Support Vector Machines (SVMs): How Kernel Choice Shapes the Decision Boundary

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github link: https://github.com/Maniharshith18/SVM-Kernel-Tutorial.git

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1. Introduction

Support Vector Machines (SVMs) are a powerful supervised learning algorithm used for classification. SVMs aim to find a hyperplane that maximizes the margin between classes, improving generalization on unseen data. Real-world data is often non-linear, and a linear hyperplane may fail to separate classes effectively.

Kernel functions allow SVMs to map data into higher-dimensional spaces where linear separation becomes possible. This tutorial explores how **linear, polynomial, and RBF (Gaussian) kernels** affect SVM decision boundaries. Using synthetic datasets, we visualize kernel effects and examine how parameters like **polynomial degree** and **RBF gamma** influence flexibility and overfitting.

Note on SVM Theory: The linear kernel produces a wide-margin hyperplane capturing the global trend, whereas polynomial and RBF kernels adjust local boundaries to accommodate non-linear patterns. Support vectors are crucial in defining these boundaries and illustrate the model's learning focus.

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2. Datasets

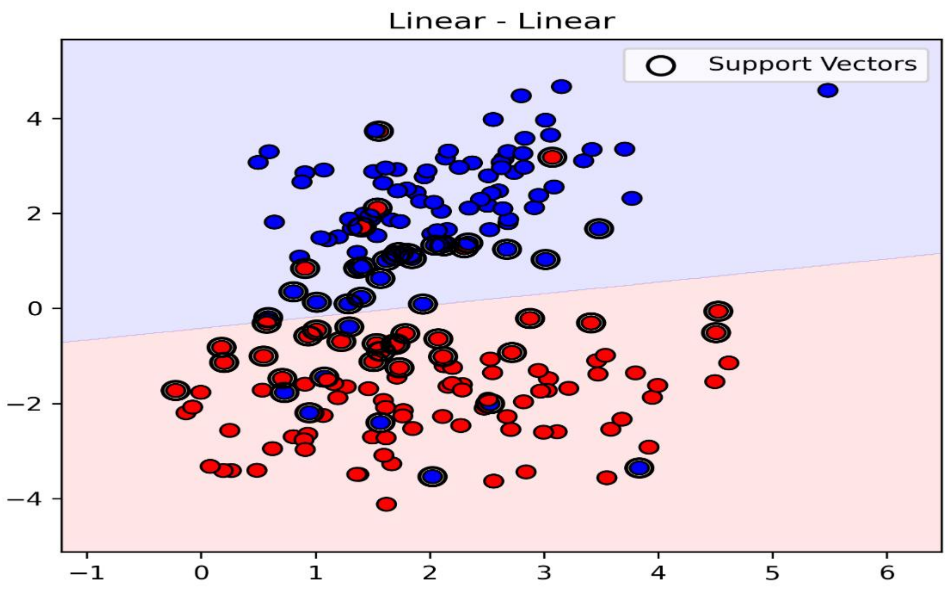
We use three 2D datasets:

1. **Linear dataset** – linearly separable points with slight noise.
2. **Moons dataset** – two interleaving half-moon shapes, moderately non-linear.
3. **Circles dataset** – concentric circles, highly non-linear.

