

Useful mathematical tools

MIGUEL A. S. CASQUILHO

Technical University of Lisbon, 1049-001 Lisboa, Portugal

Some useful mathematical tools are presented: the Newton-Raphson method; surrogate Gaussian distributions; and notes on the Monte Carlo (simulation) method.

Key words: *Newton-Raphson method, Gaussian distribution, Monte Carlo, Simulation.*

1. Introduction

Useful mathematical tools (some of which you may have forgotten) are presented: the Newton-Raphson method; surrogate Gaussian distributions; and some notes on the Monte Carlo simulation method. Pertinent illustrations are included.

2. The Newton-Raphson method

The Newton-Raphson method is a well-known numerical method to find (approximate) zeros (or “roots”) of a function. It is an iterative algorithm, which, when successful, converges (usually) rapidly (quadratically, i.e., doubling the number of correct figures in each iteration), but may fail as any other root-finding algorithm.

The method tries to solve an equation in the form of Eq. {1}

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

through the iterative procedure of Eq. {2},

$$x^* = x - \frac{f(x)}{f'(x)} \tag{2}$$

from an initial estimate of x , usually called the *initial guess*. Although the notation x^* is often used to indicate the solution to a problem (Eq. {1}), here it is used to mean the next, (hopefully) improved value of the variable, which, in the end, will indeed be the solution.

The bibliographical sources of the method are so numerous that no specific recommendation is made in this opuscle.

Eq. {2} shows that: if we know the solution, i.e., the x for which it is $f(x) = 0$, then, of course, the next x is the same as the current one, so the process is terminated; and if the derivative is null in the solution, i.e., $f'(x) = 0$, the method fails (which happens, namely, for multiple roots). Failure to converge may, of course, happen in any iterative numerical method. Anyway, the convergence of the Newton-Raphson method, when it arises, is typically quite rapid (few iterations).

Illustration 2-A

Solve

$$f(x) = ax + b = 0 \quad \{3\}$$

from $x = 1$.

Resolution Applying the algorithm, it is

$$f'(x) = a \quad \{4\}$$

$$x^* = x - \frac{ax + b}{a} = x - x - \frac{b}{a} = -\frac{b}{a} \quad \{5\}$$

In this case, we did not even have the opportunity to supply the initial guess to get the (exact) solution.

Illustration 2-B

Solve

$$f(x) = 2x^2 - 6x = 0 \quad \{6\}$$

from $x = \pm 5$.

Resolution Applying the algorithm, with the simple derivative, it is

$$x^* = x - \frac{2x^2 - 6x}{4x - 6} \quad \{7\}$$

Eq. {7} could be simplified to $x^* = x - x(x-3)/(2x-3)$ —not necessary—, just to show that 0 and 3 are, of course, the roots of the given equation. The function is shown in Fig. 1 and the computations in Table 1.

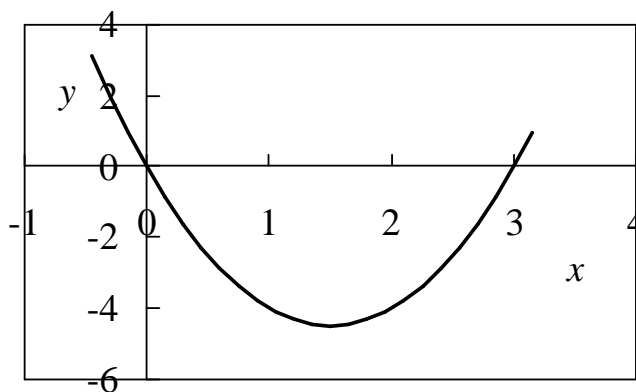


Fig. 1

Table 1

x	$f(x)$	$f'(x)$	new x	x	$f(x)$	$f'(x)$	new x
-5	80	-26	-1,92308	5	20	14	3,571429
-1,92308	18,93491	-13,6923	-0,54019	3,571429	4,081633	8,285714	3,078818
-0,54019	3,824752	-8,16076	-0,07151	3,078818	0,485331	6,315271	3,001967
-0,07151	0,439314	-6,28606	-0,00163	3,001967	0,011812	6,007869	3,000001
-0,00163	0,009768	-6,00651	-8,8E-07	3,000001	7,73E-06	6,000005	3
-8,8E-07	5,29E-06	-6	-2,6E-13	3	3,32E-12	6	3
-2,6E-13	1,55E-12	-6	-2,2E-26	3	0	6	3
-2,2E-26	1,34E-25	-6	0				
0	0	-6	0				

In this simple case, the two zeros (or “roots”, a more usual term for polynomials) were obtained from respective “reasonable” initial guesses.

