A review of important concepts in numerical optimization

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Abstract

This laboratory is focused on unconstrained optimization of a function $f(x)$ and, in particular, on understanding some of the basic conditions a minimum has to satisfy. Indeed, a minimum x^* of a function $f(x)$ has to to satisfy that $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive definite. What does this mean from a geometrical point of view? Let us analyze this with several examples.

1 One dimensional case

We begin with the one dimensional case. Assume that $x \in R$ and that

$$f(x) = x^3 - 2x + 2$$

You are asked to follow the next steps:

1. Plot this function within the range $x \in [-2, 2]$, for instance. For that purpose use the `matplotlib` from Python using the examples included within this document[1].

2. Compute analytically the points x^* that satisfy $f'(x) = 0$. Observe if the obtained result is congruent with the plot performed in the previous point.

3. We are now going to check which of the latter points x^* are a minimum (or a maximum). For that purpose let us perform a 2nd order Taylor expansion around point x^*

$$f(x^* + d) \approx f(x^*) + d\, f'(x^*) + \frac{1}{2} d^2\, f''(x^*) \quad (1)$$

   where $d \in R$ is the perturbation around x^*. Since we are dealing with a one dimensional function, $f''(x^*)$ is a real number which may be positive or negative.

   Equation (1) tells us that the function $f(x)$ can be approximated around x^* (with a small value of d) using a quadratic function. The value of the second derivative will tell us if the point x^* is a minimum or a maximum.

   In order for x^* to be a minimum, you need $f''(x^*)$ to be positive. In other words, you need $f''(x^*)$ to be convex at that point. This can be expressed in another way: you need $d^2 f''(x^*) > 0$ for any $d \neq 0$. The latter sentence is obvious (and may seem stupid) in one dimension but has a high importance in higher dimensions.

[1] You may find a gallery here: `http://matplotlib.org/gallery.html`.

4. You may also plot $f''(x)$ for the range $x \in [-2, 2]$. If $f''(x)$ is positive the function can be approximated with a convex 2nd order Taylor expansion at x. On the other hand, if $f''(x)$ is negative the function is said to be concave at that point.

2 Two dimensional case

2.1 A simple two-dimensional function

We are now going to focus on simple two-dimensional functions, $\mathbf{x} \in R^2$, $x = (x_1, x_2)^T$ (vectors are expressed column-wise). Let us begin with the next quadratic expression

$$f(\mathbf{x}) = x_1^2 + x_2^2$$

Follow the next steps:

1. Plot this function. It should be noted that this function has a minimum at $(x_1, x_2) = (0, 0)$.
2. Analytically compute the gradient of the function, $\nabla f(\mathbf{x})$, and compute the point $\mathbf{x}^*$ at which $\nabla f(\mathbf{x}^*) = 0$.
3. Let $\mathbf{d} \in R^2$ be the perturbation around $\mathbf{x}^*$. The Taylor expansion, up to second order, of a function of several variables can be compactly expressed as

$$f(\mathbf{x}^* + \mathbf{d}) \approx f(\mathbf{x}^*) + \mathbf{d}^T \, \nabla f(\mathbf{x}^*) + \frac{1}{2}\mathbf{d}^T \, \nabla^2 f(\mathbf{x}^*) \, \mathbf{d} \tag{2}$$

   Analyze the previous expression and be sure to understand the operations that are done at each of the terms.

   Compute the Hessian matrix, $\nabla^2 f(\mathbf{x})$, at the point $\mathbf{x} = \mathbf{x}^*$. You should obtain

$$\nabla^2 f(\mathbf{x}^*) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

   The latter matrix is giving us information about the shape of the quadratic approximation at $\mathbf{x} = \mathbf{x}^*$ in a similar way as has been done for the one dimensional case.

   For the one-dimensional case it is easy to check if we have a minimum, $f''(x^*) > 0$, or a maximum, $f''(x^*) < 0$. For a higher dimensional problem we are sure that the quadratic approximation is convex and that we have a minimum if

$$\mathbf{d}^T \, \nabla^2 f(\mathbf{x}^*) \, \mathbf{d} > 0 \quad \mathbf{d} \neq \mathbf{0} \tag{3}$$

   We have a maximum if

$$\mathbf{d}^T \, \nabla^2 f(\mathbf{x}^*) \, \mathbf{d} < 0 \quad \mathbf{d} \neq 0 \tag{4}$$

   The previous conditions can be verified by computing the eigenvalues of $\nabla^2 f(\mathbf{x}^*)$. If all eigenvalues are strictly positive, equation (3) is satisfied. If all eigenvalues are strictly negative, equation (4) is satisfied. For this example, which are the eigenvalues of the Hessian matrix? Do we have a minimum or a maximum at x^*?

