Computational Statistics $\qquad$ Sep 22, 2021

Optimization Methods

Model problem: unconstrained convex optimization

Find $\displaystyle \arg\min_{\vec{x} \in \mathbb{R}^n} f(\vec{x})$

Newton's Method would solve $\nabla f(\vec{x}) = \vec{0}$

using the iteration $\vec{x}^{(k+1)} = \vec{x}^{(k)} - H^{-1}(\vec{x}^{(k)}) \nabla f(\vec{x}^{(k)})$

Hessian $H_{ij} = \dfrac{\partial^2 f}{\partial x_i \partial x_j}$

f convex $\Rightarrow$ H is symmetric positive definite.

BFGS (Broyden-Fletcher-Goldfarb-Shanno)

The idea is to construct a sequence of approximations to the true Hessian:

$$\vec{x}^{(k+1)} = \vec{x}^{(k)} - \left(H^{(k)}\right)^{-1} \nabla f(\vec{x}^{(k)})$$

$$\Leftrightarrow \quad H^{(k)} \underbrace{\left(\vec{x}^{(k+1)} - \vec{x}^{(k)}\right)}_{\vec{s}^{(k)}} = -\nabla f(\vec{x}^{(k)})$$

$$\Leftarrow\Rightarrow \quad \vec{x}^{(k+1)} = \vec{x}^{(k)} + \vec{s}^{(k)}$$

What properties should $H^{(k)}$ have?

- As $k \to \infty$, $H^{(k)} \to H(\vec{x}^{(k)})$ for a truly quadratic convex function f
- $H^{(k)}$ and $\left(H^{(k)}\right)^{-1}$ should be cheap to store/apply/update
- $H^{(k)}$ should be SPD (sym. pos. def.)

If f were quadratic, then

$$\nabla f(\vec{x}) = \nabla f(\vec{x}^{(k)}) + H(\vec{x} - \vec{x}^{(k)})$$

so $$\nabla f(\vec{x}^{(k+1)}) = \nabla f(\vec{x}^{(k)}) + H(\vec{x}^{(k+1)} - \vec{x}^{(k)})$$

$$\Rightarrow \underbrace{\nabla f(\vec{x}^{(k+1)}) - \nabla f(\vec{x}^{(k)})}_{\vec{g}^{(k)}} = H \underbrace{(\vec{x}^{(k+1)} - \vec{x}^{(k)})}_{\text{step size } \vec{s}^{k}}$$

SECANT CONDITION

$$g^{(k)} = H \vec{s}^{(k)}$$

One approach to finding $H^{(k+1)}$ is to minimize the change from $H^{(k)}$:

minimize $\| H^{(k+1)} - H^{(k)} \|$ subject to previous

constraints: $\vec{g}^{(k)} = H^{(k+1)} \vec{s}^{(k)}$

and $H^{(k+1)T} = H^{(k+1)}$

Equivalently minimize $\| H^{(k+1)-1} - H^{(k)-1} \|$

subject to $H^{-1} \vec{g}^{(k)} = \vec{s}^{(k)}$ and $H^{-1} = H^{-T}$

Choosing this norm $\|\cdot\|$ to be a particular weighted Frobenius norm

$$\| A \|_F^2 = \sum_{i,j} |a_{ij}|^2$$

gives the BFGS update formula for $H^{(k+1)}$:

$$H^{(k+1)} = H^{(k)} + \underbrace{\frac{\vec{g}\vec{g}^T}{\vec{g}^T \vec{s}} - \frac{H^{(k)} \vec{s} \vec{s}^T H^{(k)}}{\vec{s}^T H^{(k)} \vec{s}}}_{\text{a rank-2 update}}$$

In fact, $H^{(k+1)^{-1}}$ can be be computed fast using the Sherman-Morrison-Woodbury formula.

The algorithm is then:

1. Set $\vec{x}^{(0)}$, $\vec{H}^{(0)} = I$ (or other good guess), and compute $\nabla f(\vec{x}^{(0)})$

2. Compute $\vec{x}^{(1)} = \vec{x}^{(0)} - \vec{H}^{(0)^{-1}} \nabla f(\vec{x}^{(0)})$

   or equivalently: solve $\vec{H}^{(0)} \vec{s}^{(0)} = -\nabla f(\vec{x}^{(0)})$

   compute $\vec{x}^{(1)} = \vec{x}^{(0)} + \vec{s}^{(0)}$

3. Stop if $\|\vec{s}^{(0)}\|$ is small.

4. Otherwise compute $\nabla f(\vec{x}^{(1)})$, $H^{(1)}$ via the BFGS update, and repeat going back to (2) for $\vec{x}^{(k+1)}$, etc.

Numerical Linear Algebra

Products	BLAS libraries		Solutions
- vector-vector	BLAS 1	$O(n)$ flops	- $A\vec{x} = \vec{b}$
- matrix-vector	BLAS 2	$O(n^2)$ flops	- minimize $\|A\vec{x} - \vec{b}\|_2$ (Least sq.)
- matrix-matrix	BLAS 3	$O(n^3)$ flops	

Contained in LAPACK

Factorizations

- $A = LU$ - $A = USV^T$
- $A = QR$

Eigencomputations

- Find all $\lambda_i, \vec{v}_i$ such that $A\vec{v}_i = \lambda \vec{v}_i$.

Condition number of a problem

The sensitivity of the "problem" at the solution.

Ex: For a function $y = f(x)$, how sensitive is y to x?

① In an <u>absolute</u> sense,

$$|y - y'| = \underbrace{C(x)}_{\text{absolute condition number}} |x - x'|$$

$$\Rightarrow \quad C(x) = \frac{|y - y'|}{|x - x'|}$$

and for $x \simeq x'$, $C(x) \simeq f'(x)$.

