Lecture 18

Scribe ?

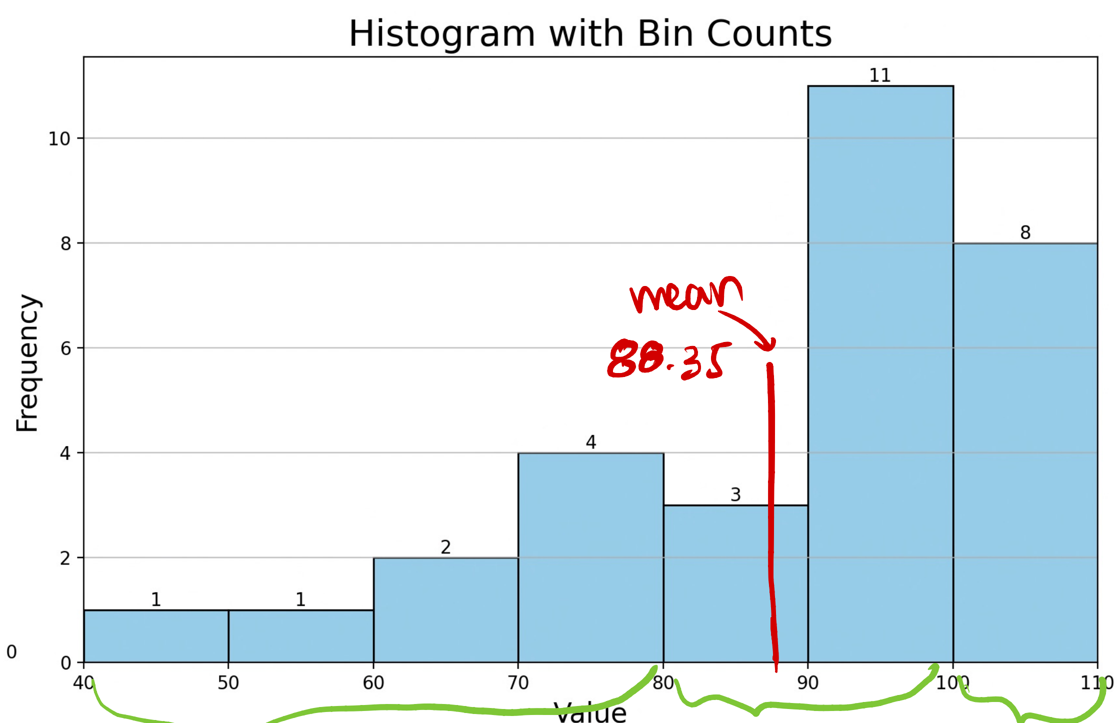
Last time

- Convergence guarantee
- Computational complexity
- Quasi-Newton intro.

Today

- Exam results.
- Modified Newton
- 3 variants

Distribution of the exam



Need to figure out what we are missing.

You are doing very well. Probably missed an ingredient.

Excellent!

The midterm weight can be anything between 15% - 40%.

Lots of room for improvement:

- Final can be worth 65%.
- Scribe and come to OH. (Easy 10% for participation).

New idea from last class

Instead of using Taylor's approximation, consider

$$m_k(x) = f_k + g_k^T(x - x_k) + \frac{1}{2}(x - x_k)^T B_k (x - x_k)$$

Thus, a natural strategy is to consider

x_{k+1} is such that $\nabla m_k(x_{k+1}) = 0$.

which in turn reduces to

$$x_{k+1} = x_k - \overbrace{B_k^{-1} g_k}^{p_k}.$$

when B_k is invertible.

Natural questions:

- How do we pick B_k so that we have descent?

▷ Can we make it cheaper per-iteration?

We will focus on the first question in this lecture.

Let's look at the geometry of a Newton step.

$\nabla^2 f(x_k)$ is a symmetric, real matrix (and let's assume nonsingular).

