Chapter 11 Quasi-Newton Methods

- Motivation It takes $\mathcal{O}\left(d^3\right)$ to calculate $\nabla^2 f(x)^{-1}$ or solve for $\nabla^2 f\left(\mathbf{x}_t\right) \Delta \mathbf{x}=-\nabla f\left(\mathbf{x}_t\right)$.

The secant method

- Motivation $\frac{f(x_t)-f(x_{t-1})}{x_t-x_{t-1}} \approx f'\left(x_t\right)$, so $x_{t+1}:=x_t-\frac{f(x_t)}{f'(x_t)} \approx x_{t+1}:=x_t-f'\left(x_t\right) \frac{x_t-x_{t-1}}{f'(x_t)-f'(x_{t-1})}$
- In optimization regime, we want to find a similar matrix s.t. $\nabla f\left(\mathbf{x}_t\right)-\nabla f\left(\mathbf{x}_{t-1}\right)=H_t\left(\mathbf{x}_t-\mathbf{x}_{t-1}\right)$ and so $\mathbf{x}_{t+1}=\mathbf{x}_t-H_t^{-1} \nabla f\left(\mathbf{x}_t\right)$.
  - This is called *secant condition*

Quasi-Newton methods

- Definition If H_t symmetric, and follows secant condition, the update method is *quasi-newton*.
- Lemma Exercise 71 $f \in C^2$ and $\nabla^2 f \neq 0$, then Newton's method is a Quasi-Newton method iff $f(\mathbf{x})=\frac{1}{2} \mathbf{x}^{\top} M \mathbf{x}-\mathbf{q}^{\top} \mathbf{x}+c$ with M invertable symmetric.
  - Proof
    - Newtwon is quasi $\Leftrightarrow \nabla f(y)-\nabla f(x)=\nabla^2 f(y)(y-x), \forall x, y$, take derivative w.r.t x, we get $\nabla^2 f(x)=\nabla^2 f(y), \forall x, y$ and this means f is a quadratic funciton, its invertable since every secant condition there is a solution. The other direciton is straightforward.

Greenstadt's Approach

- We already have $H_{t-1}^{-1}, x_{t-1}, x_t$, we need H_t^{-1}, idea is $H_t^{-1}=H_{t-1}^{-1}+E_t$, and we want to minimized the general change $\left\|A E A^{\top}\right\|_F^2$.
- Denote $H:=H_{t-1}^{-1}, H^{\prime}:=H_t^{-1}, E:=E_t, \boldsymbol{\sigma}:=\mathbf{x}_t-\mathbf{x}_{t-1}, \mathbf{y}=\nabla f\left(\mathbf{x}_t\right)-\nabla f\left(\mathbf{x}_{t-1}\right)$, and $\mathbf{r}=\boldsymbol{\sigma}-H \mathbf{y}$,
  - then the update formula is $H^{\prime}=H+E$, such that $H^{\prime} \mathbf{y}=\boldsymbol{\sigma}$ or equivalently $E \mathbf{y}=\mathbf{r}$,
  - so the overall minimization is $\operatorname{minimize} \quad \frac{1}{2}\left\|A E A^{\top}\right\|_F^2, \text{ subject to } E \mathbf{y}=\mathbf{r}$ and $E^{\top}-E=0$.

