Numerical Algorithms (MU4IN910)

Lecture 4: Introduction to optimization (2/2)

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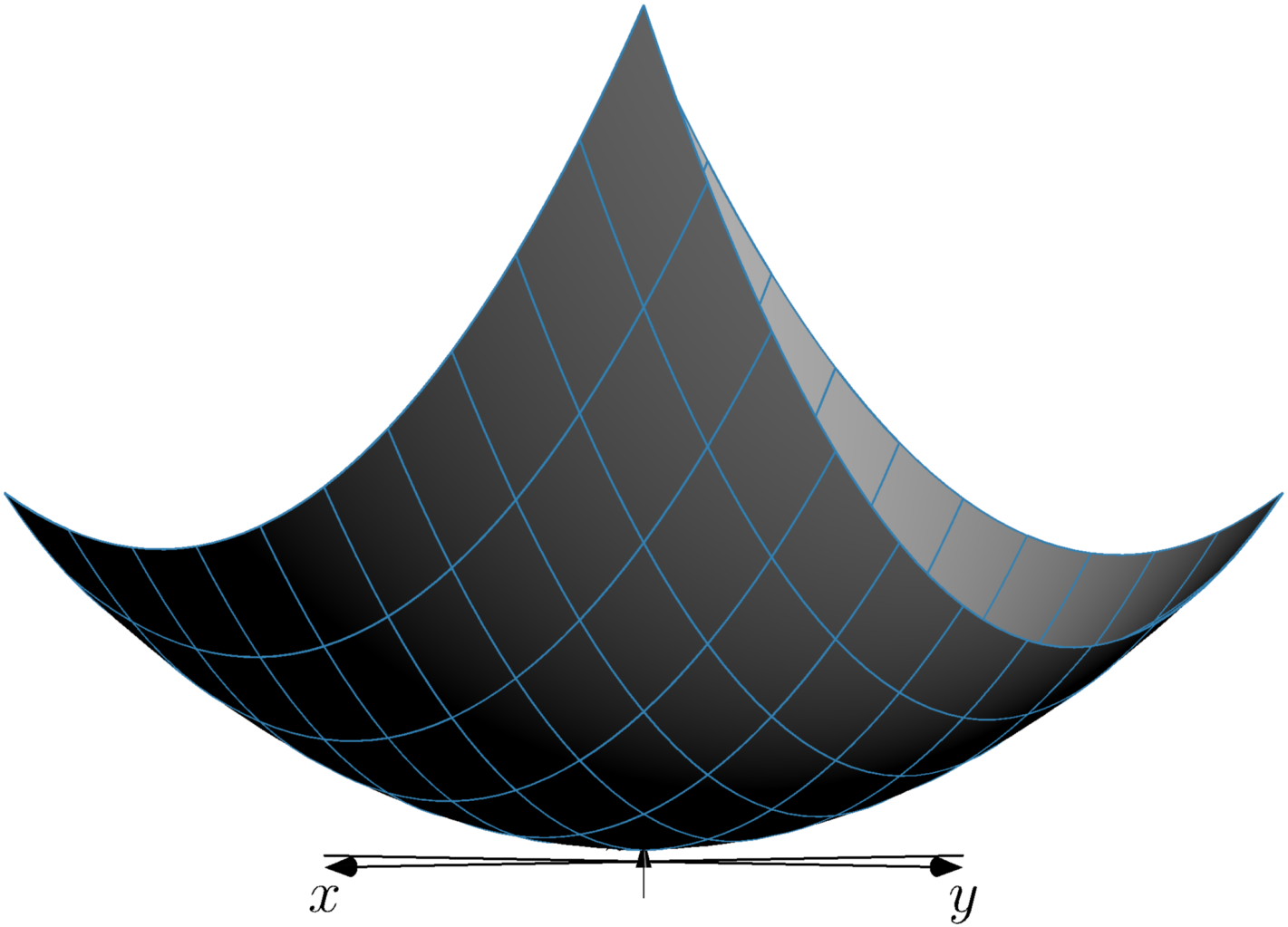
Back to tutorial: $f(x, y) = 3x^2 + 2y^2 + 2xy + x + y + 10$



Summary of the previous lecture

- Generalities on the problems of optimization
  - Notion of critical point
  - Necessary and sufficient condition of optimality
  - Lagrange multipliers
- Optimization in dimension 1
  - Golden section search
  - Method of quadratic interpolation
  - Newton's method

Outline

- Direct search method
- Steepest descent method
- Newton's method
- Quasi-Newton's method
- Conjugate gradient method (nonlinear)

