Computational Quantum Physics

Week 6

Due on Week 7

Exercise 1: **Eigenproblem**

Consider a random Hermitian matrix A of size N.

(a) Diagonalize A and store the N eigenvalues λ_i in increasing order.

(b) Compute the normalized spacings between eigenvalues
$s_i = \Delta\lambda_i/\bar{\Delta\lambda}$ where

$$\Delta\lambda_i = \lambda_{i+1} - \lambda_i,$$

and $\bar{\Delta\lambda}$ is the average $\Delta\lambda_i$.

(c) Optional: Compute the average spacing $\bar{\Delta\lambda}$ locally, i.e., over a different number of levels around λ_i (i.e. $N/100, N/50, N/10 \ldots N$) and compare the results of next exercise for the different choices.

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Normal Gaussian – distributed elements

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Exercise 1: **Eigenproblem**

Consider a random Hermitian matrix A of size N.

(a) Diagonalize A and store the N eigenvalues λ_i in increasing order.

Compile using lapack library (-llapack)

```
call dsyev('V','U', N, matr, lda, eig, wkopt, lwork, iinfo)
```

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and $\bar{\Delta\lambda}$ is the average $\Delta\lambda_i$.

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Exercise 2: **Random Matrix Theory**

Study $P(s)$, the distribution of the s_i defined in the previous exercise, accumulating values of s_i from different random matrices of size at least $N = 1000$.

(a) Compute $P(s)$ for a random HERMITIAN matrix.

(b) Compute $P(s)$ for a DIAGONAL matrix with random real entries.

(c) Fit the corresponding distributions with the function:

$$P(s) = a s^{\alpha} \exp(-b s^{\beta})$$

and report α, β, a, b.

(d) Optional: Compute and report the average $\langle r \rangle$ of the following quantity

$$r_i = \frac{\min(\Delta\lambda_i, \Delta\lambda_{i+1})}{\max(\Delta\lambda_i, \Delta\lambda_{i+1})}$$

for the cases considered above. Compare the average $\langle r \rangle$ that you obtain in the different cases.

Hint: if necessary neglect the first matrix eigenvalue.

Exercise 2: **Random Matrix Theory**

Study $P(s)$, the distribution of the s_i defined in the previous exercise, accumulating values of s_i from different random matrices of size at least $N = 1000$.

Difference between

- Histogram
- Normalized histogram
- Probability distribution

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(a) Compute $P(s)$ for a random HERMITIAN matrix.

Complex vs real?

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OPT: Same eigenvalues distribution?

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(b) Compute $P(s)$ for a DIAGONAL matrix with random real entries.

(c) Fit the corresponding distributions with the function:

$$P(s) = as^{\alpha} \exp(-bs^{\beta})$$

and report α, β, a, b.

(d) Optional: Compute and report the average $\langle r \rangle$ of the following quantity

$$r_i = \frac{\min(\Delta\lambda_i, \Delta\lambda_{i+1})}{\max(\Delta\lambda_i, \Delta\lambda_{i+1})}$$

for the cases considered above. Compare the average $\langle r \rangle$ that you obtain in the different cases.

Hint: if necessary neglect the first matrix eigenvalue.

```
INTEGER :: i,j,k,iinfo,lwork
DOUBLE PRECISION , ALLOCATABLE, DIMENSION(:) :: work, wkopt

allocate(wkopt(1))


lwork=-1

call dsyev('V','U', N, matr, lda, eig, wkopt, lwork, iinfo)

lwork = int(wkopt(1))
allocate(work(lwork))
call dsyev('V','U',N, matr, lda, eig, work, lwork, iinfo)


deallocate(work)
deallocate(wkopt)
```