NUEN 647
Uncertainty Quantification for Nuclear Engineering
Assignment 1

Due on Tuesday, October 4, 2016

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Contents

Complete the exercises in the Chapter 2 notes. Be sure to include discussion of results where appropriate. You may use any tools that are approrpriate to solving the problem.

Problem 1

Show that the transformation in equation 1 results in a standard normal random variable by computing the mean and variance of z.

$$z = \frac{x-\mu}{\sigma} \tag{1}$$

An important special case of the expectation value is the mean which is the expected value of x. It is often denoted as μ,

$$\mu = E[x] = \int_{-\infty}^{\infty} x f(x) dx$$

where x is a realization of a random sample and $f(x)$ is the probability density function (PDF) for the random variable. For a normal distribution,

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

For the sake of the transformation, the value of z substitutes for x, the realization of a random sample (not the PDF because we are transforming that distribution). Therefore, the mean for z is:

$$\mu_z = \int_{-\infty}^{\infty} \frac{x-\mu}{\sigma} \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}} dx$$

If $u = (x-\mu)^2$ and $\frac{du}{2} = (x-\mu)dx$ (note that the limits change from $(-\infty, \infty)$ to (∞, ∞) - but that seems fishy to me so I will change it back after integration).

$$\mu_z = \int_{\infty}^{\infty} \frac{1}{2\sigma^2\sqrt{2\pi}} e^{\frac{-u}{2\sigma^2}} du = \left| \frac{-1}{\sqrt{2\pi}} e^{\frac{-u}{2\sigma^2}} \right|_{\infty}^{\infty}$$

$$\mu_z = \left| \frac{-1}{\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}} \right|_{-\infty}^{\infty} = \frac{-1}{\sqrt{2\pi}} (e^{-\infty} - e^{-\infty}) = \boxed{0}$$

The variance is defined as:

$$Var(X) = E[(X-\mu)^2]$$

Substituting Eq. 1 for X, (but not for the pdf - I could be wrong about that)

$$Var(X) = E[(\frac{x-\mu}{\sigma} - \mu)^2] = E\left[\left(\frac{x-\mu-\mu\sigma}{\sigma}\right)^2\right] = \frac{1}{\sigma^2}(E[x^2] - 2\mu E[x] - 2\mu\sigma E[x] + \mu^2 E[1] + \mu^2\sigma^2 + 2\mu^2\sigma)$$

Noting that above it was proven that $E[x] = \mu$ and given that the definition of $E[1] = 1$ and assuming that $E[x^2] = \sigma^2 + \mu^2$ (will solve on next page)

$$\frac{1}{\sigma^2}(\sigma^2 + \mu^2 - 2\mu^2 - 2\mu^2\sigma + \mu^2 + \mu^2\sigma^2 + 2\mu^2\sigma) = \frac{1}{\sigma^2}(\sigma^2 + \mu^2\sigma^2) = \boxed{1 + \mu^2 = 1}$$

This is assuming that $\mu = 0$. Which was shown above.

$$E[x^2] = \int_{-\infty}^{\infty} \frac{x^2}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

If $t = \frac{(x-\mu)}{\sqrt{2}\sigma}$ and $\sqrt{2}\sigma dt = dx$ and $x = t\sqrt{2}\sigma + \mu$ then (limits of integration don't change)

$$E[x^2] = \int_{-\infty}^{\infty} \frac{\left(t\sqrt{2}\sigma + \mu\right)^2}{\sqrt{\pi}} e^{-t^2} dt = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \left(2\sigma^2 \left(t^2 e^{-t^2}\right) + 2\sqrt{2}\sigma\mu \left(te^{-t^2}\right) + \mu^2 \left(e^{-t^2}\right)\right)$$

According to wolfram alpha

$$\int_{-\infty}^{\infty} t^2 e^{-t^2} = \frac{\sqrt{\pi}}{2}$$

$$\int_{-\infty}^{\infty} te^{-t^2} = 0$$

$$\int_{-\infty}^{\infty} e^{-t^2} = \sqrt{\pi}$$

Which simplifies the above to $\sigma^2 + \mu^2$.

Problem 2

Consider the random variables $X \sim U(-1, 1)$ and $Y \sim X^2$. Are these independent random variables? What is their covariance?

If two random variables, X and Y, are independent, they satisfy the following condition: ^{link}

- $P(X|Y) = P(X)$, for all values of X and Y.

