Variational Monte Carlo method

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Importance Sampling

- The expectation value of some function $h(x)$ can be calculated using an importance sampling probability distribution function (PDF) $f(x)$:

$$\langle h \rangle = \int h(x)dx = \int f(x)\left[\frac{h(x)}{f(x)}\right]dx$$

- The resulting expectation value is more precise than without importance sampling

Markov Chains and Metropolis Algorithm

- A Markov chain is a discrete set of states $\{s_1, \dots, s_N\}$ with a rule that defines the transition probability between states
- To generate this set of random numbers from a known PDF we use the Metropolis algorithm:
  - Generate a starting state s_i with probability P_i
  - Generate a random step s_j
  - Metropolis question:
    - If $P_j > P_i$, the transition is accepted
    - If $P_j < P_i$, we evaluate the state with probability P_j/P_i, meaning that:
      - If $\frac{P_j}{P_i} > rand()$, the transition is accepted
      - If $\frac{P_j}{P_i} < rand()$, the transition is rejected and the state s_i becomes the next step in the Markov chain
- Thermalization: while carrying out a random walk starting from s_i, we can choose to only collect the state s_{i+n}, discarding the intermediate steps. This minimizes the correlations among successive states

Markov Chains and Metropolis Algorithm

```
xOld = step * (np.random.rand() - 0.5)
list_x.append(xOld)

for k in range(0,NX):
  xNew = xOld + step*(np.random.rand()-0.5)
  if ((WF(xNew,BestPar)/WF(xOld,BestPar))**2>1 or (WF(xNew,BestPar)/WF(xOld,BestPar))**2 > np.random.rand() ):
    xOld = xNew
    list_x.append(xOld)
    NAcc = NAcc +1
  else:
    xOld = xOld
    list_x.append(xOld)
```

An example of Metropolis algorithm to generate a random set of coordinates. The probability is given by the 1D harmonic oscillator wave function

Variational Principle

- Given a Hamiltonian H and a trial wave function Ψ, an upper bound to the ground state energy is

$$\langle H \rangle = \frac{\int \Psi^* H \Psi dx}{\int |\Psi|\text{^}2 dx}$$

- We can define a PDF and a local energy:

$$f(x) = \frac{|\Psi(\mathrm{x})|^2}{\int |\Psi(x)|^2 dx} \qquad E_L(x) = \frac{1}{\Psi(x)} H\, \Psi(x)$$

- The expectation value becomes

$$\langle H \rangle = \int f(x) E_L(x) dx$$

Variational Monte Carlo

- Consider $f(x)$ as the importance sampling distribution function
- The values of $E_L(x)$ in the integral of $\langle H \rangle$ are weighted by the Metropolis algorithm
- We use the variational Monte Carlo method in order to find the best parameters to represent the 1D harmonic oscillator and the He4 ground state wave functions
- The ground state is found by searching the energy minimum, varying the parameters of a chosen trial wave function

Variational Monte Carlo

- To overcome fluctuations around the minimum we use a technique called correlated sampling: assume a fixed parameter β (or set) near the minimum, and compute the energy for a random parameter α with the following equality:

$$E_\alpha = \frac{\int |\Psi(\beta,x)|^2 \left[\frac{|\Psi(\alpha,x)|^2}{|\Psi(\beta,x)|^2} E_L(\alpha,x)\right] dx}{\int |\Psi(\beta,x)|^2 \left[\frac{|\Psi(\alpha,x)|^2}{|\Psi(\beta,x)|^2}\right] dx}$$

- This way, the importance sampling function is fixed and is $|\Psi(\beta,x)|^2$.

1D Harmonic Oscillator

- Hamiltonian:

$$H = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right)$$

- Trial wave function:

$$\Psi(\alpha, x) = e^{-\alpha^2 x^2/2}$$

- Local energy:

$$E_L(\alpha, x) = \frac{H\Psi(x)}{\Psi(x)} = \frac{1}{2}[\alpha^2 + x^2(1 - \alpha^4)]$$

- We want to find the minimum of:

$$\bar{E}_{gs} = \int_{-\infty}^{+\infty} |\Psi|^2 E_L(x) dx$$

1D Harmonic Oscillator

- Start by defining the local energy and the wave function, and by initializing the necessary parameters:

```
NAcc = 0
NP = 900
NX = 10000
step = 1.0
step1 = 0.3

# parameter variables for VMC
BestPar = 1
Par = 0.4
Par_new = 0

np.random.seed(12231)

# wave function
def WF(x,alpha):
  return exp(-0.5*alpha*alpha*x*x)

# local energy
def LocalEnergy(x,alpha):
  return 0.5*x*x*(1-alpha**4) + 0.5*alpha*alpha
```

