CME 307 / MS&E 311: Optimization

Newton and quasi-Newton methods

Professor Udell

Management Science and Engineering
Stanford

April 24, 2023

Questions from Ed

- well-conditioned vs ill-conditioned
- why approximate Hessian with $\frac{1}{t}\,\mathbf{I}$?

Outline

Minimize quadratic approximation

$$\text{minimize} \quad f(x)$$

Suppose $f : \mathbf{R} \to \mathbf{R}$ is twice differentiable. For any $x \in \mathbf{R}$, approximate f about x:

$$\begin{aligned} f(x) &\approx f(x^{(k)}) + \nabla f(x^{(k)})^T (x - x^{(k)}) \\ &\quad + \frac{1}{2}(x - x^{(k)})^T \nabla^2 f(x^{(k)})(x - x^{(k)}) \\ &\approx f(x^{(k)}) + \nabla f(x^{(k)})^T s + \frac{1}{2} s^T B_k s =: m_k(x) \end{aligned}$$

where $s = x - x^{(k)}$ is the **search direction** and $B_k \approx \nabla^2 f(x^{(k)})$ is the **Hessian approximation**.

If $B_k \succeq 0$, m_k is convex. to minimize,

$$B_k s + \nabla f(x^{(k)}) = 0$$

if B_k is invertible,

$$s = -B_k^{-1} \nabla f(x^{(k)})$$

Why do we need $B_k \succ 0$?

$$x^{(k+1)} = \operatorname*{argmin}_x m_k(x) = \operatorname*{argmin}_x f(x) + \nabla f(x^{(k)})^T s + \frac{1}{2} s^T B_k s$$

Why do we need $B_k \succ 0$?

$$x^{(k+1)} = \operatorname*{argmin}_x m_k(x) = \operatorname*{argmin}_x f(x) + \nabla f(x^{(k)})^T s + \frac{1}{2} s^T B_k s$$

Q: What happens if B_k is indefinite?

Why do we need $B_k \succ 0$?

$$x^{(k+1)} = \operatorname*{argmin}_x m_k(x) = \operatorname*{argmin}_x f(x) + \nabla f(x^{(k)})^T s + \frac{1}{2} s^T B_k s$$

Q: What happens if B_k is indefinite?
A: Go in the direction of negative curvature; but not clear how far to go.

Why do we need $B_k \succ 0$?

$$x^{(k+1)} = \operatorname*{argmin}_x m_k(x) = \operatorname*{argmin}_x f(x) + \nabla f(x^{(k)})^T s + \frac{1}{2} s^T B_k s$$

Q: What happens if B_k is indefinite?
A: Go in the direction of negative curvature; but not clear how far to go.
Q: What happens if B_k is not invertible?

Why do we need $B_k \succ 0$?

$$x^{(k+1)} = \operatorname*{argmin}_x m_k(x) = \operatorname*{argmin}_x f(x) + \nabla f(x^{(k)})^T s + \frac{1}{2} s^T B_k s$$

Q: What happens if B_k is indefinite?
A: Go in the direction of negative curvature; but not clear how far to go.
Q: What happens if B_k is not invertible?
A: Not clear how far to go in flat directions.

Why do we need $B_k \succ 0$?

$$x^{(k+1)} = \operatorname*{argmin}_x m_k(x) = \operatorname*{argmin}_x f(x) + \nabla f(x^{(k)})^T s + \frac{1}{2} s^T B_k s$$

Q: What happens if B_k is indefinite?
A: Go in the direction of negative curvature; but not clear how far to go.
Q: What happens if B_k is not invertible?
A: Not clear how far to go in flat directions.

in practice

- **make it psd.** modify B_k to be positive definite
- **trust region method.** minimize nonconvex m_k over a ball

Which quadratic approximation?

- **Gradient descent.** use $B_k = \frac{1}{t} I$ for some $t > 0$.

$$s = -t \nabla f(x)$$

- **Newton's method.** use $B_k = \nabla^2 f(x)$.

$$s = -(\nabla^2 f(x))^{-1} \nabla f(x)$$

- **Quasi-Newton methods.** use $B_k \approx \nabla^2 f(x^{(k)})$.

$$s = -B_k^{-1} \nabla f(x)$$

global convergence as long as $m_k(x) \geq f(x)$ for all x. but how fast?

