Week 11, March 18-22: Resampling Techniques, Bootstrap and Blocking

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Overview of week 11, March 18-22

Topics.

- Resampling Techniques and statistics: Bootstrap and Blocking
- Discussion of onebody densities
- Video of lecture TBA
- Handwritten notes

Teaching Material, videos and written material.

- Overview video on the Bootstrap method
- Marius Johnson's Master thesis on the Blocking Method

Why resampling methods ?

Statistical analysis.

- Our simulations can be treated as *computer experiments*. This is particularly the case for Monte Carlo methods
- The results can be analysed with the same statistical tools as we would use analysing experimental data.
- As in all experiments, we are looking for expectation values and an estimate of how accurate they are, i.e., possible sources for errors.

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Statistical analysis

- As in other experiments, many numerical experiments have two classes of errors:
  1. Statistical errors
  2. Systematical errors
- Statistical errors can be estimated using standard tools from statistics
- Systematical errors are method specific and must be treated differently from case to case.

Statistics, wrapping up from last week

Let us analyze the problem by splitting up the correlation term into partial sums of the form:

$$f_d = \frac{1}{n-d}\sum_{k=1}^{n-d}(x_k - \bar{x}_n)(x_{k+d} - \bar{x}_n)$$

The correlation term of the error can now be rewritten in terms of f_d

$$\frac{2}{n}\sum_{k<l}(x_k - \bar{x}_n)(x_l - \bar{x}_n) = 2\sum_{d=1}^{n-1} f_d$$

The value of f_d reflects the correlation between measurements separated by the distance d in the sample samples. Notice that for $d = 0$, f is just the sample variance, $\mathrm{var}(x)$. If we divide f_d by $\mathrm{var}(x)$, we arrive at the so called *autocorrelation function*

$$\kappa_d = \frac{f_d}{\mathrm{var}(x)}$$

which gives us a useful measure of pairwise correlations starting always at 1 for $d = 0$.

Statistics, final expression

The sample error can now be written in terms of the autocorrelation function:

$$\begin{aligned}
\mathrm{err}_X^2 &= \frac{1}{n}\mathrm{var}(x) + \frac{2}{n}\cdot\mathrm{var}(x)\sum_{d=1}^{n-1}\frac{f_d}{\mathrm{var}(x)} \\
&= \left(1 + 2\sum_{d=1}^{n-1}\kappa_d\right)\frac{1}{n}\mathrm{var}(x) \\
&= \frac{\tau}{n}\cdot\mathrm{var}(x) \qquad (1)
\end{aligned}$$

and we see that err_X can be expressed in terms the uncorrelated sample variance times a correction factor τ which accounts for the correlation between measurements. We call this correction factor the *autocorrelation time*:

$$\tau = 1 + 2\sum_{d=1}^{n-1} \kappa_d \tag{2}$$

Statistics, effective number of correlations

For a correlation free experiment, τ equals 1.

We can interpret a sequential correlation as an effective reduction of the number of measurements by a factor τ. The effective number of measurements becomes:

$$n_{\mathrm{eff}} = \frac{n}{\tau}$$

To neglect the autocorrelation time τ will always cause our simple uncorrelated estimate of $\mathrm{err}_X^2 \approx \mathrm{var}(x)/n$ to be less than the true sample error. The estimate of the error will be too *good*. On the other hand, the calculation of the full autocorrelation time poses an efficiency problem if the set of measurements is very large.

Can we understand this? Time Auto-correlation Function

The so-called time-displacement autocorrelation $\phi(t)$ for a quantity $\mathbf{M}$ is given by

$$\phi(t) = \int dt' \left[\mathbf{M}(t') - \langle \mathbf{M} \rangle\right] \left[\mathbf{M}(t'+t) - \langle \mathbf{M} \rangle\right],$$

which can be rewritten as

$$\phi(t) = \int dt' \left[\mathbf{M}(t')\mathbf{M}(t'+t) - \langle \mathbf{M} \rangle^2\right],$$

where $\langle \mathbf{M} \rangle$ is the average value and $\mathbf{M}(t)$ its instantaneous value. We can discretize this function as follows, where we used our set of computed values $\mathbf{M}(t)$ for a set of discretized times (our Monte Carlo cycles corresponding to moving all electrons?)