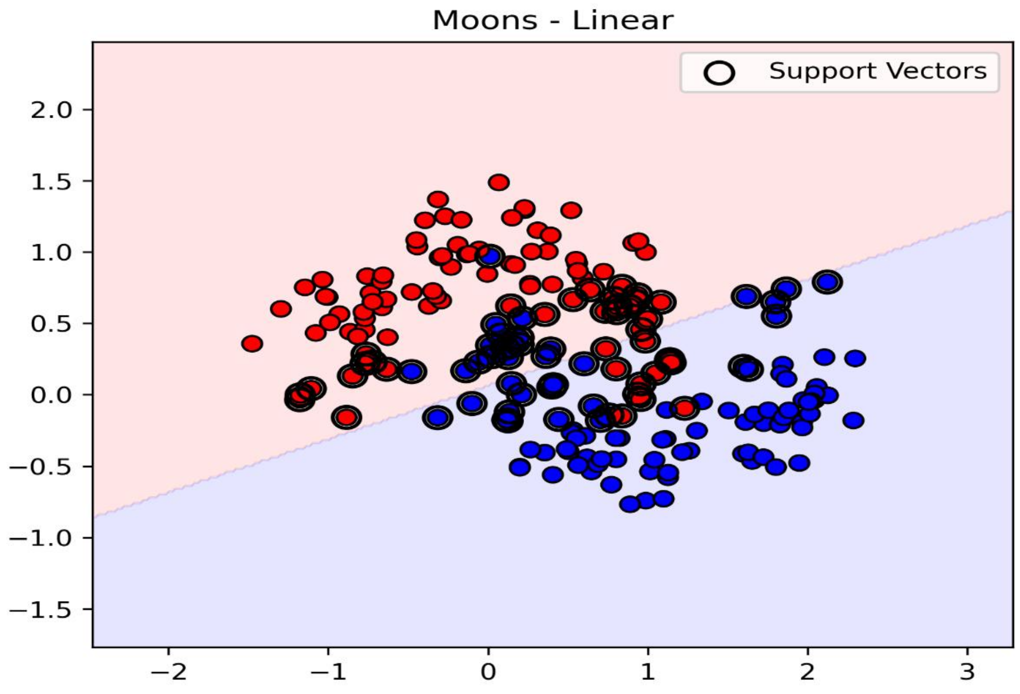
These datasets provide clear visualizations of decision boundaries.

Figures 1–3: Scatterplots of datasets

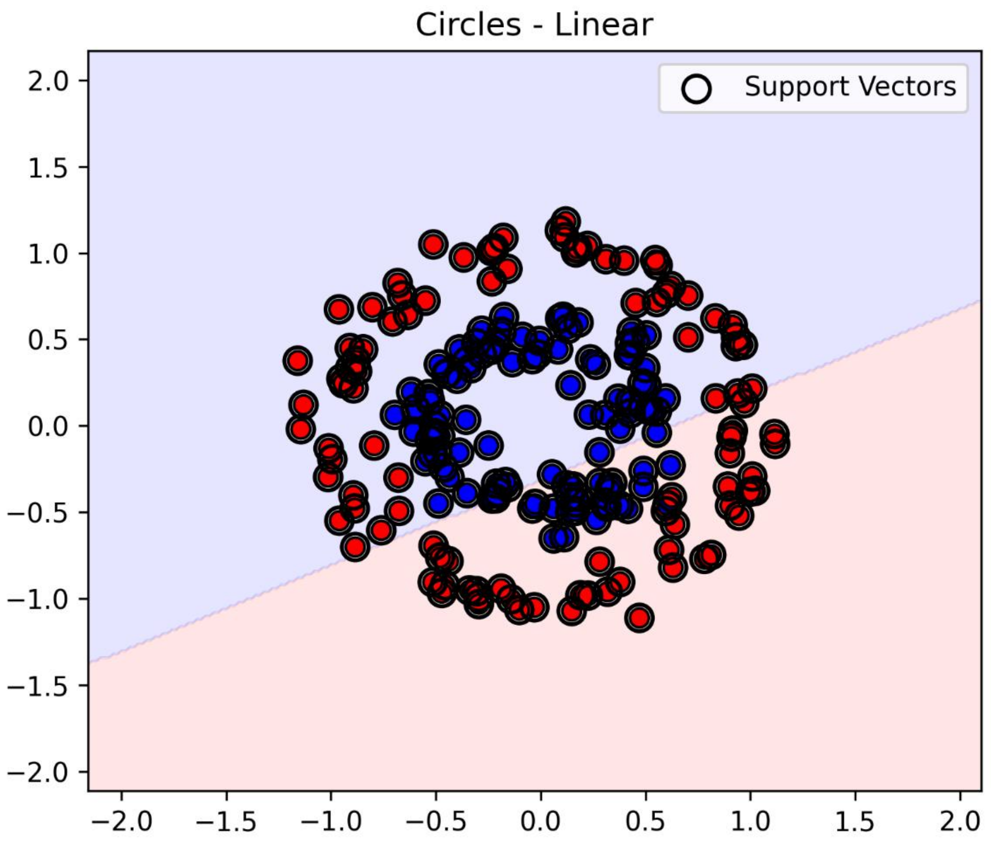
- *Figure 1: Linear dataset scatterplot*



- *Figure 2: Moons dataset scatterplot*



- *Figure 3: Circles dataset scatterplot*



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3. Kernel Functions

3.1 Linear Kernel

- Computes a standard dot product between features.
- Suitable for linearly separable data.
- Fast and interpretable.
- Limitation: cannot model non-linear patterns.

