Optimization

1. Unconstraint optimization problems

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Outline

Optimization problems

- Finance is all about *optimization*.
- Optimization helps to:
  - (i) maximize profits,
  - (ii) minimize costs,
  - (iii) control risk.
- Optimization problems facing financial professionals may include:
  - (i) Optimally allocate assets in a portfolio.
  - (ii) Build and interest rate curve based on benchmark rate observations.
  - (iii) Fit an implied volatility model to option market data.
  - (iv) Fit a time series model into observed data.
  - (v) Unwind a large position in a way that minimizes transaction costs.
  - (vi) Design an optimal hedging strategy of a portfolio of assets.
  - (vii) Optimally fit a predictive model into observed data.
  - (viii) Optimally exercise an American option.

Optimization problems

- Optimization is part of *applied mathematics*.
- That means that optimization problems are formulated in terms of properties of suitably defined functions.
- Depending on the context, solving an optimization problem draws on different disciplines of mathematics.
- A very limited number of optimization problems can be solved in “closed form”, i.e. a ready to use explicit formula. Typically, solving an optimization problem requires designing an *algorithm* and implementing it in *computer code*.
- Not all algorithms are equal: we strongly prefer algorithms with good performance characteristics.

Optimization problems

- Typically, *optimization problems* are formulated in terms of an *objective function* $f(x)$, $x \in \Omega \subset \mathbb{R}^n$ (depending on context, also known as a *loss function*, a *cost function*, etc.). The variables x are the *parameters* of the problem, and n is the *dimension* of the problem.
- The set $\Omega \subset \mathbb{R}^n$ defines constraints on the optimization problem, and its elements are called *feasible points*.
- More complex problems (such as multi-stage problems) may involve multiple objective functions.
- An optimization problem consists in finding a value x^* of the parameters such that $f(x) > f(x^*)$ for all values of x in a neighborhood of x^*. Such an x^* is called a *local minimizer* of $f(x)$.
- A *global minimizer* has the property that $f(x) > f(x^*)$ for *all* values of $x \in \Omega$.

Unconstrained optimization problems

- Finding global minimizers is typically much harder than finding local minimizer, as an objective function may have multiple local minima within Ω.
- In the case of a *convex* objective function, its local minimum is necessarily global, and there is no difference between the two problems. We will return to convex optimization later.
- A problem in which finding a maximum is required can be reduced to the case of a minimization problem by considering the objective function $\tilde{f}(x) = -f(x)$. In these lectures we will usually consider minimization problems.
- An optimization problem with $\Omega = \mathbb{R}^n$ are called *unconstrained*.

Necessary optimality conditions

- Let x^* be an unconstrained local minimizer of an objective function $f(x)$, $x \in \mathbb{R}^n$, and assume that $f(x)$ is continuously differentiable in a vicinity of x^*. Then:
  (i) Its gradient at x^* is zero,
  $$\nabla f(x^*) = 0. \tag{1}$$
  (ii) If, additionally, $f(x)$ is twice continuously differentiable near x^*, then the Hessian at x^* is positive semidefinite:
  $$\nabla^2 f(x^*) \geq 0. \tag{2}$$
- The proof is quite quick: Choose a direction $d \in \mathbb{R}^n$ and define a function $g(t) = f(x^* + td)$, $t \in \mathbb{R}$. Since x^* is a local minimizer,
$$\begin{aligned} 0 &\leq \lim_{t \to 0+} \frac{g(t) - g(0)}{t} \\ &= g'(0) \\ &= \nabla f(x^*)^{\mathrm{T}} d. \end{aligned}$$

Necessary optimality conditions

- Since d is arbitrary, this is possible only if $\nabla f(x^*) = 0$.
- If $f(x)$ is twice continuously differentiable, then from Taylor's theorem:

$$\begin{aligned} g(t) &= g(0) + g'(0)t + \frac{1}{2}\, g''(0)t^2 + o(t^2) \\ &= g(0) + \frac{1}{2}\, d^{\mathrm{T}} \nabla^2 f(x^*) d\, t^2 + o(t^2). \end{aligned}$$

- Therefore,

$$\begin{aligned} 0 &\leq \lim_{t \to 0} \frac{g(t) - g(0)}{t^2} \\ &= d^{\mathrm{T}} \nabla^2 f(x^*) d + \lim_{t \to 0} \frac{o(t^2)}{t^2} \\ &= d^{\mathrm{T}} \nabla^2 f(x^*) d, \end{aligned}$$

and we are done.

