Lecture 10 Nonlinear Programming Algorithms

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ChE 597: Computational Optimization Purdue University

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Outline of this lecture

- Equality-constrained Newton's method (only has equality constraints Ax = b
- Interior point method
 - Barrier Method
 - Primal-Dual Interior-Point Method

Convex objective function with linear equality constraints

Consider a problem with equality constraints, as in

$$\min_{x} f(x) \text{ subject to } Ax = b \qquad A \neq 2 \circ$$

Options:

• Eliminating equality constraints: write $x = Fy + x_0$, where F spans null space of A, and $Ax_0 = b$. Solve in terms of y as an unconstrained optimization problem.

$$\min f(x)$$
 s.t. $Ax = b$ \Leftrightarrow $\min_{y} f(Fy + x_0)$

 Equality-constrained Newton: in many cases, this is the most straightforward option

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Equality-constrained Newton's method

In equality-constrained Newton's method, we start with $x^{(0)}$ such that $Ax^{(0)}=b$. At each iteration, we solve a quadratic approximation of the problem

$$\min_{v} \quad \widehat{f}(x+v) = f(x) + \nabla f(x)^{T} v + (1/2) v^{T} \nabla^{2} f(x) v$$
s.t.
$$A(x+v) = b \quad A \cdot V = 0$$

Since we kept Ax = b, the constraint is equivalent to Av = 0. We know from KKT conditions that v satisfies

$$\begin{bmatrix} \nabla^2 f(x) & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x_{\mathsf{nt}} \\ w \end{bmatrix} = \begin{bmatrix} -\nabla f(x) \\ 0 \end{bmatrix}$$

for some dual variables w. Hence Newton direction v is again given by solving a linear system in the Hessian (albeit a bigger one). We can perform backtracking line search on the direction $\Delta x_{\rm nt}$

$$x^+ = x + t\Delta x_{\rm nt}$$

where t is the appropriate step size after the line search.

Newton's method for equality constrained minimization

given starting point $x \in \text{dom } f$ with Ax = b, tolerance $\epsilon > 0$. **repeat**

- Compute the Newton step and decrement $\Delta x_{\rm nt}$, $\lambda(x)$.
- Stopping criterion. quit if $\frac{\lambda^2}{2} \leq \epsilon$.
- *Line search.* Choose step size *t* by backtracking line search.
- Update $x^+ := x + t\Delta x_{nt}$.

until stopping criterion is met where the decrement is defined as

$$\lambda(x) = \left(\Delta x_{\mathsf{nt}}^{\mathsf{T}} \nabla^2 f(x) \Delta x_{\mathsf{nt}}\right)^{1/2}$$

which is the same as the standard Newton's method.

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General convex NLP

Consider the convex optimization problem

$$\min_{x}$$
 $f(x)$
subject to $h_{i}(x) \leq 0, i = 1, ..., m$
 $Ax = b$

We will assume that f, h_1, \ldots, h_m are convex, twice differentiable, each with domain \mathbb{R}^n .

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Log barrier function Ignoring equality constraints for now, our problem can be written as

where t > 0 is a large number

equality constraints for now, our proble
$$\min_{x} f(x) + \sum_{i=1}^{m} I_{-}(h_{i}(x))$$

Where I represents the indicator function (discontinuous)

 $I_{-}(u) = \begin{cases} 0 & u \leq 0 \\ +\infty & u > 0 \end{cases}$

 $\min_{x} f(x) - \frac{1}{t} \sum_{i=1}^{m} \log \left(-h_{i}(x)\right)$

This approximation is more accurate for larger t. But for any value

of t, the log barrier approaches ∞ if any $h_i(x) \to 0$

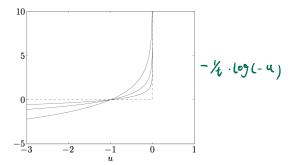
We can approximate the sum of indicators by the log barrier:

min f(x)

Interpretation of log barrier function

$$\min_{x} f(x) - \frac{1}{t} \sum_{i=1}^{m} \log \left(-h_i(x)\right)$$

where t > 0 is a large number



The dashed lines show the function $I_{-}(u)$, and the solid curves show $\widehat{I}_{-}(u) = -(1/t)\log(-u)$, for t = 0.5, 1, 2. The curve for t = 2 gives the best approximation.

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Log barrier calculus

For the log barrier function

$$\phi(x) = -\sum_{i=1}^{m} \log \left(-h_i(x)\right)$$

we have for its gradient:

$$\nabla \phi(x) = -\sum_{i=1}^{m} \frac{1}{h_i(x)} \nabla h_i(x)$$

and for its Hessian:

$$\nabla^2 \phi(x) = \sum_{i=1}^m \frac{1}{h_i(x)^2} \nabla h_i(x) \nabla h_i(x)^T - \sum_{i=1}^m \frac{1}{h_i(x)} \nabla^2 h_i(x)$$

The Hessian is always PSD for $h_i(x) < 0$. Thus, the barrier problem is convex.

