

Nonlinear problems & constraints

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Newton-Raphson Method

Let's consider we have a problema of the type

$$f(x) = 0$$

Our goal is to find “x” such that such equation is verified.

Newton method is a technique to find the solution of such type of problems with optimal convergence rate.

Newton-Raphson method

The idea is that if f is smooth, we can assume that

$$0 = f(x) \approx f(x_i + dx) \approx f(x_i) + \frac{\partial f}{\partial x} dx + O(dx^2)$$

This means that given an initial guess x_i

We can find a correction dx as

$$-\frac{\partial f}{\partial x} dx = f(x_i)$$

A practical example

Let's imagine we want to find the solution of

$$x^2 = 2$$

Of course we know the solution ... $x = \sqrt{2}$,

however ... can we solve this by NR?

A practical example

First of all we need to cast the problema in residual form

$$f(x) = 2 - x^2$$

NR only finds zeros!!

$$\begin{aligned} LHS &= -\frac{\partial f}{\partial x} = 2x \\ RHS &= 2 - x^2 \end{aligned}$$

A practical example

Let's assume that our first guess is $x_0 = 1.0$

x	LHS	RHS	dx
1.0	2.0	1.0	0.5
1.5	3.0	-0.25	-0,0833333
1,41666	2,8333333	-0,006943	-0,00245
1,414

Does it always converge?

Let's try to compute the cubic root of 2:

$$f(x) = 2 - x^3$$

We start also from $x_0 = 1.0$

x	LHS	RHS	dx
1	3	1	0,33333333
1,33333333	4	-0,37037037	-0,09259259
1,24074074	3,72222222	0,08995707	0,02416757
1,26490831	3,79472493	-0,02384449	-0,00628359
1,25862472	3,77587417	0,00616702	0,00163327
1,26025799	3,78077398	-0,00160502	-0,00042452
1,25983347	3,77950041	0,00041704	0,00011034
1,25994381	3,77983144	-0,00010841	-2,868E-05
1,25991513	3,7797454	2,8177E-05	7,4546E-06

Does it always converge?

However if we start from $x_0 = 5.0$, which is farther away from the solution, we get

x	LHS	RHS	dx
5	15	-123	-8,2
-3,2	-9,6	34,768	-3,62166667
-6,82166667	-20,465	319,447187	-15,6094399
-22,4311065	-67,2933196	11288,3131	-167,747901
-190,179007	-570,537022	6878406,75	-12056,0218
-12246,2008	-36738,6023	1,8366E+12	-49989811,2
-50002057,4	-150006172	1,2502E+23	-8,334E+14
-8,334E+14	-2,5002E+15	5,7885E+44	-2,3152E+29
-2,3152E+29	-6,9456E+29	1,241E+88	-1,7867E+58

CONCLUSION

Newton Raphson:

- Converges very fast
 - Approximatimatively doubles accurate digits at each iteration
- May diverge equally fast if initial guess is not good enough
- It is not very robust...

Multidimensional case

Let's suppose we want to solve the following set of equations:

$$\begin{aligned}x^2 + y^2 &= 1 \\x - y &= 0\end{aligned}$$

This represents the intersection of a unit circle with a line. Solutions are $(1,1)$, $(-1,-1)$

Multidimensional case

To apply NR we must cast this in residual form.

$$R(x, y) := \begin{pmatrix} 1 - x^2 - y^2 \\ y - x \end{pmatrix}$$

We need now to compute the gradient of R:

$$LHS := \begin{pmatrix} -\partial R_0/\partial x & -\partial R_0/\partial y \\ -\partial R_1/\partial x & -\partial R_1/\partial y \end{pmatrix}$$

Multidimensional case

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$$LHS := \begin{pmatrix} -\frac{\partial R_0}{\partial x} & -\frac{\partial R_0}{\partial y} \\ -\frac{\partial R_1}{\partial x} & -\frac{\partial R_1}{\partial y} \end{pmatrix}$$

NR iteration

The NR iteration thus proceeds as follows:

1. Choose a starting guess (x_i, y_i)
2. Evaluate $RHS(x_i, y_i)$ & $LHS(x_i, y_i)$
3. Solve $LHS \begin{pmatrix} dx \\ dy \end{pmatrix} = RHS$
4. Update solution $\begin{pmatrix} x_{i+1} \\ y_{i+1} \end{pmatrix} = \begin{pmatrix} x_i + dx \\ y_i + dy \end{pmatrix}$
5. check converged & eventually go back to 1