Illustration 2-C

Solve

$$\sin x = 1/2 \quad \{8\}$$

from $x = 0$. (We know that $x = \arcsin(1/2) = \pi/6 = 0.523\dots$)

Resolution First, drive Eq. {8} to the convenient form (Eq. {2}).

$$f(x) = (\sin x) - 1/2 = 0 \quad \{9\}$$

Thus,

$$f'(x) = \cos x \quad \{10\}$$

$$\tilde{x} = x - \frac{\sin x - 1/2}{\cos x} \quad \{11\}$$

The computations are shown in Table 2.

Table 2

x	$f(x)$	$f'(x)$	Dx	new x
0	-0,5	1	0,5	0,5
0,5	-0,02057	0,877583	0,023444	0,523444
0,523444	-0,00013	0,866103	0,000154	0,523599
0,523599	-6E-09	0,866025	6,87E-09	0,523599
0,523599	0	0,866025	0	0,523599

Illustration 2-D

Solve

$$x + \arctan x = 1 \quad \{12\}$$

from $x = 0$.

Resolution Drive Eq. {12} to the convenient form.

$$f(x) = x + \arctan x - 1 = 0 \quad \{13\}$$

$$f'(x) = 1 + \frac{1}{1+x^2}$$

Then,

$$\tilde{x} = x - \frac{x + \arctan x - 1}{1 + 1/(1+x^2)} \quad \{14\}$$

The function f is shown in Fig. 2 and the computations in Table 3.

Table 3

x	$f(x)$	$f'(x)$	Δx	new x
0	-1	2	0,5	0,5
0,5	-0,0363	1,8	0,020196	0,520196
0,520196	-0,00013	1,787027	7,32E-05	0,520269
0,52027	-1,7E-09	1,78698	9,67E-10	0,520269
0,520269	0	1,78698	0	0,520269

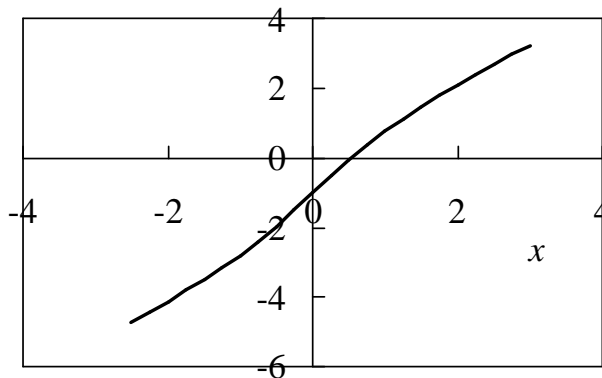


Fig. 2

Illustration 2-E

Solve

$$\Phi(z) = 0.25 \quad \{15\}$$

from $z = 0$. This will be useful in the *simulation* of a Gaussian variable.

Resolution Remember that Φ is the usual notation for the Gaussian integral,

$$\Phi(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^z \exp\left(-\frac{1}{2}x^2\right) dx \quad \{16\}$$

Applying the algorithm, with the right-hand side constant of Eq. {15} denoted by P , $P = 0.25$, it is

$$f(z) = \Phi(z) - P$$

$$f'(z) = \phi(z) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}z^2\right)$$

Then,

$$z^* = z - \frac{\Phi(z) - P}{\phi(z)} \quad \{17\}$$

The computations are shown in Table 4.

Table 4

x	$f(x)$	$f'(x)$	Δx	new x
0	0,25	0,398942	-0,62666	-0,62666
-0,62666	0,015442	0,327821	-0,04711	-0,67376
-0,67376	0,000231	0,317932	-0,00073	-0,67449
-0,67449	5,67E-08	0,317777	-1,8E-07	-0,67449
-0,67449	3,44E-15	0,317777	-1,1E-14	-0,67449
-0,67449	0	0,317777	0	-0,67449

Illustration 2-F

In a production, it is desired to have a certain Gaussian weight lying between $L = 1000$ g and $U = 1040$ g for $P = 95$ % of the items produced. The process mean is “known” to be $\mu = 1018$ g. Compute an adequate process standard deviation, σ .