② In a <u>relative</u> sense:

$$\frac{|y - y'|}{|y|} \simeq K(x) \underbrace{\left| \frac{x - x'}{x} \right|}_{\text{relative change in } x}$$

$$\Rightarrow \quad K(x) = \left| \frac{y - y'}{y} \right| \left| \frac{x'}{x - x'} \right|$$

$$= \left| \frac{f(x) - f(x')}{x - x'} \right| \left| \frac{x}{f(x)} \right| = \left| \frac{f'(x)\, x}{f(x)} \right|$$

We will now discuss the analogue for linear systems:

When solving $A\vec{x} = \vec{b}$, what is the sensitivity of $\vec{x} = A^{-1}\vec{b}$ to changes in $\vec{b}$?

Norms for vector

Def: $\|\cdot\|$ is a norm if:

① $\|\vec{u}\| \geq 0$, $\|\vec{u}\| = 0$ iff $\vec{u} = \vec{0}$.

② $\|\alpha \vec{u}\| = |\alpha| \, \|\vec{u}\|$

③ $\|\vec{u} + \vec{v}\| \leq \|\vec{u}\| + \|\vec{v}\|$

Matrix norms

Def: ① $\|A\| \geq 0$

② $\|\alpha A\| = |\alpha| \, \|A\|$

③ $\|A+B\| \leq \|A\| + \|B\|$

④ $\|AB\| \leq \|A\| \cdot \|B\|$ (sometimes).

If $\|\vec{u}\|$ is any vector norm, the the induced matrix norm is

$$\|A\| = \max_{\|\vec{u}\|=1} \|A\vec{u}\| = \max_{\vec{u} \neq \vec{0}} \frac{\|A\vec{u}\|}{\|\vec{u}\|}$$

$\Rightarrow$ For any $\|\vec{u}\|$, $\|A\vec{u}\| \leq \|A\| \, \|\vec{u}\|$

The most commonly used matrix norm is the induced 2-norm:

Thm $\|A\|_2 = \sqrt{\max\limits_j \lambda_j}$ of $A^T A$.

Pf: $\|A\|_2 = \max\limits_{\|\vec{u}\|=1} \|A\vec{u}\|_2$

SPD

$D = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix}$

$\|A\vec{u}\|_2^2 = (A\vec{u}, A\vec{u}) = (\vec{u}, A^T A \vec{u})$

$\Rightarrow \quad = (\vec{u}, PDP^T\vec{u}) = (P^T\vec{u}, DP^T\vec{u})$

since P is orthogonal, $\|P^T\vec{u}\|_2 = \|\vec{u}\|_2$.

$$\Rightarrow \max_{\|\vec{u}\|=1} \|A u\|_2^2 = \max_{\|\vec{u}\|=1} \left(P^T \vec{u}, D P^T \vec{u} \right)$$

$$= \max_{\|\vec{v}\|=1} (\vec{v}, D\vec{v})$$

$$= \max_{\|\vec{v}\|=1} \left(\lambda_1 v_1^2 + \lambda_2 v_2^2 + \dots + \lambda_n v_n^2 \right).$$

$$= \max_j \lambda_j .$$

By our definition earlier: the condition number of solving $A\vec{x} = \vec{b}$ is the sensitivity of $\vec{x}$ to changes in $\vec{b}$.

Let $\|\vec{b} - \vec{b}'\|$ be small, and $\vec{x} = A^{-1}\vec{b}$, $\vec{x}' = A^{-1}\vec{b}'$.

Then $\|\vec{x} - \vec{x}'\| = \|A^{-1}\vec{b} - A^{-1}\vec{b}'\|$

$$= \|A^{-1}(\vec{b} - \vec{b}')\|$$

$$\le \underbrace{\|A^{-1}\|}_{\text{absolute condition number.}} \cdot \|\vec{b} - \vec{b}'\|$$

Now the relative condition number is:

$$\frac{\|\vec{x} - \vec{x}'\|}{\|\vec{x}\|} \le \|A^{-1}\| \frac{\|\vec{b} - \vec{b}'\|}{\|\vec{x}\|}$$

$$= \|A^{-1}\| \frac{\|\vec{b} - \vec{b}'\|}{\|b\|} \frac{\|b\|}{\|\vec{x}\|}$$

$$= \|A^{-1}\| \frac{\|\vec{b} - \vec{b}'\|}{\|b\|} \frac{\|A\vec{x}\|}{\|\vec{x}\|}$$

Relative condition number

$K(A)$

$$\le \|A\| \, \|A^{-1}\| \frac{\|\vec{b} - \vec{b}'\|}{\|\vec{b}\|}$$

Consequences of $K(A)$:

$$\frac{\|\vec{x}-\vec{x}'\|}{\|\vec{x}\|} \le K(A) \frac{\|\vec{b}-\vec{b}'\|}{\|\vec{b}\|}$$

True linear system is $A\vec{x}=\vec{b}$.

Imagine that $\vec{b}'$ is the floating point representation of $\vec{b}$:

$$\vec{b}' = \text{round}(\vec{b}).$$

If machine precision is ϵ, this means $\frac{\|\vec{b}-\vec{b}'\|}{\|b\|} \sim \mathcal{O}(\epsilon)$

10^{-16}

$$\Rightarrow \frac{\|\vec{x}-\vec{x}'\|}{\|\vec{x}\|} \le K(A)\cdot\epsilon.$$

$\Rightarrow$ The number of significant digits lost in solving $A\vec{x}=\vec{b}$ is $\sim -\log_{10}(K(A)\cdot\epsilon)$.

This doesn't mean that $\frac{\|\vec{x}-\vec{x}'\|}{\|\vec{x}\|}$ cannot be smaller, but it puts a bound on how bad it can be.