Solving with Lagrange multiplier

- Fact 11.2 If $f(E):=\frac{1}{2}\|A E B\|_F^2$, then $\nabla f(E)=A^{\top} A E B B^{\top}$ if define $\nabla f(E)=\left(\frac{\partial f(E)}{\partial E_{ij}}\right)$.
  - Proof
    - By this def, we have $\nabla_E \operatorname{Tr}(A E) \nabla_E=\operatorname{Tr}\left(E^{\top} A^{\top}\right)=A^{\top}$, so $f(E):=\frac{1}{2}\|A E B\|_F^2=\frac{1}{2} \operatorname{Tr}\left(B^{\top} E^{\top} A^{\top} A E B\right)$, then $\nabla f(E)=\nabla_E \frac{1}{2} \operatorname{Tr}\left(E^{\top} A^{\top} A E_0 B B^{\top}\right)+\nabla_E \frac{1}{2} \operatorname{Tr}\left(B B^{\top} E_0^{\top} A^{\top} A E\right)=A^{\top} A E B B^{\top} / 2+\left(B B^{\top} E^{\top} A^{\top} A\right)^{\top} / 2$ $=A^{\top} A E B B^{\top}$
- Denote $\boldsymbol{\lambda} \in \mathbb{R}^d$ as the multiplier for d constrains of $E \mathbf{y}=\mathbf{r}$, and $\Gamma \in \mathbb{R}^{d \times d}$ as the multiplier for $d \times d$ constraints of $E^{\top}-E=0$.
- For each equation of $\partial_{E_{ij}} f=\boldsymbol{\lambda}^{\top} f_1+\operatorname{Tr}\left(\Gamma f_2\right)$, λ part yields a term of $\lambda_i y_i$ and Γ yields a term of $\Gamma_{ji}-\Gamma_{ij}$
- Lemma 11.3 The above equation gives the optimial condtional of $W E^{\star} W=\boldsymbol{\lambda} \mathbf{y}^{\top}+\Gamma^{\top}-\Gamma$, where $W:=A^{\top} A$ is symmetric and posi definite.

Solving Greenstadt family

- The minimization has now turn into three linear equation (i) $E \mathbf{y}=\mathbf{r}$, (ii) $E^{\top}-E=0$ and (iii) $W E W=\boldsymbol{\lambda} \boldsymbol{y}^{\top}+\Gamma^{\top}-\Gamma$
- To eliminate Γ, by plug (iii) into (ii) we get $M\left(\boldsymbol{\lambda} \mathbf{y}^{\top}-\mathbf{y} \boldsymbol{\lambda}^{\top}+2 \Gamma^{\top}-2 \Gamma\right) M=0$, where $M=W^{-1}$, so $\Gamma^{\top}-\Gamma=\frac{1}{2}\left(\mathbf{y} \boldsymbol{\lambda}^{\top}-\boldsymbol{\lambda} \mathbf{y}^{\top}\right)$
  - then $E=\frac{1}{2} M\left(\boldsymbol{\lambda} \mathbf{y}^{\top}+\mathbf{y} \boldsymbol{\lambda}^{\top}\right) M$
- Then to eliminate $\boldsymbol{\lambda}$, we plug in the secant condition (i) we get $\boldsymbol{\lambda}=\frac{1}{\mathbf{y}^{\top} M \mathbf{y}}\left(2 M^{-1} \mathbf{r}-\mathbf{y} \boldsymbol{\lambda}^{\top} M \mathbf{y}\right)$
  - multiply with $\mathbf{y}^{\top} M$, we get $z=\boldsymbol{\lambda}^{\top} M \mathbf{y}=\frac{\mathbf{y}^{\top} \mathbf{r}}{\mathbf{y}^{\top} M \mathbf{y}}$, so $\boldsymbol{\lambda}=\frac{1}{\mathbf{y}^{\top} M \mathbf{y}}\left(2 M^{-1} \mathbf{r}-\frac{\left(\mathbf{y}^{\top} \mathbf{r}\right)}{\mathbf{y}^{\top} M \mathbf{y}} \mathbf{y}\right)$
- Plug this into E, we get $E=\frac{1}{2} M\left(\boldsymbol{\lambda} \mathbf{y}^{\top}+\mathbf{y} \boldsymbol{\lambda}^{\top}\right) M=\frac{1}{\mathbf{y}^{\top} M \mathbf{y}}\left(\mathbf{r} \mathbf{y}^{\top} M+M \mathbf{y} \mathbf{r}^{\top}-\frac{\left(\mathbf{y}^{\top} \mathbf{r}\right)}{\mathbf{y}^{\top} M \mathbf{y}} M \mathbf{y} \mathbf{y}^{\top} M\right)$, by definition $\mathbf{r}=\boldsymbol{\sigma}-H \mathbf{y}$, we get
  - $E^{\star}=\frac{1}{\mathbf{y}^{\top} M \mathbf{y}}\left(\boldsymbol{\sigma} \mathbf{y}^{\top} M+M \mathbf{y} \boldsymbol{\sigma}^{\top}-H \mathbf{y} \mathbf{y}^{\top} M-M \mathbf{y} \mathbf{y}^{\top} H-\frac{1}{\mathbf{y}^{\top} M \mathbf{y}}\left(\mathbf{y}^{\top} \boldsymbol{\sigma}-\mathbf{y}^{\top} H \mathbf{y}\right) M \mathbf{y} \mathbf{y}^{\top} M\right)$

