Computational Methods

Optimization

Unconstrained Optimization

Optimization

- Optimization problems are concerned with finding the minimum or maximum of an objective function
  - Find x^* such that $f(x^*) \leq f(x)$ for all x in S
    - Maximization of $f(x)$ is the same as minimization of $-f(x)$
  - Least squares problem is a special case where the function to be minimized is the residual
- Optimization problems can also include a set of constraints that limit the set of feasible points, S
  - Unconstrained optimization does not have any constraints
  - Equality constraints are of the form $g(x) = 0$
  - Inequality constraints are of the form $h(x) \leq 0$

Optimization

- General continuous optimization problem is defined by the objective function and the constraints

  Find *min f(x)*

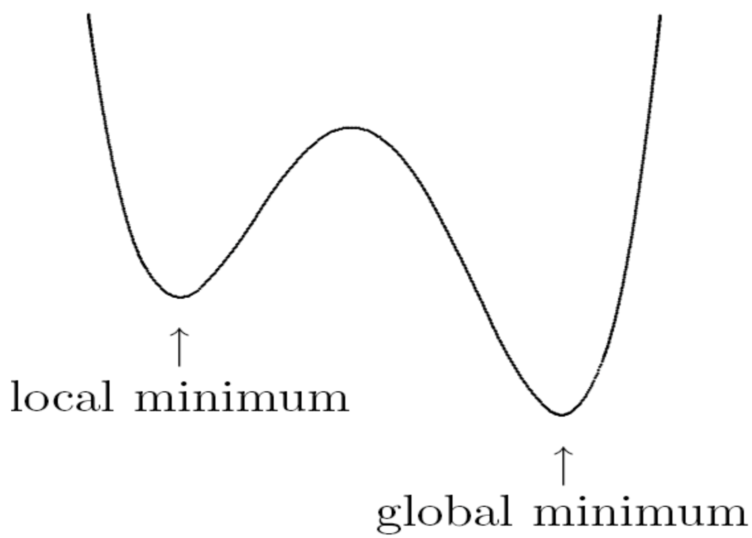
  Subject to $g_i(x) = 0$ and $h_j(x) \leq 0$

  $$f : \Re^n \rightarrow \Re \ , \ g : \Re^n \rightarrow \Re^m \ , \ h : \Re^n \rightarrow \Re^l$$

  - Linear programming characterizes optimization problems where the objective function and the constraints are linear
  - Nonlinear programming characterizes optimization problems where at least one of the constraints or the objective function are nonlinear

Global vs. Local Optimization

- A global optimum is a point that is an optimum for all feasible points (points matching the constraints)
- A local optimum is a point that is an optimum only for the feasible points in some neighborhood around the point



Global vs. Local Optimization

- Global optimization is in general a very difficult problem and existing methods for global optimality are limited to specific function types
  - Even verifying that an optimum is a global optimum is very difficult in general
- Most optimization methods are designed to find local optima
  - To increase the chance of finding global optima, local optimization methods can be run multiple times from different starting points

Existence of Solution

- Not every function has an optimum
  - E.g. Polynomials of odd order do not have global optima since they they tend to $\pm\infty$ for x towards $\pm\infty$
- Some conditions exist under which the existence of a global minimum can be ensured
  - If objective function $f(x)$ is continuous on a closed and bounded set S of feasible points, then $f(x)$ has a global minimum on S
  - If $f(x)$ is coercive on a closed, unbounded set S of feasible points, then it has a global minimum on S
    - Coercive: $\lim_{\|x\| \to \infty} f(x) = \infty$

Uniqueness of Solution

- If function *f(x)* is convex on the set of feasible points, *S*, then any minimum on S is a global minimum on *S*
  - In a convex function every minimum must have the same function value (all minima form a "plateau")
- If function *f(x)* is strictly convex on the set of feasible points, *S*, then it has a unique global minimum on *S*
  - A strictly convex function can only have one minimum

Optimality Conditions

- First-Order optimality condition
  - Any extremum of a continuous, differentiable function *f (x)* has to be either on the boundary of the feasible set or a critical point, i.e. a solution to the nonlinear system
    $\nabla f(x) = 0$
    - Not every critical point is an extrema (e.g. saddle points)
- Second-Order optimality condition
  - If *f(x)* is twice differentiable, the Hessian matrix (matrix of partial second derivatives) permits to identify extrema
    - Critical point x^* is a minimum if $H_f(x^*)$ is positive definite
    - Critical point x^* is a maximum if $H_f(x^*)$ is negative definite

