

lintegrate: A C/Python numerical integration library for working in log-space

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Summary

There are many situations in which the integral of a function must be evaluated numerically between given limits. For C codes, there is a range of numerical integration (sometimes called numerical quadrature) functions provided within the GNU Scientific Library (GSL) (Galassi et al., 2009). However, in situations where the integrand has an extremely large dynamic range these GSL functions can fail due to numerical instability. One way to get around numerical instability issues is to work with the natural logarithm of the function. The logarithm of the function cannot simply be integrated as this will not produce the logarithm of the integral of the original function. lintegrate provides a range of C integration functions, equivalent to functions in GSL, that allow the integration of a function when only working with the natural logarithm of the integral of the original function is computationally practical. The result that is returned is the natural logarithm of the integral of the underlying function. lintegrate also provides a Python (vanRossum, 1995) module for accessing some of these functions in Python.

Statement of need

A particular case where the natural logarithm of a function is generally numerically favourable is when evaluating likelihoods in statistical applications. For example, the Gaussian likelihood of a model $m(\vec{\theta})$, defined by a set of model parameters $\vec{\theta}$ and given a data set d consisting N points, is

$$L(\vec{\theta}) \propto \exp\left(-\sum_{i=1}^{N} \frac{(d_i - m_i(\vec{\theta}))^2}{2\sigma_i^2}\right),\tag{1}$$

where σ_i^2 is an estimate of the noise variance for point *i*. Evaluating the exponent for a range of $\vec{\theta}$ values will often lead to a numbers that breach the limits of values that are storable as double precision floating point numbers and/or have an extremely large dynamic range. In these cases, when performing marginalisation (i.e., integration) over some subset of the parameters $\vec{\theta}$, e.g.,

$$Z = \int^{\theta_1} L(\vec{\theta}) \pi(\theta_1) \mathrm{d}\theta_1, \tag{2}$$

where $\pi(\theta_1)$ is the prior probability distribution for the parameter θ_1 , it is not possible to work directly with Equation 1. Instead, it helps to work with the natural logarithm of the likelihood:

$$\ln L(\vec{\theta}) = C - \sum_{i=1}^{N} \frac{(d_i - m_i(\vec{\theta}))^2}{2\sigma_i^2}.$$
(3)

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Software

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lintegrate allows the calculation of the logarithm of Z in Equation 2, while working with the natural logarithm of integrands such as in Equation 3.

lintegrate was originally developed to marginalise probability distributions for the hierarchical Bayesian inference of pulsar ellipticity distributions in Pitkin et al. (2018). In Nash & Durkan (2019) and Strauss & Oliva (2021), lintegrate has been used to calculate the "true" value of integrals to compare against values learned or inferred through other methods as a form of validation.

Availability and development

lintegrate is open source code, released under a GPL-3.0 license. The source code is publically hosted on GitHub, while release versions of the Python library are available through PyPI and conda-forge. Documentation of the C library functions and Python interface can be found on Read the Docs, including the API and example usage.

Contributions to the code are welcome via the GitHub issues tracker or Pull Requests. Continuous integration is set up to run a test suite on the code when any changes are made.

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