Numerical Optimization 07: 2nd order methods

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Overview

Newton's method

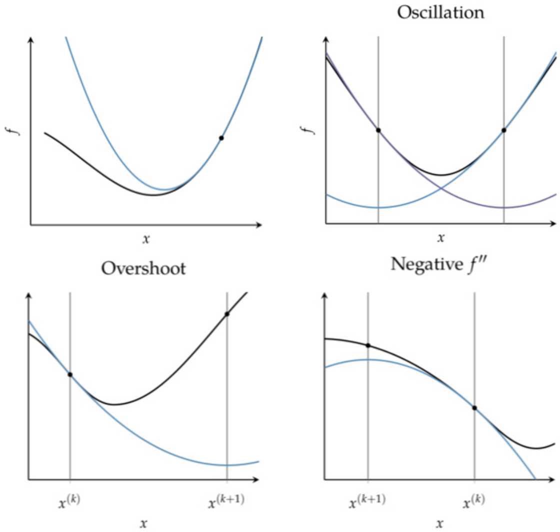
In optimization, knowing the first-order information can help determine the direction to travel, but does not help to determine how far to step to the local minimum. A better way is to use the second-order information.
In univariable optimization, the quadratic approximation about a point (x^k) come from

$$q(x) = f(x^k) + (x - x^k)f`(x^k) + \frac{(x - x^k)^2}{2} f``(x^k)$$

Setting the derivative to zero,

$$\frac{\partial q(x)}{\partial x} = f`(x^k) + (x - x^k)f``(x^k) = 0$$
$$x^{k+1} = x^k - \frac{f`(x^k)}{f``(x^k)}$$

Various cases



Extension to multivariate optimization

If f is a multivariate function

$$f(\boldsymbol{x}) = f(\boldsymbol{x}^k) + (\boldsymbol{g}^k)^T(\boldsymbol{x} - \boldsymbol{x}^k) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^{\boldsymbol{k}})^T \boldsymbol{H}^k(\boldsymbol{x} - \boldsymbol{x}^k)$$

Setting the gradient to be zero,

$$\nabla q(\boldsymbol{x}^k) = \boldsymbol{g}^k + \boldsymbol{H}^k(\boldsymbol{x} - \boldsymbol{x}^k)$$

Quiz

The Booth's function is

$$f(\boldsymbol{x}) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2$$

use the Newton's method to find the minimum when $\boldsymbol{x}$ =[9, 8]

Newton's method with line search

Newtons method can also be used to supply a descent direction to line search or can be modified to use a step factor. Smaller steps toward the minimum or line searches along the descent direction can increase the methods robustness. The descent direction is:

$$\boldsymbol{d}^k = -(\boldsymbol{H}^k)^{-1}\boldsymbol{g}^k$$

Secant Method

Newton's method for univariate function minimization needs to know the first and second derivatives. However, the second derivative is not easy to compute for some cases. The secant method use estimates of H as follows

$$f''(x^k) \approx \frac{f'(x^k) - f'(x^{k-1})}{x^k - x^{k-1}}$$

The secant method requires an additional initial design point. It suffers from the same problems as Newton's method when quadratic function is not a good approximation.

Summary

- Incorporating second-order information in descent methods often speeds convergence.
- Newtons method is a root-finding method that leverages second-order information to quickly descend to a local minimum.
- The secant method approximate Newtons method when the second-order information is not directly available.