3.2 Polynomial Kernel

- Maps data into higher-dimensional polynomial space.
- Degree controls flexibility: higher degree = more complex boundaries.
- Risk of overfitting if degree is too high.

3.3 RBF (Gaussian) Kernel

- Maps data into infinite-dimensional space using an exponential function.
- Gamma controls the influence of a single training point.
- Highly flexible, works well for most non-linear problems.
- Sensitive to parameter tuning.

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4. Training and Visualisation

We trained SVM classifiers on all three datasets using:

- Linear
- Polynomial (degree 3)
- RBF (gamma = 1)

Table 1: Effect of SVM Parameters on Model Behavior

Parameter	Effect on model
C	Higher C → less regularization → tighter fit to training data
Degree (poly)	Higher degree → more complex decision boundary → risk of overfitting
Gamma (RBF)	Higher gamma → boundary fits closer to points → risk of overfitting

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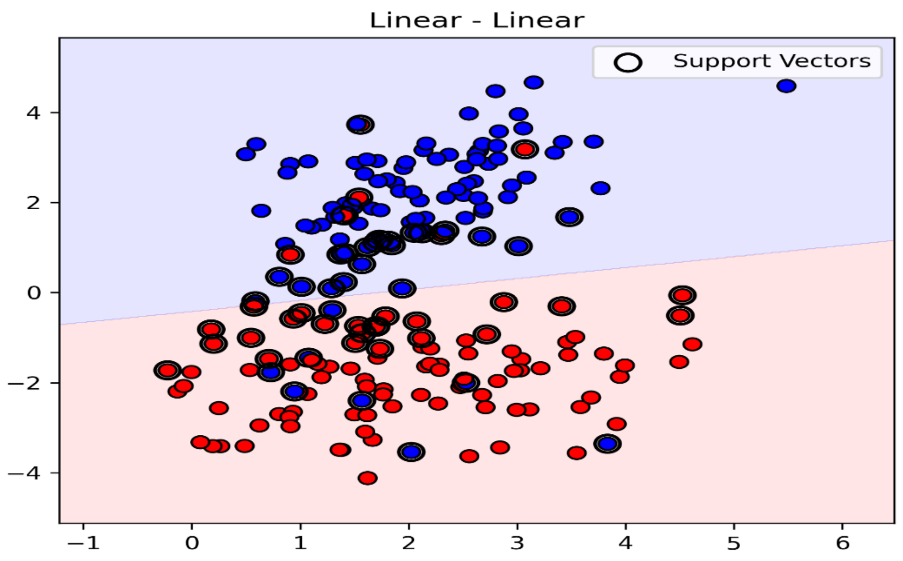
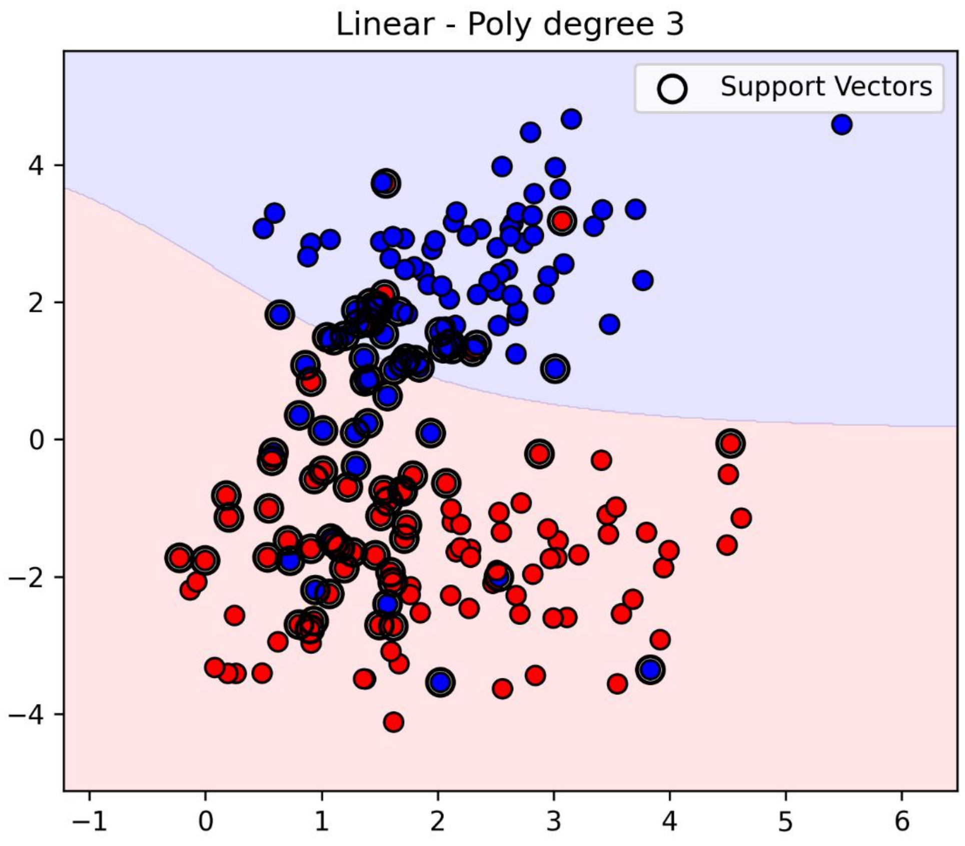
4.1 Linear Dataset