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Central path

Consider barrier problem:

$$f(x) + \frac{1}{4}\phi(x)$$

$$\min_{x}$$
 $tf(x) + \phi(x)$ subject to $Ax = b$

The central path is defined by solution $x^*(t)$ with respect to t > 0

- This is a convex optimization problem with on equality constraints. It can be solved by the equality-constrained Newton's method.
- Hope is that, as $t \to \infty$, we will have $x^*(t) \to x^*$, solution to our original problem
- Why don't we just set t to be some huge value, and solve the above problem? Directly seek solution at end of central path?
- Problem is that this is seriously inefficient in practice
- Much more efficient to traverse the central path, as we will see

How to estimate the duality gap of the orignal problem?

- The barrier problem give us a strictly feasible primal solution $x^*(t)$ to the original problem.
- If we would like to estimate how far the $f(x^*(t))$ is from the optimum, we will need the dual variables of the original problem because we need that to estimate duality gap.
- Idea: use the KKT conditions of the barrier problem to construct a dual feasible solution to the original problem.

min
$$tf(x) = \frac{1}{2}og(-hi(x))$$

 $f(t) = \frac{1}{2}og(-hi(x))$
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 $g(u,v) = \min_{x} f(x) + \sum_{i=1}^{m} u_i h_i(x) + V(1-Ax)$ $u_i^*(t) = -\frac{1}{t \cdot h_i(x^*(t))} \qquad V^*(t) = w/t$

KKT conditions of barrier and the orignal problem

KKT conditions of the barrier problem.

$$t \nabla f(x^*(t)) - \sum_{i=1}^m \frac{1}{h_i(x^*(t))} \nabla h_i(x^*(t)) + A^T w = 0,$$

 $Ax^*(t) = b, \quad h_i(x^*(t)) < 0, \quad i = 1, ..., m$

for some $w \in \mathbb{R}^m$.

Since we know $x^*(t)$ is optimal, it satisfies the KKT conditions of the barrier problem.

Claim Given $x^*(t)$ and corresponding w, we define

$$u_i^*(t) = -\frac{1}{th_i(x^*(t))}, \quad i = 1, \dots, m, \quad v^*(t) = w/t$$

 $u^{\star}(t)$ and $v^{\star}(t)$ are dual feasible for the original problem, i.e., $g(u^{\star}(t), v^{\star}(t)) \neq -\infty$,where $u_i^{\star}(t)$ is the dual variable for $h_i(x) \leq 0$, $v^{\star}(t)$ are the dual variable for Ax = b

Proof The Lagrangian of the original problem is

$$L(x, u, v) = f(x) + \sum_{i=1}^{m} u_i h_i(x) + v^T (Ax - b)$$

- Note that $u_i^*(t) > 0$ since $h_i(x^*(t)) < 0$ for all i = 1, ..., m (the signs are correct)
- The next step is to check whether g(u, v) is finite at $(u^*(t), v^*(t))$.

$$g((u^{*}(t), v^{*}(t))) = \min_{x} f(x) + \sum_{i=1}^{m} u_{i}^{*}(t) h_{i}(x) + v^{*}(t)^{T} (Ax - b)$$

By definition (from the KKT condition of the barrier problem)

$$\nabla f(x^{*}(t)) + \sum_{i=1}^{m} u_{i}(x^{*}(t)) \nabla h_{i}(x^{*}(t)) + A^{T}v^{*}(t) = 0$$

That is, $x^*(t)$ minimizes Lagrangian $L(x, u^*(t), v^*(t))$ over x, so $g(u^*(t), v^*(t)) > -\infty$

Duality gap

This allows us to bound suboptimality of $f(x^*(t))$, with respect to original problem, via the duality gap. We compute

$$g(u^{*}(t), v^{*}(t)) = f(x^{*}(t)) + \sum_{i=1}^{m} u_{i}^{*}(t)h_{i}(x^{*}(t)) + v^{*}(t)^{T}(Ax^{*}(t) - b)$$

$$= f(x^{*}(t)) + \sum_{i=1}^{m} -\frac{1}{th_{i}(x^{*}(t))}h_{i}(x^{*}(t))$$

$$= f(x^{*}(t)) - m/t$$

$$\int_{0}^{p+t} e^{tht} dt \int_{0}^{t} e^{th} dt \int$$

That is, we know that $f(x^*(t)) - f^* \leq m/t$ This will be very useful as a stopping criterion; it also confirms the hope that $x^*(t) \to x^*$ as $t \to \infty$