References

- **Scientific Computing, An Introductory Survey, Michael .T. Heath, Revised Second Edition, SIAM, 2018** (the lecture is mainly based on this book and on the associated slides)
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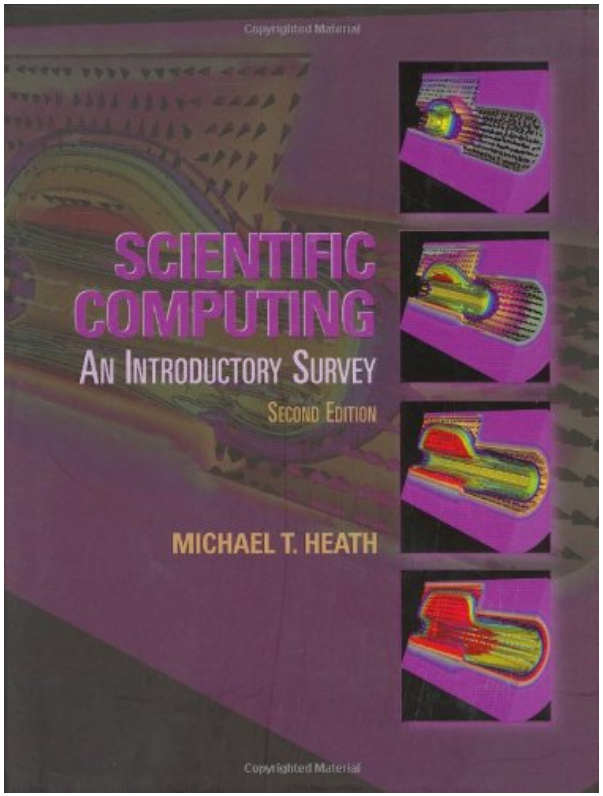
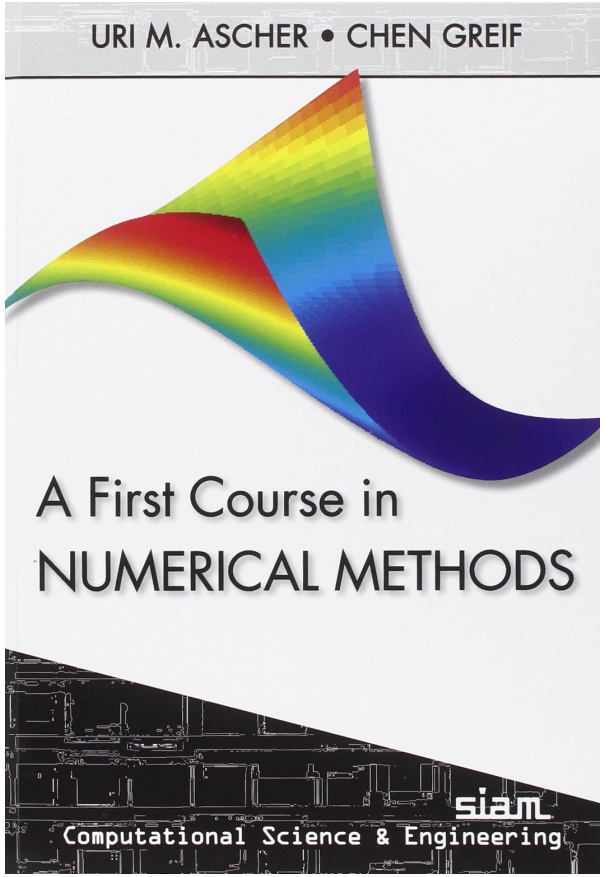
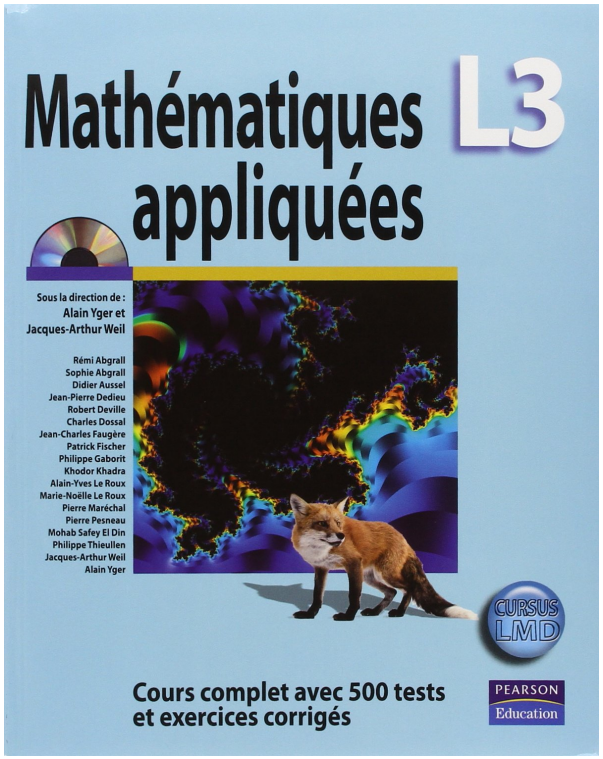