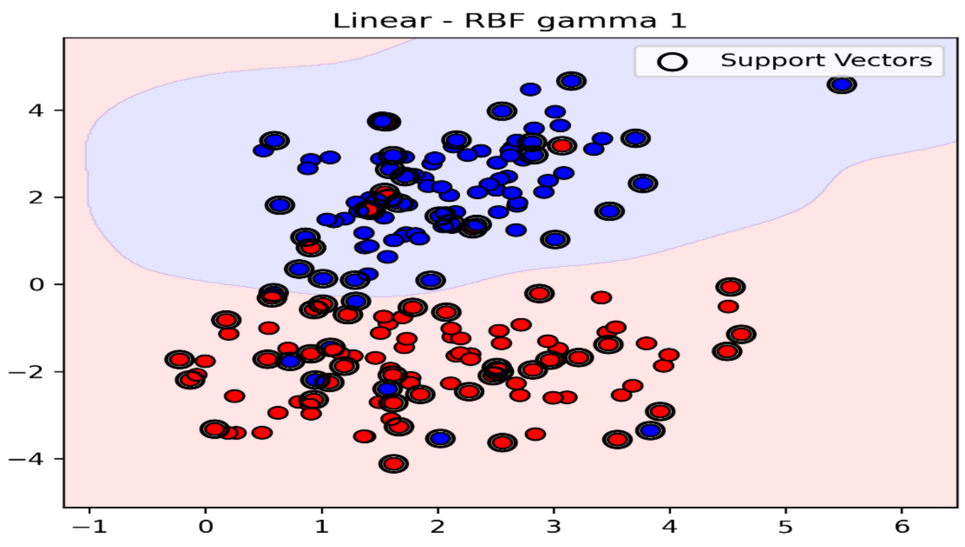
- *Figure 5: Linear dataset – Linear kernel*



