

## Mathematical Concepts 2

### Solution 1:

#### Matrix Calculus

$$(a) \frac{\partial \|\mathbf{x} - \mathbf{c}\|_2^2}{\partial \mathbf{x}} = \frac{\partial \|\mathbf{u}\|_2^2}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}} = \frac{\partial \mathbf{u}^\top \mathbf{u}}{\partial \mathbf{u}} \frac{\partial \mathbf{x} - \mathbf{c}}{\partial \mathbf{x}} = \frac{\partial \mathbf{u}^\top \mathbf{I} \mathbf{u}}{\partial \mathbf{u}} (\mathbf{I} - \mathbf{0}) = \mathbf{u}^\top (\mathbf{I} + \mathbf{I}^\top) = 2(\mathbf{x} - \mathbf{c})^\top$$

$$(b) \frac{\partial \|\mathbf{x} - \mathbf{c}\|_2}{\partial \mathbf{x}} = \frac{\partial \sqrt{\|\mathbf{x} - \mathbf{c}\|_2^2}}{\partial \mathbf{x}} = \frac{0.5}{\sqrt{\|\mathbf{x} - \mathbf{c}\|_2^2}} \frac{\partial \|\mathbf{x} - \mathbf{c}\|_2^2}{\partial \mathbf{x}} \stackrel{(a)}{=} \frac{(\mathbf{x} - \mathbf{c})^\top}{\|\mathbf{x} - \mathbf{c}\|_2}$$

$$(c) \frac{\partial \mathbf{u}^\top \mathbf{v}}{\partial \mathbf{x}} = \frac{\partial \mathbf{u}^\top \mathbf{I} \mathbf{v}}{\partial \mathbf{x}} = \mathbf{u}^\top \mathbf{I} \frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \mathbf{v}^\top \mathbf{I}^\top \frac{\partial \mathbf{u}}{\partial \mathbf{x}} = \mathbf{u}^\top \frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \mathbf{v}^\top \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$$

$$(d) \frac{\partial \mathbf{Y}^\top \mathbf{u}}{\partial \mathbf{x}} = \frac{\partial \begin{pmatrix} \mathbf{y}_1^\top \mathbf{u} \\ \vdots \\ \mathbf{y}_d^\top \mathbf{u} \end{pmatrix}}{\partial \mathbf{x}} \stackrel{(c)}{=} \begin{pmatrix} \mathbf{y}_1^\top \frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{u}^\top \frac{\partial \mathbf{y}_1}{\partial \mathbf{x}} \\ \vdots \\ \mathbf{y}_d^\top \frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{u}^\top \frac{\partial \mathbf{y}_d}{\partial \mathbf{x}} \end{pmatrix}$$

(e) Note for  $\mathbf{y} : \mathbb{R}^d \rightarrow \mathbb{R}^d, \mathbf{x} \mapsto \mathbf{y}(\mathbf{x})$  the  $i$ -th column of  $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$  is  $\frac{\partial \mathbf{y}}{\partial x_i}$ . With this it follows that

$$\begin{aligned} \frac{\partial^2 \mathbf{u}^\top \mathbf{v}}{\partial \mathbf{x} \partial \mathbf{x}^\top} &= \frac{\partial}{\partial \mathbf{x}} \left( \frac{\partial \mathbf{u}^\top \mathbf{v}}{\partial \mathbf{x}^\top} \right) \\ &= \frac{\partial}{\partial \mathbf{x}} \left[ \left( \frac{\partial \mathbf{u}^\top \mathbf{v}}{\partial \mathbf{x}} \right)^\top \right] \\ &\stackrel{(c)}{=} \frac{\partial (\mathbf{u}^\top \frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \mathbf{v}^\top \frac{\partial \mathbf{u}}{\partial \mathbf{x}})^\top}{\partial \mathbf{x}} \\ &= \frac{\partial \left( \left( \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \right)^\top \mathbf{u} + \left( \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \right)^\top \mathbf{v} \right)}{\partial \mathbf{x}} \\ &\stackrel{(d)}{=} \begin{pmatrix} \mathbf{u}^\top \frac{\partial^2 \mathbf{v}}{\partial x_1 \partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial x_1}^\top \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \\ \vdots \\ \mathbf{u}^\top \frac{\partial^2 \mathbf{v}}{\partial x_d \partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial x_d}^\top \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \end{pmatrix}^\top + \begin{pmatrix} \mathbf{v}^\top \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial \mathbf{x}} + \frac{\partial \mathbf{u}}{\partial x_1}^\top \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \\ \vdots \\ \mathbf{v}^\top \frac{\partial^2 \mathbf{u}}{\partial x_d \partial \mathbf{x}} + \frac{\partial \mathbf{u}}{\partial x_d}^\top \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \end{pmatrix}^\top \\ &= \begin{pmatrix} \mathbf{u}^\top \frac{\partial^2 \mathbf{v}}{\partial x_1 \partial \mathbf{x}} \\ \vdots \\ \mathbf{u}^\top \frac{\partial^2 \mathbf{v}}{\partial x_d \partial \mathbf{x}} \end{pmatrix}^\top + \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \left( \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \right)^\top + \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \left( \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \right)^\top + \begin{pmatrix} \mathbf{v}^\top \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial \mathbf{x}} \\ \vdots \\ \mathbf{v}^\top \frac{\partial^2 \mathbf{u}}{\partial x_d \partial \mathbf{x}} \end{pmatrix}^\top \end{aligned}$$

