Overview of Optimization Problems

slides credit: Steven Johnson

Why optimization?

- In some sense, *all engineering design* is optimization: choosing design parameters to improve some objective
- Much of *data analysis* is also optimization: extracting some model parameters from data while minimizing some error measure (e.g. fitting)
- Most *business decisions* = optimization: varying some *decision parameters* to maximize profit (e.g. investment portfolios, supply chains, etc.)

A general optimization problem

$$\min_{x \in \mathbb{R}^n} f_0(x)$$

subject to m constraints

$$f_i(x) \leq 0$$

$$i = 1, 2, \ldots, m$$

x is a *feasible point* if it satisfies all the constraints

feasible region = set of all feasible x

minimize an objective function f_0 with respect to n design parameters x
(also called *decision parameters*, *optimization variables*, etc.)

— note that *maximizing* $g(x)$ corresponds to $f_0(x) = -g(x)$

note that an *equality constraint*

$$h(x) = 0$$

yields two inequality constraints

$$f_i(x) = h(x) \text{ and } f_{i+1}(x) = -h(x)$$

(although, in practical algorithms, equality constraints typically require special handling)

Important considerations

- *Global* versus *local* optimization
- *Convex* vs. non-convex optimization
- Unconstrained or box-constrained optimization, and other special-case constraints
- Special classes of functions (linear, etc.)
- Differentiable vs. non-differentiable functions
- Gradient-based vs. derivative-free algorithms
- …
- Zillions of different algorithms, usually restricted to various special cases, each with strengths/weaknesses

Global vs. Local Optimization

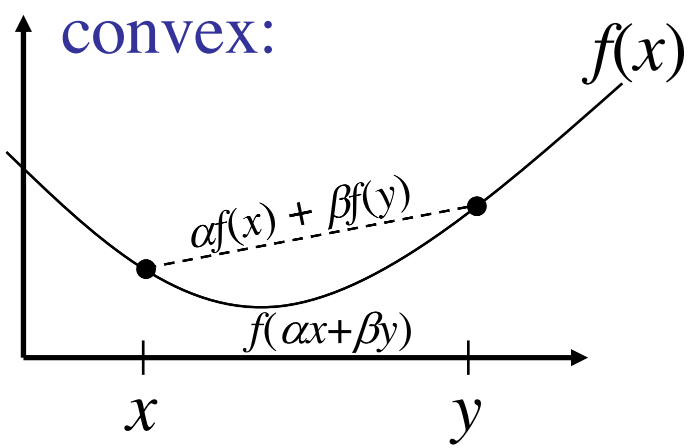
- For *general nonlinear* functions, *most* algorithms only guarantee a local optimum
  - that is, a feasible x_o such that $f_0(x_o) \leq f_0(x)$ for all feasible x within some neighborhood $\|x - x_o\| < R$ (for some small R)
- A *much harder* problem is to find a global optimum: the minimum of f_0 for *all* feasible x
  - exponentially increasing difficulty with increasing n, practically impossible to *guarantee* that you have found global minimum without knowing some special property of f_0
  - many available algorithms, problem-dependent efficiencies
    - *not* just genetic algorithms or simulated annealing (which are popular, easy to implement, and thought-provoking, but usually *very slow*!)
    - for example, non-random systematic search algorithms (e.g. DIRECT), partially randomized searches (e.g. CRS2), repeated local searches from different starting points ("multistart" algorithms, e.g. MLSL), …

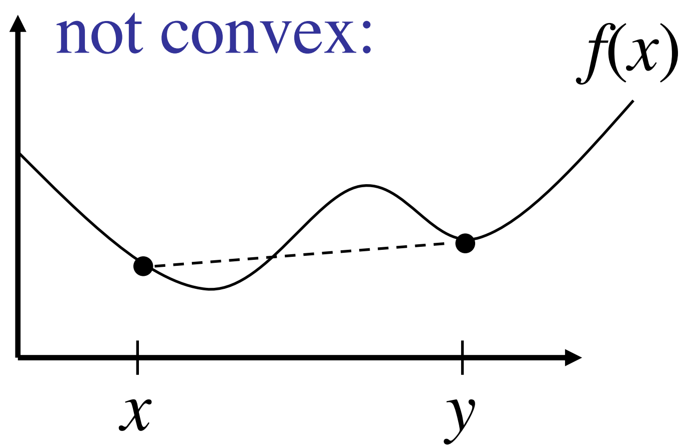
Convex Optimization

[good reference: *Convex Optimization* by Boyd and Vandenberghe, free online at www.stanford.edu/~boyd/cvxbook]

