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.