$$\phi(t) = \frac{1}{t_{\mathrm{max}} - t} \sum_{t'=0}^{t_{\mathrm{max}}-t} \mathbf{M}(t')\mathbf{M}(t'+t) - \frac{1}{t_{\mathrm{max}} - t} \sum_{t'=0}^{t_{\mathrm{max}}-t} \mathbf{M}(t') \times \frac{1}{t_{\mathrm{max}} - t} \sum_{t'=0}^{t_{\mathrm{max}}-t} \mathbf{M}(t'+t).$$

Time Auto-correlation Function

One should be careful with times close to t_{max}, the upper limit of the sums becomes small and we end up integrating over a rather small time interval. This means that the statistical error in $\phi(t)$ due to the random nature of the fluctuations in $\mathbf{M}(t)$ can become large.

One should therefore choose $t \ll t_{\mathrm{max}}$.

Note that the variable $\mathbf{M}$ can be any expectation values of interest.

The time-correlation function gives a measure of the correlation between the various values of the variable at a time t' and a time $t' + t$. If we multiply the values of $\mathbf{M}$ at these two different times, we will get a positive contribution if they are fluctuating in the same direction, or a negative value if they fluctuate in the opposite direction. If we then integrate over time, or use the discretized version of, the time correlation function $\phi(t)$ should take a non-zero value if the fluctuations are correlated, else it should gradually go to zero. For times a long way apart the different values of $\mathbf{M}$ are most likely uncorrelated and $\phi(t)$ should be zero.

Time Auto-correlation Function

We can derive the correlation time by observing that our Metropolis algorithm is based on a random walk in the space of all possible spin configurations. Our probability distribution function $\hat{\mathbf{w}}(t)$ after a given number of time steps t could be written as

$$\hat{\mathbf{w}}(t) = \hat{\mathbf{W}}^{\mathbf{t}}\hat{\mathbf{w}}(0),$$

with $\hat{\mathbf{w}}(0)$ the distribution at $t = 0$ and $\hat{\mathbf{W}}$ representing the transition probability matrix. We can always expand $\hat{\mathbf{w}}(0)$ in terms of the right eigenvectors of $\hat{\mathbf{v}}$ of $\hat{\mathbf{W}}$ as

$$\hat{\mathbf{w}}(0) = \sum_i \alpha_i \hat{\mathbf{v}}_i,$$

resulting in

$$\hat{\mathbf{w}}(t) = \hat{\mathbf{W}}^t\hat{\mathbf{w}}(0) = \hat{\mathbf{W}}^t \sum_i \alpha_i \hat{\mathbf{v}}_i = \sum_i \lambda_i^t \alpha_i \hat{\mathbf{v}}_i,$$

with λ_i the i^{th} eigenvalue corresponding to the eigenvector $\hat{\mathbf{v}}_i$.

Time Auto-correlation Function

If we assume that λ_0 is the largest eigenvector we see that in the limit $t \to \infty$, $\hat{\mathbf{w}}(t)$ becomes proportional to the corresponding eigenvector $\hat{\mathbf{v}}_0$. This is our steady state or final distribution.

We can relate this property to an observable like the mean energy. With the probabilty $\hat{\mathbf{w}}(t)$ (which in our case is the squared trial wave function) we can write the expectation values as

$$\langle \mathbf{M}(t) \rangle = \sum_\mu \hat{\mathbf{w}}(t)_\mu \mathbf{M}_\mu,$$

or as the scalar of a vector product

$$\langle \mathbf{M}(t) \rangle = \hat{\mathbf{w}}(t)\mathbf{m},$$

with $\mathbf{m}$ being the vector whose elements are the values of $\mathbf{M}_\mu$ in its various microstates μ.

