Lecture 6: Optimization

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- \blacktriangleright Lectures: cover the material no code, mostly theory
- \blacktriangleright Labs: Cover examples and code, work on problem sets. Run through Week 10
- ▶ Problem Sets: you have four more to go
- \triangleright Take Home Exam: we will be announcing the dates shortly!
- ▶ Office Hours (Jacob): Fridays 11:00 12:00, Location: 31 Buccleuch Place, 2.11

Numerical Optimization is Essential

- Nearly every economics problem that we write down involves some sort of optimization problem
	- \triangleright Utility maximization: Demand for several goods, consumption vs. savings, leisure vs. consumption,
	- \blacktriangleright Profit maximization
	- \blacktriangleright Planners' problem
	- \triangleright Best response in a game (nash equilibria)
	- \blacktriangleright etc...
- \triangleright But optimization shows up in lots of other places!
	- \triangleright Most (all?) estimators in statistics/econometrics are parameters that solve an appropriate minimization problem
- It shouldn't surprise you that when we can't solve these problems analytically, we turn to a numerical analysis of the problem

Types of Optimization Problems

 \blacktriangleright Local vs. Global

 \blacktriangleright Univariate vs. Multivariate

 \blacktriangleright Linear vs. Nonlinear

 \triangleright Constrained vs. Unconstrained

Section 1

[Unconstrained Optimization: Univariate](#page-4-0)

Problem Setup

Suppose we're given some function $f : \mathbb{R} \to \mathbb{R}$, and we're asked to solve:

$$
\min_{x \in \mathbb{R}} f(x) \tag{1}
$$

- \triangleright We haven't been told anything yet about f.
	- \blacktriangleright It's not necessarily differentiable
	- \triangleright We certainly don't have enough to get an analytic solution
- \blacktriangleright This problem seems simple, but a surprising number of economic problems can be solved with just univariate optimization
- Inter These methods also form the building blocks for some multivariate algorithms, so it is important to have fast methods to solve problems like this

Bracketing Method

- ▶ Suppose that $f : \mathbb{R} \to \mathbb{R}$ is continuous and,
- ► Suppose we've found points a, b and $c \in \mathbb{R}$ such that

 $f(a) > f(b)$ and $f(c) > f(b)$ (2)

- \triangleright We know that somewhere in (a, c) there is a minimum value $Why?$ Well, since f is continuous, and $[a, c]$ is compact, we know a minimum exists, and since $f(b) < f(a)$ and $f(b) < f(c)$, it cannot attain its minimum at the boundary
- Can we refine this to find a minimum?
- \triangleright Note: ideally, we want to find m_1 since it is the global minimum

