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SCIENCE

Homework.

Deep learning

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1 Matrix calculus

1.1 Problem № 1

Find the gradient $\nabla f(x)$, if $f(X) = \det(X^{-1} + A)$

Solution:

$$\begin{aligned} df(X) &= \det(X^{-1} + A) \langle (X^{-1} + A)^{-T}, d(X^{-1} + A) \rangle = \det(X^{-1} + A) \langle (X^{-1} + A)^{-T}, dX^{-1} \rangle = \\ &= \det(X^{-1} + A) \langle (X^{-1} + A)^{-T}, -X^{-1} dX X^{-1} \rangle \\ &= -\det(X^{-1} + A) \langle X^{-T} (X^{-1} + A)^{-T} X^{-T}, dX \rangle \end{aligned}$$

Answer: $\nabla_X f(x) = -\det(X^{-1} + A) X^{-T} (X^{-1} + A)^{-T} X^{-T}$

1.2 Problem № 2

Find $\nabla f(x)$ and $\nabla^2 f(x)$ for:

- $f : \mathbb{R}_{++} \rightarrow \mathbb{R}$, $f(t) = \|(A + tI_n)^{-1}b\|$, where $A \in \mathbb{S}_+^n$, $b \in \mathbb{R}^n$
- $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $f(x) = \frac{1}{2} \|xx^T - A\|_F^2$, where $A \in \mathbb{S}^n$

Solution:

$$C = (A + tI_n)^{-1}, \quad \frac{dC}{dt} = -CCdt$$

$$df(t) = d(\|Cb\|) = \frac{1}{2\|Cb\|} d\langle Cb, Cb \rangle = \frac{-1}{\|Cb\|} \langle CCb, Cb \rangle dt$$

$$\begin{aligned} d^2 f(t) &= \frac{1}{\|Cb\|} (\langle CCb, CCb \rangle + 2\langle CCCb, Cb \rangle) dt' dt - \frac{1}{2\|Cb\|^3} \langle CCb, Cb \rangle d\langle Cb, Cb \rangle dt' = \\ &= \frac{3}{\|Cb\|} \langle CCb, CCb \rangle dt' dt - \frac{1}{\|Cb\|^3} (\langle CCb, Cb \rangle)^2 dt' dt \end{aligned}$$

Let's solve the next one:

$$\begin{aligned} df &= d\langle xx^T - A, xx^T - A \rangle = \langle dxx^T + xdx^T, xx^T - A \rangle = \\ &= \text{tr}(x^T(xx^T - A)^T dx) + \text{tr}(dx^T(xx^T - A)^T x) = 2 \cdot \langle (xx^T - A)x, dx \rangle \\ d^2 f &= 2 \cdot \langle (xx^T - A)dx_2 + 2 \cdot dx_2 xx^T, dx_1 \rangle = \langle 2x^T x I + 4xx^T - 2A, dx_1 dx_2^T \rangle \end{aligned}$$

Answer:

- $\nabla f(t) = -\frac{\langle CCb, Cb \rangle}{\|Cb\|}$, $\nabla^2 f(t) = \frac{3}{\|Cb\|} \langle CCb, CCb \rangle - \frac{1}{\|Cb\|^3} (\langle CCb, Cb \rangle)^2$, where $C = (A + tI_n)^{-1}$
- $\nabla f = 2(xx^T - A)x$, $\nabla^2 f = 2x^T x I + 4xx^T - 2A$

1.3 Problem № 3

Find $\nabla_b L$ and $\nabla_A L$, if we know $\nabla_x L$

Solution: $Ax = b$, $x = A^{-1}b$, $\frac{\partial x}{\partial b} = A^{-T}$

$$\nabla_b L = \frac{\partial L}{\partial x} \frac{\partial x}{\partial b} = A^{-T} \nabla_x L$$

$$dL = \frac{\partial L}{\partial x} - A^{-1} dA A^{-1} b = -(A^{-T} \frac{\partial L}{\partial x} b^T A - T)$$

$$\nabla_A L = \frac{\partial L}{\partial x} \frac{\partial x}{\partial A} = -A^{-T} \nabla_x L b^T A^{-T}$$

Answer: $\nabla_A L = -A^{-T} \nabla_x L b^T A^{-T}$, $\nabla_b L = A^{-T} \nabla_x L$

1.4 Problem № 4

For each of the following functions, find all the stationarity points and specify the parameter values at which they exist.

