Numerical Optimization

Lecture Notes #14
Practical Newton Methods — Hessian Modifications

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Outline

1. Recap
   - Robust Inexact Newton Methods
2. Hessian Modifications
   - Eigenvalue Modification
   - $\mathbf{B} = \mathbf{A} + \tau\mathbf{I}$
   - Gershgorin Modification

Quick Recap: Building Robust Inexact Newton Methods

We looked at combining a modified version of the linear CG-solver (or preferably a PCG(M)-solver) with a line-search algorithm to produce an almost "unbreakable" approximate Newton method.

The modification to the CG-solver comprise of an additional termination criterion for the case where the local Hessian ($\nabla^2 f(\bar{\mathbf{x}}_k)$) is not positive definite, and we get a CG-internal search direction for which $\bar{\mathbf{p}}^T \nabla^2 f(\bar{\mathbf{x}}_k)\bar{\mathbf{p}} \leq 0$, *i.e* the search takes into a part of space with negative curvature.

The worst we do (in a particular iteration) is to take a steepest descent step.

Potential Outstanding Problem: $\bar{\mathbf{p}}^T \nabla^2 f(\bar{\mathbf{x}}_k)\bar{\mathbf{p}}$ small and positive $\rightsquigarrow$ long step.

Quick Recap: Building Robust Inexact Newton Methods

We also discussed how to specify the **forcing sequence** $\{\eta^{(k)}\}$ for the tolerance termination criterion ($\|\bar{\mathbf{r}}_k\| \leq \eta^{(k)}\|\nabla f(\bar{\mathbf{x}}_k)\|$) so that the overall convergence rate of the resulting algorithm is quadratic (when $B_k = \nabla^2 f(x_k)$) or super-linear (when $B_k \approx \nabla^2 f(x_k)$).

We also hinted at a different approach to dealing with non-positive definite Hessians in the direct-linear-solver-framework — a modification of the Hessian ($\nabla^2 f(\bar{\mathbf{x}}_k) + E_k$) so that the resulting matrix is sufficiently positive definite; today we take a closer look at this approach.

Hessian Modifications

Old Default Project: `modelhess()`

We look at modifying the Hessian matrix $\nabla^2 f(\bar{\mathbf{x}}_k)$ by either explicitly or implicitly adding a matrix E_k (usually a multiple of the identity matrix) so that the resulting matrix

$$B_k = \nabla^2 f(\bar{\mathbf{x}}_k) + E_k$$

is **sufficiently positive definite** (all the eigenvalues of B_k are bounded away from zero.)

There are a number of different approaches, we look at a few...

- Eigenvalue Modification
- Direct and Indirect modification of the Hessian

Eigenvalue Modification

Since $\nabla^2 f(\bar{\mathbf{x}}_k)$ is symmetric we can always find an orthonormal matrix Q_k and a diagonal matrix $\Lambda_k = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ so that (dropping the subscripts k)

$$\nabla^2 f(\bar{\mathbf{x}}) = Q \Lambda Q^T = \sum_{i=1}^{n} \lambda_i \bar{\mathbf{q}}_i \bar{\mathbf{q}}_i^T.$$

For simplicity of argument, let us assume $Q = I$ (we can get to this scenario by an appropriate change of variables.)

Example:

$$\nabla f(\bar{\mathbf{x}}) = \begin{bmatrix} 1 \\ -3 \\ 2 \end{bmatrix}, \quad \nabla^2 f(\bar{\mathbf{x}}) = \text{diag}(10, 3, -1) \;\Rightarrow\; \bar{\mathbf{p}}^N = \begin{bmatrix} -0.1 \\ 1 \\ 2 \end{bmatrix}$$

and $\nabla f(\bar{\mathbf{x}})^T \bar{\mathbf{p}}^N = 0.90$, hence $\bar{\mathbf{p}}^N$ is **not a descent direction**.

(continued...)

