

Formulas

1. Kernel definition

$$k(x, x') = \phi(x)^\top \phi(x')$$

2. Regularized least-squares error (primal)

$$J(w) = \frac{1}{2} \sum_{n=1}^N (w^\top \phi(x_n) - t_n)^2 + \frac{\lambda}{2} w^\top w$$

3. Dual representation of w

$$w = \sum_{n=1}^N a_n \phi(x_n)$$

4. Coefficients a_n

$$a_n = -\frac{1}{\lambda} (w^\top \phi(x_n) - t_n)$$

5. Primal \rightarrow dual objective

$$J(a) = \frac{1}{2} a^\top \Phi \Phi^\top \Phi \Phi^\top a - a^\top \Phi \Phi^\top t + \frac{1}{2} t^\top t + \frac{\lambda}{2} a^\top \Phi \Phi^\top a$$

6. Gram matrix

$$K_{nm} = \phi(x_n)^\top \phi(x_m) = k(x_n, x_m)$$

7. Objective in kernel form

$$J(a) = \frac{1}{2} a^\top K K a - a^\top K t + \frac{1}{2} t^\top t + \frac{\lambda}{2} a^\top K a$$

8. Dual solution

$$a = (K + \lambda I_N)^{-1} t$$

9. **Prediction formula**

$$y(x) = k(x)^\top (K + \lambda I_N)^{-1} t, \quad k(x)_n = k(x_n, x)$$

10. **Kernel via explicit features**

$$k(x, x') = \sum_{i=1}^M \phi_i(x) \phi_i(x')$$

11. **Polynomial-square kernel**

$$k(x, z) = (x^\top z)^2$$

12. **Linear kernel special case**

$$\phi(x) = x \implies k(x, x') = x^\top x'$$

13. **Stationary kernel**

$$k(x, x') = k(x - x')$$

14. **Homogeneous (RBF) kernel**

$$k(x, x') = k(\|x - x'\|)$$

15. **Feature map for $(x^\top z)^2$**

$$\phi(x) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)^\top$$

Derivations

Derivation of the Gram Matrix from Regularized Least Squares

Step	Equation	Reason
1	$J(w) = \frac{1}{2} \sum_{n=1}^N (w^\top \phi(x_n) - t_n)^2 + \frac{\lambda}{2} w^\top w$	Primal regularized least-squares objective
2	$\nabla_w J = \sum_{n=1}^N (w^\top \phi(x_n) - t_n) \phi(x_n) + \lambda w = 0$	Stationarity: set derivative to zero
3	$w = -\frac{1}{\lambda} \sum_{n=1}^N (w^\top \phi(x_n) - t_n) \phi(x_n) = \sum_{n=1}^N a_n \phi(x_n)$	Define dual coefficients $a_n = -\frac{1}{\lambda} (w^\top \phi(x_n) - t_n)$
4	$\Phi = \begin{bmatrix} \phi(x_1)^\top \\ \vdots \\ \phi(x_N)^\top \end{bmatrix}, \quad w = \Phi^\top a$	Stack feature vectors into design matrix
5	$\sum_{n=1}^N (w^\top \phi(x_n) - t_n)^2 = w^\top \left(\sum_{n=1}^N \phi(x_n) \phi(x_n)^\top \right) w - 2 w^\top \left(\sum_{n=1}^N t_n \phi(x_n) \right) + \sum_{n=1}^N t_n^2$	Expand $(x - y)^2 = x^2 - 2xy + y^2$
6	$\sum_{n=1}^N \phi(x_n) \phi(x_n)^\top = \Phi^\top \Phi, \quad \sum_{n=1}^N t_n \phi(x_n) = \Phi^\top t, \quad \sum_{n=1}^N t_n^2 = t^\top t$	Rewrite sums in matrix form
7	$J(w) = \frac{1}{2} w^\top (\Phi^\top \Phi) w - w^\top \Phi^\top t + \frac{1}{2} t^\top t + \frac{\lambda}{2} w^\top w$	Collect terms after substitution and include regularization

