Unconstrained Optimization Algorithms

Descent Direction

Second-Order Methods

Newton's Method

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and minimize q w.r.t. s by setting $\nabla q(s) = 0$. We obtain:

$$H_k s = -\nabla f_k$$

Denote by s_k the solution, and set $x_{k+1} = x_k + s_k$.

Newton's Method

Algorithm 1 Newton's Method

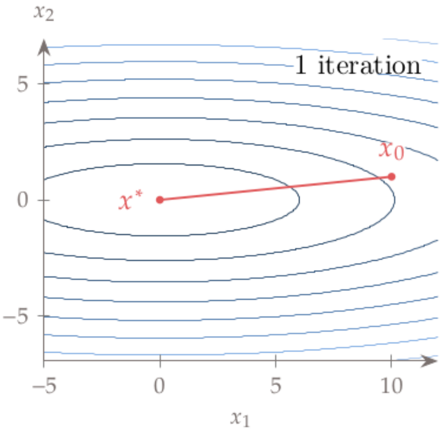
Input: x_0 starting point, $\varepsilon > 0$

Output: x^* approximation to a stationary point

```
1: k ← 0
2: while ‖∇f_k‖_∞ > ε do
3:     p_k ← −H_k^{−1} ∇f(x_k)
4:     x_{k+1} ← x_k + p_k
5:     k ← k + 1
6: end while
```

Newton's Method - Example

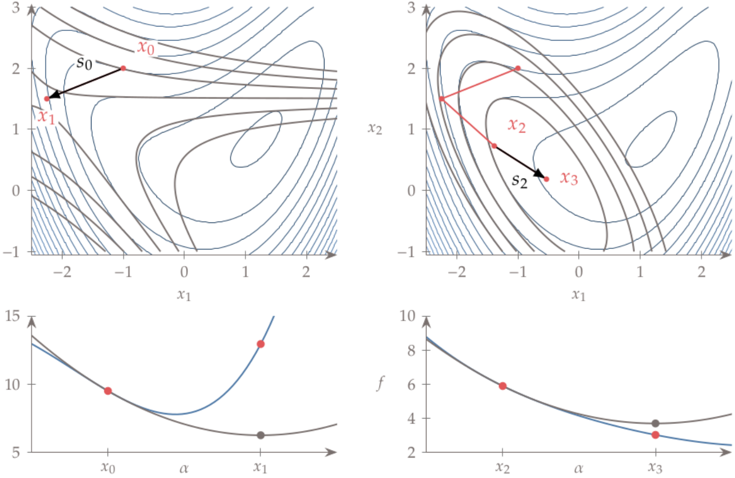
Newton's method finds the minimum of a quadratic function in a single step.



Note that the Newton's method is scale-invariant!

$$f(x_1, x_2) = (1 - x_1)^2 + (1 - x_2)^2 + \frac{1}{2}\left(2x_2 - x_1^2\right)^2$$

Stopping: $||\nabla f||_\infty \leq 10^{-6}$.



$k = 0$ $k = 2$

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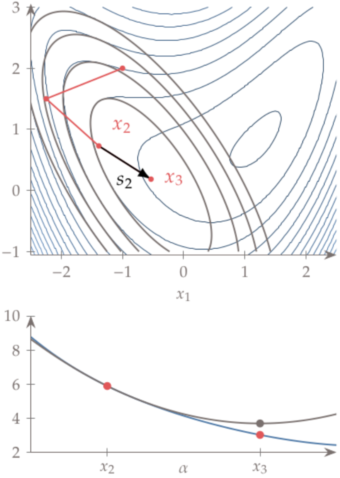
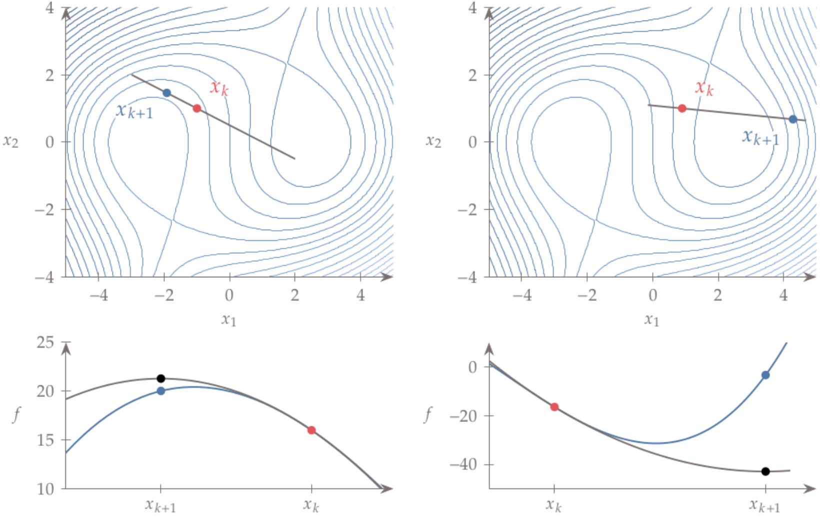


$k = 2$ $k = 8$

Convergence Issues



Negative curvature

Overshoot

Also, the computation of the Hessian is costly.

Local Quadratic Convergence of Newton's Method

Theorem 1

Assume f is defined and twice differentiable and assume that ∇f is L-smooth on $\mathcal{N}$.

Let x_* be a minimizer of $f(x)$ in $\mathcal{N}$ and assume that $\nabla^2 f(x_*)$ is positive definite.

If $\|x_0 - x_*\|$ is sufficiently small, then $\{x_k\}$ converges quadratically to x_*.

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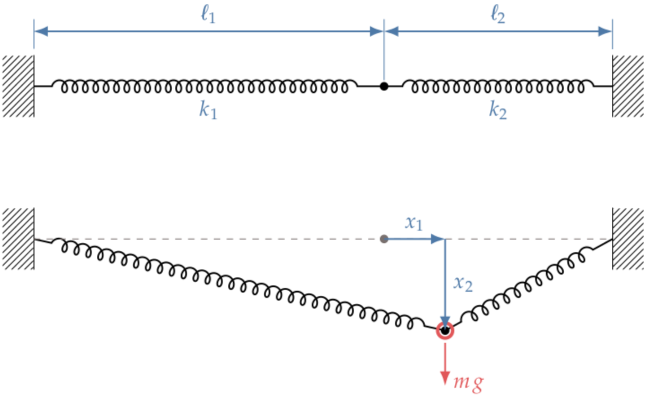
However, what happens if we start far away from a minimizer?

Newton's Method with Line Search

Algorithm 2 Newton's Method with Line Search

Input: x_0 starting point, $\varepsilon > 0$
Output: x^* approximation to a stationary point

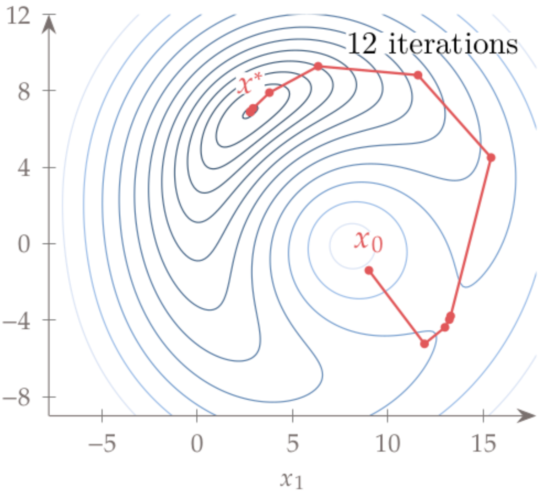
$k \leftarrow 0$
$\alpha_{\text{init}} \leftarrow 1$
while $\|\nabla f_k\|_\infty > \varepsilon$ **do**
    $p_k \leftarrow -H_k^{-1} \nabla f(x_k)$
    $\alpha_k \leftarrow \text{linesearch}(p_k, \alpha_{\text{init}})$
    $x_{k+1} \leftarrow x_k + \alpha_k p_k$
    $k \leftarrow k + 1$
end while



$$
\begin{aligned}
f(x_1, x_2) = &\frac{1}{2} k_1 \left(\sqrt{(\ell_1 + x_1)^2 + x_2^2} - \ell_1 \right)^2 \\
&+ \frac{1}{2} k_2 \left(\sqrt{(\ell_2 - x_1)^2 + x_2^2} - \ell_2 \right)^2 - mg x_2
\end{aligned}
$$

Here $\ell_1 = 12, \ell_2 = 8, k_1 = 1, k_2 = 10, mg = 7$

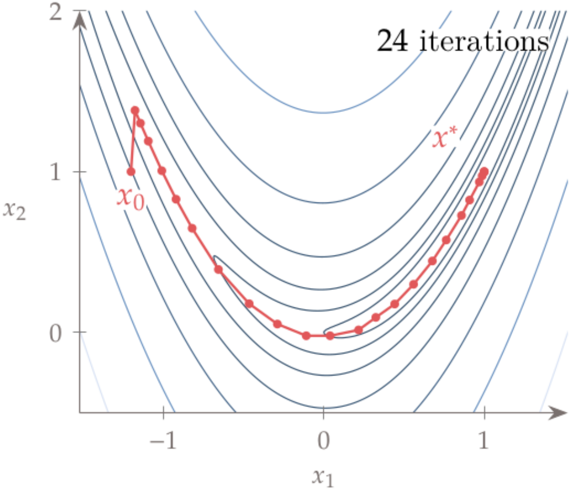
Two Spring Problem - Newton's Method



Gradient descent, line search, stop. cond. $||\nabla f||_\infty \leq 10^{-6}$.
Compare this with 32 iterations of gradient descent.

Rosenbrock Function - Newton's Method

Rosenbrock: $f(x_1, x_2) = (1 - x_1)^2 + 100\left(x_2 - x_1^2\right)^2$



Gradient descent, line search, stop. cond. $||\nabla f||_\infty \le 10^{-6}$.
Compare this with 10,662 iterations of gradient descent.