Sensitivity and Conditioning

- Sensitivity analysis for the scalar case using Taylor series expansion
  - Absolute forward error: $\Delta x = \hat{x} - x^*$
  - Absolute backward error:

$$f(x^* + \Delta x) = f(x^*) + f'(x^*)\Delta x + \frac{1}{2} f''(x^*)\Delta x^2 + O(\Delta x^3) \approx f(x^*) + \frac{1}{2} f''(x^*)\Delta x^2$$

$$f(\hat{x}) - f(x^*) \approx \frac{1}{2} f''(x^*)\Delta x^2$$

  - Sensitivity of optimization:

$$|\Delta x| \approx \sqrt{2|f(\hat{x}) - f(x^*)| / |f''(x^*)|}$$

Unconstrained Optimization

- Unconstrained optimization has many similarities to the problem of solving equations and solution methods are similar
  - Direct search methods iteratively narrow down the neighborhood of the solution (like bisection method for equation solving
  - Iterated approximation methods use a fixed-point formulation and the derivative (or an approximation of it) to achieve the solution

Direct Search Methods for One-Dimensional Optimization

- Golden Section search iteratively narrows down the interval within which the solution has to exist
  - To ensure existence of the solution within the interval, the function is assumed to be unimodal in the interval
    - *f(x)* is unimodal in an interval if it has a minimum, x*, in the interval and is strictly increasing in both directions from this point
      - Any continuous, twice differentiable function has a (potenitally small) interval around each minimum for which the function is unimodal
  - To divide the interval two points, x_1, x_2, within the interval are used and their function values indicate which end of the interval can be discarded
    - The side of the point with the higher function value is discarded

Golden Section Search

- Golden Section achieves a reduction of the interval by a constant factor and requires only one function evaluation in each iteration by carefully choosing the locations of the interior points
  - Interior points in interval [a,b] are chosen at

$$x_1 = a + \frac{3-\sqrt{5}}{2}(b-a) \quad , \quad x_2 = a + \frac{\sqrt{5}-1}{2}(b-a)$$

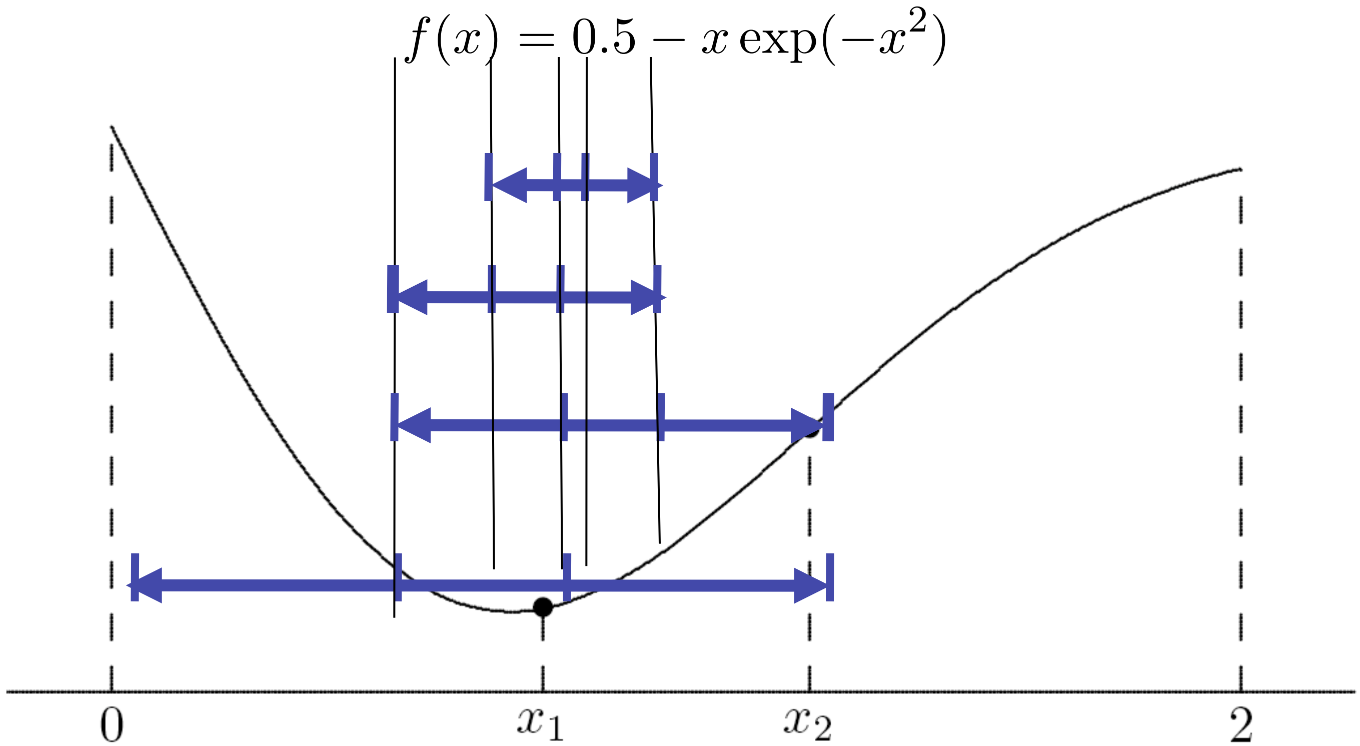
    - If one side of the interval is discarded the other point stays at a correct location in the new interval. E.g. if left is discarded:

$$x_2 = a + \frac{\sqrt{5}-1}{2}(b-a) = x_1 + \frac{2\sqrt{5}-4}{2}\frac{1}{1-(3-\sqrt{5})/2}(b-x_1) = x_1 + \frac{(2\sqrt{5}-4)2}{2(-1+\sqrt{5})}(b-x_1)$$

$$= x_1 + \frac{-3+4\sqrt{5}-5}{2(-1+\sqrt{5})}(b-x_1) = x_1 + \frac{(3-\sqrt{5})(-1+\sqrt{5})}{2(-1+\sqrt{5})}(b-x_1) = x_1 + \frac{3-\sqrt{5}}{2}(b-x_1)$$

Example

- Golden Section search on $f(x) = 0.5 - xe^{-x^2}$ and initial interval [0,2]



Successive Parabolic Interpolation

- Golden Section search is safe but converges only at a linear rate with constant 0.618
- Successive parabolic interpolation uses only one point in the interval, calculating the next (and which interval point to remove)
  - Take 3 points and their function values and interpolate them using a parabola
    - Minimum of parabola is added as a new point
    - Oldest of the points is dropped
  - Achieves superlinear convergence with $r \approx 1.324$

Newton's Method

- As in the case of solving nonlinear equations, a better convergence rate can be achieved using information about the function

$$f(x+\Delta x) \approx f(x) + f'(x)\Delta x + \frac{f''(x)}{2}\Delta x^2$$

  - Necessary first-order condition yields

$$\frac{\partial f(x+\Delta x)}{\partial \Delta x} = f'(x) + f''(x)\Delta x = 0 \quad \Rightarrow \quad \Delta x = -\frac{f'(x)}{f''(x)}$$

  - Yields Newton's method for *f'(x)=0*

$$x_{t+1} = x_t - \frac{f'(x_t)}{f''(x_t)}$$

    - Has quadratic convergence rate and converges if started close enough to the solution

Safeguard Methods

- As in nonlinear equation solving there are interval search methods that are guaranteed to converge slowly and methods with higher convergence rates but without guarantees that they will convergence
- Safeguard methods combine multiple methods to achieve both guaranteed convergence and a good convergence rate
  - Golden selection search and successive parabolic interpolation can be combined if no derivatives are available
  - Golden selection search and Newton's method can be combined if derivatives are available

Multi-Dimensional Optimization

- As for the one-dimensional case, two basic methods for optimization of multi-dimensional functions exist
  - Direct search methods
  - Iterative descent methods
- Direct search methods for multi-dimensional data introduce additional problems
  - Definition of an equivalent to a bracket is not easily possible in the multi-dimensional case

Nelder-Mead Method

- Nelder-Mead is a direct search method for the multi-variate case
  - Does not use a "bracket" but a simplex with $n+1$ points for a function with n variables
    - Points of the simplex form the points of interest defining a region
      - No guarantee that the solution lies within this region
    - Next search volume can lie partially outside the previous one
  - Next simplex is created by replacing the worst point of the existing simplex with a new point
    - New point is improved point on the line connecting the old point and the centroid of the remaining points in the simplex
    - If no better point is found, simplex is shrunk towards best point