We might take an spectral decomposition:

$$\nabla^2 f(x_k) = V \underbrace{\Lambda}_{\text{Diagonal.}} \underbrace{V^T}_{\text{orthogonal}} \quad \leftarrow \text{cost } O(d^3).$$

$$\Lambda = \underbrace{\begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_d \end{pmatrix}}_{\text{Eigenvalues}} = \begin{pmatrix} \Lambda_+ & \\ & \Lambda_- \end{pmatrix}$$

$$V = \underbrace{\begin{pmatrix} | & & | \\ v_1 & \cdots & v_d \\ | & & | \end{pmatrix}}_{\text{Eigenvectors}} = \begin{pmatrix} V_+ & V_- \end{pmatrix}$$

Now we can decompose the Newton step:

$$p_k = -(V \Lambda V^T)^{-1} \nabla f(x_k)$$

$$= -V \Lambda^{-1} V^T \nabla f(x_k)$$

$$= -\begin{pmatrix} V_+ \\ V_- \end{pmatrix} \begin{pmatrix} \Lambda_+^{-1} & \\ & \Lambda_-^{-1} \end{pmatrix} \begin{bmatrix} V_+^T \nabla f(x_k) \\ V_-^T \nabla f(x_k) \end{bmatrix}$$

invert diagonals

$$= \underbrace{-V_+ \Lambda_+^{-1} V_+^T \nabla f(x_k)}_{p_k^+} \underbrace{- V_- \Lambda_-^{-1} V_- \nabla f(x_k)}_{p_k^-}$$

Claim: p_k^+ is a "descent" direction $(\nabla f(x_k)^T p_k^+ \leq 0)$.

We can easily check

$$\nabla f(x)^T p_k^+ = -\nabla f(x_k)^T V_+ \Lambda_+^{-1} V_+^T \nabla f(x_k) \nabla f(x_k) \leq 0.$$

Symmetrically p_k^- satisfies $\nabla f(x_k)^T p_k^- \geq 0$.

Thus if all eigenvalues are positive $\Rightarrow$ Descent
all eigenvalues are negative $\Rightarrow$ Ascent
mixture $\Rightarrow$ Could do anything.

Lemma: If $B_k \succ 0$ and $g_k \neq 0$, then $p_k = \arg\min_p \{g_k^T p + p^T B_k p\}$

$\Rightarrow \quad g_k^T p_k < 0.$

In particular, if $g_k = \nabla f(x_k)$, then p_k is a descent direction.

Proof: Since B_k is positive definite, then $p \mapsto g_k^T p + p^T B_k p$ is strongly convex, then p_k is well-defined.
Then $p_k = -B_k g_k$, thus

$$g_k^T p_k = -g_k^T B_k g_k < 0 \qquad \square$$

Warning: This doesn't guarantee that we have $f(x_{k+1}) \leq f(x_k)$ via

$$x_{k+1} \leftarrow x_k - B_k^{-1} \nabla f(x_k).$$

We only have

$$f(x_k + \alpha p_k) = f(x_k) + \underbrace{\alpha \nabla f(x_k)^T p_k}_{<0} + o(\alpha^2).$$

Thus we need an stepsize!
Linesearch could we applied. The Armijo condition reduces to: for some $\eta \in (0,1)$

$$f(x_k - \alpha_k p_k) \leq f(x_k) + \eta \alpha_k g_k^T p_k$$

with α_k exponentially shrinking until this holds.

Modified Newton's Method

Consider the following template

Loop $k = 0, 1, \ldots$

Compute $\nabla f(x_k)$ and $\nabla^2 f(x_k)$

3 methods today. → Build $B_k \succ 0$ (Based on $\nabla^2 f(x_k)$)

Compute $p_k \leftarrow B_k^{-1} \nabla f(x_k)$

Pick α_k ensuring descent (Armijo)

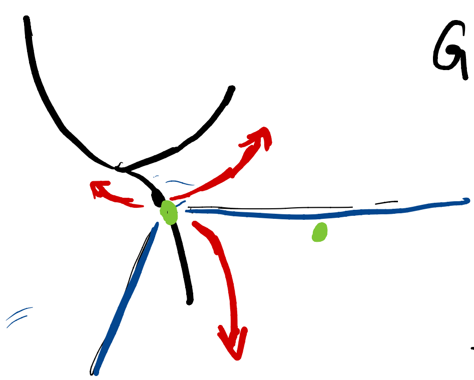
$x_{k+1} \leftarrow x_k + p_k$

End loop.