Interpretation: Perturbed KKT conditions

We can now reinterpret central path $(x^*(t), u^*(t), v^*(t))$ as solving the perturbed KKT conditions:

$$\nabla f(x) + \sum_{i=1}^{m} u_i \nabla h_i(x) + A^T v = 0$$

$$u_i \cdot h_i(x) = -1/t, \quad i = 1, \dots, m$$

$$h_i(x) \le 0, \quad i = 1, \dots, m, \quad Ax = b$$

$$u_i \ge 0, \quad i = 1, \dots, m$$

Only difference between these and actual KKT conditions for our original problem is second line: these are replaced by

$$u_i \cdot h_i(x) = 0, \quad i = 1, \ldots, m$$

i.e., complementary slackness, in actual KKT conditions

Barrier Method

The barrier method solves a sequence of problems

$$\min_{x}$$
 $tf(x) + \phi(x)$ subject to $Ax = b$

for increasing values of t>0, until duality gap satisfies $m/t\leq\epsilon$.

- 1. We fix $t^{(0)} > 0, \mu > 1$. We use Newton to compute $x^{(0)} = x^*(t)$, solution to barrier problem at $t = t^{(0)}$.
- 2. For $k=1,2,3,\ldots$, solve the barrier problem at $t=t^{(k)}$, using Newton initialized at $x^{(k-1)}$, to yield $x^{(k)}=x^{\star}(t)$
- 3. Stop if $m/t \le \epsilon$, else update $t^{(k+1)} = \mu t$

Step 2 is called a centering step (since it brings $x^{(k)}$ onto the central path)

Choice of parameters

- Choice of μ : if μ is too small, then many outer iterations might be needed; if μ is too big, then Newton's method (each centering step) might take many iterations
- Choice of $t^{(0)}$: if $t^{(0)}$ is too small, then many outer iterations might be needed; if $t^{(0)}$ is too big, then the first Newton solve (first centering step) might require many iterations

Fortunately, the performance of the barrier method is often quite robust to the choice of μ and $t^{(0)}$ in practice (However, note that the appropriate range for these parameters is scale dependent)

Barrier versus primal-dual interior point method

Overview:

- Both can be motivated in terms of perturbed KKT conditions
- Primal-dual interior-point methods take one Newton step, and move on (no separate inner and outer loops)
- Primal-dual interior-point iterates are not necessarily feasible
- Primal-dual interior-point methods are often more efficient, as they can exhibit better than linear convergence
- Primal-dual interior-point methods are less intuitive

Interpretation: Perturbed KKT conditions
$$g(x) = g(x) + g(x)$$

We can now reinterpret central path $(x^*(t), u^*(t), v^*(t))$ as solving the perturbed KKT conditions:

$$\nabla f(x) + \sum_{i=1}^{m} u_{i} \nabla h_{i}(x) + A^{T} v = 0$$

$$u_{i} \cdot h_{i}(x) = -1/t, \quad i = 1, \dots, m$$

$$h_{i}(x) \leq 0, \quad i = 1, \dots, m, \quad Ax = b$$

$$u_{i} > 0, \quad i = 1, \dots, m$$

Only difference between these and actual KKT conditions for our original problem is second line: these are replaced by

$$u_i \cdot h_i(x) = 0, \quad i = 1, \ldots, m$$

i.e., complementary slackness, in actual KKT conditions

Perturbed KKT as nonlinear system

Can view this as a nonlinear system of equations, written as

$$r(x, u, v) = \begin{pmatrix} \nabla f(x) + Dh(x)^T u + A^T v \\ -\operatorname{diag}(u)h(x) - (1/t)1 \\ Ax - b \end{pmatrix} = 0$$

where

$$h(x) = \begin{pmatrix} h_1(x) \\ \cdots \\ h_m(x) \end{pmatrix}, \quad Dh(x) = \begin{bmatrix} \nabla h_1(x)^T \\ \cdots \\ \nabla h_m(x)^T \end{bmatrix}$$

Newton's method, recall, is generally a root-finder for a nonlinear system F(y)=0. Approximating $F(y+\Delta y)\approx F(y)+DF(y)\Delta y$ leads to

$$\Delta y = -(DF(y))^{-1}F(y)$$

What happens if we apply this to r(x, u, v) = 0 above?

$$u : k : (x) = -\frac{1}{4}$$
 Newton on perturbed KKT, v1

Approach 1: from middle equation (relaxed comp slackness), note that $u_i = -1/(th_i(x))$, i = 1, ..., m. So after eliminating u, we get

$$r(x,v) = \begin{pmatrix} \nabla f(x) + \sum_{i=1}^{m} \left(-\frac{1}{th_{i}(x)} \right) \nabla h_{i}(x) + A^{T}v \\ Ax - b \end{pmatrix} = 0$$