$$\Phi\left(\frac{U - \mu}{\sigma}\right) - \Phi\left(\frac{L - \mu}{\sigma}\right) = P \quad \{18\}$$

Resolution This is a problem of a function of σ . (Anyway, σ —unlike μ — is a parameter to which it is problematic to set values !)

$$f(\sigma) = \Phi\left(\frac{U - \mu}{\sigma}\right) - \Phi\left(\frac{L - \mu}{\sigma}\right) - P \quad \{19\}$$

To apply the algorithm, we differentiate with respect to σ (chain rule).

$$\begin{aligned} f'(\sigma) &= \frac{d}{d\sigma} \left[\Phi\left(\frac{U - \mu}{\sigma}\right) - \Phi\left(\frac{L - \mu}{\sigma}\right) - \underbrace{P}_{\text{const.}} \right] = \\ &= \left[\phi\left(\frac{U - \mu}{\sigma}\right) \right] \frac{d}{d\sigma} \left(\frac{U - \mu}{\sigma} \right) - \left[\phi\left(\frac{L - \mu}{\sigma}\right) \right] \frac{d}{d\sigma} \left(\frac{L - \mu}{\sigma} \right) \end{aligned} \quad \{20\}$$

which becomes

$$f'(\sigma) = -\frac{U - \mu}{\sigma^2} \phi\left(\frac{U - \mu}{\sigma}\right) + \frac{L - \mu}{\sigma^2} \phi\left(\frac{L - \mu}{\sigma}\right) \quad \{21\}$$

The function, f (solid line), and the derivative, f' (dashed line), are shown in Fig. 3 and the computations in Table 5. So, it is $\sigma = 10.008$ g, with $\Phi[(L - \mu)/\sigma] = 3.6$ % and $\Phi[(U - \mu)/\sigma] = 98.6$ % (and $P = 98.6 - 3.6 = 95$ %).

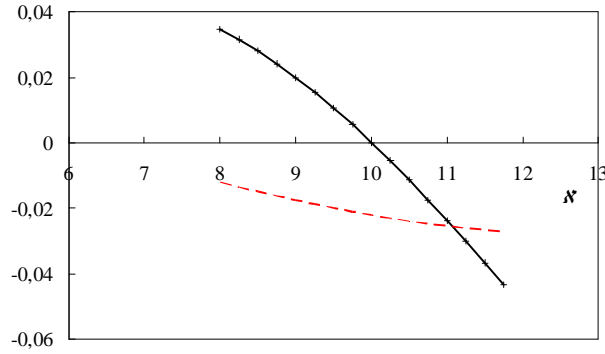


Fig. 3

Table 5

x	$(L - m)/x$	$(U - m)/x$	$f(x)$	$f'(x)$	Dx	x new
7	-2,57143	3,142857	0,044099	-0,00666	6,626194	13,62619
13,62619	-1,32099	1,614537	-0,09646	-0,029	-3,32595	10,30024
10,30024	-1,74753	2,135872	-0,00662	-0,02315	-0,2858	10,01444
10,01444	-1,7974	2,196827	-0,00015	-0,02207	-0,00689	10,00755
10,00755	-1,79864	2,19834	-9,4E-08	-0,02205	-4,3E-06	10,00755
10,00755	-1,79864	2,198341	-3,6E-14	-0,02205	-1,6E-12	10,00755
10,00755	-1,79864	2,198341	0	-0,02205	0	10,00755

Illustration 2-G

In a production, it is desired to have a certain Gaussian weight between $L = 1000$ and $U = 1040$ g in $P = 90\%$ of the items produced. The process standard deviation is “known” to be $\sigma = 10$ g. Compute an adequate process mean, μ . (The problem becomes impossible for too high a probability. Indeed, handling only μ —without σ —is a poor tool for Quality.)

$$\Phi\left(\frac{U - \mu}{\sigma}\right) - \Phi\left(\frac{L - \mu}{\sigma}\right) = P \quad \{22\}$$

Resolution This is a problem of a function of μ .

$$f(\mu) = \Phi\left(\frac{U - \mu}{\sigma}\right) - \Phi\left(\frac{L - \mu}{\sigma}\right) - P \quad \{23\}$$

To apply the algorithm, we differentiate with respect to μ .

