

Conjugate gradient methods and other optimization methods

Morten Hjorth-Jensen^{1,2}

¹Department of Physics, University of Oslo

²Department of Physics and Astronomy and National Superconducting Cyclotron Laboratory, Michigan State University

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Motivation

Our aim with this part of the project is to be able to

- find an optimal value for the variational parameters using only some few Monte Carlo cycles
- use these optimal values for the variational parameters to perform a large-scale Monte Carlo calculation

To achieve this will look at methods like *Steepest descent* and the *conjugate gradient method*. Both these methods allow us to find the minima of a multi-variable function like our energy (function of several variational parameters). Alternatively, you can always use Newton's method. In particular, since we will normally have one variational parameter, Newton's method can be easily used in finding the minimum of the local energy.

Simple example and demonstration

Let us illustrate what is needed in our calculations using a simple example, the harmonic oscillator in one dimension. For the harmonic oscillator in one-dimension we have a trial wave function and probability

$$\psi_T(x) = e^{-\alpha^2 x^2} \quad P_T(x)dx = \frac{e^{-2\alpha^2 x^2} dx}{\int dx e^{-2\alpha^2 x^2}}$$

with α being the variational parameter. We obtain then the following local energy

$$E_L[\alpha] = \alpha^2 + x^2 \left(\frac{1}{2} - 2\alpha^2 \right),$$

which results in the expectation value for the local energy

$$\langle E_L[\alpha] \rangle = \frac{1}{2}\alpha^2 + \frac{1}{8\alpha^2}$$

Simple example and demonstration

The derivative of the energy with respect to α gives

$$\frac{d\langle E_L[\alpha] \rangle}{d\alpha} = \alpha - \frac{1}{4\alpha^3}$$

and a second derivative which is always positive (meaning that we find a minimum)

$$\frac{d^2\langle E_L[\alpha] \rangle}{d\alpha^2} = 1 + \frac{3}{4\alpha^4}$$

The condition

$$\frac{d\langle E_L[\alpha] \rangle}{d\alpha} = 0,$$

gives the optimal $\alpha = 1/\sqrt{2}$, as expected.

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Exercise 1: Find the local energy for the harmonic oscillator

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a) Derive the local energy for the harmonic oscillator in one dimension and find its expectation value.

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b) Show also that the optimal value of optimal $\alpha = 1/\sqrt{2}$.

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c) Repeat the above steps in two dimensions for N bosons or electrons. What is the optimal value of α ?

Variance in the simple model

We can also minimize the variance. In our simple model the variance is

$$\sigma^2[\alpha] = \frac{1}{2}\alpha^4 - \frac{1}{4} + \frac{1}{32\alpha^4},$$

with first derivative

$$\frac{d\sigma^2[\alpha]}{d\alpha} = 2\alpha^3 - \frac{1}{8\alpha^5}$$

and a second derivative which is always positive

$$\frac{d^2\sigma^2[\alpha]}{d\alpha^2} = 6\alpha^2 + \frac{5}{8\alpha^6}$$

Computing the derivatives

In general we end up computing the expectation value of the energy in terms of some parameters $\alpha_0, \alpha_1, \dots, \alpha_n$ and we search for a minimum in this multi-variable parameter space. This leads to an energy minimization problem *where we need the derivative of the energy as a function of the variational parameters.*

In the above example this was easy and we were able to find the expression for the derivative by simple derivations. However, in our actual calculations the energy is represented by a multi-dimensional integral with several variational parameters. How can we then obtain the derivatives of the energy with respect to the variational parameters without having to resort to expensive numerical derivations?

Expressions for finding the derivatives of the local energy

To find the derivatives of the local energy expectation value as function of the variational parameters, we can use the chain rule and the hermiticity of the Hamiltonian.

Let us define

$$\bar{E}_\alpha = \frac{d\langle E_L[\alpha] \rangle}{d\alpha}.$$

as the derivative of the energy with respect to the variational parameter α (we limit ourselves to one parameter only). In the above example this was easy and we obtain a simple expression for the derivative. We define also the derivative of the trial function (skipping the subindex T) as

$$\bar{\psi}_\alpha = \frac{d\psi[\alpha]}{d\alpha}.$$

Derivatives of the local energy

The elements of the gradient of the local energy are then (using the chain rule and the hermiticity of the Hamiltonian)

$$\bar{E}_\alpha = 2 \left(\left\langle \frac{\bar{\psi}_\alpha}{\psi[\alpha]} E_L[\alpha] \right\rangle - \left\langle \frac{\bar{\psi}_\alpha}{\psi[\alpha]} \right\rangle \langle E_L[\alpha] \rangle \right).$$

From a computational point of view it means that you need to compute the expectation values of

$$\left\langle \frac{\bar{\psi}_\alpha}{\psi[\alpha]} E_L[\alpha] \right\rangle,$$

and

$$\left\langle \frac{\bar{\psi}_\alpha}{\psi[\alpha]} \right\rangle \langle E_L[\alpha] \rangle$$

*

Exercise 2: General expression for the derivative of the energy

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a) Show that

$$\bar{E}_\alpha = 2 \left(\left\langle \frac{\bar{\psi}_\alpha}{\psi[\alpha]} E_L[\alpha] \right\rangle - \left\langle \frac{\bar{\psi}_\alpha}{\psi[\alpha]} \right\rangle \langle E_L[\alpha] \rangle \right).$$

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b) Find the corresponding expression for the variance.

Brief reminder on Newton-Raphson's method

Let us quickly remind ourselves how we derive the above method.

Perhaps the most celebrated of all one-dimensional root-finding routines is Newton's method, also called the Newton-Raphson method. This method requires the evaluation of both the function f and its derivative f' at arbitrary points. If you can only calculate the derivative numerically and/or your function is not of the smooth type, we normally discourage the use of this method.

