N-dimensional nonlinear equations

N-d solve

$\downarrow$

N-d optimization

Solving Nonlinear Equations

What is the goal here?

$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}\right) = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} f_1(x_1, \ldots, x_n) \\ \vdots \\ f_n(x_1, \ldots, x_n) \end{bmatrix}$$

find

Newton's method

What does Newton's method look like in n dimensions?

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

$$0$$

$$f(x_0 + s) =$$

$$= f(x_0) + Js$$

$$-Js = f(x_0)$$

$$s = -J^{-1} f(x_0)$$

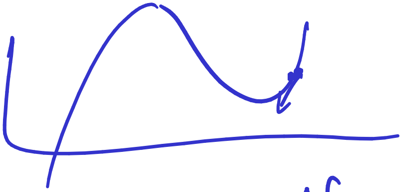
$$x_1 = x_0 + s$$

Newton: Example

Set up Newton's method to find a root of

$$\mathbf{f}(x,y) = \begin{pmatrix} x + 2y - 2 \\ x^2 + 4y^2 - 4 \end{pmatrix}.$$

Demo: Newton's method in n dimensions



$$x_k = x_{k-1} - J^{-1}_{x_{k-1}} f(x_{k-1})$$

$$J = \begin{bmatrix} \partial f_1/\partial x & \partial f_1/\partial y \\ \partial f_2/\partial x & \partial f_2/\partial y \end{bmatrix}$$

$$J = \begin{bmatrix} 1 & 2 \\ 2x & 8y \end{bmatrix}$$

Secant in n dimensions?

> What would the secant method look like in n dimensions?

1D: $x_{k+1} = x_k - \dfrac{f(x_k)}{\text{estimate of derivative at } x_k}$

$$= x_k - \frac{f(x_k)}{\dfrac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}}$$

nD

$J \Rightarrow x_{k+1} = x_k - J^{-1} f(x_k)$

$J x_k - J x_{k-1} = f(x_k) - f(x_{k-1})$

unknown

Broyden's method

minimize norm of $J_{k+1} - J_k$

Solving : • approximate function
with a linear expansion
• find zero of linear fun

Optimize : - approximate with quadratic
• minimize quadratic

Outline

Optimization

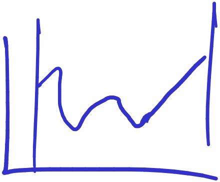
State the problem.

$$\min f(x) \quad \text{s.t.} \quad g(x) > 0, \; h(x) = 0$$

objective function

constraints

1D case



local minima: $f'(x) = 0$

Optimization: What could go wrong?

What are some potential problems in optimization?

Optimization: What is a solution?

How can we tell that we have a (at least local) minimum? (Remember calculus!)

$f'(x) = 0$

Newton's Method

Let's steal the idea from Newton's method for equation solving:
Build a simple version of f and minimize that.

solve $g(x) = f'(x) = 0$

apply Newton to $g(x)$

$$x_k = x_{k-1} - \frac{g(x_{k-1})}{g'(x_{k-1})}$$

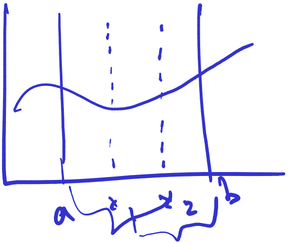
$$= x_{k-1} - \frac{f'(x_{k-1})}{f''(x_{k-1})}$$

Demo: Newton's method in 1D

In-class activity: Optimization Methods

Golden Section Search

Would like a method like bisection, but for optimization.
In general: No invariant that can be preserved.
Need *extra assumption*.

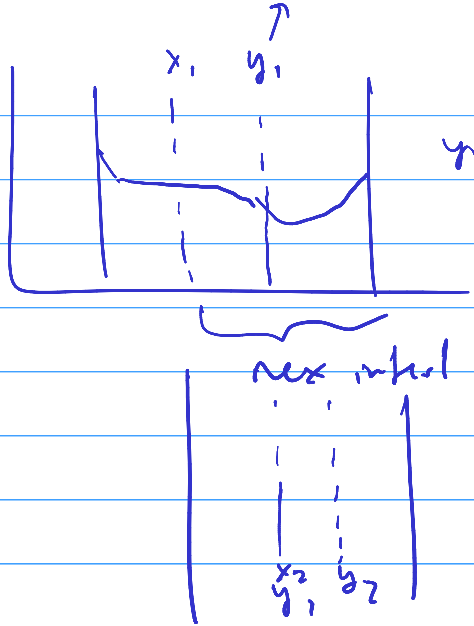


$g(x) = x + a$

$x + a > 0$

x^* - solution

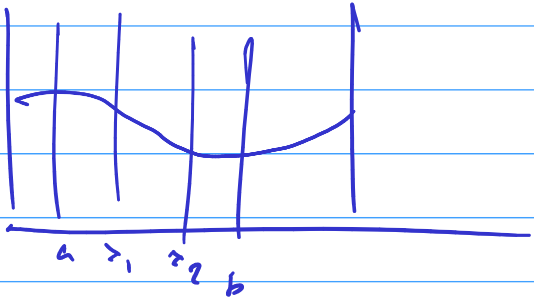
f is unimodal



$y_1 - x_1 \quad \frac{1+\sqrt{5}}{2}$

if $f(x_1) > f(x_2) \rightarrow (x_1, b)$

if $f(x_1) \leq f(x_2) \rightarrow (a, x_2)$



Demo: Golden Section Search Proportions

Outline

Optimization in n dimensions: What is a solution?

How can we tell that we have a (at least local) minimum? (Remember calculus!)

$$\nabla f = 0 \rightarrow \text{critical point}$$

$$+ \quad H_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & & \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & & \end{bmatrix} \quad \text{positive definite}$$

$$\Rightarrow \text{local minima}$$

Steepest Descent

Given a scalar function $f : \mathbb{R}^n \to \mathbb{R}$ at a point $\boldsymbol{x}$, which way is down?

x_0 - starting guess

$-\nabla f(x_0)$

line search along

along $-\nabla f(x_k) + x_k$

CS 450 - Numerical Algorithms

CS 554 - Parallel Numerical Algorithms

CS 555

CS 598 - Andreas

Fast integral methods