$$f'(\mu) = \frac{d}{d\mu} \left[\Phi\left(\frac{U - \mu}{\sigma}\right) - \Phi\left(\frac{L - \mu}{\sigma}\right) - P \right] \quad \{24\}$$

or

$$f'(\mu) = \left[\phi\left(\frac{U - \mu}{\sigma}\right) \right] \frac{d}{d\mu} \left(\frac{U - \mu}{\sigma} \right) - \left[\phi\left(\frac{L - \mu}{\sigma}\right) \right] \frac{d}{d\mu} \left(\frac{L - \mu}{\sigma} \right) \quad \{25\}$$

which becomes

$$f'(\mu) = -\frac{1}{\sigma} \left[\phi\left(\frac{U-\mu}{\sigma}\right) - \phi\left(\frac{L-\mu}{\sigma}\right) \right] \quad \{26\}$$

The function, f (solid line), and the derivative, f' (dashed line), are shown in Fig. 4 and the computations in Table 6. So, it is $\mu = 1013.0$ g, $\Phi[(L-\mu)/\sigma] = 0.3\%$ and $\Phi[(U-\mu)/\sigma] = 90.3\%$. (Another solution is 1027.0 g.)

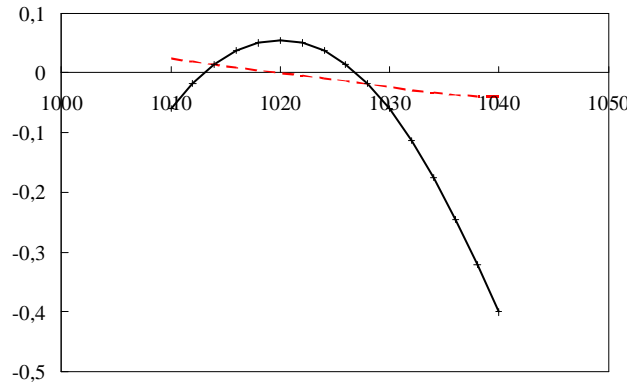


Fig. 4

Table 6

x	$(L-x)/s$	$(U-x)/s$	$f(x)$	$f'(x)$	Dx	x new
1019	-1,9	2,1	0,053419	0,002163	-24,6942	994,3058
994,3058	0,569419	4,569419	-0,61547	0,033922	18,14332	1012,449
1012,449	-1,24491	2,755087	-0,00952	0,017484	0,544236	1012,993
1012,993	-1,29934	2,700663	-0,00037	0,016111	0,02323	1013,017
1013,017	-1,30166	2,69834	-6,8E-07	0,016053	4,22E-05	1013,017
1013,017	-1,30166	2,698336	-2,2E-12	0,016053	1,39E-10	1013,017
1013,017	-1,30166	2,698336	-1E-15	0,016053	6,22E-14	1013,017
1013,017	-1,30166	2,698336	9,99E-16	0,016053	-6,2E-14	1013,017
1013,017	-1,30166	2,698336	-1E-15	0,016053	6,22E-14	1013,017
1013,017	-1,30166	2,698336	9,99E-16	0,016053	-6,2E-14	1013,017
1013,017	-1,30166	2,698336	-1E-15	0,016053	6,22E-14	1013,017

In case of non-convergence, other algorithms, such as bisection (if a “safe” interval for the solution is known), can be used.

3. The multivariate Newton-Raphson method

The Newton-Raphson method is applicable to systems of multivariate functions (of which the univariate is, of course, a particular case), as in Eq. {27},

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \quad \{27\}$$

meaning

$$\begin{cases} f_1(x_1, x_2, \dots, x_n) = 0 \\ f_2(x_1, x_2, \dots, x_n) = 0 \\ \dots \dots \\ f_n(x_1, x_2, \dots, x_n) = 0 \end{cases} \quad \{28\}$$

through the iterative procedure of Eq. {29},

$$\mathbf{x}^* = \mathbf{x} - \mathbf{J}^{-1}\mathbf{f} \quad \{29\}$$

where \mathbf{J} is the Jacobian (Eq. {30}) of \mathbf{f} :

$$\mathbf{J} = \frac{\partial(f_1, f_2, \dots, f_n)}{\partial(x_1, x_2, \dots, x_n)} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_n} \\ \dots & \dots & \dots & \dots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \dots & \frac{\partial f_n}{\partial x_n} \end{bmatrix} \quad \{30\}$$

Now, the convergence of the method becomes much more problematic.

