The BFGS Optimization Algorithm

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Outline

Problem Setup

- Given $f : \mathbb{R}^n \to \mathbb{R}$, say we are interested is minimizing the function, which is,

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x}).$$

- From calculus, $\nabla f(\boldsymbol{x}) = \mathbf{0}$ and solve analytically if it can be done.
- This problem arises everywhere especially nowadays with Machine Learning where $f(\boldsymbol{x})$ is usually a cost function we are trying to minimize.

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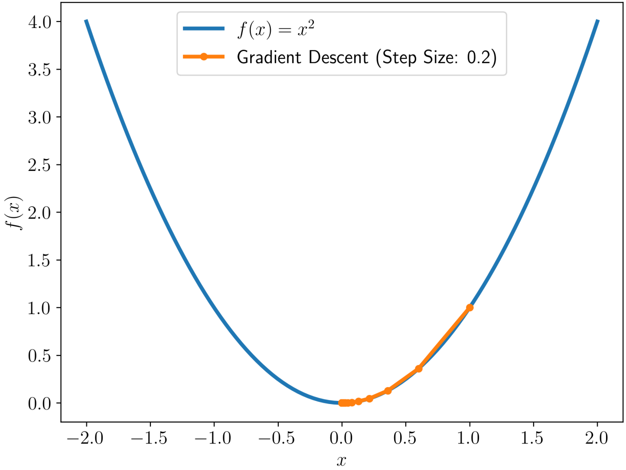
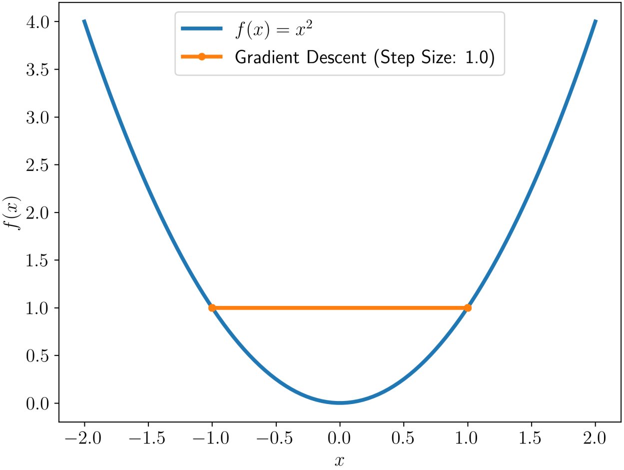


Figure: Gradient Descent on x^2

Gradient Descent



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The good this about this problem is that it is one-dimensional. But we still have to realize the function we are evaluating underneath might be expensive to evaluate.

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There is 2 conditions usually that we need to follow,
Sufficient Decrease:

$$f(\boldsymbol{x} - \alpha_k \nabla f(\boldsymbol{x}_k) \leq f(x_k) + c_1 \alpha_k \|\nabla f\|^2.$$

and curvature condition,

$$\nabla f\left(x_k + \alpha_k p_k\right)^T p_k \geq c_2 \nabla f_k^T p_k$$

These two together make the Wolfe conditions of sufficient decrease.

A picture is worth thousand words

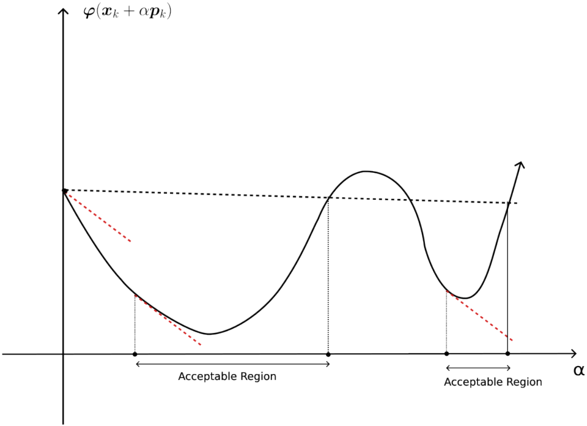

Figure: Strong Wolfe Condition acceptance regions

Steepest Descent & Newton

- As we know steepest descent has it's own problems such as "zig-zag" behaviour as discussed in class. Thus we would like a better method.
- We also learnt about Newton Update for minimizing scalar functions which is given by

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - H_f(\boldsymbol{x}_k)^{-1}\nabla f(\boldsymbol{x}_k).$$

  Where H_f is the hessian of f w.r.t $\boldsymbol{x}$
- This is computationally quite expensive as it requires solving a linear system which takes $\mathcal{O}(n^3)$ time to solve. Where n is problem dimension.

Quasi-Newton

- We would like to develop a Hessian which doesn't take $O(n^3)$ time to solve.
- Before we do that some notation. All the algorithms we saw before now take the form
$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k.$$
Where $\boldsymbol{p}_k$ is a descent direction. We define $y_k = \nabla f(\boldsymbol{x}_{k+1}) - \nabla f(\boldsymbol{x}_k)$ and $s_k = x_{k+1} - x_k$. We would like to mimic the Newton search direction, which is $\boldsymbol{p}_k^{Newton} = -H_f(x_k)^{-1}\nabla f(\boldsymbol{x})$. We would like a approximate hessian $B_k \approx H_f(x_k)$ which doesn't take $\mathcal{O}(n^2)$ to compute.
- These lead us to the BFGS update, introduced by Broyden, Fletcher, Goldfarb and Shanno over the course of 4 papers.

