

Solutions to exercises 4

1. Minimize $f(x, y) = (x + y)^2 + 4(x - y)^2$ by using the conjugate gradient method, starting from $(x_0, y_0) = (-5, -3)$.

$$\begin{aligned}\nabla f(x, y) &= (10x - 6y, -6x + 10y) \\ x_0 &= (-5, -3) \Rightarrow g_0 = h_0 = (32, 0) \\ x_1 &= x_0 + \lambda_0 h_0\end{aligned}$$

Minmizing along $f(-5 + 32\lambda_0, -3)$ gives $\lambda_0 = 1/10$ so

$$\begin{aligned}x_1 &= (-1.8, -3) \\ g_1 &= (0, 19.2) \\ h_1 &= g_1 + \frac{g_1^2}{g_0^2} h_0 = (11.52, 19.2)\end{aligned}$$

Minimizing along $f(-1.8 + 11.52\lambda_1, -3 + 19.2\lambda_1)$ gives $\lambda_1 = 0.15625$ and

$$\begin{aligned}x_2 &= x_1 + \lambda_1 h_1 = (0, 0) \\ g_2 &= (0, 0)\end{aligned}$$

Hence we have reached the minimum.

2. Minimize $f(x, y) = x^2 + y^2$ subject to the constraint that $u(x, y) = (x+y)^2 + 4(x-y)^2 - 1 = 0$ by using the Lagrange multiplier method. Describe also how the problem can be solved by introducing a soft constraint.

We construct $\tilde{f}(x, y, \lambda) = f(x, y) + \lambda u(x, y)$ and solve the equation system

$$\frac{\delta \tilde{f}}{\delta x} = 0, \frac{\delta \tilde{f}}{\delta y} = 0, \frac{\delta \tilde{f}}{\delta \lambda} = 0.$$

We get four solutions: $(x, y, \lambda) = (1/2, 1/2, -1/2), (-1/2, -1/2, -1/2), (-1/4, 1/4, -1/8)$ and $(1/4, -1/4, -1/8)$. The two first solutions corresponds to maxima rather than minima.

The soft constraint is implemented by constructing $\tilde{f}(x, y) = f(x, y) + \lambda u(x, y)^2$, minimizing for a fixed λ , increasing λ , re-minimizing and repeat until λ goes to infinity. Solving $\nabla \tilde{f}(x, y) = 0$ we get the following solutions for (x, y) :

$$\begin{aligned}(0, 0) \\ \left(-\frac{\sqrt{4\lambda-1}}{4\sqrt{\lambda}}, -\frac{\sqrt{4\lambda-1}}{4\sqrt{\lambda}}\right) &\rightarrow (-1/2, -1/2) \\ \left(\frac{\sqrt{4\lambda-1}}{4\sqrt{\lambda}}, \frac{\sqrt{4\lambda-1}}{4\sqrt{\lambda}}\right) &\rightarrow (1/2, 1/2) \\ \left(-\frac{\sqrt{16\lambda-1}}{16\sqrt{\lambda}}, \frac{\sqrt{16\lambda-1}}{16\sqrt{\lambda}}\right) &\rightarrow (-1/4, 1/4) \\ \left(\frac{\sqrt{16\lambda-1}}{16\sqrt{\lambda}}, -\frac{\sqrt{16\lambda-1}}{16\sqrt{\lambda}}\right) &\rightarrow (1/4, -1/4)\end{aligned}$$

3. The entropy $S[p]$ of a discrete probability distribution p_i is defined as

$$S[p] = -\langle \ln p \rangle = -\sum_i p_i \ln p_i .$$

Assign an energy E_i to each state i . Find the normalized distribution p_i that maximizes the entropy for a given average energy

$$\langle E \rangle = \sum_i E_i p_i = \bar{E} .$$

We construct $\tilde{S}(p, \lambda_1, \lambda_2) = S[p] + \lambda_1(\bar{E} - \sum_i E_i p_i) + \lambda_2(1 - \sum_i p_i)$ and solve the equation system

$$\begin{aligned} \frac{\delta \tilde{S}}{\delta p_i} &= -\ln p_i - 1 - \lambda_1 E_i - \lambda_2 = 0 \\ \frac{\delta \tilde{S}}{\delta \lambda_1} &= \bar{E} - \sum_i E_i p_i = 0 \\ \frac{\delta \tilde{S}}{\delta \lambda_2} &= 1 - \sum_i p_i = 0 \end{aligned}$$

Which can be reduced to the two equations for λ_1 and λ_2 :

$$\begin{aligned} e^{-\lambda_2 - 1} \sum_i E_i e^{-\lambda_1 E_i} &= \bar{E} \\ e^{-\lambda_2 - 1} \sum_i e^{-\lambda_1 E_i} &= 1 \end{aligned}$$

and a final equation:

$$\frac{\sum_i E_i e^{-\lambda_1 E_i}}{\sum_i e^{-\lambda_1 E_i}} = \bar{E}$$