1. 用基于精确线搜索的最速下降法求解下述无约束优化问题

$$\min f(x_1, x_2) = x_1^2 + x_2^2 - x_1 + 2x_2$$

其中初始点为 $y_0 = (0,0)^t$,精度为 $\varepsilon = 0.001$.

Answer. $\nabla f(x) = (2x_1 - 1, 2x_2 + 2)^t$ 第一次迭代

- $d^{(0)} = -\nabla f(x^{(0)}) = (1, -2)^t$
- $\lambda = \underset{\lambda>0}{\operatorname{arg\,min}} \varphi(\lambda) = \underset{\lambda>0}{\operatorname{arg\,min}} f(x^{(0)} + \lambda d^{(0)}) = \frac{1}{2}$
- $x^{(1)} = (\frac{1}{2}, -1)^t$

 $d^{(1)} = (0,0)^t, ||d|| = 0 \le \varepsilon$,所以 $x^* = (\frac{1}{2}, -1)^t, f^* = 0$.

2. 考虑二次函数 $f(x) = \frac{1}{2}x^tAx + b^tx + c$,其中 $A \in \mathbb{R}^{n \times n}$ 为对称正定矩阵,设函数的极小值点为 x^* ,并设 $x_0 = x^* + ts$,其中 s 为函数 f 的 Hesse 矩阵的某特征值的特征向量.若以 x_0 为初始点,试证明基于精确线搜索的最速下降法与牛顿法等价.

Proof.
$$\nabla f(x) = Ax + b, \nabla^2 f(x) = A$$

使用牛顿法: $x^{(1)} = x^{(0)} - (\nabla^2 f(x))^{-1} \nabla f(x) = x^{(0)} - A^{-1} (Ax^{(0)} + b) = -A^{-1}b$

使用最速下降法: $d^{(0)} = -\nabla f(x^{(0)}) = -Ax^{(0)} - b, f(x^{(1)}) = \frac{1}{2}x^{(1)t}Ax^{(1)} + b^tx^{(1)} + c$, 令 $f(x^1)$ 最小可得 $x^{(1)} = -A^{-1}b$

故最谏下降法与牛顿法等价.

3. 用共轭梯度法求解下列问题

$$\min \frac{1}{2}x_1^2 + x_2^2$$

取初始点 $x^{(1)} = (4,4)^t$

Answer. $f(x) = \frac{1}{2}x_1^2 + x_2^2, \nabla f(x) = (x_1, 2x_2)^t.$

第一次迭代: $g_1 = (4,8)^t$, $d^{(1)} = -g_1 = (-4,-8)^t$, $x^{(2)} = x^{(1)} + \lambda_1 d^{(1)} = (\frac{16}{9},-\frac{4}{9})^t$

第二次迭代: $g_2 = (\frac{16}{9}, -\frac{8}{9}), d^{(2)} = -g_2 + \beta_1 d^{(1)} = (-\frac{160}{81}, \frac{40}{81}), x^{(3)} = x^{(2)} + \lambda_2 d^{(2)} = (0, 0)^t$

第三次迭代: $g_3 = (0,0), ||g_3|| = 0$, 故 $\bar{x} = (0,0), f^* = 0$.

4. 总结最速下降法、牛顿法及共轭梯度法的基本思想和计算步骤.

Answer. 带精确线搜索的最速下降法

- 1. 给定初始点 $x^{(1)} \in E^n$,允许误差 $\varepsilon > 0$,置 k = 1.
- 2. 取搜索方向: $d^{(k)} = -\nabla f(x^{(k)})$

- 3. 若 $\|d^{(k)}\| \le \varepsilon$, 则停止计算;否则,从 $x^{(k)}$ 出发,沿 $d^{(k)}$ 进行一维搜索,求 λ_k ,使 $f(x^{(k)} + \lambda_k d^{(k)}) = \min_{\lambda>0} f(x^{(k)} + \lambda d^{(k)})$
- 4. 令 $x^{(k+1)} = x^{(k)} + \lambda_k d^{(k)}$, 置 k := k+1, 返回 2

牛顿法计算步骤:

- 1. 给定初始点 $x^{(0)} \in E^n$,允许误差 $\varepsilon > 0$,置 k = 0
- 2. 若 $\|\nabla f(x^{(k)})\| < \varepsilon$, 则停止计算;
- 3. $x^{(k+1)} = x^{(k)} (\nabla^2 f(x^{(k)}))^{-1} \nabla f(x^{(k)})$, $\mathbb{Z} k := k+1$, $\mathbb{Z} = 2$.

