Ackley Function - Übung für SuS – May2024

The aim is to try out Monte Carlo simulation and even simulated annealing with Ackleys function.

There will be three parts

* Just implement Ackley's function and check your implementation
* Write a program to do Monte Carlo on the function (a week later)
  + Use the program to generate some results (another week later)
* Implement simulated annealing (later in semester)

This description is just for the first part.

# Introduction

Before one writes a monte carlo program, one must have the cost function correctly implemented. This week, we just do the cost function. Next week, we do the monte carlo programming. If you do not like programming, there will be a link in moodle to an example implementation. It is not in python, but it is easy to read.

## Ackley Function

We usually discuss energy calculations for molecules, but it is easier to work with a toy function. We want a function for which we know where the minimum is and what the local minima look like.

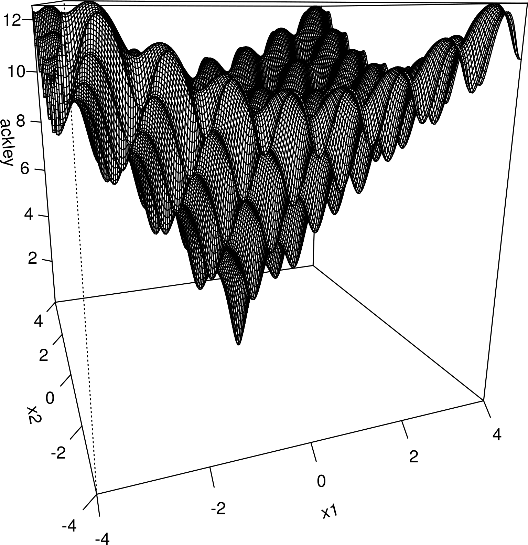
Ackley's function can be calculated in dimensions. You can work with a 1-dimensional problem or a 100-dimensional problem.

The function is:

is the number of dimensions and are the values in each dimension. , and are constants.

To understand the philosophy, consider the form in one dimension

If you set , , , you get values in a nice range. Look at the last term . It is a boring constant, but makes the function go to zero when **.**

One can plot the function in two dimensions to get an overview. It does have lots of minima, but it also has an overall curvature. If you start near -4, there is a global decrease as you move towards **0**.

## Number of dimensions

The Ackley function works in dimensions. Do not be confused by the number of dimensions. An atomic system also leads to a high dimensional sampling/optimisation problem.

You think of an atomic system in a 3D world, but think in terms of parameters. If you have particles, each has parameters. You need dimensions to describe your system.

# To Do

You can program in any language you like, if I can read it. I can read a lot of languages.

* Write a function with a name like ackley(). This function takes one or two parameters (depending on the language)  
   x – an array/vector/list of   
   n – the number of elements in x -   
  In a language like C, you need the second argument. In a language like C++, go or python, the data type knows how many elements it has and you do not need to pass in n.  
  Your function calculates the value of Ackley's function for a given array of .
* Write a test wrapper, that loops over x values from -4 to 4 in some dimension(s) and prints out the values in csv format or some space-separated format that you can feed to your favourite plotting program. Set the step size so you have something like approximately 150 points.
* Run a test loop in one dimension (-4..4). Plot it and upload a picture.
* Either
  + Run a test loop where you have 5 dimensions and you vary the middle dimension from -4 to 4 and make an plot OR
  + Run a test loop where you loop over two dimensions (-4..4) and make a 2D plot which should look like the figure above.
* Check that your function returns zero when or

In the next part, we will put this function in Monte Carlo program.