Outline

Convergence rates

- **linear convergence.**

$$\lim_{k\to\infty} \frac{\|x^{(k)} - x^\star\|}{\|x^{(k-1)} - x^\star\|} = c \in (0, 1)$$

- **superlinear convergence.**

$$\lim_{k\to\infty} \frac{\|x^{(k)} - x^\star\|}{\|x^{(k-1)} - x^\star\|} = 0$$

- **quadratic convergence.**

$$\lim_{k\to\infty} \frac{\|x^{(k)} - x^\star\|}{\|x^{(k-1)} - x^\star\|^2} < M$$

Newton's method converges quadratically

Theorem (Local rate of convergence)

Suppose f is twice ctsly differentiable and $\nabla^2 f(x)$ is L-Lipschitz in a neighborhood of a strict local minimizer $x^\star \in \operatorname{argmin} f(x)$. Then Newton's method converges to $x^\star$ quadratically near $x^\star$.

recall an operator F is L-Lipschitz if

$$\|F(x) - F(y)\| \leq L\|x - y\|$$

Taylor's theorem

since f is twice continuously differentiable,

$$\nabla f(y) - \nabla f(x) = \int_0^1 \nabla^2 f(x + t(y - x))(y - x)dt$$

source: https://www.cambridge.org/core/books/optimization-for-data-analysis/C02C3708905D236AA354D1CE1739A6A2

Newton's method converges quadratically (I)

proof: $x^\star$ is strict local min, so $\nabla f(x^\star) = 0$ and $\nabla^2 f(x^\star) \succ 0$.

$$
\begin{aligned}
x^{(k+1)} - x^\star &= x^{(k)} + s^{(k)} - x^\star \\
&= x^{(k)} - x^\star - B_k^{-1} \nabla f(x^{(k)}) \triangleright \text{(Newton's method)} \\
&= (B^{(k)})^{-1} \left(B^{(k)}(x^{(k)} - x^\star) - \nabla f(x^{(k)}) \right)
\end{aligned}
$$

by taylor's theorem,
$\nabla f(x^{(k)}) = \int_0^1 \nabla^2 f(x^\star + t(x^{(k)} - x^\star))(x^{(k)} - x^\star) dt$, so

$$
\begin{aligned}
B^{(k)}(x^{(k)} - x^\star) - \nabla f(x^{(k)}) &= \int_0^1 \left(\nabla^2 f(x^{(k)}) - \nabla^2 f(x^\star + t(x^{(k)} - x^\star)) \right) (x^{(k)} - x^\star) d \\
\|B^{(k)}(x^{(k)} - x^\star) - \nabla f(x^{(k)})\| &\leq \int_0^1 \|\nabla^2 f(x^{(k)}) - \nabla^2 f(x^\star + t(x^{(k)} - x^\star))\| \|x^{(k)} - x^\star\| d \\
&\leq \int_0^1 Lt \|x^{(k)} - x^\star\|^2 dt \\
&\leq \frac{L}{2} \|x^{(k)} - x^\star\|^2
\end{aligned}
$$

Newton's method converges quadratically (II)

now choose $r \in \mathbf{R}$ small enough that for $\|x^{(k)} - x^\star\| \le r$,

$\|(\nabla^2 f(x^{(k)}))^{-1}\| \le 2\|(\nabla^2 f(x^\star))^{-1}\| \triangleright$(possible since $\nabla^2 f(x^\star) \succ 0$)

then complete the proof:

$$\begin{aligned} \|x^{(k+1)} - x^\star\| &\le \frac{L}{2}\|(\nabla^2 f(x^{(k)}))^{-1}\|\|x^{(k)} - x^\star\|^2 \\ &\le \underbrace{L\|(\nabla^2 f(x^\star))^{-1}\|}_{\text{constant}}\|x^{(k)} - x^\star\|^2 \end{aligned}$$

