Unconstrained Optimization: Search Directions

AE 6310: Optimization for the Design of Engineered Systems

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Search Directions

Now that we have discussed how to search along a given line, we need to understand how to choose search directions.

Consider a first-order Taylor series expansion of the function $f(\boldsymbol{x})$ along a search direction in the neighborhood of the point $\boldsymbol{x_{k-1}}$ (the initial point of our line search):

$$f(\boldsymbol{x_{k-1}} + \alpha \boldsymbol{s_k}) = f(\boldsymbol{x_{k-1}}) + \alpha \boldsymbol{s}_{\boldsymbol{k}}^T \nabla f(\boldsymbol{x_{k-1}})$$

$\boldsymbol{s_k}$ is the search direction, which is typically chosen to obey $||\boldsymbol{s_k}|| = 1$.

Descent Directions

The rate of change of f along the search direction is therefore,

$$\frac{df(\boldsymbol{x})}{d\alpha} = \boldsymbol{s}_{\boldsymbol{k}}^{T} \nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})$$

We typically seek to find a *descent direction*, i.e. one that decreases the value of the objective function for positive α.

The condition for a descent direction is,

$$\frac{df(\boldsymbol{x})}{d\alpha} = \boldsymbol{s}_{\boldsymbol{k}}^{T} \nabla f(\boldsymbol{x}_{\boldsymbol{k-1}}) < 0$$

Descent Directions

We can also write this as

$$\boldsymbol{s}_{\boldsymbol{k}}^{T} \nabla f(\boldsymbol{x}_{\boldsymbol{k-1}}) = ||\boldsymbol{s}_{\boldsymbol{k}}|| \cdot ||\nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})|| \cos\theta < 0$$

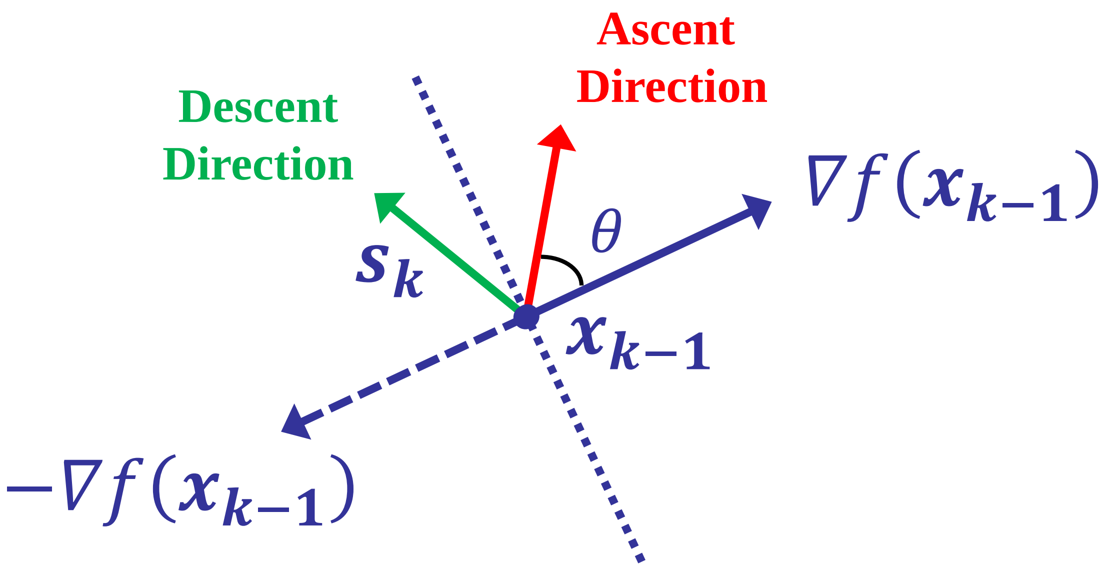
where θ is the angle between the vectors $\boldsymbol{s}_{\boldsymbol{k}}$ and $\nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})$.

