Week 6: Importance Sampling and Metropolis-Hastings' algorithm

Morten Hjorth-Jensen Email morten.hjorth-jensen@fys.uio.no[1,2]

[1]Department of Physics and Center fo Computing in Science Education, University of Oslo, Oslo, Norway
[2]Department of Physics and Astronomy and Facility for Rare Ion Beams, Michigan State University, East Lansing, Michigan, USA

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Overview of week 6, February 5-9, 2024

Topics.

- Short repetition from last week
- Mathematical and computational details of importance sampling and Fokker-Planck and Langevin equations

Teaching Material, videos and written material.

- These lecture notes
- Video of lecture TBA
- Handwritten notes tba

Importance sampling and overview of what needs to be coded, reminder from last week

For a diffusion process characterized by a time-dependent probability density $P(x,t)$ in one dimension the Fokker-Planck equation reads (for one particle /walker)

$$\frac{\partial P}{\partial t} = D\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} - F\right)P(x,t),$$

where F is a drift term and D is the diffusion coefficient.

Importance sampling

The new positions in coordinate space are given as the solutions of the Langevin equation using Euler's method, namely, we go from the Langevin equation

$$\frac{\partial x(t)}{\partial t} = DF(x(t)) + \eta,$$

with η a random variable, yielding a new position

$$y = x + DF(x)\Delta t + \xi\sqrt{\Delta t},$$

where ξ is gaussian random variable and Δt is a chosen time step. The quantity D is, in atomic units, equal to $1/2$ and comes from the factor $1/2$ in the kinetic energy operator. Note that Δt is to be viewed as a parameter. Values of $\Delta t \in [0.001, 0.01]$ yield in general rather stable values of the ground state energy.

Importance sampling

The process of isotropic diffusion characterized by a time-dependent probability density $P(\mathbf{x}, t)$ obeys (as an approximation) the so-called Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \sum_i D\frac{\partial}{\partial \mathbf{x_i}}\left(\frac{\partial}{\partial \mathbf{x_i}} - \mathbf{F_i}\right)P(\mathbf{x}, t),$$

where $\mathbf{F_i}$ is the i^{th} component of the drift term (drift velocity) caused by an external potential, and D is the diffusion coefficient. The convergence to a stationary probability density can be obtained by setting the left hand side to zero. The resulting equation will be satisfied if and only if all the terms of the sum are equal zero,

$$\frac{\partial^2 P}{\partial {\mathbf{x_i}}^2} = P\frac{\partial}{\partial \mathbf{x_i}}\mathbf{F_i} + \mathbf{F_i}\frac{\partial}{\partial \mathbf{x_i}}P.$$

Importance sampling

The drift vector should be of the form $\mathbf{F} = g(\mathbf{x})\frac{\partial P}{\partial \mathbf{x}}$. Then,

$$\frac{\partial^2 P}{\partial {\mathbf{x_i}}^2} = P\frac{\partial g}{\partial P}\left(\frac{\partial P}{\partial \mathbf{x}_i}\right)^2 + Pg\frac{\partial^2 P}{\partial \mathbf{x}_i^2} + g\left(\frac{\partial P}{\partial \mathbf{x}_i}\right)^2.$$

The condition of stationary density means that the left hand side equals zero. In other words, the terms containing first and second derivatives have to cancel each other. It is possible only if $g = \frac{1}{P}$, which yields

$$\mathbf{F} = 2\frac{1}{\Psi_T}\nabla\Psi_T,$$

which is known as the so-called *quantum force*. This term is responsible for pushing the walker towards regions of configuration space where the trial wave function is large, increasing the efficiency of the simulation in contrast to the Metropolis algorithm where the walker has the same probability of moving in every direction.

