Mathematical Concepts 3

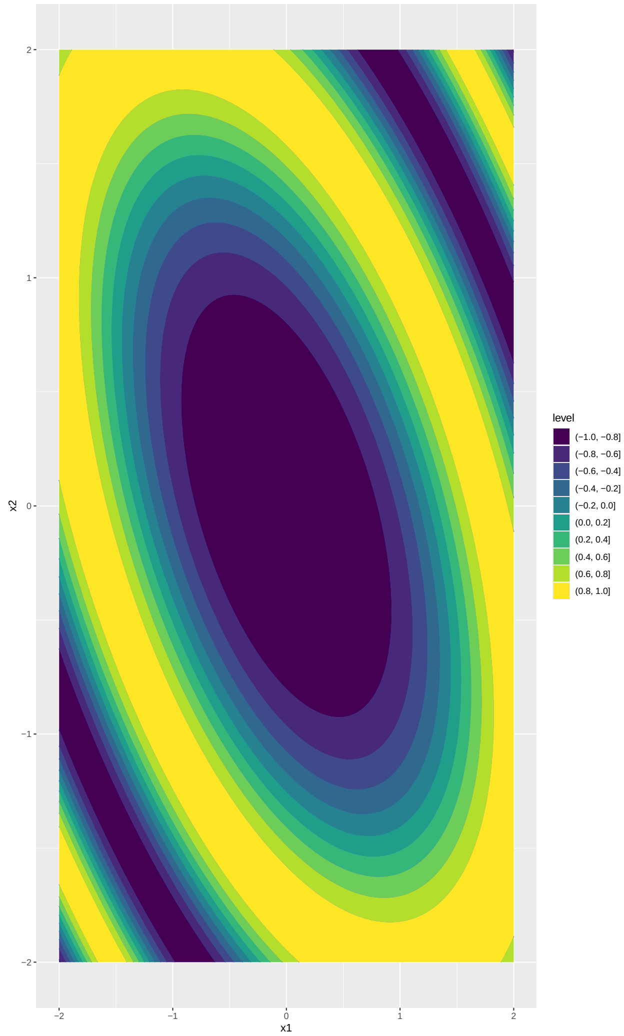
Solution 1:
Optimality in 2d

(a)
```
library(ggplot2)

f <- function(x, y) - cos(x^2 + y^2 + x*y)
x = seq(-2, 2, by=0.01)
xx = expand.grid(X1 = x, X2 = x)

fxx = f(xx[, 1], xx[, 2])
df = data.frame(X1 = xx$X1, X2 = xx$X2, fxx = fxx)

ggplot(df, aes(x = X1, y = X2, z = fxx)) +
  geom_contour_filled() +
  xlab("x1") +
  ylab("x2")
```



(b) $\nabla f = (\sin(x_1^2 + x_2^2 + x_1x_2)(2x_1 + x_2), \sin(x_1^2 + x_2^2 + x_1x_2)(2x_2 + x_1))^\top$

(c) $\nabla^2 f = \begin{pmatrix} \cos(u)(2x_1 + x_2)^2 + 2\sin(u) & \cos(u)(2x_1 + x_2)(2x_2 + x_1) + \sin(u) \\ \cos(u)(2x_1 + x_2)(2x_2 + x_1) + \sin(u) & \cos(u)(2x_2 + x_1)^2 + 2\sin(u) \end{pmatrix}$ with $u = x_1^2 + x_2^2 + x_1x_2$.

(d) Let $u : \mathbb{R}^2 \to \mathbb{R}, (x_1, x_2) \mapsto x_1^2 + x_2^2 + x_1x_2$, such that $f(\mathbf{x}) = \cos(u(\mathbf{x}))$.
$\implies \nabla^2 f(\mathbf{x}) = \cos(u(\mathbf{x}))\nabla u(\mathbf{x})\nabla u(\mathbf{x})^\top + \sin(u(\mathbf{x}))\nabla^2 u(\mathbf{x})$
$\nabla u(\mathbf{x}) = (2x_1 + x_2, x_1 + 2x_2)^\top$
$\nabla^2 u(\mathbf{x}) = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$
For $\mathbf{x} \in S_{\bar{r}}$, it holds that $u(\mathbf{x}) \geq 0$, since

$$0 \leq \frac{1}{2}(x_1 + x_2)^2 = \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 + x_1x_2 \leq x_1^2 + x_2^2 + x_1x_2 = u(\mathbf{x}),$$

and that $u(\mathbf{x}) < \pi/4$. This implies that $\cos(u(\mathbf{x})) > 0$ and $\sin(u(\mathbf{x})) \geq 0$.
$\nabla u(\mathbf{x})\nabla u(\mathbf{x})^\top$ is positive semi-definite since

$$\mathbf{v}^\top \nabla u(\mathbf{x})\nabla u(\mathbf{x})^\top \mathbf{v} = (\mathbf{v}^\top \nabla u(\mathbf{x}))^2 \geq 0.$$

