

- (1) Let  $Q \in \mathbb{R}^{n \times n}$  be symmetric and positive definite, and let  $d_1, d_2, \dots, d_n \in \mathbb{R}^n$  be a basis of  $Q$ -conjugate vectors. Show that

$$Q^{-1} = \sum_{i=1}^n \frac{d_i d_i^T}{d_i^T Q d_i}.$$

**Solution:** Let  $M := \sum_{i=1}^n \frac{d_i d_i^T}{d_i^T Q d_i}$ . Then, for every  $x \in \mathbb{R}^n$ , we have  $x = \sum_{j=1}^n \lambda_j d_j$  for a unique set of coefficients  $\lambda_1, \dots, \lambda_n$  since  $d_1, d_2, \dots, d_n$  form a basis of  $\mathbb{R}^n$ . But then

$$Mx = \sum_{i=1}^n \frac{d_i}{d_i^T Q d_i} (d_i^T Q \sum_{j=1}^n \lambda_j d_j) = \sum_{i=1}^n \frac{d_i}{d_i^T Q d_i} (\sum_{j=1}^n \lambda_j d_i^T Q d_j) = \sum_{i=1}^n \frac{d_i}{d_i^T Q d_i} \lambda_i d_i^T Q d_i = \sum_{j=1}^n \lambda_j d_j = x,$$

which implies that  $M = Q^{-1}$ .

- (2) Let  $A \in \mathbb{R}^{m \times n}$  and  $b \in \mathbb{R}^m$ , and suppose that  $\text{Nul}(A) = \{0\}$ . Consider the function

$$f(x) := \frac{1}{2} \|Ax - b\|_2^2.$$

Show how to apply the CG algorithm to minimize  $f$  on  $\mathbb{R}^n$  under the assumption that  $A$  is not available but  $Ax$  and  $A^T y$  can be obtained for arbitrary vectors  $x \in \mathbb{R}^n$  and  $y \in \mathbb{R}^m$ , respectively.

**Solution:**

**Initialization:**  $x_0 \in \mathbb{R}^n$ ,  $r_0 = Ax_0 - b$ ,  $d_0 = -g_0 = -A^T r_0$ .

For  $k = 0, 1, 2, \dots$

$$\begin{aligned} \alpha_k &:= -r_k^T A d_k / \|A d_k\|_2^2 \\ x_{k+1} &:= x_k + \alpha_k d_k \\ r_{k+1} &:= A x_{k+1} - b \\ g_{k+1} &:= A^T r_{k+1} \quad (\text{STOP if } g_{k+1} = 0) \\ \beta_k &:= (A g_{k+1})^T (A d_k) / \|A d_k\|_2^2 \\ d_{k+1} &:= -g_{k+1} + \beta_k d_k \\ k &:= k + 1. \end{aligned}$$

- (3) Apply the conjugate gradient algorithm initialized at  $x^0 = (0, 0, 0)^T$  to solve the problem  $\min_{x \in \mathbb{R}^3} \frac{1}{2} x^T H x + g^T x$ , where

$$H = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} \quad \text{and} \quad g = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}.$$

**Solution:** Later.

- (4) Let  $f(x) := \frac{1}{2} x^T H x + g^T x$ , where  $H \in \mathcal{S}_{++}^n$  and  $g \in \mathbb{R}^n$ . Let  $\{x^0, \dots, x^n\}$  be the iterates of the conjugate gradient algorithm applied to  $f$  initiated at  $x^0 = 0$ .

- (a) Show that  $f(x^k) - f(x^{k+1}) = \frac{1}{2} \frac{\langle g^k, d^k \rangle^2}{\langle Hd^k, d^k \rangle}$ , which establishes that  $f(x^k) > f(x^{k+1})$  whenever  $d^k \neq 0$ .

**Solution:** Since  $t_k = -\frac{\langle g^k, d^k \rangle}{(d^k)^T H d^k}$ , we have

$$f(x^{k+1}) = f(x^k) + t_k \langle g^k, d^k \rangle + \frac{t_k^2}{2} (d^k)^T H d^k = f(x^k) - \frac{\langle g^k, d^k \rangle^2}{(d^k)^T H d^k}.$$

- (b) Show that the sequence  $\{\beta_k\}$  generated by the CG-algorithm satisfies  $\beta_k = \frac{\langle g^{k+1}, g^{k+1} - g^k \rangle}{\|g^k\|^2}$ .