BFGS (Broyden, Fletcher, Goldfarb and Shanno)

- Definition BFGS is when $M = H' = H_t^{-1}$, $M\mathbf{y} = H'\mathbf{y} = \boldsymbol{\sigma}$, even we don't know H', but it never appears in the solution, so $E^\star = \frac{1}{\mathbf{y}^\top\boldsymbol{\sigma}}\left(-H\mathbf{y}\boldsymbol{\sigma}^\top - \boldsymbol{\sigma}\mathbf{y}^\top H + \left(1 + \frac{\mathbf{y}^\top H\mathbf{y}}{\mathbf{y}^\top\boldsymbol{\sigma}}\right)\boldsymbol{\sigma}\boldsymbol{\sigma}^\top\right)$, where $H = H_{t-1}^{-1}, \boldsymbol{\sigma} = \mathbf{x}_t - \mathbf{x}_{t-1}, \mathbf{y} = \nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1})$.
  - Iteration cost is $O(d^2)$
- Lemma Exercise 74.1 If f convex, $\mathbf{y}^\top\sigma > 0$, unless $\mathbf{x}_t = \mathbf{x}_{t-1}$ or $f(\lambda\mathbf{x}_t + (1-\lambda)\mathbf{x}_{t-1}) = \lambda f(\mathbf{x}_t) + (1-\lambda)f(\mathbf{x}_{t-1})$ for all $\lambda \in (0,1)$.
  - Proof By property of convexity $\mathbf{y}^\top\sigma = (\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1}))^\top(\mathbf{x}_t - \mathbf{x}_{t-1}) \geq 0$
- Observation 11.6 $H' = \left(I - \frac{\boldsymbol{\sigma}\mathbf{y}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}\right)H\left(I - \frac{\mathbf{y}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}\right) + \frac{\boldsymbol{\sigma}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}$
  - Proof
    - $E^\star + H = H + \frac{1}{\mathbf{y}^\top\boldsymbol{\sigma}}\left(-H\mathbf{y}\boldsymbol{\sigma}^\top - \boldsymbol{\sigma}\mathbf{y}^\top H + \left(1 + \frac{\mathbf{y}^\top H\mathbf{y}}{\mathbf{y}^\top\boldsymbol{\sigma}}\right)\boldsymbol{\sigma}\boldsymbol{\sigma}^\top\right) = \frac{\boldsymbol{\sigma}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}} + H(I - \frac{\mathbf{y}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}) - \boldsymbol{\sigma}\mathbf{y}^\top H + \frac{\boldsymbol{\sigma}\mathbf{y}^\top H\mathbf{y}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}} =$ QED
- Lemma Exercise 74.2 If $H \succeq 0$ and $\mathbf{y}^\top\sigma > 0$, then also H' is positive definite.
  - Proof
    - Since $C := \left(I - \frac{\mathbf{y}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}\right) = \left(I - \frac{\boldsymbol{\sigma}\mathbf{y}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}\right)^\top$, so $H' = C^\top HC + \frac{\boldsymbol{\sigma}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}$, $C^\top HC$ is semi positive definite and so is $\frac{\boldsymbol{\sigma}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}$.
    - When $z \perp \boldsymbol{\sigma}^\top$, we have $Cz = z \neq 0$, so the two quadratic form will not be zero at the same time, this means positive definiteness.
- Remark Usually Newton or Quasi-Newton are performed with *scaled steps* $\mathbf{x}_{t+1} = \mathbf{x}_t - \alpha_t H_t^{-1}\nabla f(\mathbf{x}_t)$, either line search or backtracking line search (when $\alpha_t = 1$ is not good enough, do $\alpha_t/2$).

