# Imprementation details

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## Computing $\log(A)$ without preconditioning

We consider the computation of $\log(A)$ for HPD matrices using the Gauss–Legendre (GL) quadrature to

$$\log(A) = \int_{-1}^{1} F(t; A)\,\mathrm{d}t \qquad \left(F(t; A) = (A - I)[(1 - t)I + (1 + t)A]^{-1}\right). \tag{1}$$

Initially, we scale the matrix $A$ to $\tilde{A} := cA$ with $c = 1/\sqrt{\lambda_{\max}\lambda_{\min}}$ to optimize the convergence rate. The scaling changes the extreme eigenvalues of $\tilde{A}$ to $\sqrt{\kappa}$ and $1/\sqrt{\kappa}$, where $\kappa$ is the condition number of $A$.

Subsequently, we select the number of abscissas $m$ according to the given error tolerance $\varepsilon$. Here, the error of the GL quadrature for $\log\left(\tilde{A}\right)$ can be estimated as that for scalar logarithms:

$$\left\|\log\left(\tilde{A}\right) - \sum_{k=1}^{m} F\left(t_k; \tilde{A}\right)\right\|_2 = \max_{\lambda\in\Lambda}\left|\log(c\lambda) - \sum_{k=1}^{m} F(t_k; c\lambda)\right|, \tag{2}$$

where $\Lambda$ is the spectrum of $A$. When $m$ is sufficiently large, the error associated with the extreme eigenvalues will dominate. Thus, we presume the error of the $m$-point GL quadrature for $\log\left(\tilde{A}\right)$ as

$$\left\|\log\left(\tilde{A}\right) - \sum_{k=1}^{m} F\left(t_k; \tilde{A}\right)\right\|_2 \approx \left|\log\left(\sqrt{\kappa}\right) - \sum_{k=1}^{m} F\left(t_k; \sqrt{\kappa}\right)\right|. \tag{3}$$

In our implementation, for the error tolerance $\varepsilon$, we find the minimum $m$ satisfying

$$\left|\log\left(\sqrt{\kappa}\right) - \sum_{k=1}^{m} F\left(t_k; \sqrt{\kappa}\right)\right| \le \varepsilon. \tag{4}$$

Then we compute $\log(A)$ with the $m$-point GL quadrature.

## Computing $\log(A)$ with the preconditioning

When we use the preconditioning, $\log(A)$ is computed via

$$\log(A) = \log\left(c'\tilde{A}\tilde{P}_1\right) - \log\left(c'\tilde{P}_1\right) - \log(c)I, \tag{5}$$

where $c' = \sqrt{\left(\kappa^{1/2} + 1\right)\left(\kappa^{-1/2} + 1\right)}$. In practice, it is not necessary to explicitly compute the inverse in $\tilde{P}_1$. For the computation of $\log\left(c'\tilde{A}\tilde{P}_1\right)$, the integrand can be rewritten as

$$\begin{aligned}
F\left(t; c'\tilde{A}\tilde{P}_1\right) &= \left[c'\tilde{A}\tilde{P}_1 - I\right]\left[(1 - t)I + (1 + t)c'\tilde{A}\tilde{P}_1\right]^{-1} \\
&= \left[c'\tilde{A}\left(\tilde{A} + I\right)^{-1} - I\right]\left[(1 - t)I + (1 + t)c'\tilde{A}\left(\tilde{A} + I\right)^{-1}\right]^{-1} \\
&= \left[c'\tilde{A} - \left(\tilde{A} + I\right)\right]\left[(1 - t)\left(\tilde{A} + I\right) + (1 + t)c'\tilde{A}\right]^{-1} \\
&= \left[(c' - 1)\tilde{A} - I\right]\left[((c' - 1)t + 1 + c')\tilde{A} + (1 - t)I\right]^{-1},
\end{aligned} \tag{6}$$

and the integrand $F\left(t; c'\tilde{P}_1\right)$ can be rewritten as

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\begin{aligned}
F\left(t; c'\tilde{P}_1\right) &= \left[c'\tilde{P}_1 - I\right]\left[(1-t)I + (1+t)c'\tilde{P}_1\right]^{-1} \\
&= \left[c'\left(\tilde{A}+I\right)^{-1} - I\right]\left[(1-t)I + (1+t)c'\left(\tilde{A}+I\right)^{-1}\right]^{-1} \\
&= \left[c'I - \left(\tilde{A}+I\right)\right]\left[(1-t)\left(\tilde{A}+I\right) + (1+t)c'I\right]^{-1} \\
&= \left[-\tilde{A} + (c'-1)I\right]\left[(1-t)\tilde{A} + ((c'-1)t + c' + 1)I\right]^{-1}.
\end{aligned} \tag{7}
$$

# Imprementation of the DE formula

The DE formula exploits the trapezoidal rule after applying a specialized change of variables. Because the convergence analysis in the non-reviewed report [1] is conducted using the variable transformation $\tanh(\pi \sinh(x)/2)$, we also use $\tanh(\pi \sinh(x)/2)$ while the original paper [2] uses the change of variables $t = t(x) = \tanh(\sinh(x))$.

In the experiments, in order to use the different change of variables and bound the absolute error, we modifed the $m$-point DE formula algorithm [2, Alg. 1] as follows:

- $F_{\mathrm{DE}}(x) = \cosh(x)\,\mathrm{sech}^2(\sinh(x)))[(1 + \tanh(\sinh(x)))(A - I) + 2I]^{-1}$
  $\rightarrow \quad F_{\mathrm{DE}}(x) = \frac{\pi \cosh(x)\,\mathrm{sech}^2(\pi \sinh(x)/2)}{2}[(1 + \tanh(\pi \sinh(x)/2))(A - I) + 2I]^{-1}$
- $\theta = |\log(\rho(A))| \quad \rightarrow \quad \theta = 1$
- $l = \mathrm{asinh}(\mathrm{atanh}(2a - 1)) \quad \rightarrow \quad l = \mathrm{asinh}(2\,\mathrm{atanh}(2a - 1)/\pi)$
- $r = \mathrm{asinh}(\mathrm{atanh}(2b - 1)) \quad \rightarrow \quad r = \mathrm{asinh}(2\,\mathrm{atanh}(2b - 1)/\pi)$

# Bibliography


[1] F. Tatsuoka, T. Sogabe, T. Kemmochi, and S.-L. Zhang, “On the convergence rate of the double exponential formula for the computation of the matrix logarithm (in Japanese),” *RIMS Kokyuroku*, vol. 2167, pp. 1–9, 2020, [Online]. Available: http://hdl.handle.net/2433/261512

[2] F. Tatsuoka, T. Sogabe, Y. Miyatake, and S.-L. Zhang, “Algorithms for the computation of the matrix logarithm based on the double exponential formula,” *J. Comput. Appl. Math.*, vol. 373, p. 11–12, 2020, doi: 10.1016/j.cam.2019.112396.