

Recap. $\nabla f(x)$

$$f(x) = \frac{1}{2} \|Ax - y\|^2$$

$$\hookrightarrow \nabla f(x) = A^T (Ax - y)$$

$$F: \mathbb{R}^p \rightarrow \mathbb{R}^q \quad \nabla F(x) \in \mathbb{R}^{q \times p}$$

$$\widetilde{\mathbb{R}^p} \xrightarrow{\text{linear}} \mathbb{R}^q$$

$$q=1 \quad \nabla f(x) = \nabla F(x)^T$$

chain rule:

$$\nabla(f \circ g) = \nabla f \circ \nabla g$$

Ex. $f(x) = \ell(Bx)$

$$\nearrow f(x + \varepsilon \delta) = f(x) + \varepsilon \dots$$

$$\hookrightarrow \text{chain rule } f = \ell \circ B$$

$$\nabla f(x) = B^T \cdot \nabla \ell(Bx)$$

$$\nabla f = B^T \circ \nabla \ell \circ B$$

Exercise sheet 1.3



$$\|x\|_p = (\sum |x_i|^p)^{1/p}$$

$$\|x + \varepsilon \delta\|_p$$

$$\Leftrightarrow \|x\|_p = (g(x))^{1/p}$$

Ex. $\|x\|_2 = \sqrt{x_1^2 + x_2^2}$



1.4

$$\langle X, Y \rangle_{\mathbb{R}^{n \times p}} = \sum_{ij} X_{ij} Y_{ij}$$

$$\langle X, \text{flatten} \rangle_{\mathbb{R}^{np}}$$

$$\langle X, Y \rangle_{\mathbb{R}^{n \times p}} = \text{trace}(XY^T) = \text{tr}(YX^T) = \text{tr}(X^T Y)$$

$$X, Y \in \mathbb{R}^{n \times p}$$

$$XY^T \in \mathbb{R}^{n \times n}$$

$$X^T Y \in \mathbb{R}^{p \times p}$$

$$Z \in \mathbb{R}^{n \times n} \quad \text{tr}(Z) = \sum Z_{ii}$$

$$\textcircled{1} (XY^T)_{ij} = \sum_k X_{ik} Y_{jk}$$

$$\text{tr}(XY^T) = \sum_i (XY^T)_{ii}$$

$$= \sum_i \sum_k X_{ik} Y_{ik}$$

$$= \sum_{ik} X_{ik} Y_{ik} = \langle X, Y \rangle$$

Application: $\langle AB, C \rangle_{\mathbb{R}^{n \times p}} = \langle B, A^T C \rangle$

$$\langle Ab, c \rangle = \langle b, A^T c \rangle$$

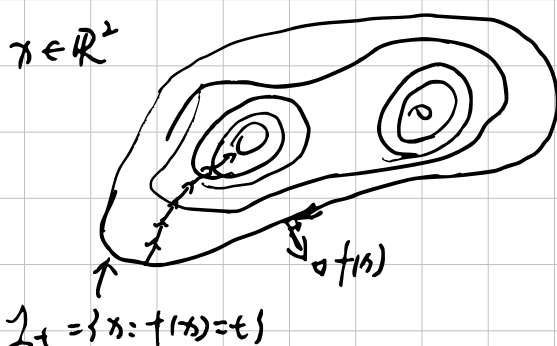
Batch Gradient descent:

$$\min_{x \in \mathbb{R}^d} f(x)$$

$$x_0 \leftarrow \text{init}$$

$$x_{k+1} = x_k - \tau_k \nabla f(x_k)$$

\hookrightarrow learning rate τ_k ??



$$\tau_k \rightarrow 0 \quad \frac{x_{k+1} - x_k}{\tau_k} = \nabla f(x_k)$$

$\tau \rightarrow 0 \downarrow$

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

$$\frac{dx}{dt} \quad \uparrow \quad \text{Gradient flow ordinary diff. Eq. (ODE)}$$