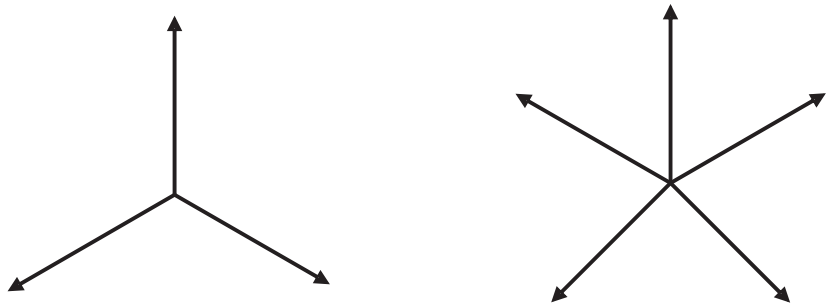


Optimization in dimension $n \geq 2$

Pattern search method

Idea:

- Suppose we are given an initial guess x at the solution and a set of at least n$n+1$ directions v_i, $i = 1, \ldots, n+1$ that form a positive basis for $\mathbb{R}^n$: this means that any vector can be expressed as a linear combination of these vectors, where the coefficients in the combination are positive numbers.

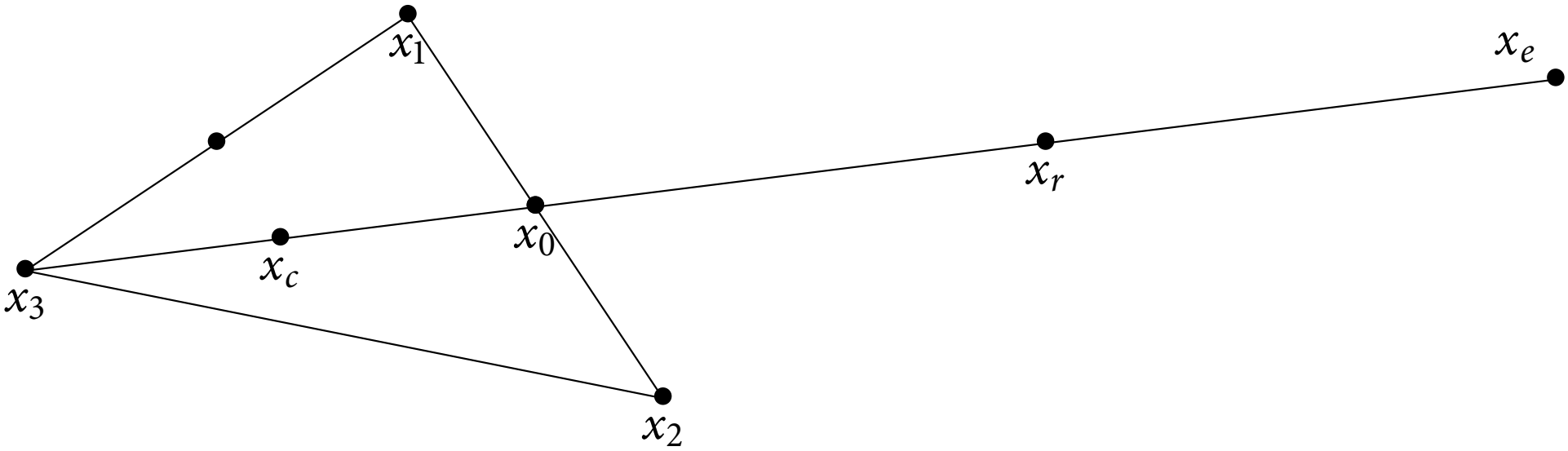


- At each step, we do a line search in each of the directions to obtain $f(x + \alpha_i v_i)$ and replace x by the point with the smallest function value.
- This is a remarkably simple algorithm, but works well in practice and is provably convergent!
- Another desirable property is that it is easy to parallelize, and this is crucial to making a no-derivative algorithm effective when n is large.

Nelder-Meade algorithm

1. Choice of $N+1$ points of the N-dimensional space of the unknowns, forming a simplex: $\{x_1, x_2, \ldots, x_{N+1}\}$,
2. Compute the values of the function f at these points, sort the points so as to have $f(x_1) \leq f(x_2) \leq \cdots \leq f(x_{N+1})$. In fact, it is enough to know the first and the last two.
3. Compute x_0, center of gravity of all points except x_{N+1}.
4. Compute $x_r = x_0 + (x_0 - x_{N+1})$ (reflection of x_{N+1} from x_0).
5. If $f(x_r) < f(x_N)$, compute $x_e = x_0 + 2(x_0 - x_{N+1})$ (simplex expansion). If $f(x_e) < f(x_r)$, replace x_{N+1} by x_e, otherwise, replace x_{N+1} by x_r. Return to step 2.
6. If $f(x_N) < f(x_r)$, compute $x_c = x_{N+1} + 1/2(x_0 - x_{N+1})$ (simplex contraction). If $f(x_c) \leq f(x_N)$, replace x_{N+1} by x_c and return to step 2, otherwise go to step 7.
7. Shrink toward x_1: replace x_i by $x_1 + 1/2(x_i - x_1)$ for $i \geq 2$. Return to step 2.