Global Convergence of Line Search

Denote by θ_k the angle between p_k and $-\nabla f_k$, i.e., satisfying

$$\cos\theta_k = \frac{-\nabla f_k^T p_k}{\|\nabla f_k\| \, \|p_k\|}$$

Recall that f is L-smooth for some $L > 0$ if

$$\|\nabla f(x) - \nabla f(\tilde{x})\| \leq L\|x - \tilde{x}\|, \qquad \text{for all } x, \tilde{x} \in \mathbb{R}^n$$

Theorem 2 (Zoutendijk)

Consider $x_{k+1} = x_k + \alpha_k p_k$, where p_k is a descent direction *and α_k satisfies the* strong Wolfe conditions*. Suppose that f is bounded below, continuously differentiable, and* L-smooth*. Then*

$$\sum_{k \geq 0} \cos^2\theta_k \, \|\nabla f_k\|^2 < \infty.$$

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Thus, under the assumptions of Zoutendijk's theorem, we obtain

$$\frac{1}{M^2}\sum_{k\geq 0}\|\nabla f_k\|^2 \leq \sum_{k\geq 0}\cos^2\theta_k\,\|\nabla f_k\|^2 < \infty$$

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What if H_k is not positive definite or is (nearly) singular?

Eigenvalue Modification

Consider $H_k = \nabla^2 f(x_k)$ and consider its diagonal form:

$$H_k = QDQ^T$$

Where D contains the eigenvalues of H_k on the diagonal, i.e., $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$ and Q is an orthogonal matrix.

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Observe that

- H_k is not positive definite iff $\lambda_i \leq 0$ for some i
- $||H_k||$ grows with $\max\{\lambda_1, \ldots, \lambda_n\}$ going to infinity.
- $\left|\left|H_k^{-1}\right|\right|$ grows with $\min\{\lambda_1, \ldots, \lambda_n\}$ going to 0
  (i.e., the matrix becomes close to a singular matrix)

We want to prevent all three cases, i.e., make sure that for some reasonably large $\delta > 0$ we have $\lambda_i \geq \delta$ but not too large.

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Two questions are in order:

- What is a reasonably large δ?
- How to modify H_k so the minimum is large enough?

Sufficiently Large Eigenvalues

Consider an example:

$$\nabla f(x_k) = (1, -3, 2) \qquad \text{and} \qquad \nabla^2 f(x_k) = \mathrm{diag}(10, 3, -1)$$

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Thus, a very long vector almost parallel to the third dimension.

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Even though f decreases along p_k, it is far from the minimum of the quadratic approximation of f.

Note that the original Newton's direction is
$-\mathrm{diag}(1/10, 1/3, -1)(1, -3, 2)^\top = (-1/10, 1, 2)$ which is completely different.

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Various methods for computing ΔH_k have been devised in literature. Typically, it is based on some computationally cheaper decomposition than spectral decomposition (e.g., Cholesky).

Modified Newton's Method

Algorithm 3 Newton's Method with Line Search

Input: x_0 starting point, $\varepsilon > 0$

Output: x^* approximation to a stationary point

$k \leftarrow 0$
while $\|\nabla f_k\|_\infty > \varepsilon$ **do**
  $H_k \leftarrow \nabla^2 f(x_k)$
  if H_k is **not** sufficiently positive definite **then**
    $H_k \leftarrow H_k + \Delta H_k$ so that H_k is sufficiently pos. definite
  end if
  Solve $H_k p_k = -\nabla f(x_k)$ for p_k
  Set $x_{k+1} = x_k + \alpha_k p_k$, here α_k sat. the Wolfe cond.
  $k \leftarrow k + 1$
end while

Convergence of Modified Newton's Method

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In a sense, Newton's method is an impractical "ideal" with which other methods are compared.

The efficiency issues (and the necessity of second-order derivatives) will be mitigated by using quasi-Newton methods.

Quasi-Newton Methods

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Recall that Newton's method step p_k in $x_{k+1} = x_k + p_k$ comes from minimization of

$$q(p) = f_k + \nabla f_k^\top p + \frac{1}{2} p^\top H_k p$$

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Quasi-Newton methods use first derivatives to approximate the Hessian H_k in Newton's method with a matrix $\tilde{H}_k$.

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First, it should be *symmetric positive definite*.

To always yield decrease direction.

Quasi-Newton Methods

Suppose we have just obtained the new point x_{k+1} after a line search starting from x_k in the direction p_k.

Consider the Hessian $H_{k+1} = \nabla^2 f(x_{k+1})$ and its approximation denoted by $\tilde{H}_{k+1}$.

We aim to use $\tilde{H}_{k+1}$ in the next step, that is, in the equation $\tilde{H}_{k+1} p = -\nabla f_{k+1}$ yielding p_{k+1}.

What conditions should $\tilde{H}_{k+1}$ satisfy so that it functions as the "true" Hessian H_{k+1}?

First, it should be *symmetric positive definite*.

To always yield decrease direction.

Second, extrapolating from the single variable secant method, we demand

$$\tilde{H}_{k+1}(x_{k+1} - x_k) = \nabla f_{k+1} - \nabla f_k$$

This is the *secant condition*.

Secant Condition

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The notation is usually simplified by

$$s_k = x_{k+1} - x_k \qquad y_k = \nabla f_{k+1} - \nabla f_k$$

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Does it have a symmetric positive definite solution?

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As a corollary, we obtain the following:

Theorem 3

Assume that we use line search satisfying strong Wolfe conditions. Then in every step, the secant condition

$$\tilde{H}_{k+1} s_k = y_k$$

has a symmetric positive definite solution $\tilde{H}_{k+1}$.

Now, we can obtain an approximate Hessian $\tilde{H}_{k+1}$ by solving the secant condition $\tilde{H}_{k+1} s_k = y_k$.

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Indeed, there are $n(n+1)/2$ degrees of freedom in a symmetric matrix, and the secant conditions represent only n conditions.

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Moreover, we want to obtain $\tilde{H}_{k+1}$ from $\tilde{H}_k$ by

$$\tilde{H}_{k+1} = \tilde{H}_k + \text{something}$$

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To have a nice iterative algorithm.

We also want $\tilde{H}_{k+1}$ to be symmetric positive definite.

We strive to choose $\tilde{H}_{k+1}$ "close" to $\tilde{H}_k$.

Symmetric Rank One Update (SR1)

Note that the information about the solution is present in s_k and y_k, so it is natural to compose the solution using these vectors.

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$$\tilde{H}_{k+1} = \tilde{H}_k + \frac{uu^\top}{u^\top s_k}$$

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Now, the secant condition is satisfied:

$$\tilde{H}_{k+1} s_k = \tilde{H}_k s_k + \frac{uu^\top s_k}{u^\top s_k} = \tilde{H}_k s_k + u = \tilde{H}_k s_k + \left(y_k - \tilde{H}_k s_k \right) = y_k$$

By the way, the matrix $\frac{uu^\top}{u^\top s_k}$ is of rank one and is a unique symmetric rank one matrix which makes $\tilde{H}_{k+1}$ satisfy the secant condition.

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By the way, the matrix $\frac{uu^\top}{u^\top s_k}$ is of rank one and is a unique symmetric rank one matrix which makes $\tilde{H}_{k+1}$ satisfy the secant condition.

To obtain a quasi-Newton method, it suffices to initialize $\tilde{H}_0$, typically to the identity I, and use $\tilde{H}_k$ instead of the Hessian $H_k = \nabla^2 f_k$ in Newton's method.

Symmetric Rank One Update

Algorithm 4 SR1

$k \leftarrow 0$
$\alpha_{\text{init}} \leftarrow 1$
$\tilde{H}_0 \leftarrow I$
while $\|\nabla f_k\|_\infty > \tau$ **do**
  Solve for p_k in $\tilde{H}_k p_k = -\nabla f_k$
  $\alpha \leftarrow \text{linesearch}(p_k, \alpha_{\text{init}})$
  $x_{k+1} \leftarrow x_k + \alpha p_k$
  $s \leftarrow x_{k+1} - x_k$
  $y \leftarrow \nabla f_{k+1} - \nabla f_k$
  $u \leftarrow y - \tilde{H}_k s$
  $\tilde{H}_{k+1} \leftarrow \tilde{H}_k + \frac{uu^\top}{u^\top s}$
  $k \leftarrow k + 1$
end while

Note that the denominator $u^\top s_k$ can be 0, in which case the update is impossible. The usual strategy is to skip the update and set $\tilde{H}_{k+1} = \tilde{H}_k$.

Example

We will look at a three-dimensional quadratic problem $f(x) = \frac{1}{2}x^\top Qx - c^\top x$ with

$$Q = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix} \quad \text{and} \quad c = \begin{pmatrix} -8 \\ -9 \\ -8 \end{pmatrix},$$

whose solution is $x_* = (-4, -3, -2)^\top$. Use the exact line search.

The initial guesses are $\tilde{H}_0 = I$ and $x_0 = (0, 0, 0)^\top$.

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At the initial point, $\|\nabla f(x_0)\|_\infty = \|-c\|_\infty = 9$, so this point is not optimal.The first search direction is

$$p_0 = \begin{pmatrix} -8 \\ -9 \\ -8 \end{pmatrix}.$$

The exact line search gives $\alpha_0 = 0.3333$.

Example

The new estimate of the solution, the update vectors, and the new Hessian approximation are:

$$x_1 = \begin{pmatrix} -2.66 \\ -3.00 \\ -2.66 \end{pmatrix}, \nabla f_1 = \begin{pmatrix} 2.66 \\ 0 \\ -2.66 \end{pmatrix}, s_0 = \begin{pmatrix} -2.66 \\ -3.00 \\ -2.66 \end{pmatrix}, y_0 = \begin{pmatrix} -5.33 \\ -9.00 \\ -10.66 \end{pmatrix},$$

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and

$$\tilde{H}_1 = I + \frac{(y_0 - Is_0)(y_0 - Is_0)^\top}{(y_0 - Is_0)^\top s_0} = \begin{pmatrix} 1.1531 & 0.3445 & 0.4593 \\ 0.3445 & 1.7751 & 1.0335 \\ 0.4593 & 1.0335 & 2.3780 \end{pmatrix}.$$

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At this new point $\|\nabla f(x_1)\|_\infty = 2.66$ so we keep going, obtaining the search direction

$$p_1 = \begin{pmatrix} -2.9137 \\ -0.5557 \\ 1.9257 \end{pmatrix},$$

and the step length $\alpha_1 = 0.3942$.

