Kernel Methods

CMSC 173 - Machine Learning

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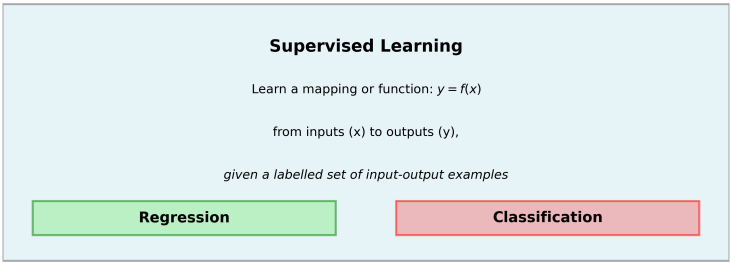
Outline

Review: Supervised Learning Framework

Supervised Learning: Learning from Labeled Examples



Core Concept

Given labeled training data, learn $f : \mathcal{X} \to \mathcal{Y}$.

Regression Tasks

- Continuous output

Classification Tasks

- Discrete labels

Comparison of Supervised Learning Methods

Method	Model	Loss Function
Linear Regression	$y = w^T x + b$	$\sum_{i=1}^{N}(y_i - w^T x_i - b)^2$ Sum-of-squares loss
Logistic Regression	$P(y = 1\|x) = \sigma(w^T x + b)$ $\sigma(z) = \frac{1}{1+e^{-z}}$	$-\sum_{i=1}^{N} y_i \log(\sigma(w^T x_i + b))$ $+(1 - y_i)\log(1 - \sigma(w^T x_i + b))$ Cross-entropy loss
Support Vector Machine	$y = \text{sign}(w^T x + b)$	$\frac{1}{2}\|w\|^2 + C\sum_i \max(0, 1 - y_i(w^T x_i + b))$ Hinge loss + L2 regularization

Today's Focus

We'll explore how **Support Vector Machines** use the **kernel trick** to solve non-linear problems while maintaining computational efficiency.

Introduction & Motivation

What are Kernel Methods?

Definition

Kernel methods are a class of algorithms that use kernel functions to operate in high-dimensional feature spaces without explicitly computing the coordinates in that space.

Key Idea:

- Transform data to higher dimensions where it becomes linearly separable
- Use **kernel trick** to avoid explicit transformation
- Compute inner products efficiently in feature space

Why Kernel Methods?

Many real-world problems are **not linearly separable** in their original feature space.

Common Applications:

- **Classification:** Support Vector Machines
- **Regression:** Support Vector Regression
- **Dimensionality Reduction:** Kernel PCA
- **Clustering:** Kernel K-means

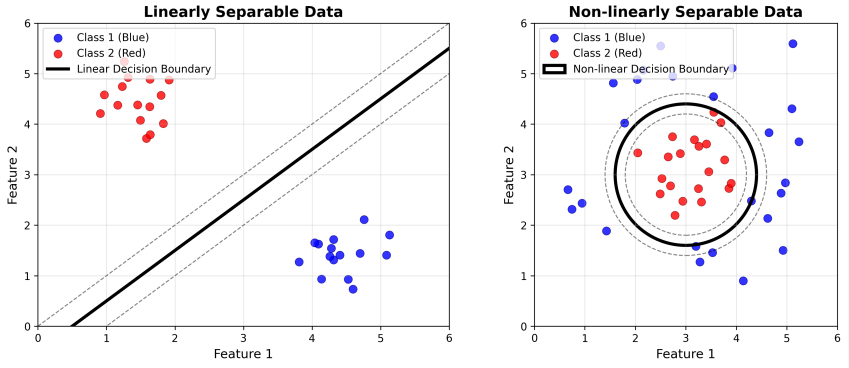
Advantages:

- Handle non-linear relationships
- Computational efficiency via kernel trick
- Strong theoretical foundations
- Flexible and powerful

Examples:

- Image classification
- Text analysis
- Bioinformatics
- Time series analysis

Linear vs Non-linear Separability



Linearly Separable Data

Characteristics:

- Classes form distinct clusters
- Linear boundary separates perfectly
- Decision rule: $w^T x + b = 0$

Advantages:

- Simple and interpretable

Non-linearly Separable Data

Characteristics:

- Complex data patterns (e.g., concentric circles)
- No linear boundary can separate
- Requires non-linear decision boundary

Solution: Kernel Methods

- Transform to higher dimensions

Historical Context: From Perceptron to SVM

Rosenblatt's Perceptron (1957)

The Perceptron Algorithm

Frank Rosenblatt introduced the first learning algorithm for binary classification in 1957.

Perceptron Model:

$$f(x) = \text{sign}(w^T x + b) \tag{1}$$

$$\text{Output} = \begin{cases} +1 & \text{if } w^T x + b \geq 0 \\ -1 & \text{if } w^T x + b < 0 \end{cases} \tag{2}$$

Learning Rule:

$$w^{(t+1)} = w^{(t)} + \eta \cdot y_i \cdot x_i \tag{3}$$

$$b^{(t+1)} = b^{(t)} + \eta \cdot y_i \tag{4}$$

Update only when misclassified

Perceptron Convergence Theorem

If data is linearly separable, the perceptron algorithm will converge to a solution in finite steps.

