Modern Optimization Techniques

2. Unconstrained Optimization / 2.4. Quasi-Newton Methods

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Outline

1. Excursion: Inverting Matrices

2. The Idea of Quasi-Newton Methods

3. BFGS and L-BFGS

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1. Excursion: Inverting Matrices

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Matrix Inversion

Given a square matrix $A \in \mathbb{R}^{N \times N}$,
its **inverse** A^{-1} is a matrix such that:

$$AA^{-1} = \mathbf{I}$$

where

- $\mathbf{I}$ is the identity matrix
- if no such matrix A^{-1} exists, A is called **singular** (aka **non-invertible**)

Matrix Inversion — Easy cases

1. **small matrices:**
   - for $A \in \mathbb{R}^{2\times 2}$ the inverse can be computed analytically:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad A^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

   - slightly more complex closed formula for $A \in \mathbb{R}^{3\times 3}$

2. **orthogonal matrices:**
   - $A \in \mathbb{R}^{N\times N}$ is **orthogonal** if $A^T A = \mathbf{I}$
   - thus $A^{-1} = A^T$
   - example:

$$A := \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

Matrix Inversion — Easy cases

3. **diagonal matrices:**
   - $A \in \mathbb{R}^{N \times N}$ is **diagonal** if $A_{n,m} = 0$ for all $n \neq m$
   - thus $A = \text{diag}(a_1, a_2, \ldots, a_N)$ with

$$\text{diag}(a_1, \ldots, a_N) := \begin{pmatrix} a_1 & 0 & \ldots & 0 \\ 0 & a_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & a_N \end{pmatrix}$$

   - $A^{-1} = \text{diag}(\frac{1}{a_1}, \frac{1}{a_2}, \ldots, \frac{1}{a_N})$

General Matrix Inversion

Generally, inverting a matrix $A \in \mathbb{R}^{N \times N}$ is equivalent to solving a linear system of equations with n different right sides:

$$AA^{-1} = I \iff Ax^n = e^n, \quad e^n := \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \leftarrow n\text{-th position} \;, \quad n = 1, \ldots,$$

via $A^{-1} = (x^1, x^2, \ldots, x^N)$

If an inverse is used only once to compute $x := A^{-1}b$ for a vector $b \in \mathbb{R}^N$, it usually is faster to solve the linear system of equations $Ax = b$ instead.

General Matrix Inversion / Complexity

Inverting matrices and solving systems of linear equations can be accomplished two ways:

1. algebraic algorithms ("direct algorithms")
    - like Gaussian elimination, LU decomposition, QR decomposition
    - complexity generally $O(N^3)$
    - there exist specialized matrix inversion algorithms with lower costs
        - Strassen algorithm $O(N^{2.807})$
        - Coppersmith–Winograd algorithm $O(N^{2.376})$
        - but they are impractical and not used in implementations
2. optimization algorithms ("iterative algorithms")
    - Gauss-Seidel, Gradient-descent type of algorithms

Inverse of a Rank-One Update

Lemma (Inverse of a Rank-One Update – Sherman-Morrison formula)

For $A \in \mathbb{R}^{N \times N}$ invertible and $a, b \in \mathbb{R}^N$:

$$(A + ab^T)^{-1} = A^{-1} - \frac{A^{-1}ab^TA^{-1}}{1 + b^TA^{-1}a}$$

Meaning:

- the inverse of a rank-one update can be computed fast
  - in $O(N^2)$ instead of in $O(N^3)$
  - if the inverse of the original matrix is available

Inverse of a Rank-One Update / Proof

Show that the right side has the property of the inverse:

$$
\begin{aligned}
(A + ab^T)(A^{-1} - \frac{A^{-1}ab^TA^{-1}}{1 + b^TA^{-1}a})
&= I + ab^TA^{-1} - \frac{ab^TA^{-1} + ab^TA^{-1}ab^TA^{-1}}{1 + b^TA^{-1}a})\\
&= I + ab^TA^{-1} - \frac{a(1 + b^TA^{-1}a)b^TA^{-1}}{1 + b^TA^{-1}a})\\
&= I + ab^TA^{-1} - ab^TA^{-1} = I
\end{aligned}
$$