Example

This gives the new estimates:

$$x_2 = \begin{pmatrix} -3.81 \\ -3.21 \\ -1.90 \end{pmatrix}, \quad \nabla f_2 = \begin{pmatrix} 0.36 \\ -0.65 \\ 0.36 \end{pmatrix}, \quad s_1 = \begin{pmatrix} -1.14 \\ -0.21 \\ 0.75 \end{pmatrix}, \quad y_1 = \begin{pmatrix} -2.29 \\ -0.65 \\ 3.03 \end{pmatrix}$$

and

$$\tilde{H}_2 = \begin{pmatrix} 1.6568 & 0.6102 & -0.3432 \\ 0.6102 & 1.9153 & 0.6102 \\ -0.3432 & 0.6102 & 3.6568 \end{pmatrix}.$$

At the point x_2, $\|\nabla f(x_2)\|_\infty = 0.65$ so we keep going, with

$$p_2 = \begin{pmatrix} -0.4851 \\ 0.5749 \\ -0.2426 \end{pmatrix},$$

and $\alpha = 0.3810$.

Example

This gives

$$x_3 = \begin{pmatrix} -4 \\ -3 \\ -2 \end{pmatrix}, \quad \nabla f_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad s_2 = \begin{pmatrix} -0.18 \\ 0.21 \\ -0.09 \end{pmatrix}, \quad y_2 = \begin{pmatrix} -0.36 \\ 0.65 \\ -0.36 \end{pmatrix},$$

and $\tilde{H}_3 = Q$. Now $\|\nabla f(x_3)\|_\infty = 0$, so we stop.

Properties of SR1

Does symmetric rank one update satisfy our demands?

We want every $\tilde{H}_k$ to be a symmetric positive definite solution to the secant condition.

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Still, the symmetric rank one approximation is used in practice, especially in trust region methods.

However, for line search, let us try a bit “richer” solution to the secant condition.

Symmetric Rank Two Update

Consider

$$\tilde{H}_{k+1} = \tilde{H}_k - \frac{\left(\tilde{H}_k s_k\right)\left(\tilde{H}_k s_k\right)^\top}{s_k^\top \tilde{H}_k s_k} + \frac{y_k y_k^\top}{y_k^\top s_k}$$

Once again, verifying $\tilde{H}_{k+1} s_k = y_k$ is not difficult.

Lemma 1

Assume that $\tilde{H}_k$ is symmetric positive definite.
Then $\tilde{H}_{k+1}$ is symmetric positive definite iff $y_k^\top s_k > 0$.

We know that line search satisfying the strong Wolfe conditions preserves $y_k^\top s_k > 0$.

Thus, starting with a symmetric positive definite $\tilde{H}_0$ (e.g., a scalar multiple of I), every $\tilde{H}_k$ is symmetric positive definite and satisfies the secant condition.

BFGS

Algorithm 5 BFGS v1

$k \leftarrow 0$
$\alpha_{\text{init}} \leftarrow 1$
$\tilde{H}_0 \leftarrow I$
while $\|\nabla f_k\|_\infty > \tau$ **do**
  Solve for p_k in $\tilde{H}_k p_k = -\nabla f_k$
  $\alpha \leftarrow \text{linesearch}(p_k, \alpha_{\text{init}})$
  $x_{k+1} \leftarrow x_k + \alpha p_k$
  $s \leftarrow x_{k+1} - x_k$
  $y \leftarrow \nabla f_{k+1} - \nabla f_k$
  $\tilde{H}_{k+1} \leftarrow \tilde{H}_k - \frac{(\tilde{H}_k s)(\tilde{H}_k s)^\top}{s^\top \tilde{H}_k s} + \frac{yy^\top}{y^\top s}$
  $k \leftarrow k + 1$
end while

Note that we still have to solve a linear system for p_k.

Example

Consider the quadratic problem $f(x) = \frac{1}{2}x^\top Qx - c^\top x$ with

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Choose $\tilde{H}_0 = I$ and $x_0 = (0, 0, 0)^T$.

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At iteration 0, $\|\nabla f(x_0)\|_\infty = 9$, so this point is not optimal.

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The search direction is

$$p_0 = \begin{pmatrix} -8 \\ -9 \\ -8 \end{pmatrix}$$

and $\alpha_0 = 0.3333$.

Example

The new estimate of the solution and the new Hessian approximation are

$$x_1 = \begin{pmatrix} -2.6667 \\ -3.0000 \\ -2.6667 \end{pmatrix} \quad \text{and} \quad \tilde{H}_1 = \begin{pmatrix} 1.1021 & 0.3445 & 0.5104 \\ 0.3445 & 1.7751 & 1.0335 \\ 0.5104 & 1.0335 & 2.3270 \end{pmatrix}.$$

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At iteration 1, $\|\nabla f(x_1)\|_\infty = 2.6667$, so we continue. The next search direction is

$$p_1 = \begin{pmatrix} -3.2111 \\ -0.6124 \\ 2.1223 \end{pmatrix}$$

and $\alpha_1 = 0.3577$.

Example

This gives the estimates.

$$x_2 = \begin{pmatrix} -3.8152 \\ -3.2191 \\ -1.9076 \end{pmatrix} \quad \text{and} \quad \tilde{H}_2 = \begin{pmatrix} 1.6393 & 0.6412 & -0.3607 \\ 0.6412 & 1.8600 & 0.6412 \\ -0.3607 & 0.6412 & 3.6393 \end{pmatrix}.$$

At iteration 2, $\|\nabla f(x_2)\|_\infty = 0.6572$, so we continue, computing

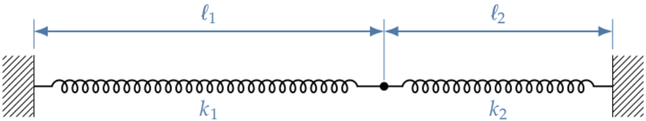
$$p_2 = \begin{pmatrix} -0.5289 \\ 0.6268 \\ -0.2644 \end{pmatrix}$$

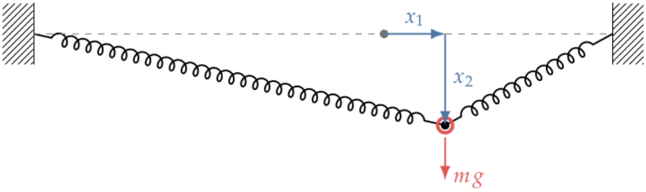
and $\alpha_2 = 0.3495$. This gives

$$x_3 = \begin{pmatrix} -4 \\ -3 \\ -2 \end{pmatrix} \quad \text{and} \quad \tilde{H}_3 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix}.$$

Now $\|\nabla f(x_3)\|_\infty = 0$, so we stop.

Notice that we got the same x_1, x_2, x_3 as for SR1. This follows from using the exact line search and the quadratic problem. It does not hold in general.

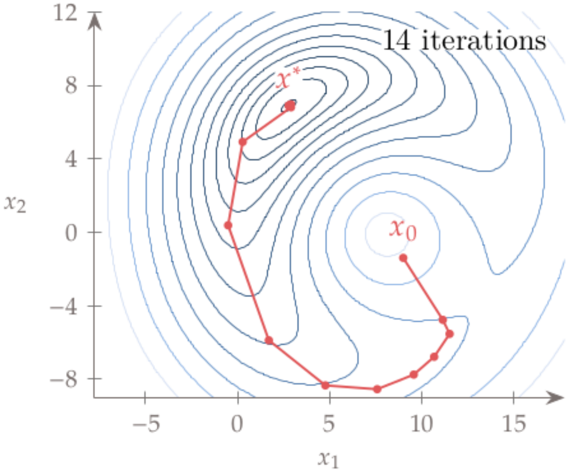




$$f(x_1, x_2) = \frac{1}{2}k_1\left(\sqrt{(\ell_1 + x_1)^2 + x_2^2} - \ell_1\right)^2 + \frac{1}{2}k_2\left(\sqrt{(\ell_2 - x_1)^2 + x_2^2} - \ell_2\right)^2 - mgx_2$$

Here $\ell_1 = 12, \ell_2 = 8, k_1 = 1, k_2 = 10, mg = 7$

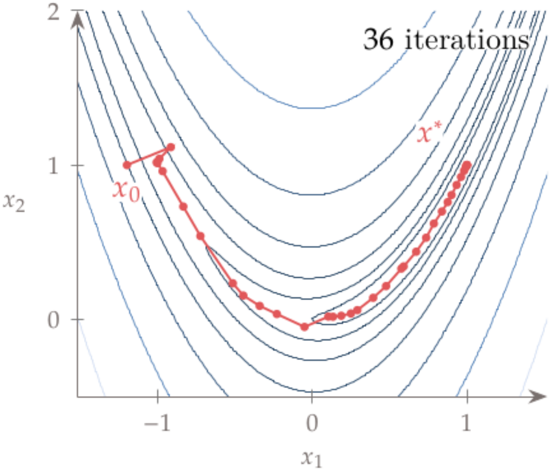
Two Spring Problem - BFGS



Gradient descent, line search, stop. cond. $||\nabla f||_\infty \leq 10^{-6}$.
Compare this with 32 iterations of gradient descent and 12 iterations of Newton's method.

Rosenbrock Function - BFGS

Rosenbrock: $f(x_1, x_2) = (1 - x_1)^2 + 100\left(x_2 - x_1^2\right)^2$



Gradient descent, line search, stop. cond. $||\nabla f||_\infty \leq 10^{-6}$.
Compare with 10,662 iterations of gradient descent and 24 iterations of Newton's method.

Sherman–Morrison–Woodbury Formula

Problem: SR1 and BFGS solve $\tilde{H}_k p = -\nabla f_k$ repeatedly. What if we could iteratively update H_k^{-1}?

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Ideally, we would like to compute $\tilde{H}_k^{-1}$ iteratively along the optimization, i.e.,

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$$\tilde{H}_{k+1}^{-1} = \tilde{H}_k^{-1} + \text{something}$$

To get such a "something" we use the following Sherman–Morrison–Woodbury (SMW) formula:

$$\left(A + UV^T\right)^{-1} = A^{-1} - A^{-1} U \left(I + V^T A^{-1} U\right)^{-1} V^T A^{-1}$$

Here A is a $(n \times n)$-matrix, U, V are $(n \times m)$-matrices with $m \leq n$.

Rank 1 – Iterative Inverse Hessian Approximation

Applying SMW to the rank one update

$$\tilde{H}_{k+1} = \tilde{H}_k + \frac{\left(y_k - \tilde{H}_k s_k\right)\left(y_k - \tilde{H}_k s_k\right)^\top}{\left(y_k - \tilde{H}_k s_k\right)^\top s_k}$$

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yields

$$\tilde{H}_{k+1}^{-1} = \tilde{H}_k^{-1} + \frac{\left(s_k - \tilde{H}_k^{-1} y_k\right)\left(s_k - \tilde{H}_k^{-1} y_k\right)^\top}{\left(s_k - \tilde{H}_k^{-1} y_k\right)^\top y_k}$$

Yes, only y and s swapped places.

