An $O(n)$ Method for Max Entry of $ST^{-1}S$

If $T = LDL^T$ then

$$ST^{-1}S \;=\; S(LDL^T)^{-1}S = SL^{-T}D^{-1}L^{-1}S = -(XS)^T(XS)$$

where $X = D^{-1/2}L^{-1}$. So the problem is to find which column of XS has the largest 2-norm. If

$$S = \begin{bmatrix} 0 & -\alpha_1 & 0 & 0 & 0 \\ \alpha_1 & 0 & -\alpha_2 & 0 & 0 \\ 0 & \alpha_2 & 0 & -\alpha_3 & 0 \\ 0 & 0 & \alpha_3 & 0 & -\alpha_4 \\ 0 & 0 & 0 & \alpha_4 & 0 \end{bmatrix}$$

then

$$XS = \left[\; \alpha_1 X(:,2) \;\middle|\; -\alpha_1 X(:,1) + \alpha_2 X(:,3) \;\middle|\; -\alpha_2 X(:,2) + \alpha_3 X(:,4) \;\middle|\; -\alpha_3 X(:,3) + \alpha_4 X(:,5) \;\middle|\; -\alpha_4 X(:,4) \;\right]$$

So for $k = 1{:}n$ we have to compute

$$\gamma_k = \begin{cases} |\alpha_1|^2 \| \, X(:,2) \, \|_2^2 & \text{if } k = 1 \\[2ex] \| -\alpha_{k-1}X(:,k-1) + \alpha_k X(:,k+1) \, \|_2^2 & \text{if } k = 2{:}n-1 \\[2ex] |\alpha_{n-1}|^2 \| \, X(:,n-1) \, \|_2^2 & \text{if } k = n \end{cases}$$

i.e.,

$$\gamma_k = \begin{cases} |\alpha_1|^2 \| \, X(:,2) \, \|_2^2 & \text{if } k = 1 \\[2ex] |\alpha_{k-1}|^2 \| \, X(:,k-1) \, \|_2^2 + |\alpha_k|^2 \| \, X(:,k+1) \, \|_2^2 - 2\alpha_{k-1}\alpha_k X(:,k-1)^T X(:,k+1) & \text{if } k = 2{:}n-1 \\[2ex] |\alpha_{n-1}|^2 \| \, X(:,n-1) \, \|_2^2 & \text{if } k = n \end{cases}$$

The function `maxElement` must return the largest γ_i. Each $X(:,k)$ can be computed in $O(n)$ flops and so there is an obvious $O(n^2)$ implementation.

But the matrix X has some critical patterns and if they are exploited we can obtain an $O(n)$ implementation of `maxElement`. Let's look at the inverse of

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -e_1 & 1 & 0 & 0 & 0 \\ 0 & -e_2 & 1 & 0 & 0 \\ 0 & 0 & -e_3 & 1 & 0 \\ 0 & 0 & 0 & -e_4 & 1 \end{bmatrix} \;=\; I - \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ e_1 & 1 & 0 & 0 & 0 \\ 0 & e_2 & 1 & 0 & 0 \\ 0 & 0 & e_3 & 1 & 0 \\ 0 & 0 & 0 & e_4 & 1 \end{bmatrix} \;=\; I - E$$

then $L^{-1} = I + E + E^2 + \cdots + E^{n-1}$, e.g.,

$$L^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ e_1 & 1 & 0 & 0 & 0 \\ e_1e_2 & e_2 & 1 & 0 & 0 \\ e_1e_2e_3 & e_2e_3 & e_3 & 1 & 0 \\ e_1e_2e_3e_4 & e_2e_3e_4 & e_3e_4 & e_4 & 1 \end{bmatrix}$$

If $D = \mathrm{diag}(d_1, \ldots, d_n)$ then

$$X \; = \; D^{-1/2}L^{-1} \; = \; \begin{bmatrix} 1/\sqrt{d_1} & 0 & 0 & 0 & 0 \\ e_1/\sqrt{d_2} & 1/\sqrt{d_2} & 0 & 0 & 0 \\ e_1e_2/\sqrt{d_3} & e_2/\sqrt{d_3} & 1/\sqrt{d_3} & 0 & 0 \\ e_1e_2e_3/\sqrt{d_4} & e_2e_3/\sqrt{d_4} & e_3/\sqrt{d_4} & 1/\sqrt{d_4} & 0 \\ e_1e_2e_3e_4/\sqrt{d_5} & e_2e_3e_4/\sqrt{d_5} & e_3e_4/\sqrt{d_5} & e_4/\sqrt{d_5} & 1/\sqrt{d_5} \end{bmatrix}$$

Note that $\| X(:,n) \|^2 = 1/d_n$ and for $k = 1{:}n-1$

$$\begin{aligned} \| X(:,k) \|_2^2 \; = \; \| X(k{:}n,k) \|_2^2 \;\; &= \;\; \frac{1}{d_k} \; + \; \| X(k+1{:}n,k) \|_2^2 \\ &= \;\; \frac{1}{d_k} \; + \; e_k^2 \cdot \| X(k+1{:}n,k+1) \|_2^2 \; = \; \frac{1}{d_k} \; + \; e_k^2 \cdot \| X(:,k+1) \|_2^2 \end{aligned}$$

Thus, if $\mu_k = \| X(:,k) \|_2^2$ then we can compute $\mu_1, \ldots, \mu_n$ in $O(n)$ flops:

```
μ_n = 1/d_n
for k = n − 1: − 1:1
      μ_k = (1/d_k) + e_k^2 μ_{k+1}
end
```

Looking back at the recipe for the γ_k, we need a quick method of evaluating $X(:,k-1)^T X(:,k+1)$, $k = 2{:}n-1$. Here it is:

$$X(:,k-1)^T X(:,k+1) = e_{k-1}e_k \| X(:,k+1) \|_2^2 \; = \; e_{k-1}e_k\mu_{k+1}$$

So the recipe for the γ_k transforms to

$$\gamma_k = \begin{cases} |\alpha_1|^2\mu_2 & \text{if } k = 1 \\ |\alpha_{k-1}|^2\mu_{k-1} + |\alpha_k|^2\mu_{k+1} - 2\alpha_{k-1}\alpha_k e_{k-1}e_k\mu_{k+1} & \text{if } k = 2{:}n-1 \\ |\alpha_{n-1}|^2\mu_{n-2} & \text{if } k = n \end{cases}$$