Multidimensional case

For the specific case at hand, this gives

$$LHS := \begin{pmatrix} 2x & 2y \\ 1 & -1 \end{pmatrix}$$

x	y	lhs	inv	rhs	dx
1	0	2 0 1 -1	0,5 0 0,5 -1	0 -1	0 1
ITERATION 1					
1	1	2 2 1 -1	0,25 0,5 0,25 -0,5	-1 0	-0,25 -0,25
ITERATION 2					
0,75	0,75	1,5 1,5 1 -1	0,33333333 0,5 0,33333333 -0,5	-0,125 0	-0,04166667 -0,04166667
ITERATION 3					
0,70833333	0,70833333	1,41666667 1,41666667 1 -1	0,35294118 0,5 0,35294118 -0,5	-0,00347222 0	-0,00122549 -0,00122549
ITERATION 4					
0,70710784	0,70710784	1,41421569 1,41421569 1 -1	0,35355286 0,5 0,35355286 -0,5	-3,0037E-06 0	-1,0619E-06 -1,0619E-06
ITERATION 5					
0,70710678	0,70710678	1,41421356 1,41421356 1 -1	0,35355339 0,5 0,35355339 -0,5	-2,2553E-12 0	-7,9737E-13 -7,9737E-13
ITERATION 6					
0,70710678	0,70710678	1,41421356 1,41421356 1 -1	0,35355339 0,5 0,35355339 -0,5	0 0	0 0
ITERATION 7					

FEM problems

Let's now focus on the FEM. A typical, potentially nonlinear, FEM problem gives:

$$RHS(\mathbf{u}) = \mathbf{b} - \mathbf{K}(\mathbf{u})\mathbf{u}$$

If we apply NR technique

$$LHS(\mathbf{u}) := - \frac{\partial \mathbf{b} - \mathbf{K}(\mathbf{u})\mathbf{u}}{\partial \mathbf{u}} = - \frac{\partial \mathbf{K}(\mathbf{u})}{\partial \mathbf{u}} \mathbf{u} - \mathbf{K}(\mathbf{u})$$

Normally not done this way since $\frac{\partial \mathbf{K}(\mathbf{u})}{\partial \mathbf{u}}$ is a third order tensor

PICARD's method

It is common to simplify the previous to:

$$RHS(\mathbf{u}) = \mathbf{b} - \mathbf{K}(\mathbf{u})\mathbf{u}$$

$$LHS(\mathbf{u}) = -\frac{\partial \mathbf{K}(\mathbf{u})}{\partial \mathbf{u}}\mathbf{u} - \mathbf{K}(\mathbf{u})$$

Giving rise to a method called **PICARD's method**. Note that this is equivalent to doing:

$$\mathbf{K}(\mathbf{u}_{old})\mathbf{u} = \mathbf{b}$$

PICARD's method

- Conceptually simple
- No need to compute the exact Jacobian
- Convergence more robust than NR (often it converges starting from a worst initial approximation to the solution)

On the bad side:

- Slow convergence

APPLICATION OF CONSTRAINTS

Let's consider a simple linear problem

1D laplacian problem (a value of 5 would be applied on a node u_0)

$$\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 5 \\ 0 \\ 0 \end{pmatrix}$$

For whatever reason we want to impose that $u_3 = u_1 + 1$

HOW DO WE DO IT?

Application of constraint

Since the constraint is linear in the unknowns, we can express it as

$$(-1 \quad 0 \quad 1) \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = 1$$

Which is normally written in matrix form as

$$\mathbf{H}\mathbf{u} = \mathbf{e} \text{ (we'll assume } e = 1)$$

If we assume that the previous problem is expressed as $\mathbf{K}\mathbf{u} = \mathbf{b}$

Lagrange Multipliers

A “recipe” exists for imposing the constraint while respecting the linear problem of interest: it consists in writing the following problem

$$\begin{pmatrix} \mathbf{K} & \mathbf{H}^t \\ \mathbf{H} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{e} \end{pmatrix}$$

we'll assume $e = 1$ in doing the math

Doing the maths

K with constraints

2	-1	0	-1
-1	2	-1	0
0	-1	1	1
-1	0	1	0

inverse

1	1	1	0
1	1,5	1	0,5
1	1	1	1
0	0,5	1	-0,5

RHS

5
0
0
1

SOLUTION

5u1
5,5u2
6u3
-0,5lambda

Is there a systematic way to do it?

YES!!