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Underlying Idea

- Approximate the Hessian with a matrix H that is fast to invert.

$$H \approx \nabla^2 f(x)$$

  - Use a low-rank update

$$H^{(0)} := I$$

$$H^{\text{next}} = H + \sum_{k=1}^{K} a_k b_k^T$$

    - fast to invert using K-times inverses of rank-one updates

$$(H^{-1})^{(0)} = I$$

$$(H^{-1})^{\text{next}} = H^{-1} + \ldots$$

- Compute the next direction using the inverse of the Hessian approximation:

$$\Delta x = -H^{-1} \nabla f(x)$$

Properties of the Hessian $\nabla^2 f(x)$

- it fulfills the **secant condition**

$$H(y - x) = \nabla f(y) - \nabla f(x)$$

  approximately:

$$\nabla^2 f(x)(y - x) \approx \nabla f(y) - \nabla f(x) \quad \text{for } y \approx x$$

  - due to first order Taylor expansion of ∇f:

$$\nabla f(y) \approx \nabla f(x) + \nabla^2 f(x)(y - x)$$

  - if H fulfills the secant condition,
    then the second order approximation of f by ∇f and H around x
    has gradient $\nabla f(y)$ at y

- it is symmetric

- it is positive semidefinite

- it is positive definite
  - for a strongly convex objective function

Properties of the Hessian $\nabla^2 f(x)$

- if H fulfills the secant condition,
  then the second order approximation of f by ∇f and H around x has gradient $\nabla f(y)$ at y

proof:

$$F(y) := f(x) + \nabla f(x)^T (y - x) + \frac{1}{2}(y - x)^T H (y - x)$$
$$\nabla F(y) = \nabla f(x) + H(y - x) = \nabla f(y)$$

Hessian Approximations

Idea: search for a matrix H that

- has some of the properties of the Hessian and
- is fast to compute
  - e.g., by a low-rank update from the previous approximation:

$$H^{(0)} := I$$

$$H^{\text{next}} = H + \sum_{k=1}^{K} a_k b_k^T, \quad a_k, b_k \in \mathbb{R}^N$$

Symmetric Rank-One Update

Lemma (Symmetric Rank-One Update)

There exists exactly one low-rank update such that

i) *H fulfils the secant condition*

$$H^{next} s = g, \quad s := x^{next} - x, \quad g := \nabla f(x^{next}) - \nabla f(x)$$

ii) *H is symmetric and*

iii) *is a rank-one update:*

$$a_1 = b_1 := \frac{g - Hs}{((g - Hs)^T s)^{\frac{1}{2}}}$$

$$H^{next} = H + \frac{(g - Hs)(g - Hs)^T}{(g - Hs)^T s}$$

Symmetric Rank-One Update / Proof

If H and H^{next} are symmetric, then $a_1 b_1^T$ must be also symmetric.

$$a_1 b_1^T \stackrel{!}{=} (a_1 b_1^T)^T = b_1 a_1^T \quad | \cdot a_1$$

$$a_1 b_1^T a_1 \stackrel{!}{=} b_1 a_1^T a_1 \quad \rightsquigarrow b_1 = \beta a_1, \quad \beta \in \mathbb{R}, \beta \neq 0$$

$$H^{\text{next}} \underset{iii}{=} H + \beta a_1 a_1^T$$

$$H^{\text{next}} s \underset{i}{=} g$$

$$\beta a_1 a_1^T s = g - Hs \quad \rightsquigarrow \quad a_1 = \gamma(g - Hs), \quad \gamma \in \mathbb{R}$$

$$\beta\gamma(g - Hs)\gamma(g - Hs)^T s = g - Hs$$

$$\beta\gamma^2(g - Hs)^T s = 1$$

$$\beta = 1, \quad \gamma = ((g - Hs)^T s)^{-\frac{1}{2}}, \quad a_1 = \frac{g - Hs}{((g - Hs)^T s)^{\frac{1}{2}}}$$