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$$\tilde{H}_{k+1} = \tilde{H}_k + \frac{\left(y_k - \tilde{H}_k s_k\right)\left(y_k - \tilde{H}_k s_k\right)^\top}{\left(y_k - \tilde{H}_k s_k\right)^\top s_k}$$

yields

$$\tilde{H}_{k+1}^{-1} = \tilde{H}_k^{-1} + \frac{\left(s_k - \tilde{H}_k^{-1} y_k\right)\left(s_k - \tilde{H}_k^{-1} y_k\right)^\top}{\left(s_k - \tilde{H}_k^{-1} y_k\right)^\top y_k}$$

Yes, only y and s swapped places.

This allows us to avoid solving $\tilde{H}_k p_k = -\nabla f_k$ for p_k in every iteration.

Rank One Update V2

Algorithm 6 Rank 1 update v1

$k \leftarrow 0$

$\alpha_{\text{init}} \leftarrow 1$

$\tilde{H}_0 \leftarrow I$

while $\|\nabla f_k\|_\infty > \tau$ **do**

    $p_k \leftarrow -\tilde{H}_k^{-1} \nabla f_k$

    $\alpha \leftarrow \text{linesearch}(p_k, \alpha_{\text{init}})$

    $x_{k+1} \leftarrow x_k + \alpha p_k$

    $s \leftarrow x_k - x_{k-1}$

    $y \leftarrow \nabla f_k - \nabla f_{k-1}$

    $\tilde{H}_{k+1}^{-1} \leftarrow \tilde{H}_k^{-1} + \frac{\left(s - \tilde{H}_k^{-1} y\right)\left(s - \tilde{H}_k^{-1} y\right)^\top}{\left(s - \tilde{H}_k^{-1} y\right)^\top y}$

    $k \leftarrow k + 1$

end while

BFGS

Applying SMW to the BFGS Hessian update

$$\tilde{H}_{k+1} = \tilde{H}_k - \frac{\left(\tilde{H}_k s_k\right)\left(\tilde{H}_k s_k\right)^\top}{s_k^\top \tilde{H}_k s_k} + \frac{y_k y_k^\top}{y_k^\top s_k}$$

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yields

$$\tilde{H}_{k+1}^{-1} = \left(I - \frac{s_k y_k^\top}{s_k^\top y_k}\right) \tilde{H}_k^{-1} \left(I - \frac{y_k s_k^\top}{s_k^\top y_k}\right) + \frac{s_k s_k^\top}{s_k^\top y_k}$$

We avoid solving the linear system for p_k.

BFGS V2

Algorithm 7 BFGS v2

$k \leftarrow 0$
$\alpha_{\text{init}} \leftarrow 1$
$\tilde{H}_0 \leftarrow I$
while $\|\nabla f_k\|_\infty > \tau$ **do**
    $p_k \leftarrow -\tilde{H}_k^{-1} \nabla f_k$
    $\alpha \leftarrow \text{linesearch}(p_k, \alpha_{\text{init}})$
    $x_{k+1} \leftarrow x_k + \alpha p_k$
    $k \leftarrow k + 1$
    $s \leftarrow x_k - x_{k-1}$
    $y \leftarrow \nabla f_k - \nabla f_{k-1}$
    $\tilde{H}_{k+1}^{-1} \leftarrow \left(I - \frac{sy^\top}{s^\top y}\right) \tilde{H}_k^{-1} \left(I - \frac{ys^\top}{s^\top y}\right) + \frac{ss^\top}{s^\top y}$
end while

Limited Memory BFGS Idea

Let us denote by $s_0, \ldots, s_k$ and $y_0, \ldots, y_k$ the values of the variables s and y, resp., during the iterations $1, \ldots, k$ of BFGS.

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So, the matrix $\tilde{H}_k$ does not have to be stored if the algorithm remembers the values $s_0, \ldots, s_k$ and $y_0, \ldots, y_k$.

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This is the basic idea behind limited-memory BFGS which stores only the running window $s_{k-m}, \ldots, s_k$ and $y_{k-m}, \ldots, y_k$ and computes $\tilde{H}_k$ using these values as if initialized by $\tilde{H}_{k-m-1} = I$.

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The space complexity becomes nm, which is beneficial when n is large.

Another View on BFGS (Optional)

We search for $\tilde{H}_{k+1}^{-1}$ where $\tilde{H}_{k+1}$ satisfies $\tilde{H}_{k+1} s_k = y_k$. Search for a solution $\tilde{V}$ for $\tilde{V} y_k = s_k$.

The idea is to use $\tilde{V}$ close to $\tilde{H}_k^{-1}$ (in some sense):

$$\min_{\tilde{H}} \left\| \tilde{V} - \tilde{H}_k^{-1} \right\|$$

$$\text{subject to} \quad \tilde{V} = \tilde{V}^\top, \quad \tilde{V} y_k = s_k$$

Here the norm is *weighted Frobenius norm*:

$$\|A\| \equiv \left\| W^{1/2} A W^{1/2} \right\|_F,$$

where $\|\cdot\|_F$ is defined by $\|C\|_F^2 = \sum_{i=1}^n \sum_{j=1}^n c_{ij}^2$. The weight W can be chosen as any matrix satisfying the relation $W y_k = s_k$.

BFGS is obtained with $W = \bar{G}_k^{-1}$ where $\bar{G}_k$ is the average Hessian defined by $\bar{G}_k = \left[\int_0^1 \nabla^2 f\left(x_k + \tau \alpha_k p_k\right) d\tau \right]$

Solving this gives precisely the BFGS formula for $\tilde{H}_{k+1}^{-1}$.

Global Convergence of Line Search

Denote by θ_k the angle between p_k and $-\nabla f_k$, i.e., satisfying

$$\cos\theta_k = \frac{-\nabla f_k^T p_k}{\|\nabla f_k\| \, \|p_k\|}$$

Recall that f is L-smooth for some $L > 0$ if

$$\|\nabla f(x) - \nabla f(\tilde{x})\| \leq L\|x - \tilde{x}\|, \qquad \text{for all } x, \tilde{x} \in \mathbb{R}^n$$

Theorem 4 (Zoutendijk)

Consider $x_{k+1} = x_k + \alpha_k p_k$, *where* p_k *is a* descent direction *and* α_k *satisfies the* strong Wolfe conditions. *Suppose that* f *is bounded below, continuously differentiable, and* L-smooth. *Then*

$$\sum_{k\geq 0} \cos^2\theta_k \, \|\nabla f_k\|^2 < \infty.$$

Global Convergence of Quasi-Newton's Method

Assume that all α_k satisfy strong Wolfe conditions.

Assume that the approximations to the Hessians $\tilde{H}_k$ are positive definite with a uniformly bounded condition number:

$$\left|\left|\tilde{H}_k\right|\right| \left|\left|\tilde{H}_k^{-1}\right|\right| \leq M \quad \text{for all } k$$

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Thus, under the assumptions of Zoutendijk's theorem, we obtain

$$\frac{1}{M^2}\sum_{k\geq 0}\|\nabla f_k\|^2 \leq \sum_{k\geq 0}\cos^2\theta_k\,\|\nabla f_k\|^2 < \infty$$

which implies that $\lim_{k\to\infty}||\nabla f_k|| = 0$.

Behavior of BFGS

- It may happen that $\tilde{H}_k$ becomes a poor approximation of the Hessian H_k. If, e.g., $y_k^\top$ is tiny, then $\tilde{H}_{k+1}$ will be huge.

  However, it has been proven experimentally that if $\tilde{H}_k$ wrongly estimates the curvature of f and this estimate slows down the iteration, then the approximation will tend to correct the bad Hessian approximations.

  The above self-correction works only if an appropriate line search is performed (strong Wolfe conditions).

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  The above self-correction works only if an appropriate line search is performed (strong Wolfe conditions).
- There are more sophisticated ways of setting the initial Hessian approximation H_0.

  See Numerical Optimization, Nocedal & Wright, page 201.

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- There is even a memory-limited variant (L-BFGS) that uses only information from past m steps, and its single iteration complexity is $\mathcal{O}(mn)$.
- Compared with Newton's method, no second derivatives are computed.
- Local superlinear convergence can be proved under specific conditions.

  Compare with local quadratic convergence of Newton's method and linear convergence of gradient descent.

Limited-Memory BFGS

Limited-Memory BFGS (L-BFGS)

When the number of design variables is extensive, working with the whole Hessian inverse approximation matrix might not be practical.

This motivates limited-memory quasi-Newton methods,

In addition, these methods also improve the computational efficiency of medium-sized problems (hundreds or thousands of design variables) with minimal sacrifice in accuracy.

L-BFGS

Recall that we compute iteratively the approximation to the inverse Hessian by

$$H_{k+1}^{-1} = \left(I - \frac{s_k y_k^\top}{s_k^\top y_k}\right) H_k^{-1} \left(I - \frac{y_k s_k^\top}{s_k^\top y_k}\right) + \frac{s_k s_k^\top}{s_k^\top y_k}$$

However, eventually, we are interested in

$$p_k = H_k^{-1} \nabla f$$

Note that given the sequences $s_1, \ldots, s_k$ and $y_1, \ldots, y_k$ and H_0^{-1} we can recursively compute H_{k+1}^{-1} for every k.

What if we limit the sequences in memory to just m last elements:

$$s_{k-m+1}, s_{k-m+2}, \ldots, s_k \qquad y_{k-m+1}, y_{k-m+2}, \ldots, y_k$$

In practice, m between 5 and 20 is usually sufficient. We also initialize the recurrence with the last iterate:

L-BFGS

Let us rewrite the BFGS update formula as follows:

$$\tilde{H}_{k+1}^{-1} = V_k^T \tilde{H}_k^{-1} V_k + \rho_k s_k s_k^\top$$

where

$$\rho_k = s_k^\top y_k \qquad \text{and} \qquad V_k = I - \rho_k s_k y_k^\top$$

$$s_k = x_{k+1} - x_k \qquad \text{and} \qquad y_k = \nabla f_{k+1} - \nabla f_k$$

By substitution, we obtain

$$\begin{aligned}
\tilde{H}_k^{-1} = &\left(V_{k-1}^T \cdots V_{k-m}^T\right) \tilde{H}_k^0 \left(V_{k-m} \cdots V_{k-1}\right) \\
&+ \rho_{k-m} \left(V_{k-1}^T \cdots V_{k-m+1}^T\right) s_{k-m} s_{k-m}^T \left(V_{k-m+1} \cdots V_{k-1}\right) \\
&+ \rho_{k-m+1} \left(V_{k-1}^T \cdots V_{k-m+2}^T\right) s_{k-m+1} s_{k-m+1}^T \left(V_{k-m+2} \cdots V_k \right. \\
&+ \cdots \\
&+ \rho_{k-1} s_{k-1} s_{k-1}^T
\end{aligned}$$

L-BFGS Algorithm

Algorithm 8 L-BFGS two-loop recursion

Input: : $s_{k-1}, \dots, s_{k-m}$ and $y_{k-1}, \dots, y_{k-m}$

Output: : p_k the search direction $-\tilde{H}_k^{-1} \nabla f_k$

$q \leftarrow \nabla f_k$

for $i = k-1, k-2, \dots, k-m$ **do**

  $\alpha_i \leftarrow \rho_i s_i^T q$

  $q \leftarrow q - \alpha_i y_i$

end for

$r \leftarrow H_k^0 q$

for $i = k-m, k-m+1, \dots, k-1$ **do**

  $\beta \leftarrow \rho_i y_i^T r$

  $r \leftarrow r + s_i(\alpha_i - \beta)$

end for

stop with result $\tilde{H}_k^{-1} \nabla f_k = r$

L-BFGS Algorithm

Algorithm 9 L-BFGS

Choose starting point x_0, integer $m > 0$

$k \leftarrow 0$

repeat

  Choose H_k^0 e.g. $\frac{s_{k-1}^\top y_{k-1}}{y_{k-1}^\top y_{k-1}}$

  Compute $p_k \leftarrow -H_k \nabla f_k$ using the previous algorithm

  Compute $x_{k+1} \leftarrow x_k + \alpha_k p_k$, where α_k is chosen to satisfy the strong Wolfe conditions

  if $k > m$ **then**

    Discard the vector pair $\{s_{k-m}, y_{k-m}\}$ from storage

  end if

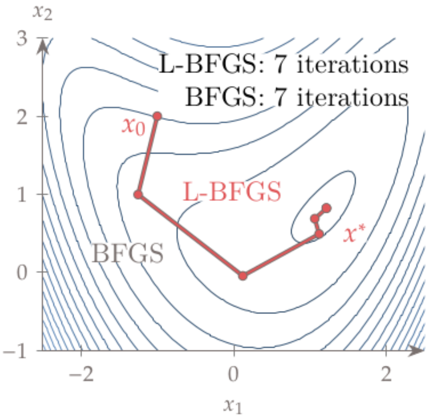
  Compute and save $s_k \leftarrow x_{k+1} - x_k$, $y_k \leftarrow \nabla f_{k+1} - \nabla f_k$

  $k \leftarrow k + 1$

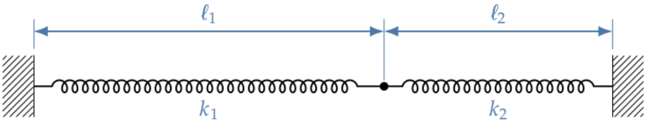
until convergence

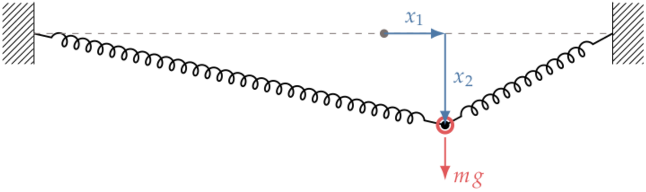
$$f(x_1, x_2) = (1 - x_1)^2 + (1 - x_2)^2 + \frac{1}{2}\left(2x_2 - x_1^2\right)^2$$

Stopping: $||\nabla f||_\infty \leq 10^{-6}$.



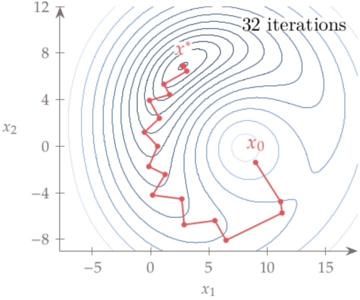
In L-BFGS, the memory length m was 5. The results are similar.



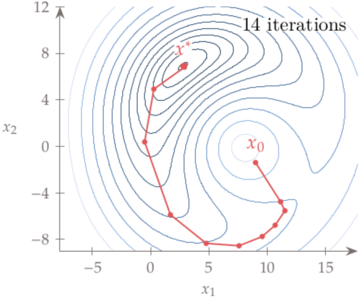


$$
\begin{aligned}
f(x_1, x_2) =& \frac{1}{2} k_1 \left(\sqrt{(\ell_1 + x_1)^2 + x_2^2} - \ell_1 \right)^2 \\
&+ \frac{1}{2} k_2 \left(\sqrt{(\ell_2 - x_1)^2 + x_2^2} - \ell_2 \right)^2 - mg x_2
\end{aligned}
$$

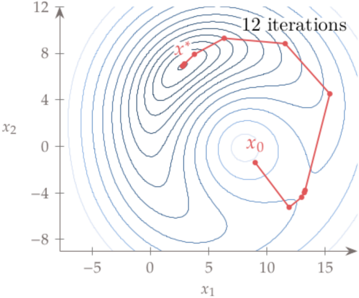
Here $\ell_1 = 12, \ell_2 = 8, k_1 = 1, k_2 = 10, mg = 7$



Steepest descent

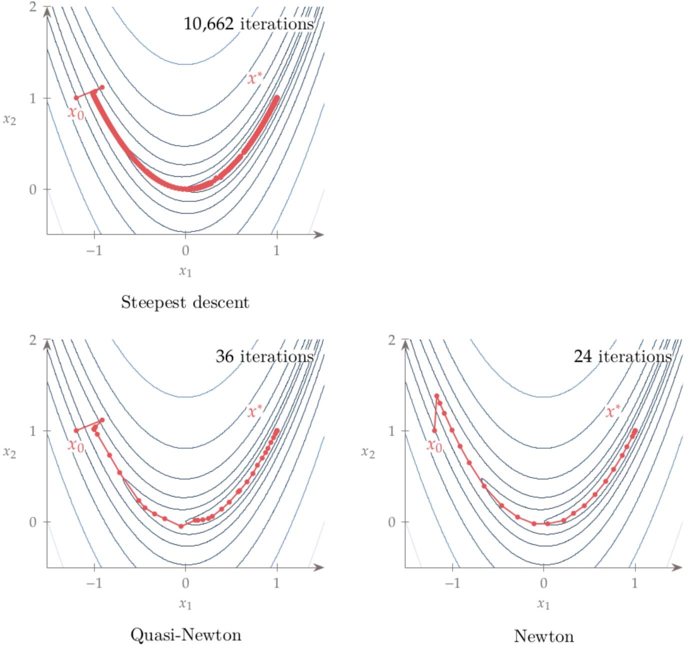


Quasi-Newton



Newton

Rosenbrock: $f(x_1, x_2) = (1 - x_1)^2 + 100\left(x_2 - x_1^2\right)^2$



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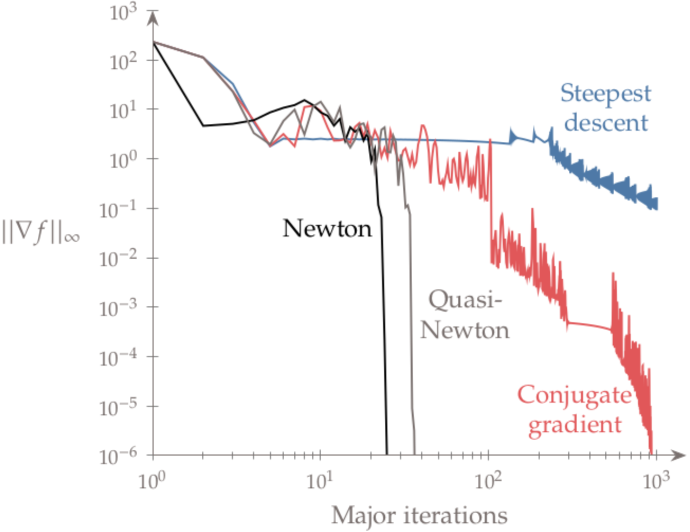


Computational Complexity

Algorithm	Computational Complexity
Steepest Descent	$O(n)$ per iteration
Newton's Method	$O(n^3)$ to compute Hessian and solve system
BFGS	$O(n^2)$ to update Hessian approximation

Table: Summary of the computational complexity for each optimization algorithm.

- Steepest Descent: Simple but often slow, requiring many iterations.
- Newton's Method: Fast convergence but expensive per iteration.
- BFGS: Quasi-Newton, no Hessian needed, good speed and iteration count balance.

Constrained Optimization

Constrained Optimization Problem

Recall that the constrained optimization problem is

$$\begin{array}{rll} \text{minimize} & f(x) & \\ \text{by varying} & x & \\ \text{subject to} & g_i(x) \leq 0 & i = 1, \ldots, n_g \\ & h_j(x) = 0 & j = 1, \ldots, n_h \end{array}$$

x^* is now a *constrained minimizer* if

$$f(x^*) \leq f(x) \quad \text{for all} \quad x \in \mathcal{F}$$

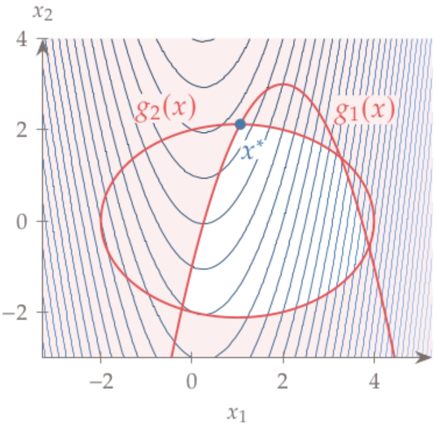
where $\mathcal{F}$ is the feasibility region

$$\mathcal{F} = \{x \mid g_i(x) \leq 0, h_j(x) = 0, i = 1, \ldots, n_g, j = 1, \ldots, n_h\}$$

Thus, to find a constrained minimizer, we have to inspect unconstrained minima of f inside of $\mathcal{F}$ and points along the boundary of $\mathcal{F}$.