Generic "descent" algorithm

$$x_{k+1} = x_k - \tau_k d_k$$

$$f(x_{k+1}) = f(x_k) - \tau_k \langle d_k, \nabla f(x_k) \rangle + o(\tau_k)$$

$$\Delta_k = f(x_{k+1}) - f(x_k) \leq 0 \quad ! < 0 \text{ if } x_k \text{ is not minimum}$$

$$\Delta_k = -\tau_k \langle d_k, \nabla f(x_k) \rangle + o(\tau_k)$$

For $\Delta_k < 0$, for τ_k small enough

$$\Leftrightarrow \langle d_k, \nabla f(x_k) \rangle > 0$$

either $\nabla f(x_k) = 0$ stop
or $\nabla f(x_k) \neq 0$



$$d_k = + \nabla f(x_k)$$

$$\hookrightarrow \Delta_k = -\tau_k \|\nabla f(x_k)\|^2 + o(\tau_k)$$

$$d_k = H_k \cdot \nabla f(x_k)$$

\hookrightarrow sym & positive matrix

$$H_k = U \cdot \text{diag}(\lambda) U^T$$

> 0 eigenvalues

$$H_k = [\partial^2 f(x_k)]^{-1} \quad \text{Newton method}$$

\uparrow convex

$$\langle d_k, \nabla f(x_k) \rangle = \langle H_k \nabla f(x_k), \nabla f(x_k) \rangle$$

$$= \langle U \text{diag}(\lambda) U^T \nabla f(x_k), \nabla f(x_k) \rangle$$

$$= \langle \text{diag}(\sqrt{\lambda}) U^T \nabla f(x_k), \text{diag}(\sqrt{\lambda}) U^T \nabla f(x_k) \rangle$$

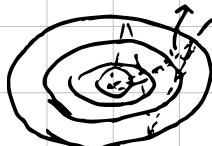
$$= \|\text{diag}(\sqrt{\lambda}) U^T \nabla f(x_k)\|^2 > 0$$

$$f(x) = a x_1^2 + b x_2^2 \quad x^* = 0$$

$$a = b = 1$$

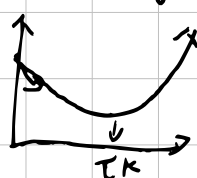


$a \ll b$
 $\tau_{\text{small}} (\text{slow})$
 $\tau_{\text{large}} (\text{slow?})$



$$h(\tau) = f(x_k - \tau \nabla f(x_k)) \quad h'(0) = -\|\nabla f(x_k)\|^2$$

$\tau \geq 0$



Armijo-Goldstein rule

Numerical tours (website)

Theory $f(x) = \frac{1}{2} \|Ax - y\|^2 + \frac{\lambda}{2} \|x\|^2$

$f(x) = \frac{1}{2} \underbrace{\langle Cx, x \rangle}_{\text{quad}} - \underbrace{\langle b, x \rangle}_{\text{linear}}$

$C = A^T A + \lambda Id$

$b = A^T y$

Ridge $f(x) = \frac{1}{2} \|Ax - y\|^2 + \frac{\lambda}{2} \|x\|^2$

$\nabla f(x) = A^T(Ax - y) + \lambda x$

General: $f(x) = \frac{1}{2} \langle Cx, x \rangle - \langle b, x \rangle$

$\nabla f(x) = Cx - b$

If $\ker(A) = \ker(C) = \{0\}$ (overdetermined)

\boxed{A} then $x^* = C^{-1}b = (A^T A + \lambda Id)^{-1} (A^T y)$

Operator norm / ∞ -norm / algebra norm

$\|H\|_{op}, \|H\|$

Def: $\|H\|_{op} = \sup_{x \neq 0} \frac{\|Hx\|}{\|x\|}$

$\|Hx\|_2 \leq \|H\|_{op} \|x\|_2$

$\|H\|_{op}$ is the lipsh constant of

$\begin{matrix} \eta & \hookrightarrow & H\eta \\ \ell^2 & & \ell^2 \end{matrix}$

$\|AB\|_{op} \leq \|A\|_{op} \cdot \|B\|_{op}$

Prop: $\|H\|_{op} = \sup_i \sqrt{\lambda_i(H^T H)}$

eigenvalue
singular value

If H is symmetry, $\|H\|_{op} = \sup_i |\lambda_i(H)|$

Proof: $\|Hx\|^2 = \langle Hx, Hx \rangle = \langle \underbrace{H^T H}_{\text{sym}} x, x \rangle$