- $f : E \rightarrow \mathbb{R}$, $f(x) = \langle a, x \rangle - \ln(1 - \langle b, x \rangle)$,
where $a, b \in \mathbb{R}^n$, $a, b \neq 0$, $E = \{x \in \mathbb{R}^n | \langle b, x \rangle < 1\}$
- $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $f(x) = \langle c, x \rangle \exp(-\langle Ax, x \rangle)$, where $c \in \mathbb{R}^n$, $c \neq 0$, $A \in \mathbb{S}^n$
- $f : \mathbb{S}_{++}^n \rightarrow \mathbb{R}$, $f(X) = \langle X^{-1}, I_n \rangle - \langle A, X \rangle$, where $A \in \mathbb{S}^n$

Solution: $f : E \rightarrow \mathbb{R}$, $f(x) = \langle a, x \rangle - \ln(1 - \langle b, x \rangle)$

$$\nabla f = a + \frac{b}{1 - \langle b, x \rangle} = 0$$

We can easily add two equations:

$$\langle a, a \rangle + \frac{\langle a, b \rangle}{1 - \langle b, x \rangle} = 0$$

$$\langle a, b \rangle + \frac{\langle b, b \rangle}{1 - \langle b, x \rangle} = 0$$

$$\langle b, x \rangle = \frac{\langle a, b \rangle}{\langle a, a \rangle} + 1$$

$$\langle b, x \rangle = \frac{\langle b, b \rangle}{\langle a, b \rangle} + 1$$

And here from that we get:

$$\frac{\langle b, b \rangle}{\langle a, b \rangle} = \frac{\langle a, b \rangle}{\langle a, a \rangle}$$

And from that we get conditions on a and b:

$$\langle a, b \rangle^2 = \langle a, a \rangle \langle b, b \rangle$$

$$f : \mathbb{R}^n \rightarrow \mathbb{R}, f(x) = \langle c, x \rangle \exp(-\langle Ax, x \rangle), \text{ where } c \in \mathbb{R}^n, c \neq 0, A \in \mathbb{S}^n$$

$$\nabla f = c \exp(-\langle Ax, x \rangle) - 2\langle c, x \rangle \exp(-\langle Ax, x \rangle) x^T A = 0$$

$$c - 2\langle c, x \rangle x^T A =$$

Multiply it on c:

$$\langle cA^{-1}, c \rangle = 2\langle c, x \rangle^2$$

And from that we get:

$$x = \frac{cA^{-1}}{2\langle c, x \rangle} = \frac{\pm cA^{-1}}{\sqrt{2\langle cA^{-1}, c \rangle}}$$

$$f : \mathbb{S}_{++}^n \rightarrow \mathbb{R}, f(X) = \langle X^{-1}, I_n \rangle - \langle A, X \rangle, \text{ where } A \in \mathbb{S}^n$$

$$\begin{aligned} \nabla f(X) &= \langle -X^{-1}dXX^{-1}, I \rangle - \langle A, dX \rangle = -\text{tr}(X^{-T}dX^T X^{-T}) - \text{tr}(A^T dX) = \\ &= -\langle X^{-1}X^{-1} + A, dX \rangle \end{aligned}$$

From that we get that: $XX = (-A)^{-1}$, $X = \sqrt{(-A)^{-1}}$

In course of optimization I had the same problem and I have already found answer in the internet: $X = Q^T \Lambda^{-0.5} Q$, where $A = -Q^T \Lambda Q$, we could prove it by putting X into equation and show that it's true.

Answer:

- $\langle a, b \rangle^2 = \langle a, a \rangle \langle b, b \rangle$, it means that $a = b \cdot t$, where $t \in \mathbb{R}$ and x such that:
 $\langle b, x \rangle = \frac{\langle b, b \rangle}{\langle a, b \rangle} + 1$
- $x = \frac{\pm cA^{-1}}{\sqrt{2\langle cA^{-1}, c \rangle}}$
- $X = Q^T \Lambda^{-0.5} Q$

1.5 Problem № 5

X – symmetric matrix and $X = Q^T \Lambda Q$, we know $\nabla_Q f$, $\nabla_\Lambda f$. Find $\nabla_X f = ?$

Solution:

$$\begin{aligned} df(X) &= df(Q^T \Lambda Q) = \langle \nabla_Q f, d_Q(Q^T \Lambda Q) \rangle + \langle \nabla_\Lambda f, d_\Lambda(Q^T \Lambda Q) \rangle = \\ &= \langle \nabla_Q f, Q^T \Lambda dQ \rangle + \langle \nabla_Q f, dQ^T \Lambda Q \rangle + \langle \nabla_\Lambda f, Q^T d\Lambda Q \rangle \\ &= \langle \Lambda Q \nabla_Q f, dQ \rangle + \langle \Lambda Q \nabla_Q f^T, dQ \rangle + \langle Q \nabla_\Lambda f Q^T, d\Lambda \rangle = \langle \nabla_X f, dX \rangle = \end{aligned}$$

$$\begin{aligned}
&= \langle \nabla_X f, dQ^T \Lambda Q + Q^T d\Lambda Q + Q^T \Lambda dQ \rangle = \\
&= \langle Q \nabla_X f Q^T, d\Lambda \rangle + \langle \Lambda Q \nabla_X f^T, dQ \rangle + \langle \Lambda Q \nabla_X f, dQ \rangle
\end{aligned}$$

From that we get two equations:

$$Q \nabla_X f Q^T = Q \nabla_\Lambda f Q^T$$

and

$$\Lambda Q \nabla_Q f + \lambda Q \nabla_Q f^T = \Lambda Q \nabla_X f + \Lambda Q \nabla_X f^T$$

and it's trivial that: $\nabla_X f = \nabla_\Lambda f$

Answer: $\nabla_X f = \nabla_\Lambda f$