Outline

Quasi-Newton methods

what's the problem with Newton's method? $\nabla^2 f(x)$ is

- expensive to compute
- expensive to invert
- not always positive definite

Quasi-Newton methods

what's the problem with Newton's method? $\nabla^2 f(x)$ is

- expensive to compute
- expensive to invert
- not always positive definite

quasi-Newton method: use a matrix $B_k \approx \nabla f^2(x^{(k)})$ (or $H_k = B_k^{-1}$) that is

- easy to update
- easy to invert

update B_k at each iteration to improve/maintain approximation

Quasi-Newton methods

what's the problem with Newton's method? $\nabla^2 f(x)$ is

- expensive to compute
- expensive to invert
- not always positive definite

quasi-Newton method: use a matrix $B_k \approx \nabla f^2(x^{(k)})$ (or $H_k = B_k^{-1}$) that is

- easy to update
- easy to invert

update B_k at each iteration to improve/maintain approximation

can still get superlinear convergence!

BFGS

BFGS is the most popular quasi-Newton method. idea:

- take step with length $\alpha_k > 0$ chosen by line search
$$x^{(k+1)} = x^{(k)} + \alpha_k(-B_k^{-1}\nabla f(x^{(k)})) =: x^{(k)} + s^{(k)}$$
- new model will be
$$m_{k+1}(x) = f(x^{(k+1)}) + \nabla f(x^{(k+1)})^T p + \frac{1}{2} p^T B_{k+1} p$$
where $p = x - x^{(k+1)}$

want gradient of m_{k+1} to match f at $x^{(k)}$ and $x^{(k+1)}$:

- match at $x^{(k+1)}$ by construction
- match at $x^{(k)}$ if
$$\begin{aligned} \nabla f(x^{(k)}) &= \nabla m_{k+1}(x^{(k)} - x^{(k+1)}) = \nabla f(x^{(k+1)}) \\ \nabla f(x^{(k+1)}) - \nabla f(x^{(k)}) &= B_{k+1}(x^{(k+1)} - x^{(k)}) \\ y^{(k)} &= B_{k+1}s^{(k)} \triangleright \text{(secant equation)} \end{aligned}$$
where $y^{(k)} = \nabla f(x^{(k+1)}) - \nabla f(x^{(k)})$, $s^{(k)} = x^{(k+1)} - x^{(k)}$.

Secant equation

$$y^{(k)} = B_{k+1} s^{(k)}$$

where $y^{(k)} = \nabla f(x^{(k+1)}) - \nabla f(x^{(k)})$, $s^{(k)} = x^{(k+1)} - x^{(k)}$.

- need $s^{(k)T} y^{(k)} > 0$ (otherwise B_{k+1} is not positive definite)
- (*) if f is strongly convex, then $s^{(k)T} y^{(k)} > 0$ for all k (pf on next slide)
- for nonconvex f, can enforce $s^{(k)T} y^{(k)} > 0$ by using a line search that satisfies Wolfe conditions:

$$\begin{aligned} f(x^{(k)} + \alpha p^{(k)}) - f(x^{(k)}) &\geq \alpha c_1 \nabla f(x^{(k)})^T p^{(k)} \\ \nabla f(x^{(k)} + \alpha p^{(k)})^T p^{(k)} &\geq c_2 \nabla f(x^{(k)})^T p^{(k)} \end{aligned}$$

  where $p^{(k)} = -B_k^{-1} \nabla f(x^{(k)})$ is search direction and $c_1, c_2 \in (0,1)$ are constants.

Proof of (*)

Lemma (*)

if f is strongly convex, then $y^{(k)T}s^{(k)} > 0$ for all k

Proof of (*)

Lemma (*)

if f is strongly convex, then $y^{(k)T}s^{(k)} > 0$ for all k

proof: for f μ-strongly convex, for any $v, w \in \mathbf{R}^n$,

$$\begin{aligned}
f(v) &\geq f(w) + \nabla f(w)^T(v-w) + \frac{\mu}{2}\|v-w\|^2 \\
f(w) &\geq f(v) + \nabla f(v)^T(w-v) + \frac{\mu}{2}\|w-v\|^2 \\
0 &\geq (\nabla f(v) - \nabla f(w))^T(v-w) + \mu\|v-w\|^2 \\
\Longrightarrow\ (y^{(k)})^T s^{(k)} &\geq \mu\|s^{(k)}\|^2 > 0
\end{aligned}$$

setting $v = x^{(k+1)}$, $w = x^{(k)}$ and using $s^{(k)} = x^{(k+1)} - x^{(k)}$, $y^{(k)} = \nabla f(x^{(k+1)}) - \nabla f(x^{(k)})$.

BFGS update

- $B_{k+1} \in \mathbf{S}^n_+$ has $n(n+1)/2$ degrees of freedom
- secant equation gives n-dimensional linear system for B_{k+1}
  $\implies$ many solutions!
- BFGS update chooses rank 2 update

$$B_{k+1} = B_k + \frac{y^{(k)} y^{(k)T}}{y^{(k)T} s^{(k)}} - \frac{B_k s^{(k)} s^{(k)T} B_k}{s^{(k)T} B_k s^{(k)}}$$

- equivalently, can update the inverse Hessian approximation $H_k = B_k^{-1}$:

$$H_{k+1} = (I - \rho^{(k)} s^{(k)} y^{(k)T}) H_k (I - \rho^{(k)} y^{(k)} s^{(k)T})^T + \rho^{(k)} s^{(k)} s^{(k)T}$$

  where $\rho^{(k)} = \frac{1}{y^{(k)T} s^{(k)}}$ (uses Sherman-Morrison-Woodbury)
- each iteration uses $O(n^2)$ flops

Sherman Morrison Woodbury formula

Lemma

Sherman-Morrison-Woodbury formula for a matrix $H = A + UCV$ *(where dimensions match)*

$$H^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

can derive from formula for 2x2 (block) matrix inverse
special case: $H = A + uv^T$ *for* $u, v \in \mathbf{R}^n$*:*

$$H^{-1} = A^{-1} - \frac{A^{-1}uv^TA^{-1}}{1 + v^TA^{-1}u}$$

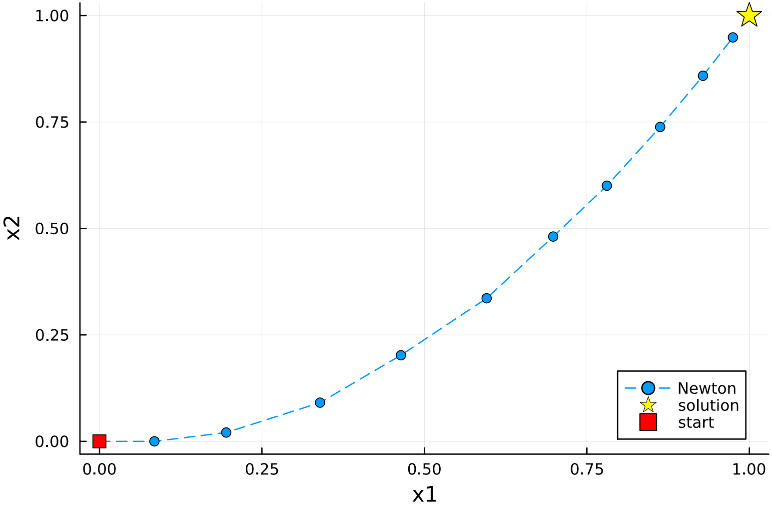
also called **matrix inversion lemma** or any subset of names

