Week 10 March 6-10: Resampling Techniques, Bootstrap and Blocking

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Overview of week 10, March 6-10

Topics

- Top down approach first, what we need to code
- Resampling Techniques and statistics: Bootstrap and Blocking
- Video of Lecture TBA
- Handwritten notes

Teaching Material, videos and written material

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

The top-down approach, part 1

Last week we discussed how to implement a gradient descent method like the simplest possible gradient descent with a simple learning rate as parameter to tune. We repeat the codes here.

```
# 2-electron VMC code for 2dim quantum dot with importance sampling
# Using gaussian rng for new positions and Metropolis- Hastings
# Added energy minimization
# Common imports
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



# 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 anal
```

What have we done?

The exact energy is 3.0 for an oscillator frequency $\omega = 1$ (with $\hbar = 1$). We note however that with this learning rate and number of iterations, the energies and the derivatives are not yet converged. 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 $f(\mathrm{x})$ where x is a vector in R^n, and f is a differentiable scalar function. There are no constraints on the values that x can take.

The algorithm begins at an initial estimate for the optimal value 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

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

where B_k is an approximation to the Hessian matrix, which is updated iteratively at each stage, and $\nabla f(\mathrm{x}_k)$ is the gradient of the function evaluated at x_k. A line search in the direction p_k is then

Code part 2

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):
```

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
```

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.

Statistical analysis

- As in other experiments, many numerical experiments have two classes of errors:
  - Statistical errors
  - 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

The *probability distribution function (PDF)* is a function $p(x)$ on the domain which, in the discrete case, gives us the probability or relative frequency with which these values of X occur:

$$p(x) = \text{prob}(X = x)$$

In the continuous case, the PDF does not directly depict the actual probability. Instead we define the probability for the stochastic variable to assume any value on an infinitesimal interval around x to be $p(x)dx$. The continuous function $p(x)$ then gives us the *density* of the probability rather than the probability itself. The probability for a stochastic variable to assume any value on a non-infinitesimal interval $[a, b]$ is then just the integral:

$$\text{prob}(a \leq X \leq b) = \int_a^b p(x)dx$$

Qualitatively speaking, a stochastic variable represents the values of numbers chosen as if by chance from some specified PDF so that

Statistics, moments

A particularly useful class of special expectation values are the *moments*. The n-th moment of the PDF p is defined as follows:

$$\langle x^n \rangle \equiv \int x^n p(x)\, dx$$

The zero-th moment $\langle 1 \rangle$ is just the normalization condition of p. The first moment, $\langle x \rangle$, is called the *mean* of p and often denoted by the letter μ:

$$\langle x \rangle = \mu \equiv \int x p(x)\, dx$$

Statistics, central moments

A special version of the moments is the set of *central moments*, the n-th central moment defined as:

$$\langle (x - \langle x \rangle)^n \rangle \equiv \int (x - \langle x \rangle)^n p(x)\, dx$$

The zero-th and first central moments are both trivial, equal 1 and 0, respectively. But the second central moment, known as the *variance* of p, is of particular interest. For the stochastic variable X, the variance is denoted as σ_X^2 or $\mathrm{var}(X)$:

$$\begin{aligned}
\sigma_X^2 \quad = \quad \mathrm{var}(X) &= \langle (x - \langle x \rangle)^2 \rangle = \int (x - \langle x \rangle)^2 p(x)\, dx && (1)\\
&= \int \left(x^2 - 2x\langle x \rangle^2 + \langle x \rangle^2 \right) p(x)\, dx && (2)\\
&= \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2 && (3)\\
&= \langle x^2 \rangle - \langle x \rangle^2 && (4)
\end{aligned}$$

The square root of the variance, $\sigma = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$ is called the

Statistics, covariance

Another important quantity is the so called covariance, a variant of the above defined variance. Consider again the set $\{X_i\}$ of n stochastic variables (not necessarily uncorrelated) with the multivariate PDF $P(x_1, \ldots, x_n)$. The *covariance* of two of the stochastic variables, X_i and X_j, is defined as follows:

$$\begin{aligned} \mathrm{cov}(X_i, X_j) &\equiv \langle (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) \rangle \\ &= \int \cdots \int (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle)\, P(x_1, \ldots, x_n)\, dx_1 \ldots dx_n \end{aligned} \tag{5}$$

with

$$\langle x_i \rangle = \int \cdots \int x_i\, P(x_1, \ldots, x_n)\, dx_1 \ldots dx_n$$

