Written solutions for these problems were to be handed in for grading on Tues. 28 Nov. 2000.

A real symmetric matrix $H = H^T$ is called "Positive Definite" just when $x^THx > 0$ for every nonzero vector x of the same dimension as H. Positive definite matrices have applications to Mechanics, Statistics, Psychology, Differential Geometry and many other areas.

1. Explain why the inverse H^{-1} exists and is positive definite.

Solution: H cannot be singular since " $Hx = o$ " implies " $x^THx = 0$ ", whence " $x = o$ ". Therefore H^{-1} exists. And $H^{-1T} = H^{-1}$ is symmetric since $I = I^T = (H^{-1}H)^T = HH^{-1T}$. Finally, H^{-1} is positive definite because $xH^{-1}x = (H^{-1}x)^TH(H^{-1}x) > 0$ whenever $x \neq o$.

A second proof exploits the factorization of any real symmetric $H = Q\Lambda Q^T$ in which Q is an *Orthogonal* (so $Q^T = Q^{-1}$) matrix of eigenvectors and Λ is a real diagonal matrix of H's eigenvalues. These are the *Stationary Values* (including maximum and minimum) of the quotient x^THx/x^Tx as x runs through all nonzero real vectors of H's dimension. When H is positive definite too that quotient is positive, and so are H's eigenvalues; then likewise for $H^{-1} = Q\Lambda^{-1}Q^T$. Choleski factorization of $H = U^TU$ provides a third proof: $H^{-1} = U^{-1}U^{-1T}$.

2. Explain why the equation $Y^2 = H$, though it may have many solutions Y, has just one symmetric positive definite solution Y; it is called the positive definite square root of H and written $Y = \sqrt{H}$.

Solution: There are several ways to construct $Y := \sqrt{H}$. One way exploits the eigenvector-value factorization $H = Q\Lambda Q^T$ already mentioned above; $Y := Q\sqrt{\Lambda}Q^T$ in which $\sqrt{\Lambda}$ is computed elementwise. A second way sets $Y := (2/\pi)\int_0^\infty (I + \xi^2H^{-1})^{-1}\, d\xi$, confirmed by using the same factorization. A third way sets $Y_0 := I$ and runs an iteration $Y_{n+1} := (Y_n + H\cdot Y_n^{-1})/2$ for $n = 0, 1, 2, \ldots$ which can be proved to converge to the limit $Y = \sqrt{H}$ most easily by using that factorization again. If (as seems unlikely) a general formula exists to compute $\sqrt{H}$ using only finitely many rational arithmetic operations and square roots, nobody has found it. No matter how $\sqrt{H}$ may be constructed, we come now to the task of proving it unique.

Suppose V and Y are both real symmetric and positive definite, and $V^2 = Y^2 = H$. Then $x^T(V+Y)(V-Y)x = x^T(YV-VY)x = 0$ for all x. To infer that $V = Y$ let μ be an extreme (maximum or minimum) value of the quotient $x^T(V-Y)x/x^Tx$ as x runs over all nonzero vectors x. Then setting the quotient's derivative to zero yields $(V-Y)x = \mu x$; each extreme value μ must be an eigenvalue of $V-Y$ with an eigenvector x for which we find that $0 = x^T(V+Y)(V-Y)x = \mu x^T(V+Y)x$. Since V and Y are positive definite, $x^T(V+Y)x > 0$; therefore every extreme value $\mu = 0$, whence $x^T(V-Y)x = 0$ for all x, which implies $V-Y = O$ thus: $4z^T(V-Y)x = (x+z)^T(V-Y)(x+z) - (x-z)^T(V-Y)(x-z) = 0$ for all x and z.

The existence and uniqueness of a positive definite matrix's positive definite square root is worth noting because square roots of a matrix are not so simple in general, not even for 2-by-2 matrices. For instance, $\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ has no square root; $\begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}$ has just two; $\begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix}$ has four; and $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ has infinitely many. Can you see why?