BFGS Derivation Outline

We start by defining a convex quadratic model as at step k as:

$$m_k(p) = f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^\top + \frac{1}{2}\boldsymbol{p}^\top B_k \boldsymbol{p}.$$

The unique minimizer of this quadratic is

$$p_k = -B_k^{-1}\nabla f(\boldsymbol{x}_k).$$

Now instead of recomputing B_{k+1} for next iteration we proceed as follows,
We would like to have $\nabla m_{k+1}(\mathbf{0}) = \nabla f(\boldsymbol{x}_k)$ and
$\nabla m_{k+1}(-\alpha_k \boldsymbol{p}_k) = \nabla f(\boldsymbol{x}_k)$ to provide a good approximation to the objective function f around those points.
The first one we get for free,

$$\nabla m_{k+1}(\mathbf{0}) = \nabla f(\boldsymbol{x}_k).$$

The second one simplifies to,

$$B_{k+1}s_k = y_k.$$

This is the secant equation for the second derivative.

BFGS Derivation Outline

The key benefit of BFGS is that it computes the inverse Hessian directly. Which means we directly find H_{k+1} such that,

$$B_{k+1}s_k = y_k \implies H_k y_k = s_k.$$

We also would like to make the minimal update on H_k to get H_{k+1} and as mentioned earlier it is positive definite,
Which results in the following constrained optimization problem,

$$\min_{H \in \mathbb{R}^{n \times n}} \|W^{1/2}(H - H_k)W^{1/2}\|_F \qquad \text{subject to } \; H = H^T \; \text{ and } Hy_k = s_k.$$

Which gives the formula: $H_{k+1} = \left(I - \rho_k s_k y_k^T\right) H_k \left(I - \rho_k y_k s_k^T\right) + \rho_k s_k s_k^T$
Which is the BFGS update.
Great thing about it is that it is a small rank-2 update and still keeps the matrix positive definite.

Algorithm 1 (BFGS Algorithm)

Require: Given starting point x_0, convergence tolerance $\epsilon > 0$, inverse Hessian approximation H_0;

1: $k \leftarrow 0$;
2: **while** $\|\nabla f_k\| > \epsilon \quad \& \quad k <$ maxIter **do**
3: Compute search direction
4: $p_k = -H_k \nabla f_k$;
5: Set $x_{k+1} = x_k + \alpha_k p_k$ where α_k is computed from a line search procedure to satisfy the Wolfe conditions;
6: Define $s_k = x_{k+1} - x_k$ and $y_k = \nabla f_{k+1} - \nabla f_k$;
7: Compute H_{k+1} ;
8: $k \leftarrow k + 1$;
9: **end while**

Rosenbrock Example

- Test function: $f(x, y) = (a - x)^2 + b(y - x^2)^2$
- Typical parameters: $a = 1, b = 100$
- Illustrates curved valley and optimization challenge

Rosenbrock Example Results

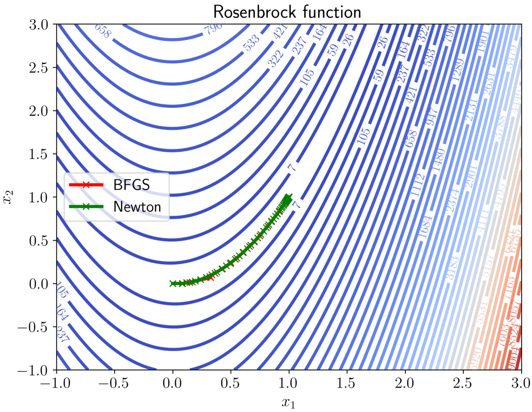

Figure: BFGS optimization path on Rosenbrock function

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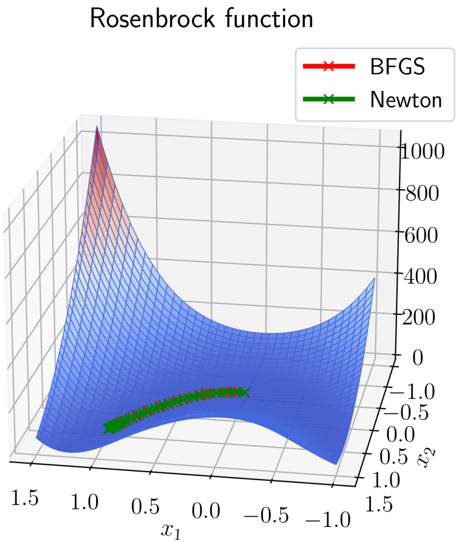

Results

Function	BFGS	Newton	LBFGS	GD
Adjiman Function (2-D)	nan	4.61e-05	5.50e-16	7.70e-01
Rosenbrock N-D (100-D)	9.28e-11	5.13e-04	9.24e-11	2.92e+00
Paviani Function (10-D)	nan	nan	nan	8.72e-02
Csendes Function (10-D)	9.57e-11	1.21e-03	9.16e-11	7.48e-02
Griewank Function (2-D)	nan	1.26e-15	6.65e-11	8.31e-09
Hosaki Function (2-D)	nan	3.17e-05	nan	8.66e-02
Brent Function (2-D)	9.00e-11	2.51e-05	9.90e-11	3.67e+00
Giunta Function (2-D)	2.22e-15	9.40e-05	2.67e-15	1.29e-08
Styblinski-Tang Function (2-D)	2.93e-14	1.12e-04	6.39e-14	9.96e-11
Trid 6 Function (6-D)	nan	2.47e-05	nan	4.08e+00

Conclusion

- Introduced BFGS as an quasi Newton optimzer.
- Provided description of Wolfe conditions, and an outline of BFGS derivation.
- Compared BFGS against other methods.