Algorithm 1 Bracketing Algorithm

```
Require: a < b < c such that f(a) > f(b) and f(c) > f(b)1: while c - a > \epsilon do . For \epsilon > 0<br>2: if b - a < c - b then . \epsilon > 0 . Choose a test point
2: if b - a < c - b then<br>3: d \leftarrow (b + c)/2d \leftarrow (b+c)/24: else
5: d \leftarrow (a+b)/2<br>6: end if
       6: end if
7: if d > b then
8: if f(d) > f(b) then
9: (a, b, c) \leftarrow (a, b, d) \rightarrow d is our new c
10: else if f(d) < f(b) then
11: (a, b, c) \leftarrow (b, d, c) \triangleright d is our new candidate
12: end if
19: end if
20: end while
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- \blacktriangleright If we continue this process, the algorithm will eventually converge.
	- \blacktriangleright At every step, we always choose a and c so that we are bracketing a minimum
	- \triangleright Our candidate point *b* always has $f(b) < f(a)$ and $f(c)$.
- \blacktriangleright The convergence rate is quite slow compared to other algorithms, but it will always work for any continuous, bounded function on a finite interval.
- \triangleright Notice, however, that we missed the true global minimum of the function.
- \blacktriangleright The bracketing algorithm is guaranteed to find a local minimum, but not necessarily the global minimum.
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Other Gradient Free Algorithms

Bracketing is slow, but we can often do better, even without derivative based methods

- Golden-section search
	- \blacktriangleright This is the same as the bracketing algorithm, but chooses our candidate and test points differently

Instead of choosing the midpoint of the intervals, we choose $b = c - (b - a)/\phi$ and $d = a + (c - b)/\phi$ where $\phi = (1 + \sqrt{5})/2$

Note that ϕ is the golden ratio

- \triangleright This keeps the size of the intervals at a constant ratio, which ensures that we are doing a better job of sampling the interval for the minimum (and avoids taking a large number of steps that are inefficiently close together)
- \triangleright Still has slow convergence, but it's guaranteed just like in the bracketing case.

Other Gradient Free Algorithms

\blacktriangleright Successive Parabolic Interpolation

- \triangleright Generates new candidate points by fitting a parabola to the last three points and choosing the minimum of the parabola as the new candidate
- In general, this is a much faster algorithm than the bracketing methods, however it can often fail to converge if the function is not well behaved
- ▶ Brent's method: combines SPI with Golden Section Search
	- \triangleright Attempts to take steps with successive parabolic interpolation
	- \blacktriangleright Falls back to the Golden-section search method if that fails.
	- \blacktriangleright This means it retains the best case properties of SPI, and often is your best bet for derivative free optimization over a single variable.

Newton's Method

 \triangleright We can do much better, however, if we are willing to use the derivatives of f

In Consider a point x_k **, and let's do a second order Taylor approximation of f around** x_k **:**

$$
p_k(x) := f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2}f''(x_k)(x - x_k)^2
$$
\n(3)

Suppose that $f''(x_k) > 0$: then $p_k(x)$ is convex, and the minimum of $p_k(x)$ is at

$$
x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}
$$
 (4)

- If p_k is a good global approximation of f, then x_{k+1} should be close to the true minimum Or at least, closer than x_k
- If we start with a good enough guess x_0 , the sequence defined by this procedure will converge to the true minimum of f

Note, however, that with a bad guess, Newton's method does not need to converge at all

Section 2

[Unconstrained Optimization: Multivariate](#page-18-0)

Problem

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$, and we want to solve the problem

$$
\max_{x \in \mathbb{R}^n} f(x) \tag{5}
$$

 \triangleright We know that if f is differentiable, a necessary condition for optimality is that:

$$
Df(x) = 0 \tag{6}
$$

If you haven't seen this notation before, read $Df(x)^T = \nabla f(x)$ if $f: \mathbb{R}^n \to \mathbb{R}$, or as $f'(x)$ if $n = 1$.

In general, if $f: \mathbb{R}^n \to \mathbb{R}^m$, then $Df(x)$ is an $m \times n$ matrix, where $(Df(x))_{ij} = \frac{\partial f_i}{\partial x_j}$

\blacktriangleright There are several main approaches here

- 1. Newton's Method: Attack eq. (6) directly as a root finding problem. This will require calculating the Hessian $D^2f(x)$
- 2. Gradient Based: Use information encoded in the gradient $Df(x)$ to either climb down the hill towards the minimum, or to approximate $D^2 f(x)$.
- 3. Gradient Free: Many different approaches.