Eigenvalue Modification

Idea#1: Replace negative eigenvalues by some positive number δ, *e.g.* $\delta = \sqrt{\epsilon^{\text{mach}}}$

In 32-bit double precision (and Matlab) $\epsilon^{\text{mach}} \approx 10^{-16}$, so $\delta = 10^{-8}$ seems like a reasonable choice(?) We can express the Hessian modification as

$$B_k = \sum_{i=1}^{2} \lambda_i \bar{\mathbf{q}}_i \bar{\mathbf{q}}_i^T + \delta \bar{\mathbf{q}}_3 \bar{\mathbf{q}}_3^T \quad \left[= \sum_{i=1}^{n} \max(\lambda_i, \delta) \bar{\mathbf{q}}_i \bar{\mathbf{q}}_i^T \right]$$

We now have

$$B_k = \text{diag}(10, 3, 10^{-8}) \;\Rightarrow\; \bar{\mathbf{p}} \approx \begin{bmatrix} -0.1 \\ 1 \\ -200,000,000 \end{bmatrix}$$

We notice that $\bar{\mathbf{p}}$ is approximately parallel to $\bar{\mathbf{q}}_3$, and **huge**...

Eigenvalue Modification

The long step length violates the spirit of Newton's method — recall that the quadratic convergence properties come from a **local** argument with the Taylor expansion.

Idea#2: Replace negative eigenvalues by $-\lambda_i$

Now $B_k = \text{diag}(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_n|)$, and in our example we get

$$\bar{\mathbf{p}} = \begin{bmatrix} -0.1 \\ 1 \\ -2 \end{bmatrix}, \quad \nabla f(\bar{\mathbf{x}})^T \bar{\mathbf{p}} = -7.1, \; \textbf{descent direction!}$$

This seems to work?!?

It may reorder the eigenvalues (and thus the "importance"/ ordering of subspaces), *i.e.*

$$\lambda_1 < \lambda_2 < \lambda_3, \quad \text{but} \quad |\lambda_2| < |\lambda_1| < |\lambda_3|.$$

Eigenvalue Modification

Let's reconsider Idea#1, what went wrong? When we solve $B\bar{\mathbf{p}} = -\nabla f(\bar{\mathbf{x}})$ we get

$$\bar{\mathbf{p}} = -B^{-1}\nabla f(\bar{\mathbf{x}}) = -\sum_{i=1}^{2} \frac{1}{\lambda_i}\bar{\mathbf{q}}_i(\bar{\mathbf{q}}_i^T\nabla f(\bar{\mathbf{x}})) - \frac{\mathbf{1}}{\delta}\bar{\mathbf{q}}_\mathbf{3}(\bar{\mathbf{q}}_\mathbf{3}^\mathbf{T}\nabla \mathbf{f}(\bar{\mathbf{x}})),$$

it's clearly the right-most term that makes us violate the spirit of Newton's method.

We could simply just drop this term (*i.e.* ignore the subspace corresponding to negative eigenvalues), or

Select δ so that we ensure that the step length is not excessive (**trust-region** flavor!).

Bad news: There is no accepted "best" way of modifying the Hessian in this manner.

Eigenvalue Modification

If we for a moment "forget" about the issue of selecting δ so that the step length is reasonable, we can ask the question **"what is the smallest change to A, which gives us an positive definite matrix B?"**

The answer depends on how we measure... Two standard measures are the **Frobenius norm** $\|A\|_F$, and the **Euclidean norm** $\|A\|$

$$\|A\|_F^2 = \sum_{i,j} a_{ij}^2, \quad \|A\| = \max_{\|\bar{\mathbf{x}}\|=1} \bar{\mathbf{x}}^T A\bar{\mathbf{x}} = \max|\mathrm{eig}(A)|.$$

If we use the Frobenius norm, the smallest change is of the type **"change negative eigenvalues to small positive ones:"**

$$B = A + \Delta A, \text{ where } \Delta A = Q\,\mathrm{diag}(\tau_i)\,Q^T, \ \tau_i = \begin{cases} 0 & \lambda_i \geq \delta \\ \delta - \lambda_i & \lambda_i < \delta \end{cases}$$

Eigenvalue Modification

If, on the other hand, we use the Euclidean norm the smallest change includes a multiple of the identity matrix, *i.e.* **"shift the eigenvalue spectrum, so all eigenvalues are positive:"**

$$B = A + \Delta A, \quad \text{where} \quad \Delta A = \tau I, \quad \tau = \max(0,\, \delta - \lambda_{\min}(A))$$

We recognize this type of modification to A from our discussion on **"Nearly exact solutions to the subproblem"** for trust-region methods (Lecture #9)...

Both constant-diagonal — $\tau\mathbf{I}$ — and "Frobenius-style" — $\mathbf{Q}\,\mathrm{diag}(\tau_\mathbf{i})\,\mathbf{Q}^\mathbf{T}$ — modifications are used in production software. Generally they do not rely on an exact spectral decomposition (full computation of the eigenvalues) of the Hessian, but use a cousin of Gaussian Elimination (usually the Cholesky factorization) which allows introduction of modifications indirectly.