Sufficient optimality conditions

- Let the objective function $f(x)$, $x \in \mathbb{R}^n$, be twice continuously differentiable in an open set $O \subset \mathbb{R}^n$. Suppose that a point $x^* \in O$ satisfies the conditions
  (i)
  $$\nabla f(x^*) = 0. \tag{3}$$
  (ii) the Hessian at x^* is (strictly) positive definite:
  $$\nabla^2 f(x^*) > 0. \tag{4}$$
- Then x^* is a strict local minimizer of $f(x)$.

Example: quadratic objective function

- Let $A \in \mathrm{Mat}_n(\mathbb{R})$ be a positive definite matrix, $b \in \mathbb{R}^n$, and consider the objective function:
$$f(x) = \frac{1}{2}\, x^{\mathrm{T}} A x - x^{\mathrm{T}} b. \tag{5}$$
- The first order optimality condition reads
$$A x^* = b,$$
i.e.
$$x^* = A^{-1} b. \tag{6}$$
- The Hessian
$$\nabla^2 f(x) = A \tag{7}$$
is positive definite (and constant). Therefore, (6) is a strict minimizer of (5).

Easy objective function: quadratic function

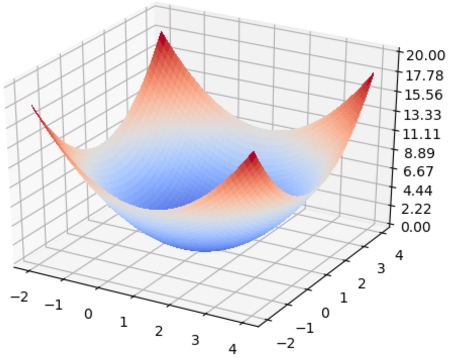
- An objective function that is easy to optimize is a quadratic function:

$$f(x, y) = (x - 1)^2 + (y - 1)^2. \tag{8}$$

- Inspection shows that it has a unique global minimum at $x = 1, y = 1$.
- This minimum is trivial to find analytically, and numerical algorithms usually have an easy time to find it.

Easy objective function: quadratic function

- The figure below shows a 3D graph of the quadratic function.



Hard objective function: Rosenbrock function

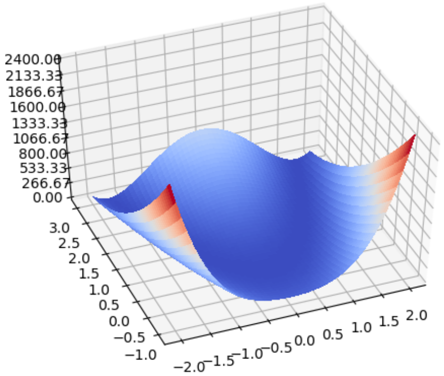
- A function, frequently used as a performance benchmark for testing optimization algorithms, is the *Rosenbrock function*:

$$f(x, y) = (x - 1)^2 + 100(y - x^2)^2. \tag{9}$$

- Inspection shows that it has a unique global minimum at $x = 1, y = 1$.
- This minimum, even though trivial to find analytically, lies inside a steep parabolic valley, and numerical algorithms struggle to find it.

Hard objective function: Rosenbrock function

- The figure below shows a 3D graph of the Rosenbrock function. Note the parabolic valley going through the point $(1, 1)$.



Sensitivity

- Suppose that we have a differentiable objective function that is parameterized by a set of parameters $\alpha \in \mathbb{R}^p$, i.e. the objective function is of the form $f(x, \alpha)$. Assume that for each α there is a local minimizer $x^*(\alpha)$, and that $x^*(\alpha)$ is a differentiable function of α.
- The first order optimality condition reads

$$\nabla_x f(x^*(\alpha), \alpha) = 0.$$

- Taking the gradient with respect to α and using the chain rule yields

$$\nabla_\alpha x^*(\alpha) \nabla_x^2 f(x^*(\alpha), \alpha) + \nabla_{x\alpha}^2 f(x^*(\alpha), \alpha) = 0,$$

where $\nabla_\alpha x(\alpha)$ is a $p \times n$ matrix of first derivatives $\partial x_i(\alpha)/\partial \alpha_k)$. Assuming invertibility of the Hessian, this yields

$$\nabla_\alpha x^*(\alpha) = -\nabla_{x\alpha}^2 f(x^*(\alpha), \alpha)\big(\nabla_x^2 f(x^*(\alpha), \alpha)\big)^{-1}. \tag{10}$$