 \triangleright We can do the same 2nd order approximation as before:

$$
p_k(x) = f(x_k) + Df(x_k)(x - x_k) + \frac{1}{2}(x - x_k)^T D^2 f(x_k)(x - x_k)
$$
(7)

If we differentiate this with respect to x , and set it equal to zero, we can obtain:

$$
x^* = x_k - (D^2 f(x_k))^{-1} Df(x_k)
$$
 (8)

- Newton's method: set $x_{k+1} = x^*(x_k)$ and keep iterating until convergence
- \triangleright You can prove that this will converge if you start with a good enough guess (close to the true minimum)
- **Problems: Newton's method takes itself too seriously**
	- **F** Treats a **local** 2nd order approximation as though it's good **globally**
	- \triangleright With a bad initial guess, tends to take extremely large step sizes, which take you even farther away from the true optimum, and the whole thing breaks down

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Newton's Method with Line Searches

- In What if instead of taking the approximation p_k so seriously, we just used it to get a good search direction?
- Remember that the FOCs for eq. (7) are $D^2 f(x_k)(x^* x_k) = -Df(x_k)$
- **I** Let's define our search direction $s_k = (x^* x_k)$ as the solution to this system of linear equations
	- In Write our update step as $x_{k+1} = x_k + \alpha s_k$
	- \triangleright When $\alpha = 1$, this is just regular Newton's Method
- ▶ What if we solve the **univariate** problem

 $\max_{\alpha_k \geq 0} f(x_k + \alpha_k s_k)$

and set $x_{k+1} = x_k + \alpha_k^* s_k$? This is called a **Line Search**

Use your favorite derivative free method from before (usually you want Brent's method)

- It tends to be much less sensitive to the initial conditions than regular Newton's method
- ▶ You can plug this line search idea back in to most search algorithms: as long as they give you a proposed point, you can try searching in that direction instead

Other Methods (non-exhaustive)

- 1. Gradient Descent: take successive steps downhill (follow the gradient) until you converge
- 2. Simplex Based Methods: (Nelder-Mead) uses a local simplicial approximation of the objective and a set of heuristic rules to "approximate" the gradient and follow it downhill
- 3. Quasi-Newton Methods: Instead of calculating the Hessian $D^2f(x)$ directly, build up an approximation using information just from the derivative.
	- \triangleright There are many options in this space, but you probably want to be using L-BFGS.
- 4. Conjugate Gradient: extremely efficient algorithm but it only works if the hessian $D^2f(x)$ is positive definite (i.e., the function is convex)
- 5. Global Methods:
	- ▶ Simulated Annealing/Monte Carlo Markov Chains: Take random steps, with a probability of sometimes stepping downhill (to help escape local minima)
	- ▶ Differential Evolution: Track many different candidate points, and sometimes "mutate" coordinates from the best ones to get better potential test points
	- \blacktriangleright And many many more...

Section 3

[A brief aside: Differentiation](#page-26-0)

Why do we need gradients?

 \triangleright We've seen already that derivatives show up all over the place.

 \blacktriangleright Any time we have a maximization problem

 $\max_{x \in \mathbb{R}^n} f(x)$

we know that the solution x^* satisfies $Df(x^*)=0$

- ▶ You need to calculate the gradient to use gradient descent, L-BFGS, or any other gradient based method
- \blacktriangleright You even need second derivatives $D^2f(x)$ (also called the Hessian) if you want to use Newton's method or other similar approaches

- 1. Write them down in closed form
	- \triangleright Nice if you can, but requires a lot of work
	- \blacktriangleright Hard if you're rapidly iterating on a model
	- \blacktriangleright Extremely error prone
- 2. Finite differences
	- \triangleright Evaluate the function multiple times at small perturbations to the point of intersection
	- \triangleright Usually quite robust
	- \blacktriangleright Requires very little work, but is often the slowest approach
- 3. Automatic Differentiation
	- \blacktriangleright Have the computer differentiate your program for you
	- \blacktriangleright Usually works, and calculates exact derivatives
	- \triangleright Relies on programming language and compiler features sometimes you're limited in how you write your code, especially in python

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Finite Differences

The basic theory of finite differences is pretty simple

► Recall the definition of a derivative for $f : \mathbb{R} \to \mathbb{R}$:

$$
Df(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}
$$

 \triangleright Rather than actually taking the limit, we can try to do this with a really small perturbation:

$$
Df(x) \approx \frac{f(x+h) - f(x)}{h}
$$

where h is small.

Benefits:

- In principle, this is pretty easy to implement (although you shouldn't there are lot's of issues with numerical stability, so you should use someone else's package rather than writing it yourself)
- \blacktriangleright Conceptually straightforward
- When implemented properly, can be fairly robust

Finite Differences: Drawbacks

All that being said, you probably want to avoid finite differences for your actual code. Why?

\blacktriangleright It adds a source of approximation error

This can be a serious issue for poorly conditioned problems, or problems with very high curvature in f (i.e. $D^2f(x)$ is large)

It is really slow compared to other options – it requires a lot more evaluations of your function, which can be quite costly

Consider what we need to do when $f : \mathbb{R}^n \to \mathbb{R}$ where *n* is nontrivially large:

$$
Df_i(x) \approx \frac{f(x + h_i e_i) - f(x)}{h_i} \quad \forall i = 1, \dots, n
$$

where $e_i = (0, \ldots, 0, 1, 0 \ldots, 0)$ is the *i*th basis vector for \mathbb{R}^n

- In This requires two function evaluations of f for every dimension of x
- \triangleright So if $n = 10$, you have to evaluate f at least 21 times every time you want the derivative
- \triangleright You can see how this gets very expensive very fast as n gets large

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- In This requires two function evaluations of f for every dimension of x In practice, it actually involves three, since people tend to use two sided finite differences to reduce the approximation error, or adaptive schemes which require even more function evaluations
- \triangleright So if $n = 10$, you have to evaluate f at least 21 times every time you want the derivative
- \triangleright You can see how this gets very expensive very fast as n gets large
- In practice you can do much, much better by having the computer write your derivatives for you
- \blacktriangleright How does this work in practice?
	- \triangleright Start with the chain rule:

$$
D(f \circ g)(x) = Df(g(x)) \cdot Dg(x)
$$

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Autodifferentiation: Benefits/Drawbacks

Benefits:

- Extremely easy you just call a package and it calculates your derivatives for you
- No approximation error (unlike finite differences)
- \triangleright Much less error prone than writing derivatives by hand
- \blacktriangleright It works especially well for large complicated functions

Drawbacks:

- \triangleright You need to have derivatives written for every primitive function that you use. This means that sometimes you're constrained in the functions you can write without breaking autodiff
- In some cases, you can achieve better performance writing derivatives by hand
- \triangleright Bad performance when the function you're differentiating involves an iterative procedure
	- Interpretiate, you should never attempt to autodifferentiate the solution to an optimization
	- Instead, you can exploit results (like the Envelope Theorem) to get the derivative to those problems in closed form, or just use finite differences

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Practical Guide to Differentiation

What packages should I use and when??

Finite Differences

- In Julia, consider either FiniteDiff.jl or FiniteDifferences.jl
	- \triangleright Both have similar functionality, and will probably work for you
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Section 4

[Constrained Optimization](#page-45-0)

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\max_{x \in \mathbb{R}^n} f(x)
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s.t. $g(x) = 0$ (9)

for some functions $f : \mathbb{R}^n \to \mathbb{R}$ (objective) and $g : \mathbb{R}^n \to \mathbb{R}^m$ (constraints).

 \triangleright Extremely general formulation – most interesting problems in economics involve some form of constrained optimization

- In An risk-averse investor chooses a portfolio of assets, subject to a budget constraint
- **I** A social planner chooses a set of labor and consumption allocations to maximize welfare, subject to incentive compatibility constraints (what is the optimal tax rate?)
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Best Approach: Reformulate the Problem

Oftentimes you can simply reformulate the constraint/problem and choose an easier domain to search over instead

- \triangleright Simplex Constraints (probabilities sum to 1): suppose $g(x) = \sum x_i 1$ and we know $0 \leq x_i \leq 1$
	- ► Use a [known bijection](https://en.wikipedia.org/wiki/Logit-normal_distribution#Multivariate_generalization) from $\mathbb{R}^{n-1} \to \Delta^n$