Nelder-Meade algorithm



Steepest Descent Method

- Let $f : \mathbb{R}^n \to \mathbb{R}$ be real-valued function of n real variables
- At any point x where gradient vector is nonzero, negative gradient, $-\nabla f(x)$, points downhill toward lower values of f
- In fact, $-\nabla f(x)$ is locally direction of steepest descent: f decreases more rapidly along direction of negative gradient than along any other
- Steepest descent method: starting from initial guess x_0, successive approximate solutions given by

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

where α_k is a line search parameter that determines how far to go in given direction $-\nabla f(x_k)$

Steepest Descent Method (cont'd)

- Given descent direction, such as negative gradient, determining appropriate value for α_k at each iteration is one-dimensional minimization problem

$$\min_{\alpha_k \geq 0} f(x_k - \alpha_k \nabla f(x_k))$$

  that can be solved by methods already discussed in dimension 1

- Steepest descent method is very reliable: it can always make progress provided gradient is nonzero

- But method is myopic in its view of function's behavior, and resulting iterates can zigzag back and forth, making very slow progress toward solution

- In general, convergence rate of steepest descent is only linear, with constant factor that can be arbitrarily close to 1

Steepest Descent Method: example

- Use steepest descent method to minimize

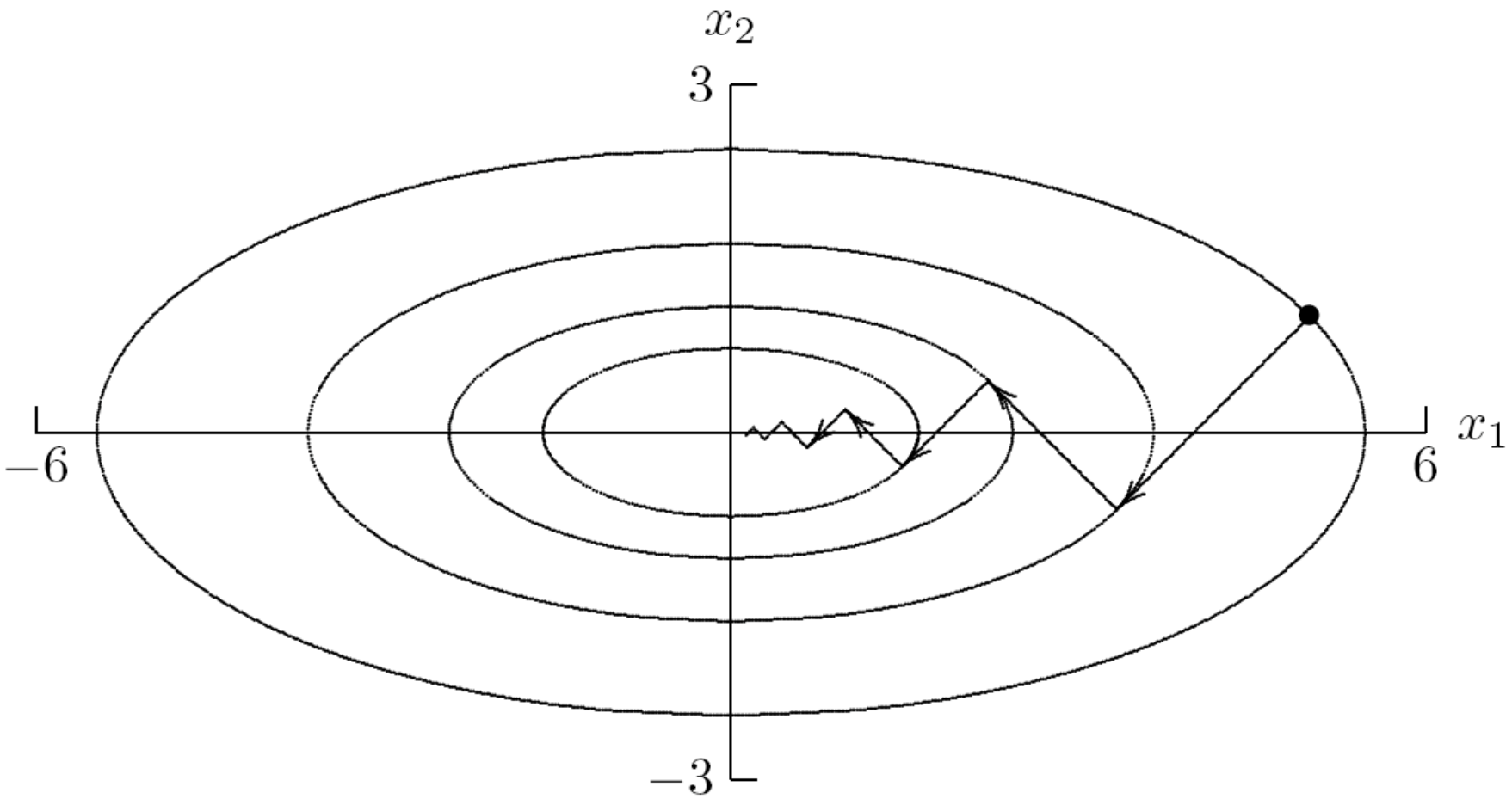
$$f(x) = 0.5x_1^2 + 2.5x_2^2$$

- Gradient is given by $\nabla f(x) = \begin{pmatrix} x_1 \\ 5x_2 \end{pmatrix}$
- Taking $x_0 = \begin{pmatrix} 5 \\ 1 \end{pmatrix}$, we have $\nabla f(x_0) = \begin{pmatrix} 5 \\ 5 \end{pmatrix}$
- Perform line search along negative gradient direction

$$\min_{\alpha_0} f(x_0 - \alpha_0 \nabla f(x_0))$$

Exact minimum along line is given by $\alpha_0 = 1/3$ so next approximation is $x_1 = \begin{pmatrix} 3.333 \\ -0.667 \end{pmatrix}$

Steepest Descent Method: example (cont'd)



Finite difference method

Principle:

- We want to approximate the gradient by finite difference

$$(\nabla f(x))_i \approx \frac{f(x + te_i) - f(x)}{t}$$

  for small t and e_i the ith standard unit vector

- Small accuracy on the gradient

- It is better to use automatic differentiation methods: it is a set of techniques to evaluate the derivative of a function specified by a computer program.

Newton's method

- We know that a minimum x^* satisfies $\nabla f(x^*) = 0$. We can then solve the equation $\nabla f(x) = 0$ with Newton's method.