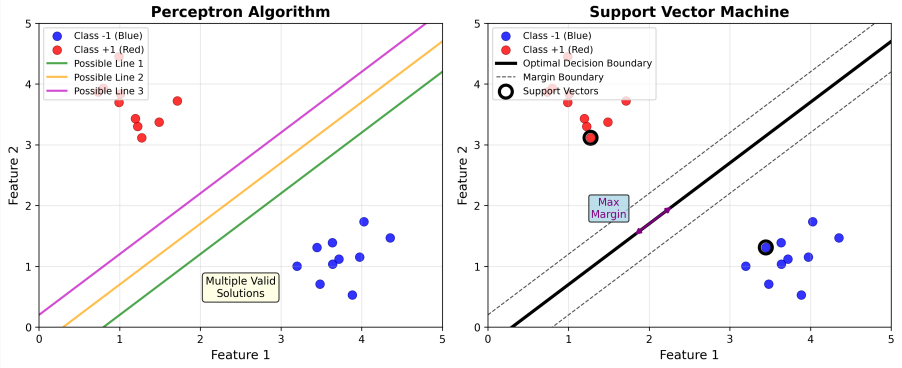
Historical Impact:

- **1957:** Perceptron introduced
- **1969:** Limitations exposed (XOR problem)
- **1980s-1990s:** SVM development
- **Key insight:** Maximum margin principle

Motivation for SVMs:

- Address perceptron limitations
- Better generalization bounds
- Handle non-linearly separable data

Perceptron vs SVM: A Visual Comparison



Perceptron Approach

- **Goal:** Find any separating hyperplane
- **Method:** Iterative weight updates
- **Result:** Multiple valid solutions
- **Issue:** No optimality criterion

SVM Approach

- **Goal:** Find optimal separating hyperplane
- **Method:** Maximize margin width
- **Result:** Unique optimal solution
- **Benefit:** Better generalization

Key Insight

SVMs choose the hyperplane that maximizes the distance to the nearest data points (**support vectors**),

From Linear to Non-linear: Evolution of Ideas

Timeline of Development:

- **1957:** Rosenblatt's Perceptron
- **1969:** Minsky & Papert limitations
- **1979:** Least squares SVM ideas
- **1992:** Boser, Guyon, Vapnik kernel trick
- **1995:** Cortes & Vapnik soft margin
- **1996:** Schölkopf kernel methods

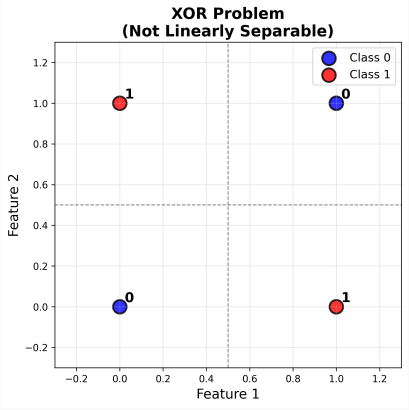
Minsky & Papert (1969)

Showed that perceptrons cannot solve non-linearly separable problems like XOR, leading to the "AI winter."

The Kernel Revolution

The kernel trick (1992) revived interest by enabling non-linear classification while maintaining computational efficiency.

The XOR Problem:



Problem Statement

- Input: $(0,0) \to 0$, $(0,1) \to 1$
- Input: $(1,0) \to 1$, $(1,1) \to 0$
- No linear separator exists

Kernel Solution: Transform to 3D space:

Support Vector Machines

Support Vector Machines: Overview

Core Concept

SVM finds the optimal hyperplane that separates classes with the **maximum margin**.

Key Components:

- **Decision boundary:** Hyperplane separating classes
- **Margin:** Distance between boundary and closest points
- **Support vectors:** Points defining the margin

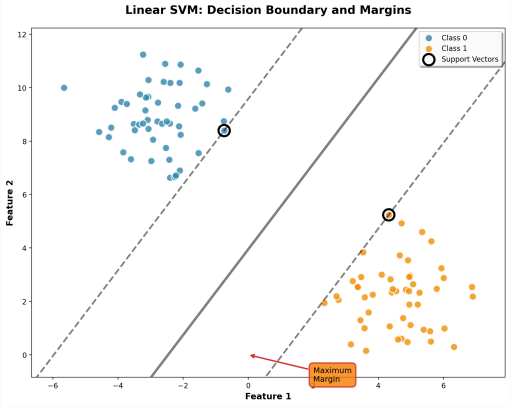
Mathematical Formulation:

$$\text{Hyperplane:} \quad w^T x + b = 0 \tag{5}$$

$$\text{Margin:} \quad \frac{2}{\|w\|} \tag{6}$$

Goal

Maximize margin while correctly classifying all training points.



Why Maximum Margin?

- **Generalization:** Better performance on unseen data
- **Robustness:** Less sensitive to noise
- **Uniqueness:** Single optimal solution

Large-Margin Classifiers

Geometric Interpretation of Margin

Margin Definition:

For a hyperplane $w^T x + b = 0$:

$$\text{Distance from point } x_i \text{ to hyperplane:} \quad (7)$$

$$d_i = \frac{|w^T x_i + b|}{\|w\|} \quad (8)$$

Margin Width:

$$\text{Margin} = \min_i d_i = \frac{1}{\|w\|} \quad (9)$$

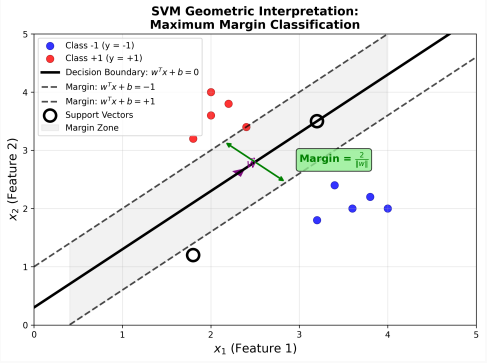
Canonical Form

Scale w and b so that for the closest points:

$$w^T x_i + b = \pm 1$$

Then margin becomes $\frac{2}{\|w\|}$.

Visual Interpretation:



Key Elements

- **Decision boundary:** $w^T x + b = 0$
- **Margin boundaries:** $w^T x + b = \pm 1$
- **Support vectors:** Closest points
- **Margin width:** $\frac{2}{\|w\|}$

Quadratic Optimization Problem

SVM Optimization: Primal Problem

Hard Margin SVM:

Primal Problem

$$\min_{w,b} \quad \frac{1}{2}\|w\|^2 \tag{10}$$

$$\text{subject to} \quad y_i(w^T x_i + b) \geq 1, \quad i = 1, \ldots, n \tag{11}$$

Interpretation:

- **Objective:** Minimize $\|w\|^2 \Rightarrow$ Maximize margin $\frac{2}{\|w\|}$
- **Constraints:** All points correctly classified with margin ≥ 1

Problem Type:

- Quadratic objective function
- Linear constraints
- Convex optimization problem
- Unique global optimum

Soft Margin SVM:

Primal Problem with Slack Variables

$$\min_{w,b,\xi} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n} \xi_i \tag{12}$$

$$\text{subject to} \quad y_i(w^T x_i + b) \geq 1 - \xi_i \tag{13}$$

$$\xi_i \geq 0, \quad i = 1, \ldots, n \tag{14}$$

Slack Variables ξ_i:

- $\xi_i = 0$: Point correctly classified with margin ≥ 1
- $0 < \xi_i < 1$: Point correctly classified but within margin
- $\xi_i \geq 1$: Point misclassified

Regularization Parameter C:

- Large C: Penalty for violations (hard margin)
- Small C: Allow more violations (soft margin)
- Controls bias-variance tradeoff

SVM Optimization: Dual Problem

Lagrangian Formulation:

Lagrangian

$$L = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i \tag{15}$$

$$- \sum_{i=1}^{n}\alpha_i[y_i(w^T x_i + b) - 1 + \xi_i] \tag{16}$$

$$- \sum_{i=1}^{n}\mu_i\xi_i \tag{17}$$

KKT Conditions:

$$\frac{\partial L}{\partial w} = 0 \Rightarrow w = \sum_{i=1}^{n}\alpha_i y_i x_i \tag{18}$$

$$\frac{\partial L}{\partial b} = 0 \Rightarrow \sum_{i=1}^{n}\alpha_i y_i = 0 \tag{19}$$

$$\frac{\partial L}{\partial \xi_i} = 0 \Rightarrow \alpha_i + \mu_i = C \tag{20}$$

Dual Problem:

Dual Formulation

$$\max_{\alpha} \quad \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^T x_j \tag{21}$$

$$\text{subject to} \quad \sum_{i=1}^{n}\alpha_i y_i = 0 \tag{22}$$

$$0 \le \alpha_i \le C, \quad i = 1, \ldots, n \tag{23}$$

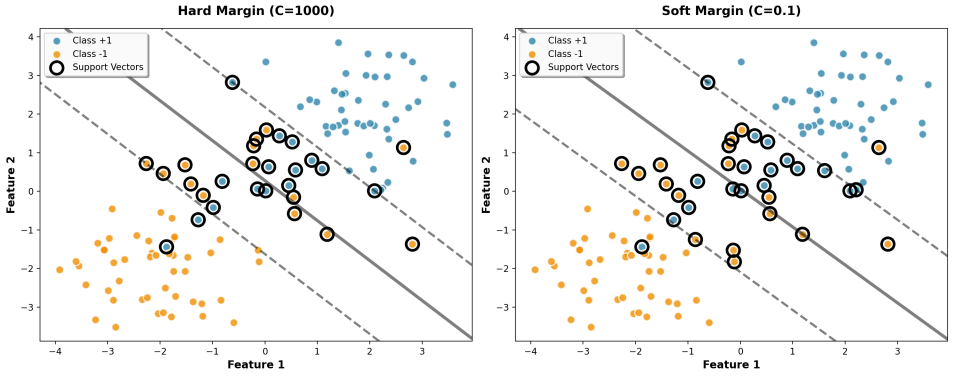
Key Insights:

- Only depends on **inner products** $x_i^T x_j$
- Sparse solution: many $\alpha_i = 0$
- Support vectors: $\alpha_i > 0$

Kernel Trick Preview

Replace $x_i^T x_j$ with $K(x_i, x_j)$ to work in higher dimensions!

Hard vs Soft Margin SVMs



Hard Margin (C = 1000)

- No training errors allowed
- Requires linearly separable data
- May overfit to training data
- Complex decision boundary

Soft Margin (C = 0.1)

- Allows some training errors
- Works with non-separable data
- Better generalization
- Smoother decision boundary

Nonlinear SVM using Kernels

The Kernel Trick

Feature Mapping:

Transform input space $\mathcal{X}$ to feature space $\mathcal{H}$:

$$\phi : \mathcal{X} \to \mathcal{H}$$

Example: Polynomial Features

$$x = (x_1, x_2) \tag{24}$$

$$\phi(x) = (1, x_1, x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2) \tag{25}$$

Kernel Function

Instead of computing $\phi(x_i)^T\phi(x_j)$ explicitly:

$$K(x_i, x_j) = \phi(x_i)^T\phi(x_j)$$

Key Insight

We can compute inner products in high-dimensional space without explicitly mapping to that space!

Computational Advantage:

Without Kernel Trick:

- Map: $\mathcal{O}(d')$ where d' is feature space dimension
- Inner product: $\mathcal{O}(d')$
- Total: $\mathcal{O}(d')$ per pair

With Kernel Trick:

- Direct kernel computation: $\mathcal{O}(d)$ where d is input dimension
- No explicit mapping needed
- Total: $\mathcal{O}(d)$ per pair

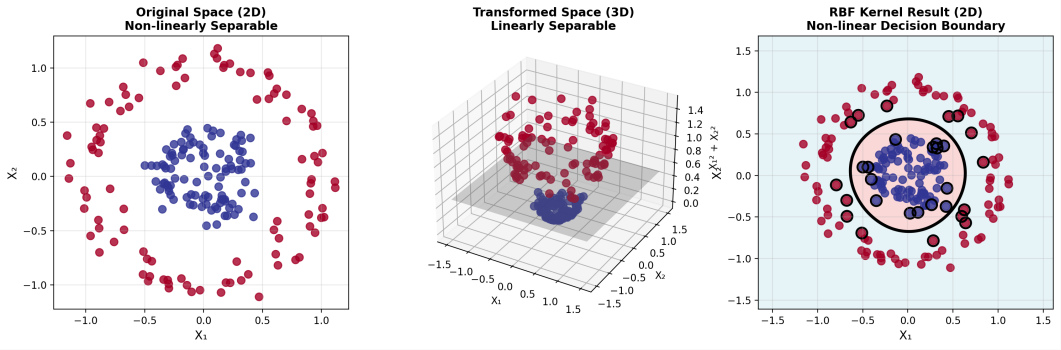
Example: Polynomial Kernel

$$K(x, x') = (x^Tx' + 1)^2 \tag{26}$$

$$= 1 + 2x^Tx' + (x^Tx')^2 \tag{27}$$

This implicitly computes inner product in a $(d+1)(d+2)/2$ dimensional space using only $\mathcal{O}(d)$ operations!

