Source task and conventions

Prove both variance and maximal-variance assertions for the uncentred data matrix.

Conventional solution and proof

Let the columns be $x_1, \dots, x_m \in \mathbb{R}^N$, $\bar{x} = m^{-1} \sum_i x_i$, and $Z = X - \bar{x}\mathbf{1}^\top$. The projected observations are $s_i = u^\top x_i$ and their mean is $\bar{s} = u^\top \bar{x}$. Thus

$$\frac{1}{m} \sum_i (s_i - \bar{s})^2 = \frac{1}{m} \sum_i u^\top (x_i - \bar{x})(x_i - \bar{x})^\top u = u^\top C u, \qquad C = ZZ^\top / m.$$

This proves (a), with the book's divisor m. For (b), C is symmetric positive semidefinite because $v^\top C v = \|Z^\top v\|^2 / m \geq 0$. By the real spectral theorem, $C = Q \operatorname{diag}(\lambda_1, \dots, \lambda_N) Q^\top$, $\lambda_1 \geq \cdots \geq 0$. For $\|u\| = 1$, writing $a = Q^\top u$ gives $u^\top C u = \sum_j \lambda_j a_j^2 \leq \lambda_1 \sum_j a_j^2 = \lambda_1$. Equality holds precisely when u lies in the top eigenspace. The leading left singular vector of Z is such a vector. If the top eigenvalue is repeated, the direction is not unique; if $Z = 0$, every unit direction is optimal.

Structural or analytic derivation

The orthogonal decomposition $Z = uu^\top Z + (I - uu^\top)Z$ gives

$$\|Z - uu^\top Z\|_F^2 = \|Z\|_F^2 - m u^\top C u.$$

Hence maximal variance and minimal rank-one projection residual are the same optimization problem. The equality follows column by column from Pythagoras, so it also proves the variational interpretation without differentiating a constrained objective.