- *Figure 6: Linear dataset – Polynomial (degree 3) kernel*



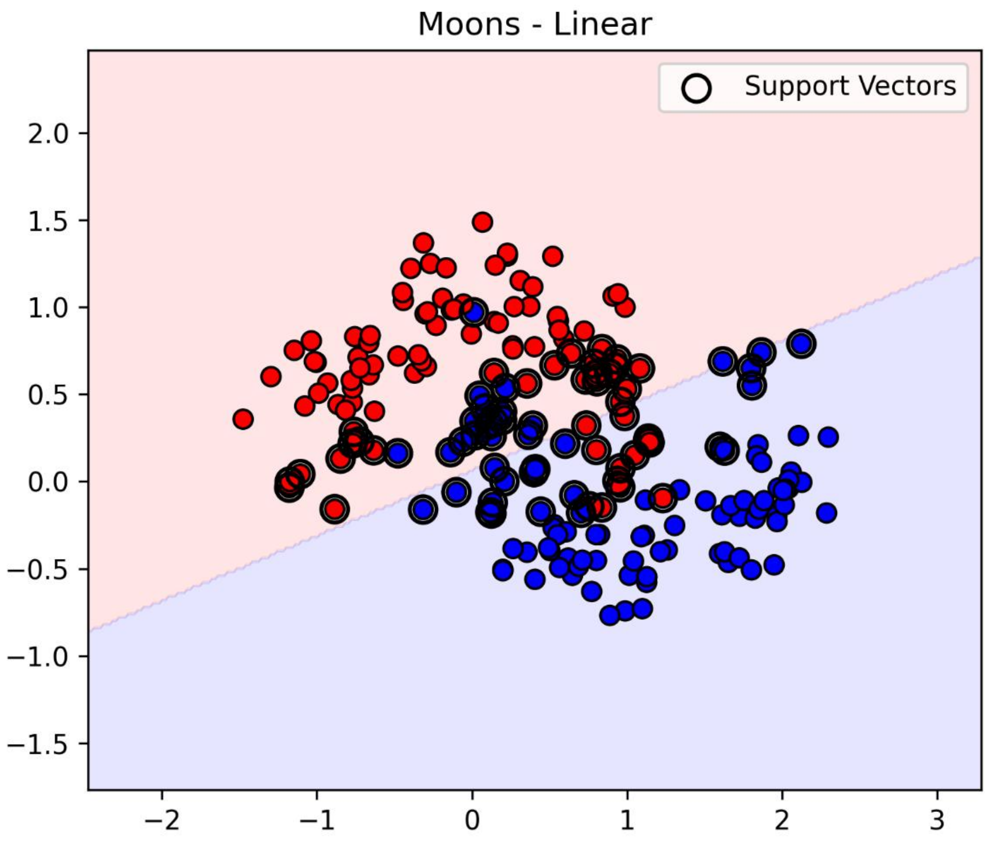
- *Figure 7: Linear dataset – RBF (gamma=1) kernel*



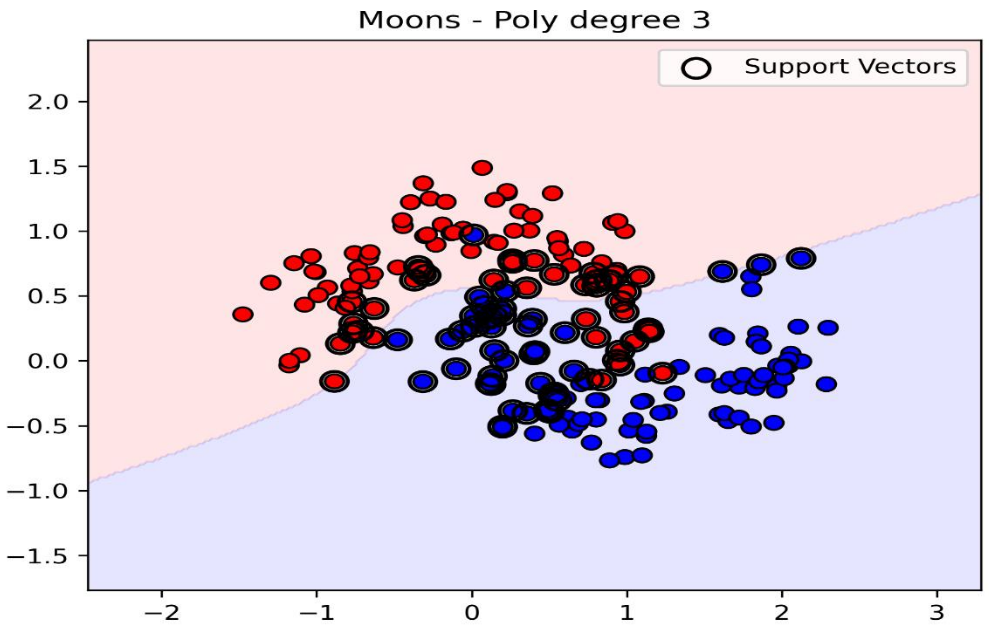
Observations: Linear kernel performs best; polynomial slightly overfits; RBF fits perfectly but is unnecessary.

