1 Quadratic Objectives and Quasi-Newton

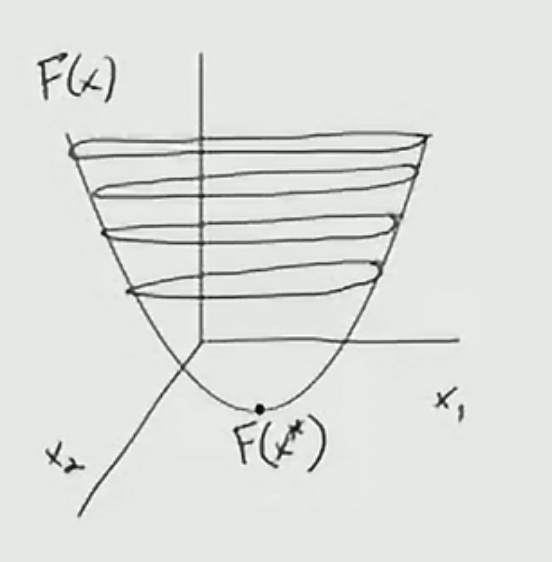
We now want to consider quadratic functions in m-dimensions,

$$a \in \mathbb{R}, \qquad b \in \mathbb{R}^m, \qquad A \in \mathbb{R}^{m \times m} \quad \text{(Symmetric.)}$$

The function of interest is

$$F(x) = a - b^T x + \frac{1}{2} x^T A x, \qquad x \in \mathbb{R}^m.$$

If A is positive definite, then $F(x)$ is convex and it has a minimum x^*.



Note that the constant a does not change the location of the minimum. In other words[1],

$$x^* = \arg\min_{x \in \mathbb{R}^m} F(x) = \arg\min_{x \in \mathbb{R}^m} \left(-b^T x + \frac{1}{2} x^T A x \right).$$

The given derivative is then

$$F(x) = a - \sum_{i=1}^{m} b_i x_i + \frac{1}{2} \underbrace{\sum_{i=1}^{m} \sum_{j=1}^{m} x_i A_{ij} x_j}_{\text{Corresponds to } x^T (Ax)}.$$

Its gradient is given by

$$\begin{aligned}
\frac{\partial F}{\partial x_k} &= \frac{d}{dx_k} \left(a - \sum_{i=1}^{m} b_i x_i + \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} x_i A_{ij} x_j \right) \\
&= -b_k + \frac{1}{2} \sum_{j=1}^{m} A_{kj} x_j + \frac{1}{2} \sum_{i=1}^{m} x_i A_{ik} \\
&= -b_k + 2 \left(\frac{1}{2} \right) \sum_{j=1}^{m} A_{kj} x_j \\
&= -b_k + \left(\frac{1}{2} \right) \sum_{j=1}^{m} A_{kj} x_j \qquad (1 \le k \le m).
\end{aligned}$$

[1] $\arg\min_{x \in \mathbb{R}^m} F(x)$ returns the x value corresponding to the smallest $F(x)$.

Note that the above two sums basically produce the same results, but with different indexing. So, we were able to combine them.

$$\nabla F = \begin{bmatrix} \frac{\partial F}{\partial x_1} \\ \vdots \\ \frac{\partial F}{\partial x_m} \end{bmatrix} = \begin{bmatrix} -b_1 + \sum_{j=1}^m A_{ij} x_j \\ \vdots \\ -b_m + \sum_{j=1}^m A_{mj} x_j \end{bmatrix} = -b + Ax = g(x).$$

For $1 \le i \le m$ and $1 \le k \le m$, the Hessian matrix is given by

$$\frac{\partial^2 F}{\partial x_k \partial x_i} = \frac{d}{dx_i} \left(-b_k + \sum_{j=1}^m A_{kj} x_j \right) = A_{ki}.$$

Thus, we can write $\nabla^2 F = A = H(x)$, the entire Hessian matrix.

1.1 Computing a Minimum

Suppose the function is convex. If we have A and we can solve for it, then to compute the minimum, we can set the gradient equal to zero:

$$0 = g(x) = -b + Ax \implies Ax = b \implies A^{-1} b = x.$$

But, in reality, A might be too big, in which case we might consider iteratively solving the minimization problem. In any case, the line-search for quadratic functions can be computed explicitly, by fixing $x^{(k)} \in \mathbb{R}^m$ and $P \in \mathbb{R}^m$, and doing

$$\min_\alpha F(x^{(k)} + \alpha P).$$

We want to compute the directional derivative, which can be done by solving

$$\begin{aligned} 0 &= \frac{d}{d\alpha} F(x^{(k)} + \alpha P) \\ &= P^T \nabla F(x^{(k)} + \alpha P) \\ &= P^T \Big(A(x^{(k)} + \alpha P) - b \Big) \\ &= P^T (Ax^{(k)} - b) + \alpha P^T A P - P^T (Ax^{(k)} - b) \\ &= \alpha P^T A P. \end{aligned}$$

or just

$$\alpha_k = \frac{P^T (b - Ax^{(k)})}{P^T a P}.$$

α_k is the solution to the line-search problem. The "residue" is given by $r^{(k)} = b - Ax^{(k)}$.

(Example.) The steepest descent for quadratics is given by

$$P^{(k)} = -g(x^{(k)}) = -(Ax^{(k)} - b).$$

A very brief algorithm is shown below, which takes

- $x^{(0)}$, the starting point, and
- M, the number of iterations,

as the arguments.

Algorithm 1 Steepest Descent

```
function STEEPEST(x^(0), M)
    k ← 0
    while k < M do
        x^(k+1) = x^(k) + α_k P^(k)
    end while
end function
```

1.2 Quasi-Newton Methods

An effective class of methods to now consider is the **Quasi-Newton**. For general nonlinear $F : \mathbb{R}^m \to \mathbb{R}$, we want to only use the gradient function $g(x)$. In other words, we don't need the Hessian matrix here, as computing a Hessian matrix can be quite expensive. So, we can either *approximate* the Hessian matrix[2], $H(x_k) \approx B_k$, or approximate the inverse of the Hessian matrix $(H(x_k))^{-1} \approx \hat{H}_k$. These approximations satisfy the secant condition,

$$s_k = x_{k+1} - x_k \in \mathbb{R}^m.$$

$$y_j = g_{j+1} - g_j \in \mathbb{R}^m.$$

We can make use of an algorithm that makes use of this concept. This algorithm, known as the Davidon-Fletcher-Powell Method, takes the following arguments:

- $x_0 \in \mathbb{R}^m$, the starting point;
- g, the gradient of F;
- F, the function itself;
- M, the maximum number of iterations; and
- ϵ, the tolerance.

The algorithm is as follows:

Algorithm 2 Davidon-Fletcher-Powell Method

```
function DFP(x_0, g, F, M, ε)
    k ← 0
    H_k ← I
    while ||g(x_k)||_2 > ε and k ≤ M do
        P_k ← −H_k g(x_k)
        α_k ← min_α F(x_k + α P_k)            ▷ Line-Search Algorithm
        s_k ← α_k P_k
        x_{k+1} ← x_k + s_k
        y_k ← g(x_{k+1}) − g(x_k)
        H_k ← H_k + (s_k s_k^T)/(y_k^T s_k) − (H_k y_k y_k^T H_k)/(y_k^T H_k y_k)
        k ← k + 1
    end while
end function
```

[2] $H(x_k)$ just means that we're evaluating the Hessian matrix at point x_k.