COP - Example

$$\begin{array}{ll} \underset{x_1, x_2}{\text{minimize}} & f(x_1, x_2) = x_1^2 - \frac{1}{2}x_1 - x_2 - 2 \\ \text{subject to} & g_1(x_1, x_2) = x_1^2 - 4x_1 + x_2 + 1 \leq 0 \\ & g_2(x_1, x_2) = \frac{1}{2}x_1^2 + x_2^2 - x_1 - 4 \leq 0 \end{array}$$



Equality Constraints

Let us restrict our problem only to the equality constraints:

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{by varying} \quad & x \\ \text{subject to} \quad & h_j(x) = 0 \quad j = 1, \ldots, n_h \end{aligned}$$

Assume that f and h_j have continuous second derivatives.

Now, we try to imitate the theory from the unconstrained case and characterize minima using gradients.

This time, we must consider the gradient of f and h_j.

Half-Space of Decrease

Consider the first-order Taylor approximation of f at x

$$f(x+p) \approx f(x) + \nabla f(x)^\top p$$

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Note that if x^* is an unconstrained minimum of f, then

$$f(x^* + p) \geq f(x^*)$$

for all p small enough.

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Note that if x^* is an unconstrained minimum of f, then

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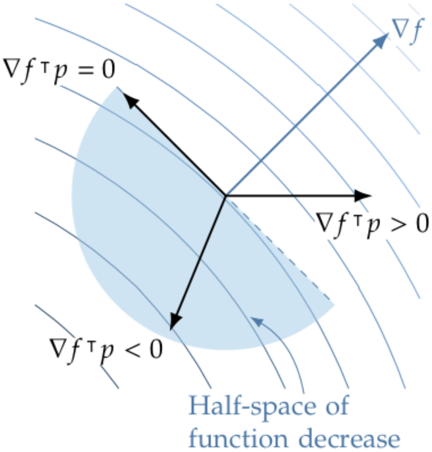
for all p small enough.

Together with the Taylor approximation, we obtain

$$f(x^*) + \nabla f(x^*)^\top p \geq f(x^*)$$

and hence

$$\nabla f(x^*)^\top p \geq 0$$



The hyperplane defined by $\nabla f^\top p = 0$ contains directions p of *zero variation* in f.

In the unconstrained case, x^* is minimizer only if $\nabla f(x^*) = 0$ because otherwise there would be a direction p satisfying $\nabla f(x^*)p < 0$, a *decrease direction*.

Decrease Direction in COP

In COP, p is a decrease direction in $x \in \mathcal{F}$ if $\nabla f(x)^\top p < 0$ and if p is a *feasible direction*!

I.e., point into the feasible region.

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I.e., point into the feasible region. How do we characterize feasible directions?

Consider Taylor approximation of h_j for all j:

$$h_j(x + p) \approx h_j(x) + \nabla h_j(x)^\top p$$

Decrease Direction in COP

In COP, p is a decrease direction in $x \in \mathcal{F}$ if $\nabla f(x)^\top p < 0$ and if p is a *feasible direction*!

I.e., point into the feasible region. How do we characterize feasible directions?

Consider Taylor approximation of h_j for all j:

$$h_j(x + p) \approx h_j(x) + \nabla h_j(x)^\top p$$

Assuming $x \in \mathcal{F}$, we have $h_j(x) = 0$ for all j and thus

$$h_j(x + p) \approx \nabla h_j(x)^\top p$$

Decrease Direction in COP

In COP, p is a decrease direction in $x \in \mathcal{F}$ if $\nabla f(x)^\top p < 0$ and if p is a *feasible direction*!

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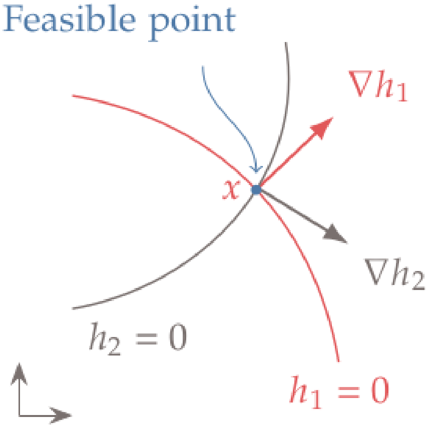
Assuming $x \in \mathcal{F}$, we have $h_j(x) = 0$ for all j and thus

$$h_j(x + p) \approx \nabla h_j(x)^\top p$$

As p is a feasible direction iff $h_j(x + p) = 0$, we obtain that

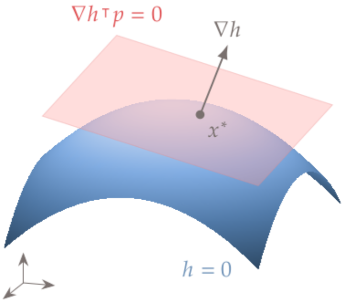
$$p \text{ is a } \textit{feasible direction} \quad \text{iff} \quad \nabla h_j(x)^\top p = 0 \text{ for all } j$$

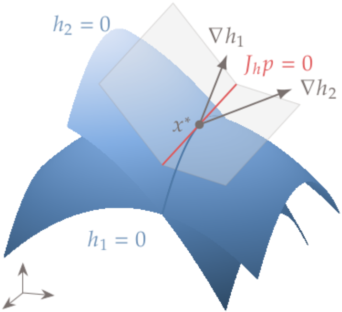
Feasible Points and Directions



Here, the only feasible direction at x is $p = 0$.

Feasible Points and Directions





Here the feasible directions at x^* point along the red line, i.e.,

$$\nabla h_1(x^*)p = 0 \qquad \nabla h_2(x^*)p = 0$$

Necessary Condition for Constrained Minima

Consider a direction p. Observe that

- If $h_j(x)^\top p \neq 0$, then moving a short step in the direction p violates the constraint $h_j(x) = 0$.

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To be a minimizer, x^* must be feasible and every direction satisfying $h_j(x^*)^\top p = 0$ for all j must also satisfy $\nabla f(x^*)^\top p \geq 0$.

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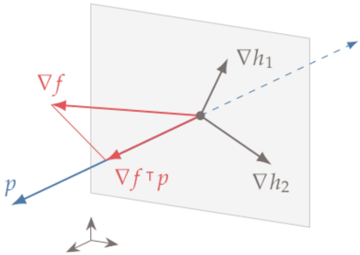
If x^* is a *constrained minimizer*, then

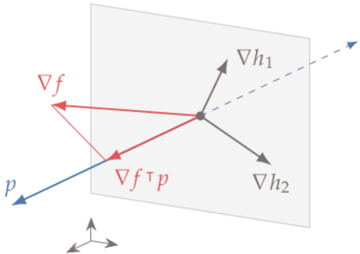
$$\nabla f(x^*)^\top p = 0 \text{ for all } p \text{ satisfying } (\forall j : \nabla h_j(x^*)^\top p = 0)$$

Lagrange Multipliers



Left: f increases along p. **Right:** f does not change along p.

Lagrange Multipliers



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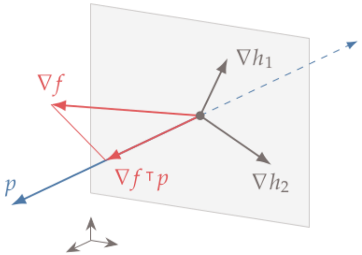
Observe that at an optimum, ∇f lies in the space spanned by the gradients of constraint functions.

Lagrange Multipliers



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Observe that at an optimum, ∇f lies in the space spanned by the gradients of constraint functions.

There are *Lagrange multipliers* λ_1, λ_2 satisfying

$$\nabla f(x^*) = -(\lambda_1 \nabla h_1 + \lambda_2 \nabla h_2)$$

The minus sign is arbitrary for equality constraints but will be significant when dealing with inequality constraints.

Lagrange Multipliers

We know that if x^* is a constrained minimizer, then.

$$\nabla f(x^*)^\top p = 0 \text{ for all } p \text{ satisfying } (\forall j : \nabla h_j(x^*)^\top p = 0)$$

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$$\nabla f(x^*)^\top p = 0 \text{ for all } p \text{ satisfying } (\forall j : \nabla h_j(x^*)^\top p = 0)$$

But then, from the geometry of the problem, we obtain

Theorem 5

Consider the COP with only equality constraints and f and all h_j twice continuously differentiable.
Assume that x^* is a constrained minimizer and that x^* is regular,
which means that $\nabla h_j(x^*)$ are linearly independent.
Then there are $\lambda_1, \ldots, \lambda_{n_h} \in \mathbb{R}$ satisfying

$$\nabla f(x^*) = -\sum_{j=1}^{n_h} \lambda_j \nabla h_j(x^*)$$

The coefficients $\lambda_1, \ldots, \lambda_{n_h}$ are called *Lagrange multipliers*.

Lagrangian Function

Try to transform the constrained problem into an unconstrained one by moving the constraints $h_j(x) = 0$ into the objective.

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Note that the stationary point of $\mathcal{L}$ gives us the Lagrange multipliers:

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Now putting $\nabla \mathcal{L}(x) = 0$, we obtain precisely the above properties of the constrained minimizer:

$$h(x) = 0 \qquad \text{and} \qquad \nabla f(x) = -\sum_{j=1}^{n_h} \lambda_j \nabla h_j(x)$$

However, we cannot use the unconstrained optimization methods here because searching for a minimizer in x asks for a maximizer in λ.

$$
\begin{array}{ll}
\underset{x_1, x_2}{\text{minimize}} & f(x_1, x_2) = x_1 + 2x_2 \\
\text{subject to} & h(x_1, x_2) = \frac{1}{4}x_1^2 + x_2^2 - 1 = 0
\end{array}
$$

The Lagrangian function

$$
\mathcal{L}(x_1, x_2, \lambda) = x_1 + 2x_2 + \lambda \left(\frac{1}{4}x_1^2 + x_2^2 - 1 \right)
$$

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Differentiating this to get the first-order optimality conditions,

$$\frac{\partial \mathcal{L}}{\partial x_1} = 1 + \frac{1}{2}\lambda x_1 = 0 \qquad \frac{\partial \mathcal{L}}{\partial x_2} = 2 + 2\lambda x_2 = 0$$

