

6.867 : Homework 1

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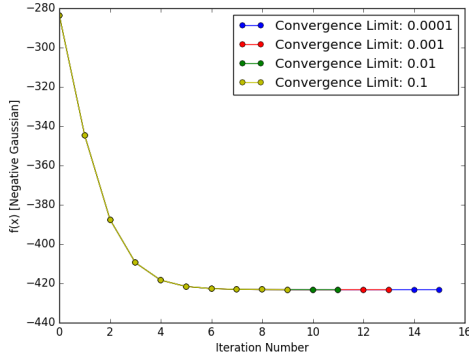


Fig. 1: As convergence limit, ϵ , increases, the iteration stops earlier. From this view, the four solutions differ very little.

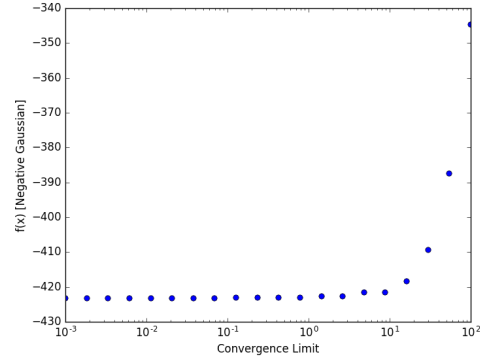


Fig. 2: The final value returned by GD can differ substantially if convergence limit is set too loosely.

I. GRADIENT DESCENT

In this section, we implemented Gradient Descent in Python to find the minimum of a function.

A. Part 1

Our Gradient Descent (GD) implementation begins with an initial guess, x_0 , of the argument x_{min} that minimizes the function, $f(x)$. The implementation is applied to two functions, a negative Gaussian and a quadratic bowl. The gradient, df/dx , can be calculated in closed form (for simple functions), and the next estimate of x_{min} is updated according to the rule $x_{i+1} = x_i - \alpha \cdot \frac{\partial f(x_i)}{\partial x}$. Here, α is the step size, or learning rate, which controls how much the gradient affects the next estimate. The rule is applied until either a pre-determined maximum number of iterations, n_{iters} , occurs, or the function's value at the current iteration differs from the previous iteration's estimate by less than ϵ . Each of these parameters, $(\alpha, n_{iters}, \text{ and } \epsilon)$ impact the GD solution in different ways.

In Fig. 3, the initial guess, x_0 , is varied to show that a close initial guess leads to convergence in only a few steps. As the norm of difference between initial and final estimates grows, the number of iterations increases. For certain initial guesses, we observed that the algorithm did not converge in some maximum number of iterations. For the negative Gaussian, this is because the gradient is very small far from the mean.

The convergence limit determines when the GD algorithm stops, seen in Fig. 2. The error increases if ϵ is too large, as on the right of Fig. 1.

In GD, the norm of the gradient decreases as the solution converges, which is shown for the quadratic bowl function in Fig. 5.

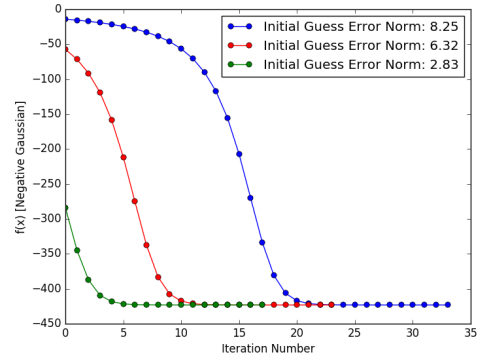


Fig. 3: When initial guess is far from true minimum, it takes many iterations (blue) to converge. As initial guess approaches final solution, number of iterations decreases.

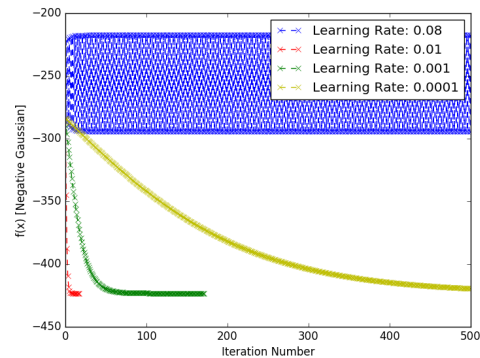


Fig. 4: If learning rate, α , is too large (blue), the solution will oscillate or diverge each iteration. If α is too small, it will take many iterations to converge (yellow). Convergence takes only a few iterations for proper α (red).

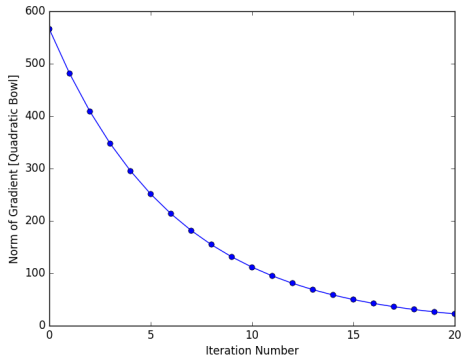


Fig. 5: Norm of gradient decreases with each iteration in GD. This example minimizes the Quadratic Bowl function.

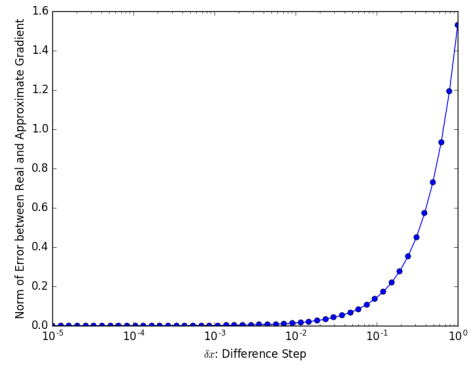


Fig. 6: Norm of gradient approximation error increases as δx increases. This plot is for the Negative Gaussian evaluated at (3,4).

B. Part 2

For more complicated functions, the gradient is not always as easy to compute. Instead, we can use finite difference approximation instead of a the closed form gradient. The gradient approximation for a function of two variables is:

$$\nabla f = \begin{bmatrix} f_x & f_y \end{bmatrix} \approx \begin{bmatrix} \frac{f(x+\delta x, y) - f(x, y)}{\delta x} & \frac{f(x, y+\delta y) - f(x, y)}{\delta y} \end{bmatrix} \quad (1)$$

While Section I-B shows that the error is rather small across a range of (x,y) values for the two functions, the choice of difference step δx is what led to this small error. In Fig. 6, the norm of the difference between the real and approximate gradient gets quite large when δx is also large.

| Gradient vs Finite Difference ($\delta x = 0.01$) | | | | |
|---|---------------------|----------------------|----------------------|------------|
| Function | Gradient | Approximation | Error | Error Norm |
| Neg. Gaussian: $f(3, 4)$ | [-4.2258, -3.6221] | [-4.2375, -3.6299] | [-0.01178, -0.00785] | 0.0141 |
| Neg. Gaussian: $f(12, 4)$ | [11.455, -34.365,] | [11.472, -34.440,] | [0.017, -0.074,] | 0.0764 |
| Quad. Bowl: $f(6, 2)$ | [-330, -350] | [-329.95, -349.95] | [0.05 0.05] | 0.0707 |
| Quad. Bowl: $f(10^3, 90)$ | [10050, 5500] | [10050.05, 5500.05] | [0.05, 0.05] | 0.0707 |