Deep Learning & Applied AI

Matrix meta-mechanics

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Matrix manipulation

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These notes may be updated as we go on with the course.

Transpose and inverse

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The same holds for the inverse:

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A matrix $\mathbf{A}$ is orthogonal if:

$$\mathbf{A}^{-1} = \mathbf{A}^\top ,$$

Thus, $\mathbf{A}^\top \mathbf{A} = \mathbf{I}$ whenever $\mathbf{A}$ is orthogonal.

Products

Matrix-vector product:

$$\mathbf{X}\mathbf{y} = \begin{pmatrix} | & | & \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots \\ | & | & \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \end{pmatrix} = y_1 \begin{pmatrix} | \\ \mathbf{x}_1 \\ | \end{pmatrix} + y_2 \begin{pmatrix} | \\ \mathbf{x}_2 \\ | \end{pmatrix} + \cdots$$

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For example, a matrix full of ones is just $\mathbf{1}\mathbf{1}^\top$.

Diagonal matrices

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From the other side:

$$\begin{pmatrix} | & | & \\ \mathbf{y}_1 & \mathbf{y}_2 & \cdots \\ | & | & \end{pmatrix} \begin{pmatrix} d_1 & & \\ & d_2 & \\ & & \ddots \end{pmatrix} = \begin{pmatrix} | & | & \\ d_1\mathbf{y}_1 & d_2\mathbf{y}_2 & \cdots \\ | & | & \end{pmatrix}$$

Trace

The trace of $\mathbf{A}$ is the sum of its diagonal elements:

$$\mathrm{tr}(\mathbf{A}) = \sum_i a_{ii}$$

It is a linear mapping, since:

$$\mathrm{tr}(\mathbf{A} + \mathbf{B}) = \mathrm{tr}(\mathbf{A}) + \mathrm{tr}(\mathbf{B})$$
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It is invariant to cyclic permutations:

$$\operatorname{tr}(\mathbf{ABC}) = \operatorname{tr}(\mathbf{CAB}) = \operatorname{tr}(\mathbf{BCA})$$

Norms

The (squared) Frobenius norm for a matrix $\mathbf{X}$ is:

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If $\mathbf{X}$ is a vector, this reduces to:

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For example, for matrices $\mathbf{A}$ and $\mathbf{B}$ we can derive the distance:

$$\begin{aligned}\|\mathbf{A}-\mathbf{B}\|_F^2 &= \mathrm{tr}((\mathbf{A}-\mathbf{B})^\top(\mathbf{A}-\mathbf{B})) \\ &= \mathrm{tr}(\mathbf{A}^\top\mathbf{A}) - 2\mathrm{tr}(\mathbf{A}^\top\mathbf{B}) + \mathrm{tr}(\mathbf{B}^\top\mathbf{B}),\end{aligned}$$

where we used the linearity of the trace and its invariance to transposition.

Ones

A vector $\mathbf{1}$ of ones can be used to calculate sums easily.

Sum up the elements of $\mathbf{A}$ along each row:

$$\mathbf{A}\mathbf{1}$$

Sum up along each column:

$$\mathbf{1}^\top \mathbf{A} = (\mathbf{A}^\top \mathbf{1})^\top$$

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Note the following relationship:

$$\mathbf{x}^\top \mathbf{A}\mathbf{x} = \mathrm{tr}(\mathbf{x}^\top \mathbf{A}\mathbf{x}) = \mathrm{tr}(\mathbf{x}\mathbf{x}^\top \mathbf{A}) = \mathrm{tr}(\mathbf{X}\mathbf{A})$$

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Constructing the matrix $\mathbf{x}\mathbf{x}^\top$ from the vector $\mathbf{x}$ is also called lifting.

Permutation matrices

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix}$$

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Their product is still a permutation matrix.

Their convex combination is a doubly stochastic matrix:

$$\alpha \mathbf{P} + (1-\alpha)\mathbf{Q} = \mathbf{D} \quad \text{with } \alpha \in [0,1]$$

that is, we get $\mathbf{D}\mathbf{1} = \mathbf{1}$ and $\mathbf{D}^\top \mathbf{1} = \mathbf{1}$.

Gradients of traces

The following expression appears frequently in practice:

$$\nabla \mathrm{tr}(\mathbf{A}) = \nabla \sum_i a_{ii}$$

which requires the computation of the partial derivatives:

$$\frac{\partial}{\partial a_{ij}} \sum_i a_{ii}$$

A common pitfall is the following invalid operation:

$$\underbrace{\nabla \mathrm{tr}(\mathbf{A})}_{\substack{\text{gradient of a}\\ \text{scalar function}}} \Rightarrow \mathrm{tr}(\underbrace{\nabla \mathbf{A}}_{\text{undefined}})$$

Also observe that $\nabla \mathrm{tr}(\mathbf{A})$ is a matrix, while $\mathrm{tr}(\cdots)$ is a scalar.

Suggested reading

For a review of matrix calculus, read Chapters 0.0 – 0.2 of the book:

R. Horn & C. Johnson, "Matrix Analysis - 2nd ed". Cambridge University Press, 2013