$(H^T H = U \text{diag}(\lambda) U^T)$

$\rightarrow \begin{aligned} &= \langle U \text{diag}(\lambda) U^T x, x \rangle \\ &= \langle \text{diag}(\lambda) \underbrace{U^T x}_z, \underbrace{U^T x}_z \rangle \\ &= \sum_i \lambda_i z_i^2 \\ &\leq \max(\lambda) \sum_i z_i^2 \\ &\quad \underbrace{\|U^T x\|^2}_{= \|x\|^2} \end{aligned}$

$\|Hx\|^2 \leq \max(\lambda) \|x\|^2$

$\|Hx\| \leq \sqrt{\max \lambda_i(H^T H)} \|x\|$

$U = (u_1, u_2, \dots, u_n)$

$\lambda_1, \lambda_2, \dots, \lambda_n$

$x = u_1$

$\|H u_1\| = \sqrt{\max(\lambda)} \|u_1\|$

$= \|H\|_{op}$

Theory of GD \rightarrow strongly cvx
 C is invertible FAST
 over determined

\rightarrow C might be non-inv slow
 under-determined

"Nice" case: C is inv

$$0 < \lambda_1(C) \leq \lambda_2(C) \leq \dots \leq \lambda_d(C)$$

$$\mu = \lambda_1(C) \quad L = \|C\|_{op}$$

$$\kappa = \frac{L}{\mu} \geq 1 \quad \text{conditioning}$$

$$\kappa = 1 \quad \lambda_1 = \lambda_2 = \dots = \lambda_d \quad C = \lambda Id$$



$$\kappa \gg 1 \quad \mu \rightarrow 0$$

$$f(x) = \frac{1}{2} \langle Cx, x \rangle - \langle b, x \rangle$$

$$\nabla f(x) = Cx - b$$

$$x^* = C^{-1}b$$

$$0 = Cx^* - b$$

Fixed LR $\tau_k = \tau$

$$x_{k+1} = x_k - \tau \nabla f(x_k)$$

$$\begin{cases} x_{k+1} = x_k - \tau (Cx_k - b) & \Delta_k = x_k - x^* \\ x^* = x^* - \tau (Cx^* - b) & \quad \quad \quad = 0 \end{cases}$$

$$\Delta_{k+1} = \Delta_k - \tau C \Delta_k$$

$$\Delta_{k+1} = (Id - \tau C) \Delta_k$$

$$\Delta_k = (Id - \tau C)^k \Delta_0$$

$$\|\Delta_k\| \leq \underbrace{\|Id - \tau C\|}_{\rho}^k \underbrace{\|\Delta_0\|}_{\|x_0 - x^*\|}$$

$\rho > 1 \rightarrow$ explodes \rightarrow no convergence

$\rho < 1 \rightarrow$ "linear convergence" ρ^k

$$\|\Delta_k\|$$

$$\|\Delta_k\| \leq \rho^k \|\Delta_0\|$$

\rightarrow

$$\log(\|\Delta_k\|)$$

stop $\log(\rho) < 0$

$$\|\Delta_k\| \leq \rho^k \|\Delta_0\| \rightarrow \log(\|\Delta_k\|) \leq k \log(\rho) + \text{cte}$$

Summary:

$$\rho_\tau = \|Id - \tau C\|_{op}$$

$$\rho_\tau = \max_i |\lambda_i(Id - \tau C)|$$

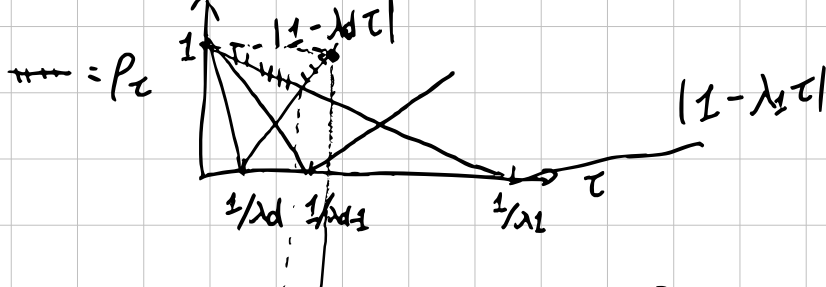
Remark: $\lambda_i(B + Id) = \lambda_i(B) + 1$

$$\lambda_i(Id - \tau C) = 1 - \tau \lambda_i(C)$$

$$\rho_\tau = \max |1 - \tau \lambda_1(C)|, |1 - \tau \lambda_2(C)|, |1 - \tau \lambda_d(C)|$$

$$\lambda_1 \leq \lambda_2 \leq \dots$$

$$1 - \tau \lambda_1 = 0 \quad \tau = \frac{1}{\lambda_1}$$



$$\frac{2}{\lambda_d} = \tau_{critical} = \frac{2}{L}$$

$$\tau_{opt} = \frac{2}{\lambda_1 + \lambda_d} = \frac{2}{L + \mu}$$

Thm: If $0 < \mu = \lambda_1(C) \leq \lambda_2(C) \leq \dots \leq \lambda_d(C) = L$