Time Auto-correlation Function

We rewrite this relation as

$$\langle \mathbf{M}(t) \rangle = \hat{\mathbf{w}}(t)\mathbf{m} = \sum_i \lambda_i^t \alpha_i \hat{\mathbf{v}}_i \mathbf{m}_i.$$

If we define $m_i = \hat{\mathbf{v}}_i \mathbf{m}_i$ as the expectation value of $\mathbf{M}$ in the i^{th} eigenstate we can rewrite the last equation as

$$\langle \mathbf{M}(t) \rangle = \sum_i \lambda_i^t \alpha_i m_i.$$

Since we have that in the limit $t \to \infty$ the mean value is dominated by the the largest eigenvalue λ_0, we can rewrite the last equation as

$$\langle \mathbf{M}(t) \rangle = \langle \mathbf{M}(\infty) \rangle + \sum_{i \neq 0} \lambda_i^t \alpha_i m_i.$$

We define the quantity

$$\tau_i = -\frac{1}{log \lambda_i},$$

and rewrite the last expectation value as

$$\langle \mathbf{M}(t) \rangle = \langle \mathbf{M}(\infty) \rangle + \sum_{i \neq 0} \alpha_i m_i e^{-t/\tau_i}.$$

Time Auto-correlation Function

The quantities τ_i are the correlation times for the system. They control also the auto-correlation function discussed above. The longest correlation time is obviously given by the second largest eigenvalue τ_1, which normally defines the correlation time discussed above. For large times, this is the only correlation time that survives. If higher eigenvalues of the transition matrix are well separated from λ_1 and we simulate long enough, τ_1 may well define the correlation time. In other cases we may not be able to extract a reliable result for τ_1. Coming back to the time correlation function $\phi(t)$ we can present a more general definition in terms of the mean magnetizations $\langle \mathbf{M}(t) \rangle$. Recalling that the mean value is equal to $\langle \mathbf{M}(\infty) \rangle$ we arrive at the expectation values

$$\phi(t) = \langle \mathbf{M}(0) - \mathbf{M}(\infty) \rangle \langle \mathbf{M}(t) - \mathbf{M}(\infty) \rangle,$$

resulting in

$$\phi(t) = \sum_{i,j \neq 0} m_i \alpha_i m_j \alpha_j e^{-t/\tau_i},$$

which is appropriate for all times.

Correlation Time

If the correlation function decays exponentially

$$\phi(t) \sim \exp(-t/\tau)$$

then the exponential correlation time can be computed as the average

$$\tau_{\exp} = -\langle \frac{t}{log|\frac{\phi(t)}{\phi(0)}|} \rangle.$$

If the decay is exponential, then

$$\int_0^\infty dt\phi(t) = \int_0^\infty dt\phi(0)\exp(-t/\tau) = \tau\phi(0),$$

which suggests another measure of correlation

$$\tau_{\text{int}} = \sum_k \frac{\phi(k)}{\phi(0)},$$

called the integrated correlation time.

Resampling methods: Jackknife and Bootstrap

Two famous resampling methods are the **independent bootstrap** and **the jackknife**.

The jackknife is a special case of the independent bootstrap. Still, the jackknife was made popular prior to the independent bootstrap. And as the popularity of the independent bootstrap soared, new variants, such as **the dependent bootstrap**.

The Jackknife and independent bootstrap work for independent, identically distributed random variables. If these conditions are not satisfied, the methods will fail. Yet, it should be said that if the data are independent, identically distributed, and we only want to estimate the variance of $\overline{X}$ (which often is the case), then there is no need for bootstrapping.

Resampling methods: Jackknife

The Jackknife works by making many replicas of the estimator $\widehat{\theta}$. The jackknife is a resampling method, we explained that this happens by scrambling the data in some way. When using the jackknife, this is done by systematically leaving out one observation from the vector of observed values $\hat{x} = (x_1, x_2, \cdots, X_n)$. Let $\hat{x}_i$ denote the vector

$$\hat{x}_i = (x_1, x_2, \cdots, x_{i-1}, x_{i+1}, \cdots, x_n),$$

which equals the vector $\hat{x}$ with the exception that observation number i is left out. Using this notation, define $\widehat{\theta}_i$ to be the estimator $\widehat{\theta}$ computed using $\vec{X}_i$.