- Then, find a set of steps with the Metropolis algorithm, by using $|\Psi(\alpha, x)|^2 = e^{-\alpha^2 x^2}$ to define the probabilities for each step x_i

```
xOld = step * (np.random.rand() - 0.5)
list_x.append(xOld)

for k in range(0,NX):
  xNew = xOld + step*(np.random.rand()-0.5)
  if ((WF(xNew,BestPar)/WF(xOld,BestPar))**2>1 or (WF(xNew,BestPar)/WF(xOld,BestPar))**2 > np.random.rand() ):
    xOld = xNew
    list_x.append(xOld)
    NAcc = NAcc +1
  else:
    xOld = xOld
    list_x.append(xOld)
```

To construct the Markov chain, we use the value of α in the minimum, which is $\alpha = 1$

1D Harmonic Oscillator

- Then, start the Markov chain to find the energy minimum, starting from $\alpha = 0.4$ (the expected value in the minimum is $\alpha = 1$)
- Algorithm:
  - Generate each value of α as a random step

```
Par_new = Par + (np.random.rand()-0.5)*step1
```

  - Calculate the energy and variance using correlated sampling

```
for j in range(0,NX):
  E_loc = E_loc + LocalEnergy(list_x[j],Par_new)*(WF(list_x[j],Par_new)/WF(list_x[j],BestPar))**2
  E_loc_2 = E_loc_2 +(LocalEnergy(list_x[j],Par_new)*(WF(list_x[j],Par_new)/WF(list_x[j],BestPar))**2)**2
  D = D + (WF(list_x[j], Par_new)/WF(list_x[j], BestPar))**2

E_mean = E_loc/D
Var2 = (E_loc_2/D - (E_loc/D)**2)/D
```

1D Harmonic Oscillator

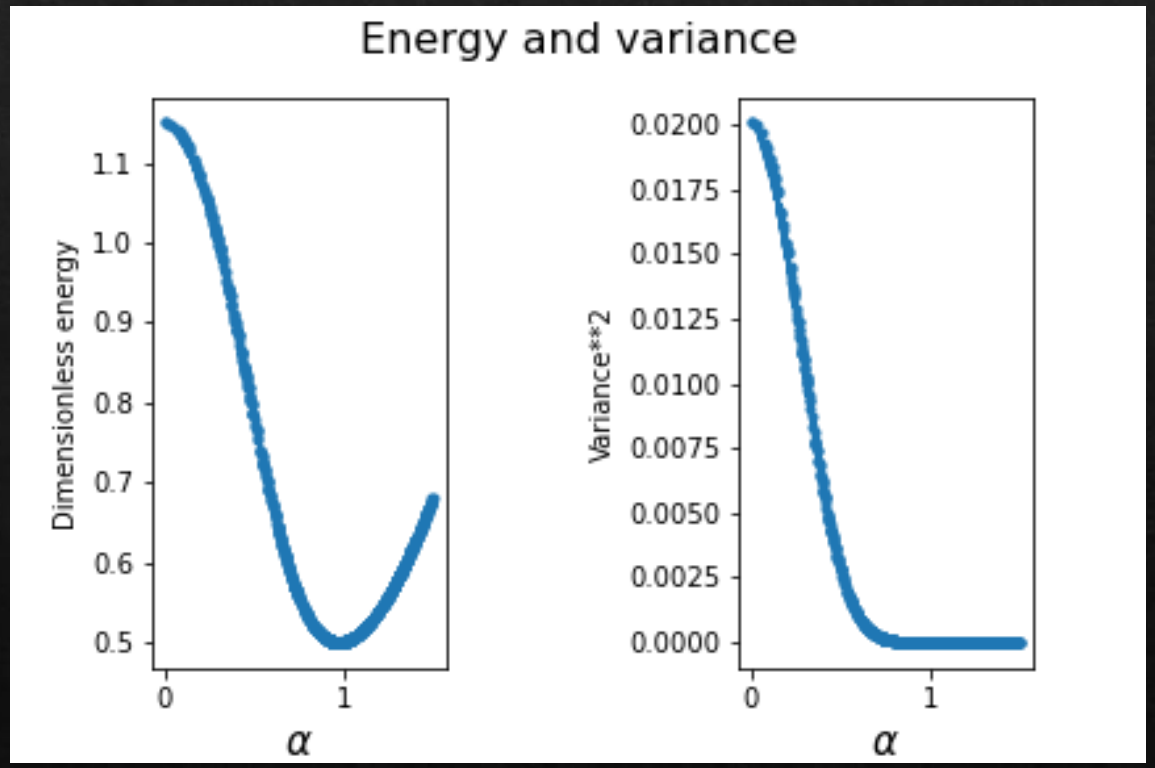
- Ask the Metropolis question:
  - If $\bar{E}_{gs}(\alpha_{old}) > \bar{E}_{gs}(\alpha_{new})$, the move is accepted; if instead $\bar{E}_{gs}(\alpha_{old}) > \bar{E}_{gs}(\alpha_{new})$, we evaluate the step α_{new} using as probability $\frac{\bar{E}_{gs}(\alpha_{new})}{\bar{E}_{gs}(\alpha_{old})}$
  - We also store the value of the minimum energy and update it in every cycle

```
if (list_Eall[l-1]>E_mean or list_Eall[l-1]/E_mean>np.random.rand()):

  if (minimumE>E_mean):
    minimumE = E_mean
    minimumAlpha = Par
    minimumVariance2 = Var2
  else:
    minimumE = minimumE
    minimumAlpha = minimumAlpha
    minimumVariance2 = minimumVariance2

  Par = Par_new
  list_alpha.append(Par)
  list_Eall.append(E_mean)
  list_E.append(E_mean)
  list_variance2.append(Var2)

else:
  Par = Par
  list_Eall.append(list_Eall[l-1])
```