All the functions f_i (i=0…m) are *convex*:

$$f_i(\alpha x + \beta y) \leq \alpha f_i(x) + \beta f_i(y) \quad \text{where} \quad \begin{array}{c} \alpha + \beta = 1 \\ \alpha, \beta \in [0,1] \end{array}$$





For a convex problem (convex objective & constraints)
any local optimum *must* be a global optimum
$\Rightarrow$ efficient, robust solution methods available

Important Convex Problems

- LP (linear programming): the objective and constraints are *affine*: $f_i(x) = a_i^T x + \alpha_i$
- QP (quadratic programming): affine constraints + convexquadratic objective $x^T A x + b^T x$
- SOCP (second-order cone program): LP + *cone* constraints $||Ax+b||_2 \leq a^T x + \alpha$
- SDP (semidefinite programming): constraints are that $\Sigma A_k x_k$ is positive-semidefinite

all of these have very efficient, specialized solution methods

Important special constraints

- Simplest case is the *unconstrained* optimization problem: m=0
  - e.g., line-search methods like steepest-descent, nonlinear conjugate gradients, Newton methods …
- Next-simplest are *box constraints* (also called *bound constraints*): $x_k^{\min} \le x_k \le x_k^{\max}$
  - easily incorporated into line-search methods and many other algorithms
  - many algorithms/software *only* handle box constraints
- …
- Linear equality constraints $Ax=b$
  - for example, can be explicitly eliminated from the problem by writing $x=Ny+\xi$, where ξ is a solution to $A\xi=b$ and N is a basis for the nullspace of A

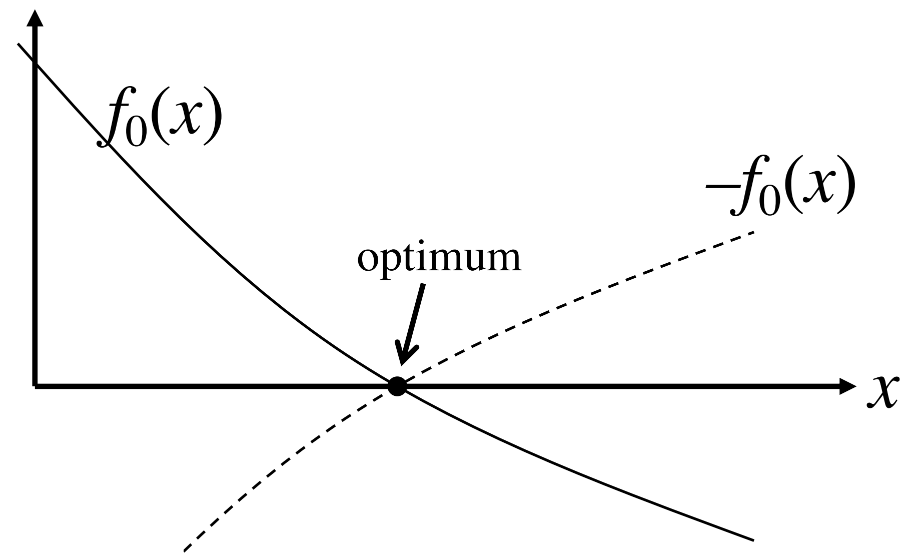
Derivatives of f_i

- Most-efficient algorithms typically require user to supply the gradients $\nabla_x f_i$ of objective/constraints
  - you should *always* compute these analytically
    - rather than use finite-difference approximations, better to just use a derivative-free optimization algorithm
    - in principle, one can always compute $\nabla_x f_i$ with about the same cost as f_i, using adjoint methods
  - gradient-based methods can find (local) optima of problems with millions of design parameters
- Derivative-free methods: only require f_i values
  - easier to use, can work with complicated "black-box" functions where computing gradients is inconvenient
  - *may* be only possibility for nondifferentiable problems
  - need $> n$ function evaluations, bad for large n

Removable non-differentiability

consider the *non*-differentiable *unconstrained* problem:

$$\min_{x \in \mathbb{R}^n} |f_0(x)|$$



equivalent to *minimax* problem:

$$\min_{x \in \mathbb{R}^n} (\max\{f_0(x), -f_0(x)\})$$

…still nondifferentiable…

…equivalent to *constrained* problem with a "temporary" variable *t*:

differentiable!

$$\min_{x \in \mathbb{R}^n, t \in \mathbb{R}} t \quad \text{subject to:} \quad \begin{array}{l} t \geq f_0(x) \\ t \geq -f_0(x) \end{array}$$