Symmetric Rank-One Update / Inverse

Lemma (Symmetric Rank-One Update / Inverse)

The inverse H^{-1} of the approximate Hessian in the symmetric rank-one update is

$$(H^{-1})^{next} = H^{-1} + \frac{(s - H^{-1}g)(s - H^{-1}g)^T}{(s - H^{-1}g)^T g}$$

Symmetric Rank-One Update / Inverse / Proof

Apply Morrison-Sherman to the rank-one update of the Hessian approximation:

$$
\begin{aligned}
(H^{-1})^{\text{next}} &= H^{-1} - \frac{H^{-1}(g-Hs)(g-Hs)^T H^{-1}}{(g-Hs)^T s(1+\frac{(g-Hs)^T H^{-1}(g-Hs)}{(g-Hs)^T s})} \\
&= H^{-1} - \frac{(H^{-1}g-s)(H^{-1}g-s)^T}{\underbrace{(g-Hs)^T s + (g-Hs)^T H^{-1}(g-Hs)}_{\substack{=(g-Hs)^T(s+H^{-1}g-s) \\ =(g-Hs)^T H^{-1} g \\ =(H^{-1}g-s)^T g}}} \\
&= H^{-1} + \frac{(s-H^{-1}g)(s-H^{-1}g)^T}{(s-H^{-1}g)^T g}
\end{aligned}
$$

Newton's Method (Review)

$$
\begin{array}{l}
\textbf{min-newton}(f, \nabla f, \nabla^2 f, x^{(0)}, \mu, \epsilon, K): \\
\quad \text{for } k := 1, \ldots, K: \\
\quad\quad \Delta x^{(k-1)} := -\nabla^2 f(x^{(k-1)})^{-1} \nabla f(x^{(k-1)}) \\
\quad\quad \text{if } -\nabla f(x^{(k-1)})^T \Delta x^{(k-1)} < \epsilon: \\
\quad\quad\quad \text{return } x^{(k-1)} \\
\quad\quad \mu^{(k-1)} := \mu(f, x^{(k-1)}, \Delta x^{(k-1)}) \\
\quad\quad x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)} \\
\quad \text{return "not converged"}
\end{array}
$$

where

- f objective function
- ∇f, $\nabla^2 f$ gradient and Hessian of objective function f
- $x^{(0)}$ starting value
- μ step length controller
- ϵ convergence threshold for Newton's decrement
- K maximal number of iterations

Quasi-Newton Method / SR1

min-qnewton-sr1$(f, \nabla f, x^{(0)}, \mu, \epsilon, K)$:
  $A^{(0)} := I$
  for $k := 1, \ldots, K$:
    $\Delta x^{(k-1)} := -A^{(k-1)} \nabla f(x^{(k-1)})$
    if $-\nabla f(x^{(k-1)})^T \Delta x^{(k-1)} < \epsilon$:
      return $x^{(k-1)}$
    $\mu^{(k-1)} := \mu(f, x^{(k-1)}, \Delta x^{(k-1)})$
    $x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)}$
    $s^{(k)} := x^{(k)} - x^{(k-1)}$
    $g^{(k)} := \nabla f(x^{(k)}) - \nabla f(x^{(k-1)})$
    $A^{(k)} := A^{(k-1)} + \frac{(s^{(k)} - A^{(k-1)} g^{(k)})(s^{(k)} - A^{(k-1)} g^{(k)})^T}{(s^{(k)} - A^{(k-1)} g^{(k)})^T g^{(k)}}$
  return "not converged"

where

- $A = H^{-1}$ the inverse of the approximative Hessian

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Positive Definite Hessian Approximations