$\mathbf{B} = \mathbf{A} + \tau\mathbf{I}$

In adding a multiple of the identity matrix, we would like to identify a scalar τ so that

$$\tau = \max\Big(0,\, \delta - \lambda_{\min}(A)\Big).$$

Usually we do not have access to $\lambda_{\min}(A)$, so we have to use some clever heuristic to get an estimate and generate

$$\begin{cases} \tau = 0 & \text{if } \lambda_{\min}(A) \geq \delta \\ \tau \geq \delta - \lambda_{\min}(A) & \text{if } \lambda_{\min}(A) < \delta \end{cases}$$

It is important not to select a value of τ that is unnecessarily large, since this biases the direction toward the steepest descent direction.

$\mathbf{B} = \mathbf{A} + \tau\mathbf{I}$

The following algorithm uses the fact that

$$|\lambda_i| \leq \|A\|_F, \quad \forall i = 1, 2, \ldots, n$$

it is quite expensive since a new factorization is attempted in each loop, further the generated τ may be unnecessarily large.

Algorithm

```
β = ||A||_F, k=0
if( min(a_ii) > 0 ) { τ_0 = 0 } else { τ_0 = β/2 } endif
while( k < maxiter )
  ATTEMPT (Incomplete) Cholesky Factorization
  LL^T = A + τ_k I
  if( successful_factorization ), return(L)
  else, τ_{k+1} = max(2τ_k, β/2)
  endif
end(while)
```


$\mathbf{B} = \mathbf{A} + \text{diag}(\bar{\mathbf{d}}^{\text{add}})$ — Breaking Cholesky

It is more efficient to let the Cholesky factorization routine directly modify the matrix A so that the factorization succeeds.

What can go wrong in Cholesky factorization?

We look at the Cholesky factorization in LDL^T-form — set $M = LD^{1/2}$ to get to MM^T form.

Algorithm: Cholesky Factorization, LDL^T-form

```
for j = 1:n
  c_jj = a_jj - sum_{s=1}^{j-1} d_s l_js^2
  d_j = c_jj                   --- The diagonal entries in D (must be ≥ δ)
  for i = (j+1):n
    c_ij = a_ij - sum_{s=1}^{j-1} d_s l_is l_js
    l_ij = c_ij/d_j            --- We don't want l_ij to be too large
  end
end
```


$\mathbf{B} = \mathbf{A} + \text{diag}(\bar{\mathbf{d}}^{\text{add}})$ — Modifying Cholesky

If we want to require that the matrix LDL^T is sufficiently positive definite, we simply modify the elements d_j:

$$\mathbf{d_j} = \mathbf{c_{jj}} \quad \rightarrow \quad \mathbf{d_j} = \max(\mathbf{c_{jj}}, \delta)$$

Usually, we also want to have a bound on the size of the off-diagonal entries of $M = LD^{1/2}$, *i.e.* $|m_{ij}| \leq \beta$ $(i > j)$, we set

$$\theta_j = \max_{j<i\leq n} |c_{ij}|$$

and let

$$d_j = c_{jj} \quad \rightarrow \quad d_j = \max\left(c_{jj}, \delta, \left[\frac{\theta_j}{\beta}\right]^2\right)$$

we have

$$|m_{ij}| = |l_{ij}\sqrt{d_j}| = \frac{|c_{ij}|}{\sqrt{d_j}} \leq \frac{|c_{ij}|\beta}{\theta_j} \leq \beta.$$

$\mathbf{B} = \mathbf{A} + \text{diag}(\bar{\mathbf{d}}^{\text{add}})$ — Modifying Cholesky

Finally, we throw in an absolute value on the c_{jj} term for good measure, and come up with

$$d_j = \max\left(|c_{jj}|, \delta, \left[\frac{\theta_j}{\beta}\right]^2\right), \quad d_j^{\text{add}} = d_j - c_{jj}$$

This exactly what the module `choldecomp()` in the old default project does! (With some modifications for computational efficiency — the algorithm generates the factorization directly in LL^T-form)

Old Default Project

choldecomp()	
Implementation	**Theory (here)**
`maxoffl`	β
`minl`	$\sqrt{\delta}$
`maxadd`	$\max(\textbf{diag}(\bar{\mathbf{d}}^{\text{add}}))$

Gershgorin Modification

choldecomp() and modelhess()

Theorem (Gershgorin's circle theorem)

tells us where the eigenvalues of a matrix are located:

$$|\lambda_i - a_{ii}| \leq \sum_{j \neq i} |a_{ij}|, \quad i = 1, \ldots, n.$$

Now given a matrix A, let $\mathbf{b_1}$ be the smallest value which makes $A + b_1 I$ positive definite from the Gershgorin circle theorem.

