Sample Problems

Problem 1:

Calculate

$$f(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

for $x = 1.0$ and $x = 4.5$

This function is the error function, erf, and is implemented in S15AEF.

Problem 2:

Given the matrix G of pair-wise correlations:

$$G = \begin{pmatrix} 1 & -0.3368 & -0.1746 & 0.1282 & -0.8092 \\ -0.3368 & 1 & -0.3935 & 0.0696 & -0.2727 \\ -0.1746 & 0.0696 & 1 & 0.1563 & 0.1223 \\ -0.3935 & 0.1563 & -0.2727 & 1 & 0.2291 \\ 0.1282 & -0.8092 & 0.1223 & 0.2291 & 1 \end{pmatrix}$$

calculate a square, semi-positive definite, symmetric matrix Σ ,with unit diagonal, that is the nearest to G in the Frobenius norm, i.e.

$$\sqrt{trace\left((G - \Sigma)^T (G - \Sigma)\right)}$$

is minimised.

One solution to this can be obtained via the algorithm of Qi and Sun and is implemented in G02AAF.

Problem 3:

Solve the two equations:

Maximise $\dfrac{(2x^2+4x+1)}{e^{x/2}}$ subject to $0 \le x \le 10$

and

Maximise $\dfrac{\left(0.5x^3+6x^2+2x\right)}{e^x}$ subject to $0 \le x \le 10$

One way of solving these two equations is via quadratic interpolation, as implemented in E04ABA.

Using the thread safe, “A” version of this routine means that you can make use of the IUSER and RUSER arrays and so only need implement one user defined function to solve both.