The PDF for X is:

$$f_X(x) = \frac{1}{(1-(-1))} = 0.5 \quad x \in [-1, 1]$$

The PDF for Y is: ^{link}

$$f_Y(y) = \frac{1}{2\sqrt{y}} \quad y \in [0, 1]$$

If the covariance is non zero, then these two variables are independant. The covariance of two random variables can be given by: ^{link}

$$\sigma_{XY} = E(XY) - \mu_X\mu_Y = \int_{-1}^{1} dx \int_{0}^{1} dy \;\; xyf(x, y) - \mu_X\mu_Y$$

Because $\mu_X = 0$ this reduces to

$$\sigma_{XY} = E(XY) = \int_{-1}^{1} dx \int_{0}^{1} dy \;\; xyf(x, y)$$

Where $f(x, y)$ is:

$$f(x, y) = f(y|x)f_X(x)$$

From the definition of Y, $f(y|x)$ is 0 except when $y = x^2$. I think this would be.

$$f(y|x) = \delta(y - x^2)$$

Which means,

$$f(x, y) = 0.5\delta(y - x^2)$$

I am not 100% sure to do here, but after using wolfram, I think its 0.25.

Problem 3

Show that a general covariance matrix must be positive definite, i.e. $\vec{x}^T \Sigma \vec{x} > 0$ for any vector $\vec{x}$ that is not all zeros.

Given that $\vec{Y}$ is a vector of random variables and $\vec{\mu}_Y$ is a vector of the mean values for the random variables found in $\vec{Y}$.

$$\begin{aligned}\vec{x}^T \Sigma \vec{x} &= \vec{x}^T E[(\vec{Y} - \vec{\mu}_Y)(\vec{Y} - \vec{\mu}_Y)^T]\vec{x} \\ &= E[\vec{x}^T (\vec{Y} - \vec{\mu}_Y)(\vec{Y} - \vec{\mu}_Y)^T \vec{x}]\end{aligned}$$

The last step above puts a constant inside the expectation value integral. Notice

$$\vec{x}^T (\vec{Y} - \vec{\mu}_Y) = (\vec{Y} - \vec{\mu}_Y)^T \vec{x}$$

and that both are scaler functions of the random variables. Therefore,

$$\begin{aligned}\vec{x}^T \Sigma \vec{x} &= E[(\vec{x}^T (\vec{Y} - \vec{\mu}_Y))^2] \\ &= E[g(Y)^2] = \sigma_f^2\end{aligned}$$

The expectation value for a multivariate distribution is defined as

$$E[g(Y)] = \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \; ... \int_{-\infty}^{\infty} dy_p \; g(y) f(y)$$

Where $f(y)$ is the multivariate PDF for the random variables of $\vec{Y}$. To prove that the covariance matrix is positive definite the above integral must be proved to be positive with $g(x) = (\vec{x}^T (\vec{Y} - \vec{\mu}_Y))^2$. Explicitly,

$$\begin{aligned}E[g(Y)] &= \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \; ... \int_{-\infty}^{\infty} dy_p \; (\vec{x}^T (\vec{Y} - \vec{\mu}_Y))^2 f(y) \\ &= \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \; ... \int_{-\infty}^{\infty} dy_p \; ((y_1 - \mu_1)x_1 + (y_2 - \mu_2)x_2 + \; ... \; + (y_p - \mu_p)x_p)^2 f(y)\end{aligned}$$

Problem 4

Use rejection sampling to sample from a Gamma random variable $X \sim \mathscr{G}(\alpha, \beta)$ where

$$f(x) = \frac{\theta^{\alpha-1} e^{-\theta/\beta}}{\Gamma(\alpha)\beta^{-\alpha}} \quad \alpha, \beta > 0$$

Let $\alpha = 1$ and $\beta = 0.5$. From rejection sampling with a $N = 10^4$, compute a rejection rate for the sampling procedure. Now draw a triangle around the function and do rejection sampling. Compare the rejection rate from the triangle versus the rectangle. You may consider that the PDF is zero if $f(x) < 10^{-6}$.

Python script for rejection sampling.