Statistics, more covariance

If we consider the above covariance as a matrix $C_{ij} = \mathrm{cov}(X_i, X_j)$, then the diagonal elements are just the familiar variances, $C_{ii} = \mathrm{cov}(X_i, X_i) = \mathrm{var}(X_i)$. It turns out that all the off-diagonal elements are zero if the stochastic variables are uncorrelated. This is easy to show, keeping in mind the linearity of the expectation value. Consider the stochastic variables X_i and X_j, $(i \neq j)$:

$$\begin{aligned}
\mathrm{cov}(X_i, X_j) &= \langle (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) \rangle && (6)\\
&= \langle x_i x_j - x_i \langle x_j \rangle - \langle x_i \rangle x_j + \langle x_i \rangle \langle x_j \rangle \rangle && (7)\\
&= \langle x_i x_j \rangle - \langle x_i \langle x_j \rangle \rangle - \langle \langle x_i \rangle x_j \rangle + \langle \langle x_i \rangle \langle x_j \rangle \rangle && (8)\\
&= \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle - \langle x_i \rangle \langle x_j \rangle + \langle x_i \rangle \langle x_j \rangle && (9)\\
&= \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle && (10)
\end{aligned}$$

Statistics, independent variables

If X_i and X_j are independent, we get $\langle x_i x_j \rangle = \langle x_i \rangle \langle x_j \rangle$, resulting in $\mathrm{cov}(X_i, X_j) = 0 \quad (i \neq j)$.
Also useful for us is the covariance of linear combinations of stochastic variables. Let $\{X_i\}$ and $\{Y_i\}$ be two sets of stochastic variables. Let also $\{a_i\}$ and $\{b_i\}$ be two sets of scalars. Consider the linear combination:

$$U = \sum_i a_i X_i \qquad V = \sum_j b_j Y_j$$

By the linearity of the expectation value

$$\mathrm{cov}(U, V) = \sum_{i,j} a_i b_j \mathrm{cov}(X_i, Y_j)$$

Statistics, more variance

Now, since the variance is just $\mathrm{var}(X_i) = \mathrm{cov}(X_i, X_i)$, we get the variance of the linear combination $U = \sum_i a_i X_i$:

$$\mathrm{var}(U) = \sum_{i,j} a_i a_j \mathrm{cov}(X_i, X_j) \tag{11}$$

And in the special case when the stochastic variables are uncorrelated, the off-diagonal elements of the covariance are as we know zero, resulting in:

$$\mathrm{var}(U) = \sum_i a_i^2 \mathrm{cov}(X_i, X_i) = \sum_i a_i^2 \mathrm{var}(X_i)$$

$$\mathrm{var}(\sum_i a_i X_i) = \sum_i a_i^2 \mathrm{var}(X_i)$$

which will become very useful in our study of the error in the mean value of a set of measurements.

Statistics and stochastic processes

A *stochastic process* is a process that produces sequentially a chain of values:

$$\{x_1, x_2, \dots x_k, \dots\}.$$

We will call these values our *measurements* and the entire set as our measured *sample*. The action of measuring all the elements of a sample we will call a stochastic *experiment* since, operationally, they are often associated with results of empirical observation of some physical or mathematical phenomena; precisely an experiment. We assume that these values are distributed according to some PDF $p_X(x)$, where X is just the formal symbol for the stochastic variable whose PDF is $p_X(x)$. Instead of trying to determine the full distribution p we are often only interested in finding the few lowest moments, like the mean μ_X and the variance σ_X.

