Multidimensional Optimization

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Session Outline

- Problem Definition
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- Multidimensional Optimization
  - Methods without Using Derivatives
  - Methods with Using Derivatives
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We have a (possibly) non-linear, but deterministic function $f(x)$ that depends on one or more independent variables.

$f(x)$ is probably expensive to evaluate, and we may or may not be able to efficiently and/or accurately (!) compute its gradient or Hessian.

Problem: find a minimum of $f(x)$ with as few evaluations as possible.

Examples of real-life problems
- MLE, model fitting, cost minimization, performance maximization

How do we recognize what we are looking for?
- local vs. global optima
- trying to find the longest straw in the haystack
One-dimensional Optimization: Golden Section Search

- Analogy with bisection root search.

- Given an initial bracket of a minimum \([a, b, c]\), i.e. \(a < b < c\), and \(f(b) < f(a)\), and \(f(b) < f(c)\), we take a guess at a point \(x\) either in \((a, b)\) or in \((b, c)\). We evaluate \(f(x)\) and update our bracket accordingly.
  - e.g. \(x\) is in \((a, b)\): if \(f(x) < f(b)\) then the new bracket is \([a, x, b]\), else the new bracket is \([x, b, c]\).

- We repeat this until the bracket is small enough.
  - e.g. suppose that \(b\) is a fraction \(w\) of the way between \(a\) and \(c\), so \(w = (b-a)/(c-a)\). Let the next trial point be a fraction \(z\) before \(b\), so \(z = (b-x)/(c-a)\). Hence the size of the next bracket is either \(w\) or \(1-w+z\). Minimizing the worst case probability yields \(z = 2w-1\). \(z\) is positive only if \(x\) is in the larger segment \((w > \frac{1}{2})\). If \(z\) is “optimal” then so was \(w\), which suggests that \(z / w = 1-w\), which in turn gives \(w^2+w-1=0\), i.e. \(w \approx 0.61803\).

- Optimal choice of \(x\) is \((1-w)\) fraction into the larger interval from the middle.
A Note on Accuracy

- Convergence is linear: count of successive significant figures grows linearly with iterations.

- Do not set tolerance in $x$ to lower than the square root of your numerical precision.
  
  - Close to a minimum at $b$, $f(x) \approx f(b) + \frac{1}{2}f''(b)(x - b)^2$, because the first derivative vanishes.
  
  - The second term above is $\epsilon$ times smaller than the first, i.e. $\epsilon|f(b)| > \frac{1}{2}f''(b)(x - b)^2$ if
    
    $$|x - b| < \sqrt{\epsilon \ |b| \ \sqrt{\left( \frac{2 |f(b)|}{b^2 f''(b)} \right)}}$$
    
    , where the final square root is a number of order one for most functions.
  
  - Unless you know a better estimate for the final square root, apply the limit suggested above.
One-dimensional Optimization: Fancier Methods

- Parabolic interpolation: try to fit a parabola through \([a,b,c]\) and jump to its minimum as a guess for \(x\).
  - Caveats: parabolic interpolation may converge to a maximum, or the fit might not be feasible because of collinearity.
- An ideal scheme can avoid unnecessary evaluations, switch between a robust and slow (e.g. Golden Section) technique and parabolic interpolations as \(f(x)\) permits, and carefully define a stopping criterion.
- Brent's method is good at all the above at the expense of maintaining six function points instead of three and defining robust rules for acceptance of guesses.
One-dimensional Optimization: Fancier Methods (Cont’d)

- What if we can also use derivatives?

- Keeping the bracketing idea and updating the bracket based on function as opposed to derivative information is more robust.

- You can try to fit a higher order polynomial to function and derivative information.

- You can also try to select the interval to look at based on the derivative at the middle point.

- The latter idea combined with extrapolation to zero of the derivative and robust rules for acceptance of the results as in Brent’s method appears to work well.
Multidimensional Optimization: An Overview

- Methods without using derivatives
  - Downhill simplex
  - Line methods in general
  - Direction set methods (line methods)

- Methods with using derivatives
  - Conjugate gradient methods (line methods)
  - Quasi-Newton methods
  - Levenberg-Marquardt method

- Methods using random numbers
  - Simulated annealing
  - Genetic algorithm
  - Ant colony optimization
Downhill Simplex

- Definitely not the best in the number of required function evaluations, but can be used for initial trials. Also, sometimes more robust than other methods.

- A simplex is a geometrical figure consisting of N+1 vertices and all their interconnecting line segments or polygonal faces, etc. in N dimensions.

- We are now interested in simplexes with a finite inner N-dimensional volume (>0).

