CS 450: Numerical Anlaysis[1]

Numerical Optimization

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[1] *These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book "Scientific Computing: An Introductory Survey" by Michael T. Heath (slides).*

Numerical Optimization

- Our focus will be on *continuous* rather than *combinatorial* optimization:

equality   inequality

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{subject to} \quad \boldsymbol{g}(\boldsymbol{x}) = \mathbf{0} \quad \text{and} \quad \boldsymbol{h}(\boldsymbol{x}) \leq \mathbf{0}$$

constraints

$\Downarrow$

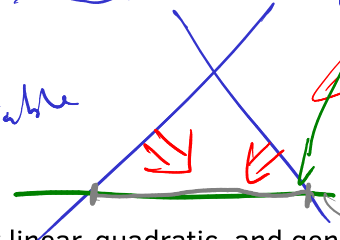
feasible region

$\{x : x \in \mathbb{R}^n, g(x) = 0, h(x) \leq 0\}$

$f : \mathbb{R}^n \to \mathbb{R}$

$\downarrow$

is differentiable



- We consider linear, quadratic, and general nonlinear optimization problems:

$\downarrow$

f, g, h are affine functions

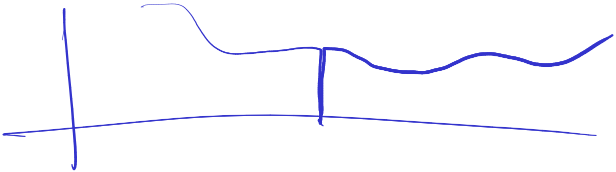
quadratic $\to$ f is quadratic, g, h are linear

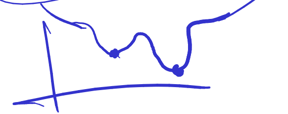
$H_f(x) = H_f(x')$

$\frac{1}{2}x^T A x - b^T x$

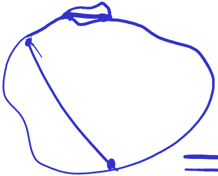
Local Minima and Convexity

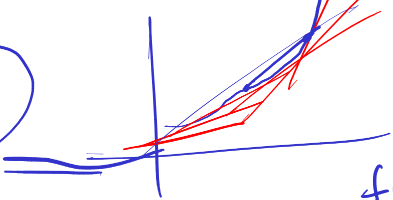
- Without knowledge of the analytical form of the function, numerical optimization methods at best achieve convergence to a *local* rather than *global* minimum:





- A set is *convex* if it includes all points on any line, while a function is (strictly) convex if its (unique) local minimum is always a global minimum:





S is convex if

$\forall x, y \in S$, $\alpha x + (1-\alpha) y \in S$

f is convex if

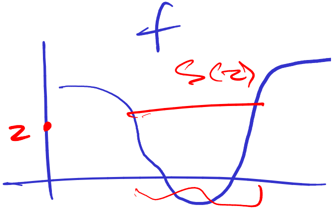
$f(\alpha x + (1-\alpha) y) \leq \alpha f(x) + (1-\alpha) f(y)$

Existence of Local Minima

- *Level sets* are all points for which f has a given value, *sublevel sets* are all points for which the value of f is less than or equal to a given value:

$$L(z) = \{x : f(x) = z\}$$

$$S(z) = \{x : f(x) \leq z\}$$



- If there exists a closed and bounded sublevel set in the domain of feasible points, then f has has a global minimum in that set:

need to find z, s.t. $S(z)$ $\underbrace{\text{has finite size}}_{\text{bounded}}$

and $\underbrace{\text{includes its own boundary}}_{\text{closed}}$

Optimality Conditions

- If x is an interior point in the feasible domain and is a local minima,

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} \frac{df}{dx_1}(\boldsymbol{x}) & \cdots & \frac{df}{dx_n}(\boldsymbol{x}) \end{bmatrix}^T = \mathbf{0}:$$