Illustration 3-A

Solve

$$\begin{cases} x_1 + x_2^2 = 3 \\ x_1/x_2 = -2 \end{cases} \quad \{31\}$$

from (1, 1).

Resolution This must be driven to the form of Eq. {28}:

$$\begin{cases} f_1 = x_1 + x_2^2 - 3 = 0 \\ f_2 = x_1/x_2 + 2 = 0 \end{cases} \quad \{32\}$$

To apply the algorithm, we need the Jacobian.

$$\mathbf{J} = \begin{bmatrix} 1 & 2x_2 \\ 1/x_2 & -x_1/x_2^2 \end{bmatrix} \quad \{33\}$$

Its inverse

$$\mathbf{J}^{-1} = \frac{1}{\det \mathbf{J}} \begin{bmatrix} j_{11} & j_{12} \\ j_{21} & j_{22} \end{bmatrix}^{-1} \quad \{34\}$$

becomes, in the 2-dimensional case,

$$\mathbf{J}^{-1} = \frac{1}{j_{11}j_{22} - j_{12}j_{21}} \begin{bmatrix} j_{22} & -j_{12} \\ -j_{21} & j_{11} \end{bmatrix} \quad \{35\}$$

or

$$\mathbf{J}^{-1} = \begin{bmatrix} 1 & 2x_2 \\ 1/x_2 & -x_1/x_2^2 \end{bmatrix}^{-1} = \frac{1}{-x_1/x_2^2 - 2} \begin{bmatrix} -x_1/x_2^2 & -2x_2 \\ -1/x_2 & 1 \end{bmatrix} \quad \{36\}$$

The computations are shown in Table 7. So, it is $\mathbf{x}^* = (-6, 3)$ (perhaps not unique).

Table 7

$x_{1,2}$	$f_{1,2}$	\mathbf{J}	det	\mathbf{J}^{-1}	$\mathbf{J}^{-1}\mathbf{f}$	$x_{1,2}$ new	norm(f)
1	-1	1 2	-3	0,333333 0,666667	1,666667 -0,66667		
1	3	1 -1		0,333333 -0,33333	-1,33333 2,33333	3,162278	
-0,66667	1,777778	1 4,666667	-1,87755	-0,06522 2,485507	4,144928 -4,81159		
2,333333	1,714286	0,428571 0,122449		0,228261 -0,53261	-0,50725 2,84058	2,46967	
-4,81159	0,257299	1 5,681159	-1,40369	-0,42482 4,047315	1,129668 -5,94126		
2,84058	0,306122	0,352041 0,596314		0,250797 -0,71241	-0,15355 2,994135	0,399892	
-5,94126	0,023579	1 5,988269	-1,33727	-0,49558 4,477978	0,058617 -5,99988		
2,994135	0,0157	0,333986 0,662729		0,249752 -0,74779	-0,00585 2,999986	0,028328	
-5,99988	3,42E-05	1 5,999971	-1,33334	-0,49999 4,499955	0,000121 -6		
2,999986	3,06E-05	0,333335 0,66666		0,25 -0,75	-1,4E-05 3	4,59E-05	
-6	2,08E-10	1 6	-1,33333	-0,5 4,5	5,58E-10 -6		
3	1,47E-10	0,333333 0,666667		0,25 -0,75	-5,8E-11 3		

This problem could be solved analytically:

$$x_2^2 - 2x_2 - 3 = 0 \quad \{37\}$$

$$x_2 = \frac{2 \pm \sqrt{4 + 4 \times 3}}{2} = 1 \pm 2 = \begin{cases} -1 \\ 3 \end{cases} \quad \{38\}$$

$$x_1 = -2x_2 = \begin{cases} 2 \\ -6 \end{cases}$$

i.e., $\mathbf{x}^* = (-6, 3)$ (in Table 7) or $\mathbf{x}^* = (2, -1)$.

Illustration 3-B

Solve

$$\begin{cases} x_1^2 + 3 \cos x_2 = 1 \\ x_2 + 2 \sin x_1 = 2 \end{cases} \quad \{39\}$$

from (0, 1).