	- \triangleright See UnitSimplex transformation in TransformVariables.jl

In Consumption Savings with Labor Choice:

$$
\max_{c,n} u(c,n) + V(b')\ns.t.c + b' \leq wn
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Choose consumption share of income rather than consumption directly to ensure that $c > 0$ always

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Best Approach: Reformulate the Problem (cont.)

- ► Linear Equality Constraints: Suppose $g(x) = Ax b$ where A is an $m \times n$ matrix
	- In Let M be any matrix whose columns span the nullspace of A (i.e, $AM = 0$, where M is $n \times p$) and let \hat{x} be any solution to $Ax = b$
	- Search over $z \in \mathbb{R}^p$, and solve the reformulated problem

 $\max_{z \in \mathbb{R}^p} f(Mz + \hat{x})$

Notice that by construction, $A(Mz + \hat{x}) = A\hat{x} = b$, so this lets us search in an unconstrained way while ensuring that the constraint always holds

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- It's much much easier to solve unconstrained problems (or problems with simple box-bounds) than problems with nonlinear constraints
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\mathcal{L}(x,\lambda):=f(x)-\lambda\cdot g(x)
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where $\lambda \in \mathbb{R}^m$.

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This can be an extremely effective strategy, as long as the problem is not too large, since it requires you to solve a system of equations involving the dense hessian $D^2f(x)$ (which is $O(n^3)$)

Penalty Methods

Intuition here is simple: make it painful for the optimizer to violate the constraints

 \triangleright Consider the following unconstrained problem:

$$
\max_{x \in R^n} f(x) - P \sum_{i=1}^m g_i(x)^2 \tag{11}
$$

for some penalty parameter P

Note: if you're solving a minimization problem, add the penalty term rather than subtract it

As $P \to \infty$, the solution to this problem converges to the true solution

For inequality constraints $g(x) \le 0$, replace $g(x)$ with $g^+(x)$ where $g_i^+(x) = \max\{g_i(x), 0\}$

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In This makes our solution algorithms converge very slowly, and can introduce numerical instabilities to our problem

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Penalty Methods: Solution

Instead of starting with a very large P , instead solve a sequence of problems where P gets larger and larger

 \triangleright Choose a sequence P_k which starts small and diverges to ∞ :

Let
$$
P_k = \gamma P_{k-1}
$$
 for some $\gamma > 1$, with $P_0 = 1$

► Common choice is to use $\gamma = 10$ but you may need to vary it by problem

 \blacktriangleright Let x_k be the solution to

$$
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In The trick: use x_k as the initial guess for the $k + 1$ th problem

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Augmented Lagrangian Method

- \triangleright Similar to the penalty method approach, but we use the Lagrangian of the problem, rather than just the penalty functions, to enforce the constraint
- \triangleright Consider the sequence of problems for $k = 0, \ldots, \infty$:

$$
\max_{x \in \mathbb{R}^n} \underbrace{f(x)}_{\text{Main Objective}} -\frac{P_k}{2} \sum_{i=1}^m g_i(x)^2 - \sum_{i=1}^m \lambda_i^k g_i(x)
$$
(13)

where $P_k \to \infty$ is a sequence of increasing penalties Note: if you're solving a minimization problem, add the penalty term rather than subtract it

- \triangleright We can't pick λ_i as part of the optimization: the true optimum is a saddle point of the Lagrangian, not a minimum
- \blacktriangleright Use the following update rule for λ_i :

$$
\lambda_i^{k+1} = \lambda_i^k + P_k g_i(x_k) \tag{14}
$$

At every iteration, we're updating λ_i with exactly the "contribution" of the penalty function in the previous iteration

 \triangleright You don't need to keep going until P_k is really large – you can stop if λ has converged!

Section 5

[Special Cases](#page-66-0)

Recall some definitions:

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if for any $\lambda \in (0,1)$, and any points $x, y \in \mathbb{R}^n$ $f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y)$

A set
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A \subset \mathbb{R}^n
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 is convex if for every $x, y \in A$, and every $\lambda \in (0, 1)$,

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- 1. It has sharp implications about where the extrema can be
- 2. There are usually a set of specialized methods you can use once you know that your problem is convex (which tend to perform much better)