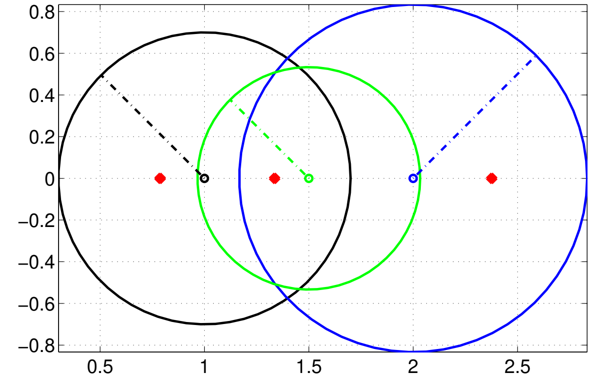
Let $\mathbf{b_2}$ = maxadd from choldecomp(), and let $\mu = \min(\mathbf{b_1}, \mathbf{b_2})$. Now, $A + \mu I$ is guaranteed to be positive definite.

Old Default Project

This is essentially modelhess(). In addition modelhess() returns the LL^T-decomposition of $A + \mu I$, and there are tests prior to the first call to choldecomp() which takes care of negative diagonal elements of A and large off-diagonal elements of A.

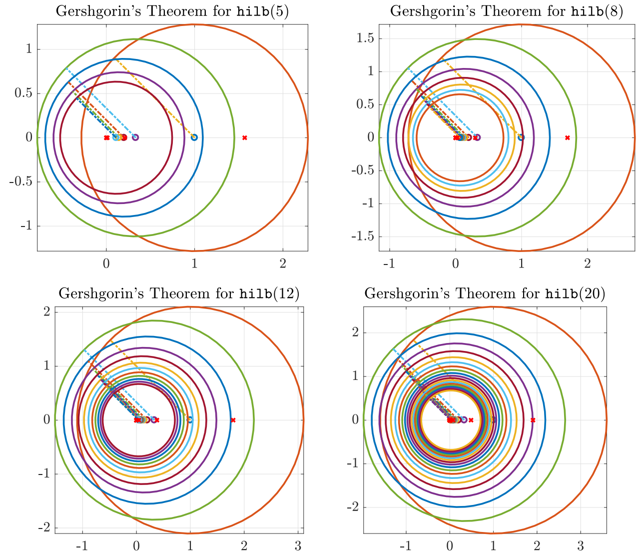
Note that modelhess() is similar to the algorithm on slide #13, but requires *at most* two calls to a Cholesky factorization algorithm.

Gershgorin's Circle Theorem: Illustration



$$A = \begin{bmatrix} 1 & 1/2 & 1/5 \\ 1/2 & 2 & 1/3 \\ 1/5 & 1/3 & 3/2 \end{bmatrix}, \quad \lambda(A) = \{0.7875,\ 1.3363,\ 2.3762\}$$

Gershgorin's Circle Theorem: Illustration



Project Expectation and Deliverables

Clarified

- Solve a larger optimization problem (see *e.g.* the "examples of past projects" handout from last time.
- You can look at different types of methods; performance for different test functions, etc... **BEST:** something relevant to your thesis project.
- **Deliverables:**
  - *Project Proposal* — 1 page, Due 11/16/2018
  - *Presentation* — 12–15 minutes, in-class (starting 12/10/2018)
  - *email* — presentation + code(s). (after presentation)

Next...

- Practical Newton Methods: Trust-Region Newton Methods
- Calculating Derivatives: Finite Differencing & Automatic Differentiation
- Quasi-Newton Methods...

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Recap
Hessian Modifications
Eigenvalue Modification
$\mathbf{B} = \mathbf{A} + \tau\mathbf{I}$
Gershgorin Modification

Index

matrix norm
- Euclidean, 10
- Frobenius, 10

theorem
- Gershgorin's circle theorem, 17

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