$\nabla^2 u(\mathbf{x})$ is positive definite since

$$\mathbf{v}^\top \nabla^2 u(\mathbf{x})\mathbf{v} = 2v_1^2 + 2v_1v_2 + 2v_2^2 = v_1^2 + v_2^2 + (v_1 + v_2)^2 \geq 0$$

and equality only holds if $\mathbf{v} = \mathbf{0}$.
So, in total, for $\mathbf{x} \in S_{\bar{r}}$, we have that

$$\nabla^2 f(\mathbf{x}) = \underbrace{\cos(u(\mathbf{x}))}_{>0} \underbrace{\nabla u(\mathbf{x})\nabla u(\mathbf{x})^\top}_{\text{p.s.d.}} + \underbrace{\sin(u(\mathbf{x}))}_{\geq 0} \underbrace{\nabla^2 u(\mathbf{x})}_{\text{p.d.}}.$$

$\Rightarrow \nabla^2 f(\mathbf{x})$ is positive semi-definite.
$\Rightarrow f_{|S_{\bar{r}}}$ is convex.

(e) For $\mathbf{x} \in S_{\bar{r}}$, it holds that $\nabla f(\mathbf{x}) = -\underbrace{\cos(u(\mathbf{x}))}_{>0} \nabla u(\mathbf{x})$ and thus

$$\nabla f(\mathbf{x}) = \mathbf{0} \iff \nabla u(\mathbf{x}) = \mathbf{0} \iff \mathbf{x} = \mathbf{0}.$$

It follows that $\mathbf{x} = \mathbf{0}$ is a local minimum.

(f) $f(\mathbf{0}) = -1$ and $\cos : \mathbb{R} \to [-1, 1]$. From this it follows that $\mathbf{0}$ must be a global minimum of f since no element of the image of f is smaller than -1.

Solution 2:
Optimality in d dimensions

(a) $\mathsf{Var}(\mathbf{w}^\top \mathbf{X} - \mathbf{Y}) = \mathsf{Var}(\mathbf{w}^\top \mathbf{X}) + \mathsf{Var}(\mathbf{Y}) - 2\mathsf{Cov}(\mathbf{w}^\top \mathbf{X}, \mathbf{Y}) = \mathbf{w}^\top \Sigma_{\mathbf{X}} \mathbf{w} + \mathsf{Var}(\mathbf{Y}) - 2\mathbf{w}^\top \Sigma_{\mathbf{XY}}$. This is a quadratic form in $\mathbf{w}$ and $\Sigma_{\mathbf{X}}$ is p.s.d. (since it is a covariance matrix) $\Rightarrow f$ is convex.

(b) $\nabla f = 2\Sigma_{\mathbf{X}}\mathbf{w} - 2\Sigma_{\mathbf{XY}}, \nabla^2 f = 2\Sigma_{\mathbf{X}}$

(c) $\nabla f \overset{!}{=} \mathbf{0} \iff 2\Sigma_{\mathbf{X}}\mathbf{w} - 2\Sigma_{\mathbf{XY}} = 0 \iff \Sigma_{\mathbf{X}}\mathbf{w} = \Sigma_{\mathbf{XY}}$. This system of linear equations has a unique solution if $\Sigma_{\mathbf{X}}$ is non-singular. If $\Sigma_{\mathbf{X}}$ is non-singular it follows that $\mathbf{w} = \Sigma_{\mathbf{X}}^{-1}\Sigma_{\mathbf{XY}}$. In this case $\Sigma_{\mathbf{X}}$ is p.d. since no eigenvalue can be zero, f is strictly convex and the local minimum is global.

(d) First condition: Since $\mathbf{w}$ exists $\Sigma_{\mathbf{X}}$ must be non-singular.
Then $\Sigma_{\mathbf{X}}^{-1}\Sigma_{\mathbf{XY}} = \mathbb{E}\left((\mathbf{X} - \mathbb{E}(\mathbf{X})(\mathbf{X} - \mathbb{E}(\mathbf{X}))^\top\right)^{-1} \mathbb{E}\left((\mathbf{X} - \mathbb{E}(\mathbf{X}))(\mathbf{Y} - \mathbb{E}(\mathbf{Y}))^\top\right)$
Second condition: If $\mathbb{E}(\mathbf{X}) = \mathbf{0}, \mathbb{E}(\mathbf{Y}) = \mathbf{0}$ then
$\Sigma_{\mathbf{X}}^{-1}\Sigma_{\mathbf{XY}} = \left(\mathbb{E}(\mathbf{X}\mathbf{X}^\top)\right)^{-1} \mathbb{E}(\mathbf{X}\mathbf{Y}^\top)$.
$n(\mathbf{x}_{1:n}^\top \mathbf{x}_{1:n})^{-1}$ is a consistent estimator of $\left(\mathbb{E}(\mathbf{X}\mathbf{X}^\top)\right)^{-1}$ and
$\frac{1}{n}\mathbf{x}_{1:n}^\top y_{1:n}$ is a consistent estimator of $\mathbb{E}(\mathbf{X}\mathbf{Y}^\top)$.
$\Rightarrow$ The least squares estimator $(\mathbf{x}_{1:n}^\top \mathbf{x}_{1:n})^{-1}\mathbf{x}_{1:n}^\top y_{1:n}$ is a consistent estimator of $\left(\mathbb{E}(\mathbf{X}\mathbf{X}^\top)\right)^{-1} \mathbb{E}(\mathbf{X}\mathbf{Y}^\top)$.