The equations

The Newton-Raphson formula consists geometrically of extending the tangent line at a current point until it crosses zero, then setting the next guess to the abscissa of that zero-crossing. The mathematics behind this method is rather simple. Employing a Taylor expansion for x sufficiently close to the solution s , we have

$$f(s) = 0 = f(x) + (s - x)f'(x) + \frac{(s - x)^2}{2}f''(x) + \dots$$

For small enough values of the function and for well-behaved functions, the terms beyond linear are unimportant, hence we obtain

$$f(x) + (s - x)f'(x) \approx 0,$$

yielding

$$s \approx x - \frac{f(x)}{f'(x)}.$$

Having in mind an iterative procedure, it is natural to start iterating with

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

Simple geometric interpretation

The above is Newton-Raphson's method. It has a simple geometric interpretation, namely x_{n+1} is the point where the tangent from $(x_n, f(x_n))$ crosses the x -axis. Close to the solution, Newton-Raphson converges fast to the desired result. However, if we are far from a root, where the higher-order terms in the series are important, the Newton-Raphson formula can give grossly inaccurate results. For instance, the initial guess for the root might be so far from the true root as to let the search interval include a local maximum or minimum of the function. If an iteration places a trial guess near such a local extremum, so that the first derivative nearly vanishes, then Newton-Raphson may fail totally

Extending to more than one variable

Newton's method can be generalized to systems of several non-linear equations and variables. Consider the case with two equations

$$\begin{aligned} f_1(x_1, x_2) &= 0 \\ f_2(x_1, x_2) &= 0, \end{aligned}$$

which we Taylor expand to obtain

$$\begin{aligned} 0 = f_1(x_1 + h_1, x_2 + h_2) &= f_1(x_1, x_2) + h_1 \partial f_1 / \partial x_1 + h_2 \partial f_1 / \partial x_2 + \dots \\ 0 = f_2(x_1 + h_1, x_2 + h_2) &= f_2(x_1, x_2) + h_1 \partial f_2 / \partial x_1 + h_2 \partial f_2 / \partial x_2 + \dots \end{aligned}$$

Defining the Jacobian matrix \hat{J} we have

$$\hat{J} = \begin{pmatrix} \partial f_1 / \partial x_1 & \partial f_1 / \partial x_2 \\ \partial f_2 / \partial x_1 & \partial f_2 / \partial x_2 \end{pmatrix},$$

we can rephrase Newton's method as

$$\begin{pmatrix} x_1^{n+1} \\ x_2^{n+1} \end{pmatrix} = \begin{pmatrix} x_1^n \\ x_2^n \end{pmatrix} + \begin{pmatrix} h_1^n \\ h_2^n \end{pmatrix},$$

where we have defined

$$\begin{pmatrix} h_1^n \\ h_2^n \end{pmatrix} = -\hat{J}^{-1} \begin{pmatrix} f_1(x_1^n, x_2^n) \\ f_2(x_1^n, x_2^n) \end{pmatrix}.$$

We need thus to compute the inverse of the Jacobian matrix and it is to understand that difficulties may arise in case \hat{J} is nearly singular.

It is rather straightforward to extend the above scheme to systems of more than two non-linear equations. In our case, the Jacobian matrix is given by the Hessian that represents the second derivative of cost function.

Steepest descent

The basic idea of gradient descent is that a function $F(\mathbf{x})$, $\mathbf{x} \equiv (x_1, \dots, x_n)$, decreases fastest if one goes from \mathbf{x} in the direction of the negative gradient $-\nabla F(\mathbf{x})$.

It can be shown that if

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma_k \nabla F(\mathbf{x}_k),$$

with $\gamma_k > 0$.

For γ_k small enough, then $F(\mathbf{x}_{k+1}) \leq F(\mathbf{x}_k)$. This means that for a sufficiently small γ_k we are always moving towards smaller function values, i.e a minimum.

More on Steepest descent

The previous observation is the basis of the method of steepest descent, which is also referred to as just gradient descent (GD). One starts with an initial guess \mathbf{x}_0 for a minimum of F and computes new approximations according to

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma_k \nabla F(\mathbf{x}_k), \quad k \geq 0.$$

The parameter γ_k is often referred to as the step length or the learning rate within the context of Machine Learning.

The ideal

Ideally the sequence $\{\mathbf{x}_k\}_{k=0}$ converges to a global minimum of the function F . In general we do not know if we are in a global or local minimum. In the special case when F is a convex function, all local minima are also global minima, so in this case gradient descent can converge to the global solution. The advantage of this scheme is that it is conceptually simple and straightforward to implement. However the method in this form has some severe limitations:

In machine learning we are often faced with non-convex high dimensional cost functions with many local minima. Since GD is deterministic we will get stuck in a local minimum, if the method converges, unless we have a very good initial guess. This also implies that the scheme is sensitive to the chosen initial condition.

Note that the gradient is a function of $\mathbf{x} = (x_1, \dots, x_n)$ which makes it expensive to compute numerically.

The sensitiveness of the gradient descent

The gradient descent method is sensitive to the choice of learning rate γ_k . This is due to the fact that we are only guaranteed that $F(\mathbf{x}_{k+1}) \leq F(\mathbf{x}_k)$ for sufficiently small γ_k . The problem is to determine an optimal learning rate. If the learning rate is chosen too small the method will take a long time to converge and if it is too large we can experience erratic behavior.

Many of these shortcomings can be alleviated by introducing randomness. One such method is that of Stochastic Gradient Descent (SGD), see below.

Convex functions

Ideally we want our cost/loss function to be convex(concave).

First we give the definition of a convex set: A set C in \mathbb{R}^n is said to be convex if, for all x and y in C and all $t \in (0, 1)$, the point $(1 - t)x + ty$ also belongs to C . Geometrically this means that every point on the line segment connecting x and y is in C as discussed below.

The convex subsets of \mathbb{R} are the intervals of \mathbb{R} . Examples of convex sets of \mathbb{R}^2 are the regular polygons (triangles, rectangles, pentagons, etc...).

Convex function

Convex function: Let $X \subset \mathbb{R}^n$ be a convex set. Assume that the function $f : X \rightarrow \mathbb{R}$ is continuous, then f is said to be convex if

$$f(tx_1 + (1 - t)x_2) \leq tf(x_1) + (1 - t)f(x_2)$$

for all $x_1, x_2 \in X$ and for all $t \in [0, 1]$. If \leq is replaced with a strict inequality in the definition, we demand $x_1 \neq x_2$ and $t \in (0, 1)$ then f is said to be strictly convex. For a single variable function, convexity means that if you draw a straight line connecting $f(x_1)$ and $f(x_2)$, the value of the function on the interval $[x_1, x_2]$ is always below the line as illustrated below.

