

Assignment 3

https://github.com/jchryssanthacopoulos/quantum_information/tree/main/assignment_3

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Exercise 1: Matrix Multiplication Scaling



- Matrix multiplication program extended to parse command-line arguments using `get_command_argument`
- Python script written in Jupyter notebook to make subprocess calls to Fortran program to get runtimes

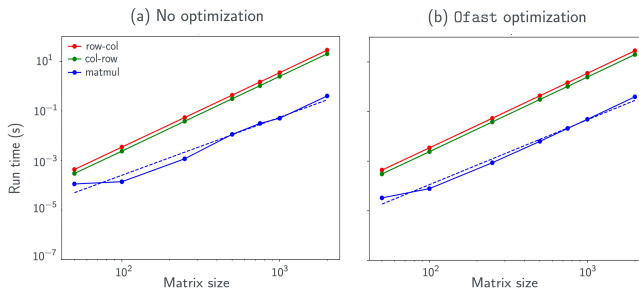
```
$ compiled/exercise_1_00 \  
--mat_mul_method matmul --num_rows 3 \  
--num_cols 3 --num_inner_dim 4 --debug  
mat_mul_method = matmul  
num_rows = 3  
num_cols = 3  
num_inner_dim = 4  
Running in debug mode ...  
Matrix A =  
  0.43  0.39  0.04  0.17  
  0.42  0.95  0.88  0.55  
  0.01  0.19  0.47  0.62  
Matrix B =  
  0.10  0.37  0.73  
  0.96  0.39  0.38  
  0.03  0.53  0.23  
  0.21  0.36  0.69  
Product =  
  0.45  0.39  0.59  
  1.10  1.19  1.25  
  0.33  0.55  0.62  
Elapsed time = 7.000000000E-06
```

```
def get_run_time(mat_mul_method, flag, mat_dim):  
    """Get the run time for the given matrix multiplication method,  
    optimization flag, and matrix dimension.  
    """  
    run_params = [  
        f"{program_base_name}_{flag}",  
        "--mat_mul_method", mat_mul_method,  
        "--num_rows", str(mat_dim),  
        "--num_cols", str(mat_dim),  
        "--num_inner_dim", str(mat_dim)  
    ]  
  
    output = subprocess.run(  
        run_params, stdout=subprocess.PIPE, encoding='ascii'  
    )  
  
    lines = output.stdout.split('\n')  
  
    return float(lines[4].split('=')[1])
```

Exercise 1: Matrix Multiplication Scaling



Linear fit of log run time to log matrix size
performed with numpy's polyfit



Method	O0	O1	O2	O3	Ofast
row-col	3.01	3.01	3.00	3.00	3.00
col-row	3.02	3.01	3.02	3.00	3.01
matmul	2.34	2.64	2.57	2.66	2.61

Table: Polynomial time complexity, given by coefficient a in fit $\log T = a \log N + b$

Exercise 2: Eigenproblem



- Hermitian matrix created with random number generator
- Eigenvalues computed using zheev

```
function rand_hermitian_matrix(n) result(H)
  integer n
  integer ii, jj
  complex*16 H(n, n)

  do ii = 1, n
    do jj = 1, ii
      if (ii /= jj) then
        ! sample random complex numbers off the diagonal
        H(ii, jj) = cmplx(rand(0)*2 - 1, rand(0)*2 - 1)
        H(jj, ii) = conjg(H(ii, jj))
      else
        ! sample real numbers on the diagonal
        H(ii, ii) = rand(0)*2 - 1
      end if
    end do
  end do
end function
```

```
! compute eigenvalues in ascending order
call zheev('N', 'U', ndim, H, ndim, eigvals, work, lwork, rwork, info)

! compute eigenvalue spacings and average
ave_delta_eigvals = (eigvals(ndim) - eigvals(1)) / (ndim - 1)
do ii = 1, ndim - 1
  norm_eigval_spacings(ii) = (eigvals(ii + 1) - eigvals(ii)) / ave_delta_eigvals
end do
```

```
$ compiled/exercise_2 --ndim 2 -d
mat_type = hermitian
output_filename = histogram.csv
ndim = 2
nsamples = 1
nbins = 100
min_val = 0.000
max_val = 5.000
Sampled Hermitian matrix =
-1.0000 +0.0000i  -0.7369 -0.5112i
-0.7369 +0.5112i  -0.0827 +0.0000i
Eigenvalues = -1.5486887628051993      0.46600424589846079
Normalized eigenvalue spacings = 1.0000000000000000
Average eigenvalue spacing = 2.0146930087036603
```

Exercise 3: Random Matrix Theory



- Distribution of normalized spacings $P(s)$ produced for Hermitian and diagonal matrix
- Fit to $P(s) = as^\alpha \exp(bs^\beta)$ performed using scipy's `curve_fit` function

```
def func(x, a, b, alpha, beta):  
    return a * x ** alpha * np.exp(b * x ** beta)  
popt, pcov = curve_fit(func, bin_centers, norm_count)  
popt  
  
array([13.79272512, -2.82466922,  2.59653888,  1.32155578])
```

Matrix	a	b	α	β
hermitian	13.792 ± 2.266	-2.825 ± 0.166	2.597 ± 0.091	1.322 ± 0.043
diagonal	1.017 ± 0.007	-1.018 ± 0.008	0.005 ± 0.002	0.987 ± 0.005

Exercise 3: Random Matrix Theory



- Histograms produced with matrix size $N = 1000$ and number of bins $n_{\text{bins}} = 100$
- Results agree with random matrix theory (cf. Edelman and Rao, *Random Matrix Theory*, *Acta Numerica*, 2005, pp. 41)