If $0 < \tau < \frac{2}{L}$, then $\exists \rho < 1$

$$\text{s.t. } \|x_k - x^*\| \leq \rho^k \|x_0 - x^*\|$$

A "good" (optimal for the proof)

$$\text{choice is } \tau = \frac{2}{L + \mu}$$

$$\rho_{opt} = \frac{L - \mu}{L + \mu} = \frac{\kappa - 1}{\kappa + 1}$$

$$\kappa = \frac{L}{\mu}$$

$$\kappa \rightarrow +\infty \quad \rho_{opt} \rightarrow 1$$

$$\kappa \rightarrow 1 \quad \rho_{opt} \rightarrow 0$$

Underdetermined $\mu = 0$, $\kappa = +\infty$

Thm: If $0 < \tau_{min} \leq \tau_k \leq \frac{2}{L}$

x_k will converge to some sol $^\circ$ x^*

$$f(x_k) - f(x^*) \leq \underbrace{\text{dist}(x_0, \argmin(f))}_{\substack{\delta \propto \tau \times k \\ \sim \text{true e? } 2 \geq 4}}$$

General case: $C \rightarrow$ Hessian

Def: $f: \mathbb{R}^d \rightarrow \mathbb{R}$

$$\partial^2 f(x) = \left(\frac{\partial^2 f}{\partial x_i \partial x_j}(x) \right)_{i,j=1}^d \in \mathbb{R}^{d \times d}$$

$$\partial^2 f(x)^T = \partial^2 f(x)$$

Prop: f is cvx $\Leftrightarrow \partial^2 f(x) \succeq 0$

$$\lambda_i(\partial^2 f(x)) \geq 0$$

Def: f is twice differentiable at x

quad

$$f(x + \varepsilon \delta) = \underbrace{f(x)}_{\text{cte}} + \underbrace{\varepsilon \langle \nabla f(x), \delta \rangle}_{\text{linear}} + \underbrace{\frac{\varepsilon^2}{2} \langle \partial^2 f(x) \delta, \delta \rangle}_{o(\varepsilon^2)}$$

$$\hookrightarrow \sum_{i,j} \frac{\partial^2 f}{\partial x_i \partial x_j}(x) \times \delta_i \times \delta_j$$

$$\nabla f(x + \varepsilon \delta) = \nabla f(x) + \varepsilon \partial^2 f(x) \times \delta + o(\varepsilon)$$

Thm 1: $0 < \mu \leq \lambda_i(\partial^2 f(x)) \leq L$ f is convex

\downarrow strong convexity

\downarrow smoothness

$\uparrow \mu \geq 0$

Remark: if $f(x) = \frac{1}{2} \langle Cx, x \rangle - \langle b, x \rangle$

$$\nabla f(x) = Cx - b$$

$$\partial^2 f(x) = C$$

$$\mu = \inf_x \lambda_i(\partial^2 f(x))$$

$$L = \sup_x \lambda_i(\partial^2 f(x)) \quad L \neq \lambda_{\max}(\partial^2 f(x))$$

Same thm: $0 < \tau < \frac{2}{L} \Rightarrow$ conv

$$\|x_k - x^*\| \leq \rho^k \|x_0 - x^*\|$$

Thm 2: same $\mu = 0$, $\tau < \frac{2}{L}$

$$x_k \rightarrow x^*$$

$$f(x_k) - f(x^*) \leq o(1/k)$$

$$\partial^2 f(x) \leq L Id$$

$$\mu \in \lambda_i(\partial^2 f(x)) \leq L$$

$$[f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{\mu}{2} \|x - x_k\|^2] \leq f(x)$$

$$\leq f(x)$$

$$\leq [f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{L}{2} \|x - x_k\|^2]$$

$$GD \sim 1/k$$

$$\text{Vesterov} \sim 1/k^2 \quad \text{optimal}$$