Numerical integration in many dimensions. III

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Extending a previous line of work, a powerful computational method is found for numerical integration in many dimensions of functions of the form $F(f_1(x_1,x_2)+f_2(x_2,x_3)+f_3(x_3,x_4)+\cdots+f_d(x_d,x_1))$.

I. INTRODUCTION

In a previous paper[1] a method for fast and accurate machine computation of d-dimensional integrals, where the integrand was of the form $F(f_1(x_1)+f_2(x_2)+\cdots+f_d(x_d))$ was presented. The first step was to introduce an integral transform representation of the function F so that its argument appeared in an exponential, then each of the d integrations over the coordinates x_i could be done separately, with the final product then numerically integrated over the transform variable. If n lattice points were needed for the adequate numerical evaluation of each one-dimensional integral, then this method would require of the order of n^2d operations: This is enormously better than the n^d operations that would be required in a direct integration method. Now this method of approach is extended to a more complicated integrand, in which the argument of the general function F has the coordinates x_i linked together in a chain.

II. THE METHOD

Consider the integral over the d-dimensional product space

$$I=\left(\prod_{i=1}^{d}\int g_i(x_i)dx_i\right)F\left(\sum_{i=1}^{d}f_i(x_i,x_{i+1})\right), \tag{1}$$

where $x_{d+1}=x_1$. Start, as before, with some integral transform

$$F(s)=\int d\sigma\,\hat{F}(\sigma)e^{su(\sigma)}, \tag{2}$$

where the integration takes place along some suitable contour. Then we have

$$I=\int d\sigma\,\hat{F}(\sigma)J(\sigma), \tag{3}$$

where

$$J(\sigma)=\left(\prod_{i=1}^{d}\int g_i(x_i)dx_i\right)\exp\left(u(\sigma)\sum_{i=1}^{d}f_i(x_i,x_{i+1})\right). \tag{4}$$

Now introduce the numerical quadrature rule of choice for each x_i:

$$\int h(x)dx\cong\sum_{j=1}^{n}w_jh(z_j). \tag{5}$$

We assume, only for simplicity of notation, that we use the same quadrature rule (points z_j and weights w_j) for each x_i integration variable.

Now comes the coup. Notice, that with the definition

$$A^{i}_{jj'}(\sigma)=w_j\,g_i(z_j)\exp[u(\sigma)f_i(z_j,z_{j'})], \tag{6}$$

we can write the multiple integration in terms of the matrices A^i:

$$J(\sigma)=\mathrm{Trace}\,A^1(\sigma)A^2(\sigma)\cdots A^d(\sigma). \tag{7}$$

There are n^2 elements in each of d matrices, and these must be evaluated for each of n values of σ. The multiplication of two matrices requires n^3 multiplications of numbers. Therefore the total amount of computer time for this method is of the order of n^3d function evaluations plus n^4d additional multiplications. For n of the order of 10, this means that we can evaluate integrals with d into the hundreds or more for pennies.

Once again, a problem that seemed to increase exponentially with the number of dimensions has been reduced to a procedure that increases only linearly. The choice of the integral transform is of course important, and the reader is referred to Ref. 1, where several examples are given.

III. FURTHER COMMENTS

If the entire integrand is symmetric in all variables (all functions f_i and g_i given by a single f and g), then there is only a single matrix A; and then

$$J=\sum_{j=1}^{n}(\lambda_j)^d, \tag{8}$$

where the λ_j are the eigenvalues of the matrix A (for each value of σ). Thus we can even take the limit as d goes to infinity, with the answer given in terms of the largest eigenvalue of A.

If the structure of the integrand is that of an *open* chain [i.e., if the function $f_d(x_d,x_1)$ is absent in (1)], then the problem is simplified a bit. The work of multiplying the matrices is reduced by a factor of n.

The technique used here for handling the multiple sum over chain-linked variables leads to the study of some well-known problems in statistical mechanics. I have applied this approach to the Ising model in one, two, and three dimensions; and these results will be published separately.

[1] C. Schwartz, J. Math. Phys. **26**, 951 (1985).

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