- We can also approximate f by

$$f(x+h) \approx f(x) + \nabla f(x)h + \frac{1}{2}h^T H_f(x)h$$

  and minimize the quadratic approximation with respect to h

- In the two cases, we obtain the following iteration

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

Newton's method (cont'd)

- We do not explicitly invert Hessian matrix, but instead we solve the linear system

$$H_f(x_k)s_k = -\nabla f(x_k)$$

and we compute

$$x_{k+1} = x_k + s_k$$

- Convergence rate of Newton's method for minimization is normally quadratic

- As usual, Newton's method is unreliable unless started close enough to solution to converge

Newton's method: example

- Use Newton's method to minimize

$$f(x) = 0.5x_1^2 + 2.5x_2^2$$

- Gradient and Hessian are given by

$$\nabla f(x) = \begin{pmatrix} x_1 \\ 5x_2 \end{pmatrix} \quad \text{and} \quad H_f(x) = \begin{pmatrix} 1 & 0 \\ 0 & 5 \end{pmatrix}$$

- Taking $x_0 = \begin{pmatrix} 5 \\ 1 \end{pmatrix}$, we have $\nabla f(x_0) = \begin{pmatrix} 5 \\ 5 \end{pmatrix}$
- The linear system for Newton step is

$$\begin{pmatrix} 1 & 0 \\ 0 & 5 \end{pmatrix} s_0 = \begin{pmatrix} -5 \\ -5 \end{pmatrix}$$

and so $x_1 = x_0 + s_0 = \begin{pmatrix} 5 \\ 1 \end{pmatrix} + \begin{pmatrix} -5 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ which is exact solution for this problem (as expected for quadratic function)

Newton's method (cont'd)

- In principle, line search parameter is unnecessary with Newton's method, since quadratic model determines length, as well as direction, of step to next approximate solution
- When started far from solution, however, it may still be advisable to perform line search along direction of Newton step s_k to make method more robust
- Once iterates are near solution, then $\alpha_k = 1$ should suffice for subsequent iterations

Newton's method (cont'd)

- If objective function f has continuous second partial derivatives, then Hessian matrix H_f is symmetric, and near minimum it is positive definite
- Thus, linear system for step to next iterate can be solved in only about half of work required for LU factorization using Cholesky factorization
- Far from minimum, $H_f(x_k)$ may not be positive definite, so Newton step sk may not be descent direction for function, i.e., we may not have

$$\nabla f(x_k)^T s_k < 0$$

- In this case, alternative descent direction can be computed, such as negative gradient or direction of negative curvature, and then perform line search