1D Harmonic Oscillator: results

- From these graphs we see that the minimum energy is around $\alpha = 1$, and the value at the minimum is approximately $\bar{E}_{gs} = 0.5$

- The variance gets smaller as the value of α approaches the minimum



Ground State of Helium – 4

- Hamiltonian:

$$H = -\frac{h^2}{2m}\frac{d^2}{d\boldsymbol{r}^2} + V(r_1, \dots, r_4)$$

- Trial wave function:

$$\Psi(r_1, \dots, r_4, \gamma, a, \beta) = \prod_{i<j}^{4} \left(e^{-\gamma\, r_{ij}^2} + a\, e^{-(\beta+\gamma) r_{ij}^2} \right)$$

- Local energy:

$$E_L(r_1, \dots, r_4, \gamma, a, \beta) = -\frac{h^2}{2m}\left(\frac{d^2\Psi}{d\boldsymbol{r}^2}\right)\frac{1}{\Psi} + V(r_1, \dots, r_4)$$

Ground State of Helium – 4

- The potential is an effective potential that reproduces the spin-isospin-independent interaction between two nucleons at low energies [3]:

$$V(r) = 1000\, e^{-3\, r^2} - 163.35\, e^{-1.05\, r^2} - 21.5\, e^{-0.6\, r^2} - 83\, e^{-0.8\, r^2} - 11.5\, e^{-0.4\, r^2}$$

- The trial wave function, with 3 free parameters, is a Jastrow correlation factor multiplying an uncorrelated state:

$$\Psi(r_1, \dots, r_4) = \prod_{i<j}^{4} \left(1 + a\, e^{-\beta r_{ij}^2}\right) e^{-\alpha^2 (r_1^2 + \cdots + r_4)/2}$$

which can be written as the product:

$$\prod_{i<j}^{4} g(r_{ij}) = \prod_{i<j}^{4} \left(e^{-\gamma\, r_{ij}^2} + a\, e^{-(\beta+\gamma) r_{ij}^2}\right)$$

