Financial Modeling and Information Technology

Budapest Technology Centre

Multidimensional Optimization

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Session Outline

- Problem Definition
- One-dimensional Optimization
- Multidimensional Optimization
 - Methods without Using Derivatives
 - Methods with Using Derivatives
 - Heuristics Using Random Numbers
- Tips&Tricks, Suggestions
- References



Problem Definition

- 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 fraction 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 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 > ½). If z is "optimal" then so was w, which suggests that z / w = 1-w, which in turn gives w²+w-1=0, i.e. w ≈ 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 ε times smaller than the first, i.e. $\varepsilon |f(b)| > \frac{1}{2}f''(b)(x b)^2$ if
 - $|x b| < \sqrt{\epsilon} |b| \sqrt{(2 |f(b)| / \{b^2 f''(b)\})}$, 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. P₀ is an initial starting point, and P_i = P₀ + Δ_ie_i, where e_i are the unit vectors and Δ_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.

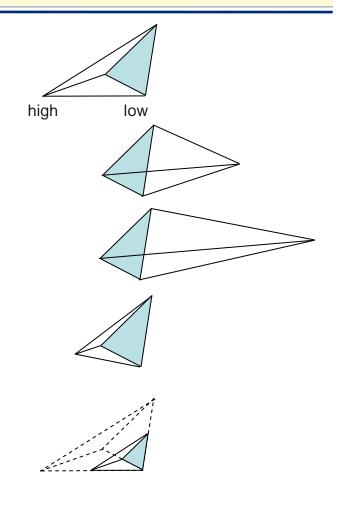
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Downhill Simplex (Cont'd)

• 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



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Downhill Simplex (Cont'd)

- 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 onedimensional minimization routine to minimize $f(\lambda) = f(\mathbf{P} + \lambda \mathbf{n})$. 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.

Direction Set Methods (Line Methods)

- 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: $f(x) = f(p) + b x + \frac{1}{2} x A x + ...$, 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

 $0 = \mathbf{u} \mathbf{A} \mathbf{v}$, i.e., the change in the gradient along \mathbf{v} is perpendicular to \mathbf{u} (note that \mathbf{u} and \mathbf{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 P₀. (3) For i = 0,...N-1 move P_i to the minimum along direction u_i and call this point P_{i+1}. (5) For i = 0,...N-2 set u_i := u_{i+1}. (6) Set u_{N-1} := P_N P₀. (7) Move P_N to the minimum along direction u_{N-1}, and call this point P₀. (8) Repeat from step (3).
- N iterations, that is, N(N + 1) line minimizations will exactly minimize a quardatic form.
- Problem: throwing away \mathbf{u}_0 in favor of \mathbf{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.

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Conjugate Gradient Methods (Line Methods with Derivatives)

• Let us now return to $f(\mathbf{x}) \approx c + \mathbf{b} \mathbf{x} + \frac{1}{2} \mathbf{x} \mathbf{A} \mathbf{x}$. 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(N²) 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 \mathbf{g}_0 be our first auxiliary vector. Let the first direction be $\mathbf{h}_0 = \mathbf{g}_0$.
- Let $\mathbf{g}_{i+1} = \mathbf{g}_i \lambda_i \mathbf{A} \mathbf{h}_i$, and let $\mathbf{h}_{i+1} = \mathbf{g}_{i+1} + \gamma_i \mathbf{h}_i$, where

 $\lambda_i = \mathbf{g}_i \ \mathbf{g}_i \ / \ (\mathbf{h}_i \ \mathbf{A} \ \mathbf{h}_i \), \ \text{and} \ \gamma_i = \mathbf{g}_{i+1} \ \mathbf{g}_{i+1} \ / \ (\mathbf{g}_i \ \mathbf{g}_i) \qquad [\text{improvement:} \ \gamma_i = (\mathbf{g}_{i+1} - \mathbf{g}_i) \ \mathbf{g}_{i+1} \ / \ (\mathbf{g}_i \ \mathbf{g}_i)].$

- The generated sequence will satisfy $\mathbf{g}_i \mathbf{g}_j = 0$, $\mathbf{h}_i \mathbf{A} \mathbf{h}_j = 0$ and $\mathbf{g}_i \mathbf{h}_j = 0$ for j < i.
- Problem: as opposed to the case of solving the linear system of equations, here we don't know A.
- Solution: let $\mathbf{g}_i = -grad f(\mathbf{p}_i)$ and we go along the direction \mathbf{h}_i to the local minimum of $f(\mathbf{x})$ at

 \mathbf{p}_{i+1} . Let then $\mathbf{g}_{i+1} = -grad f(\mathbf{p}_{i+1})$. This is equivalent to our choice of \mathbf{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.