Conditions on convex functions

In the following we state first and second-order conditions which ensures convexity of a function f . We write D_f to denote the domain of f , i.e the subset of \mathbb{R}^n where f is defined. For more details and proofs we refer to: [S. Boyd and L. Vandenberghe. Convex Optimization. Cambridge University Press.](#)

First order condition. Suppose f is differentiable (i.e $\nabla f(x)$ is well defined for all x in the domain of f). Then f is convex if and only if D_f is a convex set and

$$f(y) \geq f(x) + \nabla f(x)^T(y - x)$$

holds for all $x, y \in D_f$. This condition means that for a convex function the first order Taylor expansion (right hand side above) at any point is a global under estimator of the function. To convince yourself you can make a drawing of $f(x) = x^2 + 1$ and draw the tangent line to $f(x)$ and note that it is always below the graph.

Second order condition. Assume that f is twice differentiable, i.e the Hessian matrix exists at each point in D_f . Then f is convex if and only if D_f is a convex set and its Hessian is positive semi-definite for all $x \in D_f$. For a single-variable function this reduces to $f''(x) \geq 0$. Geometrically this means that f has nonnegative curvature everywhere.

This condition is particularly useful since it gives us an procedure for determining if the function under consideration is convex, apart from using the definition.

More on convex functions

The next result is of great importance to us and the reason why we are going on about convex functions. In machine learning we frequently have to minimize a loss/cost function in order to find the best parameters for the model we are considering.

Ideally we want the global minimum (for high-dimensional models it is hard to know if we have local or global minimum). However, if the cost/loss function is convex the following result provides invaluable information:

Any minimum is global for convex functions. Consider the problem of finding $x \in \mathbb{R}^n$ such that $f(x)$ is minimal, where f is convex and differentiable. Then, any point x^* that satisfies $\nabla f(x^*) = 0$ is a global minimum.

This result means that if we know that the cost/loss function is convex and we are able to find a minimum, we are guaranteed that it is a global minimum.

Some simple problems

1. Show that $f(x) = x^2$ is convex for $x \in \mathbb{R}$ using the definition of convexity.
Hint: If you re-write the definition, f is convex if the following holds for all $x, y \in D_f$ and any $\lambda \in [0, 1]$ $\lambda f(x) + (1 - \lambda)f(y) - f(\lambda x + (1 - \lambda)y) \geq 0$.
2. Using the second order condition show that the following functions are convex on the specified domain.
 - $f(x) = e^x$ is convex for $x \in \mathbb{R}$.
 - $g(x) = -\ln(x)$ is convex for $x \in (0, \infty)$.
3. Let $f(x) = x^2$ and $g(x) = e^x$. Show that $f(g(x))$ and $g(f(x))$ is convex for $x \in \mathbb{R}$. Also show that if $f(x)$ is any convex function then $h(x) = e^{f(x)}$ is convex.
4. A norm is any function that satisfy the following properties
 - $f(\alpha x) = |\alpha|f(x)$ for all $\alpha \in \mathbb{R}$.
 - $f(x + y) \leq f(x) + f(y)$
 - $f(x) \leq 0$ for all $x \in \mathbb{R}^n$ with equality if and only if $x = 0$

Using the definition of convexity, try to show that a function satisfying the properties above is convex (the third condition is not needed to show this).

Standard steepest descent

Before we proceed, we would like to discuss the approach called the **standard Steepest descent**, which again leads to us having to be able to compute a matrix. It belongs to the class of Conjugate Gradient methods (CG).

The success of the CG method for finding solutions of non-linear problems is based on the theory of conjugate gradients for linear systems of equations. It belongs to the class of iterative methods for solving problems from linear algebra of the type

$$\hat{A}\hat{x} = \hat{b}.$$

In the iterative process we end up with a problem like

$$\hat{r} = \hat{b} - \hat{A}\hat{x},$$

where \hat{r} is the so-called residual or error in the iterative process.

When we have found the exact solution, $\hat{r} = 0$.

Gradient method

The residual is zero when we reach the minimum of the quadratic equation

$$P(\hat{x}) = \frac{1}{2}\hat{x}^T \hat{A}\hat{x} - \hat{x}^T \hat{b},$$

with the constraint that the matrix \hat{A} is positive definite and symmetric. This defines also the Hessian and we want it to be positive definite.

Steepest descent method

We denote the initial guess for \hat{x} as \hat{x}_0 . We can assume without loss of generality that

$$\hat{x}_0 = 0,$$

or consider the system

$$\hat{A}\hat{z} = \hat{b} - \hat{A}\hat{x}_0,$$

instead.

Steepest descent method

One can show that the solution \hat{x} is also the unique minimizer of the quadratic form

$$f(\hat{x}) = \frac{1}{2}\hat{x}^T \hat{A}\hat{x} - \hat{x}^T \hat{b}, \quad \hat{x} \in \mathbf{R}^n.$$

This suggests taking the first basis vector \hat{r}_1 (see below for definition) to be the gradient of f at $\hat{x} = \hat{x}_0$, which equals

$$\hat{A}\hat{x}_0 - \hat{b},$$

and $\hat{x}_0 = 0$ it is equal $-\hat{b}$.

Final expressions

We can compute the residual iteratively as

$$\hat{r}_{k+1} = \hat{b} - \hat{A}\hat{x}_{k+1},$$

which equals

$$\hat{b} - \hat{A}(\hat{x}_k + \alpha_k \hat{r}_k),$$

or

$$(\hat{b} - \hat{A}\hat{x}_k) - \alpha_k \hat{A}\hat{r}_k,$$

which gives

$$\alpha_k = \frac{\hat{r}_k^T \hat{r}_k}{\hat{r}_k^T \hat{A}\hat{r}_k}$$

leading to the iterative scheme

$$\hat{x}_{k+1} = \hat{x}_k - \alpha_k \hat{r}_k,$$

Code examples for steepest descent

Simple codes for steepest descent and conjugate gradient using a 2×2 matrix, in c++, Python code to come

```
#include <cmath>
#include <iostream>
#include <fstream>
#include <iomanip>
#include "vectormatrixclass.h"
using namespace std;
// Main function begins here
int main(int argc, char * argv[]){
    int dim = 2;
    Vector x(dim),xsd(dim), b(dim),x0(dim);
    Matrix A(dim,dim);

    // Set our initial guess
    x0(0) = x0(1) = 0;
    // Set the matrix
    A(0,0) = 3;    A(1,0) = 2;    A(0,1) = 2;    A(1,1) = 6;
    b(0) = 2; b(1) = -8;
    cout << "The Matrix A that we are using: " << endl;
    A.Print();
```

```

    cout << endl;
    xsd = SteepestDescent(A,b,x0);
    cout << "The approximate solution using Steepest Descent is: " << endl;
    xsd.Print();
    cout << endl;
}