Statistics and sample variables

In practical situations a sample is always of finite size. Let that size be n. The expectation value of a sample, the *sample mean*, is then defined as follows:

$$\bar{x}_n \equiv \frac{1}{n}\sum_{k=1}^{n} x_k$$

The *sample variance* is:

$$\mathrm{var}(x) \equiv \frac{1}{n}\sum_{k=1}^{n}(x_k - \bar{x}_n)^2$$

its square root being the *standard deviation of the sample*. The *sample covariance* is:

$$\mathrm{cov}(x) \equiv \frac{1}{n}\sum_{kl}(x_k - \bar{x}_n)(x_l - \bar{x}_n)$$

Statistics, sample variance and covariance

Note that the sample variance is the sample covariance without the cross terms. In a similar manner as the covariance in Eq. (5) is a measure of the correlation between two stochastic variables, the above defined sample covariance is a measure of the sequential correlation between succeeding measurements of a sample. These quantities, being known experimental values, differ significantly from and must not be confused with the similarly named quantities for stochastic variables, mean μ_X, variance $\mathrm{var}(X)$ and covariance $\mathrm{cov}(X, Y)$.

Statistics, law of large numbers

The law of large numbers states that as the size of our sample grows to infinity, the sample mean approaches the true mean μ_X of the chosen PDF:

$$\lim_{n\to\infty} \bar{x}_n = \mu_X$$

The sample mean $\bar{x}_n$ works therefore as an estimate of the true mean μ_X.
What we need to find out is how good an approximation $\bar{x}_n$ is to μ_X. In any stochastic measurement, an estimated mean is of no use to us without a measure of its error. A quantity that tells us how well we can reproduce it in another experiment. We are therefore interested in the PDF of the sample mean itself. Its standard deviation will be a measure of the spread of sample means, and we will simply call it the *error* of the sample mean, or just sample error, and denote it by err_X. In practice, we will only be able to produce an *estimate* of the sample error since the exact value would require the knowledge of the true PDFs behind, which we usually do not have.

Statistics, more on sample error

Let us first take a look at what happens to the sample error as the size of the sample grows. In a sample, each of the measurements x_i can be associated with its own stochastic variable X_i. The stochastic variable $\overline{X}_n$ for the sample mean $\bar{x}_n$ is then just a linear combination, already familiar to us:

$$\overline{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$$

All the coefficients are just equal $1/n$. The PDF of $\overline{X}_n$, denoted by $p_{\overline{X}_n}(x)$ is the desired PDF of the sample means.

Statistics

The probability density of obtaining a sample mean $\bar{x}_n$ is the product of probabilities of obtaining arbitrary values $x_1, x_2, \ldots, x_n$ with the constraint that the mean of the set $\{x_i\}$ is $\bar{x}_n$:

$$p_{\overline{X}_n}(x) = \int p_X(x_1) \cdots \int p_X(x_n)\, \delta\left(x - \frac{x_1 + x_2 + \cdots + x_n}{n}\right) dx_n \cdots dx_1$$

And in particular we are interested in its variance $\mathrm{var}(\overline{X}_n)$.

The Central Limit Theorem

Suppose we have a PDF $p(x)$ from which we generate a series N of averages $\mathbb{E}[x_i]$. Each mean value $\mathbb{E}[x_i]$ is viewed as the average of a specific measurement, e.g., throwing dice 100 times and then taking the average value, or producing a certain amount of random numbers. For notational ease, we set $\mathbb{E}[x_i] = x_i$ in the discussion which follows. We do the same for $\mathbb{E}[z] = z$.
If we compute the mean z of m such mean values x_i

$$z = \frac{x_1 + x_2 + \cdots + x_m}{m},$$

the question we pose is which is the PDF of the new variable z.

Finding the Limit

The probability of obtaining an average value z is the product of the probabilities of obtaining arbitrary individual mean values x_i, but with the constraint that the average is z. We can express this through the following expression

$$\tilde{p}(z) = \int dx_1 p(x_1) \int dx_2 p(x_2) \cdots \int dx_m p(x_m) \delta(z - \frac{x_1 + x_2 + \cdots + x_m}{m}),$$

where the δ-function enbodies the constraint that the mean is z. All measurements that lead to each individual x_i are expected to be independent, which in turn means that we can express $\tilde{p}$ as the product of individual $p(x_i)$. The independence assumption is important in the derivation of the central limit theorem.