Kernel Trick Visualization



Original Space

Non-linearly separable data in 2D cannot be separated by a straight line.

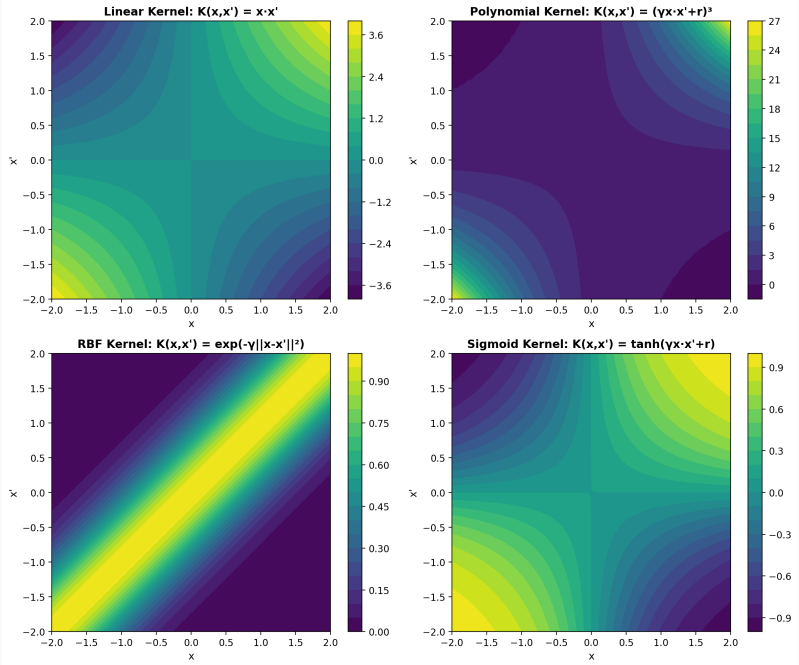
Transformed Space

Data becomes linearly separable in 3D after polynomial transformation $\phi(x) = (x_1, x_2, x_1^2 + x_2^2)$.

Kernel Result

RBF kernel achieves non-linear separation directly in original 2D space.

Common Kernel Functions



Common Kernel Functions: Definitions

Linear Kernel

$$K(x, x') = x^T x'$$

- Equivalent to no transformation
- Fastest computation
- Good baseline

RBF (Gaussian) Kernel

$$K(x, x') = \exp\left(-\gamma \|x - x'\|^2\right)$$

- Most popular kernel
- Infinite-dimensional feature space
- Smooth, localized similarity

Polynomial Kernel

$$K(x, x') = (\gamma x^T x' + r)^d$$

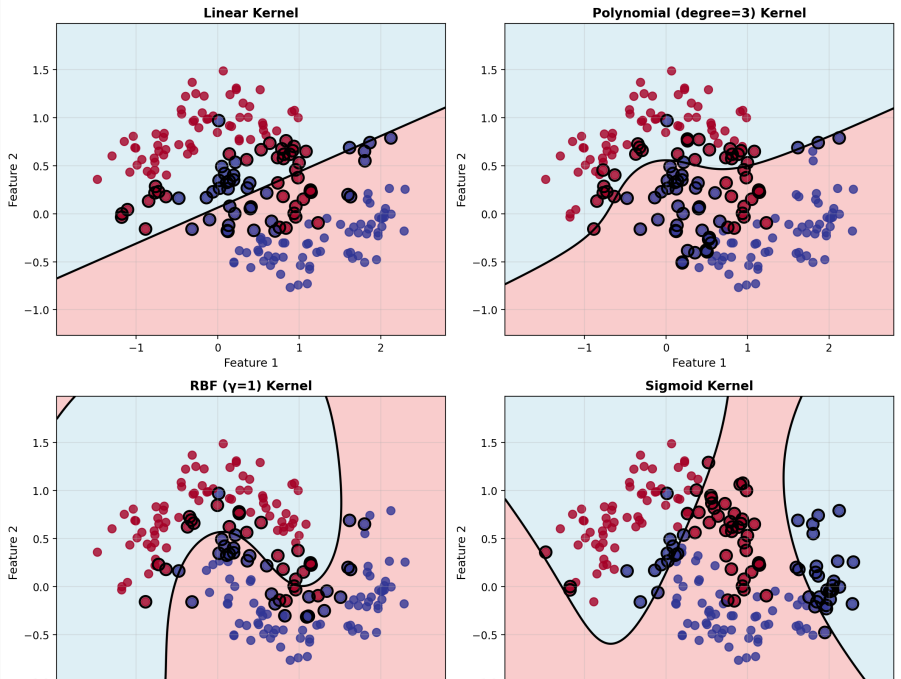
- Captures interactions to degree d
- Parameters: γ, r, d

Sigmoid Kernel

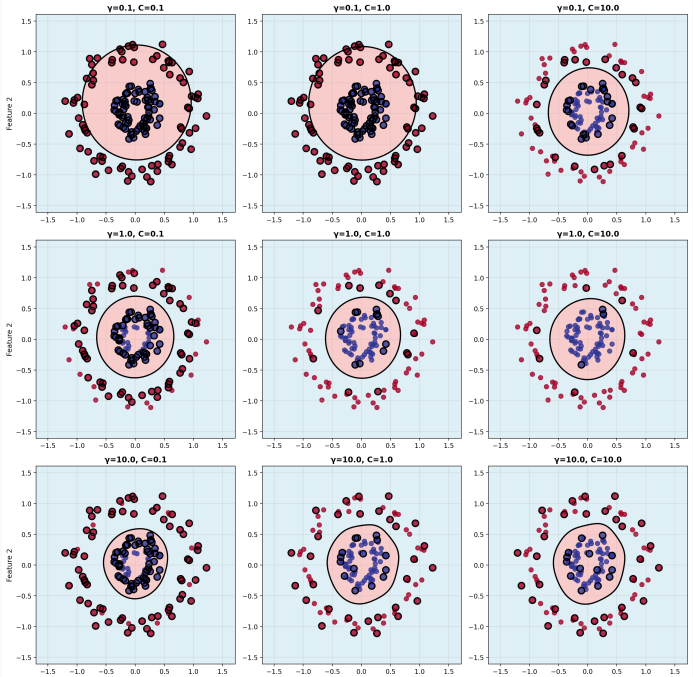
$$K(x, x') = \tanh(\gamma x^T x' + r)$$

- Neural network inspired
- Less commonly used

Comparing Different Kernels



RBF Kernel Parameter Effects



Mercer's Theorem

Mercer's Theorem: Valid Kernels

Mercer's Theorem

A function $K(x, x')$ is a valid kernel (corresponds to an inner product in some feature space) if and only if for any finite set of points $\{x_1, \ldots, x_n\}$, the kernel matrix $\mathbf{K}$ is positive semi-definite.