Resampling methods: Jackknife estimator

To get an estimate for the bias and standard error of $\widehat{\theta}$, use the following estimators for each component of $\widehat{\theta}$

$$\widehat{\text{Bias}}(\widehat{\theta},\theta) = (n-1)\left(-\widehat{\theta} + \frac{1}{n}\sum_{i=1}^{n}\widehat{\theta}_i\right) \qquad \text{and} \qquad \widehat{\sigma}^2_{\widehat{\theta}} = \frac{n-1}{n}\sum_{i=1}^{n}(\widehat{\theta}_i - \frac{1}{n}\sum_{j=1}^{n}\widehat{\theta}_j)^2.$$

Jackknife code example

```
from numpy import *
from numpy.random import randint, randn
from time import time

def jackknife(data, stat):
    n = len(data);t = zeros(n); inds = arange(n); t0 = time()
    ## 'jackknifing' by leaving out an observation for each i
    for i in range(n):
        t[i] = stat(delete(data,i) )

    # analysis
    print("Runtime: %g sec" % (time()-t0)); print("Jackknife Statistics :")
    print("original           bias      std. error")
    print("%8g %14g %15g" % (stat(data),(n-1)*mean(t)/n, (n*var(t))**.5))

    return t


# Returns mean of data samples
def stat(data):
    return mean(data)


mu, sigma = 100, 15
datapoints = 10000
x = mu + sigma*random.randn(datapoints)
# jackknife returns the data sample
t = jackknife(x, stat)
```

Resampling methods: Bootstrap

Bootstrapping is a nonparametric approach to statistical inference that substitutes computation for more traditional distributional assumptions and asymptotic results. Bootstrapping offers a number of advantages:

1. The bootstrap is quite general, although there are some cases in which it fails.

2. Because it does not require distributional assumptions (such as normally distributed errors), the bootstrap can provide more accurate inferences when the data are not well behaved or when the sample size is small.

3. It is possible to apply the bootstrap to statistics with sampling distributions that are difficult to derive, even asymptotically.

4. It is relatively simple to apply the bootstrap to complex data-collection plans (such as stratified and clustered samples).

Resampling methods: Bootstrap background

Since $\widehat{\theta} = \widehat{\theta}(\hat{X})$ is a function of random variables, $\widehat{\theta}$ itself must be a random variable. Thus it has a pdf, call this function $p(\hat{t})$. The aim of the bootstrap is to estimate $p(\hat{t})$ by the relative frequency of $\widehat{\theta}$. You can think of this as using a histogram in the place of $p(\hat{t})$. If the relative frequency closely resembles $p(\vec{t})$, then using numerics, it is straight forward to estimate all the interesting parameters of $p(\hat{t})$ using point estimators.

Resampling methods: More Bootstrap background

In the case that $\widehat{\theta}$ has more than one component, and the components are independent, we use the same estimator on each component separately. If the probability density function of X_i, $p(x)$, had been known, then it would have been straight forward to do this by:

1. Drawing lots of numbers from $p(x)$, suppose we call one such set of numbers $(X_1^*, X_2^*, \cdots, X_n^*)$.

2. Then using these numbers, we could compute a replica of $\widehat{\theta}$ called $\widehat{\theta}^*$.

By repeated use of (1) and (2), many estimates of $\widehat{\theta}$ could have been obtained. The idea is to use the relative frequency of $\widehat{\theta}^*$ (think of a histogram) as an estimate of $p(\hat{t})$.

Resampling methods: Bootstrap approach

But unless there is enough information available about the process that generated $X_1, X_2, \cdots, X_n$, $p(x)$ is in general unknown. Therefore, Efron in 1979 asked the question: What if we replace $p(x)$ by the relative frequency of the observation X_i; if we draw observations in accordance with the relative frequency of the observations, will we obtain the same result in some asymptotic sense? The answer is yes.

Instead of generating the histogram for the relative frequency of the observation X_i, just draw the values $(X_1^*, X_2^*, \cdots, X_n^*)$ with replacement from the vector $\hat{X}$.

Resampling methods: Bootstrap steps

The independent bootstrap works like this:

1. Draw with replacement n numbers for the observed variables $\hat{x} = (x_1, x_2, \cdots, x_n)$.
2. Define a vector $\hat{x}^*$ containing the values which were drawn from $\hat{x}$.
3. Using the vector $\hat{x}^*$ compute $\widehat{\theta}^*$ by evaluating $\widehat{\theta}$ under the observations $\hat{x}^*$.
4. Repeat this process k times.