Since the vector norms $||\boldsymbol{s}_{\boldsymbol{k}}||$ and $||\nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})||$ are positive, we require $\cos\theta < 0$.

$$\cos\theta < 0 \Rightarrow \quad \pi/2 < \theta < 3\pi/2$$

Descent Directions

We can visualize the situation as follows:



A descent direction forms an acute angle with $-\nabla f(\boldsymbol{x}_{k-1})$.

Steepest Descent Direction

The direction of most rapid decrease in $f(\boldsymbol{x})$ *in a small neighborhood around* $\boldsymbol{x}_{\boldsymbol{k-1}}$ can be found through the problem,

$$\min_{\boldsymbol{s}_{\boldsymbol{k}}} \ \boldsymbol{s}_{\boldsymbol{k}}^T \nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})$$

subject to $||\boldsymbol{s}_{\boldsymbol{k}}|| = 1$

Since $\boldsymbol{s}_{\boldsymbol{k}}^T \nabla f(\boldsymbol{x}_{\boldsymbol{k-1}}) = ||\boldsymbol{s}_{\boldsymbol{k}}|| \cdot ||\nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})|| \cos\theta$, the problem is solved for the value of $\boldsymbol{s}_{\boldsymbol{k}}$ for which $\theta = \pi$ and $||\boldsymbol{s}_{\boldsymbol{k}}|| = 1$:

$$\boldsymbol{s}_{\boldsymbol{k}} = \frac{-\nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})}{||\nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})||}$$

Newton Directions

Consider now a *second-order* Taylor series of the form,

$$f(\boldsymbol{x}_{\boldsymbol{k-1}} + \boldsymbol{s}_{\boldsymbol{k}}) = f(\boldsymbol{x}_{\boldsymbol{k-1}}) + \boldsymbol{s}_{\boldsymbol{k}}^T \nabla f(\boldsymbol{x}_{\boldsymbol{k-1}}) + \frac{1}{2}\boldsymbol{s}_{\boldsymbol{k}}^T H(\boldsymbol{x}_{\boldsymbol{k-1}})\, \boldsymbol{s}_{\boldsymbol{k}}$$

This is a quadratic approximation in the neighborhood of $\boldsymbol{x}_{\boldsymbol{k-1}}$. Note that α does not appear; this implies that $\alpha = 1$.

If the Hessian is positive definite, we can find a search direction that points directly toward the minimum point of this quadratic approximation.

Newton Directions

To do this, we take the derivative of the function with respect to $\boldsymbol{s}_k$ and set it equal zero,

$$\frac{df(\boldsymbol{x}_{k-1}+\boldsymbol{s}_k)}{d\boldsymbol{s}_k} = \nabla f(\boldsymbol{x}_{k-1}) + H(\boldsymbol{x}_{k-1})\,\boldsymbol{s}_k = \boldsymbol{0}$$

We can then solve for $\boldsymbol{s}_k$ to obtain,

$$\boldsymbol{s}_k = -[H(\boldsymbol{x}_{k-1})]^{-1}\,\nabla f(\boldsymbol{x}_{k-1})$$

This $\boldsymbol{s}_k$ is called the **Newton search direction.**

Newton Directions

When $H(\boldsymbol{x_{k-1}})$ is positive definite, the Newton direction is a descent direction.

When $H(\boldsymbol{x_{k-1}})$ is not positive definite, we can have two problems:

- ❖ $[H(\boldsymbol{x_{k-1}})]^{-1}$ may not exist
- ❖ Even if $[H(\boldsymbol{x_{k-1}})]^{-1}$ exists, the Newton direction may not define a descent direction

Algorithms that use Newton's method to determine search directions incorporate ways to modify $\boldsymbol{s_k}$ to deal with these problems.

Quasi-Newton Directions

An advantage of using a Newton direction is that convergence is faster (of second-order). However, the Hessian is expensive to calculate.

A common approach is therefore to approximate the Hessian and then find a **quasi-Newton search direction**. Quasi-Newton methods are sometimes called "variable metric" methods.