Trust regions: an alternative to linesearch

- We approach f by

$$f(x+h) \approx q(h) := f(x) + \nabla f(x)h + \frac{1}{2}h^T H_f(x)h$$

- We try to minimize $q(h)$ but we restrict the search to $\|h\| < r$ with r small enough
- We choose $x_{\text{new}} = x + h^*$ with h^* solution of

$$\min_{\|h\| leq r} q(h)$$

- This allows us to search for a solution only in a domain where the quadratic approximation is sufficiently accurate

Quasi-Newton Methods

- Newton's method is very fast (if it converges) but it requires the gradient and the Hessian matrix to be evaluated at each iteration. So each iteration is quite expensive!

- Can we solve

$$\min_x f(x)$$

when $\nabla f(x)$ can be computed but not $H_f(x)$?

Two main options::

- Estimate $H_f(x)$ using finite differences: discrete Newton method
- Approximate $H_f(x)$ using Quasi-Newton methods

Quasi-Newton Methods (cont'd)

- The Newton step: $x_{k+1} = x_k + s_k$ with $s_k = H_f(x_k)^{-1}\nabla f(x_k)$
- Quasi-Newton step: accumulate an approximation $B_k \approx H_f(x_k)$ using free information!
- At step k, we know $\nabla f(x_k)$ and we compute $\nabla f(x_{k+1})$ where $x_{k+1} = x_k + s_k$
- $H_f(x_k)$ satisfies

$$H_f(x_k)s_k = \lim_{t\to 0} \frac{\nabla f(x_k + ts_k) - \nabla f(x_k)}{t}$$

Let us denote $g_k = \nabla f(x_k)$. If f is quadratic then

$$H_f(x_k)s_k = g_{k+1} - g_k$$

- We will ask the same property of the approximation B_{k+1} and call this the secant equation:

$$B_{k+1}s_k = g_{k+1} - g_k$$

Quasi-Newton Methods (cont'd)

- So we know how we want B_{k+1} to behave in the direction $g_{k+1} - g_k$, and we have no new information in any other direction, so we could require

$$B_{k+1}v = B_k v \qquad \text{if} \qquad v^T s_k = 0$$

- There is a unique matrix B_{k+1} that satisfies the secant equation and the no-change conditions. It is called Broyden's method:

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

where $s_k = x_{k+1} - x_k$ and $y_k = g_{k+1} - g_k$

- B_{k+1} is formed from B_k by adding a rank-one matrix

BFGS (Broyden-Fletcher-Goldfarb-Shanno) method

- B_{k+1} is not necessarily symmetric, even if B_k is
- In order to regain symmetry, we need to sacrifice the no-change conditions. Instead, we formulate the problem in a least change sense:

$$\min_{B_{k+1}} \|B_{k+1} - B_k\|$$

  satisfying B_{k+1} symmetric and the secant condition $B_{k+1}s_k = y_k$
- The solution depends on the choice of norm
- For a certain norm, we obtain the BFGS formula

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

BFGS method (cont'd)

$x_0 =$ `initial guess`
$B_0 =$ `initial Hessian approximation`
`for` $k = 0, 1, 2, \ldots$
    `Solve` $B_k s_k = -\nabla f(x_k)$
    $x_{k+1} = x_k + s_k$
    $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$
    $B_{k+1} = B_k - (B_k s_k s_k^T B_k)/(s_k^T B_k s_k) + (y_k y_k^T)/(y_k^T s_k)$
`end`

BFGS method (cont'd)

- In practice, factorization of B_k is updated rather than B_k itself, so linear system for s_k can be solved at cost of $\mathcal{O}(n^2)$ rather than $\mathcal{O}(n^3)$ work
- Unlike Newton's method for minimization, no second derivatives are required
- Can start with $B_0 = I$, so initial step is along negative gradient, and then second derivative information is gradually built up in approximate Hessian matrix over successive iterations
- BFGS normally has superlinear convergence rate, even though approximate Hessian does not necessarily converge to true Hessian

Nonlinear conjugate gradient method

- This is a method which does not require the calculation of the of the Hessian and does not require either the storage of a matrix approximating the Hessian
- The algorithm generates a sequence of conjugate directions accumulating implicitly information on the Hessian
- For some quadratic functions, the algorithm of the conjugate gradient algorithm converges after at most n iterations, where n is the dimension of the problem

Nonlinear conjugate gradient method (cont'd)

$x_0 =$ `initial approximation`
$g_0 = \nabla f(x_0)$
$s_0 = -g_0$
`for` $k = 0, 1, 2, \ldots$
    `choose` α_k `minimizing` $f(x_k + \alpha_k s_k)$
    $x_{k+1} = x_k + \alpha_k s_k$
    $g_{k+1} = \nabla f(x_{k+1})$
    $\beta_{k+1} = (g_{k+1}^T g_{k+1})/(g_k^T g_k)$
    $s_{k+1} = -g_{k+1} + \beta_{k+1} s_k$
`end`