**Solution:**

$$\begin{aligned} \beta_k &= \frac{\langle g^{k+1}, H d^k \rangle}{\langle d^{kT}, H d^k \rangle} = \frac{\langle g^{k+1}, t_k^{-1} H(x^{k+1} - x^k) \rangle}{\langle d^k, H d^k \rangle} \\ &= \frac{\langle g^{k+1}, (H x^{k+1} + g) - (H x^k + g) \rangle}{\langle -g^k, d^k \rangle} = \frac{\langle g^{k+1}, g^{k+1} - g^k \rangle}{\langle -g^k, -g^k + \beta_{k-1} d^{k-1} \rangle} \\ &= \frac{\langle g^{k+1}, g^{k+1} - g^k \rangle}{\langle g^k, g^k \rangle}. \end{aligned}$$

- (5) Let  $A \in \mathbb{R}^{m \times n}$  and  $b \in \mathbb{R}^m$ , and consider the function

$$f(x) := \frac{1}{2} \|Ax - b\|_2^2.$$

Show that  $\nabla f(x) = A^T(Ax - b)$  and  $\nabla^2 f(x) = A^T A$ .

**Solution:**

$$\begin{aligned} f(x + \Delta x) &= \frac{1}{2} \|A(x + \Delta x) - b\|_2^2 \\ &= \frac{1}{2} \|(Ax - b) + A\Delta x\|_2^2 \\ &= \frac{1}{2} \|Ax - b\|_2^2 + \langle A^T(Ax - b), \Delta x \rangle + \frac{1}{2} \|A\Delta x\|_2^2 \\ &= f(x) + \langle A^T(Ax - b), \Delta x \rangle + \frac{1}{2} (\Delta x)^T (A^T A) (\Delta x). \end{aligned}$$

- (6) Let  $f(x) := \frac{1}{2} x^T H x + g^T x$ , where  $H \in \mathbb{R}^{n \times n}$  and  $g \in \mathbb{R}^n$ .

- (a) Show that  $\nabla f(x) = \frac{1}{2}(H + H^T)x + g$  so that if  $H \in \mathcal{S}^n$ , then  $\nabla f(x) = Hx + g$ .  
(b) Show that  $\nabla^2 f(x) = \frac{1}{2}(H + H^T)$  so that if  $H \in \mathcal{S}^n$ , then  $\nabla^2 f(x) = H$ .

**Solution:**

$$\begin{aligned} f(x + \Delta x) &= \frac{1}{2} (x + \Delta x)^T H (x + \Delta x) + g^T (x + \Delta x) \\ &= f(x) + \frac{1}{2} ((\Delta x)^T H x + x^T H \Delta x) + g^T \Delta x + \frac{1}{2} (\Delta x)^T H \Delta x \\ &= f(x) + \left\langle \frac{1}{2} (H + H^T)x + g, \Delta x \right\rangle + (\Delta x)^T \left( \frac{1}{2} (H + H^T) \right) \Delta x. \end{aligned}$$

- (7) Let  $F : \mathbb{R}^n \rightarrow \mathbb{R}^m$  be a smooth function (has as many continuous derivatives as you want), and define  $f(x) := \frac{1}{2}\|F(x)\|_2^2$ .
- (a) Show that  $\nabla f(x) = \nabla F(x)^T F(x)$ .
- (b) Show that  $\nabla^2 f(x) = \nabla F(x)^T \nabla F(x) + \sum_{j=1}^m F_j(x) \nabla^2 F_j(x)$ , where  $F_j : \mathbb{R}^n \rightarrow \mathbb{R}$  are the component functions of  $F$ ,  $j = 1, \dots, m$ .