When you are done, you can draw a histogram of the relative frequency of $\widehat{\theta}^*$. This is your estimate of the probability distribution $p(t)$. Using this probability distribution you can estimate any statistics thereof. In principle you never draw the histogram of the relative frequency of $\widehat{\theta}^*$. Instead you use the estimators corresponding to the statistic of interest. For example, if you are interested in estimating the variance of $\widehat{\theta}$, apply the etsimator $\widehat{\sigma}^2$ to the values $\widehat{\theta}^*$.

Code example for the Bootstrap method

The following code starts with a Gaussian distribution with mean value $\mu = 100$ and variance $\sigma = 15$. We use this to generate the data used in the bootstrap analysis. The bootstrap analysis returns a data set after a given number of bootstrap operations (as many as we have data points). This data set consists of estimated mean values for each bootstrap operation. The histogram generated by the bootstrap method shows that the distribution for these mean values is also a Gaussian, centered around the mean value $\mu = 100$ but with standard deviation $\sigma/\sqrt{n}$, where n is the number of bootstrap samples (in this case the same as the number of original data points). The value of the standard deviation is what we expect from the central limit theorem.

```
%matplotlib inline

from numpy import *
from numpy.random import randint, randn
from time import time
from scipy.stats import norm
import matplotlib.pyplot as plt

# Returns mean of bootstrap samples
def stat(data):
    return mean(data)

# Bootstrap algorithm
def bootstrap(data, statistic, R):
    t = zeros(R); n = len(data); inds = arange(n); t0 = time()

    # non-parametric bootstrap
    for i in range(R):
        t[i] = statistic(data[randint(0,n,n)])

    # analysis
    print("Runtime: %g sec" % (time()-t0)); print("Bootstrap Statistics :")
    print("original           bias      std. error")
    print("%8g %8g %14g %15g" % (statistic(data), std(data),\
                                 mean(t), \
```

```
                                std(t)))
    return t


mu, sigma = 100, 15
datapoints = 10000
x = mu + sigma*random.randn(datapoints)
# bootstrap returns the data sample
# the histogram of the bootstrapped  data
t = bootstrap(x, stat, datapoints)
# the histogram of the bootstrapped  data
n, binsboot, patches = plt.hist(t, bins=50, density='true',histtype='bar', color='red', alpha=0.75

# add a 'best fit' line
y = norm.pdf( binsboot, mean(t), std(t))
lt = plt.plot(binsboot, y, 'r--', linewidth=1)
plt.xlabel('Smarts')
plt.ylabel('Probability')
plt.axis([99.5, 100.6, 0, 3.0])
plt.grid(True)

plt.show()
```

Resampling methods: Blocking

The blocking method was made popular by Flyvbjerg and Pedersen (1989) and has become one of the standard ways to estimate $V(\widehat{\theta})$ for exactly one $\widehat{\theta}$, namely $\widehat{\theta} = \overline{X}$.

Assume $n = 2^d$ for some integer $d > 1$ and $X_1, X_2, \cdots, X_n$ is a stationary time series to begin with. Moreover, assume that the time series is asymptotically uncorrelated. We switch to vector notation by arranging $X_1, X_2, \cdots, X_n$ in an n-tuple. Define:

$$\hat{X} = (X_1, X_2, \cdots, X_n).$$

The strength of the blocking method is when the number of observations, n is large. For large n, the complexity of dependent bootstrapping scales poorly, but the blocking method does not, moreover, it becomes more accurate the larger n is.