BFGS convergence

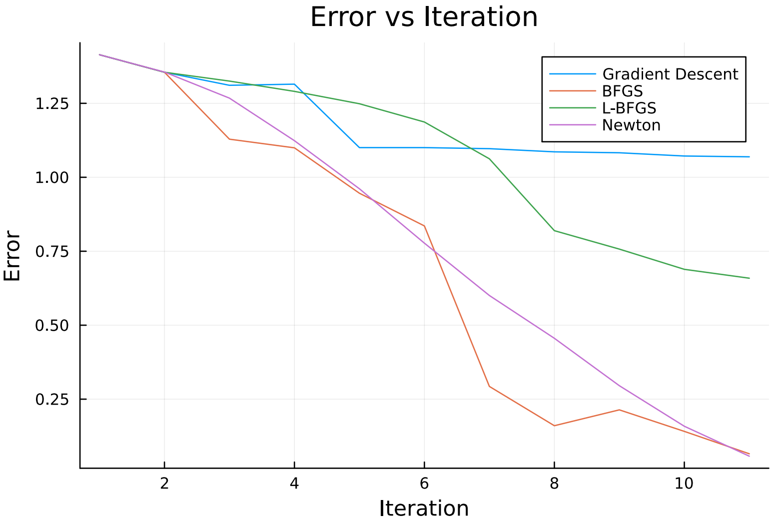
demo: try on Rosenbrock function
$f(x, y) = (1 - x)^2 + 100(y - x^2)^2$

https://github.com/stanford-cme-307/demos/blob/main/qn.jl

BFGS in practice



BFGS in practice



Limited memory quasi-Newton methods

main disadvantage of quasi-Newton method: need to store H or B

Limited-memory BFGS (L-BFGS): don't store B explicitly!

- instead, store the m (say, $m = 30$) most recent values of

$$s_j = x^{(j)} - x^{(j-1)}, \qquad y_j = \nabla f(x^{(j)}) - \nabla f(x^{(j-1)})$$

- evaluate $\delta x = B_k \nabla f(x^{(k)})$ recursively, using

$$B_j = \left(I - \frac{s_j y_j^T}{y_j^T s_j}\right) B_{j-1} \left(I - \frac{y_j s_j^T}{y_j^T s_j}\right) + \frac{s_j s_j^T}{y_j^T s_j}$$

assuming $B_{k-m} = I$

Limited memory quasi-Newton methods

main disadvantage of quasi-Newton method: need to store H or B

Limited-memory BFGS (L-BFGS): don't store B explicitly!

- instead, store the m (say, $m = 30$) most recent values of

$$s_j = x^{(j)} - x^{(j-1)}, \qquad y_j = \nabla f(x^{(j)}) - \nabla f(x^{(j-1)})$$

- evaluate $\delta x = B_k \nabla f(x^{(k)})$ recursively, using

$$B_j = \left(I - \frac{s_j y_j^T}{y_j^T s_j}\right) B_{j-1} \left(I - \frac{y_j s_j^T}{y_j^T s_j}\right) + \frac{s_j s_j^T}{y_j^T s_j}$$

  assuming $B_{k-m} = I$
- advantage: for each update, just apply rank 1 + diagonal matrix to vector!
- cost per update is $O(n)$; cost per iteration is $O(mn)$
- storage is $O(mn)$

L-BFGS: interpretations

- only remember curvature of Hessian on active subspace

$$S_k = \mathrm{span}\{s_k, \ldots, s_{k-m}\}$$

- hope: locally, $\nabla f(x^{(k)})$ will approximately lie in active subspace

$$\nabla f(x^{(k)}) = g^S + g^{S^\perp}, \quad g^S \in S_k,\ g^{S^\perp} \text{ small}$$

- L-BFGS assumes $B_k \sim I$ on $S^\perp$, so $B_k g^{S^\perp} \approx g^{S^\perp}$;
  if $g^{S^\perp}$ is small, it shouldn't matter much.

Outline

Three perspectives

- precondition the function
- change the quadratic approximation
- change the metric

Three perspectives

- precondition the function
- change the quadratic approximation
- change the metric

three names:

- preconditioned
- quasi-Newton
- variable metric

Recap: convergence analysis for gradient descent

$$\text{minimize} \quad f(x)$$

recall: we say (twice-differentiable) f is μ-strongly convex and L-smooth if

$$\mu I \preceq \nabla^2 f(x) \preceq LI$$

recall: if f is μ-strongly convex and L-smooth, gradient descent converges linearly

$$f(x^{(k)}) - p^\star \leq \frac{Lc^k}{2}\|x^{(0)} - x^\star\|^2,$$

where $c = (\frac{\kappa-1}{\kappa+1})^2$, $\kappa = \frac{L}{\mu} \geq 1$ is condition number
$\implies$ want $\kappa \approx 1$