Listing 1: Python Script for problem

```
#!/usr/bin/env python3

"""
Chem Calculations
"""

__author__     =  "Paul Mendoza"
__copyright__  =  "Copyright 2016, Planet Earth"
__credits__    = ["Sunil Chirayath",
                  "Charles Folden",
                  "Jeremy Conlin"]
__license__    =  "GPL"
__version__    =  "1.0.1"
__maintainer__ =  "Paul Mendoza"
__email__      =  "paul.m.mendoza@gmail.com"
__status__     =  "Production"

################################################################
##################### Import packages ##########################
################################################################

import os.path
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import datetime
from uncertainties import ufloat
from uncertainties.umath import *
from uncertainties import unumpy as unp
import re
import time
start_time = time.time()

import Functions as fun


################################################################
################## Examples of Calculations ####################
################################################################

```

```
#######################################################
############ Atom Fraction to Mass Fraction ###########
############          and vice versa        ###########
#######################################################

string='92235 0.285714286 0 92238 0.714285714 0'
MasstoAtom=True
Mass,Zaid=fun.StringToMass(string)
stringCalculated=fun.ConvertFractions(string,Mass,MasstoAtom,Zaid)

# if MasstoAtom:
#     print("Mass Fractions:")
#     print(string)
#     print("Atom Fractions:")
#     print(stringCalculated)
# else:
#     print("Mass Fractions:")
#     print(stringCalculated)
#     print("Atom Fractions:")
#     print(string)

#######################################################
############ Calculate grams per mol of ##############
############    a chemical formula      ##############
#######################################################

#Make sure your chemical form has no repeats
#And no parentheses
ChemicalFormula='HNO_3'
ChemicalFormulaError=[0,0,0,0,0,0,0,0] #+/- error in integers of
                                       #chemical formula
ChemicalFormula=ChemicalFormula+"    "
List=fun.ChemList(ChemicalFormula)

#Enter Modifications:
#1. Each element should be a single item in the list
#2. Format: zaid atomfraction+/-error zaid atomfraction+/-error
#   or    : zaid atomfraction error zaid atomfraction
Modifications=['92235 0.2883155436+/-0.0000000024 92238 0.7116844564+/-0.0000000024',stringCalcu

df = pd.read_csv('../Data/AtomicWeights.csv')


ModMass,ModSymbols,AtomFractions=fun.FormatMods(Modifications,df)
MolarMass=fun.DetermineMolarMass(List,df,
                                 ModSymbols,ModMass,
                                 AtomFractions,ChemicalFormulaError)

# print(MolarMass)

#######################################################
############### Calculate Molality from ##############
###############          Wt %           ##############
```

```
######################################################

gramsOmol=MolarMass
WtConcentration=ufloat(69,0.1)
Molality=1000/(gramsOmol*(100/WtConcentration-1))

######################################################
############# Convert molality/molarity ##############
######################################################

MolarityToMolality=True

gramsOmol=MolarMass

#Density in grams per cc or grams per ml
dfDen=pd.read_csv('../Data/Nitric_Acid.csv')

Temperature=ufloat(20,3) #Same degrees as dfDen!!!

Molality=Molality
Molarity=ufloat(15.43,0.06)

if MolarityToMolality:
    Molality=fun.ConvertMol(MolarityToMolality,Molarity,
                            gramsOmol,dfDen,Temperature)
else:
    Molarity=fun.ConvertMol(MolarityToMolality,Molality,
                            gramsOmol,dfDen,Temperature)


#print("Molarity = "+str(Molarity))
#print("Molality = "+str(Molality))


######################################################
############# Calculate New Concentration ############
######################################################

Vol1=1
Vol2=1

gramsOmol=gramsOmol

m1=Molality
m2=Molality*.25

Temperature=ufloat(20,3)

dfDen=pd.read_csv('../Data/Nitric_Acid.csv')

m3,p3,Vol3,Wt,M3=fun.NewConcentration(m1,m2,gramsOmol,
                                    Temperature,dfDen,
                                    Vol1,Vol2)
```

```
M1=fun.ConvertMol(False,m1,gramsOmol,dfDen,Temperature)
M2=fun.ConvertMol(False,m2,gramsOmol,dfDen,Temperature)


###################### Time To execute #################

print("--- %s seconds ---" % (time.time() - start_time))
```

This is an example citation [1].

References

[1] E. T. Tatro, S. Hefler, S. Shumaker-Armstrong, B. Soontornniyomkij, M. Yang, A. Yermanos, N. Wren, D. J. Moore, and C. L. Achim. Modulation of bk channel by microrna-9 in neurons after exposure to hiv and methamphetamine. *J Neuroimmune Pharmacol*, 2013. Tatro, Erick T Hefler, Shannon Shumaker-Armstrong, Stephanie Soontornniyomkij, Benchawanna Yang, Michael Yermanos, Alex Wren, Nina Moore, David J Achim, Cristian L R03 DA031591/DA/NIDA NIH HHS/United States U19 AI096113/AI/NIAID NIH HHS/United States Journal article Journal of neuroimmune pharmacology : the official journal of the Society on NeuroImmune Pharmacology J Neuroimmune Pharmacol. 2013 Mar 19.