FR 共轭梯度法(二次凸函数)

- 1. 给定初始点 $x^{(1)}$, 置 k=1
- 2. 计算 $g_k = \nabla f(x^{(k)})$, 若 $||g_k|| = 0$, 则停止计算, 否则进行下一步
- 3. $\diamondsuit d^{(k)} = -g_k + \beta_{k-1} d^{(k-1)}$, $\sharp \dot{p}$, \sharp
- 4. $\diamondsuit x^{(k+1)} = x^{(k)} + \lambda_k d^{(k)}$, $\sharp \mapsto \lambda_k = \frac{g_k^t g_k}{d^{(k)t} A d^{(k)}}$
- 5. 若 k=n, 则停止计算, 否则置 k=k+1, 返回步骤 2.
- 5. $\min x_1^2 + 2x_2^2 2x_1x_2 + 2x_2 + 2$, 取初始点 $x^{(1)} = (0,0)^t$.

Answer. $\nabla f(x) = (2x_1 - 2x_2, 4x_2 - 2x_1 + 2)^t$

共轭梯度法:

第一次迭代:
$$g_1 = (0,2)^t$$
, $d^{(1)} = -g_1 = (0,-2)^t$, $x^{(2)} = x^{(1)} + \lambda_1 d^{(1)} = (0,-\frac{1}{2})^t$

第二次迭代:
$$g_2 = (1,0)^t, d^{(2)} = -g_2 + \beta_1 d^{(1)} = (-1,-\frac{1}{2})^t, x^{(3)} = x^{(2)} + \lambda_2 d^{(2)} = (-1,-1)^t$$

第三次迭代: $g_3 = (0,0)^t$, $||g_3|| = 0$, 故 $\bar{x} = (-1,-1)^t$, $f^* = 1$

牛顿法:

$$x^{(2)} = x^{(1)} - G_1^{-1}g_1 = (-1, -1)^t, ||g_2|| = 0, \text{ if } \bar{x} = (-1, -1)^t.$$

6. $\min 2x_1^2 + 2x_1x_2 + 5x_2^2$,取初始点 $x^{(1)} = (2, -2)^t$.

Answer. $\nabla f(x) = (4x_1 + 2x_2, 2x_1 + 10x_2)^t$

共轭梯度法:

第一次迭代:
$$g_1 = (4, -16)^t, d^{(1)} = -g_1 = (-4, 16)^t, x^{(2)} = x^{(1)} + \lambda d^{(1)} = (\frac{57}{37}, -\frac{6}{37})$$

第二次迭代:
$$g_2 = (\frac{216}{37}, \frac{54}{37})^t, d^{(2)} = -g_2 + \beta d^{(1)}, x^{(3)} = x^{(2)} + \lambda_2 d^{(2)} = (0,0)^t$$

第三次迭代: $g_3 = (0,0), ||g_3|| = 0$, 故 $\bar{x} = (0,0)^t$.

牛顿法:

$$x^2 = x^1 - G_1^{-1}g_1 = (0,0), ||g_2|| = 0, \text{ if } \bar{x} = (0,0)^t.$$

7. $\min x_1^2 + 2x_2^2 + 2$,取 $x_0 = (1,1)^t$,用共轭梯度法.

Answer. $\nabla f(x) = (2x_1, 4x_2)^t$

第一次迭代: $g_1 = (2,4)^t, d^{(1)} = (-2,-4)^t, x^{(2)} = (\frac{4}{9},-\frac{1}{9})^t$

第二次迭代: $g_2 = (\frac{8}{9}, -\frac{4}{9})^t, d^{(2)} = -g_2 + \beta_1 d^{(1)} = \frac{20}{81}(-4, 1)^t, x^{(3)} = x^{(2)} + \lambda_2 d^{(2)} = (0, 0)^t$

第三次迭代: $g_3 = (0,0), ||g_3|| = 0$, 故最优点 $\bar{x} = (0,0)$.

8. 证明: 如果非零向量 $p_0, ..., p_l$ 满足 $p_i^t A p_j = 0, \forall i \neq j$, 其中 A 为对称正定矩阵,则这些向量线性无关.

Proof. 设 $\alpha_0 p_0 + \cdots + \alpha_l p_l = 0$

左乘 $p_i^t A$ 可得 $\alpha_0 p_i^t A p_0 + \cdots + \alpha_l p_i^t A p_l = 0$, 得到 $\alpha_i = 0$. 故 p_0, \ldots, p_l 线性无关.