Thus the Newton root-finding update $(\Delta x, \Delta v)$ is determined by

$$\begin{bmatrix} H_{\text{bar}}(x) & A^T \\ A & 0 \end{bmatrix} \begin{pmatrix} \Delta x \\ \Delta v \end{pmatrix} = -r(x, v)$$

where $H_{\text{bar}}(x) =$

$$\nabla^2 f(x) + \sum_{i=1}^m \frac{1}{th_i(x)^2} \nabla h_i(x) \nabla h_i(x)^T + \sum_{i=1}^m \left(-\frac{1}{th_i(x)} \right) \nabla^2 h_i(x)$$

This is just the KKT system solved by one iteration of Newton's method for minimizing the barrier problem

Newton on perturbed KKT, v2

Approach 2: directly apply Newton root-finding update, without eliminating u. Introduce notation

$$r_{\text{dual}} = \nabla f(x) + Dh(x)^T u + A^T v$$

 $r_{\text{cent}} = -\operatorname{diag}(u)h(x) - (1/t)t$
 $r_{\text{prim}} = Ax - b$

called the dual, central, and primal residuals at y=(x,u,v). Now root-finding update $\Delta y=(\Delta x,\Delta u,\Delta v)$ is given by

$$\begin{bmatrix} H_{\mathrm{pd}}(x) & Dh(x)^T & A^T \\ -\operatorname{diag}(u)Dh(x) & -\operatorname{diag}(h(x)) & 0 \\ A & 0 & 0 \end{bmatrix} \begin{pmatrix} \Delta x \\ \Delta u \\ \Delta v \end{pmatrix} = -\begin{pmatrix} r_{\mathrm{dual}} \\ r_{\mathrm{cent}} \\ r_{\mathrm{prim}} \end{pmatrix}$$

where
$$H_{\mathrm{pd}}(x) = \nabla^2 f(x) + \sum_{i=1}^m u_i \nabla^2 h_i(x)$$

Surrogate duality gap

For barrier method, we have simple duality gap: m/t, since we set $u_i = -1/(th_i(x))$, i = 1, ..., m and saw this was dual feasible For primal-dual interior-point method, we can construct surrogate duality gap:

$$\eta = -h(x)^T u = -\sum_{i=1}^m u_i h_i(x)$$

This would be a real duality gap if we had feasible points, i.e., $r_{prim} = 0$ and $r_{dual} = 0$, but we don't, so it's not

Primal-dual Interior-point Method

Putting it all together, we now have our primal-dual interior-point method.

- Start with $x^{(0)}$ such that $h_i(x^{(0)}) < 0$, $i = 1, \ldots, m$, and $u^{(0)} > 0$, $v^{(0)}$. Define $\eta^{(0)} = -h(x^{(0)})^T u^{(0)}$. We fix $\mu > 1$, repeat for $k = 1, 2, 3, \ldots$
 - Define $t = \mu m / \eta^{(k-1)}$
 - ullet Compute primal-dual update direction Δy
 - Use backtracking to determine step size s
 - Update $y^{(k)} = y^{(k-1)} + s \cdot \Delta y$
 - Compute $\eta^{(k)} = -h(x^{(k)})^T u^{(k)}$
 - Stop if $\eta^{(k)} \leq \varepsilon$ and $(\|r_{\mathsf{prim}}\|^2 + \|r_{\mathsf{dual}}\|^2)^{1/2} \leq \varepsilon$

Note that we stop based on surrogate duality gap, and approximate feasibility. (Line search maintains $h_i(x) < 0, u_i > 0, i = 1, ..., m$)

Backtracking line search

At each step, must ensure we arrive at $y^+ = y + s\Delta y$, i.e.,

$$x^+ = x + s\Delta x$$
, $u^+ = u + s\Delta u$, $v^+ = v + s\Delta v$

that maintains both $h_i(x) < 0$, and $u_i > 0, i = 1, \ldots, m$ A multi-stage backtracking line search for this purpose: start with largest step size $s_{\text{max}} \leq 1$ that makes $u + s\Delta u \geq 0$:

$$s_{\max} = \min \left\{ 1, \min \left\{ -u_i / \Delta u_i : \Delta u_i < 0 \right\} \right\}$$

Then, with parameters $\alpha, \beta \in (0,1)$, we set $s = 0.999s_{\text{max}}$, and

- Let $s = \beta s$, until $h_i(x^+) < 0, i = 1, ..., m$
- Let $s = \beta s$, until $||r(x^+, u^+, v^+)||_2 \le (1 \alpha s)||r(x, u, v)||_2$

Software

Crossover Gurbi to solve an LP

Crossover using barrier = x* (not
an extreme pant

Point

Gurobi/Cplex has barrier algorithm for linear programs.

- Gurobi/Cplex has barrier algorithm for linear programs.

 Barrier algorithm has no guranttee to terminate at an extreme point.
- Interior point solvers: IPOPT (open-source), Mosek, Knitro

References

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