Let's assume that:

- $f(\mathbf{u})$ is a *functional* describing our problem
- $g(\mathbf{u})$ is the the *functional* describing our constraint.

Both could be non-linear!

“Lagrangian”

We can define a functional of the type

$$\Psi(\mathbf{u}, \lambda) := f(\mathbf{u}) + \lambda g(\mathbf{u})$$

The imposition of the constraint on \mathbf{f} can be obtained by minimizing **the functional**

$$\Psi(\mathbf{u}, \lambda)$$

How?

Defining the problem

1 - DEFINE AN RHS

$$RHS(\mathbf{u}, \lambda) := \begin{pmatrix} \frac{\partial \Psi(\mathbf{u}, \lambda)}{\partial \mathbf{u}} \\ \frac{\partial \Psi(\mathbf{u}, \lambda)}{\partial \lambda} \end{pmatrix}$$

2 - MINIMIZE THE RHS (for example by NR)

$$LHS(\mathbf{u}, \lambda) := -\frac{\partial RHS(\mathbf{u}, \lambda)}{\partial (\mathbf{u}, \lambda)} = - \begin{pmatrix} \frac{\partial^2 \Psi(\mathbf{u}, \lambda)}{\partial \mathbf{u} \partial \mathbf{u}} & \frac{\partial^2 \Psi(\mathbf{u}, \lambda)}{\partial \mathbf{u} \partial \lambda} \\ \frac{\partial^2 \Psi(\mathbf{u}, \lambda)}{\partial \lambda \partial \mathbf{u}} & \frac{\partial^2 \Psi(\mathbf{u}, \lambda)}{\partial \lambda \partial \lambda} \end{pmatrix}$$

And in application to our model problem??

Our model problema was $\mathbf{Ku} = \mathbf{b}$ subjected to the constraint $\mathbf{Hu} = \mathbf{e}$

In order to apply the abstract technique we just described, we must define the functionals $f(\mathbf{u})$ and $g(\mathbf{u})$

Interestingly we don't need their exact expression!! We can FORMALLY take

- $f(\mathbf{u})$ such that $\frac{\partial f(\mathbf{u})}{\partial \mathbf{u}} = \mathbf{b} - \mathbf{Ku}$
- $g(\mathbf{u}) = \mathbf{e} - \mathbf{Hu}$

On the model problem

$$\begin{aligned} RHS(\mathbf{u}, \boldsymbol{\lambda}) &:= \begin{pmatrix} \mathbf{b} - \mathbf{K}\mathbf{u} - \mathbf{H}^t \boldsymbol{\lambda} \\ \mathbf{e} - \mathbf{H}\mathbf{u} \end{pmatrix} \\ LHS(\mathbf{u}, \boldsymbol{\lambda}) &:= \begin{pmatrix} \mathbf{K} & \mathbf{H}^t \\ \mathbf{H} & \mathbf{0} \end{pmatrix} \end{aligned}$$

Which gives the iteration

$$\begin{pmatrix} \mathbf{K} & \mathbf{H}^t \\ \mathbf{H} & \mathbf{0} \end{pmatrix} \begin{pmatrix} d\mathbf{u} \\ d\boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{b} - \mathbf{K}\mathbf{u} - \mathbf{H}^t \boldsymbol{\lambda} \\ \mathbf{e} - \mathbf{H}\mathbf{u} \end{pmatrix}$$

Which completed by

$$\mathbf{u} = \mathbf{u} + d\mathbf{u}$$

Is completely equivalent to the original problem (just take the initial guess as 0 for a proof)

Advantages & disadvantages of Lagrange Multipliers method

- **Very General & accurate**
- **Constraints are exactly enforced**

It would be “the method of choice”, however:

- **Increases the number of unknowns**
- **Problem is not any longer SPD, even if the original unconstrained problem is → typically plays badly with Iterative Solvers**
- **Zeros appear on the main diagonal**
- **User must take care not to repeat constraints. If the same condition is asked twice → linearly dependent constraints → FAILURE**
- **STABILIZATION MAY BE NEEDED TO MAKE THE PROBLEM SOLVABLE (out of scope for now)**

“penalty-based” alternatives

Penalty method – defines a new functional as

$$\Psi(\mathbf{u}) := f(\mathbf{u}) - \frac{k}{2}(\mathbf{g}(\mathbf{u}) \cdot \mathbf{g}(\mathbf{u}))$$

