(Quasi-)Newton methods

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Outline

So far you have seen:

- gradient descent
- proximal gradient descent
- accelerated gradient descent
- (proximal) coordinate descent
- conjugate gradient

Now

- Newton methods
- Quasi-Newton methods
- Methods dedicated to non-linear least squares

Quasi-Newton and in particular L-BFGS are still heavily used to tackle smooth potentially large scale optim problems in machine learning (e.g. ℓ_2 logistic regression, conditional random fields)

Newton method

It is used to find the zeros of a differentiable non-linear function g:

$$\text{Find } x \text{ such that } g(x) = 0, \text{ where } g : \mathbb{R}^n \to \mathbb{R}^n.$$

Given a starting point x_0, Newton method consists in iterating:

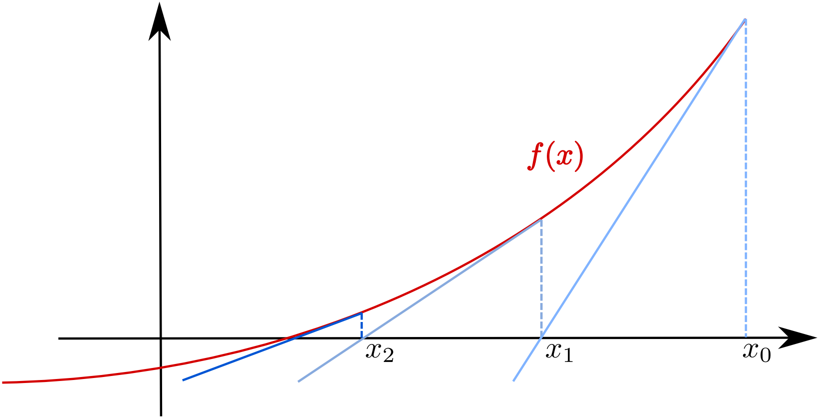
$$x_{k+1} = x_k - g'(x_k)^{-1} g(x_k)$$

where $g'(x)$ is the derivative (Jacobian) of g at point x.

We have that:

- $g'(x_k)$ is matrix in $\mathbb{R}^{n \times n}$
- each iteration requires to solve a linear system.

Newton method in 1d



Newton method?

Applying this method to the optimization problem:

$$\min_{x \in \mathbb{R}^n} f(x)$$

consists in setting $g(x) = \nabla f(x)$, i.e., looking for stationary points. The iterations read:

$$x_{k+1} = x_k - \nabla^2 f(x_k)^{-1} \nabla f(x_k) \ .$$

Newton method is particularly interesting as its convergence is quadratic locally around x^*, i.e.:

$$\|x_{k+1} - x^*\| \leq \gamma \|x_k - x^*\|^2, \gamma > 0 \ .$$

Convergence of Newton method

Theorem (Convergence of Newton method)

Let $g : \mathbb{R}^n \to \mathbb{R}^n$ assumed twice differentiable $\mathcal{C}^2$, and $x^* \in \mathbb{R}^n$ an isolated zero of g ($g(x^*) = 0$). Assuming that $g'(x^*)$ is invertible, there exists a closed ball $\mathcal{B}$ centered on x^*, such that for every $x_0 \in \mathcal{B}$, the sequence x_k obtained with Newton algorithm stays in $\mathcal{B}$ and converges towards x^*. Furthermore, there is a constant $\gamma > 0$, such that $\|x_{k+1} - x^*\| \leq \gamma \|x_k - x^*\|^2$.

Remark: Convergence of Newton is local. The method may diverge if the initial point is too far from x^* or if the Hessian is not positive definite. That is why Newton should be coupled with a line search strategy.

→ See proof in lecture notes.

Newton on quadratic function

Exercise

Show that for a quadratic function

$$f(x) = \frac{1}{2} x^\top A x - b^\top x + c,\ x \in \mathbb{R}^n$$

with A symmetric positive definite, Newton method converges in one iteration independently of the choice of x_0.

Remark: Newton is therefore not affected by the conditioning of the problem (not like Gradient descent).

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Variable metric

The idea behind variable metric methods consists in using iterations of the form

$$\begin{cases} d_k = -B_k g_k \ , \\ x_{k+1} = x_k + \rho_k d_k \ , \end{cases}$$

where $g_k = \nabla f(x_k)$, B_k is a positive definite matrix and $\rho_k \geq 0$ is a step size.