$\rightarrow$ the algorithm will be studied in detail in the course on iterative methods for solving linear systems

Truncated Newton's method

- One can reduce the amount of computation of a Newton type method by solving the linear system by an iterative method
- A small number of iterations then allows to obtain in general a solution
- The iterative method used to solve the system is often the conjugate gradient method
- These algorithms only require matrix-vector products. It is then possible to avoid the construction of the Hessian by using a finite difference method on the gradient

Nonlinear least squares

- Given data (t_i, y_i), find vector x of parameters that gives "best fit" in least squares sense to model function $f(t, x)$, where f is nonlinear function of x

- We define components of residual function

$$r_i(x) = y_i - f(t_i, x) \text{ for } i = 1, \ldots, m$$

so we want to minimize $\phi(x) = \frac{1}{2} r(x)^T r(x)$

- Gradient vector is $\nabla \phi(x) = J(x)^T r(x)$ and Hessian matrix is

$$H_\phi(x) = J(x)^T J(x) + \sum_{i=1}^{m} r_i(x) H_i(x)$$

where $J(x)$ is Jacobian of $r(x)$ and $H_i(x)$ is Hessian of $r_i(x)$

Gauss-Newton method

- Linear system for Newton step is

$$(J(x_k)^T J(x_k) + \sum_{i=1}^{m} r_i(x_k) H_i(x_k)) s_k = -J(x_k)^T r(x_k)$$

- m Hessian matrices H_i are usually inconvenient and expensive to compute
- Moreover, each H_i is multiplied by residual component r_i, which is small at solution if fit of model function to data is good
- This motivates Gauss-Newton method for nonlinear least squares, in which second-order term is dropped and linear system

$$J(x_k)^T J(x_k) s_k = -J(x_k)^T r(x_k)$$

  is solved for approximate Newton step s_k at each iteration
- This is system of normal equations for linear least squares problem

$$J(x_k) s_k \approx -r(x_k)$$

Gauss-Newton method (cont'd)

- Gauss-Newton method replaces nonlinear least squares problem by sequence of linear least squares problems whose solutions converge to solution of original nonlinear problem
- If residual at solution is large, then second-order term omitted from Hessian is not negligible, and Gauss-Newton method may converge slowly or fail to converge
- In such "large-residual" cases, it may be best to use general nonlinear minimization method that takes into account true full Hessian matrix

Levenberg-Marquardt Method

- It is possible that the matrix $J(x_k)^T J(x_k)$ is singular (but it is symmetric)
- The Levenberg-Marquardt method consists in perturbing the matrix to make it positive definite
- We solve at each step the system

$$(J(x_k)^T J(x_k) + \mu_k I)s_k = -J(x_k)^T r(x_k)$$

- The parameter μ_k is chosen so that $(J(x_k)^T J(x_k) + \mu_k I)$ is symmetric positive definite

Constrained Optimization

- We seek to solve the problem

$$\min_x f(x) \text{under } g(x) = 0$$

with $f : \mathbb{R}^n \to \mathbb{R}$, $g : \mathbb{R}^n \to \mathbb{R}^m$ with $m \leq n$

- We look for a critical point of the Lagrangian $\mathcal{L}(x, \lambda) = f(x) + \lambda^T g(x)$
- By applying Newton's method to the system nonlinear system

$$\nabla \mathcal{L}(x, \lambda) = \begin{pmatrix} \nabla f(x) + J_g(x)^T \lambda \\ g(x) \end{pmatrix} = 0$$

we obtain the linear system

$$\begin{pmatrix} B(x, \lambda) & J_g(x)^T \\ J_g(x) & 0 \end{pmatrix} \begin{pmatrix} s \\ \lambda \end{pmatrix} = - \begin{pmatrix} \nabla f(x) + J_g(x)^T \lambda \\ g(x) \end{pmatrix}$$

This technique is called sequential quadratic programming

Linear programming

- This is a problem of minimizing a linear function under linear constraints
- It can be written in the form

$$\min f(x) = c^T x \quad \text{under} \quad Ax = b \text{ and } x \geq 0$$

with $m < b$, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $c, x \in \mathbb{R}^n$

- The set of constraints forms a polyhedron of $\mathbb{R}^n$ and the minimum is reached at a vertex of this polyhedron
- The simplex method consists in going from vertices to vertices until we find the minimum

Linear programming (continued)