- There is no rank-one update with positive definite Hessian approximation H.
- There are many rank-two update schemes with positive definite Hessian approximation H.
- Most widely used: BFGS
  - developed independently by Broyden, Fletcher, Goldfarb and Shanno in 1970

$$H^{\text{next}} = H - \frac{Hs(Hs)^T}{s^T Hs} + \frac{gg^T}{g^T s}$$

BFGS

Lemma (BFGS)

The BFGS update

$$H^{next} = H - \frac{Hs(Hs)^T}{s^T Hs} + \frac{gg^T}{g^T s}$$

i) *fulfils the secant condition,*

ii) *yields symmetric H and*

iii) *yields positive definite H, if $g^T s > 0$.*

The inverse H^{-1} of the approximate Hessian is

$$(H^{-1})^{next} = H^{-1} + \frac{(s - H^{-1}g)s^T + s(s - H^{-1}g)^T}{s^T g} - \frac{(s - H^{-1}g)^T g}{(s^T g)^2} ss^T$$

$$= (I - \frac{sg^T}{s^T g})H^{-1}(I - \frac{gs^T}{s^T g}) + \frac{ss^T}{s^T g}$$

BFGS / Proof (1/3)

i) BFGS fulfils the secant condition:

$$H^{\text{next}} s = Hs - \frac{Hs(Hs)^T s}{s^T Hs} + \frac{gg^T s}{g^T s}$$
$$= Hs - Hs + g = g$$

ii) BFGS yields symmetric H: obvious.

iii) BFGS yields positive definite H:

If H is positive definite, it can be represented $H = LL^T$ with a non-singular L (Cholesky decomposition).

$$H^{\text{next}} = LWL^T$$
$$W := I - \frac{\tilde{s}\tilde{s}^T}{\tilde{s}^T \tilde{s}} + \frac{\tilde{g}\tilde{g}^T}{\tilde{g}^T \tilde{s}}, \quad \tilde{s} := L^T s, \quad \tilde{g} := L^{-1} g$$

H^{next} will be pos.def., if W is.

BFGS / Proof (2/3)

for any $v \in \mathbb{R}^N$:

$$0 \overset{?}{<} v^T W v = v^T v - \frac{(v^T \tilde{s})^2}{\tilde{s}^T \tilde{s}} + \frac{(v^T \tilde{g})^2}{\tilde{g}^T \tilde{s}}$$

$$= ||v||^2 - \frac{||v||^2 ||\tilde{s}||^2 \cos^2 \theta_1}{||\tilde{s}||^2} + \frac{(v^T \tilde{g})^2}{\tilde{g}^T \tilde{s}}$$

$$= ||v||^2 (1 - \cos^2 \theta_1) + \frac{(v^T \tilde{g})^2}{\tilde{g}^T \tilde{s}}$$

$$= ||v||^2 \sin^2 \theta_1 + \frac{(v^T \tilde{g})^2}{\tilde{g}^T \tilde{s}}$$

$$\tilde{g}^T \tilde{s} = g^T s \underset{\text{assumption}}{>} 0$$

- if $v = \lambda \tilde{s}, \lambda \in \mathbb{R}, \lambda \neq 0$:
  - $\sin^2 \theta_1 = 0$, but
  - $(v^T \tilde{g})^2 = \lambda^2 (\tilde{s}^T \tilde{g})^2 > 0$
- if $v \neq \lambda \tilde{s}, \lambda \in \mathbb{R}, \lambda \neq 0$:
  - $\sin^2 \theta_1 > 0$

BFGS / Proof (3/3)

To derive the inverse of the approximate Hessian,
apply Morrison-Sherman twice.