where $\gamma = \alpha^2/8$

Ground State of Helium – 4

- Wave function →
  - The parameters are $\mathrm{Par}[0] = \gamma$, $\mathrm{Par}[1] = \mathrm{a}$, $\mathrm{Par}[2] = \beta$
  - The function $d(R, i, j)$ is the square distance between particles
- Potential →
- Kinetic energy →
  - The second-order differential in the kinetic energy is approximated with a centered second difference, and the constant is $C = \frac{h^2}{2m} \simeq 20.72$

```
def d(R,i,j):
  return np.sum((R[:, i] - R[:, j])**2)

def WF(R, Par):
  wf = 1
  for i in range(0,A-1):
    for j in range(i+1,A):
      wf = wf * (exp(-Par[0]*d(R,i,j))+Par[1]*exp(-Par[2]*d(R,i,j)))
  return wf

def V(R):
  V = 0
  for i in range(0,A-1):
    for j in range(i+1,A):
      V = V + 1000*exp(-3*d(R,i,j))-165.35*exp(-1.05*d(R,i,j))
      -21.5*exp(-0.6*d(R,i,j))
      -83*exp(-0.8*d(R,i,j))-11.5*exp(-0.4*d(R,i,j))
  return V

def Diff (R, i, j, h, Par):
  R_P = R.copy()
  R_M = R.copy()
  R_P[i,j] = R[i,j]+h
  R_M[i,j] = R[i,j]-h
  return (WF(R_P, Par)+WF(R_M, Par)-2*WF(R, Par))/h**2

def K(R, Par):
  K = 0
  for j in range(0,A):
    for i in range(0,3):
      K = K + Diff(R, i, j, h, Par )*C
  return K
```

Ground State of Helium – 4

- As the final goal for parameters, we take the values from ref. [1]

```
BestPars = [0.08597 , -0.7191 , 2.13796 ]
```

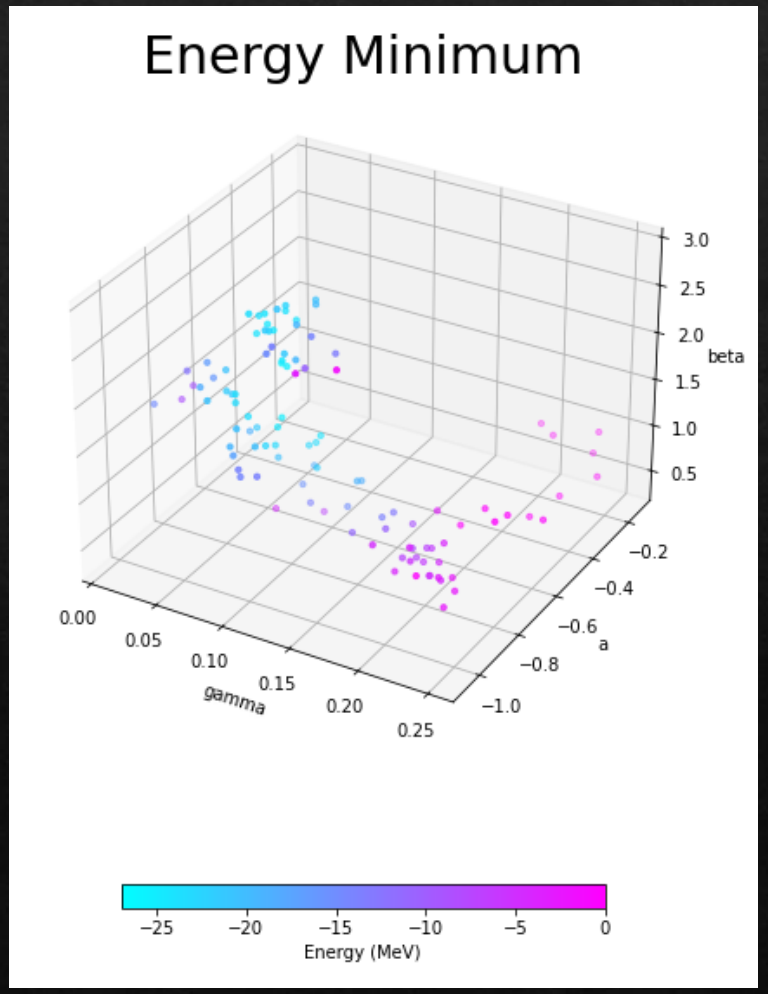
- The code structure is the same as in the 1d harmonic oscillator case, with the difference that now we are varying 3 parameters:

```
Par_new[0] = Par[0].copy() + (np.random.rand()-0.5)*step1
Par_new[1] = Par[1].copy() + (np.random.rand()-0.5)*step2
Par_new[2] = Par[2].copy() + (np.random.rand()-0.5)*step3
```

Ground State of Helium – 4: results

- Varying the parameter steps and the number of iterations of the VMC cycle, the results are visibly different

- The starting parameters that optimize the precision and the running time are:
  - step1 = 10/100
  - step2 = 25/100
  - Step3 = 50/100



References

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