Blocking Transformations

We now define blocking transformations. The idea is to take the mean of subsequent pair of elements from $\vec{X}$ and form a new vector $\vec{X}_1$. Continuing in the same way by taking the mean of subsequent pairs of elements of $\vec{X}_1$ we obtain $\vec{X}_2$, and so on. Define $\vec{X}_i$ recursively by:

$$\begin{aligned}(\vec{X}_0)_k &\equiv (\vec{X})_k \\ (\vec{X}_{i+1})_k &\equiv \frac{1}{2}\Big((\vec{X}_i)_{2k-1} + (\vec{X}_i)_{2k}\Big) \qquad \text{for all} \qquad 1 \leq i \leq d-1 \end{aligned} \tag{3}$$

The quantity $\vec{X}_k$ is subject to k **blocking transformations**. We now have d vectors $\vec{X}_0, \vec{X}_1, \cdots, \vec{X}_{d-1}$ containing the subsequent averages of observations. It turns out that if the components of $\vec{X}$ is a stationary time series, then the components of $\vec{X}_i$ is a stationary time series for all $0 \leq i \leq d-1$

We can then compute the autocovariance, the variance, sample mean, and number of observations for each i. Let $\gamma_i, \sigma_i^2, \overline{X}_i$ denote the autocovariance, variance and average of the elements of $\vec{X}_i$ and let n_i be the number of elements of $\vec{X}_i$. It follows by induction that $n_i = n/2^i$.

Blocking Transformations

Using the definition of the blocking transformation and the distributive property of the covariance, it is clear that since $h = |i-j|$ we can define

$$\begin{aligned}
\gamma_{k+1}(h) &= cov\left((X_{k+1})_i, (X_{k+1})_j\right) \\
&= \frac{1}{4} cov\left((X_k)_{2i-1} + (X_k)_{2i}, (X_k)_{2j-1} + (X_k)_{2j}\right) \\
&= \frac{1}{2}\gamma_k(2h) + \frac{1}{2}\gamma_k(2h+1) \text{ h} = 0 \qquad (4) \\
&= \frac{1}{4}\gamma_k(2h-1) + \frac{1}{2}\gamma_k(2h) + \frac{1}{4}\gamma_k(2h+1) \quad \text{else} \qquad (5)
\end{aligned}$$

The quantity $\hat{X}$ is asymptotic uncorrelated by assumption, $\hat{X}_k$ is also asymptotic uncorrelated. Let's turn our attention to the variance of the sample mean $V(\overline{X})$.

Blocking Transformations, getting there

We have

$$V(\overline{X}_k) = \frac{\sigma_k^2}{n_k} + \underbrace{\frac{2}{n_k}\sum_{h=1}^{n_k-1}\left(1 - \frac{h}{n_k}\right)\gamma_k(h)}_{\equiv e_k} = \frac{\sigma_k^2}{n_k} + e_k \quad \text{if} \quad \gamma_k(0) = \sigma_k^2. \qquad (6)$$

The term e_k is called the **truncation error**:

$$e_k = \frac{2}{n_k}\sum_{h=1}^{n_k-1}\left(1 - \frac{h}{n_k}\right)\gamma_k(h). \qquad (7)$$

We can show that $V(\overline{X}_i) = V(\overline{X}_j)$ for all $0 \leq i \leq d-1$ and $0 \leq j \leq d-1$.

Blocking Transformations, final expressions

We can then wrap up

$$n_{j+1}\overline{X}_{j+1} = \sum_{i=1}^{n_{j+1}} (\hat{X}_{j+1})_i = \frac{1}{2}\sum_{i=1}^{n_j/2} (\hat{X}_j)_{2i-1} + (\hat{X}_j)_{2i}$$
$$= \frac{1}{2}\left[(\hat{X}_j)_1 + (\hat{X}_j)_2 + \cdots + (\hat{X}_j)_{n_j}\right] = \underbrace{\frac{n_j}{2}}_{=n_{j+1}} \overline{X}_j = n_{j+1}\overline{X}_j. \quad (8)$$

By repeated use of this equation we get $V(\overline{X}_i) = V(\overline{X}_0) = V(\overline{X})$ for all $0 \leq i \leq d-1$. This has the consequence that

$$V(\overline{X}) = \frac{\sigma_k^2}{n_k} + e_k \qquad \text{for all} \qquad 0 \leq k \leq d-1. \quad (9)$$

Flyvbjerg and Petersen demonstrated that the sequence $\{e_k\}_{k=0}^{d-1}$ is decreasing, and conjecture that the term e_k can be made as small as we would like by making k (and hence d) sufficiently large. The sequence is decreasing (Master of Science thesis by Marius Jonsson, UiO 2018). It means we can apply blocking transformations until e_k is sufficiently small, and then estimate $V(\overline{X})$ by $\widehat{\sigma}_k^2/n_k$.