Sensitivity

- This expresses the *sensitivity* of the minimizer to the parameter α.
- For example, if $f(x, \alpha) = f(x) - x^{\mathrm{T}}\alpha$, $\alpha \in \mathbb{R}^n$, then

$$\nabla_\alpha x^*(\alpha) = \left(\nabla_x^2 f(x^*(\alpha))\right)^{-1}. \tag{11}$$

- Sensitivity analysis will be a helpful tool in studying constraint optimization problems.

NLS problems

- In a *nonlinear least square (NLS) problem* the objective function is of the form:

$$f(x) = \frac{1}{2} \sum_{i=1}^{m} \phi_i(x)^2, \quad x \in \mathbb{R}^n, \tag{12}$$

  with given functions $\phi_i(x)$, and $m \geq n$. The factor $\frac{1}{2}$ is introduced for convenience.
- Introducing the column vector $\phi(x) = (\phi_1(x), \ldots \phi_m(x))^{\mathrm{T}}$, we can conveniently write this objective function as

$$f(x) = \frac{1}{2} \phi(x)^{\mathrm{T}} \phi(x). \tag{13}$$

- NLS problems arise in *data fitting*: We are given a set of data points (observations) $(T_1, S_1), \ldots, (T_p, S_p)$ and a *data model* depending on a number of parameters $x_1, \ldots x_k$:

$$S = g(x, T). \tag{14}$$

  The goal is to fit the data to the model.
- The model function $g(x, T)$ can be e.g. an explicitly defined function or a suitable spline function.

NLS problems

- Assume that
$$S_i = g(x, T_i) + \varepsilon_i, \tag{15}$$
where ε_i are residuals. One way to fit the model to the data is to minimize the sum of squares of the residuals, which leads to the following objective function:
$$f(x) = \frac{1}{2}\sum_{i=1}^{m}\left(g(x, T_i) - S_i\right)^2. \tag{16}$$
- In the simplest situation, x is two-dimensional, $x = (a, b) \in \mathbb{R}^2$, and the function $g(x, T)$ is linear:
$$\begin{aligned} S &= g(a, b, T) \\ &= a + bT. \end{aligned} \tag{17}$$
- This is the *linear* least square problem that can easily be solved in the closed form.

NLS problems

- The minimizer is given by the linear regression formulas:

$$\begin{aligned} b^* &= \frac{\sum_i (S_i - \overline{S})(T_i - \overline{T})}{\sum_i (T_i - \overline{T})^2}\,, \\ a^* &= \overline{S} - b^*\,\overline{T}, \end{aligned} \tag{18}$$

  where $\overline{T} = \frac{1}{p}\sum_{i=1}^{p} T_i$, and $\overline{S} = \frac{1}{p}\sum_{i=1}^{p} S_i$.

- Except for the linear case, NLS problems cannot be solved in closed form. NLS problems tend to be hard (think about it: the Rosenbrock function can be viewed as an NLS problem), and require refined numerical algorithms.

NLS problems

- In finance, NLS problems arise when we face the task of interpolating a cross section of market data. This amounts to the problem of *curve building* in a variety of contexts. Here are a few important examples.
- Given a snapshot of benchmark swap rates of given tenors, build a smooth interpolating curve that allows us to compute the swap rate of any tenor.
- Given a snapshot of the US Treasuries, fit a smooth curve that allows to carry out rich-cheap analysis.
- Given a snapshot of benchmark credit spreads, build a smooth interpolating curve that allows us to compute the spread of any maturity.
- Given a snapshot of option prices of the same expiration (and underlying) but varying strikes, build an interpolation curve that allows us to predict volatility smile for any strike.