Quasi-Newton Method / BFGS

min-qnewton-bfgs$(f, \nabla f, x^{(0)}, \mu, \epsilon, K)$:

$A^{(0)} := I$

for $k := 1, \ldots, K$:

$\Delta x^{(k-1)} := -A^{(k-1)} \nabla f(x^{(k-1)})$

if $-\nabla f(x^{(k-1)})^T \Delta x^{(k-1)} < \epsilon$:

return $x^{(k-1)}$

$\mu^{(k-1)} := \mu(f, x^{(k-1)}, \Delta x^{(k-1)})$

$x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)}$

$s^{(k)} := x^{(k)} - x^{(k-1)}$

$g^{(k)} := \nabla f(x^{(k)}) - \nabla f(x^{(k-1)})$

$$A^{(k)} := A^{(k-1)} + \frac{(s^{(k)} - A^{(k-1)} g^{(k)})(s^{(k)})^T + s^{(k)}(s^{(k)} - A^{(k-1)} g^{(k)})^T}{(s^{(k)})^T g^{(k)}} - \frac{(s^{(k)} - A^{(k-1)} g^{(k)})^T g^{(k)}}{((s^{(k)})^T g^{(k)})^2} s^{(k)} (s^{(k)})^T$$

return "not converged"

where

- $A = H^{-1}$ the inverse of the approximative Hessian

Avoid Materialization of A

- In the previous form, BFGS still requires N^2 storage to materialize the inverse A of the approximate Hessian.

- For any vector $v \in \mathbb{R}^N$, images $A^{(K)}v$ can be computed from the recursive formula from vectors $g^{(k)}, s^{(k)}$ $(k = 1, \ldots, K)$

$$
\begin{aligned}
A^{(K+1)} &= (I - \frac{s^{(K)}(g^{(K)})^T}{(s^{(K)})^T g^{(K)}}) A^{(K)} (I - \frac{g^{(K)}(s^{(K)})^T}{(s^{(K)})^T g^{(K)}}) + \frac{s^{(K)}(s^{(K)})^T}{(s^{(K)})^T g^{(K)}} \\
&= \left(\prod_{k=K}^{\downarrow 1} (I - \frac{s^{(k)}(g^{(k)})^T}{(s^{(k)})^T g^{(k)}}) \right) A^{(0)} \left(\prod_{k=1}^{K} (I - \frac{g^{(k)}(s^{(k)})^T}{(s^{(k)})^T g^{(k)}}) \right) + \ldots
\end{aligned}
$$

Compute Image Av without Materialization of A

bfgs-image-iha$(v, (s^{(k)})_{k=1,\ldots,K}, (g^{(k)})_{k=1,\ldots,K}, (\rho^{(k)})_{k=1,\ldots,K}, A^{(0)})$:

  $q := v$

  for $k := K, \ldots, 1$:

    $\alpha_k := \rho^{(k)} (s^{(k)})^T q$

    $q := q - \alpha_k g^{(k)}$

  $r := A^{(0)} q$

  for $k := 1, \ldots, K$:

    $\beta := \rho^{(k)} (g^{(k)})^T r$

    $r := r + s^{(k)} (\alpha_k - \beta)$

  return r

where

- $v \in \mathbb{R}^N$ vector whose image to compute, usually $\nabla f(x^{(k)})$
- $(s^{(k)})_{k=1,\ldots,K}, (g^{(k)})_{k=1,\ldots,K}$ as defined earlier
- $\rho^{(k)} := 1/(g^{(k)})^T s^{(k)}$
- $A^{(0)}$ initial inverse Hessian, e.g. I.