- The simplex method is reliable and efficient in general but is exponential in the size of the problem in the worst cases
- Recently developed interior point methods allow to solve linear programming problems with polynomial complexity in the worst case
- The interior point methods navigate inside the admissible regions admissible regions by not restricting themselves only to the vertices
- Although interior point methods are of better complexity, the simplex method complexity, the simplex method remains the most commonly used method used in practice

Example

- Consider the problem

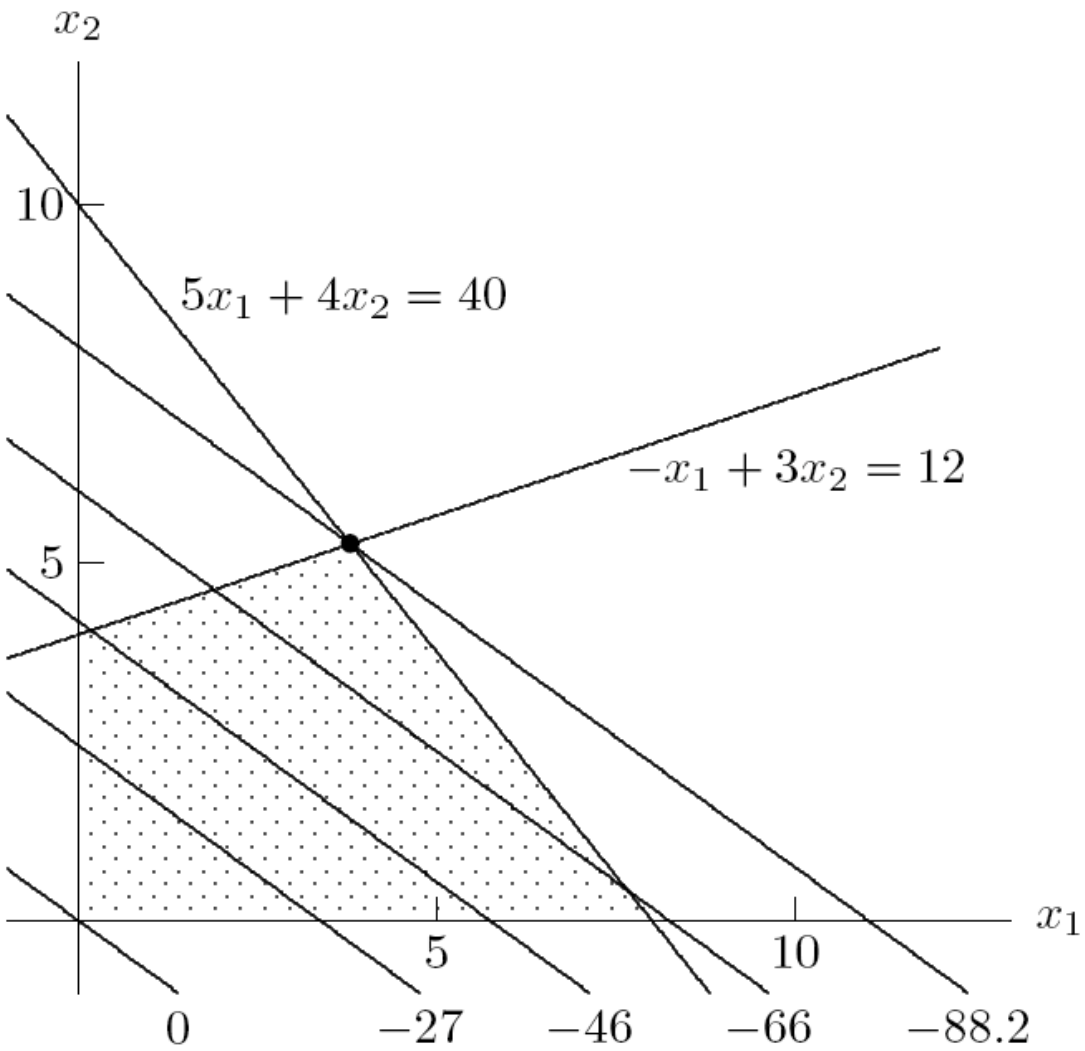
$$\min_x -8x_1 - 11x_2$$

under the conditions

$$5x_2 + 4x_2 \leq 40, \quad -x_1 + 3x_2 \leq 12, \quad x_1 \geq 0, \quad x_2 \geq 0$$

- The minimum is obtained in $x_1 = 3,79$ and $x_2 = 5,26$ where the objective function is -88.2

Example (continued)



Conclusion

- Newton's method
- Alternative methods not requiring the calculation of the hessian
  - Quasi-Newton's method
  - Newton's method by finite difference
- Alternative methods not requiring the computation of the hessian nor the storage of matrix
  - Steepest descent method
  - Nonlinear conjugate gradient method
- Alternative methods that do not require the computation of derivatives
  - Finite difference method
  - Nelder-Meade method
  - Pattern search method