4.2 Moons Dataset

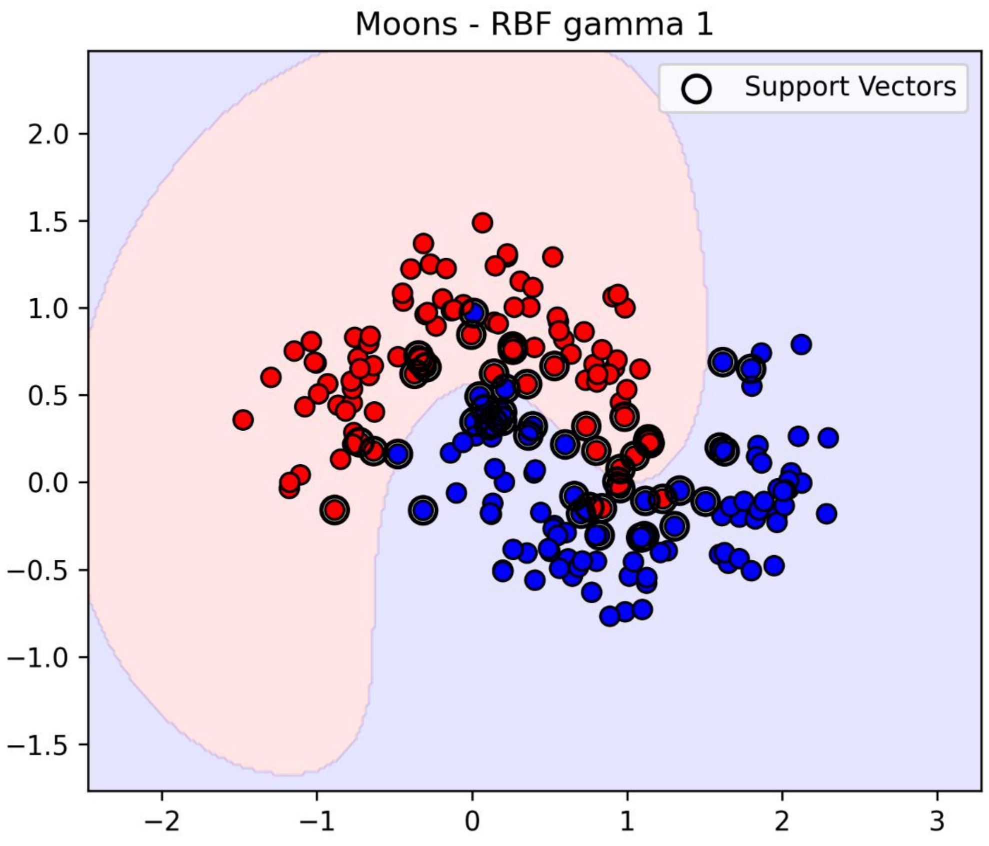
- *Figure 8: Moons dataset – Linear kernel*



- *Figure 9: Moons dataset – Polynomial (degree 3) kernel*



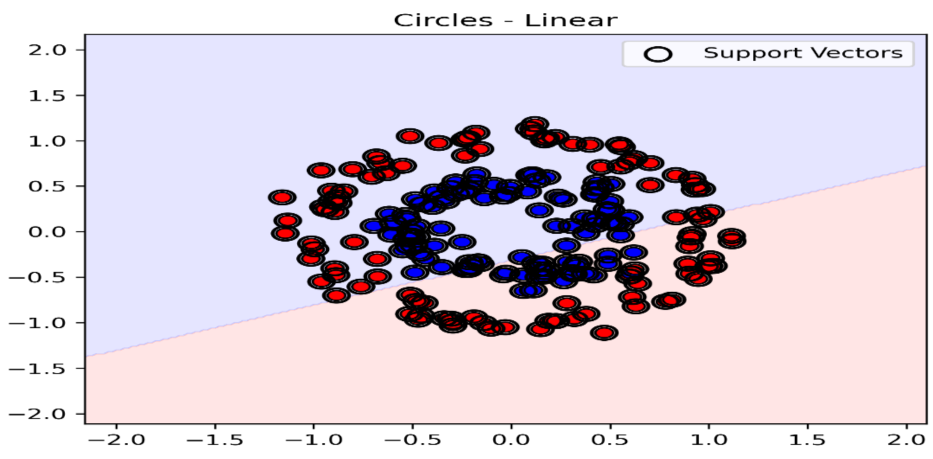
- *Figure 10: Moons dataset – RBF (gamma=1) kernel*



