Numerical Optimization: Local Descent

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May 12, 2020

Overview

Optimization involving multivariate functions

Similar to the single variable function, a common approach to optimization is to incrementally improve a design point x by taking a step that minimizes the objective value based on a local model. The local model may be obtained, for example, from a first- or second-order Taylor approximation.

- Check whether x_k satisfies the termination conditions. If it does, terminate; otherwise proceed to the next step.
- Determine the descent direction d_k using local information such as the gradient or Hessian.
- Determine the step size or learning rate α_k.
- Compute the next design point according to:

$$x_{k+1} = x_k + \alpha_k d_k$$

Line Search

Assuming that we have chosen a descent direction d. We need to choose the step factor α to obtain our next design point. One approach is to use line search, which selects the step factor that minimizes the one-dimensional function:

$$\underset{\alpha}{\text{minimize}} : f(x + \alpha d)$$

Line search is a univariate optimization problem, which was covered in the previous lecture. We can apply the univariate optimization method of our choice. To inform the search, we can use the derivative of the line search objective, which is simply the directional derivative along d at $x + \alpha d$. One needs to be cautious in choosing α. Large steps will result in faster convergence but risk overshooting the minimum. Smaller steps is more stable but very slow. A fixed step factor α is sometimes referred to as a learning rate.

Approximate line search

It is often more computationally efficient to perform more iterations of a descent method than to do exact line search at each iteration. In this case, the goal is to find a suitable step size with a small number of evaluations. Ideally, it needs to satisfy the following

- Sufficient decrease

$$f(x^{k+1}) \leq f(x^k) + \beta\alpha\nabla_{d^k} f(x^k)$$

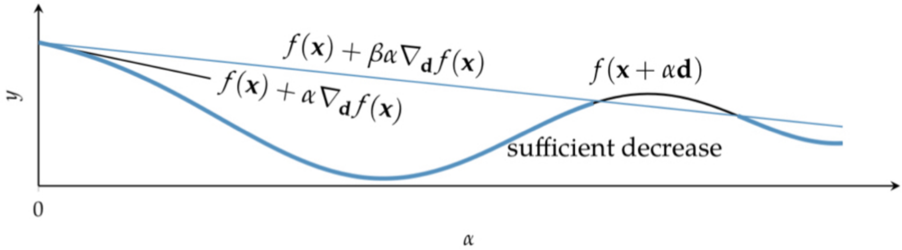
- Curvature condition

$$\nabla_{d^k} f(x^{k+1}) \geq \sigma\nabla_{d^k} f(x^k)$$

Sufficient decrease

$$f(x^{k+1}) \leq f(x^k) + \beta\alpha\nabla_{d^k} f(x^k)$$

where $\beta \in [0, 1]$. A common choice is 1e-4.

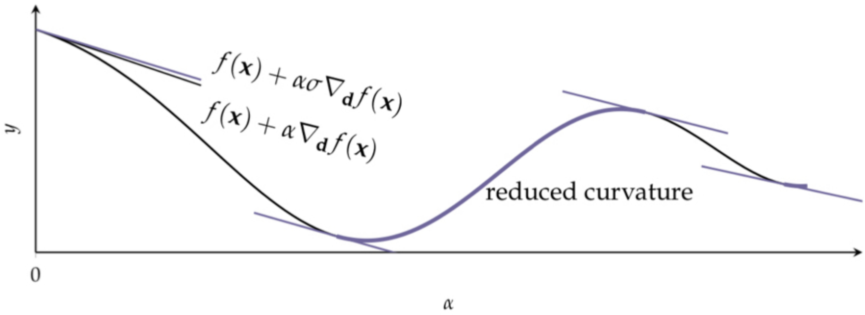


Question: what will happen if you adjust β?