Resolution This must be driven to the form of Eq. {28}:

$$\begin{cases} f_1 = x_1^2 + 3 \cos x_2 - 1 \\ f_2 = x_2 + 2 \sin x_1 - 2 \end{cases} \quad \{40\}$$

To apply the algorithm, we find the Jacobian.

$$\mathbf{J}^{-1} = \begin{bmatrix} 2x_1 & -3\sin x_2 \\ 2\cos x_1 & 1 \end{bmatrix}^{-1} = \frac{1}{2x_1 + 6\sin x_2 \cos x_2} \begin{bmatrix} 1 & 3\sin x_2 \\ -2\cos x_1 & 2x_1 \end{bmatrix} \quad \{41\}$$

The computations are shown in Table 8. So, it is $\mathbf{x}^* = (0.369, 1.279)$ (not unique).

Table 8

$x_{1,2}$	$f_{1,2}$	\mathbf{J}	det	\mathbf{J}^{-1}	$\mathbf{J}^{-1}\mathbf{f}$	$x_{1,2}$ new	norm(f)
0	0,620907	0 -2,52441	5,048826	0,198066 0,5	-0,37702 0,37702		
1	-1	2 1		-0,39613 0	-0,24596 1,245961		1,177083
0,37702 1,245961	0,099602 -0,01774	0,754039 -2,84311 1,859532 1	6,040893	0,165538 0,470644 -0,30782 0,124822	0,00814 0,368879 -0,03287 1,278835		0,101169
0,368879 1,278835	-0,00043 -2,4E-05	0,737759 -2,87304 1,865464 1	6,097318	0,164007 0,471198 -0,30595 0,120997	-8,3E-05 0,368962 0,00013 1,278705		0,000435
0,368962 1,278705	-4,6E-10 -2,5E-09	0,737924 -2,87293 1,865404 1	6,097103	0,164012 0,471196 -0,30595 0,121029	-1,2E-09 0,368962 -1,6E-10 1,278705		2,5E-09
0,368962 1,278705	0 0	0,737924 -2,87293 1,865404 1	6,097103	0,164012 0,471196 -0,30595 0,121029	0 0,368962 0 1,278705		0

Illustration 3-C

Solve

$$\begin{cases} \Phi\left(\frac{L-\mu}{\sigma}\right) = p_L \\ 1-\Phi\left(\frac{U-\mu}{\sigma}\right) = p_U \end{cases} \quad \{42\}$$

from some convenient (μ, σ) .

Resolution This must be driven to the form of Eq. {28}:

$$\begin{cases} f_1 = \Phi\left(\frac{L-\mu}{\sigma}\right) - p_L \\ f_2 = 1 - \Phi\left(\frac{U-\mu}{\sigma}\right) - p_U \end{cases} \quad \{43\}$$

To apply the algorithm, we find the Jacobian.

$$\mathbf{J} = \begin{bmatrix} -\frac{1}{\sigma}\phi\left(\frac{L-\mu}{\sigma}\right) & -\frac{L-\mu}{\sigma^2}\phi\left(\frac{L-\mu}{\sigma}\right) \\ -\frac{U-\mu}{\sigma^2}\phi\left(\frac{U-\mu}{\sigma}\right) & -\frac{1}{\sigma}\phi\left(\frac{U-\mu}{\sigma}\right) \end{bmatrix} \quad \{44\}$$

The computations are not shown here. It is $\mathbf{x}^* = (1020.879, 10.1665)$. This case appears to be one of difficult convergence. In a 2-variable case in these circumstances,

exploratory calculations can be useful to find initial guesses possibly leading to convergence.

4. Surrogate Gaussian distributions

The use of the Gaussian distribution presents some numerical difficulties, as seen above. Although many software applications silently solve these matters, numerical methods underlie the computations, namely with risks of lack of convergence and possible slowness, both of which should be avoided if numerous instances are necessary. The approximations, or surrogate distributions referred to will be based on a cosine and on a parabola. Only the final formulas are given here.

$$f(x) = \frac{\pi}{4a} \cos\left(\frac{\pi}{2} \frac{x-\mu}{a}\right) \quad \{45\}$$

$$F(x) = \frac{1}{2} + \frac{1}{2} \sin\left(\frac{\pi}{2} \frac{x-\mu}{a}\right) \quad \{46\}$$

with $x \in (\mu \pm a)$, and

$$f(x) = \frac{3}{4a} \left[1 - \left(\frac{x-\mu}{a} \right)^2 \right] \quad \{47\}$$

$$F(x) = \frac{1}{2} + \frac{3}{4} \left(\frac{x-\mu}{a} \right) - \frac{1}{4} \left(\frac{x-\mu}{a} \right)^3 \quad \{48\}$$