- We need an initial simplex when starting the algorithm.
  - e.g. $P_0$ is an initial starting point, and $P_i = P_0 + \Delta_i e_i$, where $e_i$ are the unit vectors and $\Delta_i$ are some characteristic length scales.

- The one-dimensional bracketing does not work, so we take a slightly different approach to modify the simplex in the iterations of the algorithm.
Given an initial simplex, the following list of moves is considered at each iteration:

- **reflection**: most of the time just move the point with the largest function value through the opposite face of the simplex
- **reflection and expansion**: the above combined with increasing the search step size, if reflection yields a significantly better point
- **contraction**: when in a “valley”, the simplex is contracted in the transverse direction, i.e., when the reflected point is worse than the one with the second largest function value
- **multiple contraction**: when passing through the eye of a needle it is best to contract around the point with the lowest function value, i.e., when none of the above works
• Solution at each iteration is the best point found so far.

• Stopping criteria can be tricky:
  • terminate when vector distance of last move is less than some tolerance limit (not smaller than square root of machine precision)
  • terminate when decrease of function value in the last iteration is less than some tolerance limit (can be approx. machine precision)
  • it is often a good idea to restart the algorithm where it claims to have found a minimum, because an anomalous step might cause the stopping criteria to be triggered
Line Methods in General

- Let us now build on the available one-dimensional routines.
- If we have a starting point \( P \) and a vector \( n \) in \( N \) dimensions, then (1) we can use our one-dimensional minimization routine to minimize \( f(\lambda) = f(P + \lambda n) \). Thus \( n \) is the search direction.
- We can then (2) reset our starting point to the minimum found along the search direction and (3) determine a new search direction and continue with step (1) above.
- The various line methods differ by how they choose the search direction.
• First, not too bad idea:
  • take a set of directions, e.g. the unit vectors $e_i$,
  • iterate over the set of directions and minimize along the current direction, then from there along the next direction, and so on until the function stops decreasing.

• Problem: what if the function has a narrow valley at an angle to the unit vectors?

• Let us use conjugate directions,
  • which are directions that do not impact the efficacy of minimization along themselves.
  • If we minimize along some direction $u$, then the gradient of the function must be perpendicular to $u$ at the minimum.
  • Using Taylor series: $f(x) = f(p) + b \cdot x + \frac{1}{2} x^T A x + \ldots$, where $b$ is the gradient at $p$ and $A$ is the Hessian at $p$.
  • The approximation of the gradient at $x$ is $A x + b$ (derivative with respect to $x$).
  • The gradient vanishes at $x$ that solves $A x = -b$, and change in the gradient when moving along $x$ is $A$ ($\delta x$).
  • If we move along direction $u$ to a minimum, then a new direction $v$ does not spoil our minimization as long as $0 = u^T A v$, i.e., the change in the gradient along $v$ is perpendicular to $u$ (note that $u$ and $v$ are conjugate vectors).
Direction Set Methods (Cont’d)

- If we can find a set of $N$ linearly independent, mutually conjugate directions, then $N$ line minimizations will reach exactly the minimum of a quadratic form.

- If our $f(x)$ is not exactly quadratic, we will be close, and repeated cycles will yield quadratic convergence.

- Powell’s method: (1) Initialize the set of directions $u_i$ to the basis vectors $e_i$. (2) Save your starting position as $P_0$. (3) For $i = 0,…N-1$ move $P_i$ to the minimum along direction $u_i$ and call this point $P_{i+1}$. (4) For $i = 0,…N-2$ set $u_i := u_{i+1}$. (5) Set $u_{N-1} := P_N - P_0$. (6) Move $P_N$ to the minimum along direction $u_{N-1}$, and call this point $P_0$. (7) Repeat from step (3).

- $N$ iterations, that is, $N(N + 1)$ line minimizations will exactly minimize a quadratic form.

- Problem: throwing away $u_0$ in favor of $u_{N-1}$ tends to produce linearly dependent directions.

- One (and not the best) solution: rerun step (1) after every $N$ or $N+1$ iterations.
Conjugate Gradient Methods (Line Methods with Derivatives)

- Let us now return to \( f(x) \approx c + b \cdot x + \frac{1}{2} x^T A x \). Each element of \( b \) and \( A \) can affect the location of the minimum, so the information content of this form is \( \sim N^2 \).

- When minimizing via direction sets, we collect this amount of information via \( O(N^2) \) separate line minimizations. If we can easily evaluate the gradient, we get \( N \) pieces of new information and hence \( O(N) \) carefully chosen line minimizations should suffice.

- Note that the gradient may need \( O(N) \) function evaluation time to compute, but there might be repeating computations to take advantage of. Also, each gradient evaluation spares a line minimization, which itself requires possibly many function calls.
Conjugate Gradient Methods (Cont’d)

- Steepest descent performs poorly: takes many steps in a long valley.