→ If $B_k = I_n$, it corresponds to gradient descent.
→ Setting $B_k = B$ is the fixed metric case.

Fixed metric case

When minimizing

$$\min_{x \in \mathbb{R}^n} f(x)$$

one can set $x = Cy$ with C invertible (change of variable). Let us denote $\tilde{f}(y) = f(Cy)$. This leads to:

$$\nabla \tilde{f}(y) = C^\top \nabla f(Cy) \ .$$

Gradient descent applied to $\tilde{f}(y)$ reads:

$$y_{k+1} = y_k - \rho_k C^\top \nabla f(Cy_k)$$

which means using $B = CC^\top$ as it is equivalent to:

$$x_{k+1} = x_k - \rho_k CC^\top \nabla f(x_k) \ .$$

Question: How would you choose C for quadratic problem?

Quadratic case

Theorem (Preconditioned gradient descent)

Let $f(x)$ a positive definite quadratic form with Hessian A, and B a positive definite matrix. The preconditioned gradient algorithm:

$$\begin{cases} x_0 = \textit{fixed}, \\ x_{k+1} = x_k - \rho_k B g_k, \;\; \rho_k \;\; \textit{optimal} \end{cases}$$

has a linear convergence: $\|x_{k+1} - x^*\| \leq \gamma \|x_k - x^*\|$
where:

$$\gamma = \frac{\chi(BA) - 1}{\chi(BA) + 1} < 1 \;\; .$$

$\chi(M) = \lambda_1 / \lambda_n$ is the Euclidian conditioning *i.e.*, ratio of largest and lowest eigenvalues (≥ 1).

Quadratic case

So we have a linear convergence:

$$\|x_{k+1} - x^*\| \leq \gamma \|x_k - x^*\|$$

where:

$$\gamma = \frac{\chi(BA) - 1}{\chi(BA) + 1} < 1 \ .$$

Remark

The lower the conditioning of BA, the faster is the algorithm. One cannot set $B = A^{-1}$ as it would imply having already solved the problem, but this however suggests to use B so that is approximate A^{-1}. This is the idea behind quasi-Newton methods.

B 取值应尽可能靠近inv(A)

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Quasi-Newton

A quasi-Newton method reads

$$\begin{cases} d_k = -B_k g_k \quad , \\ x_{k+1} = x_k + \rho_k d_k \quad , \end{cases}$$

or

$$\begin{cases} d_k = -H_k^{-1} g_k \quad , \\ x_{k+1} = x_k + \rho_k d_k \quad , \end{cases}$$

where B_k (resp. H_k) is a matrix which aims to approximate the inverse of the Hessian (resp. the Hessian) of f at x_k.

Question: How to achieve this?

Quasi-Newton

One can start with $B_0 = I_n$. how to update B_k at every iteration?

Idea: apply a Taylor expansion on the gradient, notice that at point x_k, the gradient and the Hessian are such that:

$$g_{k+1} = g_k + \nabla^2 f(x_k)(x_{k+1} - x_k) + \epsilon(x_{k+1} - x_k) \ .$$

If one assumes that the approximation is good enough one has:

$$g_{k+1} - g_k \approx \nabla^2 f(x_k)(x_{k+1} - x_k) \ ,$$

which leads to the quasi-Newton relation, a.k.a, the secant condition.

Quasi-Newton relation (or secant condition)

Definition (Quasi-Newton relation)

Two matrices B_{k+1} and H_{k+1} verify the quasi-Newton relation (or secant condition) if:

$$H_{k+1}(x_{k+1} - x_k) = \nabla f(x_{k+1}) - \nabla f(x_k)$$

or

$$x_{k+1} - x_k = B_{k+1}(\nabla f(x_{k+1}) - \nabla f(x_k))$$

Problem: How to update B_k keeping it positive definite?

