(\gamma_n)$, increment n and return to step 2. If this is not true, proceed to step 3.
- **3.** Perform step (5*). If $|G'(\gamma_n) 1| \ge 1/2$ then set $\gamma_{n+1} = \tilde{\gamma}_n$, increment n and return to step 2. If this is not true, calculate $\hat{\gamma}_n$, the average of γ_n and $\tilde{\gamma}_n$, and proceed to step 4.

4. Use steps (1) and (2) to calculate $G(\hat{\gamma}_n)$. If $G(\hat{\gamma}_n) - \hat{\gamma}_n$ has the same sign as $G(\gamma_n) - \gamma_n$ then set $\gamma_{n+1} = \tilde{\gamma}_n$, increment *n* and return to step 2. If this is not true, set $\gamma_{n+1} = G(\gamma_n)$, increment *n* and return to step 2.

6.3 Explanation of the algorithm

In step 2 of the algorithm, we use fixed point iteration if $G'(\gamma_n) = 1$. The Newton-Raphson iteration, even with Branin's adjustment, will calculate an infinite result if we proceed to step 3. Since $G(\gamma)$ lies within region 2 we are certain that a fixed point step will always converge, however slowly. Therefore, one may avoid the problem by using the slower method.

In steps 3 and 4, we use the calculated Newton-Raphson iteration only if we guarantee such an iteration lies within regions 2 and 3. As has been shown in section 3, if $G'(\gamma) < 1/2$ then the iteration is certainly within regions 2 and 3. By using Branin's adjustment, we also have this fact for $G'(\gamma) > 3/2$.

Step 4 checks if the Newton-Raphson iteration lies within region 4. Since we know the geometry along which the boundary of regions 3 and 4 is defined, we can calculate the following scenario: we suppose that the point $(\gamma_n, G(\gamma_n))$ lies on this boundary. The line $g_C(\gamma)$ at this point intersects the line y = x at the point $\hat{\gamma}_n$. If the fixed point lies between γ_n and $\hat{\gamma}_n$ then the point lies within region 4.

To check which side of $\hat{\gamma}_n$ the fixed point lies, we need to test $G(\hat{\gamma}_n)$. If $G(\hat{\gamma}_n) - \hat{\gamma}_n$ has the same sign as $G(\gamma_n) - \gamma_n$ then both $\hat{\gamma}_n$ and γ_n lie on the same side of the fixed point, and the iteration lies in regions 2 and 3. If not, they lie on different sides of the fixed point and so the fixed point must lie between them. In this instance, the iteration lies in region 4 and to avoid spiralling away from the fixed point one should use the fixed point iteration which, as has already been stated, is guaranteed to converge.

In this way, all possibilities are accounted for: region 1 cannot occur due to Branin's adjustment and the avoidance of $G'(\gamma_n) = 1$; region 4 is tested for extensively and whenever it occurs the algorithm uses a method that is guaranteed to converge under the assumptions listed previously.

6.4 The algorithm in higher dimensions

The algorithm may be adapted to higher dimensions with minor revisions. Firstly, step (5^*) must be replaced by the standard high dimension Newton-Raphson step (5) as seen in section 4. The Davidenko-Branin correction cannot be used here as we are not certain as to which direction is appropriate.

Most importantly, it must be noted that the sign of $G(\gamma) - \gamma$ no longer has meaning in a higher dimension. Instead, the sign of $\langle \tilde{\gamma} - \gamma, G(\gamma) - \gamma \rangle$ may be used in its place. This tests whether there is local monotonicity in $G(\gamma)$ moving between each Newton iteration. This gives a rough indication if we are heading in the right direction. However, as this depends heavily on the local behaviour of $G(\gamma)$ it is fallible. Both false negatives and false positives are possible. As there will always be a region around the root where Newton-Raphson is convergent, this algorithm need only be used until such a region has been reached. Indeed, given a problem for which it has been shown that alternating Schwarz is everywhere convergent, the unaccelerated method may be used until one is reasonably confident that one is close enough to the root for Newton-Raphson to be convergent, much like the bisection method is used on onedimensional problems.

- **1.** Select some $\gamma_0 \in \mathbb{R}^N$. Set n = 0.
- 2. Calculate $G(\gamma_n)$ using steps (1) and (2) from equation (nb:cite) and $G'(\gamma_n)$ using steps (3) and (4). Finally, calculate $\tilde{\gamma}$ using step (5).
- **3.** Calculate $G(\tilde{\gamma})$ using steps (1) and (2) (this result may be re-used for the next iteration of step 2 of this algorithm). If $\operatorname{sign}\langle \tilde{\gamma} \gamma_n, G(\gamma_n) \gamma_n \rangle = \operatorname{sign}\langle \tilde{\gamma} \gamma_n, G(\tilde{\gamma}) \tilde{\gamma} \rangle$ then set $\gamma_{n+1} = \tilde{\gamma}$, increment *n* and return to step 2. If not, calculate $\hat{\gamma}$, the average of γ_n and $\tilde{\gamma}$, and proceed to step 4.
- 4. Use steps (1) and (2) to calculate $G(\hat{\gamma})$. If $\langle \tilde{\gamma} \gamma, G(\hat{\gamma}) \hat{\gamma} \rangle$ has the same sign as $\langle \tilde{\gamma} \gamma, G(\gamma_n) \gamma_n \rangle$ then set $\gamma_{n+1} = \tilde{\gamma}_n$, increment *n* and return to step 2. If this is not true, set $\gamma_{n+1} = G(\gamma_n)$, increment *n* and return to step 2.

References

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