Gaussian Markov improvement algorithm and its derivatives

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1 Sparse matrix techniques

To compute the CEI for all solutions $\boldsymbol{x} \in \mathcal{X}$, one needs to compute the conditional mean $M(\boldsymbol{x})$ for all solutions and the conditional variance $V(\boldsymbol{x}, \tilde{\boldsymbol{x}})$ of the difference between all solutions and the current best $\tilde{\boldsymbol{x}}$. Computing $M(\boldsymbol{x})$ for all solutions requires a factorisation of $\bar{Q}$, the conditional precision matrix, and a backsolve operation. Computing $V(\boldsymbol{x}, \tilde{\boldsymbol{x}})$ for all solutions requires the conditional variance $V(\boldsymbol{x})$ of all solutions and the conditional correlation $C(\boldsymbol{x}, \tilde{\boldsymbol{x}})$ between all solutions and the current best $\tilde{\boldsymbol{x}}$. Computing $C(\boldsymbol{x}, \tilde{\boldsymbol{x}})$ for all solutions requires a factorisation of $\bar{Q}$ and a backsolve operation to obtain the column of $\bar{Q}^{-1}$ relating to $\tilde{\boldsymbol{x}}$. Computing $V(\boldsymbol{x})$ for all solutions requires each diagonal element of $\bar{Q}^{-1}$, which is more problematic.

The main bottleneck in the original GMIA algorithm is in factorising $\bar{Q}$ and using this to compute diagonal elements of $\bar{Q}^{-1}$. The original GMIA algorithm does the latter with a full inversion. Semelhago et al. (2017) show an efficient way of computing diagonal elements without full inversion. This relies on an identity for the covariance matrix given by Takahashi (1973), explained by Vanhatalo and Vehtari (2012) which gives simple expressions for desired elements of $\bar{Q}^{-1}$ which are functions of elements of the factors of $\bar{Q}$. Semelhago et al. (2017) also show how factorising can be avoided using the Sherman-Morrison-Woodbury identity, which they use to update $M(\boldsymbol{x})$ using old factors of $\bar{Q}$ when they are not updating $V(\boldsymbol{x})$.

References

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