3. Show that if H, M and $H–M$ are symmetric and positive definite, so is $M^{-1} – H^{-1}$.

Solution: Verify the identity $M^{-1} – H^{-1} = H^{-1}(H–M)H^{-1} + H^{-1}(H–M)M^{-1}(H–M)H^{-1}$, and then observe that it expresses $M^{-1} – H^{-1}$ as a sum of positive definite matrices, which must also be positive definite. Another shorter identity $M^{-1} – H^{-1} = M^{-1}((H–M)^{-1} + M^{-1})^{-1} M^{-1}$ works too but is trickier to verify. A third proof uses $Y := \sqrt{H}$ and $X := \sqrt{(Y^{-1}MY^{-1})}$ to deduce that $I – X^2 = Y^{-1}(H–M)Y^{-1}$ is positive definite, whence the same conclusion follows for $M^{-1} – H^{-1} = Y^{-1}(X^{-2} – I)Y^{-1} = (XY)^{-1}(I – X^2)(XY)^{-1T}$.

4. Show that if H, M and $H–M$ are symmetric and positive definite, so is $\sqrt{H} – \sqrt{M}$.

Solution: One proof uses $\sqrt{H} = (2/\pi)\int_0^\infty (I + \xi^2H^{-1})^{-1}\, d\xi$ and $\sqrt{M} = (2/\pi)\int_0^\infty (I + \xi^2M^{-1})^{-1}\, d\xi$ from problem 2's solution as starting points. For every $\xi > 0$ apply problem 3 twice to infer that first $(I + \xi^2M^{-1}) – (I + \xi^2H^{-1})$ and then $(I + \xi^2H^{-1})^{-1} – (I + \xi^2M^{-1})^{-1}$ are positive definite; then integrate to deduce the same for $\sqrt{H} – \sqrt{M}$. Another proof parallels the uniqueness proof of problem 2: Let the minimum of the quotient $z^T(\sqrt{H} – \sqrt{M})z/z^Tz$ be μ, the least eigenvalue of $\sqrt{H} – \sqrt{M}$, so that $(\sqrt{H} – \sqrt{M})z = \mu z$ for an eigenvector $z \neq o$. Then $\sqrt{M}z = (\sqrt{H} – \mu I)z$, whence $0 < z^T(H–M)z = z^T(H – (\sqrt{H} – \mu I)^2)z = 2\mu z^T\sqrt{H}z – \mu^2z^Tz$, and therefore $\mu > 0$.

5. Show that H, M and $H–M$ can be symmetric and positive definite when $H^2 – M^2$ is not.

Solution: The fact that a real symmetric matrix is positive definite if and only if it and its every principal submatrix have positive determinants helps to reveal the following 2-by-2 examples:

$H = \begin{bmatrix} 2 & 2 \\ 2 & 9 \end{bmatrix}$, $M = \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix}$ and $H–M = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix}$ are positive definite but $H^2 – M^2 = \begin{bmatrix} 7 & 22 \\ 22 & 69 \end{bmatrix}$ isn't.

$H = \begin{bmatrix} 3 & 3 \\ 3 & 8 \end{bmatrix}$, $M = \begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix}$ and $H–M = \begin{bmatrix} 2 & 3 \\ 3 & 5 \end{bmatrix}$ are positive definite but $H^2 – M^2 = \begin{bmatrix} 17 & 33 \\ 33 & 64 \end{bmatrix}$ isn't.

$H = \begin{bmatrix} 8 & 5 \\ 5 & 9 \end{bmatrix}$, $M = \begin{bmatrix} 1 & 0 \\ 0 & 5 \end{bmatrix}$ and $H–M = \begin{bmatrix} 7 & 5 \\ 5 & 4 \end{bmatrix}$ are positive definite but $H^2 – M^2 = \begin{bmatrix} 88 & 85 \\ 85 & 81 \end{bmatrix}$ isn't.