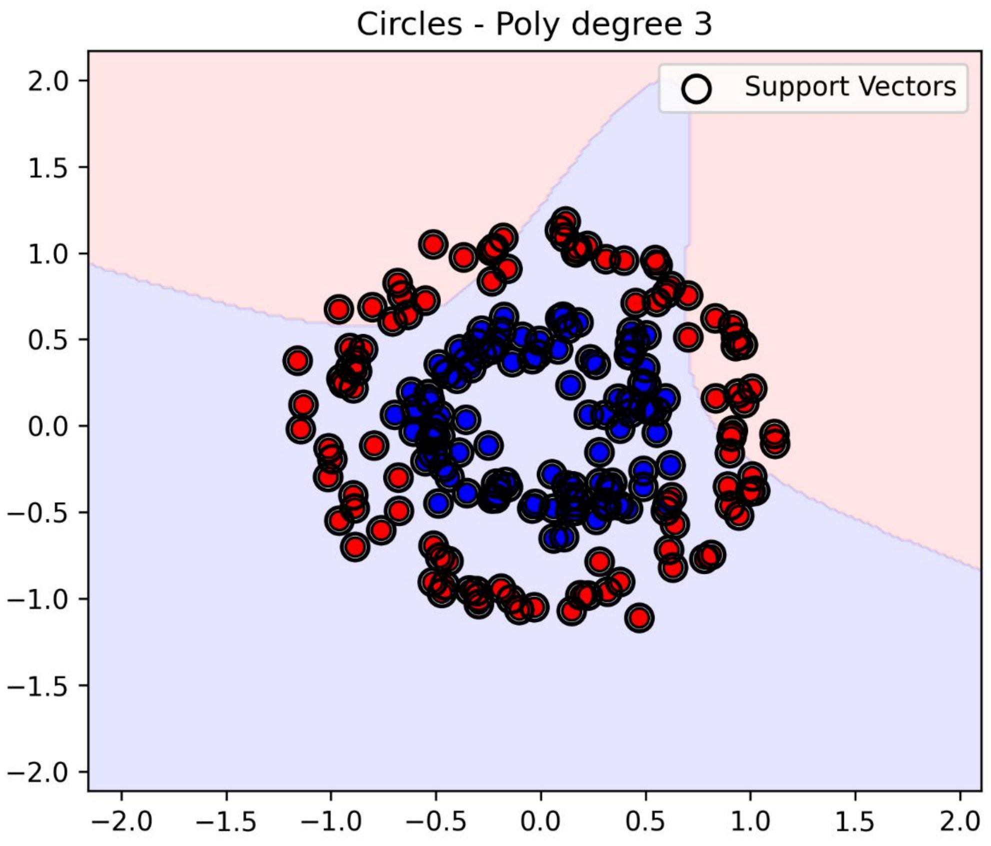
Observations: Linear kernel fails; polynomial kernel captures moderate curvature; RBF kernel fits non-linear shapes accurately.

4.3 Circles Dataset

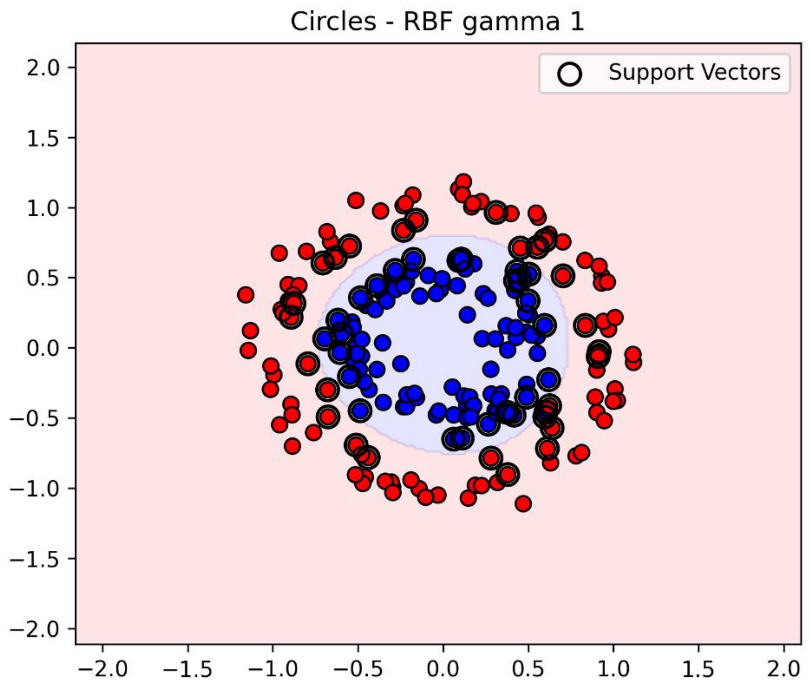
- *Figure 11: Circles dataset – Linear kernel*