```

The routine for the steepest descent method

```

Vector SteepestDescent(Matrix A, Vector b, Vector x0){
    int IterMax, i;
    int dim = x0.Dimension();
    const double tolerance = 1.0e-14;
    Vector x(dim),f(dim),z(dim);
    double c,alpha,d;
    IterMax = 30;
    x = x0;
    r = A*x-b;
    i = 0;
    while (i <= IterMax){
        z = A*r;
        c = dot(r,r);
        alpha = c/dot(r,z);
        x = x - alpha*r;
        r = A*x-b;
        if(sqrt(dot(r,r)) < tolerance) break;
        i++;
    }
    return x;
}

```

Steepest descent example

```

import numpy as np
import numpy.linalg as la

import scipy.optimize as sopt

import matplotlib.pyplot as pt
from mpl_toolkits.mplot3d import axes3d

def f(x):
    return 0.5*x[0]**2 + 2.5*x[1]**2

def df(x):
    return np.array([x[0], 5*x[1]])

fig = pt.figure()
ax = fig.gca(projection="3d")

xmesh, ymesh = np.mgrid[-2:2:50j,-2:2:50j]
fmesh = f(np.array([xmesh, ymesh]))
ax.plot_surface(xmesh, ymesh, fmesh)

```

And then as contour plot

```
pt.axis("equal")
pt.contour(xmesh, ymesh, fmesh)
guesses = [np.array([2, 2./5])]
```

Find guesses

```
x = guesses[-1]
s = -df(x)
```

Run it!

```
def f1d(alpha):
    return f(x + alpha*s)

alpha_opt = sopt.golden(f1d)
next_guess = x + alpha_opt * s
guesses.append(next_guess)
print(next_guess)
```

What happened?

```
pt.axis("equal")
pt.contour(xmesh, ymesh, fmesh, 50)
it_array = np.array(guesses)
pt.plot(it_array.T[0], it_array.T[1], "x-")
```

Conjugate gradient method

In the CG method we define so-called conjugate directions and two vectors \hat{s} and \hat{t} are said to be conjugate if

$$\hat{s}^T \hat{A} \hat{t} = 0.$$

The philosophy of the CG method is to perform searches in various conjugate directions of our vectors \hat{x}_i obeying the above criterion, namely

$$\hat{x}_i^T \hat{A} \hat{x}_j = 0.$$

Two vectors are conjugate if they are orthogonal with respect to this inner product. Being conjugate is a symmetric relation: if \hat{s} is conjugate to \hat{t} , then \hat{t} is conjugate to \hat{s} .

Conjugate gradient method

An example is given by the eigenvectors of the matrix

$$\hat{v}_i^T \hat{A} \hat{v}_j = \lambda \hat{v}_i^T \hat{v}_j,$$

which is zero unless $i = j$.

Conjugate gradient method

Assume now that we have a symmetric positive-definite matrix \hat{A} of size $n \times n$. At each iteration $i + 1$ we obtain the conjugate direction of a vector

$$\hat{x}_{i+1} = \hat{x}_i + \alpha_i \hat{p}_i.$$

We assume that \hat{p}_i is a sequence of n mutually conjugate directions. Then the \hat{p}_i form a basis of R^n and we can expand the solution $\hat{A}\hat{x} = \hat{b}$ in this basis, namely

$$\hat{x} = \sum_{i=1}^n \alpha_i \hat{p}_i.$$

Conjugate gradient method

The coefficients are given by

$$\mathbf{Ax} = \sum_{i=1}^n \alpha_i \mathbf{Ap}_i = \mathbf{b}.$$

Multiplying with \hat{p}_k^T from the left gives

$$\hat{p}_k^T \hat{A}\hat{x} = \sum_{i=1}^n \alpha_i \hat{p}_k^T \hat{A}\hat{p}_i = \hat{p}_k^T \hat{b},$$

and we can define the coefficients α_k as

$$\alpha_k = \frac{\hat{p}_k^T \hat{b}}{\hat{p}_k^T \hat{A}\hat{p}_k}$$

Conjugate gradient method and iterations

If we choose the conjugate vectors \hat{p}_k carefully, then we may not need all of them to obtain a good approximation to the solution \hat{x} . We want to regard the conjugate gradient method as an iterative method. This will us to solve systems where n is so large that the direct method would take too much time.

We denote the initial guess for \hat{x} as \hat{x}_0 . We can assume without loss of generality that

$$\hat{x}_0 = 0,$$

or consider the system

$$\hat{A}\hat{z} = \hat{b} - \hat{A}\hat{x}_0,$$

instead.

Conjugate gradient method

One can show that the solution \hat{x} is also the unique minimizer of the quadratic form

$$f(\hat{x}) = \frac{1}{2} \hat{x}^T \hat{A} \hat{x} - \hat{x}^T \hat{b}, \quad \hat{x} \in \mathbf{R}^n.$$

This suggests taking the first basis vector \hat{p}_1 to be the gradient of f at $\hat{x} = \hat{x}_0$, which equals

$$\hat{A} \hat{x}_0 - \hat{b},$$

and $\hat{x}_0 = 0$ it is equal $-\hat{b}$. The other vectors in the basis will be conjugate to the gradient, hence the name conjugate gradient method.