Where “**k**” is a large number, called **penalty parameter**

Penalty method

For our model problem:

$$\Psi(\mathbf{u}) := f(\mathbf{u}) - \frac{k}{2}((\mathbf{e} - \mathbf{H}\mathbf{u}) \cdot (\mathbf{e} - \mathbf{H}\mathbf{u}))$$

Hence, as $RHS(\mathbf{u}) := \frac{\partial \Psi(\mathbf{u}, \lambda)}{\partial \mathbf{u}}$

We get:

$$RHS(\mathbf{u}) := \mathbf{b} - \mathbf{K}\mathbf{u} - k((\mathbf{e} - \mathbf{H}\mathbf{u}) \cdot (-\mathbf{H}))$$

And after minor manipulation

$$\underline{RHS(\mathbf{u}) := \mathbf{b} - \mathbf{K}\mathbf{u} + k\mathbf{H}^t(\mathbf{e} - \mathbf{H}\mathbf{u})}$$

Penalty method

Applying NR method:

$$LHS(\mathbf{u}) := -\frac{\partial RHS(\mathbf{u})}{\partial(\mathbf{u})}$$

We get

$$LHS(\mathbf{u}) = \mathbf{K} + \mathbf{kH}^t\mathbf{H}$$

Penalty Method

In application to our problem we get
(assuming a zero initial guess)

penalty 1000

original matrix

2	-1	0
-1	2	-1
0	-1	1

penalization kH^tH

1000	0	-1000
0	0	0
-1000	0	1000

RHS

5
0
0

RHS with
penalty

-995
0
1000

modified matrix

1002	-1	-1000
-1	2	-1
-1000	-1	1001

inverse of modified matrix

1	1	1
1	1,50024988	1,00049975
1	1,00049975	1,0009995

sol

5
5,49975012
5,99950025

Penalty method

- Easy to implement and pretty general
- Equivalent constraints can be enforced multiple times without any problem.
- No additional unknowns

HOWEVER (on the bad side):

- Large “k” needed to enforce the constraints. (constraints “compete” with the stiffness matrix K) → **LEADS TO ILL CONDITIONED MATRICES**
- Inaccurate (constraints **can** be violated)

Penalty in mixed form

It is interesting (we'll see soon why) to observe that the penalty method can be recast in a form similar to the lagrange multipliers.

To do so we can start with the expression

of the residual which corresponds to the penalty method

$$\text{RHS}(\mathbf{u}) := \mathbf{b} - \mathbf{K}\mathbf{u} + \mathbf{k}\mathbf{H}^t(\mathbf{e} - \mathbf{H}\mathbf{u})$$

And introduce a new var $\lambda_k := -\mathbf{k}(\mathbf{e} - \mathbf{H}\mathbf{u})$

Penalty in mixed form

This leads to the definition of a “mixed” RHS

$$\text{RHS}(\mathbf{u}, \boldsymbol{\lambda}_k) := \begin{pmatrix} \mathbf{b} - \mathbf{K}\mathbf{u} - \mathbf{H}^t \boldsymbol{\lambda}_k \\ (\mathbf{e} - \mathbf{H}\mathbf{u}) + \frac{1}{k} \boldsymbol{\lambda}_k \end{pmatrix}$$

To which corresponds the NR iteration

$$\begin{pmatrix} \mathbf{K} & \mathbf{H}^t \\ \mathbf{H} & -\frac{1}{k} \end{pmatrix} \begin{pmatrix} d\mathbf{u} \\ d\boldsymbol{\lambda}_k \end{pmatrix} = \begin{pmatrix} \mathbf{b} - \mathbf{K}\mathbf{u} - \mathbf{H}^t \boldsymbol{\lambda}_k \\ \mathbf{e} - \mathbf{H}\mathbf{u} + \frac{1}{k} \boldsymbol{\lambda}_k \end{pmatrix}$$

Why the mixed form?

When written in mixed form, **the system conditioning is less sensitive to the value of the penalty parameter “k”**

It may make sense to use it since it allows using a larger value of k

Augmented lagrangian method

It is a combination of “Lagrange” & “Penalty” methods

$$\Psi(\mathbf{u}) := f(\mathbf{u}) - \frac{k}{2} (\mathbf{g}(\mathbf{u}) \cdot \mathbf{g}(\mathbf{u})) + \lambda_{k_{old}} \cdot \mathbf{g}(\mathbf{u})$$