HW 5 you'll prove constant stepsizes also work.

▷ Option 1

Discard nonpositive eigenvalues



Get the factorization

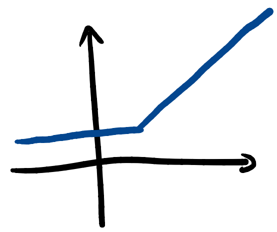
$$\nabla^2 f(x_k) = V \Lambda V^T$$

Define

$$\bar{\Lambda} = \operatorname{diag}(\bar{\lambda}_i) \quad \text{with}$$

$$\bar{\lambda}_i = \max\{\lambda_i, \varepsilon\}$$

$\varepsilon \geq 0$



Then take

$$B_k = V \bar{\Lambda} V^T.$$

The downside is that we loose the "mag

nitude" of the negative λ_i.
We move little when $\nabla f(x_k)$ is aligned with negative components.
Pretty bad unless $\nabla^2 f(x_k) \succeq \varepsilon I$, in which case was good too.

Option 2

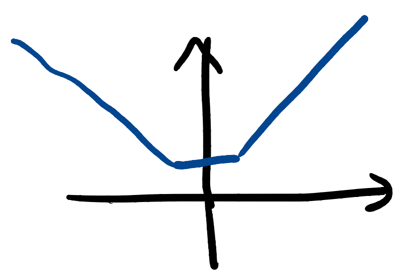
Keep eigenvalues with large magnitude, but make them positive

$$\nabla f(x_k) = V \Lambda V^T$$

Pick $\varepsilon > 0$ and set

$$\bar{\Lambda} = \operatorname{diag}(\bar{\lambda}_i) \quad \text{where} \quad \bar{\lambda}_i = \max\{|\lambda_i|, \varepsilon\}$$

$$B_k = V \bar{\Lambda} V^T.$$



$$\Rightarrow p_k = -B_k^{-1} \nabla f(x_k)$$

$$= -\left(\begin{pmatrix} V_+ & V_\varepsilon & V_- \end{pmatrix} \begin{pmatrix} \Lambda_+ & & \\ & \varepsilon I & \\ & & -\Lambda_- \end{pmatrix} \begin{pmatrix} V_+^T \\ V_\varepsilon^T \\ V_-^T \end{pmatrix} \right)^{-1} \nabla f(x_k)$$

$$= -V_+ \Lambda_+^{-1} V_+^T \nabla f(x_k) \leftarrow \text{descent}$$

$$- \frac{1}{\varepsilon} V_\varepsilon V_\varepsilon^T \nabla f(x_k)$$

"null space"

$$+ V_- \Lambda_-^{-1} V_-^T \nabla f(x_k).$$

previous ascent

Option 3

Shift the entire spectrum

Compute $\lambda_{min} = \lambda_{min}(\nabla^2 f(x_k))$

Pick $\varepsilon > 0$

If $\lambda_{min} \geq \varepsilon \Rightarrow B_k = 0$

Otherwise, set $\gamma = \varepsilon - \lambda_{min}$ and

$$B_k = \nabla f(x_k) + \gamma I.$$

Clearly

$$\lambda_i(B_k) = \lambda_i - \lambda_{min} + \varepsilon \geq \varepsilon.$$

Moreover if $p = -(\nabla^2 f(x_k) + \gamma I)^{-1} \nabla f(x_k)$

$\Rightarrow$ as $\gamma \downarrow 0$, $p \to -\nabla^2 f(x_k)$ (Newton)

$\Rightarrow$ as $\gamma \uparrow \infty$, $\frac{p}{\|p\|} \to \frac{\nabla f(x_k)}{\|\nabla f(x_k)\|}$ (Gradient descent)

Next time we will cover convergence guarantees.