Quasi-Newton Methods (Methods with Derivatives)

- Let us now again return to f(x) ≈ f(x_i)+ (x x_i) grad f(x_i) + ½ (x x_i) 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 \mathbf{H}_i to the matrix \mathbf{A}^{-1} to mimic Newton's minimum search method. That is, making the gradient at \mathbf{x} , grad $f(\mathbf{x}_i) + \mathbf{A} (\mathbf{x} \mathbf{x}_i)$, equal to zero yields the equation $\mathbf{x} \mathbf{x}_i = -\mathbf{A}^{-1}$ grad $f(\mathbf{x}_i)$, where we use \mathbf{H}_i to replace \mathbf{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 grad $f(\mathbf{x}_i)$ $(\mathbf{x} \mathbf{x}_i) = -(\mathbf{x} \mathbf{x}_i) \mathbf{A} (\mathbf{x} \mathbf{x}_i) < 0$, which means \mathbf{A} must be positive definite. There is no guarantee that the Hessian will always be positive definite, but the series \mathbf{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 (DFB) 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.

Levenberg-Marquardt Method (Methods with Derivatives)

- Let's say now that our $f(\mathbf{a}) = \chi^2(\mathbf{a}) = \sum [\{y_i y(x_i | \mathbf{a})\} / \sigma_i]^2$, i.e., we are looking for a least-square
 - fit. We again use the quadratic approximation $\chi^2(\mathbf{a}) \approx c + \mathbf{b} \mathbf{a} + \frac{1}{2} \mathbf{a} \mathbf{A} \mathbf{a}$, which suggests

using either $\mathbf{a}_{min} = \mathbf{a}_{cur} + \mathbf{A}^{-1}[-grad \chi^2(\mathbf{a}_{cur})]$, if the quadratic approximation is good enough,

or a steepest descent $\mathbf{a}_{next} = \mathbf{a}_{cur} - \text{constant} * \text{grad } \chi^2(\mathbf{a}_{cur})$, if it isn't.

• Here we do know the form of the Hessian:

 $\alpha_{kl} = \partial^2 \chi^2 / \left(\partial a_k \partial a_l\right) = 2 \sum 1/\sigma_i^2 \left[\partial y(x_i | \boldsymbol{a}) / \partial a_k * \partial y(x_i | \boldsymbol{a}) / \partial a_l - \{y_i - y(x_i | \boldsymbol{a})\} * \partial^2 y(xi | \boldsymbol{a}) / \left(\partial a_l \partial a_k\right) \right]$

- 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 $\sum \alpha_{kl} \Delta a_l = \beta_k$ (r.h.s. is the gradient) by replacing

 α_{kl} with z_{kl} , where $z_{jj} = \alpha_{kl} (1 + \lambda)$, and $z_{jk} = \alpha_{jk}$. 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 λ (=0.001),
 (2) solve the above system of equations for Δa. (3) If χ²(a + Δa) >= χ²(a), then increase λ by a significant factor, otherwise decrease λ by a significant factor. (4) Continue with step (2) after setting a := a + Δa.
- The stopping condition can be tricky. Decrease in χ^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 $f(\mathbf{x})$ 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 ~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 \mathbf{x} to $\mathbf{x}+\Delta \mathbf{x}$. (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 x as a Hamiltonian cycle in a given graph with given non-negative edge weights. Let f(x) be the sum of the weights of edges in the cycle.
 Minimizing f(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 $f(\mathbf{x})$ as much as possible to identify qualitative behavior, parameter ranges

of interest and signs of numerical errors.

- Try to use as much information about $f(\mathbf{x})$ as possible, e.g. go for LM if $f(\mathbf{x})$ is χ^2 .
- Try to match the scales of function parameters (coordinates in **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 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.

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References

Most of this presentation is based on

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

a highly recommended reference.

Q & A



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References

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