Importance sampling

The Fokker-Planck equation yields a (the solution to the equation) transition probability given by the Green's function

$$G(y,x,\Delta t) = \frac{1}{(4\pi D\Delta t)^{3N/2}}\exp\left(-(y-x-D\Delta tF(x))^2/4D\Delta t\right)$$

which in turn means that our brute force Metropolis algorithm

$$A(y,x) = \min(1,q(y,x))),$$

with $q(y,x) = |\Psi_T(y)|^2/|\Psi_T(x)|^2$ is now replaced by the Metropolis-Hastings algorithm as well as Hasting's article,

$$q(y,x) = \frac{G(x,y,\Delta t)|\Psi_T(y)|^2}{G(y,x,\Delta t)|\Psi_T(x)|^2}$$

Code example for the interacting case with importance sampling

We are now ready to implement importance sampling. This is done here for the two-electron case with the Coulomb interaction, as in the previous example. We have two variational parameters α and β. After the set up of files

```
# Common imports
import os

# Where to save the figures and data files
PROJECT_ROOT_DIR = "Results"
FIGURE_ID = "Results/FigureFiles"
DATA_ID = "Results/VMCQdotImportance"

if not os.path.exists(PROJECT_ROOT_DIR):
    os.mkdir(PROJECT_ROOT_DIR)

if not os.path.exists(FIGURE_ID):
    os.makedirs(FIGURE_ID)

if not os.path.exists(DATA_ID):
    os.makedirs(DATA_ID)

def image_path(fig_id):
    return os.path.join(FIGURE_ID, fig_id)

def data_path(dat_id):
    return os.path.join(DATA_ID, dat_id)

def save_fig(fig_id):
    plt.savefig(image_path(fig_id) + ".png", format='png')

outfile = open(data_path("VMCQdotImportance.dat"),'w')
```

we move on to the set up of the trial wave function, the analytical expression for the local energy and the analytical expression for the quantum force.

```
# 2-electron VMC code for 2dim quantum dot with importance sampling
# Using gaussian rng for new positions and Metropolis- Hastings
# No energy minimization
from math import exp, sqrt
from random import random, seed, normalvariate
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm
from matplotlib.ticker import LinearLocator, FormatStrFormatter
import sys
from numba import jit,njit


# Trial wave function for the 2-electron quantum dot in two dims
def WaveFunction(r,alpha,beta):
    r1 = r[0,0]**2 + r[0,1]**2
    r2 = r[1,0]**2 + r[1,1]**2
    r12 = sqrt((r[0,0]-r[1,0])**2 + (r[0,1]-r[1,1])**2)
    deno = r12/(1+beta*r12)
    return exp(-0.5*alpha*(r1+r2)+deno)

# Local energy  for the 2-electron quantum dot in two dims, using analytical local energy
def LocalEnergy(r,alpha,beta):

    r1 = (r[0,0]**2 + r[0,1]**2)
    r2 = (r[1,0]**2 + r[1,1]**2)
    r12 = sqrt((r[0,0]-r[1,0])**2 + (r[0,1]-r[1,1])**2)
    deno = 1.0/(1+beta*r12)
    deno2 = deno*deno
    return 0.5*(1-alpha*alpha)*(r1 + r2) +2.0*alpha + 1.0/r12+deno2*(alpha*r12-deno2+2*beta*deno-1

# Setting up the quantum force for the two-electron quantum dot, recall that it is a vector
def QuantumForce(r,alpha,beta):

    qforce = np.zeros((NumberParticles,Dimension), np.double)
    r12 = sqrt((r[0,0]-r[1,0])**2 + (r[0,1]-r[1,1])**2)
    deno = 1.0/(1+beta*r12)
    qforce[0,:] = -2*r[0,:]*alpha*(r[0,:]-r[1,:])*deno*deno/r12
    qforce[1,:] = -2*r[1,:]*alpha*(r[1,:]-r[0,:])*deno*deno/r12
    return qforce
```