Curvature condition

$$\nabla_{d^k} f(x^{k+1}) \geq \sigma \nabla_{d^k} f(x^k)$$

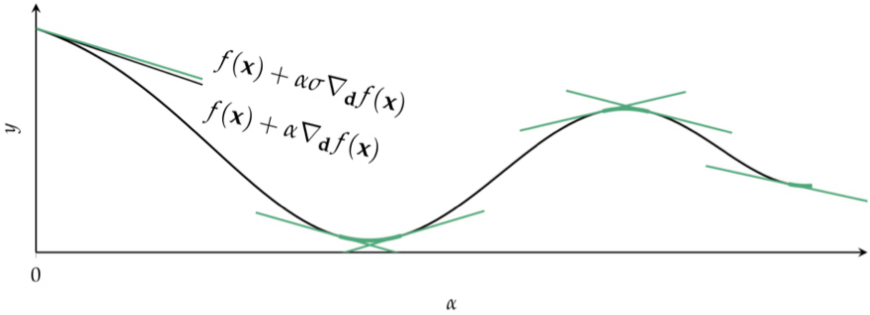
where σ controls how shallow the next directional derivative must be. It is common to set $\beta < \sigma < 1$ with $\sigma = 0.1$ in the conjugate gradient method and 0.9 in Newtons method.



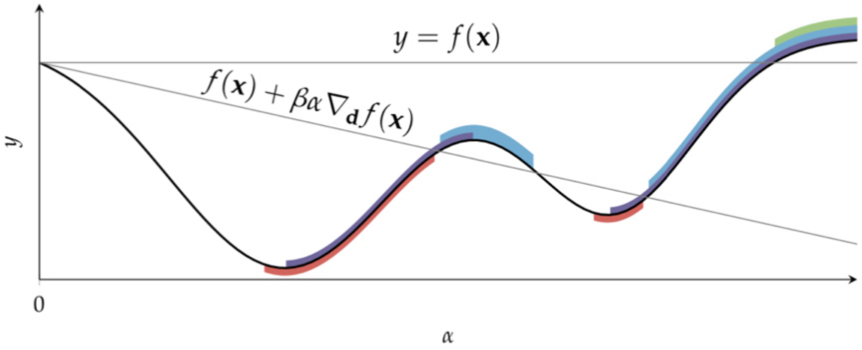
More restrictive curvature condition (strong Wolfe)

$$|\nabla_{d^k} f(x^{k+1})| \leq -\sigma \nabla_{d^k} f(x^k)$$

where σ controls how shallow the next directional derivative must be. It is common to set $\beta < \sigma < 1$ with $\sigma = 0.1$ in the conjugate gradient method and 0.9 in Newtons method.

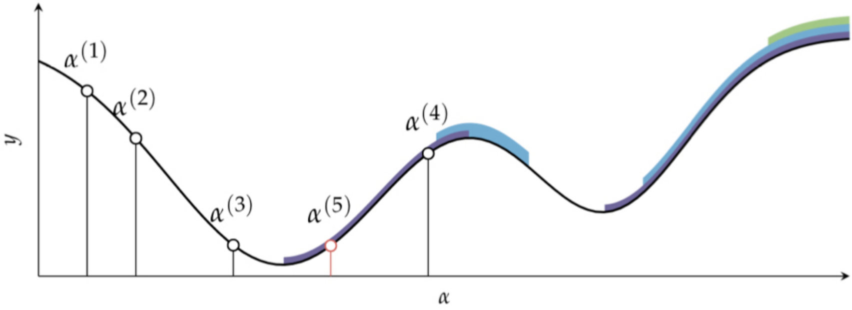


When both conditions are applied



Graphical illustration of line search

- Initial Bracket
- Fibonacci/0.618/bisection until it satisfies the conditions



Terminations conditions

- Maximum iterations.
- Absolute improvement. If the change is smaller than a given threshold, it will terminate:

$$f(x_k) - f(x_{k+1}) < \epsilon_a$$

- Relative improvement. If the change is smaller than a given threshold, it will terminate:

$$f(x_k) - f(x_{k+1}) < \epsilon_r |f(x_k)|$$

- Gradient magnitude. We can also terminate based on the magnitude of the gradient:

$$|\nabla f(x_{k+1})| < \epsilon_g$$

Summary

- Descent direction methods incrementally descend toward a local optimum.
- Univariate optimization can be applied during line search.
- Approximate line search can be used to identify appropriate descent step sizes.
- Termination conditions for descent methods can be based on multiple criteria