- Ideally, we want to proceed along a direction that is chosen to be conjugate to the previous gradient, as well as all previous directions to the extent possible.

- Conjugate gradient methods make use of the technique available for solving sparse linear systems of equations in the context of function minimization.
Conjugate Gradient Methods (Cont’d)

• Let an arbitrary vector \( g_0 \) be our first auxiliary vector. Let the first direction be \( h_0 = g_0 \).

• Let \( g_{i+1} = g_i - \lambda_i A h_i \), and let \( h_{i+1} = g_{i+1} + \gamma_i h_i \), where

\[
\lambda_i = g_i^T g_i / ( h_i^T A h_i ), \quad \text{and} \quad \gamma_i = g_{i+1}^T g_{i+1} / ( g_i^T g_i ) \quad [\text{improvement:} \quad \gamma_i = (g_{i+1} - g_i)^T g_{i+1} / (g_i^T g_i)].
\]

• The generated sequence will satisfy \( g_i^T g_j = 0, h_i^T A h_j = 0 \) and \( g_i^T h_j = 0 \) for \( j < i \).

• Problem: as opposed to the case of solving the linear system of equations, here we don’t know \( A \).

• Solution: let \( g_i = -\nabla f(p_i) \) and we go along the direction \( h_i \) to the local minimum of \( f(x) \) at \( p_{i+1} \). Let then \( g_{i+1} = -\nabla f(p_{i+1}) \). This is equivalent to our choice of \( g_{i+1} \) above, and does not require the knowledge of \( A \).
Conjugate Gradient Methods (Cont’d)

- Described method is called Fletcher-Reeves. Improvement is called Polak-Ribiere: provides smoother transition between iterations and falls back to using local gradient when additional gain is lost.
• Let us now again return to \( f(x) \approx f(x_i) + (x - x_i)^T \nabla f(x_i) + \frac{1}{2} (x - x_i)^T A (x - x_i) \). Recall that we do not know \( A \), and so our aim is to collect its information content somehow.

• Basic idea: try to construct an iterative approximation \( H_i \) to the matrix \( A^{-1} \) to mimic Newton’s minimum search method. That is, making the gradient at \( x \), \( \nabla f(x_i) + A (x - x_i) \), equal to zero yields the equation \( x - x_i = -A^{-1} \nabla f(x_i) \), where we use \( H_i \) to replace \( A^{-1} \).

• The name “Quasi”-Newton comes from not using the actual Hessian but the current approximation of its inverse only. It is actually better, because we need to descend, hence we want \( (x - x_i)^T \nabla f(x_i) = - (x - x_i)^T A (x - x_i) < 0 \), which means \( A \) must be positive definite. There is no guarantee that the Hessian will always be positive definite, but the series \( H_i \) can be defined so.
Quasi-Newton Methods (Cont’d)

- Derivation of the iterative approximation $H_i$ is somewhat involved, but the two main updating formulas are referred to as Davidon-Fletcher-Powell (DFP) and Broyden-Fletcher-Goldfarb-Shanno (BFGS), the latter being recognized as empirically superior.

- Note that it might be worth using Quasi-Newton Methods with finite difference approximations of the gradient to decrease total computation effort compared to using methods without derivatives.
• Let’s say now that our \( f(a) = \chi^2(a) = \sum \left[ \left\{ y_i - y(x_i|a) \right\} / \sigma_i \right]^2 \), i.e., we are looking for a least-square fit. We again use the quadratic approximation \( \chi^2(a) \approx c + a^T b + \frac{1}{2} a^T A a \), which suggests using either \( a_{\text{min}} = a_{\text{cur}} + A^{-1} \left[ - \nabla \chi^2(a_{\text{cur}}) \right] \), if the quadratic approximation is good enough, or a steepest descent \( a_{\text{next}} = a_{\text{cur}} - \text{constant} \times \nabla \chi^2(a_{\text{cur}}) \), if it isn’t.

• Here we do know the form of the Hessian:

\[
\alpha_{kl} = \frac{\partial^2 \chi^2}{(\partial a_k \partial a_l)} = 2 \sum \frac{1}{\sigma_i^2} \left[ \frac{\partial y(x_i|a)}{\partial a_k} \times \frac{\partial y(x_i|a)}{\partial a_l} - \left( y_i - y(x_i|a) \right) \times \frac{\partial^2 y(x_i|a)}{\partial a_l \partial a_k} \right]
\]

• Now, we neglect the second partial derivatives in the above expression, because

  • they are often small enough to be negligible in practice;

  • the term multiplying them should be a random, uncorrelated measurement error in a successful model, which can have either sign, so they will probably cancel;

  • they might lead to destabilizing in the presence of outliers.
Levenberg-Marquardt Method (Cont’d)

- Levenberg-Marquardt solves the equation $\sum a_{kl} \Delta a_l = \beta_k$ (r.h.s. is the gradient) by replacing $a_{kl}$ with $z_{kl}$, where $z_{jj} = a_{jj} (1 + \lambda)$, and $z_{jk} = a_{jk}$. This will ensure a smooth scaling between the two extremes of using the inverse Hessian and using the steepest descent.