NLS problems

- We will now develop an number of algorithms for solving NLS problems. Each of these algorithms is *recursive*, meaning that it starts with an initial guess for x^* and continues until an exit criterion is met.
- Before we move on, notice that the gradient of the objective function (12) (or (13)) is given by

$$\begin{aligned}\nabla f(x) &= \sum_{i=1}^{m} \phi_i(x)\nabla\phi_i(x)\\ &= J(x)^{\mathrm{T}}\phi(x),\end{aligned} \tag{19}$$

  where $J(x)_{ij} = \nabla_j\phi_i(x)$ is the $m \times n$ Jacobian matrix.
- Likewise, the Hessian of $f(x)$ is given by

$$\begin{aligned}\nabla^2 f(x) &= \sum_{i=1}^{m} \left(\nabla\phi_i(x)\nabla\phi_i(x)^{\mathrm{T}} + \phi_i(x)\nabla^2\phi_i(x)\right)\\ &= J(x)^{\mathrm{T}}J(x) + \sum_{i=1}^{m}\phi_i(x)\nabla^2\phi_i(x).\end{aligned} \tag{20}$$

NLS problems

- As discussed earlier, finding a local minimizer x^* of $f(x)$ requires solving the equation
$$\nabla f(x^*) = 0. \tag{21}$$
- If x is close to x^*, we can use Taylor's expansion to approximate
$$\begin{aligned} 0 &= \nabla f(x^*) \\ &\approx \nabla f(x) + \nabla^2 f(x)(x^* - x). \end{aligned}$$
- Assuming that the matrix $\nabla^2 f(x)$ is nonsingular for all x, this suggest the following *Newton method* update rule:
  - (i) Start with an initial guess x_0 for x^*.
  - (ii) For $k = 1, 2 \ldots,$
$$x_{k+1} = x_k - \nabla^2 f(x_k)^{-1} \nabla f(x_k). \tag{22}$$
- This observation is the starting point of several powerful algorithms for solving the NLS problem.

- In some ways, the scheme above is very attractive: it can be proved that if x_0 is sufficiently close to the local minimizer x^*, then the sequence x_k converges rapidly to x^*, namely quadratically in the error $\|x_{k+1} - x_k\|$.
- Notice, however, some of the practical challenges that it faces:
  (i) Finding an appropriate initial guess may be difficult.
  (ii) Expressions (19) and (20) for the gradient and Hessian of $f(x)$, respectively, require computing the first and second derivatives of the functions $\phi_i(x)$. Preferably, these derivatives should be calculated in closed form. Typically, even in the case of moderate dimensionality n of the problem, this is infeasible. It is especially true for the second derivatives.
  (iii) One may try to calculate the derivatives numerically, as finite differences. In the case of a moderate / large dimensionality of the problem, this is computationally prohibitively expensive, and the algorithm is inefficient.
  (iv) There is no guarantee that the Hessian in (22) is invertible. Even if it is, there is a cost associated with this operation at each iteration step.

Gradient descent method

- The *gradient descent method* is the simplest approximation to (22), in which assume that the Hessian is a multiple of the identity matrix.
- The scheme can thus be formulated as
  (i) Start with an initial guess x_0 for x^*.
  (ii) For $k = 1, 2 \ldots,$

$$x_{k+1} = x_k - \alpha \nabla f(x_k). \tag{23}$$

  Here the parameter $\alpha > 0$ is called the *step size* or *learning rate*.
- The value of α can be either determined by trial and error or by means of a *line search* algorithm. In the latter approach, in each step, we numerically search for a value α_k satisfying

$$\alpha_k = \arg\min_{\alpha} f(x_k - \alpha \nabla f(x_k)). \tag{24}$$

- Gradient descent methods are easy to implement, but their performance tends to be mixed. Convergence (if any) is linear and slow, and it requires many iterations.
- Among the descent methods, the gradient descent method is locally the best, as it moves the next iteration in the direction of the steepest descent of $f(x)$.

Gauss-Newton method

- The *Gauss-Newton method* is based on the assumption that the function $\phi_i(x)$ can be locally well approximated by linear functions:

$$\phi(x+h) \approx \phi(x) + J(x)h. \tag{25}$$

- This implies that

$$\begin{aligned} f(x+h) &\approx f(x) + \nabla f(x)h + \frac{1}{2}\, h^{\mathrm{T}} \nabla^2 f(x) h \\ &= f(x) + h^{\mathrm{T}} J(x)^{\mathrm{T}} \phi(x) + \frac{1}{2}\, h^{\mathrm{T}} J(x)^{\mathrm{T}} J(x) h, \end{aligned} \tag{26}$$

  where we have used expressions (19) and (20) for the gradient and Hessian of $f(x)$, respectively.
- Notice the absence of the second derivatives in (20) from the term quadratic in h. This is a consequence of the linear approximation assumption. This is a boon to the computational efficiency of algorithm.