For an elegant solution and proof of the blocking method, see the recent article of Marius Jonsson (former MSc student of the Computational Physics group).

We can improve upon this by using the algorithms provided by the **optimize** package in Python. One of these algorithms is Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm.

The optimization problem is to minimize $f(\mathbf{x})$ where $\mathbf{x}$ is a vector in R^n, and f is a differentiable scalar function. There are no constraints on the values that $\mathbf{x}$ can take.

The algorithm begins at an initial estimate for the optimal value $\mathbf{x}_0$ and proceeds iteratively to get a better estimate at each stage.

The search direction p_k at stage k is given by the solution of the analogue of the Newton equation

$$B_k\mathbf{p}_k = -\nabla f(\mathbf{x}_k),$$

where B_k is an approximation to the Hessian matrix, which is updated iteratively at each stage, and $\nabla f(\mathbf{x}_k)$ is the gradient of the function evaluated at x_k. A line search in the direction p_k is then used to find the next point x_{k+1} by minimising

$$f(\mathbf{x}_k + \alpha\mathbf{p}_k),$$

over the scalar $\alpha > 0$.

The modified code here uses the BFGS algorithm but performs now a production run and writes to file all average values of the energy.

```
# 2-electron VMC code for 2dim quantum dot with importance sampling
# Using gaussian rng for new positions and Metropolis- Hastings
# Added 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
from scipy.optimize import minimize
import sys
import os

# Where to save data files
PROJECT_ROOT_DIR = "Results"
DATA_ID = "Results/EnergyMin"

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

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

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

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


# 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

# Derivate of wave function ansatz as function of variational parameters
def DerivativeWFansatz(r,alpha,beta):

    WfDer  = np.zeros((2), np.double)
    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
    WfDer[0] = -0.5*(r1+r2)
    WfDer[1] = -r12*r12*deno2
    return  WfDer
```

```
# 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


# Computing the derivative of the energy and the energy
def EnergyDerivative(x0):


    # 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)

    energy = 0.0
    DeltaE = 0.0
    alpha = x0[0]
    beta = x0[1]
    EnergyDer = 0.0
    DeltaPsi = 0.0
    DerivativePsiE = 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)
            DerPsi = DerivativeWFansatz(PositionOld,alpha,beta)
            DeltaPsi += DerPsi
            energy += DeltaE
            DerivativePsiE += DerPsi*DeltaE

        # We calculate mean values
        energy /= NumberMCcycles
        DerivativePsiE /= NumberMCcycles
        DeltaPsi /= NumberMCcycles
        EnergyDer  = 2*(DerivativePsiE-DeltaPsi*energy)
        return EnergyDer


    # Computing the expectation value of the local energy
    def Energy(x0):
        # 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)

        energy = 0.0
        DeltaE = 0.0
        alpha = x0[0]
        beta = x0[1]
        #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
            if Printout:
               outfile.write('%f\n' %(energy/(MCcycle+1.0)))
        # We calculate mean values
        energy /= NumberMCcycles
        return energy

    #Here starts the main program with variable declarations
    NumberParticles = 2
    Dimension = 2
    # seed for rng generator
    seed()
    # Monte Carlo cycles for parameter optimization
    Printout = False
    NumberMCcycles= 10000
    # guess for variational parameters
    x0 = np.array([0.9,0.2])
    # Using Broydens method to find optimal parameters
    res = minimize(Energy, x0, method='BFGS', jac=EnergyDerivative, options={'gtol': 1e-4,'disp': True
    x0 = res.x
    # Compute the energy again with the optimal parameters and increased number of Monte Cycles
    NumberMCcycles= 2**19
    Printout = True
    FinalEnergy = Energy(x0)
    EResult = np.array([FinalEnergy,FinalEnergy])
    outfile.close()
    #nice printout with Pandas
    import pandas as pd
    from pandas import DataFrame
    data ={'Optimal Parameters':x0, 'Final Energy':EResult}
    frame = pd.DataFrame(data)
    print(frame)
```

Note that the **minimize** function returns the final values for the variable $\alpha = x0[0]$ and $\beta = x0[1]$ in the array x.

