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Notes for Lecture 4: Unconstrained Optimization

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Optimization Problems

• Canonical problem:

$$\min_{x} f(x)$$

$$s.t. \ g(x) = 0,$$

$$h(x) \le 0,$$

- $-f: \mathbb{R}^n \to \mathbb{R}$ is the objective function
- $-g: \mathbb{R}^n \to \mathbb{R}^m$ is the vector of *m* equality constraints
- $-h: \mathbb{R}^n \to \mathbb{R}^{\ell}$ is the vector of ℓ inequality constraints.
- Examples:
 - Maximization of consumer utility subject to a budget constraint
 - Optimal incentive contracts
 - Portfolio optimization
 - Life-cycle consumption
- Assumptions
 - Always assume f, g, and h are continuous
 - Usually assume f, g, and h are C^1
 - Often assume f, g, and h are C^3

- Topics
 - Unconstrained optimization
 - * Unconstrained optimization problems occur naturally maximum likelihood, minimize moment criteria
 - * They are also the foundation of constrained optimization methods
 - Nonlinear equations
 - \ast Similar to unconstrained optimization
 - \ast Not as easy as unconstrained optimization
 - Constrained optimization
 - * Optimal life-cycle problems with budget constraint
 - * Maximize profit given production constraints
 - \ast Optimal taxation given incentive compatibility constraints
 - * Econometric estimation of structural models

One-D Unconstrained Minimization: Newton's Method

$$\min_{x \in \mathbb{R}} \quad f(x),$$

• Assume f(x) is C^2 functions f(x)

– At a point a, the quadratic polynomial, p(x)

$$p(x) \equiv f(a) + f'(a) \left(x - a\right) + \frac{f''(a)}{2} (x - a)^2.$$

is the second-order approximation of f(x) at a

- Approximately minimize f by minimizing p(x)
- If f''(a) > 0, then p is convex, and $x_m = a f'(a)/f''(a)$.

– Hope: x_m is closer than a to the minimum.

• Newton's method:

Algorithm 4.2 Newton's Method in \mathbb{R}^1

Initialize. Choose initial guess x_0 and stopping parameters $\delta, \epsilon > 0$.

Step 1.
$$x_{k+1} = x_k - f'(x_k)/f''(x_k)$$
.
Step 2. If $|x_k - x_{k+1}| < \epsilon(1 + |x_k|)$ and $|f'(x_k)| < \delta$, STOP and report success; else go to step 1.

- Properties:
 - Newton's method finds critical points, that is, solutions to f'(x) = 0, not min or max.
 - If x_n converges to x^* , must check $f''(x^*)$ to check if min or max
 - Only find local extrema.
- Good news: convergence is locally quadratic.

Theorem 1 Suppose that f(x) is minimized at x^* , C^3 in a neighborhood of x^* , and that $f''(x^*) \neq 0$. Then there is some $\epsilon > 0$ such that if $|x_0 - x^*| < \epsilon$, then the x_n sequence defined in (4.1.2) converges quadratically to x^* ; in particular,

$$\lim_{n \to \infty} \frac{|x_{n+1} - x^*|}{|x_n - x^*|^2} = \frac{1}{2} \left| \frac{f'''(x^*)}{f''(x^*)} \right|$$
(4.1.3)

is the quadratic rate of convergence.

- Consumer problem example:
 - Consumer has \$1; price of x is \$2, price of y is \$3, utility function is $x^{1/2} + 2y^{1/2}$.

– If θ is amount spent on x then we have

$$\max_{\theta} \quad \left(\frac{\theta}{2}\right)^{1/2} + 2\left(\frac{1-\theta}{3}\right)^{1/2} \tag{4.1.6}$$

- Solution $\theta^* = 3/11 = .272727$
- If $\theta_0 = 1/2$, Newton iteration is

 $0.5, 0.2595917942, \ 0.2724249335, \ 0.2727271048, \ 0.272727272727$

and magnitude of the errors are

$$2.3(-1), 1.3(-2), 3.1(-4), 1.7(-7), 4.8(-14)$$

- Problems with Newton's method
 - May not converge if initial guess is too far away from solution.
 - f''(x) may be difficult to calculate.

Multidimensional Unconstrained Optimization: Comparison Methods

- Grid Search
 - Pick a finite set of points, X; for example, a Cartesian grid:

$$V = \{v_i | i = 1, ..., n\}$$
$$X = \{x \in \mathbb{R}^n | \forall i, x_i \in V\}$$

- Compute $f(x), x \in X$, and locate max
- Grid search is often the first method to use.
 - * Only involves function evaluations
 - * It is embarassingly parallelizable
 - \ast It should get you a good initial guess
- A good initial guess is not critical for grid search, but is for all good algorithms
- Grid search is slooooooow, so you should always switch to something better
- General lesson: start with a reliable but slow method to find good initial guess for a faster method

• Polytope Methods (a.k.a. Nelder-Mead, simplex, "amoeba")

Algorithm 4.3 Polytope Algorithm

- Initialize. Choose the stopping rule parameter ϵ . Choose an initial simplex $\{x^1, x^2, \cdots, x^{n+1}\}$.
- Step 1. Reorder vertices so $f(x^i) \ge f(x^{i+1}), i = 1, \cdots, n$.
- Step 2. Look for least *i* s.t. $f(x^i) > f(y^i)$ where y^i is reflection of x^i . If such an *i* exists, set $x^i = y^i$, and go to step 1. Otherwise, go to step 3.
- Step 3. Stopping rule: If the width of the current simplex is less than ϵ , STOP. Otherwise, go to step 4.
- Step 4. Shrink simplex: For $i = 1, 2, \dots, n$ set $x^i = \frac{1}{2}(x^i + x^{n+1})$, and go to step 1.



Multidimensional Optimization: Newton's Method

• Idea: Given x^k , compute local quadratic approximation, p(x), of f(x) around x^k , and let x^{k+1} be max of p(x)

Algorithm 4.4 Newton's Method in \mathbb{R}^n

- Stopping rule: Don't be too fussy!
 - Good values for ε and δ are close to the square root of machine epsilon.
 - First use sloppy ε and δ , such as 10⁽⁻³⁾.
 - Then reduce ε and δ until failure.
 - You can try to push them below square root of machine epsilon but you will probably not get too far.

Theorem 2 Suppose that f(x) is C^3 , minimized at x^* , and that $H(x^*)$ is nonsingular. Then there is some $\epsilon > 0$ such that if $||x^0 - x^*|| < \epsilon$, then the sequence defined in (4.3.1) converges quadratically to x^* .

- Problems with Newton's method:
 - May not converge
 - Computational demands may be excessive
 - * need at least $\mathcal{O}(n^2)$ time to compute $H(x^k)$, perhaps more if one does not have efficient code for H(x)
 - * need $\mathcal{O}(n^2)$ space for $H(x^k)$
 - * need $\mathcal{O}(n^3)$ time to solve $H(x^k)s^k = -(\bigtriangledown f(x^k))^\top$ for s^k
 - May converge to local solution, not global solution
 - We now consider methods which address these problems.

Direction Set Methods

- Problem: may not converge, or go to wrong kind of extremum
- Solution: if we always move uphill, we will eventually get to a local maximum

Algorithm 4.5 Generic Direction Method

- *Initialize.* Choose initial x^0 and stopping parameters δ and $\epsilon > 0$.
- Step 1. Compute a search direction s^k .
- Step 2. Solve $\lambda_k = \arg \min_{\lambda} f(x^k + \lambda s^k)$.
- Step 3. $x^{k+1} = x^k + \lambda_k s^k$.
- $Step \not 4. \qquad \text{If} \parallel x^k x^{k+1} \parallel < \epsilon (1+ \parallel x^k \parallel), \text{ go to step 5};$

else go to step 1.

- Step 5. If $\| \bigtriangledown f(x^{k+1}) \| < \delta(1 + f(x^{k+1}))$, STOP and report success; else STOP and report convergence to nonoptimal point.
- Possible direction set methods
 - Coordinate Directions
 - * Let search directions be coordinate, x_1 , x_2 , etc.
 - * Search direction $s_{2n+k} = x_k$
 - Steepest Descent: $s_k = \nabla f(x^k)$
 - Newton's Method with Line Search: $H_k s^k = -(\nabla f(x^k))^\top$
- Will converge to a local optimum IF we apply something like the Armijo rule (see website).

Quasi-Newton Methods

- Problem: Hessians are expensive to compute
- Solution: Don't need true Hessians (see Carter, 1993), so approximate them

Generic Quasi-Newton MethodInitialize.Choose initial
$$x^0$$
, Hessian $H^0(I)$ and stopping
parameters δ and $\epsilon > 0$.Step 1.Solve $H_k s^k = -(\bigtriangledown f(x^k))^\top$ for the search direction s^k .Step 2.Solve $\lambda_k = \arg \min_{\lambda} f(x^k + \lambda s^k)$ Step 3. $x^{k+1} = x^k + \lambda_k s^k$.Step 4.Compute H_{k+1} using H_k , $\bigtriangledown f(x^{k+1})$, x^{k+1} , $\bigtriangledown f(x^k)$, etc.Step 5.If $|| x^k - x^{k+1} || < \epsilon (1+ || x^k ||)$, go to step 6;else go to step 1If $|| \bigtriangledown f(x^{k+1}) || < \delta |1 + f(x^{k+1})|$. STOP and report succ

Step 6. If $\| \bigtriangledown f(x^{k+1}) \| < \delta |1 + f(x^{k+1})|$, STOP and report success; else STOP and report convergence to nonoptimal point. • Example: BFGS:

$$\begin{aligned} z_k &= x^{k+1} - x^k \\ y_k &= (\bigtriangledown f(x^{k+1}))^\top - (\bigtriangledown f(x^k))^\top \\ H_{k+1} &= H_k - \frac{H_k z_k z_k^\top H_k}{z_k^\top H_k z_k} + \frac{y_k y_k^\top}{y_k^\top z_k} \end{aligned}$$

- Preserves positive definiteness
- Uses only gradients that are already needed
- Warning: denominators may get too small; should keep them away from zero since small z_k does not necessarily stop iteration.
- Note: The Hessian iterates H_k may not converge to true Hessian at solution, even if x_k converges to solution. NEVER USE APPROXIMATE HESSIANS TO COMPUTE STANDARD ERRORS!!!!

Monopoly Example

- We look at a simple monopoly pricing example:
 - Utility function: if M is spending on other goods,

$$U(Y,Z) = (Y^{\alpha} + Z^{\alpha})^{\eta/\alpha} + M = u(Y,Z) + M,$$

- Output Y and Z implies prices of u_Y and u_Z .
- Monopoly problem is

$$\max_{Y,Z} \Pi(Y,Z) \equiv Y u_Y(Y,Z) + Z u_Z(Y,Z) - C_Y(Y) - C_Z(Z),$$
(1)

– Restate in terms of $y \equiv \ln Y$ and $z \equiv \ln Z$, $\pi(y, z) \equiv \Pi(e^y, e^z)$

$$\max_{y,z} \pi(y,z),\tag{2}$$



Example: A Dynamic Optimization Problem

- Life-cycle savings problem.
 - an individual lives for T periods
 - earns wages w_t in period $t, t = 1, \cdots, T$
 - consumes c_t in period t
 - earns interest on savings per period at rate \boldsymbol{r}
 - define S_t to be end-of-period savings:

$$S_{t+1} = (1+r)S_t + w_{t+1} - c_{t+1}.$$

- Set initial wealth: $S_0 = 0$
- utility function $\sum_{t=1}^{T} \beta^t u(c_t) + W(S_T)$
- Substitute $c_t = S_{t-1}(1+r) + w_t S_t$
- Problem now has T choices:

$$\max_{S_t} \sum_{t=1}^T \beta^t u(S_{t-1}(1+r) + w_t - S_t) + W(S_T)$$

- Newton's method looks impractical if T large. BUT
 - Hessian is tridiagonal (a sparse matrix)
 - * The choice of S_t interacts only with the choices for S_{t-1} and S_{t+1}
 - * Newton step is easy to compute.
 - \ast The normal Hessian has size T^2
 - \ast The tridiagonal matrix has size 3T
 - Sparse Hessians are common in dynamic problems because time t variables interact only with time t 1 and time t + 1 variables.
 - You must recognize this and implement Newton or quasi-Newton method with sparse Hessians, Or use software that automatically recognizes this structure AMPL, GAMS, AIMMS, CASADI (future lecture), and others.

