

### Multidimensional Optimization

Zsolt Pándi

Morgan Stanley Hungary Analytics Ltd.



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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  $f(\mathbf{x})$  that depends on one or more independent variables.
- $f(\mathbf{x})$  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  $f(\mathbf{x})$  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 ( $w > 1/2$ ). 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  
 $|x - b| < \sqrt{\epsilon |b| \sqrt{2 |f(b)| / \{ b^2 f''(b) \}}}$ , 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

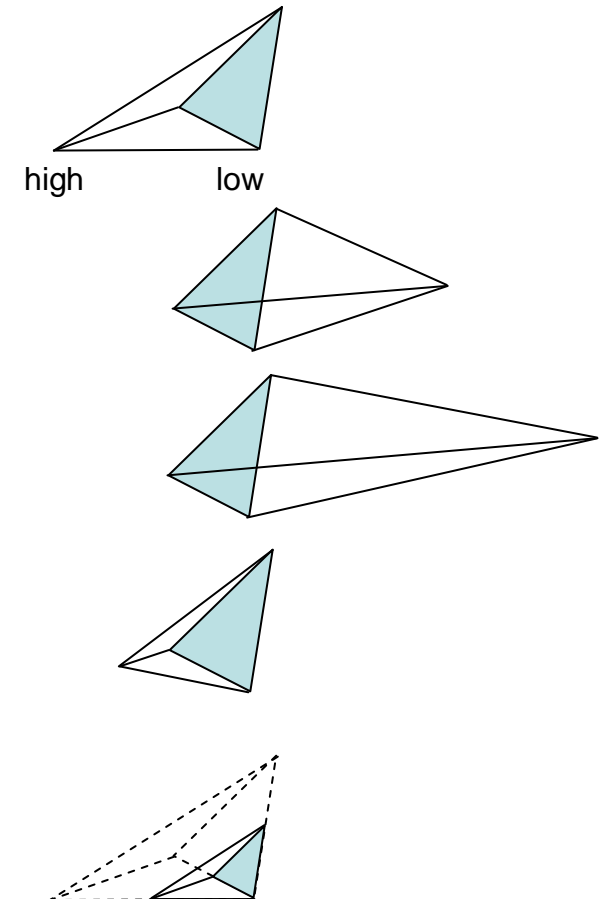


# Downhill Simplex

- 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.  $\mathbf{P}_0$  is an initial starting point, and  $\mathbf{P}_i = \mathbf{P}_0 + \Delta_i \mathbf{e}_i$ , where  $\mathbf{e}_i$  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.

## 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



## 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

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- Let us now build on the available one-dimensional routines.
- If we have a starting point  $\mathbf{P}$  and a vector  $\mathbf{n}$  in  $N$  dimensions, then (1) we can use our one-dimensional minimization routine to minimize  $f(\lambda) = f(\mathbf{P} + \lambda\mathbf{n})$ . Thus  $\mathbf{n}$  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  $\mathbf{e}_i$ ,
  - 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  $\mathbf{u}$ , then the gradient of the function must be perpendicular to  $\mathbf{u}$  at the minimum.
  - Using Taylor series:  $f(\mathbf{x}) = f(\mathbf{p}) + \mathbf{b} \mathbf{x} + \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} + \dots$ , where  $\mathbf{b}$  is the gradient at  $\mathbf{p}$  and  $\mathbf{A}$  is the Hessian at  $\mathbf{p}$ .
  - The approximation of the gradient at  $\mathbf{x}$  is  $\mathbf{A} \mathbf{x} + \mathbf{b}$  (derivative with respect to  $\mathbf{x}$ ).
  - The gradient vanishes at  $\mathbf{x}$  that solves  $\mathbf{A} \mathbf{x} = -\mathbf{b}$ , and change in the gradient when moving along  $\mathbf{x}$  is  $\mathbf{A} (\delta \mathbf{x})$ .
  - If we move along direction  $\mathbf{u}$  to a minimum, then a new direction  $\mathbf{v}$  does not spoil our minimization as long as  $0 = \mathbf{u}^T \mathbf{A} \mathbf{v}$ , 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  $f(\mathbf{x})$  is not exactly quadratic, we will be close, and repeated cycles will yield quadratic convergence.
- Powell's method: (1) Initialize the set of directions  $\mathbf{u}_i$  to the basis vectors  $\mathbf{e}_i$ . (2) Save your starting position as  $\mathbf{P}_0$ . (3) For  $i = 0, \dots, N-1$  move  $\mathbf{P}_i$  to the minimum along direction  $\mathbf{u}_i$  and call this point  $\mathbf{P}_{i+1}$ . (4) For  $i = 0, \dots, N-2$  set  $\mathbf{u}_i := \mathbf{u}_{i+1}$ . (5) Set  $\mathbf{u}_{N-1} := \mathbf{P}_N - \mathbf{P}_0$ . (6) Move  $\mathbf{P}_N$  to the minimum along direction  $\mathbf{u}_{N-1}$ , and call this point  $\mathbf{P}_0$ . (7) Repeat from step (3).
- $N$  iterations, that is,  $N(N + 1)$  line minimizations will exactly minimize a quadratic form.
- Problem: throwing away  $\mathbf{u}_0$  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.