L-BFGS (limited memory version)

- Idea Only use information from the previous m iterations, for some small value of m.
- Lemma 11.7 If an oracle can compute $\mathbf{s} = H\mathbf{g}$ for any vertor $\mathbf{g}$, then $\mathbf{s}' = H'\mathbf{g}'$ can be computed with one oracle call of $\mathbf{s} = H\mathbf{g}$, and $O(d)$ arithmetic operation, assuming $\sigma, \mathbf{y}$ known.
  - Proof
    - $H'\mathbf{g}' = \underbrace{\underbrace{\left(I - \frac{\boldsymbol{\sigma}\mathbf{y}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}\right)\underbrace{H\underbrace{\left(I - \frac{\mathbf{y}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}\right)\mathbf{g}'}_{\mathbf{g}}}_{\mathbf{s}}}_{\mathbf{w}} + \underbrace{\frac{\boldsymbol{\sigma}\boldsymbol{\sigma}^\top}{\mathbf{y}^\top\boldsymbol{\sigma}}\mathbf{g}'}_{\mathbf{h}}}_{\mathbf{z}}$
    - $\mathbf{g}, \mathbf{h}, \mathbf{s}, \mathbf{w}, \mathbf{z}$ all are compuated in $O(d)$.
- The idea is that we need $H_t^{-1}\nabla f_t$, and we can borrow from $H_{t-1}^{-1}\nabla f_t$, etc, and recurse back to $t = 0$, This gives the BFGS-step:
- Algorithm (BFGS-STEP)
  - Input $(k, \mathbf{g})$
  - If $k = 0$ then return $H_0^{-1}\mathbf{g}'$
  - Else
    - Set $\mathbf{h} = \boldsymbol{\sigma}\frac{\boldsymbol{\sigma}_k^\top\mathbf{g}'}{\mathbf{y}_k^\top\boldsymbol{\sigma}_k}$, and $\mathbf{g} = \mathbf{g}' - \mathbf{y}\frac{\boldsymbol{\sigma}_k^\top\mathbf{g}'}{\mathbf{y}_k^\top\boldsymbol{\sigma}_k}$
    - $\mathbf{s} = \text{ BFGS-STEP } (k-1, \mathbf{g})$ (*recursive call*)
    - $\mathbf{w} = \mathbf{s} - \boldsymbol{\sigma}_k\frac{\mathbf{y}_k^\top\mathbf{s}}{\mathbf{y}_k^\top\boldsymbol{\sigma}_k}$
    - $\mathbf{z} = \mathbf{w} + \mathbf{h}$
    - return z
- Remark If H_0 can be computed in $O(d)$ the total runtime is $O(td)$, this is acceptable when $t \leq d$. It's natual to think of a cut-off version
- Algorithm (L-BFGS-STEP)
  - Input $(k, l, \mathbf{g})$
  - If $l = 0$ then return $H_0^{-1}\mathbf{g}'$
  - Else
    - Set $\mathbf{h} = \boldsymbol{\sigma}\frac{\boldsymbol{\sigma}_k^\top\mathbf{g}'}{\mathbf{y}_k^\top\boldsymbol{\sigma}_k}$, and $\mathbf{g} = \mathbf{g}' - \mathbf{y}\frac{\boldsymbol{\sigma}_k^\top\mathbf{g}'}{\mathbf{y}_k^\top\boldsymbol{\sigma}_k}$
    - $\mathbf{s} = \text{ L-BFGS-STEP } (k-1, l-1, \mathbf{g})$ (*recursive call*)
    - $\mathbf{w} = \mathbf{s} - \boldsymbol{\sigma}_k\frac{\mathbf{y}_k^\top\mathbf{s}}{\mathbf{y}_k^\top\boldsymbol{\sigma}_k}$
    - $\mathbf{z} = \mathbf{w} + \mathbf{h}$

- **return** z