Nelder-Mead Method

- Nelder-Mead does not require any information about the function to be minimized
  - Only evaluation of the function is necessary
  - Convergence is only guaranteed if the function within the simplex region has a unique minimum
- Operations change location and shape of simplex
  - Reflection: mirrors simplex away from worst point
  - Expansion: expands simplex in direction of new point
  - Contraction: contracts simplex away from worst point
  - Reduction: shrinks simplex around best point

Nelder-Mead Method

- Variations of the algorithm exists which apply slightly different rules to select operation
- A common set of rules is:
  - Precomputation:
    - Sort the vertices of the simplex by function value $f(x_i)$
    - Compute centroid x_c of the best n vertices
  - Start by applying reflection to worst vertex to get reflected vertex x_r

$$x_r = x_c + \alpha(x_c - x_{n+1}) \quad , \quad often \;\; \alpha = 1$$

    - If reflected vertex is not the worst of the remaining and not the best vertex, replace previously worst vertex with reflected vertex

Nelder-Mead Method

- Else, if reflected vertex is the best vertex apply expansion

$$x_e = x_c + \beta(x_c - x_{n+1}) \quad , \quad often \;\; \beta = 2$$

  - If expansion point is better than the reflected point, replace the worst point with the expanded point
  - Else replace the worst point with the reflected point
- Else, if reflected point is the worst point apply contraction

$$x_o = x_c - \gamma(x_c - x_{n+1}) \quad , \quad often \;\; \gamma = 1/2$$

  - If contraction point is better than the original worst point, replace the worst point with the contraction point
  - Else, if the contraction point is no better than the original worst point apply reduction by shrinking all points towards the best point

$$x_i = x_1 + \eta(x_i - x_1) \quad , \quad often \;\; \eta = 1/2$$

Nelder-Mead Method

- Nelder-Mead can be applied to smooth and non-smooth functions
  - Does not need derivatives
- Computational cost of the algorithm increases fast as the number of variables increases
- No guaranteed convergence
  - The choice of the initial simplex is essential to finding the desired minimum

Iterative Descent Methods

- When derivative information of the function is available, this information can be used to accelerate optimization on smooth functions
  - Steepest descent methods
    - Strictly follow the gradient direction of the function
  - Newton's method
    - Take into account the derivative of the gradient (the Hessian)
  - Quasi-Newton methods
    - Use a local approximation of the Hessian to reduce computation and be potentially more robust

Steepest Descent with Line Search

- In steepest descent methods the direction of the update step for the iterative solution is always given by the negative gradient at the current point.

$$x_{t+1} = x_t - \alpha_t \nabla f(x_t)$$

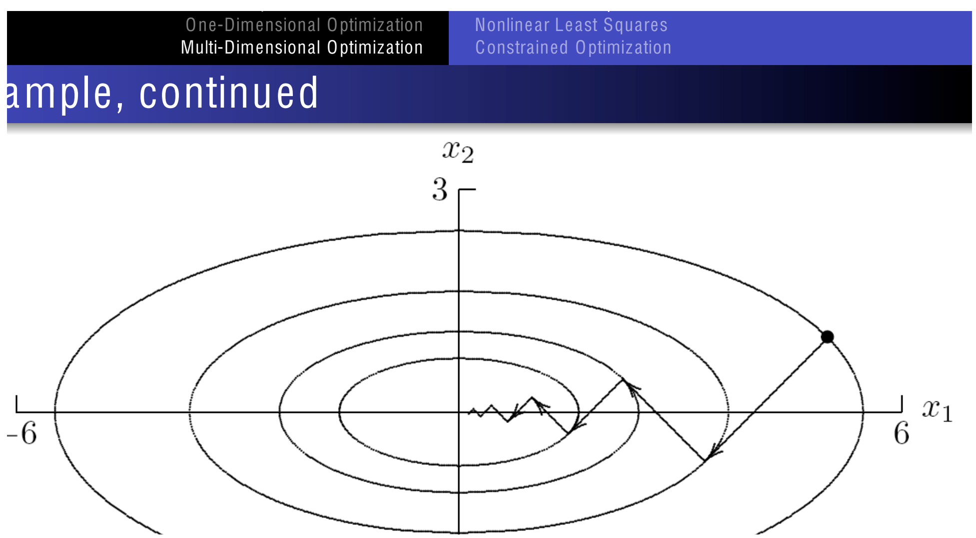
  - Pick of step size α is very important for convergence towards a solution
    - Line search can be used to determine the best α for the current point

$$\alpha_t = \arg\min_\alpha f(x_t - \alpha \nabla f(x_t))$$

      Line search can be solved a a one-dimensional minimization problem

Steepest Descent with Line Search

- Steepest descent with line search is very robust and reliable
  - Always makes progress
  - Convergence is only linear
    - Ignoring of second derivatives makes it inefficient



Newton's Method

- Rather than relying on the gradient alone (a first order approximation), Newton's method again uses a local second order approximation.

$$x_{t+1} = x_t - H_f^{-1}(x_t)\nabla f(x_t) \quad , \quad H_f(x)_{i,j} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}$$

  - To avoid the inversion, this can again be broken into a linear equation solution for the step size followed by an update

$$H_f(x_t)s_t = -\nabla f(x_t)$$

$$x_{t+1} = x_t + s_t$$

Newton's Method

- If it converges, Newton's method converges faster towards the solution
  - Quadratic convergence
  - Convergence is assured only when started close enough to a solution
    - In principle a step size is no longer necessary
    - Convergence can be improved by adding line search in the direction of the Newton step to ensure decrease in every step (damped Newton)
      - Incurs significant additional complexity

Quasi-Newton Methods

- Newton's method needs calculation of the Hessian and its inversion (solution of linear system).
  - *$O(n^3)$* computational complexity
  - Requires knowledge of the Hessian
- Quasi-Newton methods use an approximation of the Hessian (similar to Boyden's method)

$$x_{t+1} = x_t - \alpha_t B_f^{-1}(x_t)\nabla f(x_t)$$

  - Broyden–Fletcher–Goldfarb–Shannon (BFGS) Method
  - Conjugate Gradient Methods

BFGS Method

- Broyden–Fletcher–Goldfarb–Shannon (BFGS) is an extension of Broyden's Method for equation solving that maintains symmetry of approximate Hessian

$$x_{t+1} = x_t - B_f^{-1}(x_t)\nabla f(x_t)$$

  - The approximate Hessian is updated in each iteration starting with an initial estimate (often $B_0=I$)

$$B_t s_t = -\nabla f(x_t)$$

$$x_{t+1} = x_t + s_t$$

$$\Delta f'_{t+1} = \nabla f(x_{t+1}) - \nabla f(x_t)$$

$$B_{t+1} = B_t + (\Delta f'^{\,T}_{t+1}\,\Delta f'_{t+1}) \big/ (\Delta f'^{\,T}_t\, s_t) - (B_t s_t s_t^T B_t^T) \big/ (s_t^T B_t s_t)$$

Sherman-Morrison formula can be used to avoid inversion

BFGS Method

- BFGS method does not require second derivatives and is computationally much less expensive
  - Methods can be used to directly update factorization of B, making the method $O(n^2)$
  - Converges superlinearly
  - More robust than Newton's method
  - Line search can be used to add a step size
    - Can increase the convergence radius for BFGS
      - Incurs additional cost

Conjugate Gradient Method

- The Conjugate gradient method further simplifies the approximation of the Hessian by explicitly estimating its effect on the gradient

$$x_{t+1} = x_t - \alpha_t(\nabla f(x_t) - \beta_t s_{t-1})$$

$$s_t = -\nabla f(x_t) + \beta_t s_{t-1}$$

$$\beta_t = (\nabla f(x_t)^T \nabla f(x_t)) \big/ (\nabla f(x_{t-1})^T \nabla f(x_{t-1}))$$

  - Conjugate gradient is exact for a quadratic objective function after at most n iterations
    - Also works usually well for general unconstrained optimization
  - The step parameter can be formed using line search

Unconstrained Optimization

- Unconstrained Optimization allows to find the best parameters for arbitrary objective functions
  - Least squares is a special case of unconstrained optimization
- Two basic approaches exist
  - Direct search techniques
  - Iterative improvement algorithms
    - Newton's method if gradient and Hessian information is available
    - Quasi-Newton methods if no such information is to be used.