## Conjugate Gradient Methods (Line Methods with Derivatives)

- Let us now return to  $f(\mathbf{x}) \approx c + \mathbf{b} \mathbf{x} + \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x}$ . Each element of  $\mathbf{b}$  and  $\mathbf{A}$  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)

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- 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
$$\lambda_i = \mathbf{g}_i^T \mathbf{g}_i / (\mathbf{h}_i^T \mathbf{A} \mathbf{h}_i), \text{ and } \gamma_i = \mathbf{g}_{i+1}^T \mathbf{g}_{i+1} / (\mathbf{g}_i^T \mathbf{g}_i) \text{ [improvement: } \gamma_i = (\mathbf{g}_{i+1} - \mathbf{g}_i)^T \mathbf{g}_{i+1} / (\mathbf{g}_i^T \mathbf{g}_i)].$$
- The generated sequence will satisfy  $\mathbf{g}_i^T \mathbf{g}_j = 0$ ,  $\mathbf{h}_i^T \mathbf{A} \mathbf{h}_j = 0$  and  $\mathbf{g}_i^T \mathbf{h}_j = 0$  for  $j < i$ .
- Problem: as opposed to the case of solving the linear system of equations, here we don't know  $\mathbf{A}$ .
- Solution: let  $\mathbf{g}_i = -\text{grad} f(\mathbf{p}_i)$  and we go along the direction  $\mathbf{h}_i$  to the local minimum of  $f(\mathbf{x})$  at  $\mathbf{p}_{i+1}$ . Let then  $\mathbf{g}_{i+1} = -\text{grad} f(\mathbf{p}_{i+1})$ . This is equivalent to our choice of  $\mathbf{g}_{i+1}$  above, and does not require the knowledge of  $\mathbf{A}$ .

## Conjugate Gradient Methods (Cont'd)

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- 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  $f(\mathbf{x}) \approx f(\mathbf{x}_i) + (\mathbf{x} - \mathbf{x}_i)^T \text{grad } f(\mathbf{x}_i) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_i)^T \mathbf{A} (\mathbf{x} - \mathbf{x}_i)$ . Recall that we do not know  $\mathbf{A}$ , 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  $\mathbf{x}$ ,  $\text{grad } f(\mathbf{x}_i) + \mathbf{A} (\mathbf{x} - \mathbf{x}_i)$ , equal to zero yields the equation  $\mathbf{x} - \mathbf{x}_i = -\mathbf{A}^{-1} \text{grad } f(\mathbf{x}_i)$ , 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  $(\mathbf{x} - \mathbf{x}_i)^T \text{grad } f(\mathbf{x}_i) = -(\mathbf{x} - \mathbf{x}_i)^T \mathbf{A} (\mathbf{x} - \mathbf{x}_i) < 0$ , 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  $\mathbf{H}_i$  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.

## 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  $\chi^2(\mathbf{a}) \approx c + \mathbf{a}^T \mathbf{b} + \frac{1}{2} \mathbf{a}^T \mathbf{A} \mathbf{a}$ , which suggests using either  $\mathbf{a}_{\min} = \mathbf{a}_{\text{cur}} + \mathbf{A}^{-1}[-\text{grad } \chi^2(\mathbf{a}_{\text{cur}})]$ , if the quadratic approximation is good enough, or a steepest descent  $\mathbf{a}_{\text{next}} = \mathbf{a}_{\text{cur}} - \text{constant} * \text{grad } \chi^2(\mathbf{a}_{\text{cur}})$ , if it isn't.

- Here we do know the form of the Hessian:

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

- 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  $\alpha_{kl}$  with  $z_{kl}$ , where  $z_{jj} = \alpha_{jj} (1 + \lambda)$ , 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  $\mathbf{a}$ , and an initial setting of  $\lambda$  ( $=0.001$ ), (2) solve the above system of equations for  $\Delta \mathbf{a}$ . (3) If  $\chi^2(\mathbf{a} + \Delta \mathbf{a}) \geq \chi^2(\mathbf{a})$ , then increase  $\lambda$  by a significant factor, otherwise decrease  $\lambda$  by a significant factor. (4) Continue with step (2) after setting  $\mathbf{a} := \mathbf{a} + \Delta \mathbf{a}$ .
- 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  $f(\mathbf{x})$  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  $\sim \exp(-E/kT)$  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  $\mathbf{x}$  to  $\mathbf{x}+\Delta\mathbf{x}$ . (What moves to pick from? How to choose?)
  - Accept new state with probability  $\min(\exp\{-[f(\mathbf{x}+\Delta\mathbf{x})-f(\mathbf{x})]/kT\}, 1)$ .
  - Decrease T. (How fast? Repeats at the same temperature?)



# Genetic Algorithm

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

Think about  $\mathbf{x}$  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

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- 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  $\chi^2$ .
  - 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.
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# References

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Most of this presentation is based on

Press-Teukolsky-Vetterling-Flannery: Numerical Recipes, 3<sup>rd</sup> ed,

a highly recommended reference.

# Q & A



# References

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