1 singular 1/r

We want to compute by quadrature:

$$\int_a^b f(r)\,\mathrm{d}r \quad \text{with} \quad f(r) = \frac{1}{r} \quad . \tag{1}$$

For $a = 10^{-3}$ and $b = 1.0$, the analytical result is $\log(b) - \log(a) \approx 6.91$. Standard trapezoidal quadrature on 100 points leads to

$$\sum_{i=0}^{99} \frac{1/x_i + 1/x_{i+q}}{2} \Delta x \approx 10.1 \tag{2}$$

where

$$x_i = a + \frac{i}{100-1} \Delta x \text{ and } \Delta x = \frac{b-a}{100-1} \quad . \tag{3}$$

This specific quadrature can be made much more accurate by a substitution that leads to

$$\int_{s(a)}^{s(b)} \frac{1}{r} r \,\mathrm{d}s = [s]_{s(a)}^{s(b)} \quad , \tag{4}$$

for which we need

$$\mathrm{d}r = r\,\mathrm{d}s \quad . \tag{5}$$

Rephrase:

$$\frac{\mathrm{d}r}{r} = \mathrm{d}s \Leftrightarrow \int \frac{\mathrm{d}r}{r} = \int \mathrm{d}s \Leftrightarrow \log(r) = s \quad . \tag{6}$$

The quadrature for the substituded integral is then:

$$\sum_{i=0}^{99} \dots \tag{7}$$

2 nearly-singular 1/(r+eps)

We want to compute:

$$\int_a^b f(r)\,\mathrm{d}r \text{ where } f(r) \propto \frac{1}{\sqrt{r^2 + \epsilon^2}} \quad . \tag{8}$$

If we take f to be the pure kernel function, an analytical solution to this can be found:

$$\int_a^b \frac{1}{\sqrt{r^2+\epsilon^2}}\,\mathrm{d}r = \log\left(b + \sqrt{b^2+\epsilon^2}\right) - \log\left(a + \sqrt{a^2+\epsilon^2}\right) \quad . \tag{9}$$

Again do the substitution trick:

$$\int_a^b f(r)\,\mathrm{d}r = \int_{s(a)}^{s(b)} f(r)\left(\sqrt{r^2+\epsilon^2}\right)\mathrm{d}s \quad , \tag{10}$$

where we used

$$\mathrm{d}r = \left(\sqrt{r^2+\epsilon^2}\right)\mathrm{d}s \quad . \tag{11}$$

The substitution is therefore

$$s = \log\left(r + \sqrt{r^2+\epsilon^2}\right) \quad . \tag{12}$$