Kernel Matrix:

$$\mathbf{K}_{ij} = K(x_i, x_j)$$

Positive Semi-definite:

$$\mathbf{K} \succeq 0 \iff \sum_{i,j} c_i c_j K(x_i, x_j) \geq 0$$

for all real numbers $c_1, \ldots, c_n$.

Practical Implication

Not every function can be used as a kernel! Only those satisfying Mercer's condition.

Properties of Valid Kernels:

- **Symmetry:** $K(x, x') = K(x', x)$
- **Positive semi-definiteness:** Kernel matrix $\mathbf{K} \succeq 0$

Constructing New Kernels:

If K_1 and K_2 are valid kernels, then:

$$K(x, x') = K_1(x, x') + K_2(x, x') \tag{28}$$
$$K(x, x') = c \cdot K_1(x, x'), \quad c > 0 \tag{29}$$
$$K(x, x') = K_1(x, x') \cdot K_2(x, x') \tag{30}$$
$$K(x, x') = \exp(K_1(x, x')) \tag{31}$$
$$K(x, x') = f(x) K_1(x, x') f(x') \tag{32}$$

Domain-Specific Kernels:

- String kernels for text
- Graph kernels for networks
- Tree kernels for structured data

Examples of Valid and Invalid Kernels

Valid Kernels:

Linear

$$K(x, x') = x^T x'$$

Polynomial

$$K(x, x') = (x^T x' + 1)^d, \quad d \geq 1$$

RBF/Gaussian

$$K(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right)$$

Exponential

$$K(x, x') = \exp(-\gamma\|x - x'\|), \quad \gamma > 0$$

Why Valid? All can be shown to correspond to inner products in (possibly infinite-dimensional) feature spaces.

Invalid Kernels:

Negative Power

$$K(x, x') = (x^T x')^{-1}$$

Not positive semi-definite.

Logarithmic

$$K(x, x') = \log(x^T x' + 1)$$

Can produce negative eigenvalues.

Checking Validity:

1. **Theoretical:** Prove positive semi-definiteness
2. **Computational:** Check eigenvalues of kernel matrix
3. **Construction:** Build from known valid kernels

Practical Note

Most standard kernels in ML libraries are guaranteed to be valid. Custom kernels need verification.

Multiple Kernel Learning

Multiple Kernel Learning (MKL)

Motivation

Different kernels capture different aspects of data:

- RBF kernel: local similarities
- Linear kernel: global structure
- Polynomial kernel: feature interactions

Idea: Combine multiple kernels to get better performance than any single kernel.

Linear Combination:

$$K(x, x') = \sum_{m=1}^{M} \beta_m K_m(x, x')$$

where $\beta_m \geq 0$ and $\sum_{m=1}^{M} \beta_m = 1$.

Applications:

- Multi-modal data (text + images)
- Feature selection
- Domain adaptation

MKL Optimization:

Joint Optimization

$$\min_{w,b,\xi,\beta} \quad \frac{1}{2} \sum_{m=1}^{M} \frac{\|w_m\|^2}{\beta_m} + C \sum_{i=1}^{n} \xi_i \tag{33}$$

$$\text{subject to} \quad y_i \left(\sum_{m=1}^{M} w_m^T \phi_m(x_i) + b \right) \geq 1 - \xi_i \tag{34}$$

$$\xi_i \geq 0, \quad \beta_m \geq 0, \quad \sum_{m=1}^{M} \beta_m = 1 \tag{35}$$

Solution Methods:

- **Alternating optimization:** Fix β, solve for w; fix w, solve for β
- **Semi-definite programming:** Convex formulation
- **Gradient-based methods:** Efficient for large-scale

Kernel Weight Interpretation:

- β_m close to 1: Kernel m is most important

MKL Example: Combining Kernels

Example Setup:

Consider combining three kernels:

$$K_1(x, x') = x^T x' \quad \text{(Linear)} \tag{36}$$
$$K_2(x, x') = (x^T x' + 1)^2 \quad \text{(Polynomial)} \tag{37}$$
$$K_3(x, x') = \exp(-\|x - x'\|^2) \quad \text{(RBF)} \tag{38}$$

Combined Kernel:

$$K(x, x') = \beta_1 K_1(x, x') + \beta_2 K_2(x, x') + \beta_3 K_3(x, x')$$

Learning Process:

1. Start with equal weights: $\beta_1 = \beta_2 = \beta_3 = \frac{1}{3}$
2. Iteratively optimize weights and SVM parameters
3. Converge to optimal combination

Sample Results:

Kernel	Weight	Accuracy
Linear	0.1	0.78
Polynomial	0.3	0.82
RBF	0.6	0.85
Combined MKL	-	**0.89**

Advantages:

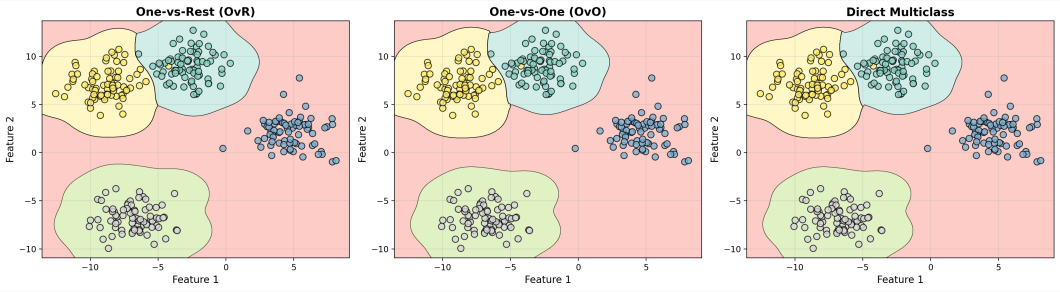
- **Better performance** than individual kernels
- **Automatic selection** of relevant kernels
- **Interpretability** through weights

Challenges:

- Increased computational complexity
- More hyperparameters to tune
- Risk of overfitting with many kernels

Multi-class Classification

Multi-class SVM Strategies



One-vs-Rest (OvR)

- Train k binary classifiers
- Each separates one class from all others
- Prediction: class with highest score

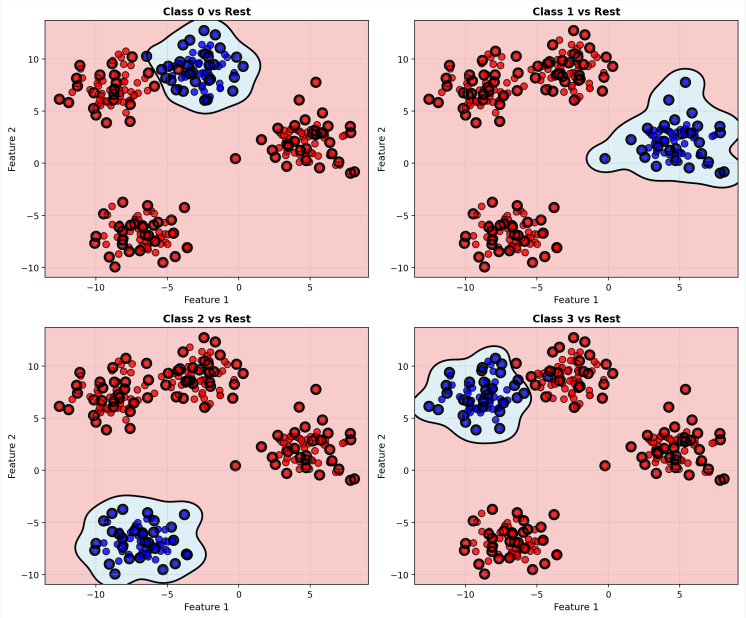
One-vs-One (OvO)

- Train $\binom{k}{2}$ binary classifiers
- Each separates pair of classes
- Prediction: majority voting

Direct Multiclass

- Single optimization problem
- Simultaneous separation
- More complex but unified

One-vs-Rest Detailed Analysis

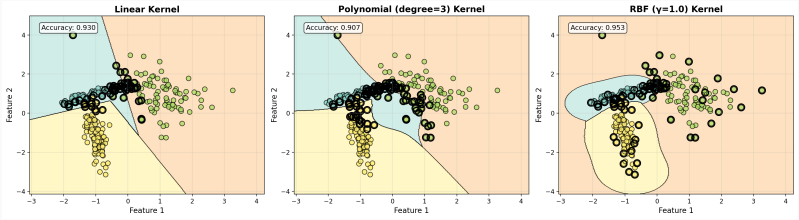


OvR Strategy:

For k classes:

Advantages:

Multi-class Kernel Comparison



Performance:

- **Linear:** High-dim data
- **Polynomial:** Feature interactions
- **RBF:** Most flexible

Selection Criteria:

- Dataset size
- Computational cost
- Cross-validation

Best Practice

Start with RBF kernel and tune C, γ via cross-validation.

Kernel Methods for Regression

Support Vector Regression (SVR)

SVR Concept

Extend SVM to regression by finding a function that deviates from target values by at most ϵ, while being as flat as possible.

Linear SVR:

$$f(x) = w^T x + b$$

Optimization Problem:

$$\min_{w,b,\xi,\xi^*} \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}(\xi_i + \xi_i^*) \tag{39}$$

$$\text{subject to} \quad y_i - w^T x_i - b \leq \epsilon + \xi_i \tag{40}$$

$$w^T x_i + b - y_i \leq \epsilon + \xi_i^* \tag{41}$$

$$\xi_i, \xi_i^* \geq 0 \tag{42}$$

ϵ-insensitive Loss:

$$L_\epsilon(y, f(x)) = \max(0, |y - f(x)| - \epsilon)$$

Key Parameters:

- ϵ: Width of insensitive zone
- C: Regularization parameter
- **Kernel parameters:** γ for RBF, etc.

Dual Formulation:

$$f(x) = \sum_{i=1}^{n}(\alpha_i - \alpha_i^*)K(x_i, x) + b \tag{43}$$

where $\alpha_i, \alpha_i^* \geq 0$ are Lagrange multipliers.

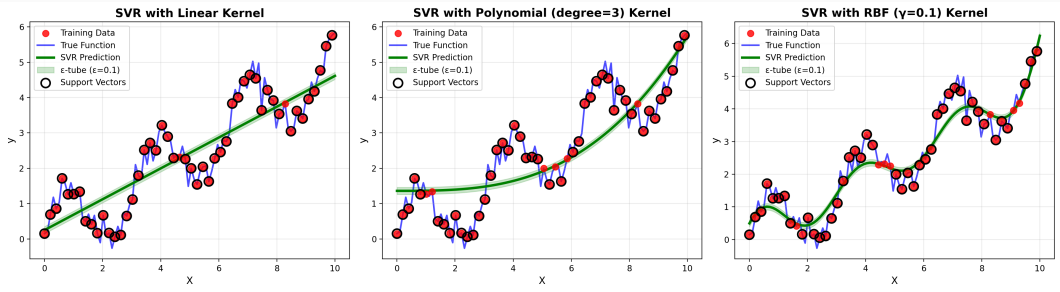
Support Vectors:

- Points outside ϵ-tube
- $\alpha_i > 0$ or $\alpha_i^* > 0$
- Determine the regression function

Sparsity

Many $\alpha_i = \alpha_i^* = 0$, leading to sparse solutions.