Update formula of Hessian

The update strategy at iteration

$$\begin{cases} d_k = -B_k g_k \ , \\ x_{k+1} = x_k + \rho_k d_k \ , \end{cases}$$

is to correct B_k with a symmetric matrix Δ_k:

$$B_{k+1} = B_k + \Delta_k$$

such that quasi-Newton relation holds:

$$x_{k+1} - x_k = B_{k+1}(g_{k+1} - g_k)$$

with B_{k+1} positive definite, assuming B_k is positive definite.
Idea: Use rank 1 or 2 matrices for Δ_k

Broyden formula (known as SR1)

Broyden formula is a rank 1 correction: $B_{k+1} = B_k + vv^\top$.
The matrix B_{k+1}, with $v \in \mathbb{R}^n$, should verify the quasi-Newton relation:

$$B_{k+1} y_k = s_k \,,$$

where $y_k = g_{k+1} - g_k$ and $s_k = x_{k+1} - x_k$. It follows that:

$$\begin{aligned} B_k y_k + vv^\top y_k &= s_k \\ \Rightarrow (y_k^\top v)^2 &= (s_k - B_k y_k)^\top y_k \end{aligned}$$

Using the equality $vv^\top = \frac{vv^\top y_k (vv^\top y_k)^\top}{(v^\top y_k)^2}$,
one can write after replacing $vv^\top y_k$ by $s_k - B_k y_k$, and $(v^\top y_k)^2$ by $y_k^\top (s_k - B_k y_k)$, the correction formula

$$B_{k+1} = B_k + \frac{(s_k - B_k y_k)(s_k - B_k y_k)^\top}{(s_k - B_k y_k)^\top y_k} \quad ,$$

also known as Broyden formula.

Broyden formula

Theorem

Let f a quadratic form positive definite. Let us consider the method that, starting for x_0, iterates:

$$x_{k+1} = x_k + s_k \quad ,$$

where the vectors s_k are linearly independent. Then the sequence of matrices starting by B_0 and defined as:

$$B_{k+1} = B_k + \frac{(s_k - B_k y_k)(s_k - B_k y_k)^\top}{(s_k - B_k y_k)^\top y_k} \quad ,$$

where $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$, converges in less than n iterations towards A^{-1}, the inverse of the Hessian of f.

→ Cf. proof in lecture notes

Remark: No guarantee that the matrices B_k are positive definite, even if the function f is quadratic and $B_0 = I_n$.

Davidon, Fletcher and Powell formula

Using a rank 2 correction, it reads:

$$B_{k+1} = B_k + \alpha u u^\top + \beta v v^\top \ .$$

Imposing the quasi-Newton relation (secant condition):

$$\begin{aligned} B_{k+1} y_k &= s_k \\ \Rightarrow B_k y_k + \alpha(u^\top y_k)u + \beta(v^\top y_k)v &= s_k \\ \Rightarrow \alpha(u^\top y_k)u + \beta(v^\top y_k)v &= s_k - B_k y_k \end{aligned}$$

This equation has not a unique solution. The choice for u and v by DFP is:

$$u = s_k \quad \text{and} \quad v = B_k y_k$$

Davidon, Fletcher and Powell formula

Solving for α and β the equation:

$$\alpha(s_k^\top y_k)s_k + \beta(y_k^\top B_k y_k)B_k y_k = s_k - B_k y_k$$

we obtain

$$\alpha = \frac{1}{s_k^\top y_k} \quad \text{and} \quad \beta = -\frac{1}{y_k^\top B_k y_k}$$

Davidon, Fletcher and Powell formula

The DFP formula is a rank 2 correction. It reads:

$$B_{k+1} = B_k + \frac{s_k s_k^\top}{s_k^\top y_k} - \frac{B_k y_k y_k^\top B_k}{y_k^\top B_k y_k} \quad . \tag{1}$$

Theorem

Let us consider the update

$$\begin{cases} d_k = -B_k g_k \quad , \\ x_{k+1} = x_k + \rho_k B_k g_k, \;\; \rho_k \;\; optimal \end{cases}$$

where B_0 is positive definite and provided as well as x_0. Then the matrices B_k defined as in (1) *are positive definite for all $k > 0$.*

→ Cf. proof in lecture notes

Davidon-Fletcher-Powell algorithm

```
Require: $\varepsilon > 0$ (tolerance), $K$ (maximum number of iterations)
$x_0 \in \mathbb{R}^n$, $B_0 > 0$ (for example $I_n$)
for $k = 0$ to $K$ do
    if $\|g_k\| < \varepsilon$ then
        break
    end if
    $d_k = -B_k \nabla f(x_k)$
    $x_{k+1} = x_k + \rho_k d_k$ (Compute optimal step size $\rho_k$)
    $s_k = \rho_k d_k$
    $y_k = g_{k+1} - g_k$
    $B_{k+1} = B_k + \frac{s_k s_k^\top}{s_k^\top y_k} - \frac{B_k y_k y_k^\top B_k}{y_k^\top B_k y_k}$
end for
return $x_{k+1}$
```

Davidon-Fletcher-Powell algorithm

This algorithm has a remarkable property when the function f is quadratic.