The Monte Carlo sampling includes now the Metropolis-Hastings algorithm, with the additional complication of having to evaluate the **quantum force** and the Green's function which is the solution of the Fokker-Planck equation.

```
# The Monte Carlo sampling with the Metropolis algo
# jit decorator tells Numba to compile this function.
# The argument types will be inferred by Numba when function is called.
@jit()
def MonteCarloSampling():

    NumberMCcycles= 100000
    # Parameters in the Fokker-Planck simulation of the quantum force
    D = 0.5
    TimeStep = 0.05
    # positions
    PositionOld = np.zeros((NumberParticles,Dimension), np.double)
    PositionNew = np.zeros((NumberParticles,Dimension), np.double)
```

```
# Quantum force
QuantumForceOld = np.zeros((NumberParticles,Dimension), np.double)
QuantumForceNew = np.zeros((NumberParticles,Dimension), np.double)

# seed for rng generator
seed()
# start variational parameter  loops, two parameters here
alpha = 0.9
for ia in range(MaxVariations):
    alpha += .025
    AlphaValues[ia] = alpha
    beta = 0.2
    for jb in range(MaxVariations):
        beta += .01
        BetaValues[jb] = beta
        energy = energy2 = 0.0
        DeltaE = 0.0
        #Initial position
        for i in range(NumberParticles):
            for j in range(Dimension):
                PositionOld[i,j] = normalvariate(0.0,1.0)*sqrt(TimeStep)
        wfold = WaveFunction(PositionOld,alpha,beta)
        QuantumForceOld = QuantumForce(PositionOld,alpha, beta)

        #Loop over MC MCcycles
        for MCcycle in range(NumberMCcycles):
            #Trial position moving one particle at the time
            for i in range(NumberParticles):
                for j in range(Dimension):
                    PositionNew[i,j] = PositionOld[i,j]+normalvariate(0.0,1.0)*sqrt(TimeStep)+
                                       QuantumForceOld[i,j]*TimeStep*D
                wfnew = WaveFunction(PositionNew,alpha,beta)
                QuantumForceNew = QuantumForce(PositionNew,alpha, beta)
                GreensFunction = 0.0
                for j in range(Dimension):
                    GreensFunction += 0.5*(QuantumForceOld[i,j]+QuantumForceNew[i,j])*\
                                  (D*TimeStep*0.5*(QuantumForceOld[i,j]-QuantumForceNew[i,j])-
                                  PositionNew[i,j]+PositionOld[i,j])

                GreensFunction = exp(GreensFunction)
                ProbabilityRatio = GreensFunction*wfnew**2/wfold**2
                #Metropolis-Hastings test to see whether we accept the move
                if random() <= ProbabilityRatio:
                   for j in range(Dimension):
                       PositionOld[i,j] = PositionNew[i,j]
                       QuantumForceOld[i,j] = QuantumForceNew[i,j]
                   wfold = wfnew
            DeltaE = LocalEnergy(PositionOld,alpha,beta)
            energy += DeltaE
            energy2 += DeltaE**2
        # We calculate mean, variance and error (no blocking applied)
        energy /= NumberMCcycles
        energy2 /= NumberMCcycles
        variance = energy2 - energy**2
        error = sqrt(variance/NumberMCcycles)
        Energies[ia,jb] = energy
        outfile.write('%f %f %f %f %f\n' %(alpha,beta,energy,variance,error))
return Energies, AlphaValues, BetaValues
```

The main part here contains the setup of the variational parameters, the energies and the variance.

```
#Here starts the main program with variable declarations
NumberParticles = 2
Dimension = 2
MaxVariations = 10
Energies = np.zeros((MaxVariations,MaxVariations))
AlphaValues = np.zeros(MaxVariations)
BetaValues = np.zeros(MaxVariations)
(Energies, AlphaValues, BetaValues) = MonteCarloSampling()
outfile.close()
# Prepare for plots
fig = plt.figure()
ax = fig.gca(projection='3d')
# Plot the surface.
X, Y = np.meshgrid(AlphaValues, BetaValues)
surf = ax.plot_surface(X, Y, Energies,cmap=cm.coolwarm,linewidth=0, antialiased=False)
# Customize the z axis.
zmin = np.matrix(Energies).min()
zmax = np.matrix(Energies).max()
ax.set_zlim(zmin, zmax)
ax.set_xlabel(r'$\alpha$')
ax.set_ylabel(r'$\beta$')
ax.set_zlabel(r'$\langle E \rangle$')
ax.zaxis.set_major_locator(LinearLocator(10))
ax.zaxis.set_major_formatter(FormatStrFormatter('%.02f'))
# Add a color bar which maps values to colors.
fig.colorbar(surf, shrink=0.5, aspect=5)
save_fig("QdotImportance")
plt.show()
```