

input: X (inputs), \mathbf{y} (targets), k (covariance function), σ_n^2 (noise level),
 \mathbf{x}_* (test input)

2: $L := \text{cholesky}(K + \sigma_n^2 I)$
 $\boldsymbol{\alpha} := L^\top \backslash (L \backslash \mathbf{y})$ } predictive mean eq. (2.25)

4: $\bar{f}_* := \mathbf{k}_*^\top \boldsymbol{\alpha}$
 $\mathbf{v} := L \backslash \mathbf{k}_*$ } predictive variance eq. (2.26)

6: $\mathbb{V}[f_*] := k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^\top \mathbf{v}$
 $\log p(\mathbf{y}|X) := -\frac{1}{2} \mathbf{y}^\top \boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{n}{2} \log 2\pi$ eq. (2.30)

8: **return:** \bar{f}_* (mean), $\mathbb{V}[f_*]$ (variance), $\log p(\mathbf{y}|X)$ (log marginal likelihood)

Algorithm 2.1: Predictions and log marginal likelihood for Gaussian process regression. The implementation addresses the matrix inversion required by eq. (2.25) and (2.26) using Cholesky factorization, see section A.4. For multiple test cases lines 4-6 are repeated. The log determinant required in eq. (2.30) is computed from the Cholesky factor (for large n it may not be possible to represent the determinant itself). The computational complexity is $n^3/6$ for the Cholesky decomposition in line 2, and $n^2/2$ for solving triangular systems in line 3 and (for each test case) in line 5.