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Effect of grid-point packing fraction on Reimann summation

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January 2, 2017

1 SIMPLE EXAMPLE

Consider functions defined on the unit square that will be integrated using Riemann summation. As an example, we will begin with $f(x, y) = \sin(\pi x)\sin(\pi y)$. This function is shown in Fig. 1.1.

The obvious way to integrate this function numerically is to partition the domain into $n \times n$ squares, evaluate the function in each square and then perform the sum:

$$S = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} f(x_i, y_i)\Delta x \Delta y$$

Riemann summation is formally equivalent to writing the function as a Fourier series and then integrating the series term by term (only the leading, constant term contributes a non-zero value). Figure 1.2 shows the simple idea of a straight-forward grid for the numerical integration. The so-called *Monkhorst-Pack* grids are the generalization of this to idea to integration domains defined by (generally) non-orthogonal basis vectors.

2 PACKING FRACTION AND NON-MP GRIDS

In his book on lattice integration methods, Ian Sloan, makes an argument (I'll include it later after I get the book back from the library) that the effectiveness of a particular integration grid is related to the packing fraction of the integration points. The heart of the argument comes from expressing the integrand as a Fourier series.

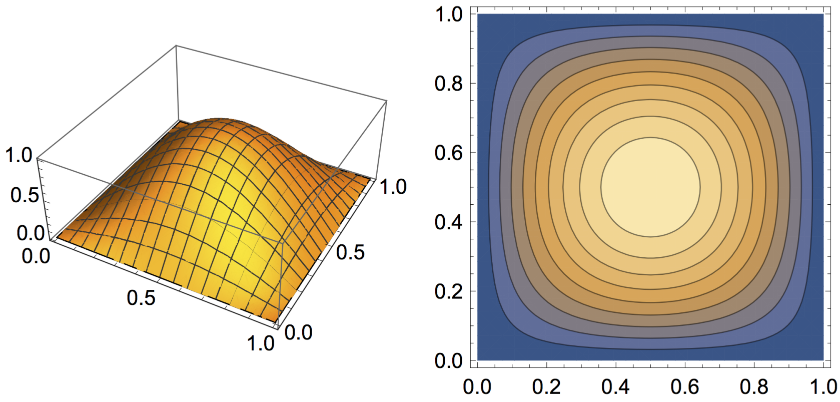

Figure 1.1: Two different visualizations of the function $f(x, y) = \sin(\pi x)\sin(\pi y)$.

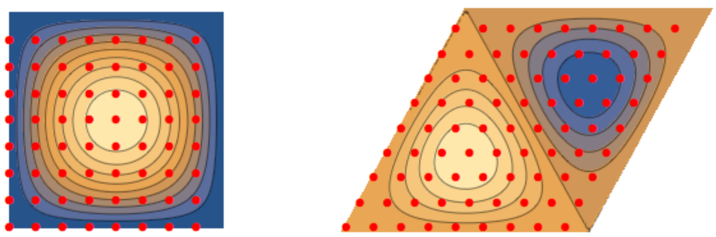

Figure 1.2: Examples of two integration grids. Left: A function defined over a square domain. The integration grid points lie on surfaces of constant Cartesian coordinates. The integration grid "tile" is, except for scale, identical to the function domain. Right: A function defined over a rhombus and the corresponding Monkhorst-Pack-type grid. The integration grid is defined by lattice vectors that are not orthogonal. Again the integration grid tile is a scaled-down replica of the domain.

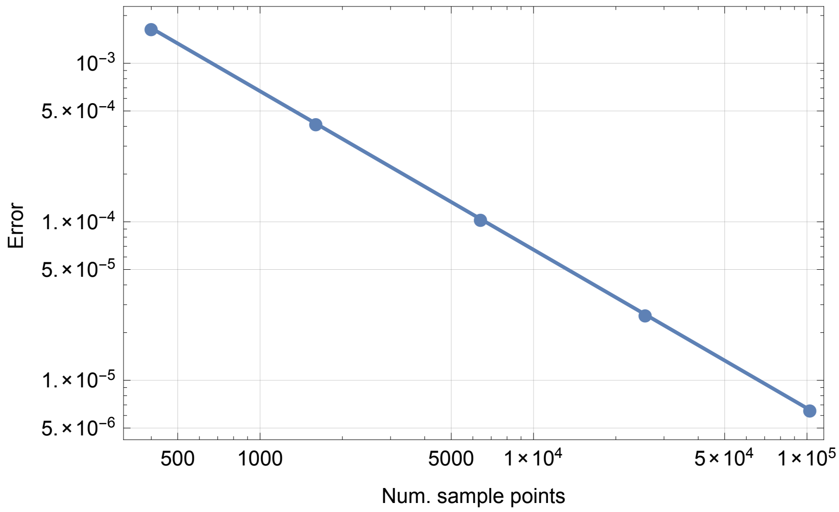

Figure 2.1: Convergence of numerical integral as a function of number of sample points. The absolute error decrease is proportional to the number of sample points.

The function shown in Fig. 1.1 has a slowly converging Fourier series because it is not smooth at the domain edges. Consequently, we expect that numerical integration will converge rather slowly. Indeed, in Fig. 2.1, we see that the absolute error in the integral decreases as $\mathcal{O}(1/N)$ where N is the number of sample points.