

Machine Learning

Matrix meta-mechanics

Emanuele Rodolà
rodola@di.uniroma1.it



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Matrix manipulation

The definition of matrix product gives rise to some **alternative viewpoints** that are often useful for practical manipulation of matrices.

These notes cover a few useful “meta-mechanics” of matrix products and other operations that are frequently encountered.

These results should be **checked!**

Do **not** trust everything blindly at the first exposure.
After the check, you can go blindfolded.

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

Transpose and inverse

A matrix \mathbf{A} is **symmetric** if:

$$\mathbf{A} = \mathbf{A}^\top$$

If the matrix is a product $\mathbf{A} = \mathbf{BC}$, the transpose applies as follows:

$$(\mathbf{BC})^\top = \mathbf{C}^\top \mathbf{B}^\top$$

The same holds for the inverse:

$$(\mathbf{BC})^{-1} = \mathbf{C}^{-1} \mathbf{B}^{-1}$$

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:

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

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Vector-matrix product; it's just a transposed version of the above:

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

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Products

Matrix-matrix product:

$$\mathbf{XY} = \begin{pmatrix} \text{---} & \mathbf{x}_1^\top & \text{---} \\ \text{---} & \mathbf{x}_2^\top & \text{---} \\ & \vdots & \end{pmatrix} \begin{pmatrix} | & | & \cdots \\ \mathbf{y}_1 & \mathbf{y}_2 & \\ | & | & \end{pmatrix} = \begin{pmatrix} \cdots & & \\ \vdots & \mathbf{x}_i^\top \mathbf{y}_j & \vdots \\ \cdots & & \end{pmatrix}$$

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Vector-vector product (**inner**):

$$\mathbf{x}^\top \mathbf{y} = \alpha$$

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Vector-vector product (**outer**):

$$\mathbf{xy}^\top = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \end{pmatrix} \begin{pmatrix} y_1 & y_2 & \cdots \end{pmatrix} = \begin{pmatrix} | & | & \cdots \\ y_1 \mathbf{x} & y_2 \mathbf{x} & \\ | & | & \end{pmatrix}$$

For example, a matrix full of ones is just $\mathbf{11}^\top$.

Diagonal matrices

Matrix-vector product:

$$\begin{pmatrix} d_1 & & \\ & d_2 & \\ & & \ddots \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} d_1 x_1 \\ d_2 x_2 \\ \vdots \end{pmatrix}$$

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From the other side:

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

Trace

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

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

It is a **linear** mapping, since:

$$\text{tr}(\mathbf{A} + \mathbf{B}) = \text{tr}(\mathbf{A}) + \text{tr}(\mathbf{B})$$

$$\text{tr}(a\mathbf{A}) = a \text{tr}(\mathbf{A})$$

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It is invariant to **cyclic permutations**:

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

Norms

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

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

$$\|\mathbf{x}\|_2^2 = \text{tr}(\underbrace{\mathbf{x}\mathbf{x}^\top}_{n \times n}) = \text{tr}(\underbrace{\mathbf{x}^\top\mathbf{x}}_{1 \times 1}) = \mathbf{x}^\top\mathbf{x}$$

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

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

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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Sum up all the elements of **A**:

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Note the following relationship:

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

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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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Permutation matrices are **orthogonal**.

Their product is still a permutation matrix.

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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:

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

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:

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

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