Theorem

When f is a quadratic form, the algorithm of Davidon-Fletcher-Powell generates a sequence of directions $s_0, \ldots, s_k$ which verify:

$$\begin{aligned} s_i A^\top s_j &= 0, \quad 0 \leq i < j \leq k, \\ B_{k+1} A s_i &= s_i, \qquad\quad 0 \leq i \leq k. \end{aligned} \tag{2}$$

Remark: This theorem says that in the quadratic case, the algorithm is like a conjugate gradient method, which therefore converges in at most n iterations.

Remark: This required to have an optimal step size.

Davidon-Fletcher-Powell algorithm

One can also notice that for $k = n - 1$

$$B_n A s_i = s_i, i = 0, \ldots, n - 1,$$

and since all s_i are linearly independent it implies $B_n = A^{-1}$.

Remark: One can show that in the general case (non-quadratic), if the direction d_k is reinitialized to $-g_k$ periodically, this algorithm converges to a local minimum $\hat{x}$ of f and that:

$$\lim_{k \to \infty} B_k = \nabla^2 f(\hat{x})^{-1} \ .$$

This implies that close to the optimum, the method behaves like a Newton method. This justifies the use of $\rho_k = 1$ when using approximate line search.

Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm

- The BFGS formula is derived from the formula of DFP by swapping the roles of s_k and y_k.
- The formula obtained allows to maintain an approximation H_k of the Hessian which satisfies the same properties: $H_{k+1} > 0$ if $H_k > 0$ and satisfying the quasi-Newton relation:

$$y_k = H_k s_k \quad .$$

- The BFGS formula therefore reads:

$$H_{k+1} = H_k + \frac{y_k y_k^\top}{y_k^\top s_k} - \frac{H_k s_k s_k^\top H_k}{s_k^\top H_k s_k} \quad .$$

Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm

```
Require: $\varepsilon > 0$ (tolerance), $K$ (maximum number of iterations)
$x_0 \in \mathbb{R}^n$, $H_0 > 0$ (for example $I_n$)
for $k = 0$ to $K$ do
    if $\|g_k\| < \varepsilon$ then
        break
    end if
    $d_k = -H_k^{-1} \nabla f(x_k)$
    $x_{k+1} = x_k + \rho_k d_k$ (optimal step size $\rho_k$ with line-search)
    $s_k = \rho_k d_k$
    $y_k = g_{k+1} - g_k$
    $H_{k+1} = H_k + \frac{y_k y_k^\top}{y_k^\top s_k} - \frac{H_k s_k s_k^\top H_k}{s_k^\top H_k s_k}$
end for
return $x_{k+1}$
```

Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm

- Direction d_k is obtained by solving a linear system.
- In practice update of H_k is done on Cholesky factorization of $H_k = C_k C_k^\top$
- So the complexity of BFGS is the same as DFP.
- Cholesky factorization allows to check that H_k stays numerically positive definite

The BFGS algorithm has the same property as the DFP method:

- in the quadratic case it produces conjugate directions
- it converges in less than n iterations and $H_n = A$
- Usually combined with Wolfe and Powell's or Goldstein's rule.

but:

- much less sensitive than DFP to the use of approximate step size (to combine with Wolfe and Powell's or Goldstein's rule).

Remark: BFGS is in scipy see scipy.optimize.fmin_bfgs.

Limited-memory BFGS (L-BFGS) algorithm

- L-BFGS is a variant of BFGS that limits memory usage. It was originally proposed by Liu and Nocedal in 1989:
- Does not store matrix of the size of the Hessian, $n \times n$ which can be prohibitive in applications such as computer vision or machine learning where n can be millions.
- L-BFGS stores only a few vectors that are used to approximate the matrix H_k^{-1}
- So the memory usage is linear in the dimension of the problem.

[Liu, D. C.; Nocedal, J. (1989). "On the Limited Memory Method for Large Scale Optimization". Mathematical Programming B. 45 (3): 503528.]