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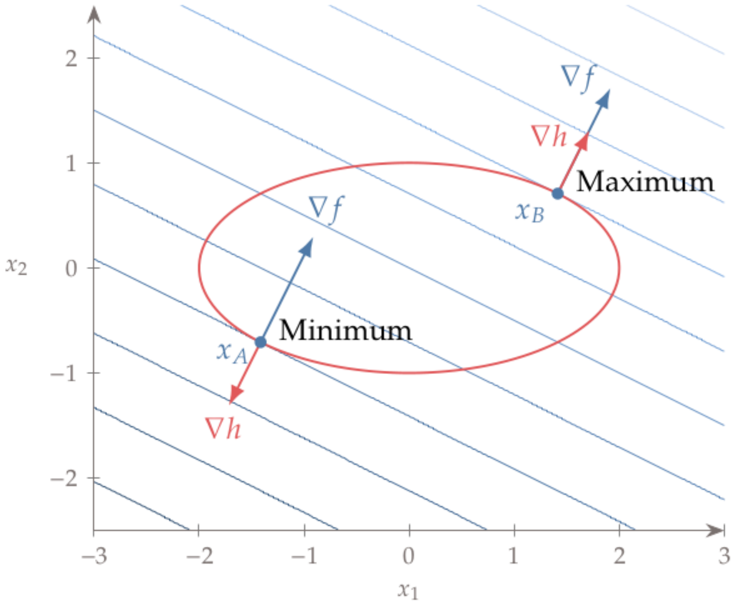
Solving these three equations for the three unknowns (x_1, x_2, λ), we obtain two possible solutions:

$$x_A = (x_1, x_2) = (-\sqrt{2}, -\sqrt{2}/2), \quad \lambda_A = \sqrt{2}$$

$$x_B = (x_1, x_2) = (\sqrt{2}, \sqrt{2}/2), \quad \lambda_A = -\sqrt{2}$$



∇f
∇h
Maximum
x_B
∇f
Minimum
x_A
∇h
2
1
0
−1
−2
x_2
−3
−2
−1
0
1
2
3
x_1

Second-Order Sufficient Conditions

As in the unconstrained case, the first-order conditions characterize any "stable" point (minimum, maximum, saddle).

Consider *Lagrangian Hessian*:

$$H_{\mathcal{L}}(x, \lambda) = H_f(x) + \sum_{j=1}^{n_h} \lambda_j H_{h_j}(x)$$

Here H_f is the Hessian of f, and each H_{h_j} is the Hessian of h_j.

The second-order sufficient conditions are as follows: Assume x^* is regular and feasible. Also, assume that there is λ s.t.

$$\nabla f(x^*) = \sum_{j=1}^{n_h} -\lambda_j \nabla h_j(x^*)$$

and that

$$p^\top H_{\mathcal{L}}(x^*, \lambda) p > 0 \text{ for all } p \text{ satisfying } (\forall j : \nabla h_j(x^*)^\top p = 0)$$

Then, x^* is a constrained minimizer of f.

$$\begin{array}{ll} \underset{x_1, x_2}{\text{minimize}} & f(x_1, x_2) = x_1 + 2x_2 \\ \text{subject to} & h(x_1, x_2) = \frac{1}{4}x_1^2 + x_2^2 - 1 = 0 \end{array}$$

The Lagrangian function

$$\mathcal{L}(x_1, x_2, \lambda) = x_1 + 2x_2 + \lambda\left(\frac{1}{4}x_1^2 + x_2^2 - 1\right)$$

Differentiating this to get the first-order optimality conditions,

$$\frac{\partial \mathcal{L}}{\partial x_1} = 1 + \frac{1}{2}\lambda x_1 = 0 \qquad \frac{\partial \mathcal{L}}{\partial x_2} = 2 + 2\lambda x_2 = 0$$
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$$x_B = (x_1, x_2) = (\sqrt{2}, \sqrt{2}/2), \quad \lambda_A = -\sqrt{2}$$

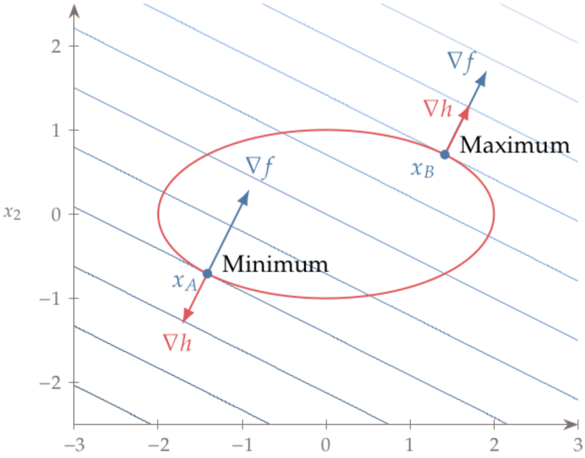
Which one is a minimum?

Second Order Conditions - Example

Compute the Hessian:

$$H_{\mathcal{L}} = \begin{pmatrix} \frac{1}{2}\lambda & 0 \\ 0 & 2\lambda \end{pmatrix}$$

The Hessian is positive definite only for the case $\lambda_A = \sqrt{2}$.



$$
\begin{aligned}
\underset{x_1, x_2}{\text{minimize}} \quad & f(x_1, x_2) = x_1^2 + 3(x_2 - 2)^2 \\
\text{subject to} \quad & h(x_1, x_2) = \beta x_1^2 - x_2 = 0,
\end{aligned}
$$

where β is a parameter. The Lagrangian for this problem is

$$
\mathcal{L}(x_1, x_2, \lambda) = x_1^2 + 3(x_2 - 2)^2 + \lambda\left(\beta x_1^2 - x_2\right).
$$

Differentiating for the first-order optimality conditions, we get

$$
\begin{aligned}
\nabla_x \mathcal{L} &= \begin{bmatrix} 2x_1(1 + \lambda\beta) \\ 6(x_2 - 2) - \lambda \end{bmatrix} = 0 \\
\nabla_\lambda \mathcal{L} &= \beta x_1^2 - x_2 = 0.
\end{aligned}
$$

Solving these three equations for the three unknowns (x_1, x_2, λ), the solution is $x_A = (0, 0)$, $\lambda_A = -12$, independent of β.

The Hessian of the Lagrangian,

$$
H_{\mathcal{L}} = \begin{bmatrix} 2(1 - 12\beta) & 0 \\ 0 & 6 \end{bmatrix}
$$

We need this to be positive definite in feasible directions.

$$\begin{array}{ll}\underset{x_1,x_2}{\text{minimize}} & f\left(x_1,x_2\right)=x_1^2+3\left(x_2-2\right)^2 \\ \text{subject to} & h\left(x_1,x_2\right)=\beta x_1^2-x_2=0,\end{array}$$

The Hessian of the Lagrangian,

$$H_{\mathcal{L}}=\left[\begin{array}{cc}2(1-12\beta) & 0 \\ 0 & 6\end{array}\right]$$

What are the feasible directions?

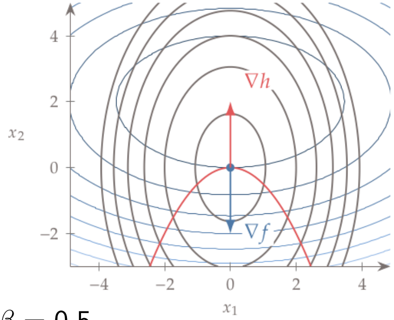
$\nabla h=(2\beta x_1,-1)$ and thus $\nabla h(x^*)=(0,-1)$.
Thus all p satisfying $\nabla h^\top p=0$ are $(\alpha,0)$ for $\alpha\in\mathbb{R}$.

Thus, for positive curvature in the feasible direction, we need

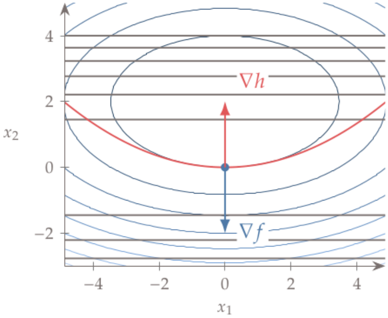
$$p^\top H_{\mathcal{L}}p=2\alpha^2(1-12\beta)>0$$

which is equivalent to $\beta<1/12$.

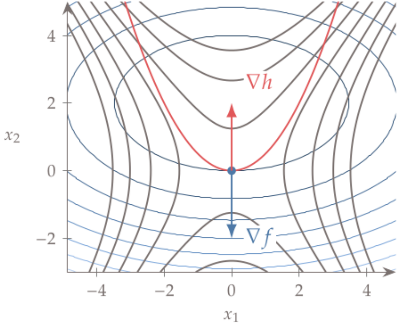
$\beta = -0.5$



$\beta = 1/12$



$\beta = 0.5$



Inequality Constraints

Recall that the constrained optimization problem is

$$
\begin{array}{rll}
\text{minimize} & f(x) & \\
\text{by varying} & x & \\
\text{subject to} & g_i(x) \leq 0 & i = 1, \dots, n_g \\
& h_j(x) = 0 & j = 1, \dots, n_h
\end{array}
$$

We say that a constraint $g_i(x) \leq 0$ is *active* for x if $g_i(x) = 0$, otherwise it is *inactive* for x.

As before, if x^* is a minimizer, any small step in a feasible direction p must not decrease f, i.e.,

$$\nabla f(x^*)^\top p \geq 0$$

How do we identify feasible directions for inequality constraints?

Feasible Directions

For inactive constraints, arbitrary direction p is feasible.

Feasible Directions

For inactive constraints, arbitrary direction p is feasible.

For active constraints $g_i(x) = 0$ we have p feasible at x if

$$g_i(x + p) \approx g_i(x) + \nabla g_i(x)^\top p \leq 0, \quad i = 1, \dots, n_g$$

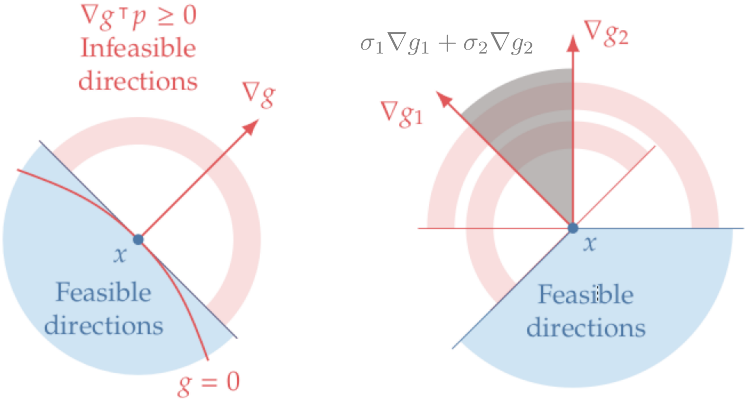
Feasible Directions

For inactive constraints, arbitrary direction p is feasible.