Conjugate gradient method

Let \hat{r}_k be the residual at the k -th step:

$$\hat{r}_k = \hat{b} - \hat{A} \hat{x}_k.$$

Note that \hat{r}_k is the negative gradient of f at $\hat{x} = \hat{x}_k$, so the gradient descent method would be to move in the direction \hat{r}_k . Here, we insist that the directions \hat{p}_k are conjugate to each other, so we take the direction closest to the gradient \hat{r}_k under the conjugacy constraint. This gives the following expression

$$\hat{p}_{k+1} = \hat{r}_k - \frac{\hat{p}_k^T \hat{A} \hat{r}_k}{\hat{p}_k^T \hat{A} \hat{p}_k} \hat{p}_k.$$

Conjugate gradient method

We can also compute the residual iteratively as

$$\hat{r}_{k+1} = \hat{b} - \hat{A} \hat{x}_{k+1},$$

which equals

$$\hat{b} - \hat{A}(\hat{x}_k + \alpha_k \hat{p}_k),$$

or

$$(\hat{b} - \hat{A} \hat{x}_k) - \alpha_k \hat{A} \hat{p}_k,$$

which gives

$$\hat{r}_{k+1} = \hat{r}_k - \hat{A} \hat{p}_k,$$

Simple implementation of the Conjugate gradient algorithm

```

Vector ConjugateGradient(Matrix A, Vector b, Vector x0){
    int dim = x0.Dimension();
    const double tolerance = 1.0e-14;
    Vector x(dim), r(dim), v(dim), z(dim);
    double c, t, d;

    x = x0;
    r = b - A*x;
    v = r;
    c = dot(r, r);
    int i = 0; IterMax = dim;
    while(i <= IterMax){
        z = A*v;
        t = c/dot(v, z);
        x = x + t*v;
        r = r - t*z;
        d = dot(r, r);
        if(sqrt(d) < tolerance)
            break;
        v = r + (d/c)*v;
        c = d; i++;
    }
    return x;
}

```

Broyden–Fletcher–Goldfarb–Shanno 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 $\alpha > 0$.

Automatic differentiation

Python has tools for so-called **automatic differentiation**. Consider the following example

$$f(x) = \sin(2\pi x + x^2)$$

which has the following derivative

$$f'(x) = \cos(2\pi x + x^2) (2\pi + 2x)$$

Using **autograd** we have

```

import autograd.numpy as np

# To do elementwise differentiation:
from autograd import elementwise_grad as egrad

# To plot:
import matplotlib.pyplot as plt

def f(x):
    return np.sin(2*np.pi*x + x**2)

def f_grad_analytic(x):
    return np.cos(2*np.pi*x + x**2)*(2*np.pi + 2*x)

# Do the comparison:
x = np.linspace(0,1,1000)

f_grad = egrad(f)

computed = f_grad(x)
analytic = f_grad_analytic(x)

plt.title('Derivative computed from Autograd compared with the analytical derivative')
plt.plot(x,computed,label='autograd')
plt.plot(x,analytic,label='analytic')

plt.xlabel('x')
plt.ylabel('y')
plt.legend()

plt.show()

print("The max absolute difference is: %g"%(np.max(np.abs(computed - analytic))))

```

Using autograd

Here we experiment with what kind of functions Autograd is capable of finding the gradient of. The following Python functions are just meant to illustrate what Autograd can do, but please feel free to experiment with other, possibly more complicated, functions as well.

```

import autograd.numpy as np
from autograd import grad

def f1(x):
    return x**3 + 1

f1_grad = grad(f1)

# Remember to send in float as argument to the computed gradient from Autograd!
a = 1.0

# See the evaluated gradient at a using autograd:
print("The gradient of f1 evaluated at a = %g using autograd is: %g"%(a,f1_grad(a)))

# Compare with the analytical derivative, that is f1'(x) = 3*x**2
grad_analytical = 3*a**2
print("The gradient of f1 evaluated at a = %g by finding the analytic expression is: %g"%(a,grad_analytical))

```


Autograd with more complicated functions

To differentiate with respect to two (or more) arguments of a Python function, Autograd need to know at which variable the function is being differentiated with respect to.

```
import autograd.numpy as np
from autograd import grad
def f2(x1,x2):
    return 3*x1**3 + x2*(x1 - 5) + 1

# By sending the argument 0, Autograd will compute the derivative w.r.t the first variable, in this case x1
f2_grad_x1 = grad(f2,0)

# ... and differentiate w.r.t x2 by sending 1 as an additional argument to grad
f2_grad_x2 = grad(f2,1)

x1 = 1.0
x2 = 3.0

print("Evaluating at x1 = %g, x2 = %g"%(x1,x2))
print("-"*30)

# Compare with the analytical derivatives:

# Derivative of f2 w.r.t x1 is: 9*x1**2 + x2:
f2_grad_x1_analytical = 9*x1**2 + x2

# Derivative of f2 w.r.t x2 is: x1 - 5:
f2_grad_x2_analytical = x1 - 5

# See the evaluated derivations:
print("The derivative of f2 w.r.t x1: %g"%( f2_grad_x1(x1,x2) ))
print("The analytical derivative of f2 w.r.t x1: %g"%( f2_grad_x1_analytical ))

print()

print("The derivative of f2 w.r.t x2: %g"%( f2_grad_x2(x1,x2) ))
print("The analytical derivative of f2 w.r.t x2: %g"%( f2_grad_x2_analytical ))
```

Note that the grad function will not produce the true gradient of the function. The true gradient of a function with two or more variables will produce a vector, where each element is the function differentiated w.r.t a variable.

More complicated functions using the elements of their arguments directly

```
import autograd.numpy as np
from autograd import grad
def f3(x): # Assumes x is an array of length 5 or higher
    return 2*x[0] + 3*x[1] + 5*x[2] + 7*x[3] + 11*x[4]**2

f3_grad = grad(f3)

x = np.linspace(0,4,5)

# Print the computed gradient:
print("The computed gradient of f3 is: ", f3_grad(x))
```

```

# The analytical gradient is: (2, 3, 5, 7, 22*x[4])
f3_grad_analytical = np.array([2, 3, 5, 7, 22*x[4]])

# Print the analytical gradient:
print("The analytical gradient of f3 is: ", f3_grad_analytical)

```

Note that in this case, when sending an array as input argument, the output from Autograd is another array. This is the true gradient of the function, as opposed to the function in the previous example. By using arrays to represent the variables, the output from Autograd might be easier to work with, as the output is closer to what one could expect from a gradient-evaluating function.