The inverses are, for Eq. {46},

$$\frac{x-\mu}{a} = \frac{2}{\pi} \arcsin(2F-1) \quad \{49\}$$

and for Eq. {48}, with $\beta = \frac{1}{3} \arccos(1-2F)$,

$$\frac{x-\mu}{a} = -\cos \beta + \sqrt{3} \sin \beta \quad \{50\}$$

5. Monte Carlo simulation

Simulation —also Monte Carlo simulation or simply Monte Carlo— is a powerful, very general purpose technique, used in many fields that deal with chance. Note that the term “simulation” is also used with the classical meaning of “imitation” or “modelling” of the behaviour of a system, e.g., by ordinary calculus or differential equations, without the intervention of chance. Monte Carlo simulation can, however, be used even to solve some types of deterministic problems.

The simulation of Gaussian variables will be used to illustrate the technique, as well as the aforementioned Newton-Raphson method.

Illustration 5-A

Compute a (random) value, x , from a Gaussian distribution with $\mu = 1020$ and $\sigma = 10$. Use a 3-digit random number of 0.891.

Resolution The usual technique is the *inversion technique*, given a (*uniform*) random number, r (conventionally, in the interval 0–1):

$$F(x; \mu, \sigma) = r \quad \{51\}$$

Using the standard Gaussian, this becomes

$$\Phi\left(\frac{x - \mu}{\sigma}\right) = r \quad \{52\}$$

This function is not analytically invertible, so, the following, Eq. {53}, is not a useful path (unless some software, such as Excel, does the task):

$$x = \mu + \sigma \Phi^{\text{inv}}(r) \quad \{53\}$$

So, Eq. {52} will be solved by the Newton-Raphson method:

$$f(x) = \Phi\left(\frac{x - \mu}{\sigma}\right) - r \quad \{54\}$$

$$f'(x) = \frac{1}{\sigma} \phi\left(\frac{x - \mu}{\sigma}\right) \quad \{55\}$$

The iteration is

$$x^* = x - \frac{\Phi\left(\frac{x - \mu}{\sigma}\right) - r}{\frac{1}{\sigma} \phi\left(\frac{x - \mu}{\sigma}\right)} \quad \{56\}$$

The initial guess $x = \mu$ appears to be a good (robust) choice. If r approaches 0 or 1, more iterations will be necessary till convergence. [Remember that $\Phi(-\infty) = 0$ and $\Phi(+\infty) = 1$, so convergence will of course be lengthier.] (Note that the Excel Gaussian pdf includes σ , so the factor $1/\sigma$ is not applied.) The computations are shown in Table 9, with $x^* = 1032.32$.

Table 9

x	$f(x)$	$f'(x)$	Δx	new x
1020	-0,391	0,039894	9,800917	1029,801
1029,801	-0,05452	0,024679	2,209207	1032,01
1032,01	-0,00587	0,019395	0,30282	1032,313
1032,313	-0,00011	0,018694	0,005691	1032,319
1032,319	-3,7E-08	0,018681	2E-06	1032,319
1032,319	-5,6E-15	0,018681	2,97E-13	1032,319
1032,319	-1,1E-15	0,018681	5,94E-14	1032,319
1032,319	-1,1E-15	0,018681	5,94E-14	1032,319

This problem can be presented in a simpler form. Let $z = \frac{x - \mu}{\sigma}$ and solve with respect to z .

$$\Phi(z) = r \quad \{57\}$$

This equation will be solved by the Newton-Raphson method:

$$f(z) = \Phi(z) - r \quad \{58\}$$

$$f'(z) = \phi(z) \quad \{59\}$$

The iteration is

$$x^* = x - \frac{\Phi(z) - r}{\phi(z)} \quad \{60\}$$

The computations are shown in Table 10, with $z^* = 1.23186$, which, through

$$x = \mu + \sigma z \quad \{61\}$$

gives $x^* = 1020 + 10 \times 1.23186 = 1032.32$, as before.