Rewriting the δ-function

If we use the integral expression for the δ-function

$$\delta(z-\frac{x_1+x_2+\cdots+x_m}{m}) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dq \exp\left(iq(z-\frac{x_1+x_2+\cdots+x_m}{m})\right)$$

and inserting $e^{i\mu q - i\mu q}$ where μ is the mean value we arrive at

$$\tilde{p}(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dq \exp\left(iq(z-\mu)\right)\left[\int_{-\infty}^{\infty} dx p(x) \exp\left(iq(\mu-x)/m\right)\right]^m,$$

with the integral over x resulting in

$$\int_{-\infty}^{\infty} dx p(x) \exp\left(iq(\mu-x)/m\right) = \int_{-\infty}^{\infty} dx p(x)\left[1+\frac{iq(\mu-x)}{m}-\frac{q^2(\mu-x)}{2m^2}\right.$$

Identifying Terms

The second term on the rhs disappears since this is just the mean and employing the definition of σ^2 we have

$$\int_{-\infty}^{\infty} dx p(x) e^{(iq(\mu-x)/m)} = 1 - \frac{q^2\sigma^2}{2m^2} + \ldots,$$

resulting in

$$\left[\int_{-\infty}^{\infty} dx p(x) \exp\left(iq(\mu - x)/m\right)\right]^m \approx \left[1 - \frac{q^2\sigma^2}{2m^2} + \ldots\right]^m,$$

and in the limit $m \to \infty$ we obtain

$$\tilde{p}(z) = \frac{1}{\sqrt{2\pi}(\sigma/\sqrt{m})} \exp\left(-\frac{(z-\mu)^2}{2(\sigma/\sqrt{m})^2}\right),$$

which is the normal distribution with variance $\sigma_m^2 = \sigma^2/m$, where σ is the variance of the PDF $p(x)$ and μ is also the mean of the PDF $p(x)$.

Wrapping it up

Thus, the central limit theorem states that the PDF $\tilde{p}(z)$ of the average of m random values corresponding to a PDF $p(x)$ is a normal distribution whose mean is the mean value of the PDF $p(x)$ and whose variance is the variance of the PDF $p(x)$ divided by m, the number of values used to compute z.
The central limit theorem leads to the well-known expression for the standard deviation, given by

$$\sigma_m = \frac{\sigma}{\sqrt{m}}.$$

The latter is true only if the average value is known exactly. This is obtained in the limit $m \to \infty$ only. Because the mean and the variance are measured quantities we obtain the familiar expression in statistics (the so-called Bessel correction)

$$\sigma_m \approx \frac{\sigma}{\sqrt{m-1}}.$$

In many cases however the above estimate for the standard deviation, in particular if correlations are strong, may be too simplistic. Keep in mind that we have assumed that the variables x

Resampling methods: Bootstrap steps

The independent bootstrap works like this:

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

When you are done, you can draw a histogram of the relative frequency of $\widehat{\beta}^*$. 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 $\widehat{\beta}^*$. Instead you use the estimators corresponding to the statistic of interest. For example, if you are interested in estimating the variance of $\widehat{\beta}$, apply the etsimator $\widehat{\sigma}^2$ to the values $\widehat{\beta}^*$.

Code example for the Bootstrap method and demonstration of central limit theorem

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.

```
import numpy as np
from time import time
from scipy.stats import norm
import matplotlib.pyplot as plt

# Returns mean of bootstrap samples
# Bootstrap algorithm
def bootstrap(data, datapoints):
```

Plotting the Histogram

```
# the histogram of the bootstrapped data (normalized data if density =
n, binsboot, patches = plt.hist(t, 50, density=True, facecolor='red',
# add a 'best fit' line
y = norm.pdf(binsboot, np.mean(t), np.std(t))
lt = plt.plot(binsboot, y, 'b', linewidth=1)
plt.xlabel('x')
plt.ylabel('Probability')
plt.grid(True)
plt.show()
```

Statistics, more technicalities

The desired variance $\mathrm{var}(\overline{X}_n)$, i.e. the sample error squared err_X^2, is given by:

$$\mathrm{err}_X^2 = \mathrm{var}(\overline{X}_n) = \frac{1}{n^2} \sum_{ij} \mathrm{cov}(X_i, X_j) \tag{12}$$

We see now that in order to calculate the exact error of the sample with the above expression, we would need the true means μ_{X_i} of the stochastic variables X_i. To calculate these requires that we know the true multivariate PDF of all the X_i. But this PDF is unknown to us, we have only got the measurements of one sample. The best we can do is to let the sample itself be an estimate of the PDF of each of the X_i, estimating all properties of X_i through the measurements of the sample.