Functions using mathematical functions from Numpy

```

import autograd.numpy as np
from autograd import grad
def f4(x):
    return np.sqrt(1+x**2) + np.exp(x) + np.sin(2*np.pi*x)

f4_grad = grad(f4)

x = 2.7

# Print the computed derivative:
print("The computed derivative of f4 at x = %g is: %g"%(x,f4_grad(x)))

# The analytical derivative is: x/sqrt(1 + x**2) + exp(x) + cos(2*pi*x)*2*pi
f4_grad_analytical = x/np.sqrt(1 + x**2) + np.exp(x) + np.cos(2*np.pi*x)*2*np.pi

# Print the analytical gradient:
print("The analytical gradient of f4 at x = %g is: %g"%(x,f4_grad_analytical))

```

More autograd

```

import autograd.numpy as np
from autograd import grad
def f5(x):
    if x >= 0:
        return x**2
    else:
        return -3*x + 1

f5_grad = grad(f5)

x = 2.7

# Print the computed derivative:
print("The computed derivative of f5 at x = %g is: %g"%(x,f5_grad(x)))

```

And with loops

```

import autograd.numpy as np
from autograd import grad
def f6_for(x):
    val = 0

```

```

    for i in range(10):
        val = val + x**i
    return val

def f6_while(x):
    val = 0
    i = 0
    while i < 10:
        val = val + x**i
        i = i + 1
    return val

f6_for_grad = grad(f6_for)
f6_while_grad = grad(f6_while)

x = 0.5

# Print the computed derivatives of f6_for and f6_while
print("The computed derivative of f6_for at x = %g is: %g"%(x,f6_for_grad(x)))
print("The computed derivative of f6_while at x = %g is: %g"%(x,f6_while_grad(x)))

import autograd.numpy as np
from autograd import grad
# Both of the functions are implementation of the sum: sum(x**i) for i = 0, ..., 9
# The analytical derivative is: sum(i*x**(i-1))
f6_grad_analytical = 0
for i in range(10):
    f6_grad_analytical += i*x**(i-1)

print("The analytical derivative of f6 at x = %g is: %g"%(x,f6_grad_analytical))

```

Using recursion

```

import autograd.numpy as np
from autograd import grad

def f7(n): # Assume that n is an integer
    if n == 1 or n == 0:
        return 1
    else:
        return n*f7(n-1)

f7_grad = grad(f7)

n = 2.0

print("The computed derivative of f7 at n = %d is: %g"%(n,f7_grad(n)))

# The function f7 is an implementation of the factorial of n.
# By using the product rule, one can find that the derivative is:

f7_grad_analytical = 0
for i in range(int(n)-1):
    tmp = 1
    for k in range(int(n)-1):
        if k != i:
            tmp *= (n - k)
    f7_grad_analytical += tmp

print("The analytical derivative of f7 at n = %d is: %g"%(n,f7_grad_analytical))

```

Note that if n is equal to zero or one, Autograd will give an error message. This message appears when the output is independent on input.

Unsupported functions

Autograd supports many features. However, there are some functions that is not supported (yet) by Autograd.

Assigning a value to the variable being differentiated with respect to

```
import autograd.numpy as np
from autograd import grad
def f8(x): # Assume x is an array
    x[2] = 3
    return x*2

f8_grad = grad(f8)

x = 8.4

print("The derivative of f8 is:",f8_grad(x))
```

Here, Autograd tells us that an 'ArrayBox' does not support item assignment. The item assignment is done when the program tries to assign $x[2]$ to the value 3. However, Autograd has implemented the computation of the derivative such that this assignment is not possible.

The syntax `a.dot(b)` when finding the dot product

```
import autograd.numpy as np
from autograd import grad
def f9(a): # Assume a is an array with 2 elements
    b = np.array([1.0,2.0])
    return a.dot(b)

f9_grad = grad(f9)

x = np.array([1.0,0.0])

print("The derivative of f9 is:",f9_grad(x))
```

Here we are told that the 'dot' function does not belong to Autograd's version of a Numpy array. To overcome this, an alternative syntax which also computed the dot product can be used:

```
import autograd.numpy as np
from autograd import grad
def f9_alternative(x): # Assume a is an array with 2 elements
    b = np.array([1.0,2.0])
    return np.dot(x,b) # The same as x_1*b_1 + x_2*b_2

f9_alternative_grad = grad(f9_alternative)

x = np.array([3.0,0.0])

print("The gradient of f9 is:",f9_alternative_grad(x))
```

```
# The analytical gradient of the dot product of vectors x and b with two elements (x_1, x_2) and (
# w.r.t x is (b_1, b_2).
```

Recommended to avoid

The documentation recommends to avoid inplace operations such as

```
a += b
a -= b
a *= b
a /= b
```

Stochastic Gradient Descent

Stochastic gradient descent (SGD) and variants thereof address some of the shortcomings of the Gradient descent method discussed above.

The underlying idea of SGD comes from the observation that a given function, which we want to minimize, can almost always be written as a sum over n data points $\{\mathbf{x}_i\}_{i=1}^n$,

$$C(\beta) = \sum_{i=1}^n c_i(\mathbf{x}_i, \beta).$$

Computation of gradients

This in turn means that the gradient can be computed as a sum over i -gradients

$$\nabla_{\beta} C(\beta) = \sum_i^n \nabla_{\beta} c_i(\mathbf{x}_i, \beta).$$

Stochasticity/randomness is introduced by only taking the gradient on a subset of the data called minibatches. If there are n data points and the size of each minibatch is M , there will be n/M minibatches. We denote these minibatches by B_k where $k = 1, \dots, n/M$.

SGD example

As an example, suppose we have 10 data points $(\mathbf{x}_1, \dots, \mathbf{x}_{10})$ and we choose to have $M = 5$ minibatches, then each minibatch contains two data points. In particular we have $B_1 = (\mathbf{x}_1, \mathbf{x}_2), \dots, B_5 = (\mathbf{x}_9, \mathbf{x}_{10})$. Note that if you choose $M = 1$ you have only a single batch with all data points and on the other extreme, you may choose $M = n$ resulting in a minibatch for each datapoint, i.e $B_k = \mathbf{x}_k$.

The idea is now to approximate the gradient by replacing the sum over all data points with a sum over the data points in one the minibatches picked at random in each gradient descent step

$$\nabla_{\beta} C(\beta) = \sum_{i=1}^n \nabla_{\beta} c_i(\mathbf{x}_i, \beta) \rightarrow \sum_{i \in B_k}^n \nabla_{\beta} c_i(\mathbf{x}_i, \beta).$$

The gradient step

Thus a gradient descent step now looks like

$$\beta_{j+1} = \beta_j - \gamma_j \sum_{i \in B_k}^n \nabla_{\beta} c_i(\mathbf{x}_i, \beta)$$

where k is picked at random with equal probability from $[1, n/M]$. An iteration over the number of minibatches (n/M) is commonly referred to as an epoch. Thus it is typical to choose a number of epochs and for each epoch iterate over the number of minibatches, as exemplified in the code below.