### Solution 2:

#### Optimality in 1d

Let  $f : [-1, 2] \rightarrow \mathbb{R}, x \mapsto \exp(x^3 - 2x^2)$

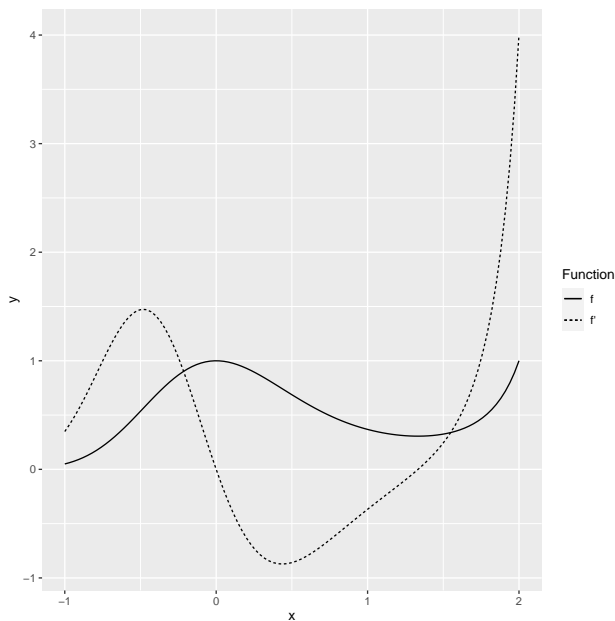
$$(a) f'(x) = \exp(x^3 - 2x^2) \cdot (3x^2 - 4x)$$

(b) `library(ggplot2)`

```
f <- function(x) exp(x^3 - 2*x^2)
df <- function(x) f(x) * (3*x^2 - 4*x)
```

```
ggplot(data.frame(x = seq(-1, 2, by=0.005)), aes(x)) +
```

```
geom_function(fun = f, aes(linetype = "f")) +  
geom_function(fun = df, aes(linetype = "f'")) +  
scale_linetype_discrete(name = "Function")
```



(c)  $f$  is continuously differentiable  $\Rightarrow$  candidates can only be stationary points and boundary points.

Find stationary points, i.e., points where

$$f'(x) = 0 \iff \underbrace{\exp(x^3 - 2x^2)}_{>0} \cdot (3x^2 - 4x) = 0 \iff 3x^2 - 4x = 0 \iff x(3x - 4) = 0.$$

$\Rightarrow x_1 = 0, x_2 = 4/3$ . The other candidates are boundary points, i.e.,  $x_3 = -1, x_4 = 2$ .

(d)  $f''(x) = \exp(x^3 - 2x^2) \cdot (3x^2 - 4x)^2 + \exp(x^3 - 2x^2) \cdot (6x - 4)$

(e)  $f''(x_1) = \exp(0) \cdot (-4) < 0$

$\Rightarrow x_1$  is a local maximum

$$f''(x_2) = \exp((4/3)^3 - 2(4/3)^2) \cdot (4) > 0$$

$\Rightarrow x_2$  is a local minimum.

The boundary points  $x_3$  and  $x_4$  are not considered as *local* optima.

(f)  $f(x_1) = \exp(0) = 1$

$$f(x_2) = \exp((4/3)^3 - 2(4/3)^2) \approx 0.3057$$

$$f(x_3) = \exp(-3) \approx 0.05$$

$$f(x_4) = \exp(0) = 1$$

$\Rightarrow x_1, x_4$  are global maxima.  $x_3$  is global minimum.