To see how this works, let's begin by creating a first-order Taylor series expansion for the gradient:

$$\nabla f(\boldsymbol{x_k}) = \nabla f(\boldsymbol{x_{k-1}}) + H(\boldsymbol{x_{k-1}})[\boldsymbol{x_k} - \boldsymbol{x_{k-1}}]$$

Quasi-Newton Directions

We can rearrange this equation as,

$$H(\boldsymbol{x}_{\boldsymbol{k-1}})[\boldsymbol{x}_{\boldsymbol{k}} - \boldsymbol{x}_{\boldsymbol{k-1}}] = \nabla f(\boldsymbol{x}_{\boldsymbol{k}}) - \nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})$$

This expression is of the form,

$$B_k \boldsymbol{p}_{\boldsymbol{k-1}} = \boldsymbol{y}_{\boldsymbol{k-1}}$$

where B_k is the Hessian (or Hessian-like) matrix and,

$$\boldsymbol{p}_{\boldsymbol{k-1}} = \boldsymbol{x}_{\boldsymbol{k}} - \boldsymbol{x}_{\boldsymbol{k-1}}$$

$$\boldsymbol{y}_{\boldsymbol{k-1}} = \nabla f(\boldsymbol{x}_{\boldsymbol{k}}) - \nabla f(\boldsymbol{x}_{\boldsymbol{k-1}})$$

Quasi-Newton Directions

Quasi-newton methods work by developing approximations for $B_k \approx H(\boldsymbol{x}_{\boldsymbol{k-1}})$ by enforcing the relation,

$$B_k \boldsymbol{p}_{\boldsymbol{k-1}} = \boldsymbol{y}_{\boldsymbol{k-1}}$$

that holds for the true Hessian $H(\boldsymbol{x}_{\boldsymbol{k-1}})$.

The approximations typically enforce additional constraints on B_k:

- Symmetry – because $H(\boldsymbol{x}_{\boldsymbol{k-1}})$ is symmetric
- Low rank of the matrix $[B_k - B_{k-1}]$– implies few rows of the Hessian change in each iteration

Quasi-Newton Directions

A common approach for generating the approximation B_k is the Broyden, Fletcher, Goldfarb, Shanno (BFGS) update formula:

$$B_{k+1} = B_k + \frac{(\boldsymbol{y_k} - B_k \boldsymbol{p_k})(\boldsymbol{y_k} - B_k \boldsymbol{p_k})^T}{(\boldsymbol{y_k} - B_k \boldsymbol{p_k})^T \boldsymbol{p_k}}$$

Set $B_1 = I$ (identity matrix) such that the initial search direction is steepest descent.

Quasi-Newton Directions

Once the approximation B_k has been found, we can use it to define the search direction in a similar way that we used the Hessian to define a Newton direction:

Newton direction:

$$\boldsymbol{s_k} = -[H(\boldsymbol{x_{k-1}})]^{-1} \nabla f(\boldsymbol{x_{k-1}})$$

Quasi-Newton direction:

$$\boldsymbol{s_k} = -B_k^{-1} \nabla f(\boldsymbol{x_{k-1}})$$

Since only B_k^{-1} is needed to define the search direction, some methods compute it directly, without the step of computing B_k .

Conjugate Directions

Let A be an $n \times n$ symmetric matrix. A set of n vectors (or directions) $\{\boldsymbol{s_i}\}$ is said to be conjugate with respect to the matrix A if,