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Convex Functions have Unique Global Minima

Theorem 1

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a strictly convex function. Then every local minima of f is a global minimum.

Proof. Suppose not. I.e, there is $x^* \neq x_m$ with $f(x^*) < f(x_m)$

- I Let x_m be a local minimum of f (there exists a neighborhood U such that if $y \in U$, then $f(y) > f(x_m)$
- ► Pick λ sufficiently small that $x' = \lambda x_m + (1 \lambda)x^* \in U$, and so $f(x') \ge f(x_m)$
- I But we also know that

$$
f(x') < \lambda f(x_m) + (1 - \lambda)f(x^*)
$$
 By strict convexity of f

$$
< \lambda f(x_m) + (1 - \lambda)f(x_m)
$$
 Since x^* is a global minimum

$$
= f(x_m)
$$

This is a contradiction, so no such x^* can exist.

г

Convex Problems have Unique Minima

Theorem 2

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a strictly convex, continuous function, and let $D \subset \mathbb{R}^n$ be a compact, convex set. Then, the constrained optimization problem

> min $f(x)$ s.t. $x \in \mathcal{D}$

has a unique minimum.

Proof. We know a minimum exists because continuous functions on compact sets always have a minimum.

Suppose we have two: x_1 and x_2 with $f(x_1) = f(x_2) \le f(x)$ for all $x \in \mathcal{D}$

Then consider $x' = \frac{x_1 + x_2}{2}$. We know $x' \in \mathcal{D}$ because \mathcal{D} is convex.

But then strict convexity implies

$$
f(x') < \frac{1}{2}f(x_1) + \frac{1}{2}f(x_2) = f(x_1)
$$

which contradicts that $f(x_1)$ was a minimum to begin with.

So what does convexity buy us?

- \blacktriangleright Peace of Mind
	- \blacktriangleright Theorem 1 means that with a convex objective, if we find a local minimum (which satisfies our constraints) then we're done. We can never do better
	- \triangleright Theorem 2 tells us that we'll never wind up with an indeterminate solution there's always a unique minimum
	- \blacktriangleright This means that if our objective is convex, we can check the interior for a single unique global minimum, and then just check points on the boundary of D if we can't find one
- \blacktriangleright Speed
	- \triangleright For general, nonlinear convex problems, consider looking into the Conjugate Gradient method
	- \triangleright Many other convex problems have special structures that specific solvers can exploit.
	- \triangleright Taking advantage of it often gets you huge speed gains, or takes an infeasible problem and makes it feasible
- \triangleright Note: All of this goes through, exactly the same, if you replace min with max and convex function with concave function

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Special Case: Linear Programs

Consider a problem of the form

$$
\min_{x \in \mathbb{R}^n} c^T x
$$
\n
$$
\text{s.t. } Ax \leq b
$$
\n
$$
x \geq 0
$$
\n
$$
(15)
$$

where $c \in \mathbb{R}^n$, $b \in \mathbb{R}^m$, and A is an $m \times n$ matrix.

- \blacktriangleright This is known as a Linear Program (LP)
- It has a linear objective function and affine (linear plus a constant) constraint set
- \triangleright Whenever you're working on a problem, you should always be on the lookout for the possibility that you can reformulate it as an LP

There are extremely efficient numerical algorithms to solve these problems

Intervaller Simplex Method: Intuition

- \triangleright The constraint set of this problem looks like a polytope (in 2-d, polygon)
- In One can show that a minimum to the problem will always lie on one of the corners, so its sufficient to just check all the corners in a smart way

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Operationalizing It All: What packages do I use in Julia?

- \triangleright Univariate Optimization: use Optim. i 1 defaults to Brent's method
- Multivariate Optimization:
	- ▶ Nelder-Mead, Newton, Conjugate Gradient, and L-BFGS: use Optim. jl

This is usually the fastest and easiest way to get off the ground, since Optim will automatically compute the derivaties you need with ForwardDiff.jl

- \blacktriangleright If you need nonlinear constraints, use NLopt. il
	- ▶ Gradient Based: MMA (Method of Moving Asymptotes) is extremely robust, but also has SLSQP and L-BFGS
	- \triangleright COBYLA and BOBYQA are good for derivative free (and BOBYQA works particularly well when your objective function looks quadratic)
	- In Allows you to embed any method inside an Augmented Lagrangian problem, which lets you do L-BFGS with nonlinear constraints, for instance

▶ Linear Programming: Use JuMP. j1

In principle, if you like using JuMP. i1, you can use it to set up and solve any of these problems. However it's particularly useful for LPs and other special convex problems