Statistics

Our estimate of μ_{X_i} is then the sample mean $\bar{x}$ itself, in accordance with the the central limit theorem:

$$\mu_{X_i} = \langle x_i \rangle \approx \frac{1}{n} \sum_{k=1}^{n} x_k = \bar{x}$$

Using $\bar{x}$ in place of μ_{X_i} we can give an *estimate* of the covariance in Eq. (12)

$$\mathrm{cov}(X_i, X_j) = \langle (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) \rangle \approx \langle (x_i - \bar{x})(x_j - \bar{x}) \rangle,$$

resulting in

$$\frac{1}{n} \sum_{l}^{n} \left(\frac{1}{n} \sum_{k}^{n} (x_k - \bar{x}_n)(x_l - \bar{x}_n) \right) = \frac{1}{n} \frac{1}{n} \sum_{kl} (x_k - \bar{x}_n)(x_l - \bar{x}_n) = \frac{1}{n} \mathrm{cov}(x)$$

Statistics and sample variance

By the same procedure we can use the sample variance as an estimate of the variance of any of the stochastic variables X_i

$$\mathrm{var}(X_i) = \langle x_i - \langle x_i \rangle \rangle \approx \langle x_i - \bar{x}_n \rangle,$$

which is approximated as

$$\mathrm{var}(X_i) \approx \frac{1}{n} \sum_{k=1}^{n} (x_k - \bar{x}_n) = \mathrm{var}(x) \tag{13}$$

Now we can calculate an estimate of the error err_X of the sample mean $\bar{x}_n$:

$$\mathrm{err}_X^2 = \frac{1}{n^2} \sum_{ij} \mathrm{cov}(X_i, X_j)$$

$$\approx \frac{1}{n^2} \sum_{ij} \frac{1}{n} \mathrm{cov}(x) = \frac{1}{n^2} n^2 \frac{1}{n} \mathrm{cov}(x)$$

$$= \frac{1}{n} \mathrm{var}(x)$$

Statistics, uncorrelated results

In the special case that the measurements of the sample are uncorrelated (equivalently the stochastic variables X_i are uncorrelated) we have that the off-diagonal elements of the covariance are zero. This gives the following estimate of the sample error:

$$\mathrm{err}_X^2 = \frac{1}{n^2}\sum_{ij}\mathrm{cov}(X_i, X_j) = \frac{1}{n^2}\sum_{i}\mathrm{var}(X_i),$$

resulting in

$$\mathrm{err}_X^2 \approx \frac{1}{n^2}\sum_{i}\mathrm{var}(x) = \frac{1}{n}\mathrm{var}(x) \tag{15}$$

where in the second step we have used Eq. (13). The error of the sample is then just its standard deviation divided by the square root of the number of measurements the sample contains. This is a very useful formula which is easy to compute. It acts as a first approximation to the error, but in numerical experiments, we cannot overlook the always present correlations.

Statistics, computations

For computational purposes one usually splits up the estimate of err_X^2, given by Eq. (14), into two parts

$$\mathrm{err}_X^2 = \frac{1}{n}\mathrm{var}(x) + \frac{1}{n}(\mathrm{cov}(x) - \mathrm{var}(x)),$$

which equals

$$\frac{1}{n^2}\sum_{k=1}^{n}(x_k - \bar{x}_n)^2 + \frac{2}{n^2}\sum_{k<l}(x_k - \bar{x}_n)(x_l - \bar{x}_n) \qquad (16)$$

The first term is the same as the error in the uncorrelated case, Eq. (15). This means that the second term accounts for the error correction due to correlation between the measurements. For uncorrelated measurements this second term is zero.

Statistics, more on computations of errors

Computationally the uncorrelated first term is much easier to treat efficiently than the second.

$$\mathrm{var}(x) = \frac{1}{n}\sum_{k=1}^{n}(x_k - \bar{x}_n)^2 = \left(\frac{1}{n}\sum_{k=1}^{n} x_k^2\right) - \bar{x}_n^2$$

We just accumulate separately the values x^2 and x for every measurement x we receive. The correlation term, though, has to be calculated at the end of the experiment since we need all the measurements to calculate the cross terms. Therefore, all measurements have to be stored throughout the experiment.