SVR Demonstration



Linear SVR

- Simple linear relationship
- Good for linear trends
- Fast computation

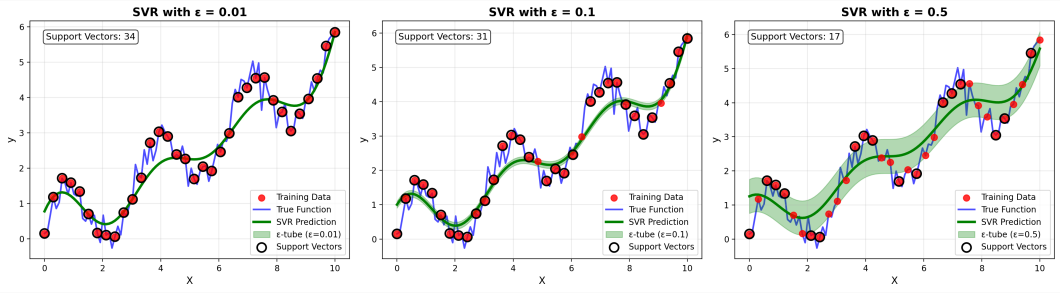
Polynomial SVR

- Captures polynomial trends
- Risk of overfitting
- Degree selection important

RBF SVR

- Most flexible
- Handles non-linear patterns
- Requires parameter tuning

Effect of ϵ Parameter in SVR



ϵ Parameter Effects:

- **Small ϵ (0.01):** Tight fit, many support vectors
- **Medium ϵ (0.1):** Balanced complexity
- **Large ϵ (0.5):** Loose fit, fewer support vectors

Trade-offs:

- **Small ϵ:** Low bias, high variance
- **Large ϵ:** High bias, low variance
- **Sparsity:** Larger $\epsilon \Rightarrow$ fewer support vectors

Selection Guidelines:

- Cross-validation for optimal ϵ
- Consider noise level in data
- Balance accuracy vs complexity

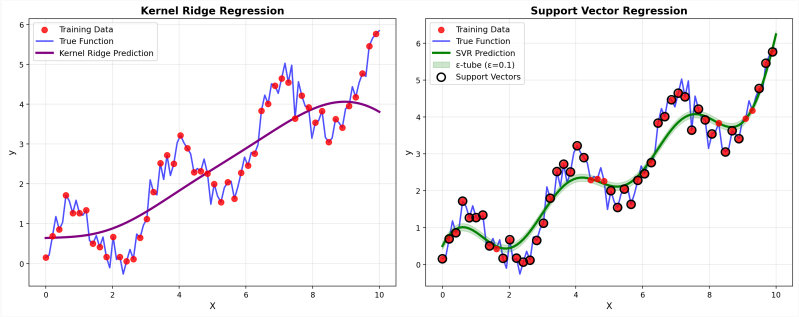
Practical Values:

- Start with $\epsilon = 0.1$
- Scale with target variable range
- Grid search with C and kernel parameters

Rule of Thumb

Support Vector Regression

Kernel Ridge Regression vs SVR



Kernel Ridge Regression vs SVR: Comparison

Kernel Ridge

Objective:

$$\min_{\alpha} \|\mathbf{K}\alpha - y\|^2 + \lambda \alpha^T \mathbf{K}\alpha$$

Solution:

$$\alpha = (\mathbf{K} + \lambda \mathbf{I})^{-1} y$$

Properties:

- Non-sparse
- Closed-form
- Fast for small data

SVR

Objective:

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + C \sum_i (\xi_i + \xi_i^*)$$

Constraints:

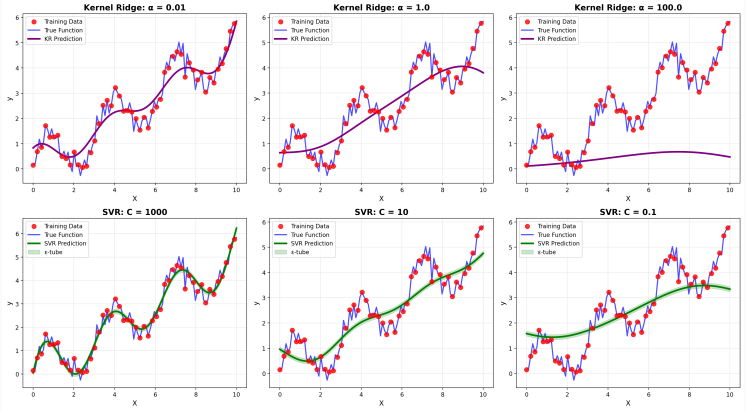
$$|y_i - f(x_i)| \leq \epsilon + \xi_i$$

Properties:

- Sparse (SVs)
- Robust to outliers
- Quadratic program

Kernel Ridge Regression

Regularization in Kernel Regression



Kernel Ridge (α):

- Small: Overfitting risk
- Medium: Balanced
- Large: Underfitting risk

SVR (C):

- High: Complex model
- Medium: Balanced
- Low: Simple model

Relationship: $C \approx \frac{1}{\alpha}$

$$\min_f \sum_i (y_i - f(x_i))^2 + \alpha \|f\|^2$$

Worked Example: RBF Kernel Computation

Problem Setup:

Given two points:

$$x_1 = (1, 2) \tag{44}$$
$$x_2 = (3, 1) \tag{45}$$

Compute RBF kernel with $\gamma = 0.5$:

$$K(x_1, x_2) = \exp(-\gamma \|x_1 - x_2\|^2)$$

Step 1: Compute distance

$$x_1 - x_2 = (1, 2) - (3, 1) = (-2, 1) \tag{46}$$
$$\|x_1 - x_2\|^2 = (-2)^2 + 1^2 = 4 + 1 = 5 \tag{47}$$

Step 2: Apply kernel

$$K(x_1, x_2) = \exp(-0.5 \times 5) \tag{48}$$
$$= \exp(-2.5) \tag{49}$$
$$\approx 0.082 \tag{50}$$

Interpretation:

- Points are moderately far apart
- Kernel value is small (0.082)
- Indicates low similarity

Compare with closer points:

For $x_1 = (1, 2)$ and $x_3 = (1.1, 2.1)$:

$$\|x_1 - x_3\|^2 = (0.1)^2 + (0.1)^2 = 0.02 \tag{51}$$
$$K(x_1, x_3) = \exp(-0.5 \times 0.02) = \exp(-0.01) \tag{52}$$
$$\approx 0.99 \tag{53}$$

Effect of γ:

- Large γ: Rapid decay, local influence
- Small γ: Slow decay, global influence

Key Insight

RBF kernel measures similarity through Euclidean distance in input space.