Where $\lambda_{k_{old}}$ is modified at every iteration as

$$\lambda_{k_{old}} = \lambda_{k_{old}} - k\mathbf{g}(\mathbf{u}_{old})$$

Augmented lagrangian method

For our model problem:

$$\Psi(\mathbf{u}) := f(\mathbf{u}) - \frac{k}{2}((\mathbf{e} - H\mathbf{u}) \cdot (\mathbf{e} - H\mathbf{u})) + \lambda_{old} \cdot (\mathbf{e} - H\mathbf{u})$$

using $RHS(\mathbf{u}) := \frac{\partial \Psi(\mathbf{u}, \lambda)}{\partial \mathbf{u}}$ we get:

$$RHS(\mathbf{u}) := \mathbf{b} - K\mathbf{u} - k((\mathbf{e} - H\mathbf{u}) \cdot (-H)) - H^t \lambda_{old}$$

And after minor manipulation

Note that this is the value to be used in the next iteration!!

$$\lambda_k = \lambda_{old} - k(\mathbf{e} - H\mathbf{u})$$

$$RHS(\mathbf{u}) := \mathbf{b} - K\mathbf{u} - H^t(\lambda_{old} - k(\mathbf{e} - H\mathbf{u}))$$

Augmented lagrangian in mixed form

Introducing an auxiliary variable

$$\lambda_k = \lambda_{old} - k(e - Hu)$$

we arrive to the iterative scheme:

- STEP1 solve for until convergence

$$\begin{pmatrix} K & H^t \\ H & -\frac{1}{k} \end{pmatrix} \begin{pmatrix} du \\ d\lambda_k \end{pmatrix} = \begin{pmatrix} b - Ku - H^t(\lambda_k) \\ e - Hu - \frac{1}{k}(\lambda_k - \lambda_{old}) \end{pmatrix}$$

- STEP2

$$\lambda_{old} = \lambda_k = \lambda_{old} - k(e - Hu)$$

- STEP3 repeat 1 and 2 until convergence in λ_{old}

Augmented lagrangian

- Easy to implement and pretty general
- Equivalent constraints can be enforced multiple times without any problem.
- Large penalty **not needed** (at convergence)

HOWEVER (on the bad side):

- A linear problem is transformed into an iterative process
- If the iterative process is stopped before convergence constraint is not respected exactly

Master-Slave elimination

An alternative approach is the so-called master-slave elimination.

We recall that our model problem was

$$\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 5 \\ 0 \\ 0 \end{pmatrix}$$

Subjected to the additional constraint:

$$u_3 = u_1 + 1$$

Master-slave elimination

The idea is to build the constraint within the unknowns. In the specific case, u_3 can be expressed in terms of u_1 and u_2 as follows

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Or in short

$$\mathbf{u} = \mathbf{T}\mathbf{u}^* + \mathbf{q}$$

Master-slave elimination

We can now substitute $\mathbf{u} = \mathbf{T}\mathbf{u}^* + \mathbf{q}$

In the original problem $\mathbf{K}\mathbf{u} = \mathbf{b}$ to get

$$\mathbf{K}(\mathbf{T}\mathbf{u}^* + \mathbf{q}) = \mathbf{b}$$

To make the problem solvable we then left multiply it by \mathbf{T}^t

$$\mathbf{T}^t\mathbf{K}(\mathbf{T}\mathbf{u}^* + \mathbf{q}) = \mathbf{T}^t\mathbf{b}$$

Or

$$\mathbf{T}^t\mathbf{K}\mathbf{T}\mathbf{u}^* = \mathbf{T}^t\mathbf{b} - \mathbf{T}^t\mathbf{K}\mathbf{q}$$

Master-slave elimination

$$\begin{aligned} & \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_1^* \\ u_2^* \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 5 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \end{aligned}$$

Simplifying this gives

$$\begin{pmatrix} 3 & -2 \\ -2 & 2 \end{pmatrix} \begin{pmatrix} u_1^* \\ u_2^* \end{pmatrix} = \begin{pmatrix} 4 \\ 1 \end{pmatrix} \rightarrow \begin{pmatrix} u_1^* \\ u_2^* \end{pmatrix} = \begin{pmatrix} 5 \\ 5.5 \end{pmatrix}$$

Once we recover the value of u_3 we can immediately verify that the solution is the same as before

Master-slave elimination

- Smaller, well conditioned systems
- Preserves symmetry and matrix properties

HOWEVER (on the bad side):

- Not very general (how to do for a generic nonlinear constraint??)
- Can be (very) difficult to implement
- User must be extremely careful in applying constraints exactly once
- User must identify variables to be eliminated

bibliography

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