Lecture 10 Nonlinear Programming Algorithms

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ChE 597: Computational Optimization
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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

$$\min_x f(x) \text{ subject to } Ax = b$$

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.

$$\min f(x) \quad s.t.\ Ax = b \quad \Leftrightarrow \quad \min_y f(Fy + x_0)$$

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

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

$$\begin{array}{ll} \min_v & \widehat{f}(x+v) = f(x) + \nabla f(x)^T v + (1/2) v^T \nabla^2 f(x) v \\ \text{s.t.} & A(x+v) = b \end{array}$$

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

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

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 Δx_{nt}

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

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

Newton's method for equality constrained minimization

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

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

until stopping criterion is met
where the decrement is defined as

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

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

General convex NLP

Consider the convex optimization problem

$$\begin{array}{ll} \min_x & f(x) \\ \text{subject to} & h_i(x) \leq 0, i = 1, \ldots, m \\ & Ax = b \end{array}$$

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

Log barrier function

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

$$\min_x f(x) + \sum_{i=1}^{m} I_-\left(h_i(x)\right)$$

Where $I_{\_}$ represents the indicator function (discontinuous)

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

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

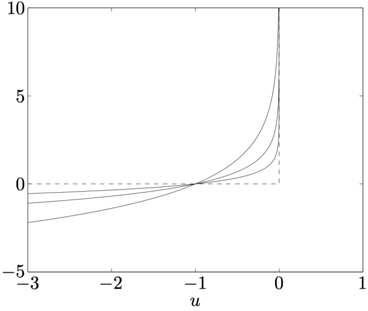
$$\min_x f(x) - \frac{1}{t} \sum_{i=1}^{m} \log\left(-h_i(x)\right)$$

where $t > 0$ is a large number
This approximation is more accurate for larger t. But for any value of t, the log barrier approaches ∞ if any $h_i(x) \to 0$

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.

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.

Central path

Consider barrier problem:

$$\begin{array}{ll} \min_x & tf(x) + \phi(x) \\ \text{subject to} & Ax = b \end{array}$$

The central path is defined by solution $x^\star(t)$ 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 $x^\star(t) \to x^\star$, 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 $x^\star(t)$ to the original problem.
- If we would like to estimate how far the $f(x^\star(t))$ 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.

KKT conditions of barrier and the orignal problem

KKT conditions of the barrier problem.

$$t\nabla f\left(x^{\star}(t)\right)-\sum_{i=1}^{m}\frac{1}{h_i\left(x^{\star}(t)\right)}\nabla h_i\left(x^{\star}(t)\right)+A^T w=0,$$
$$Ax^{\star}(t)=b,\quad h_i\left(x^{\star}(t)\right)<0,\quad i=1,\dots,m$$

for some $w\in\mathbb{R}^m$.
Since we know $x^{\star}(t)$ is optimal, it satisfies the KKT conditions of the barrier problem.
Claim Given $x^{\star}(t)$ and corresponding w, we define

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

$u^{\star}(t)$ 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 $u_i^\star(t) > 0$ since $h_i\left(x^\star(t)\right) < 0$ for all $i = 1, \ldots, m$ (the signs are correct)
- The next step is to check whether $g(u, v)$ is finite at $(u^\star(t), v^\star(t))$.

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

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

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

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

Duality gap

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

$$g(u^\star(t), v^\star(t)) = f(x^\star(t)) + \sum_{i=1}^{m} u_i^\star(t) h_i(x^\star(t)) +$$
$$v^\star(t)^T (Ax^\star(t) - b)$$
$$= f(x^\star(t)) + \sum_{i=1}^{m} -\frac{1}{t h_i(x^\star(t))} h_i\big(x^\star(t)\big)$$
$$= f(x^\star(t)) - m/t$$

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

Interpretation: Perturbed KKT conditions

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

$$\nabla f(x) + \sum_{i=1}^m u_i \nabla h_i(x) + A^T v = 0$$
$$u_i \cdot h_i(x) = -1/t, \quad i = 1, \ldots, m$$
$$h_i(x) \le 0, \quad i = 1, \ldots, m, \quad Ax = b$$
$$u_i \ge 0, \quad i = 1, \ldots, m$$

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

$$\begin{array}{ll} \min_x & tf(x) + \phi(x) \\ \text{subject to} & Ax = b \end{array}$$

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

1. We fix $t^{(0)} > 0, \mu > 1$. We use Newton to compute $x^{(0)} = x^\star(t)$, 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

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

$$\nabla f(x) + \sum_{i=1}^m u_i \nabla h_i(x) + A^T v = 0$$
$$u_i \cdot h_i(x) = -1/t, \quad i = 1, \ldots, m$$
$$h_i(x) \le 0, \quad i = 1, \ldots, m, \quad Ax = b$$
$$u_i \ge 0, \quad i = 1, \ldots, m$$

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

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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?

Newton on perturbed KKT, v1

Approach 1: from middle equation (relaxed comp slackness), note that $u_i = -1/\left(th_i(x)\right), i = 1, \ldots, m$. 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

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

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

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

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

$$\begin{aligned} r_{\text{dual}} &= \nabla f(x) + Dh(x)^T u + A^T v \\ r_{\text{cent}} &= -\operatorname{diag}(u)h(x) - (1/t)t \\ r_{\text{prim}} &= Ax - b \end{aligned}$$

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

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

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 $u_i = -1/(th_i(x)), i = 1, \ldots, m$ 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., $r_{\text{prim}} = 0$ and $r_{\text{dual}} = 0$, 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 $t = \mu m / \eta^{(k-1)}$
  - 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 $(\|r_{\text{prim}}\|^2 + \|r_{\text{dual}}\|^2)^{1/2} \leq \varepsilon$

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

Backtracking line search

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

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

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 $u + s\Delta u \geq 0$:

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

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

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

Software

- 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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- Lemaréchal, C., & Oustry, F. (1999). Semidefinite relaxations and Lagrangian duality with application to combinatorial optimization (Doctoral dissertation, INRIA).