Step	Equation	Reason
8	$J(a) = \frac{1}{2} a^\top \Phi (\Phi^\top \Phi) \Phi^\top a - a^\top \Phi \Phi^\top t + \frac{1}{2} t^\top t + \frac{\lambda}{2} a^\top \Phi \Phi^\top a$	Substitute $w = \Phi^\top a$ into $J(w)$
9	$K = \Phi \Phi^\top, \quad K_{nm} = \phi(x_n)^\top \phi(x_m)$	Define Gram matrix via matrix multiplication
10	$J(a) = \frac{1}{2} a^\top K^2 a - a^\top K t + \frac{1}{2} t^\top t + \frac{\lambda}{2} a^\top K a$	Final kernelized objective expressed entirely in terms of K

Kernel symmetry (Formula 1)

Step	Equation	Reason
1	$k(x, x') = \phi(x)^\top \phi(x')$	Definition
2	$k(x', x) = \phi(x')^\top \phi(x)$	Swap arguments
3	$k(x, x') = k(x', x)$	Dot-product symmetry: $a^\top b = b^\top a$

Primal to Dual for regularized LS (Formulas 2–8)

Step	Equation	Reason
1	$J(w) = \frac{1}{2} \sum_n (w^\top \phi_n - t_n)^2 + \frac{\lambda}{2} w^\top w$	Given (primal objective)
2	$\nabla_w J = \sum_n (w^\top \phi_n - t_n) \phi_n + \lambda w = 0$	Differentiate w.r.t. w
3	$\lambda w = - \sum_n (w^\top \phi_n - t_n) \phi_n$	Rearrange gradient = 0
4	$w = -\frac{1}{\lambda} \sum_n (w^\top \phi_n - t_n) \phi_n = \sum_n a_n \phi_n$	Define $a_n = -\frac{1}{\lambda} (w^\top \phi_n - t_n)$
5	Substitute $w = \Phi^\top a$ into $J(w) \implies$ $J(a) = \frac{1}{2} a^\top \Phi \Phi^\top \Phi \Phi^\top a - a^\top \Phi \Phi^\top t + \frac{1}{2} t^\top t + \frac{\lambda}{2} a^\top \Phi \Phi^\top a$	Replace w in objective Algebraic expansion
6	Define $K = \Phi \Phi^\top \implies$ replace in $J(a)$	Gram-matrix substitution
7	$J(a) = \frac{1}{2} a^\top K K a - a^\top K t + \frac{1}{2} t^\top t + \frac{\lambda}{2} a^\top K a$	Compact kernel form
8	$\nabla_a J = (K K + \lambda K) a - K t = 0 \implies$ $(K + \lambda I) a = t$	Differentiate w.r.t. a , factor K
9	$a = (K + \lambda I_N)^{-1} t$	Solve linear system

Prediction formula (Formula 9)

Step	Equation	Reason
1	$y(x) = w^\top \phi(x)$	Model prediction
2	$w = \Phi^\top a$	From dual representation
3	$y(x) = a^\top \Phi \phi(x)$	Substitute w
4	$\Phi \phi(x) = k(x)$ with $k(x)_n = k(x_n, x)$	Definition of kernel vector
5	$y(x) = k(x)^\top a = k(x)^\top (K + \lambda I)^{-1} t$	Substitute dual solution for a

Kernel via features (Formula 10)

Step	Equation	Reason
1	$\phi(x) \in \mathbb{R}^M$ with $\phi_i(x)$	Assume M basis functions
2	$k(x, x') = \phi(x)^\top \phi(x') = \sum_{i=1}^M \phi_i(x) \phi_i(x')$	Dot-product expansion

Squared-dot-product kernel (Formulas 11 & 15)

Step	Equation	Reason
1	$k(x, z) = (x^\top z)^2$	Given polynomial kernel
2	Expand: $(x_1 z_1 + x_2 z_2)^2 = x_1^2 z_1^2 + 2x_1 x_2 z_1 z_2 + x_2^2 z_2^2$	Algebraic square
3	Choose $\phi(x) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)^\top$	So that $\phi(x)^\top \phi(z)$ matches above

Special kernels (Formulas 12–14)

Step	Equation	Reason
1	$\phi(x) = x$	Identity mapping
2	$k(x, x') = x^\top x'$	Linear kernel
3	$k(x, x') = k(x - x')$	Stationarity definition
4	$k(x, x') = k(\ x - x'\)$	Homogeneity (radial basis) definition