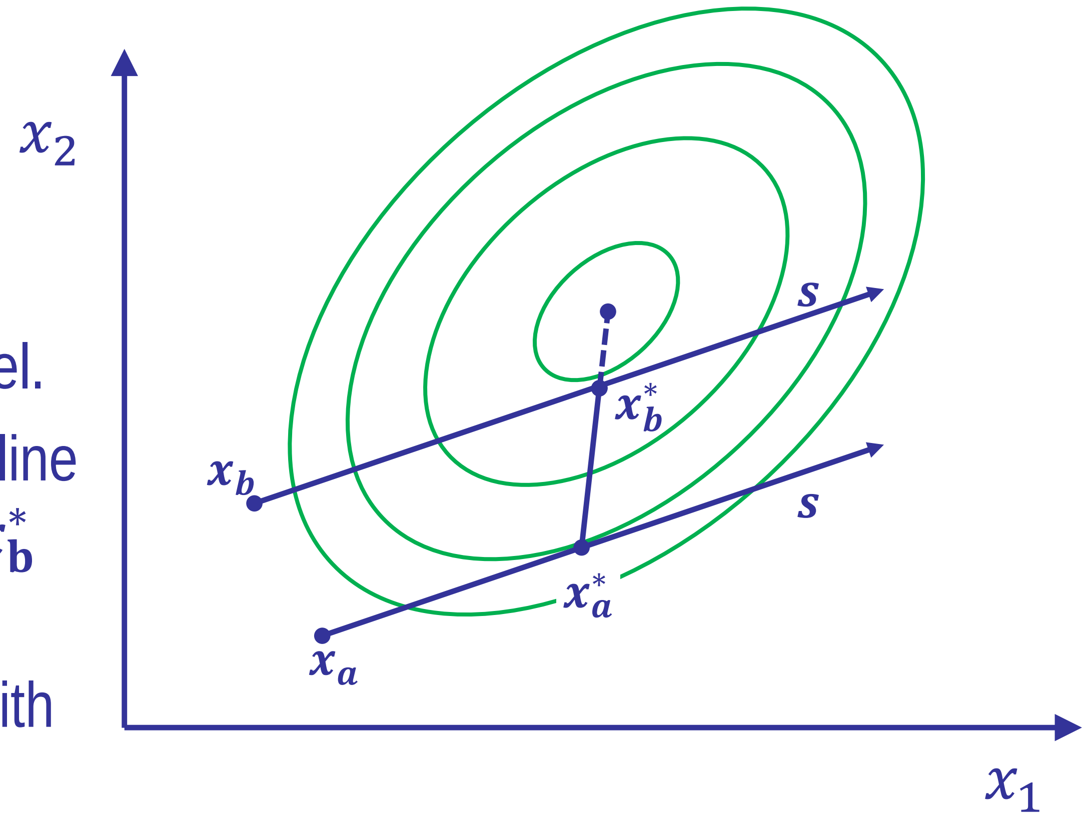
$$\boldsymbol{s}_{\boldsymbol{i}}^{T} A \boldsymbol{s}_{\boldsymbol{j}} = 0$$

for all $i \neq j,\ \ i = 1, \dots, n,\ \ \ j = 1, \dots, n.$

Conjugate Directions

Consider a quadratic function: $f(\boldsymbol{x}) = 1/2\, \boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b}^T \boldsymbol{x} + \boldsymbol{c}$

- Draw a line from a point $\boldsymbol{x_a}$ in a direction $\boldsymbol{s}$.
- Draw a 2nd line from a point $\boldsymbol{x_b}$ in the same direction $\boldsymbol{s}$. These first two lines are parallel.
- Find the minimum along each line and call these points $\boldsymbol{x}_\mathbf{a}^*$ and $\boldsymbol{x}_\mathbf{b}^*$
- The direction $(\boldsymbol{x}_\mathbf{b}^* - \boldsymbol{x}_\mathbf{a}^*)$ is <u>conjugate</u> to the direction $\boldsymbol{s}$ with respect to the matrix A.



Adapted from Rao, S., *Engineering Optimization: Theory and Practice*, 3rd Edition, Wiley Interscience, 1996.

Conjugate Directions

Note that mutually perpendicular directions (such as the coordinate directions) are conjugate with respect to the identity matrix, I_n.

Conjugate Directions: So What?

The wonder of conjugate directions is the following theorem, quoted from (Rao, 1996), which we state without proof:

Theorem: If a quadratic function $f(\boldsymbol{x}) = 1/2\,\boldsymbol{x}^T A\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x} + \boldsymbol{c}$ is minimized sequentially, once along each direction of a set of n mutually conjugate directions, the minimum of the function $f(x)$ will be found at or before the nth step, irrespective of the starting point.

Rao, S., *Engineering Optimization: Theory and Practice*, 3rd Edition, Wiley Interscience, 1996.