4. The question that may arise know is: what happens if some eigenvalues are positive and some negative? What happens if the eigenvalue is zero? For that issue you are asked to analyze the following functions:

$$f_A(\mathbf{x}) = -x_1^2 - x_2^2 \qquad f_B(\mathbf{x}) = x_1^2 - x_2^2 \qquad f_C(\mathbf{x}) = x_1^2$$

   You are recommended to draw the contour plot of the previous functions. Observe the shape they have. Then answer the following questions:

   (a) Perform a plot of the function. At which point $\mathbf{x}^*$ is the gradient zero?

   (b) At the points where the gradient is zero, what kind of information is giving us the Hessian matrix? Is this a minimum? A maximum? None of both? You may use the `eigvals` function of Python to compute the eigenvalues of the Hessian matrix (i.e. there is no need to compute them analytically).

   In a similar way as for the one dimensional case, the eigenvalues of the Hessian $\nabla^2 f(\mathbf{x})$ gives us information about the local shape of the function $f(\mathbf{x})$ at point $\mathbf{x}$. This information will be used by numerical methods to accelerate descent to the optimal point we are looking for! In this lab we will focus, however, on the optimal points.

2.2 A more complex two dimensional function

You are proposed to study the function that has been given in the lectures

$$f(x_1, x_2) = x_1^2\,(4 - 2.1\,x_1^2 + \frac{1}{3}x_1^4) + x_1 x_2 + x_2^2\,(-4 + 4x_2^2)$$

Follow these steps:

1. Plot the previous function within the range $x_1 \in [-2, 2]$ and $x_2 \in [-1, 1]$ using, for instance, a step of e.g. 0.1. Be sure that the plot is correct: just look at the plot of the lectures and compare them with the result you obtain. Observe where the minimums (and maximums) may be. There may be multiple minimums and maximums!

2. Analytically compute the gradient $\nabla f(\mathbf{x})$.

3. Numerically compute an approximation of the points $\mathbf{x}^*$ at which $\nabla f(\mathbf{x}^*) = 0$. For that issue

   (a) Evaluate $\|\nabla f(\mathbf{x})\|^2$ at the previous range using a step of e.g. 0.005 or smaller if you prefer (but not too small!). You may create a matrix that stores all the latter values to be able to analyze them in the next steps.

   (b) Using brute force, search for those points $\tilde{\mathbf{x}}$ within the previous range at which the value of $\|\nabla f(\mathbf{x})\|^2$ is strictly smaller than the value of its 8 neighbors[2]. Our purpose here is to find the those points at which the gradient is small. We thus find all the "candidate" points that may be a minimum, a maximum or a saddle point!

   (c) Which are the values of $\tilde{\mathbf{x}}$ you have obtained? Which is the value of $\|\nabla f(\mathbf{x})\|^2$ at those points?

[2] For that issue just ignore those points that are at the border of the grid.

4. Analytically compute the Hessian of $f(x_1, x_2)$ and evaluate it at the values $\tilde{\mathbf{x}}$ you have found. What kind of information is giving you the Hessian? Does it correspond to a minimum (the Hessian is positive definite)? To a maximum (the Hessian is negative definite)? Or may be a saddle point? You may use the eigvals function of Python to compute the eigenvalues of the Hessian matrix (i.e. there is no need to compute them analytically). Take into account that there may be several minimums, maximums and saddle points for the function you are analyzing.

Report

You are asked to deliver a report (PDF, notebook, or whatever else you prefer) that can be done , preferably, in *pairs of two persons* (or *individually*). The format of the document may be a (clean) Python notebook or a PDF document, for instance. Comment the experiments you have performed in section 1 and 2 as well as the results and plots you obtain. Do not expect the reader (i.e. me) to interpret the results for you. I would like to see if you are able to understand the results you have obtained.

If you want to include some parts of code, please include it within the report. Do not include it as separate files. The code, however, won't be evaluated nor executed. You may just deliver the Python notebook if you want.