Domain Problems

• Suppose $S_0 = 0$ and you want to solve

$$\max_{S_t} \sum_{t=1}^T \beta^t \log \left(S_{t-1}(1+r) + w_t - S_t \right) + W(S_T)$$

- Newton's method will take the guess S^k and compute a new guess S^{k+1} .
- Problem: S^{k+1} could imply consumption, $c_t = S_{t-1}(1+r) + w_t S_t$, will be negative at some t, causing computer to crash.
- A possible solution: Alter objective function
 - E.G.; replace $u(c) = \log c$ with, for some small $\varepsilon > 0$

$$\widetilde{u}(c) = \begin{cases} u(c), & c > \varepsilon \\ u(\varepsilon) + u'(\varepsilon)(c - \varepsilon) + u''(\varepsilon)(c - \varepsilon)^2/2, & c \le \varepsilon \end{cases}$$

- Maintains curvature
- Equals real u(c) on most of domain, which hopefully includes solution
- Not as easy to apply to multivariate functions
- General solution: add constraints (next week's topic) to keep this from happening.

Nonlinear Least Squares

• Objective function has form, $f^i: \mathbb{R}^n \to \mathbb{R}, i = 1, ..., m$.:

$$\min_{x} \frac{1}{2} \sum_{i=1}^{m} f^{i}(x)^{2} \equiv S(x),$$

- Idea: use simple approximation of Hessian
- In econometric applications
 - $f^i(x)$ are $g(\beta, y^i)$,

* $x = \beta$ is parameter vector

* y^i are the data.

* $g(\beta, y^i)$ is residual for observation i

– $S(\beta)$ is the sum of squared residuals at β .

• Let f(x) denote the column vector $(f^i(x))_{i=1}^m$.

- Let J(x) be the Jacobian of $f(x) \equiv (f^1(x), \dots, f^m(x))^\top$. - Let $f_\ell^i \equiv \frac{\partial f^i}{\partial x_\ell}$ and $f_{j\ell}^i \equiv \frac{\partial^2 f^i}{\partial x_j \partial x_\ell}$. - The gradient of S(x) is $J(x)^\top f$: $S_\ell(x) = \sum_{i=1}^m f_\ell^i(x) f^i(x)$. - The Hessian of S(x) is $J(x)^\top J(x) + G(x)$, where

$$G_{j\ell}(x) = \sum_{i=1}^{m} f_{j\ell}^i(x) f^i(x)$$

- Special structure of the gradient and Hessian.
 - $f_i^i(x)$ terms are needed to compute gradient of S(x).
 - If f(x) = 0, then Hessian is just $J(x)^{\top}J(x)$: easy to compute.
 - A problem where f(x) is small at the solution is called a *small residual problem*; otherwise, it is a *large residual problem*.
- Gauss-Newton algorithm
 - Do Newton except use $J(x)^{\top}J(x)$ for Hessian approx.

$$s^{k} = -(J(x^{k})^{\top}J(x^{k}))^{-1}(\nabla f(x^{k}))^{\top}$$
(4.5.1)

and avoid computing second derivatives of f.

- Natural to use for small residual problems.
- Works very well when it works.

- Problems.
 - $J(x)^{\top}J(x)$ is likely to be poorly conditioned, since it is the "square" of a matrix.
 - J(x) may be poorly conditioned itself, particularly in statistical contexts.
 - Gauss-Newton step may not be a descent direction.
- Solution: Levenberg-Marquardt algorithm.

– Use $J(x)^{\top}J(x) + \lambda I$ for some scalar λ (I is identity matrix):

$$s^k = -(J(x^k)^\top J(x^k) + \lambda I)^{-1} (\nabla f(x^k))^\top$$

- The λI term reduces conditioning problems by "adding a little piece of the identity matrix" - s^k will be descent direction for large λ since s^k gets closer to steepest descent direction λ .