Simple example code

```
import numpy as np

n = 100 #100 datapoints
M = 5   #size of each minibatch
m = int(n/M) #number of minibatches
n_epochs = 10 #number of epochs

j = 0
for epoch in range(1, n_epochs+1):
    for i in range(m):
        k = np.random.randint(m) #Pick the k-th minibatch at random
        #Compute the gradient using the data in minibatch Bk
        #Compute new suggestion for
        j += 1
```

Taking the gradient only on a subset of the data has two important benefits. First, it introduces randomness which decreases the chance that our optimization scheme gets stuck in a local minima. Second, if the size of the minibatches are small relative to the number of datapoints ($M < n$), the computation of the gradient is much cheaper since we sum over the datapoints in the k -th minibatch and not all n datapoints.

When do we stop?

A natural question is when do we stop the search for a new minimum? One possibility is to compute the full gradient after a given number of epochs and check if the norm of the gradient is smaller than some threshold and stop if true. However, the condition that the gradient is zero is valid also for local minima, so this would only tell us that we are close to a local/global minimum. However, we could also evaluate the cost function at this point, store the result and continue the search. If the test kicks in at a later stage we can compare the values of the cost function and keep the β that gave the lowest value.

Slightly different approach

Another approach is to let the step length γ_j depend on the number of epochs in such a way that it becomes very small after a reasonable time such that we do not move at all.

As an example, let $e = 0, 1, 2, 3, \dots$ denote the current epoch and let $t_0, t_1 > 0$ be two fixed numbers. Furthermore, let $t = e \cdot m + i$ where m is the number of minibatches and $i = 0, \dots, m - 1$. Then the function

$$\gamma_j(t; t_0, t_1) = \frac{t_0}{t + t_1}$$

goes to zero as the number of epochs gets large. I.e. we start with a step length $\gamma_j(0; t_0, t_1) = t_0/t_1$ which decays in time t .

In this way we can fix the number of epochs, compute β and evaluate the cost function at the end. Repeating the computation will give a different result since the scheme is random by design. Then we pick the final β that gives the lowest value of the cost function.

```
import numpy as np

def step_length(t,t0,t1):
    return t0/(t+t1)

n = 100 #100 datapoints
M = 5   #size of each minibatch
m = int(n/M) #number of minibatches
n_epochs = 500 #number of epochs
t0 = 1.0
t1 = 10

gamma_j = t0/t1
j = 0
for epoch in range(1,n_epochs+1):
    for i in range(m):
        k = np.random.randint(m) #Pick the k-th minibatch at random
        #Compute the gradient using the data in minibatch Bk
        #Compute new suggestion for beta
        t = epoch*m+i
        gamma_j = step_length(t,t0,t1)
        j += 1

print("gamma_j after %d epochs: %g" % (n_epochs,gamma_j))
```

Program for stochastic gradient

```
# Importing various packages
from math import exp, sqrt
from random import random, seed
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import SGDRegressor

x = 2*np.random.rand(100,1)
y = 4+3*x+np.random.rand(100,1)
```

```

xb = np.c_[np.ones((100,1)), x]
theta_linreg = np.linalg.inv(xb.T.dot(xb)).dot(xb.T).dot(y)
print("Own inversion")
print(theta_linreg)
sgdreg = SGDRegressor(n_iter = 50, penalty=None, eta0=0.1)
sgdreg.fit(x,y.ravel())
print("sgdreg from scikit")
print(sgdreg.intercept_, sgdreg.coef_)

theta = np.random.randn(2,1)

eta = 0.1
Niterations = 1000
m = 100

for iter in range(Niterations):
    gradients = 2.0/m*xb.T.dot(xb.dot(theta)-y)
    theta -= eta*gradients
print("theta frm own gd")
print(theta)

xnew = np.array([[0],[2]])
xbnew = np.c_[np.ones((2,1)), xnew]
ypredict = xbnew.dot(theta)
ypredict2 = xbnew.dot(theta_linreg)

n_epochs = 50
t0, t1 = 5, 50
m = 100
def learning_schedule(t):
    return t0/(t+t1)

theta = np.random.randn(2,1)

for epoch in range(n_epochs):
    for i in range(m):
        random_index = np.random.randint(m)
        xi = xb[random_index:random_index+1]
        yi = y[random_index:random_index+1]
        gradients = 2 * xi.T.dot(xi.dot(theta)-yi)
        eta = learning_schedule(epoch*m+i)
        theta = theta - eta*gradients
print("theta from own sdg")
print(theta)

plt.plot(xnew, ypredict, "r-")
plt.plot(xnew, ypredict2, "b-")
plt.plot(x, y, 'ro')
plt.axis([0,2.0,0, 15.0])
plt.xlabel(r'$x$')
plt.ylabel(r'$y$')
plt.title(r'Random numbers ')
plt.show()

```


Using gradient descent methods, limitations

- **Gradient descent (GD) finds local minima of our function.** Since the GD algorithm is deterministic, if it converges, it will converge to a local minimum of our energy function. Because in ML we are often dealing with extremely rugged landscapes with many local minima, this can lead to poor performance.
- **GD is sensitive to initial conditions.** One consequence of the local nature of GD is that initial conditions matter. Depending on where one starts, one will end up at a different local minima. Therefore, it is very important to think about how one initializes the training process. This is true for GD as well as more complicated variants of GD.
- **Gradients are computationally expensive to calculate for large datasets.** In many cases in statistics and ML, the energy function is a sum of terms, with one term for each data point. For example, in linear regression, $E \propto \sum_{i=1}^n (y_i - \mathbf{w}^T \cdot \mathbf{x}_i)^2$; for logistic regression, the square error is replaced by the cross entropy. To calculate the gradient we have to sum over *all* n data points. Doing this at every GD step becomes extremely computationally expensive. An ingenious solution to this, is to calculate the gradients using small subsets of the data called “mini batches”. This has the added benefit of introducing stochasticity into our algorithm.
- **GD is very sensitive to choices of learning rates.** GD is extremely sensitive to the choice of learning rates. If the learning rate is very small, the training process take an extremely long time. For larger learning rates, GD can diverge and give poor results. Furthermore, depending on what the local landscape looks like, we have to modify the learning rates to ensure convergence. Ideally, we would *adaptively* choose the learning rates to match the landscape.
- **GD treats all directions in parameter space uniformly.** Another major drawback of GD is that unlike Newton’s method, the learning rate for GD is the same in all directions in parameter space. For this reason, the maximum learning rate is set by the behavior of the steepest direction and this can significantly slow down training. Ideally, we would like to take large steps in flat directions and small steps in steep directions. Since we are exploring rugged landscapes where curvatures change, this requires us to keep track of not only the gradient but second derivatives. The ideal scenario would be to calculate the Hessian but this proves to be too computationally expensive.
- GD can take exponential time to escape saddle points, even with random initialization. As we mentioned, GD is extremely sensitive to initial condition since it determines the particular local minimum GD would eventually reach. However, even with a good initialization scheme, through

the introduction of randomness, GD can still take exponential time to escape saddle points.