**Solution:** Let  $F_i$  be the  $i^{\text{th}}$  component function of  $F$  so that  $f(x) = \frac{1}{2} \sum_{j=1}^m (F_j(x))^2$ . For each  $j = 1, \dots, m$ , we have

$$F_j(x + \Delta x) = F_j(x) + \nabla F_j(x)^T \Delta x + \frac{1}{2} \Delta x^T \nabla^2 F_j(x) \Delta x + o(\|\Delta x\|^2).$$

Hence,

$$\frac{1}{2}(F_j(x + \Delta x))^2 = \frac{1}{2}(F_j(x))^2 + \langle F_j(x) \nabla F_j(x), \Delta x \rangle + \frac{1}{2} \Delta x^T (\nabla F_j(x) \nabla F_j(x)^T + F_j(x) \nabla^2 F_j(x)) \Delta x + o(\|\Delta x\|^2).$$

Consequently,

$$\begin{aligned} f(x + \Delta x) &= \frac{1}{2} \sum_{j=1}^m (F_j(x + \Delta x))^2 \\ &= \sum_{j=1}^m \frac{1}{2} (F_j(x))^2 + \langle F_j(x) \nabla F_j(x), \Delta x \rangle + \frac{1}{2} \Delta x^T (\nabla F_j(x) \nabla F_j(x)^T + F_j(x) \nabla^2 F_j(x)) \Delta x + o(\|\Delta x\|^2) \\ &= f(x) + \langle \nabla F(x)^T F(x), \Delta x \rangle + \frac{1}{2} \Delta x^T \left( \nabla F(x)^T \nabla F(x) + \sum_{j=1}^m F_j(x) \nabla^2 F_j(x) \right) \Delta x + o(\|\Delta x\|^2), \end{aligned}$$

since

$$\nabla F(x) = \begin{bmatrix} \nabla F_1(x)^T \\ \nabla F_2(x)^T \\ \vdots \\ \nabla F_m(x)^T \end{bmatrix} \quad \text{so that} \quad \nabla F(x)^T \nabla F(x) = \sum_{j=1}^m \nabla F_j(x) \nabla F_j(x)^T.$$

- (8) Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  be twice continuously differentiable,  $V \in \mathbb{R}^{n \times k}$ , and  $\hat{x} \in \mathbb{R}^n$ , where  $k < n$ . Consider the function given by  $h(z) := f(\hat{x} + Vz)$ .
- (a) Show that  $\nabla h(z) = V^T \nabla f(\hat{x} + Vz)$ .

**Solution:**

$$\begin{aligned} h(z + \Delta z) &= f(\hat{x} + V(z + \Delta z)) = f((\hat{x} + Vz) + V\Delta z) \\ &= f(\hat{x}) + \langle \nabla f(\hat{x} + Vz), V\Delta z \rangle + o(\|V\Delta z\|) \\ &= f(\hat{x}) + \langle V^T \nabla f(\hat{x} + Vz), \Delta z \rangle + o(\|\Delta z\|). \end{aligned}$$

- (b) Show that if  $\bar{z}$  is a local solution to  $\min_z h(z)$ , then  $\nabla f(\hat{x} + V\bar{z}) \perp \text{Ran}(V)$ .

**Solution:** If  $\bar{z}$  is a local solution to  $\min_z h(z)$ , then  $0 = \nabla h(\bar{z}) = V^T \nabla f(\hat{x} + V\bar{z})$ , or equivalently,  $\nabla f(\hat{x} + V\bar{z}) \in \text{Nul}(V^T) = \text{Ran}(V)^\perp$ .

- (c) Let  $S$  be a subspace of  $\mathbb{R}^n$ . Show that if  $\bar{x} \in \hat{x} + S$  solves  $\min \{f(x) \mid x \in \hat{x} + S\}$ , then  $\nabla f(\bar{x}) \perp S$ .

**Solution:** Let the columns of the matrix  $V \in \mathbb{R}^{n \times k}$  form a basis for the subspace  $S$  where  $k = \dim S$ . Then the problem  $\min \{f(x) \mid x \in \hat{x} + S\}$  is equivalent to the problem  $\min_z f(\hat{x} + Vz)$ . By part (b), we have  $\nabla f(\bar{x}) \perp \text{Ran}(V) = S$ .