- Outline of algorithm is then: (1) given an initial guess $a$, and an initial setting of $\lambda (=0.001)$, (2) solve the above system of equations for $\Delta a$. (3) If $\chi^2(a + \Delta a) >= \chi^2(a)$, then increase $\lambda$ by a significant factor, otherwise decrease $\lambda$ by a significant factor. (4) Continue with step (2) after setting $a := a + \Delta a$.

- The stopping condition can be tricky. Decrease in $\chi^2$ less than 1 is often not significant statistically, but 0.001 will put you on the safe side. Method tends to wander around near the minimum in a flat valley.
Simulated Annealing

- Now think about $f(x)$ as a function with multiple local minima.

- Apply the analogy of liquids freezing and crystallizing from thermodynamics.
  - At high temperatures, the molecules move freely.
  - At lower temperatures this mobility is gradually lost.
  - If cooling is slow, the molecules can arrange in an ordered fashion leading to (or near to) the state of the lowest energy.
  - If cooling is fast, the result is a polycrystalline or amorphous state with higher energy.
  - The key is to keep cooling slow to allow for atoms to redistribute.
  - A state of energy $E$ is occupied with probability $\sim \exp(-E/kT)$ at temperature $T$. $k$ is Boltzmann’s constant.
Simulated Annealing (Cont’d)

- Outline of the Metropolis algorithm
  - Define an initial temperature. (How high?)
  - Generate a random move from state $x$ to $x + \Delta x$. (What moves to pick from? How to choose?)
  - Accept new state with probability $\min(\exp\{-[f(x+\Delta x) - f(x)]/kT\}, 1)$. 
  - Decrease $T$. (How fast? Repeats at the same temperature?)
Genetic Algorithm

- Think about \(-f(x)\) as a measure of success of an individual in a population (fitness function).

  Think about \(x\) as the genome of the individual.

- Define the following rules of evolution
  
  - Set up an initial population. (What size? Which individuals?)
  
  - Select the part of the current population for reproduction. (Randomized based on fitness.)
  
  - Apply crossover and mutation operators to selected subpopulation. (How to define operators? More than two parents?)
  
  - Evaluate termination criteria (Number of generations? Average fitness?) and continue with selection step, if needed.

- The details are highly problem-specific.
Ant Colony Optimization

- How do ants search for food? How do they form trails connecting the colony with the food source?
- To illustrate the concept, think about $\mathbf{x}$ as a Hamiltonian cycle in a given graph with given non-negative edge weights. Let $f(\mathbf{x})$ be the sum of the weights of edges in the cycle. Minimizing $f(\mathbf{x})$ now amounts to solving the traveling salesman problem.
Ant Colony Optimization (Cont’d)

- ACO solution to traveling salesman problem:
  - Let’s imagine a number of ants that walk on the graph.
  - We define the following rules for one iteration:
    - Each ant must visit each node exactly once.
    - The smaller the weight and the stronger the pheromone trail the more likely that an ant chooses a particular edge as a next step on its cycle.
  - We iterate over the following steps:
    - Each ant visits a Hamiltonian cycle according to the rules above.
    - Each ant lays pheromone trail on the edges it visited in the current iteration. The shorter the Hamiltonian cycle the stronger the trail.
    - All pheromone trails evaporate (weaken).
**Tips & Tricks, Suggestions**

- Get to know your f(x) as much as possible to identify qualitative behavior, parameter ranges of interest and signs of numerical errors.

- Try to use as much information about f(x) as possible, e.g. go for LM if f(x) is $\chi^2$.

- Try to match the scales of function parameters (coordinates in $\mathbf{x}$).

- Try changing your initial guess.

- When working on a constrained problem, hide the constraints from the optimizer by applying variable transforms.
  - e.g. $f(\exp(y))$ lets the optimizer work in the range $(-\infty, \infty)$ even if the domain of $f(x)$ is $\mathbb{R}^+$.

- Recall the shape of objective function value plotted against iterations taken in a random optimization method.

- There is not any single best recipe, so experiment with different approaches.
References

Most of this presentation is based on

Press-Teukolsky-Vetterling-Flannery: Numerical Recipes, 3rd ed,

a highly recommended reference.
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