Codes from numerical recipes

You can however use codes we have adapted from the text [Numerical Recipes in C++](#), see chapter 10.7. Here we present a program, which you also can find at the webpage of the course we use the functions **dfpmin** and **lnsrch**. This is a variant of the Broyden et al algorithm discussed in the previous slide.

- The program uses the harmonic oscillator in one dimensions as example.
- The program does not use armadillo to handle vectors and matrices, but employs rather my own vector-matrix class. These auxiliary functions, and the main program *model.cpp* can all be found under the [program link here](#).

Below we show only excerpts from the main program. For the full program, see the above link.

Finding the minimum of the harmonic oscillator model in one dimension

```
// Main function begins here
int main()
{
    int n, iter;
    double gtol, fret;
    double alpha;
    n = 1;
    // reserve space in memory for vectors containing the variational
    // parameters
    Vector g(n), p(n);
    cout << "Read in guess for alpha" << endl;
    cin >> alpha;
    gtol = 1.0e-5;
    // now call dfmin and compute the minimum
    p(0) = alpha;
    dfpmin(p, n, gtol, &iter, &fret, Efunction, dEfunction);
    cout << "Value of energy minimum = " << fret << endl;
    cout << "Number of iterations = " << iter << endl;
    cout << "Value of alpha at minimum = " << p(0) << endl;
    return 0;
} // end of main program
```

Functions to observe

The functions **Efunction** and **dEfunction** compute the expectation value of the energy and its derivative. They use the the quasi-Newton method of Broyden, Fletcher, Goldfarb, and Shanno (BFGS) It uses the first derivatives only. The BFGS algorithm has proven good performance even for non-smooth

optimizations. These functions need to be changed when you want to your own derivatives.

```
// this function defines the expectation value of the local energy
double Efunction(Vector &x)
{
    double value = x(0)*x(0)*0.5+1.0/(8*x(0)*x(0));
    return value;
} // end of function to evaluate

// this function defines the derivative of the energy
void dEfunction(Vector &x, Vector &g)
{
    g(0) = x(0)-1.0/(4*x(0)*x(0)*x(0));
} // end of function to evaluate
```

You need to change these functions in order to compute the local energy for your system. I used 1000 cycles per call to get a new value of $\langle E_L[\alpha] \rangle$. When I compute the local energy I also compute its derivative. After roughly 10-20 iterations I got a converged result in terms of α .

Python program for 2-electrons in 2 dimensions

```
# 2-electron VMC code for 2dim quantum dot with importance sampling
# Using gaussian rng for new positions and Metropolis- Hastings
# Added energy minimization with gradient descent using fixed step size
# To do: replace with optimization codes from scipy and/or use stochastic gradient descent
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 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 EnergyMinimization(alpha, beta):

    NumberMCcycles= 10000
    # 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()
    energy = 0.0
    DeltaE = 0.0
    EnergyDer = np.zeros((2), np.double)
    DeltaPsi = np.zeros((2), np.double)
    DerivativePsiE = np.zeros((2), np.double)
    #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 energy, EnergyDer

#Here starts the main program with variable declarations
NumberParticles = 2
Dimension = 2
# guess for variational parameters
alpha = 0.9
beta = 0.2
# Set up iteration using gradient descent method
Energy = 0
EDerivative = np.zeros((2), np.double)
eta = 0.01
Niterations = 50
#
for iter in range(Niterations):
    Energy, EDerivative = EnergyMinimization(alpha,beta)
    alphagradient = EDerivative[0]
    betagradient = EDerivative[1]
    alpha -= eta*alphagradient
    beta -= eta*betagradient

print(alpha, beta)
print(Energy, EDerivative[0], EDerivative[1])

```

Using Broyden's algorithm in scipy

The following function uses the above described BFGS algorithm. Here we have defined a function which calculates the energy and a function which computes the first derivative.

```

# 2-electron VMC code for 2dim quantum dot with importance sampling
# Using gaussian rng for new positions and Metropolis- Hastings
# Added energy minimization using the BFGS algorithm, see p. 136 of https://www.springer.com/it/b
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

# 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
    NumberMCCycles= 10000
    # 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]
NumberMCcycles= 10000
#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

# 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()
# guess for variational parameters
x0 = np.array([0.9,0.2])
# Using Broydens method
res = minimize(Energy, x0, method='BFGS', jac=EnergyDerivative, options={'gtol': 1e-4, 'disp': True})
print(res.x)

```


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

How do we proceed?

There are several paths which can be chosen. One is to extend the brute force gradient descent method with an adaptive 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.

Modified code

The modified code here uses the BFGS algorithm but performs now a production run and writes to file all average values of the energy. The [sampling functions](#) can be used to perform both a blocking analysis, or a standard bootstrap and jackknife analysis.

```
# 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

# 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*deno2)

# 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
print(x0)
# Compute the energy again with the optimal parameters and increased number of Monte Cycles
NumberMCcycles= 2**19
Printout = True
outfile = open("Energies.dat",'w')
print(Energy(x0))
outfile.close()

```

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

```

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

# Demo

# data
T0 = time()
X = loadtxt("Energies.dat")

# statistic to be estimated. Takes two args.
# arg1: the data
def stat(data):
    return mean(data)

print ("Data loaded in %g sec" % (time() - T0))
t = tsboot(X, stat, 2**12, 2**10)

```

The blocking code, based on the article of [Marius Jonsson](#) is given here

```

from numpy import log2, zeros, mean, var, sum, loadtxt, arange, array, cumsum, dot, transpose, diag
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 the above table 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 s[k]/2**(d-k)

x = loadtxt("Energies.dat")
print(block(x))

```