Practical Implementation Tips

Data Preprocessing:

- **Feature Scaling:** Critical for RBF kernels
- **Normalization:** StandardScaler or MinMaxScaler
- **Missing Values:** Handle before kernel computation

Hyperparameter Tuning:

Grid Search Example

```
param_grid = {
 'C': [0.1, 1, 10, 100],
 'gamma':  [0.001, 0.01, 0.1, 1],
 'kernel':  ['rbf', 'poly', 'linear']
}
```

Performance Considerations:

- Linear kernel: $\mathcal{O}(n \times d)$
- RBF kernel: $\mathcal{O}(n \times d)$ per evaluation
- Training complexity: $\mathcal{O}(n^2)$ to $\mathcal{O}(n^3)$

Model Selection:

1. Start with RBF kernel
2. Use cross-validation
3. Compare with linear kernel
4. Consider computational constraints

Common Pitfalls:

Avoid These

- Forgetting to scale features
- Using default parameters
- Ignoring class imbalance
- Overfitting with complex kernels

Debugging Tips:

- Check kernel matrix properties
- Visualize decision boundaries
- Monitor support vector counts
- Validate on holdout set

Software Libraries:

Parametric vs Non-parametric Models

Understanding Model Types

Parametric Models:

Definition

Fixed number of parameters independent of training set size. Make strong assumptions about functional form.

Examples:

- **Linear Regression:** $f(x) = w^T x + b$
- **Logistic Regression:** $p = \sigma(w^T x + b)$
- **Perceptron:** Fixed decision boundary
- **Neural Networks:** Fixed architecture

Characteristics:

- Fast training and prediction
- Strong inductive bias
- May underfit complex data
- Interpretable parameters

Non-parametric Models:

Definition

Number of parameters grows with training data size. Make minimal assumptions about functional form.

Examples:

- **k-NN:** Stores all training data
- **Decision Trees:** Adaptive structure
- **Kernel Methods:** Support vector representation
- **Gaussian Processes:** Infinite parameters

Characteristics:

- Flexible representation
- Can fit complex patterns
- Risk of overfitting
- Higher computational cost

Kernel Methods: The Non-parametric Perspective

Why SVMs are Non-parametric:

Key Insight

SVM decision function depends on support vectors, whose number grows with data complexity, not fixed in advance.

Decision Function:

$$f(x) = \sum_{i \in SV} \alpha_i y_i K(x_i, x) + b$$

- Number of support vectors $|SV|$ varies
- Complex data $\Rightarrow$ more support vectors
- Simple data $\Rightarrow$ fewer support vectors

Adaptive Complexity:

- Model complexity adapts to data
- Automatic feature selection
- Sparse representation via support vectors

Comparison with Other Methods:

Parametric Linear Classifier

$$f(x) = w^T x + b$$

Fixed $d + 1$ parameters regardless of training set size.

Non-parametric SVM

$$f(x) = \sum_{i=1}^{n_{sv}} \alpha_i y_i K(x_i, x) + b$$

n_{sv} support vectors determined by data.

Benefits of Non-parametric Approach:

- **Flexibility:** No assumptions about decision boundary shape
- **Universality:** Can approximate any function (with appropriate kernel)
- **Robustness:** Less sensitive to model specification

Kernel Functions and Function Spaces

Reproducing Kernel Hilbert Space (RKHS):

Mathematical Framework

Kernel K defines an infinite-dimensional feature space $\mathcal{H}$ where linear methods become non-linear in original space.

Key Properties:

$$\phi : \mathcal{X} \to \mathcal{H} \tag{54}$$

$$K(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}} \tag{55}$$

Universal Approximation:

- RBF kernels are universal approximators
- Can represent any continuous function
- Given sufficient training data

Non-parametric Power

Kernel methods can learn arbitrarily complex decision boundaries without specifying the form in advance.

Practical Implications:

Model Selection Strategy:

- **Start Simple:** Linear kernel first
- **Add Complexity:** Polynomial $\rightarrow$ RBF
- **Cross-validate:** Choose optimal kernel and parameters

Trade-offs:

Parametric Advantage

- Fast training and prediction
- Lower memory requirements
- Better interpretability

Non-parametric Advantage

- Higher representational power
- Better fit to complex data
- Fewer modeling assumptions

When to Use Kernel Methods:

- Non-linear relationships in data

Summary and Key Takeaways

Core Concepts Learned:

- **Kernel Trick:** Implicit high-dimensional mapping
- **Support Vectors:** Sparse representation
- **Margin Maximization:** Generalization principle
- **Non-linear Separation:** Via kernels

Main Algorithms:

- **SVM:** Classification with maximum margin
- **SVR:** Regression with ϵ-insensitive loss
- **Kernel Ridge:** Regularized regression
- **Multi-class:** Extensions to multiple classes

Key Kernels:

- Linear, Polynomial, RBF, Sigmoid
- Mercer's theorem for validity
- Multiple kernel learning

Practical Guidelines:

When to Use Kernel Methods

- Non-linear relationships in data
- Need for sparse solutions
- Strong theoretical guarantees required
- Medium-sized datasets

Parameter Selection:

- **C:** Start with 1.0, tune via CV
- γ: Start with $\frac{1}{\text{n\_features}}$
- ϵ: Start with 0.1 for SVR

Limitations:

- Computational complexity: $\mathcal{O}(n^2)$ to $\mathcal{O}(n^3)$
- Memory requirements: Store kernel matrix
- Parameter sensitivity
- Not suitable for very large datasets

Next Steps

Explore deep learning for automatic feature learning