When we have found the minimum, we use these optimal parameters to perform a production run of energies. The output is in turn written to file and is used, together with resampling methods like the **blocking method**, to obtain the best possible estimate for the standard deviation. The optimal minimum is, even with our guess, rather close to the exact value of 3.0 a.u.

The sampling functions can be used to perform both a blocking analysis, or a standard bootstrap and jackknife analysis.

How do we proceed?

There are several paths which can be chosen. One is to extend the brute force gradient descent method with an adapative stochastic gradient. There are several examples of this. A recent approach based on the Langevin equations seems like a promising approach for general and possibly non-convex optimization problems.

Here we would like to point out that our next step is now to use the optimal values for our variational parameters and use these as inputs to a production run.

Here we would output values of the energy and perform for example a blocking analysis of the results in order to get a best possible estimate of the standard deviation.

Resampling analysis

The next step is then to use the above data sets and perform a resampling analysis, either using say the Bootstrap method or the Blocking method. Since the data will be correlated, we would recommend to use the non-iid Bootstrap code here. The theoretical background for these resampling methods is found in the statistical analysis lecture notes

Here we have tailored the codes to the output file from the previous example. We present first the bootstrap resampling with non-iid stochastic event.

```
# Common imports
import os

# Where to save the figures and data files
DATA_ID = "Results/EnergyMin"

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

infile = open(data_path("Energies.dat"),'r')

from numpy import std, mean, concatenate, arange, loadtxt, zeros, ceil
from numpy.random import randint
from time import time


def tsboot(data,statistic,R,l):
    t = zeros(R); n = len(data); k = int(ceil(float(n)/l));
    inds = arange(n); t0 = time()

    # time series bootstrap
    for i in range(R):
        # construct bootstrap sample from
        # k chunks of data. The chunksize is l
        _data = concatenate([data[j:j+l] for j in randint(0,n-l,k)])[0:n];
        t[i] = statistic(_data)

    # analysis
    print ("Runtime: %g sec" % (time()-t0)); print ("Bootstrap Statistics :")
    print ("original           bias      std. error")
    print ("%8g %14g %15g" % (statistic(data), \
                             mean(t) - statistic(data), \
                             std(t) ))
    return t
# Read in data
X = loadtxt(infile)
# statistic to be estimated. Takes two args.
# arg1: the data
def stat(data):
    return mean(data)
t = tsboot(X, stat, 2**12, 2**10)
```

The blocking code, based on the article of Marius Jonsson is given here

```
# Common imports
import os

# Where to save the figures and data files
DATA_ID = "Results/EnergyMin"

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

infile = open(data_path("Energies.dat"),'r')

from numpy import log2, zeros, mean, var, sum, loadtxt, arange, array, cumsum, dot, transpose, dia
from numpy.linalg import inv

def block(x):
    # preliminaries
    n = len(x)
    d = int(log2(n))
    s, gamma = zeros(d), zeros(d)
    mu = mean(x)

    # estimate the auto-covariance and variances
    # for each blocking transformation
    for i in arange(0,d):
        n = len(x)
        # estimate autocovariance of x
        gamma[i] = (n)**(-1)*sum( (x[0:(n-1)]-mu)*(x[1:n]-mu) )
        # estimate variance of x
        s[i] = var(x)
        # perform blocking transformation
        x = 0.5*(x[0::2] + x[1::2])

    # generate the test observator M_k from the theorem
    M = (cumsum( ((gamma/s)**2*2**arange(1,d+1)[::-1])[::-1] )  )[::-1]

    # we need a list of magic numbers
    q =array([6.634897,9.210340, 11.344867, 13.276704, 15.086272, 16.811894, 18.475307, 20.090235,

    # use magic to determine when we should have stopped blocking
    for k in arange(0,d):
        if(M[k] < q[k]):
            break
    if (k >= d-1):
        print("Warning: Use more data")
    return mu, s[k]/2**(d-k)


x = loadtxt(infile)
(mean, var) = block(x)
std = sqrt(var)
import pandas as pd
from pandas import DataFrame
data ={'Mean':[mean], 'STDev':[std]}
frame = pd.DataFrame(data,index=['Values'])
print(frame)
```