HW1 Solutions
Computational Physics
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Gregg Stiesberg

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1.4

Results for

$$\int_0^1 \frac{1}{\frac{1}{4}+\frac{\pi}{8}} \frac{1}{(1+x^2)^2} dx$$

using `trapint()` and `simpint()`:

```
Trap, Simp:       2     0.98413086001031,    0.98802070530679
Trap, Simp:      20     0.99983794339634,    0.99999991848188
Trap, Simp:     200     0.99999837923315,    0.99999999999190
Trap, Simp:    2000     0.99999998379231,    1.00000000000000
Trap, Simp:   20000     0.99999999983792,    1.00000000000000
Trap, Simp:  200000     0.99999999999836,    0.99999999999998
Trap, Simp: 2000000     1.00000000000010,    1.00000000000016
```

I have included some extra calculation here. Notice that roundoff errors are creeping in when many intervals are used; this is telling us that we have to consider the machine precision when deciding what resolution to use in our calculations. There are proper techniques to minimize this error- see the NR book.

2.1

Using the suggested change of variables we find that

$$r(u) = \frac{1}{1-u} - 1 = \frac{u}{1-u}$$

$$\frac{dr(u)}{du} = \frac{1}{(1-u)^2}.$$

Thus the integral being evaluated will be

$$I = 4 \int_0^1 \left(e^{-\left(\frac{u}{1-u}\right)} \right) \left(\frac{u^2}{(1-u)^4} \right) du.$$

The lower integration limit is well defined; however the upper limit requires some thought, since the exponential will be zero, and the rational expression will be ∞. Thinking about the limit as $u \to 1^-$, it can be shown that the exponential will decrease faster than the reciprocal of any polynomial (this is easily seen by considering the series expansion). Therefore the exponential wins, and the proper changes to the driver code for the upper limit of integration are

```
f[N]=0.0;
dr[N]=0.0;
```

Note that it necessary to specify the value for f also, since the exponent is also approaching ∞; undefined $\times$ zero will should still be undefined. (The floating point standard probably defines these situations explicitly- see the link to the floating point article on the course web page.)

The results of the calculation are:

```
Trap, Simp:       2     1.08268226589290,    1.44357635452387
Trap, Simp:      20     1.00000051060024,    0.99992390776598
Trap, Simp:     200     1.00000000004167,    0.99999999983334
Trap, Simp:    2000     1.00000000000000,    0.99999999999998
Trap, Simp:   20000     1.00000000000000,    1.00000000000000
Trap, Simp:  200000     0.99999999999998,    0.99999999999998
```

and if the upper limit is not explicitly cared for, disaster strikes:

```
Trap, Simp:       2                 nan,                 nan
Trap, Simp:      20                 nan,                 nan
Trap, Simp:     200                 nan,                 nan
.
.
.
```

2.2

Here we have a similar calculation, with one less power of r. When the change of variables is applied, we still have the same limit to consider as $u \to 1^-$, and hence the same endpoint conditions to impose. Running the code yields

```
Trap, Simp:       2    -1.08268226589290,   -1.44357635452387
Trap, Simp:      20    -0.99916646582534,   -1.00001769724284
Trap, Simp:     200    -0.99999166666667,   -0.99999999999999
Trap, Simp:    2000    -0.99999991666667,   -1.00000000000000
Trap, Simp:   20000    -0.99999999916666,   -1.00000000000000
Trap, Simp:  200000    -0.99999999999165,   -0.99999999999997
```

2.3

Here we have an integral with pieces we have already calculated, up to constants:

$$V_{ee} = 2\int_0^\infty \left[re^{-2r} - re^{-4r} - r^2e^{-4r}\right] dr$$

The code returns

```
Trap, Simp:       2     0.39481602183658,    0.52642136244877
Trap, Simp:      20     0.31250010782537,    0.31250803836510
Trap, Simp:     200     0.31250000002083,    0.31249999991666
Trap, Simp:    2000     0.31250000000000,    0.31249999999999
Trap, Simp:   20000     0.31250000000000,    0.31250000000000
Trap, Simp:  200000     0.31250000000000,    0.31250000000000
```

which agrees with the analytic result.

-The End-