For active constraints $g_i(x) = 0$ we have p feasible at x if

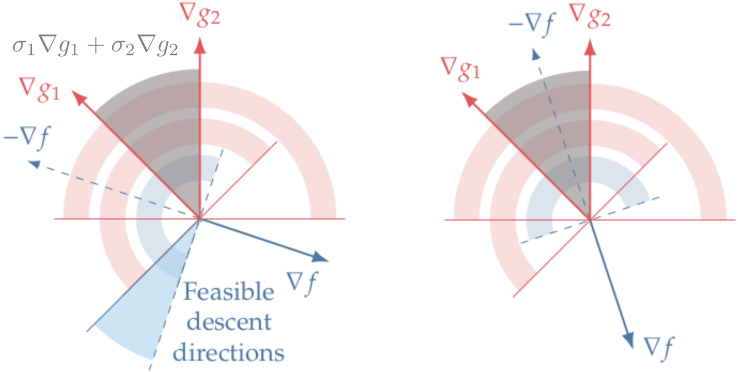
$$g_i(x+p) \approx g_i(x) + \nabla g_i(x)^\top p \le 0, \quad i = 1, \dots, n_g$$

thus p is *feasible* iff $\nabla g_i(x)^\top p \le 0$ for all active constr. $g_i(x) = 0$.



Lagrange Multipliers

When could f be decreased in a feasible direction?



Left: f decreases in the blue cone. **Right:** f does not decrease in any feasible direction.

At an optimum there are *Lagrange multipliers* $\sigma_1, \sigma_2 \geq 0$:

$$-\nabla f = \sigma_1 \nabla g_1 + \sigma_2 \nabla g_2$$

Lagrange Multipliers

We know that if x^* is a constrained minimizer, then

$$\nabla f(x)^\top p = 0 \quad \text{for all } p \text{ feasible at } x$$

Lagrange Multipliers

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One can prove the following

Theorem 6

Consider the COP with f and all g_i, h_j twice continuously differentiable.
Assume that x^* is a constrained minimizer and that x^* is regular *which means that $\nabla g_i(x^*), \nabla h_j(x^*)$ are linearly independent.*
Then there are Lagrange multipliers $\lambda_1, \ldots, \lambda_{n_h} \in \mathbb{R}$ and $\sigma_1, \ldots, \sigma_{n_g} \in \mathbb{R}$ satisfying

$$-\nabla f(x^*) = \sum_{j=1}^{n_h} \lambda_j \nabla h_j(x^*) + \sum_{i=1}^{n_h} \sigma_i \nabla g_i(x^*) \qquad \textit{where } \sigma_i \geq 0$$

Lagrangian Function

Note that inequality $g_i(x) \leq 0$ can be equivalently expressed using a *slack variable* s_i by

$$g(x) + s_i^2 = 0$$

The Lagrangian function then generalizes from equality to inequality COP as follows.

$$\mathcal{L}(x, \lambda, \sigma, s) = f(x) + h(x)^\top \lambda + (g(x) + s \odot s)^\top \sigma$$

Here, $h(x) = (h_1(x), \ldots, h_{n_h}(x))^\top$, $g(x) = (g_1(x), \ldots, g_{n_g}(x))^\top$, $s = (s_1, \ldots, s_{n_g})$, and $\odot$ is the component-wise multiplication.

Now compute the stable point of $\mathcal{L}$ by considering

$$\nabla_x \mathcal{L} = 0$$
$$\nabla_\lambda \mathcal{L} = 0$$
$$\nabla_\sigma \mathcal{L} = 0$$
$$\nabla_s \mathcal{L} = 0$$

(see the whiteboard)

KKT

If x^* is a constrained minimizer and x^* is regular. Then there are λ, σ, s satisfying

$$\begin{aligned}
\frac{\partial f}{\partial x_\ell}(x^*) + \sum_{j=1}^{n_h} \lambda_j \frac{\partial h_j}{\partial x_\ell}(x^*) + \sum_{j=1}^{n_g} \sigma_j \frac{\partial g_j}{\partial x_\ell}(x^*) &= 0 \qquad \ell = 1, \dots, n \\
h_j(x^*) &= 0 \quad j = 1, \dots, n_h \\
g_i(x^*) + s_i^2 &= 0 \quad i = 1, \dots, n_g \\
2\sigma_i s_i &= 0 \quad i = 1, \dots, n_g \\
\sigma_i &\geq 0
\end{aligned}$$

So, solving the above system allows us to identify potential constrained minimizers.

KKT

If x^* is a constrained minimizer and x^* is regular. Then there are λ, σ, s satisfying

$$\begin{aligned}
\frac{\partial f}{\partial x_\ell}(x^*) + \sum_{j=1}^{n_h} \lambda_j \frac{\partial h_j}{\partial x_\ell}(x^*) + \sum_{j=1}^{n_g} \sigma_j \frac{\partial g_j}{\partial x_\ell}(x^*) &= 0 \qquad \ell = 1, \ldots, n \\
h_j(x^*) &= 0 \quad j = 1, \ldots, n_h \\
g_i(x^*) + s_i^2 &= 0 \quad i = 1, \ldots, n_g \\
2\sigma_i s_i &= 0 \quad i = 1, \ldots, n_g \\
\sigma_i &\geq 0
\end{aligned}$$

So, solving the above system allows us to identify potential constrained minimizers.

To decide whether x^* solving KKT is a minimizer, check whether

$$p^\top H_{\mathcal{L}}(x^*, \lambda) p > 0$$

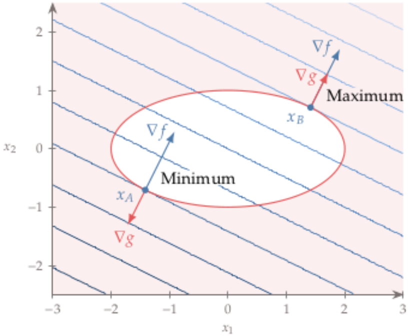
For all feasible directions p (similarly to the equality case).

Example

$$\underset{x_1,x_2}{\text{minimize}} \quad f(x_1,x_2) = x_1 + 2x_2$$
$$\text{subject to} \quad g(x_1,x_2) = \tfrac{1}{4}x_1^2 + x_2^2 - 1 \le 0.$$

The Lagrangian function for this problem is

$$\mathcal{L}(x_1,x_2,\sigma,s) = x_1 + 2x_2 + \sigma\left(\frac{1}{4}x_1^2 + x_2^2 - 1 + s^2\right)$$



Example

$$\frac{\partial \mathcal{L}}{\partial x_1} = 1 + \frac{1}{2}\sigma x_1 = 0$$
$$\frac{\partial \mathcal{L}}{\partial x_2} = 2 + 2\sigma x_2 = 0$$
$$\frac{\partial \mathcal{L}}{\partial \sigma} = \frac{1}{4}x_1^2 + x_2^2 - 1 = 0$$
$$\frac{\partial \mathcal{L}}{\partial s} = 2\sigma s = 0.$$

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\frac{\partial \mathcal{L}}{\partial s} &= 2\sigma s = 0.
\end{aligned}$$

Setting $\sigma = 0$ does not yield any solution. Setting $s = 0$ and $\sigma \neq 0$ we obtain

$$x_A = \begin{bmatrix} x_1 \\ x_2 \\ \sigma \end{bmatrix} = \begin{bmatrix} -\sqrt{2} \\ -\sqrt{2}/2 \\ \sqrt{2} \end{bmatrix}, \quad x_B = \begin{bmatrix} x_1 \\ x_2 \\ \sigma \end{bmatrix} = \begin{bmatrix} \sqrt{2} \\ \sqrt{2}/2 \\ -\sqrt{2} \end{bmatrix}$$

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Now, σ must be non-negative, so only x_A is the solution. There is no feasible descent direction at x_A. We already know that the Hessian Lagrangian is positive definite, so this is a minimizer.

$$
\begin{array}{ll}
\underset{x_1, x_2}{\text{minimize}} & f(x_1, x_2) = x_1 + 2x_2 \\
\text{subject to} & g_1(x_1, x_2) = \frac{1}{4}x_1^2 + x_2^2 - 1 \leq 0 \\
& g_2(x_2) = -x_2 \leq 0.
\end{array}
$$

The feasible region is the top half of the ellipse defined by g_1.

$$
\begin{array}{ll}
\underset{x_1,x_2}{\text{minimize}} & f(x_1, x_2) = x_1 + 2x_2 \\
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The feasible region is the top half of the ellipse defined by g_1.
The Lagrangian for this problem is

$$
\mathcal{L}(x, \sigma, s) = x_1 + 2x_2 + \sigma_1 \left(\frac{1}{4}x_1^2 + x_2^2 - 1 + s_1^2 \right) + \sigma_2 \left(-x_2 + s_2^2 \right).
$$

$$
\begin{array}{ll}
\underset{x_1, x_2}{\text{minimize}} & f(x_1, x_2) = x_1 + 2x_2 \\
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$$

Differentiating the Lagrangian with respect to all the variables, we get the first-order optimality conditions,

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial x_1} &= 1 + \frac{1}{2}\sigma_1 x_1 = 0 & \qquad \frac{\partial \mathcal{L}}{\partial \sigma_2} &= -x_2 + s_2^2 = 0 \\
\frac{\partial \mathcal{L}}{\partial x_2} &= 2 + 2\sigma_1 x_2 - \sigma_2 = 0 & \qquad \frac{\partial \mathcal{L}}{\partial s_1} &= 2\sigma_1 s_1 = 0 \\
\frac{\partial \mathcal{L}}{\partial \sigma_1} &= \frac{1}{4}x_1^2 + x_2^2 - 1 + s_1^2 = 0 & \qquad \frac{\partial \mathcal{L}}{\partial s_2} &= 2\sigma_2 s_2 = 0.
\end{aligned}
$$

Assumption	Meaning	x_1	x_2	σ_1	σ_2	s_1	s_2	Point
$s_1 = 0$	g_1 is active	-2	0	1	2	0	0	x^*
$s_2 = 0$	g_2 is active	2	0	-1	2	0	0	x_C
$\sigma_1 = 0$	g_1 is inactive							
$\sigma_2 = 0$	g_2 is inactive		-	-	-	-	-	
$s_1 = 0$	g_1 is active	$\sqrt{2}$	$\frac{\sqrt{2}}{2}$	$-\sqrt{2}$	0	0	$2^{-\frac{1}{4}}$	x_B
$\sigma_2 = 0$	g_2 is inactive							
$\sigma_1 = 0$	g_1 is inactive							
$s_2 = 0$	g_2 is active			-	-