if $\frac{df}{dx_i}(x) < 0$ then $x + \delta x \rightarrow f(x+\delta x) < f(x)$

if $\frac{df}{dx_i}(x) > 0$ $x - \delta x$

- *Critical points* $\boldsymbol{x}$ satisfy $\nabla f(\boldsymbol{x}) = \mathbf{0}$ and can be minima, maxima, or saddle points:

in scalar case, value of $f''(x)$ distinguishes

Hessian Matrix

- To ascertain whether a critical point x, for which $\nabla f(x) = \mathbf{0}$, is a local minima, consider the *Hessian matrix*:

$$H_f(x) = J_{\nabla f}(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \\ \vdots & \ddots & \\ & & \end{bmatrix}$$

$$H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}(x)$$

$$H = H^T$$

- If x^* is a minima of f, then $H_f(x^*)$ is positive semi-definite:

$$f(x) = f(x^*) + \nabla f(x^*)(x - x^*) + \frac{1}{2}(x - x^*)^T H_f(x^*)(x - x^*) + \cdots$$

$$\nabla f(x^*) = 0$$

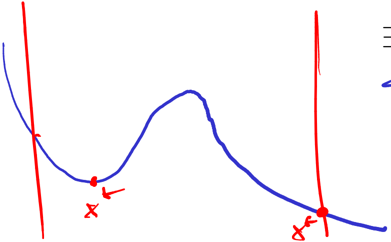
$$\lambda(H_f(x^*)) \geq 0$$

$$x^T H_f(x^*) x \geq 0$$

if $\exists s$, s.t. $s^T H_f(x^*) s < 0$

Optimality on Feasible Region Border

- Given an equality constraint $\boldsymbol{g}(\boldsymbol{x}) = \mathbf{0}$, it is no longer necessarily the case that $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$. Instead, it may be that directions in which the gradient decreases lead to points outside the feasible region:



$$\exists \boldsymbol{\lambda} \in \mathbb{R}^n, \quad -\nabla f(\boldsymbol{x}^*) = \boldsymbol{J}_{\boldsymbol{g}}^T(\boldsymbol{x}^*)\boldsymbol{\lambda}$$

- Such *constrained minima* are critical points of the Lagrangian function $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \boldsymbol{\lambda}^T \boldsymbol{g}(\boldsymbol{x})$, so they satisfy:

$$\nabla \mathcal{L}(\boldsymbol{x}^*, \boldsymbol{\lambda}) = \begin{bmatrix} \nabla f(\boldsymbol{x}^*) + \boldsymbol{J}_{\boldsymbol{g}}^T(\boldsymbol{x}^*)\boldsymbol{\lambda} \\ \boldsymbol{g}(\boldsymbol{x}^*) \end{bmatrix} = \mathbf{0}$$

Sensitivity and Conditioning

- The condition number of solving a nonlinear equations is $1/f'(x^*)$, however for a minimizer x^*, we have $f'(x^*) = 0$, so conditioning of optimization is inherently bad:

- To analyze worst case error, consider how far we have to move from a root $\boldsymbol{x}^*$ to perturb the function value by ϵ:

Golden Section Search

- Given bracket $[a, b]$ with a unique local minimum (f is *unimodal* on the interval), *golden section search* considers consider points $f(x_1), f(x_2)$, $a < x_1 < x_2 < b$ and discards subinterval $[a, x_1]$ or $[x_2, b]$:

- Since one point remains in the interval, golden section search selects x_1 and x_2 so one of them can be effectively reused in the next iteration:

Newton's Method for Optimization

Demo: *Newton's Method in 1D*

- At each iteration, approximate function by quadratic and find minimum of quadratic function:

- The new approximate guess will be given by $x_{k+1} - x_k = -f'(x_k)/f''(x_k)$:

Successive Parabolic Interpolation

- Interpolate f with a quadratic function at each step and find its minima:

- The convergence rate of the resulting method is roughly 1.324

Safeguarded 1D Optimization

- Safeguarding can be done by bracketing via golden section search:

- Backtracking and step-size control:

Demo: *Nelder-Mead Method*

General Multidimensional Optimization

- Direct search methods by simplex (*Nelder-Mead*):