Quasi-Newton Method / BFGS w/o Materialization of A

min-qnewton-bfgs-nomat$(f, \nabla f, x^{(0)}, \mu, \epsilon, K)$:
  for $k := 1, \ldots, K$:
    $\Delta x^{(k-1)} := -\text{bfgs-image-iha}(\nabla f(x^{(k-1)}, s^{(1:k-1)},$
      $g^{(1:k-1)}, \rho^{(1:k-1)}, I)$
    if $-\nabla f(x^{(k-1)})^T \Delta x^{(k-1)} < \epsilon$:
      return $x^{(k-1)}$
    $\mu^{(k-1)} := \mu(f, x^{(k-1)}, \Delta x^{(k-1)})$
    $x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)}$
    $s^{(k)} := x^{(k)} - x^{(k-1)}$
    $g^{(k)} := \nabla f(x^{(k)}) - \nabla f(x^{(k-1)})$
    $\rho^{(k)} := 1/(g^k)^T s^{(k)}$
  return "not converged"

Avoid Materialization of A

- Storing all vectors $g^{(1:K)}, s^{(1:K)}$ requires $2KN$ storage, i.e. is only memory efficient for $K \ll N$.
- Instead of computing the inverse A of the approximate Hessian by all these vectors, we could
  - forget the older ones, i.e.,
  - just store and compute the $M \ll N$ most recent ones.
- This approach is called **Limited Memory BFGS** (L-BFGS)

Quasi-Newton Method / L-BFGS

min-qnewton-lbfgs$(f, \nabla f, x^{(0)}, \mu, \epsilon, K, M)$:
  for $k := 1, \ldots, K$:
    $k_0 := \max\{1, k-1-M+1\}$
    $\Delta x^{(k-1)} := -\text{bfgs-image-iha}(\nabla f(x^{(k-1)}, s^{(k_0:k-1)},$
      $g^{(k_0:k-1)}, \rho^{(k_0:k-1)}, I)$
    if $-\nabla f(x^{(k-1)})^T \Delta x^{(k-1)} < \epsilon$:
      return $x^{(k-1)}$
    $\mu^{(k-1)} := \mu(f, x^{(k-1)}, \Delta x^{(k-1)})$
    $x^{(k)} := x^{(k-1)} + \mu^{(k-1)} \Delta x^{(k-1)}$
    $s^{(k)} := x^{(k)} - x^{(k-1)}$
    $g^{(k)} := \nabla f(x^{(k)}) - \nabla f(x^{(k-1)})$
    $\rho^{(k)} := 1/(g^k)^T s^{(k)}$
  return "not converged"

Implementations need to ensure that the old vectors $s^{(1:k_0-1)}, g^{(1:k_0-1)}$ do not consume any memory (i.e., are overwritten by the more recent ones).

Summary

- Rank One Updates $A + ab^T$ of a matrix A can be inverted fast (in $O(N^2)$; if an inverse of A is available; Sherman-Morrison formula).
- Quasi-Newton methods are Newton methods with approximated Hessian.
  - approximations should share properties of the Hessian
    - secant condition, symmetry, positive definiteness
  - maintain the inverse of the Hessian (not the Hessian itself)
- symmetric rank one update:
  - only one such rank one update (not even pos.def.)
- BFGS rank two update:
  - one out of many such rank two updates
  - pos.def.

Summary (2/2)

- Images of a vector under the inverse Hessian can be computed even without materializing the inverse Hessian:
  - compute the image recursively from the images under the rank one update steps
  - Limited Memory BFGS (L-BFGS)

Further Readings

- Quasi-Newton methods are not covered by Boyd and Vandenberghe [2004]
- BFGS:
  - [Nocedal and Wright, 2006, ch. 6]
  - [Griva et al., 2009, ch. 12.3]
    the update formulas for the inverse are in ch. 13.5.
  - [Sun and Yuan, 2006, ch. 5.1]
- L-BFGS:
  - [Nocedal and Wright, 2006, ch. 7]
  - [Griva et al., 2009, ch. 13.5]

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Igor Griva, Stephen G. Nash, and Ariela Sofer. *Linear and Nonlinear Optimization*. Society for Industrial and Applied Mathematics, 2009.

Jorge Nocedal and Stephen J. Wright. *Numerical Optimization*. Springer Science+ Business Media, 2006.

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