Limited-memory BFGS (L-BFGS) algorithm

- L-BFGS is an algorithm of the quasi-Newton family with $d_k = -B_k \nabla f(x_k)$.
- Difference is in the computation of the product between B_k and $\nabla f(x_k)$.
- Idea is to keep in memory the last low rank corrections, more specifically the last m values of $s_k = x_{k+1} - x_k$ and $y_k = g_{k+1} - g_k$.

Limited-memory BFGS (L-BFGS) algorithm

Let $\mu_k = \frac{1}{y_k^\top s_k}$, the algorithm to obtain d_k reads:

Require: m (memory size)

```
$q = g_k$
**for** $i = k - 1$ to $k - m$ **do**
    $\alpha_i = \mu_i s_i^\top q$
    $q = q - \alpha_i y_i$
**end for**
$z = B_k^0 q$
**for** $i = k - m$ to $k - 1$ **do**
    $\beta = \mu_i y_i^\top z$
    $z = z + s_i(\alpha_i - \beta)$
**end for**
$d_k = -z$
```

where B_k^0 is positive definite matrix, e.g., a diagonal matrix, so that initially setting z is fast.

Limited-memory BFGS (L-BFGS) algorithm

- Like BFGS, L-BFGS does not need exact line search to converge.
- L-BFGS is for smooth unconstrained problem but can be extended to handle simple box constraints (a.k.a. bound constraints): $l_i \leq x_i \leq u_i$ where l_i and u_i are per-variable constant lower and upper bounds. This algorithm called L-BFGS-B is due to Byrd et al. (1995).
- L-BFGS-B in scipy as `scipy.optimize.fmin_l_bfgs_b`.

[Byrd, R. H.; Lu, P.; Nocedal, J.; Zhu, C. (1995). "A Limited Memory Algorithm for Bound Constrained Optimization". SIAM J. Sci. Comput. 16 (5): 11901208. doi:10.1137/0916069.]

→ Can you solve a Lasso with L-BFGS-B?

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non-linear least-squares

The function to minimize reads:

$$f(x) = \frac{1}{2}\sum_{i=1}^{m} f_i(x)^2 \ .$$

Newton method can be applied to the minimization of f. The gradient and the Hessian matrix read in this particular case:

$$\nabla f(x) = \sum_{i=1}^{m} f_i(x)\nabla f_i(x) \ ,$$

and

$$\nabla^2 f(x) = \sum_{i=1}^{m} \nabla f_i(x)\nabla f_i(x)^\top + \sum_{i=1}^{m} f_i(x)\nabla^2 f_i(x) \ .$$

Gauss-Newton method

Close to the optimum, the $f_i(x)$ are small so the second term can be ignored. The Hessian reads:

$$H(x) \approx \sum_{i=1}^{m} \nabla f_i(x) \nabla f_i(x)^\top \ .$$

This matrix is always positive. Furthermore when m is much larger than n, this matrix is often positive definite.

The Gauss-Newton method uses this approximation of $H(x)$ in a Newton-like solver:

$$\begin{cases} x_0 = \text{fixed}, \\ H_k = \sum_{i=1}^{m} \nabla f_i(x_k) \nabla f_i(x_k)^\top, \\ x_{k+1} = x_k - H_k^{-1} \nabla f(x_k) \ . \end{cases}$$

Gauss-Newton method

To guarantee the convergence of the Gauss-Newton method, it can be combined with a line search procedure:

$$\begin{cases} x_0 = \text{fixed}, \\ H_k = \sum_{i=1}^{m} \nabla f_i(x_k) \nabla f_i(x_k)^\top, \\ x_{k+1} = x_k - \rho_k H_k^{-1} \nabla f(x_k) \end{cases} .$$

Levenberg-Marquardt method

- Levenberg-Marquardt method is a variant of Gauss-Newton that enforces that the Hessian approximation H_k is positive definite.
- The idea is simply to replace H_k by $H_k + \lambda I_n$.

$$\begin{cases} x_0 = \text{fixed}, \\ H_k = \sum_{i=1}^{m} \nabla f_i(x_k) \nabla f_i(x_k)^\top, \\ d_k = -(H_k + \lambda I_n)^{-1} \nabla f(x_k) \\ x_{k+1} = x_k + \rho_k d_k \quad . \end{cases}$$

- If λ is large, method is equivalent to a gradient method.
- The Levenberg-Marquardt method in scipy as scipy.optimize.leastsq.

References

- Wright and Nocedal, Numerical Optimization, 1999, Springer, Chapters 6 and 8.