- Steepest descent: find the minimizer in the direction of the negative gradient:

Convergence of Steepest Descent

- Steepest descent converges linearly with a constant that can be arbitrarily close to 1:

- Given quadratic optimization problem $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} + \boldsymbol{c}^T\boldsymbol{x}$ where $\boldsymbol{A}$ is symmetric positive definite, the error $\boldsymbol{e}_k = \boldsymbol{x}_k - \boldsymbol{x}^*$ satisfies

Gradient Methods with Extrapolation

- We can improve the constant in the linear rate of convergence of steepest descent by leveraging *extrapolation methods*, which consider two previous iterates (maintain *momentum* in the direction $\boldsymbol{x}_k - \boldsymbol{x}_{k-1}$):

- The *heavy ball method*, which uses constant $\alpha_k = \alpha$ and $\beta_k = \beta$, achieves better convergence than steepest descent:

Conjugate Gradient Method

- The *conjugate gradient method* is capable of making the optimal choice of α_k and β_k at each iteration of an extrapolation method:

- *Parallel tangents* implementation of the method proceeds as follows

Demo: *Conjugate Gradient Parallel Tangents as Krylov Subspace Method*

Krylov Optimization

- Conjugate Gradient finds the minimizer of $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} + \boldsymbol{c}^T\boldsymbol{x}$ within the Krylov subspace of $\boldsymbol{A}$:

Newton's Method

- Newton's method in n dimensions is given by finding minima of n-dimensional quadratic approximation:

Quasi-Newton Methods

- *Quasi-Newton* methods compute approximations to the Hessian at each step:

- The *BFGS* method is a secant update method, similar to Broyden's method:

Nonlinear Least Squares

- An important special case of multidimensional optimization is *nonlinear least squares*, the problem of fitting a nonlinear function $f_{\boldsymbol{x}}(t)$ so that $f_{\boldsymbol{x}}(t_i) \approx y_i$:

- We can cast nonlinear least squares as an optimization problem and solve it by Newton's method:

Gauss-Newton Method

- The Hessian for nonlinear least squares problems has the form:

- The *Gauss-Newton* method is Newton iteration with an approximate Hessian:

- The Levenberg-Marquardt method incorporates Tykhonov regularization into the linear least squares problems within the Gauss-Newton method.

Constrained Optimization Problems

- We now return to the general case of *constrained* optimization problems:

- Generally, we will seek to reduce constrained optimization problems to a series of unconstrained optimization problems:
  - *sequential quadratic programming*:
  - *penalty-based methods*:
  - *active set methods*:

Sequential Quadratic Programming

- *Sequential quadratic programming* (SQP) corresponds to using Newton's method to solve the equality constrained optimality conditions, by finding critical points of the Lagrangian function $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \boldsymbol{\lambda}^T \boldsymbol{g}(\boldsymbol{x})$,

- At each iteration, SQP computes $\begin{bmatrix} \boldsymbol{x}_{k+1} \\ \boldsymbol{\lambda}_{k+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{x}_{k} \\ \boldsymbol{\lambda}_{k} \end{bmatrix} + \begin{bmatrix} \boldsymbol{s}_{k} \\ \boldsymbol{\delta}_{k} \end{bmatrix}$ by solving

Inequality Constrained Optimality Conditions

- The *Karush-Kuhn-Tucker (KKT)* conditions hold for local minima of a problem with equality and inequality constraints, the key conditions are

- To use SQP for an inequality constrained optimization problem, consider at each iteration an *active set* of constraints:

Penalty Functions

- Alternatively, we can reduce constrained optimization problems to unconstrained ones by modifying the objective function. *Penalty* functions are effective for equality constraints $\boldsymbol{g}(\boldsymbol{x}) = 0$:

- The augmented Lagrangian function provides a more numerically robust approach:

Barrier Functions

- *Barrier functions* (*interior point methods*) provide an effective way of working with inequality constraints $\boldsymbol{h}(\boldsymbol{x}) \leq \mathbf{0}$: