Quantum Information and Computing

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Exercise #06

Physics of Data

Goal of the exercise: numerical handling of pure N-body wave functions.

Theory

Assume N particles each described by a d-dimensional Hilbert space ($\psi_i \in H_D$), we describe pure state of whole system :

$$|\psi> = \sum_{\alpha_1,\dots,\alpha_n} C_{\alpha_1,\dots,\alpha_n} |\alpha_1> \otimes \dots \otimes |\alpha_n> , \quad |\alpha_n> \in \{|0>, \dots, |D\text{-}1>\} , \quad (1)$$

We also describe the separable state:

$$|\psi> = \left(\sum_{\alpha_1} C_{\alpha_1} |\alpha_1>\right) \otimes \dots \otimes \left(\sum_{\alpha_n} C_{\alpha_n} |\alpha_n>\right) , (2)$$

The non-separable state is defined by D^N complex coefficients, while the separable wave function requires D . N complex coefficients.

Theory

For pure state of an N- body wave function |ψ> its density matrix is defined as:

$$\rho = |\psi><\psi| = \sum_{i,j=0}^{D^N-1} C_j^* C_i \, |i><j| \quad , (3)$$

It is positive semi-definite, Hermitian, with Tr(ρ) = 1 => $\rho^2 = \rho$

A reduced density matrix on the k^{th} subsystem is computed by tracing over all remaining subsystems:

$$\rho_k = Tr_1 \ldots Tr_{k-1} Tr_{k+1} \ldots Tr_N \rho \, , \quad Tr_i \rho = \sum_{j=0}^{d-1} < j|\rho|i > \, , (4)$$

In general:

$$\text{Dim}(\rho_k) = D^{N-1} \times D^{N-1}$$

Code development

A way to visualize the total wave function (non-separable case):

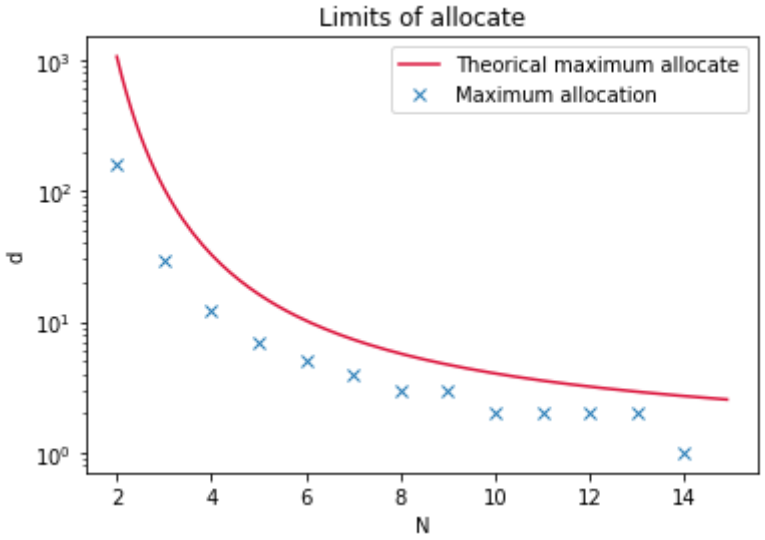
$$\Psi = a_0\,|0,0,\ldots,0> \;+a_0\,|0,0,\ldots,1> + \cdots + \\ +a_{d-1}|0,0,\ldots,d\;-1> \;+a_d|0,0,\ldots,d> + \;..$$

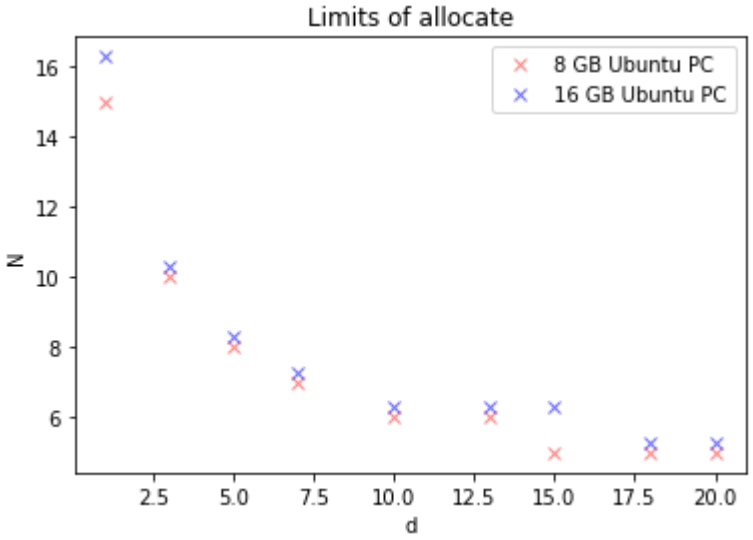
Function getting the index of the array from the eigenvectors combination and vice versa is just a base change.

```
module basechange

 contains

 function basechange_to(b_to, number, N) result(number_b_to)
   integer :: b_to, number, N, ii
   integer, dimension(N) :: number_b_to

   number_b_to = 0*number_b_to ! Allocate to 0, just to be sure
   do ii = 1, N, 1
     number_b_to(N - ii + 1) = modulo(number, b_to)
     number = number/b_to
   end do
 end function

 function basechange_from(b_from, number_from, N) result(number_b10)
   integer :: b_from, number_b10, N, ii
   integer, dimension(N) :: number_from

   do ii = 1, N, 1
     number_b10 = number_b10 + number_from(N - ii + 1)*b_from**(ii - 1)
   end do
 end function
end module
```

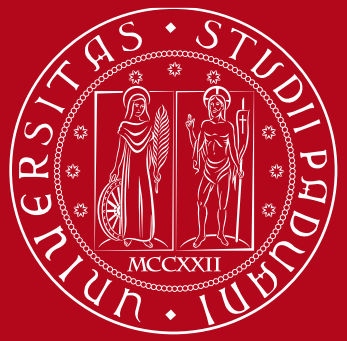
Result

Data was generated using a Ubuntu machine with 8GB of RAM.





- Traces and eigenvalues of ρ, were computed to check the correctness. The results given match the theory up to some numerical error.
- When trying to allocate too much memory, the program may give errors.
- The number of elements of ρ is d^{2N} and each element occupies 16 bytes (double complex).



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Thanks for the attention