Recap: convergence analysis for gradient descent

$$\text{minimize} \quad f(x)$$

recall: we say (twice-differentiable) f is μ-strongly convex and L-smooth if

$$\mu I \preceq \nabla^2 f(x) \preceq LI$$

recall: if f is μ-strongly convex and L-smooth, gradient descent converges linearly

$$f(x^{(k)}) - p^\star \leq \frac{Lc^k}{2}\|x^{(0)} - x^\star\|^2,$$

where $c = (\frac{\kappa-1}{\kappa+1})^2$, $\kappa = \frac{L}{\mu} \geq 1$ is condition number
$\implies$ want $\kappa \approx 1$

idea: can we minimize another function with $\kappa \approx 1$ whose solution will tell us the minimizer of f?

Preconditioning

for $D \succ 0$, the two problems

$$\text{minimize} \quad f(x) \quad \text{and} \quad \text{minimize} \quad f(Dz)$$

have solutions related by $x^\star = Dz^\star$

- gradient of $f(Dz)$ is $D^T \nabla f(Dz)$
- the second derivative (Hessian) of $f(Dz)$ is $D^T \nabla^2 f(Dz) D$

a gradient step on $f(Dz)$ with step-size $t > 0$ is

$$\begin{aligned} z^+ &= z - tD^T \nabla f(Dz) \\ Dz^+ &= Dz - tDD^T \nabla f(Dz) \\ x^+ &= x - tDD^T \nabla f(x) \end{aligned}$$

from prev analysis, gd on z converges fastest if

$$\begin{aligned} D^T \nabla^2 f(Dz) D &\approx I \\ D &\approx (\nabla^2 f(Dz))^{-1/2} \end{aligned}$$

Approximate inverse Hessian

$B = DD^T$ is called the **approximate inverse Hessian**

can fix B or update it at every iteration:

- if B is constant: called **preconditioned** method (*e.g.*, preconditioned conjugate gradient)
- if B is updated: called **(quasi)-Newton** method

how to choose B? want

- $B \approx \nabla^2 f(x)^{-1}$
- easy to compute (and update) B
- fast to multiply by B

Outline

Variable metric

definition of the gradient:

$$f(x+h) = f(x) + \langle \nabla f(x), s \rangle + \frac{1}{2}\langle s, \nabla^2 f(x) s \rangle + o(s^3)$$

wrt Euclidean inner product $\langle u, v \rangle = u^T v$

now define new inner product $\langle u, v \rangle_A = u^T A v$ for some matrix $A \in \mathbf{S}^n_{++}$.

compute the gradient and Hessian wrt this inner product:

$$\begin{aligned} f(x+h) &= f(x) + \langle \nabla f(x), s \rangle + \frac{1}{2}\langle s, \nabla^2 f(x) s \rangle + o(s^3) \\ &= f(x) + \langle A^{-1} \nabla f(x), s \rangle_A + \frac{1}{2}\langle s, A^{-1} \nabla^2 f(x) s \rangle_A + o(s^3) \end{aligned}$$

so the gradient and Hessian wrt the new inner product is

$$\nabla_A f(x) = A^{-1} \nabla f(x), \qquad \nabla_A^2 f(x) = \frac{1}{2}\left[A^{-1}\nabla^2 f(x) + \nabla^2 f(x) A^{-1}\right]$$

source: Nesterov Introductory Lectures on Convex Optimization, p. 40

Outline

Trust region methods

suppose B_k is indefinite. solution to model problem is unbounded!

$$\operatorname*{argmin}_x m_k(x) = \operatorname*{argmin}_x f(x) + \nabla f(x^{(k)})^T s + \frac{1}{2} s^T B_k s$$

trust region method limits step size by choosing $x^{(k+1)}$ to solve **trust region subproblem**

$$\begin{array}{ll} \text{minimize} & m_k(x) \\ \text{subject to} & \|x - x^{(k)}\| \leq \delta_k \end{array}$$

- nonconvex quadratic problem
- can solve with generalized eigenvalue solver

source: https://www.math.uwaterloo.ca/ hwolkowi/henry/reports/pre-views.d/trsalgorithm10.pdf