Table 10

x	$f(x)$	$f'(x)$	Δx	new x
0	-0,391	0,398942	0,980092	0,980092
0,980092	-0,05452	0,246787	0,220921	1,201012
1,201012	-0,00587	0,19395	0,030282	1,231294
1,231294	-0,00011	0,186937	0,000569	1,231864
1,231864	-3,7E-08	0,186806	2E-07	1,231864
1,231864	-4,7E-15	0,186806	2,5E-14	1,231864
1,231864	0	0,186806	0	1,231864
1,231864	0	0,186806	0	1,231864

Illustration 5-B

Compute a (random) value, x , from a truncated Gaussian distribution with $\mu = 1020$ and $\sigma = 10$, between $a = 995$ and $b = 1035$. Use a random number of 0.891.

Resolution Remark that a is at a “distance” of $(995 - 1020)/10 = -2,5\sigma$ and b at $(1035 - 1020)/10 = 1,5\sigma$ from the mean (compare to the typical 3σ), so the truncation is “effective”. The pdf (probability density function), f_T , and cdf (cumulative distribution function), F_T , now are

$$f_T(x; \mu, \sigma, a, b) = \frac{1}{\sigma} \frac{\phi(x')}{\Delta\Phi} \quad \{62\}$$

$$F_T(x) = \frac{\Phi(x') - \Phi(a')}{\Delta\Phi} \quad \{63\}$$

where it is $x' = \frac{x - \mu}{\sigma}$, etc., and $\Delta\Phi = \Phi(b') - \Phi(a')$. The equation to be solved, using z , is, thus,

$$G_T(z) = \frac{\Phi(z) - \Phi(a')}{\Delta\Phi} = r \quad \{64\}$$

Using the Newton-Raphson method, this becomes

$$f(z) = \frac{\Phi(z) - \Phi(a')}{\Delta\Phi} - r \quad \{65\}$$

$$f'(z) = \frac{\phi(z)}{\Delta\Phi} \quad \{66\}$$

The computations are shown in Table 11, with $z^* = 0,9627$, thence $x^* = 1029,62$. Due to truncation, this value is nearer the mean when compared to the previous illustration. The Gaussian and its truncated are shown in Fig. 5.

Table 11

z	$f(z)$	$f'(z)$	Δz	new z
0	-0,35831	0,430366	0,832581	0,832581
0,832581	-0,03742	0,304308	0,122984	0,955564
0,955564	-0,00194	0,272622	0,007114	0,962678
0,962678	-6,6E-06	0,270768	2,44E-05	0,962703
0,962703	-7,7E-11	0,270762	2,85E-10	0,962703
0,962703	0	0,270762	0	0,962703
0,962703	0	0,270762	0	0,962703

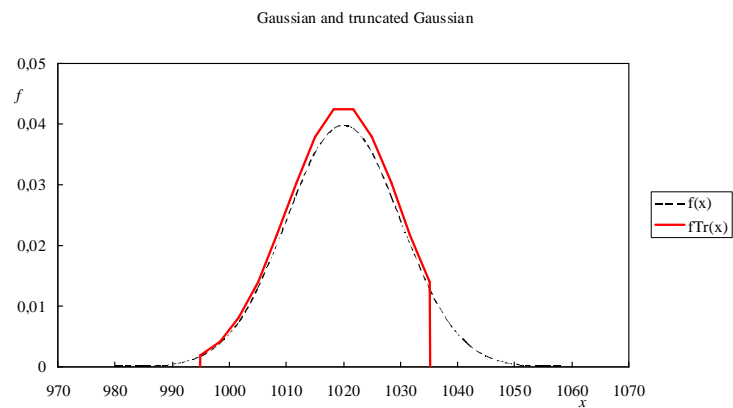


Fig. 5

6. Conclusions

Expectedly useful mathematical tools were presented: the Newton-Raphson method to solve uni-variate equations; the same method to solve systems of multi-variate equations; surrogate Gaussian distributions to try to ease simulation; and some notes on the Monte Carlo simulation method. Pertinent illustrations were included.

Acknowledgements

This work was done at “Centro de Processos Químicos do IST” (Chemical Process Research Center of IST), in the Department of Chemical Engineering, Technical University of Lisbon. Computations were done on the central system of CIIST (Computing Center of IST).

References

- MACTUTOR (The MacTutor History of Mathematics archive) (2010), <http://www-history.mcs.st-andrews.ac.uk/history/>, accessed 27.th Oct.

