APPENDIX

Gradient Matrices

In Chapter 7 we use the gradient of a scalar with respect to a matrix. Before presenting a detailed discussion, we need an index arithmetic for matrix manipulations.

A matrix $A \in R^{n \times m}$ is denoted by A_{nm}, where n and m are free indices. If in an expression a specific index appears twice, it means a summation with respect to this index. For example, if $B \in \mathbf{R}^{m \times r}$ and $C \in \mathbf{R}^{r \times n}$ then the product BC is denoted by $[BC]_{mn} = B_{mi}C_{in}$, which means $BC = \sum_{i=1}^{r} B_{mi}C_{in}$. Another example is $\mathrm{tr}(A) = A_{ii}$, which means $\sum_{i=1}^{n} A_{ii}$. In matrix transposition, we change the indices order. That is, if $B \in \mathbf{R}^{n \times d}$ and $C \in \mathbf{R}^{n \times k}$, then $B'C = Q$ is written $B_{id}C_{ik} = Q_{dk}$. Note that since each element in index arithmetic is a scalar, we can change the order as needed. We now define the gradient of a scalar z with respect to a matrix F.

Definition A.1 Given a scalar z and a matrix F, $\frac{\partial z}{\partial F} = B$, where $B_{ij} = \frac{\partial z}{\partial F_{ij}}$.

Theorem A.1

(i) $\frac{\partial}{\partial F}\mathrm{tr}(F' MF) = 2MF$, if M symmetric,

(ii) $\frac{\partial}{\partial F}\mathrm{tr}(BFC) = B'C'$, if $B, F, C \in \mathbf{R}^{n \times n}$,

(iii) $\frac{\partial}{\partial F}\mathrm{tr}(F) = I$, if $F \in \mathbf{R}^{n \times n}$.

Proof We prove only (i). Parts (ii), (iii) are proved along the same lines. $F'MF$ is denoted by $F_{ij}M_{ik}F_{kj}$. Thus, for any a, b we write

$$\begin{aligned} \frac{\partial}{\partial F_{ab}}(F_{ij}M_{ik}F_{kj}) &= M_{ak}F_{kb} + F_{ib}M_{ia} \\ &= M_{ak}F_{kb} + M_{ia}F_{ib} \\ &= (M + M')F \\ &= 2MF . \end{aligned}$$

We now turn to more complicated derivatives.

Theorem A.2 Let $F \in \mathbf{R}^{m \times p}$, $A \in \mathbf{R}^{n \times n}$, $B \in \mathbf{R}^{n \times m}$, $C \in \mathbf{R}^{p \times n}$, and let $\Lambda \in \mathbf{R}^{n \times n}$, $P \in \mathbf{R}^{n \times n}$ be symmetric. Then,

(i) $\frac{\partial}{\partial F}\mathrm{tr}\left[(BFC)^{i}\right] = iB^{i}(C'F'B')^{i-1}C'$;

(ii) $\frac{\partial}{\partial F}\mathrm{tr}\,[\Lambda(BFC)^{i}] = \sum_{j=0}^{i-1} B'(C'F'B')^{j}\Lambda(C'F'B')^{i-1-j}C'$;

(iii) $\frac{\partial}{\partial F}\mathrm{tr}\,[\Lambda(BFC)^{i}P] = \sum_{j=0}^{i-1} B'(C'F'B')^{j}P\Lambda(C'F'B')^{i-1-j}C'$;

(iv) $$\frac{\partial}{\partial F}\operatorname{tr}\,[\Lambda(BFC)^i P(C'F'B')^j] = \sum_{k=0}^{i-1} B'(C'F'B')^k \Lambda(BFC)^j P(C'F'B')^{i-1-k} C'$$

$$+ \sum_{k=0}^{j-1} B'(C'F'B')^k \Lambda(BFC)^i P(C'F'B')^{j-1-k} C';$$

(v) $$\frac{\partial}{\partial F}\operatorname{tr}\,[\Lambda(A + BFC)^i P(A' + C'F'B')^j] =$$

$$= \sum_{k=0}^{i-1} B'(A' + C'F'B')^k \Lambda(A + BFC)^j P(A' + C'F'B')^{i-1-k} C'$$

$$+ \sum_{k=0}^{j-1} B'(A' + C'F'B')^k \Lambda(A + BFC)^i P(A' + C'F'B')^{j-1-k} C'.$$

Proof We prove (v). The rest are special cases of (v). Write

$$J = \operatorname{tr}\left[\Lambda(A + BFC)^i P(A' + C'F'B')^j\right]$$

$$= \Lambda_{ab}(A_{be} + B_{bc}F_{cd}C_{de}) \cdot \ldots \cdot (A_{lo} + B_{lm}F_{mn}C_{no}) \cdot \ldots \cdot P_{qr} \cdot$$

$$\cdot (A_{ur} + C_{sr}F_{ts}B_{ut}) \cdot \ldots \cdot (A_{av} + C_{wv}F_{xw}B_{ax}) .$$

We now take the derivative of J with respect to F_{yz} and obtain an $m\times p$ matrix. Consider the following two cases. (a) F is between Λ and P, and (b) F appears following P. In case (a), we consider the $k+1$ term $(k + 1 \leq i)$, $A_{lo} + B_{lm}F_{mn}C_{no}$, and take the derivative with respect to F_{yz}. The result is zero except for $m = y$, $n = z$, in which case the result is $B_{ly}\,C_{zo}$. More specifically, we obtain

$$\Lambda_{ab}(A_{be} + B_{bc}F_{cd}C_{de}) \cdot \ldots \cdot (B_{ly}C_{zo}) \cdot \ldots \cdot P_{qr} \cdot (A_{ur} + C_{sr}F_{ts}B_{ut}) \ldots \cdot (A_{av} + C_{wv}F_{xw}B_{ax}) .$$

Now, rearranging the terms, in cyclic order moving backwards from B_{ly}, we end at C_{zo}, and obtain

$$B'(A' + C'F'B')^k \Lambda(A + BFC)^j P(A' + C'F'B')^{i-1-k} C' .$$

Since we take a derivative for each $k = 0, 1, \ldots, i - 1$, we take the sum over k, and obtain the first sum in (v). Likewise, in case (b), we consider the $k + 1$ term $(k + 1 \leq j)$, $A_{ur} + C_{sr}F_{ts}B_{ut}$, so that the derivative with respect to F_{yz}, yields $C_{zr}B_{uy}$. Rearranging terms forwards in cyclic order starting at B_{uy}, yields

$$B'(A' + C'F'B')^k \Lambda(A + BFC)^i P(A' + C'F'B')^{j-1-k} C' .$$

Taking the sum as above, we obtain the second sum in (v). This completes the proof.

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