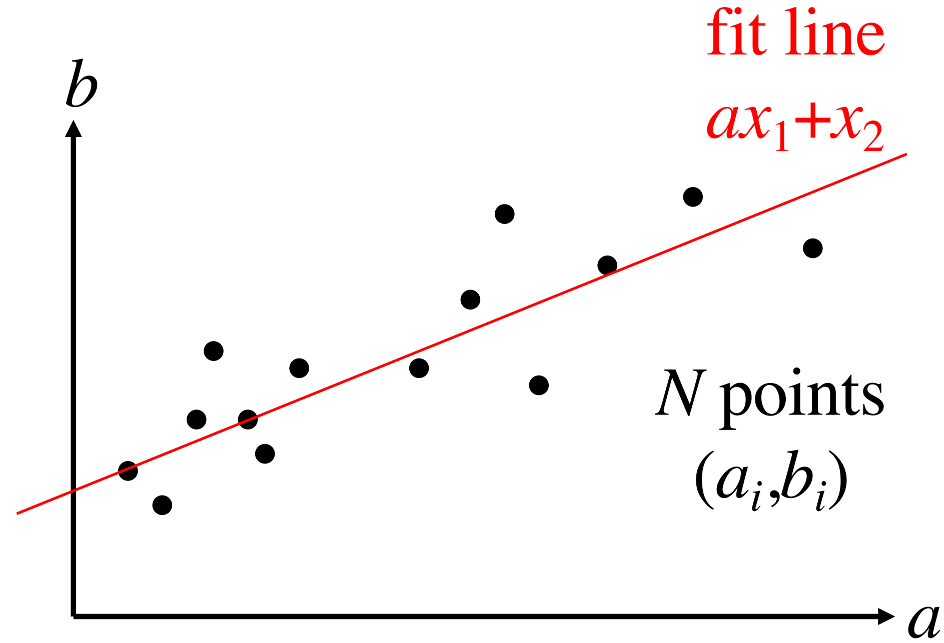
i.e. $f_1(x,t) = f_0(x) - t$
$f_2(x,t) = -f_0(x) - t$

Example: Chebyshev linear fitting

find the fit that minimizes the *maximum error*:

$$\min_{x_1,x_2}\left(\max_i |x_1 a_i + x_2 - b_i|\right) = \min_{x\in\mathbb{R}^2} \|Ax - b\|_\infty$$

… nondifferentiable minimax problem



equivalent to a *linear programming* problem (LP):

$$\min_{x_1,x_2,t} t$$

subject to $2N$ constraints:

$$t \geq x_1 a_i + x_2 - b_i$$
$$t \geq -x_1 a_i - x_2 + b_i$$

equivalently:

$$t \geq |x_1 a_i + x_2 - b_i|$$

Relaxations of Integer Programming

If x is integer-valued rather than real-valued (e.g. $x \in \{0,1\}^n$), the resulting *integer programming* or *combinatorial optimization* problem becomes *much harder* in general.

However, useful results can often be obtained by a *continuous relaxation* of the problem — e.g., going from $x \in \{0,1\}^n$ to $x \in [0,1]^n$ … at the very least, this gives an lower bound on the optimum f_0

"Penalty terms" or "projection filters" (SIMP, RAMP, etc.) can be used to obtain x that ≈ 0 or ≈ 1 almost everywhere.

[See e.g. Sigmund & Maute, "Topology optimization approaches," *Struct. Multidisc. Opt.* **48**, pp. 1031–1055 (2013).]

Stochastic Optimization

$$\min_{x \in \mathbb{R}^n} E[f(x, \xi)]$$

where $E[\cdots]$ is expected value averaging over random vars ξ

Deep-learning example:

Fitting ("learning") to a huge "training set" by sampling a random subset ξ:

$$f(x, \xi) = \sum_{k \in \xi} f_k(x)$$

$\nabla_x f$ often exists, but typically can't use standard gradient-descent because of randomness.

A popular algorithm: Adam [Kingma & Ba, 2014]
"stochastic gradient descent"

Some Sources of Software

- NLopt: implements many nonlinear optimization algorithms
  callable from many languages (C, Python, R, Matlab, …)
  (global/local, constrained/unconstrained, derivative/no-derivative)
  http://github.com/stevengj/nlopt

- Python: scipy.optimize, pyOpt, …; Julia: JuMP, Optim,…

- Decision tree for optimization software:
  http://plato.asu.edu/guide.html
  — lists many (somewhat older) packages for many problems

- CVX: general convex-optimization package http://cvxr.com
  … also Python CVXOPT, R CVXR, Julia Convex