Gauss-Newton method

- Effectively, we thus approximate the Hessian of $f(x)$ as follows:

$$\nabla^2 f(x) \approx J(x)^{\mathrm{T}} J(x). \tag{27}$$

  This approximation guarantees that Hessian is always positive semidefinite. Also, it turns out that dropping the second derivatives does not, in practice, affect the convergence of the process.

- We now choose the optimal h by minimizing the quadratic function in h on the right hand side of (26). This yields the condition

$$J(x)^{\mathrm{T}} J(x) h = -J(x)^{\mathrm{T}} \phi(x). \tag{28}$$

- The function $f(x)$ descents along the direction of h as

$$\begin{aligned} h^{\mathrm{T}} \nabla f(x) &= J(x)^{\mathrm{T}} h \\ &= -h^{\mathrm{T}} J(x)^{\mathrm{T}} J(x) h \\ &\leq 0. \end{aligned}$$

Gauss-Newton method

- The Gauss-Newton scheme can be thus formulate as follows. We start at x_0 and iterate:
$$x_{k+1} = x_k - \big(J(x_k)^{\mathrm{T}} J(x_k)\big)^{-1} J(x_k)^{\mathrm{T}} \phi(x_k). \tag{29}$$
The key step of the method is solving equation (31), which amounts to inverting the matrix $J(x_k)^{\mathrm{T}} J(x_k)$. In case if $J(x)$ is poorly conditioned, this inverse may not exist.
- It may be beneficial to refine the method by introducing the learning rate α,
$$x_{k+1} = x_k - \alpha\big(J(x_k)^{\mathrm{T}} J(x_k)\big)^{-1} J(x_k)^{\mathrm{T}} \phi(x_k), \tag{30}$$
which can be either set *a priori* or determined at each step by conducting a line search. Under suitable technical assumptions, this method is guaranteed to converge.
- Unlike the Newton method, the Gauss-Newton method typically converges linearly in *h*.

Levenberg-Marquardt method

- The *Levenberg-Marquardt method* is a clever hybrid of the gradient descent and Gauss-Newton methods.
- Namely, we introduce a *damping parameter* $\mu > 0$, and determine the step size by solving the equation

$$\big(J(x)^{\mathrm{T}}J(x) + \mu I\big)h = -J(x)^{\mathrm{T}}\phi(x). \tag{31}$$

- Notice that the presence of μ has the following effects on the problem:
  (i) The matrix $J(x)^{\mathrm{T}}J(x) + \mu I$ is strictly positive definite, and the existence of its inverse is guaranteed.
  (ii) For small values of μ, the iteration step is similar to the iteration step in the Gauss-Newton method.
  (iii) For large values of μ, the iteration step is similar to the iteration step in the gradient descent method.
- The value of μ will be updated throughout the iteration process, and it renders line search unnecessary.

Levenberg-Marquardt method

- In order to initialize μ, one usually chooses it be of the order of magnitude of maximum diagonal term of the matrix $J(x_0)^{\mathrm{T}} J(x_0)$,

$$\mu_0 = \beta \max_i \left(J(x_0)^{\mathrm{T}} J(x_0) \right)_{ii}, \tag{32}$$

  where $\beta \approx 10^{-3}$ is determined empirically.

- The update process is determined bu the *gain ratio*, defined as the ratio of the projected change in $f(x)$ to the change in $f(x)$ projected by the quadratic approximation (26):

$$\rho = -\frac{f(x_k) - f(x_k + h)}{h^{\mathrm{T}} J(x_k)^{\mathrm{T}} \phi(x_k) + \frac{1}{2}\, h^{\mathrm{T}} J(x_k)^{\mathrm{T}} J(x_k) h}, \tag{33}$$

  which can also be expressed as

$$\rho = 2\, \frac{f(x_k) - f(x_k + h)}{h^{\mathrm{T}} \left(\mu h - J(x_k)^{\mathrm{T}} \phi(x_k) \right)}. \tag{34}$$

Levenberg-Marquardt method

- Note that the denominator in (34) is always positive (why?)
- Large value of ρ indicates that the quadratic approximation to $f(x)$ is accurate. We should decrease the value of μ in order to make the process more Gauss-Newton like, and accelerate the convergence.
- On the other hand, a small value of ρ (also negative) indicates that the approximation is poor and we are on the wrong path. In this case, the value of μ should be increased to make the process more gradient descent like, and also decrease the step size.
- The updates of μ are done in terms of a scaling factor λ (frequently chosen as $\lambda = 2$): if the gain ratio is positive, the value of μ is reduced by a factor depending on ρ, otherwise it is scaled up according to $\mu \to \lambda\mu$.

Levenberg-Marquardt method

- An important element of a search algorithm is a set of *exit criteria*, which stop the algorithm once it has converged or it failed to converge.
  1. (i) Ideally, the search should stop if $\nabla f(x^*) = J(x^*)^{\mathrm{T}}\phi(x^*) = 0$. We can implement it numerically by choosing a small $\varepsilon_1 > 0$, and require that all components of the vector $\nabla f(x_k)$ have absolute values less than ε_1. This is equivalent to stating that

$$\|J(x_k)^{\mathrm{T}}\phi(x_k)\|_\infty \leq \varepsilon_1. \qquad (35)$$

     Here, the L^∞*-norm* $\|X\|_\infty$ of a vector X is defined as $\max_i |X_i|$.
  2. (ii) Another criterion guarantees exit, if the changes in x_k are slow. We choose another small number ε_2 and verify if

$$\|x_{k+1} - x_k\| \leq \varepsilon_2(\|x_k\| + \varepsilon_2). \qquad (36)$$

  3. (iii) Lastly, in order to avoid running an infinite loop, one has to choose the maximum number of iterations k_{max}

Levenberg-Marquardt method

- Let us now summarize the Levenberg-Marquardt method in an algorithmic form:

```
choose $x_0$, initialize $\mu$ according to (32), and $\lambda = 2$
$done = (\|J(x_0)^{\mathrm{T}}\phi(x_0)\|_\infty \leq \varepsilon_1)$
while ($not\ done$ and $k \leq k_{max}$)
    $h = -(J(x_k)^{\mathrm{T}}J(x_k) + \mu I)^{-1}J(x_k)\phi(x_k)$
    if $\|h\| \leq \varepsilon_2(\|x_k\| + \varepsilon_2)$
        $done = true$
    else
        calculate $\rho$ according to (33)
        if $\rho > 0$
            $x_{k+1} = x_k + h$
            $done = (\|J(x_{k+1})^{\mathrm{T}}\phi(x_{k+1})\|_\infty \leq \varepsilon_1)$
            update $\mu \to \mu \max(1/3, 1 - (2\rho - 1)^3)$, and $\lambda = 2$
        else
            update $\mu \to \lambda\mu$, and $\lambda \to 2\lambda$
```

Levenberg-Marquardt method

- The Levenberg-Marquard method is implemented in `scipy`.

Data fitting without NLS

- Data fitting problems in finance often lead to optimization problems which are not of the NLS type.
- For example, in models requiring maximum likelihood estimation (MLE) from historical data, the objective function is typically not a sum squares of the residuals between the data and the model. Instead, it is the probability of the observed data given given the (unknown) parameters of the probability distribution.
- For example, many problems lead to the task of minimizing the Kullback-Leibler divergence between the observed frequencies p and a probability model $q(x)$,

$$KL(p\|q(x)) = \sum_{i=1}^{m} p_i \log \frac{p_i}{q_i(x)} \,. \tag{37}$$

  This objective function clearly is not of the NLS form.
- Quasi-Newton methods have been designed to problems like this. The most popular among them is the *BGFS method* (for Broyden, Fletcher, Goldfarb, and Shanno)and its variations.

BFGS method

- Our goal is to find a local minimizer of an objective function $f(x)$, not necessary expressed as a sum of squares. We initialize the search with x_0 and iterate.
- At the $(k+1)$-th step of iteration we approximate the value of $f(x_{k+1})$ by an expression quadratic in the direction of the step from x_k. Namely, for x in the vicinity of x_k, we can write

$$f(x) \approx f(x_k) + \nabla f(x_k)^{\mathrm{T}} h + \frac{1}{2}\, h^{\mathrm{T}} B_k h, \tag{38}$$

  where B_k is a positive definite matrix.
- Naively, B_k should be the Hessian at x_k, but, as we know, this leads to serious performance issues, and the challenge is to choose B_k smartly.
- The minimizer of (38) is

$$h = -B_k^{-1} \nabla f(x_k), \tag{39}$$

  and x_{k+1} is given by

$$x_{k+1} = x_k + \alpha_k h. \tag{40}$$

BFGS method

- The value of the multiplier α_k is determined from the line search:

$$\alpha_k = \arg\min_{\alpha} f(x_k - \alpha \nabla f(x_k)). \tag{41}$$

- In the BFGS method, the matrix B_k is constructed iteratively as follows. Given B_k, we require that the updated value B_{k+1} satisfies the *secant equation*

$$B_{k+1}(x_{k+1} - x_k) = \nabla f(x_{k+1}) - \nabla f(x_k) \tag{42}$$

  (remember B_k is supposed to mimic the Hessian!).
- This can be written as

$$B_{k+1} s_k = y_k, \tag{43}$$

  where $s_k = x_{k+1} - x_k$ and $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$.

BFGS method

- Premultiplying (43) by s_k^{T}, we see that the following *curvature condition* has to be satisfied:
$$s_k^{\mathrm{T}} y_k > 0. \tag{44}$$
If the curvature condition is satisfied, the secant equation (43) has a unique solution.
- For non-convex functions, the curvature condition is not always satisfied. In such a case, it has to be enforced by means of choosing an appropriate step size α_k.
- We will now assume that the updated B_{k+1} equals to B_k plus two positive definite rank 1 matrices:
$$B_{k+1} = B_k + auu^{\mathrm{T}} + bvv^{\mathrm{T}}, \tag{45}$$
where $a, b \in \mathbb{R}$, and $u, v \in \mathbb{R}^n$.
- How do we choose the parameters above?

BFGS method

- This in itself is an optimization in which we minimize the Frobenius norm between the symmetric matrices B_{k+1} and B_k under the constraint that the secant equation holds. The solution turns out to be

$$
\begin{aligned}
u &= y_k,\\
v &= B_k s_k\\
a &= \frac{1}{s_k^{\mathrm{T}} y_k},\\
b &= -\frac{1}{s_k^{\mathrm{T}} B_k s_k},
\end{aligned}
$$

which leads to the following update equation for B_{k+1}:

$$
B_{k+1} = B_k - \frac{B_k s_k s_k^{\mathrm{T}} B_k}{s_k^{\mathrm{T}} B_k s_k} + \frac{y_k y_k^{\mathrm{T}}}{s_k^{\mathrm{T}} y_k}. \tag{46}
$$

BFGS method

- We are now almost ready, except for the choice of the initial matrix B_0. Unfortunately, there is no standard recipe for the choice of B_0.
- One possible choice is the Hessian of $f(x)$ calculated at the initial guess x_0 (either in closed form, or using finite differences.)
- Another choice is a multiple of the identity matrix, $B_0 = aI$, where a is user determined.
- For the exit criterion we use $\|\nabla f(x_k)\|_\infty < \varepsilon$, where ε is user determined.

BFGS method

- Let us now summarize the BFGS method in an algorithmic form:

```
initialize $x_0$ and $B_0$
while $(\|\nabla f(x_k)\|_\infty > \varepsilon)$ and $k \leq k_{max}$
    compute the search direction (39)
    carry out the line search (41)
    set $s_k = \alpha_k h$, update $x_{k+1} = x_k + s_k$, and calculate $y_k$
    update $B_k$ to $B_{k+1}$ according to equation (46)
```

BFGS method

- The algorithm above requires inverting the matrix B_k at each step of the iteration.
- There is a version of the BFGS method, which operates in terms of the inverses $H_k = B_k^{-1}$ only.
- Namely, one can verify (with some pain) that the update equation (46) can be formulated in terms of the inverses as follows:

$$H_{k+1} = \Big(I - \frac{s_k y_k^{\mathrm{T}}}{s_k^{\mathrm{T}} y_k}\Big) H_k \Big(I - \frac{y_k s_k^{\mathrm{T}}}{s_k^{\mathrm{T}} y_k}\Big) + \frac{s_k s_k^{\mathrm{T}}}{s_k^{\mathrm{T}} y_k}\,. \tag{47}$$

- The BFGS method is implemented in the Python package `scipy`.

Global optimization

- In many applications, the objective function has multiple local minima, or at least the existence of a unique global minimum cannot be guaranteed.
- Furthermore, objective functions can be non-differentiable, noisy, exhibit flat directions, etc.
- In situations like this, analytic methods or Newton-like methods are not applicable.
- A number of approaches for solving such optimization problems have been proposed. We will focus on a particularly neat stochastic search method, namely *differential evolution*.

Hard objective function: Ackley function

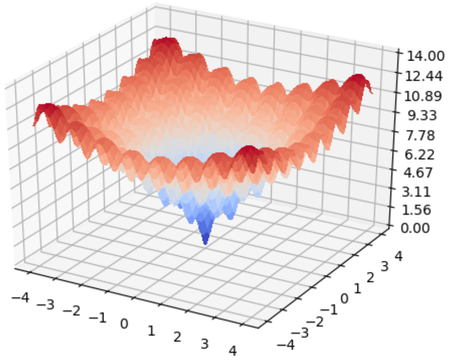
- Another function, frequently used as a performance benchmark for testing optimization algorithms, is the *Ackley function*:

$$\begin{aligned} f(x, y) = 20 + e - 20 \exp\Big(- 0.2\sqrt{0.5(x^2 + y^2)}\Big) \\ - \exp\Big(0.5\big(\cos(2\pi x) + \cos(2\pi y)\big)\Big). \end{aligned} \tag{48}$$

- Inspection shows that it has a unique global minimum at $x = 0, y = 0$.
- This minimum, even though trivial to find analytically, is hidden among plenty of local minima and maxima, which makes Newton-type methods impractical.

Hard objective function: Ackley function

- The figure below shows a 3D graph of the Ackley function. Note the multitude of local minima and maxima.



Differential evolution

- As before, let $f(x)$, $x \in \mathbb{R}^n$ be an objective function. We do not require $f(x)$ to be differentiable.
- Each of the components of x is restricted to a finite interval:

$$L_i \leq x_i \leq U_i. \tag{49}$$

  The limits are chosen by the user. Tighter limits lead to a better performance of the algorithm.
- We select the population size $N \geq 4$, and randomly generate the initial population: $x_{1,0}, \ldots, x_{N,0}$.
- We will evolve this population through a number of generations G according to the rules motivated by genetics.

Differential evolution

- *Mutation*. We choose a constant *mutation factor* $F \in [0, 2]$, determined by the user.
- For a given vector $x_{i,G}$ (we start with $G = 0$), we randomly select three vectors $x_{r_1,G}$, $x_{r_2,G}$, $x_{r_3,G}$, such that the four indices i, r_1, r_2, r_3 are all distinct.
- We form the *donor (mutant) vectors*:

$$v_{i,G+1} = x_{r_1,G} + F(x_{r_2,G} - x_{r_3,G}), \tag{50}$$

  for each element of the population $i = 1, \dots, N$.

Differential evolution

- *Crossover*. We choose a user determined *crossover constant* $CR \in [0, 1]$.
- For each $i = 1, \ldots, N$ we form a *trial vector* $u_{i,G+1}$ constructed as follows.
  (i) Generate random numbers $u_j \sim U(0, 1), j = 1 \ldots, n$.
  (ii) Generate a random integer r from the range $1, \ldots, n$.
  (iii) For $j = 1 \ldots, n$, set

$$u_{j,i,G+1} = \begin{cases} v_{j,i,G+1}, & \text{if } u_j \leq CR \text{ or } j = r, \\ x_{j,i,G}, & \text{if } u_j > CR \text{ and } j \neq r. \end{cases} \tag{51}$$

Differential evolution

- *Selection*. The target vector $x_{i,G}$ is now compared with the trial vector $u_{i,G+1}$, and the one with the lower value of the objective function is passed on to the next generation.
- Namely, for $i = 1, \ldots, N$,

$$x_{i,G+1} = \begin{cases} u_{i,G+1}, & \text{if } f(u_{i,G+1}) < f(x_{i,G}) \\ x_{i,G} & \text{otherwise.} \end{cases} \tag{52}$$

Differential evolution

- Choosing the right parameters for the differential evolution requires trial and error. Usually, $F = 0.5$, and $CR = 0.1$ work well. Population size N should be a function of the dimensionality of the problem. A useful rule of thumb is $N = 5n$.
- Implementation of differential evolution requires exit criteria imposed by the user. One of them is the maximum number of generations G_{max}.
- Another criterion is the average rate of improvement of $\min_i f(x_{i,G})$ from generation to generation. Once this rate falls below a user chosen level ε, the algorithm should stop.

References

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