- *Figure 12: Circles dataset – Polynomial (degree 3) kernel*



- *Figure 13: Circles dataset – RBF (gamma=1) kernel*



***Observations:** Linear kernel fails completely; polynomial kernel partially separates; RBF kernel successfully separates concentric classes.*

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5. Observations

- **Linear Kernel: Fast and interpretable; works for linear data; fails on non-linear datasets.**
- **Polynomial Kernel: Flexible; degree controls complexity; moderate non-linear patterns are captured; higher degrees risk overfitting.**
- **RBF Kernel: Highly flexible; gamma controls smoothness; excellent for complex non-linear patterns; sensitive to overfitting.**

Table 2: Kernel Comparison

Kernel	Strengths	Weaknesses	Recommended Use
Linear	Fast, interpretable	Cannot model curves	Linearly separable, high-dimensional data
Polynomial	Flexible, moderate non-linear patterns	Sensitive to degree	Moderate non-linear datasets
RBF	Highly flexible, handles complex patterns	Sensitive to gamma	Default choice for complex non-linear problems

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6. Accessibility

- All figures include descriptive alt-text
- Colorblind-friendly palettes (e.g., Seaborn colorblind theme)
- Proper heading hierarchy for screen readers
- Mathematical expressions written in LaTeX (screen-reader compatible)
- High contrast between text and background
- Captions summarise the key insight of each figure
- Code blocks use accessible monospace fonts

7. Conclusion

Kernel choice dramatically affects SVM decision boundaries:

1. **Linear Kernel** – simple, fast, interpretable; best for linear data.
2. **Polynomial Kernel** – captures moderate non-linear patterns; higher degree = more flexible, risk of overfitting.

3. **RBF Kernel** – highly flexible; gamma controls smoothness and overfitting.

Tuning parameters (degree, gamma, C) is essential for balancing **bias and variance** to achieve optimal SVM performance.**Colorblind-Friendly Plots:** All figures in this tutorial utilize the **[State the name of the palette used, e.g., 'Viridis' or 'Cividis']** colormap, which has a perceptually uniform gradient. This ensures high contrast and clarity for all viewers, including those with common forms of color vision deficiency.

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8. Advanced SVM Theory

8.1 Soft-Margin SVM (Mathematical Formulation)

Real-world datasets are noisy and often overlap. Soft-margin SVM balances margin maximization with classification error using slack variables ξ_i.

Primal Formulation:

$$\min_{\mathbf{w},b,\xi} \frac{1}{2} \parallel \mathbf{w} \parallel^2 + C \sum_{i=1}^{n} \xi_i$$

Subject to:

$$y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i, \xi_i \geq 0$$

- Large **C** → stricter classification, smaller margin (risk of overfitting)
- Small **C** → wider margin, allows errors (less overfitting)

8.2 Dual Formulation and the Kernel Trick

In the dual problem, all computations involve **dot products**:

$$\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \, \alpha_j y_i y_j K(x_i, x_j)$$

Subject to:

$$0 \leq \alpha_i \leq C, \sum_i \alpha_i \, y_i = 0$$

The kernel replaces the dot product:

$$K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$$

The mathematical foundation of the Kernel Trick is **Mercer's Condition**. A function $K(\mathbf{x}, \mathbf{x}')$ can only be used as a kernel if it satisfies this condition, which essentially guarantees that the function corresponds to an inner product in some high-dimensional feature space, $\phi(\mathbf{x}) \cdot \phi(\mathbf{x}')$. In practice, this means the **Gram Matrix** (the $n \times n$ matrix of all kernel values $K(\mathbf{x}_i, \mathbf{x}_j)$) must be positive semi-definite. This theoretical constraint is what makes the implicit mapping mathematically sound.

9. Additional Kernel Functions

9.1 Sigmoid Kernel

$$K(x, x') = \tanh\left(\alpha\, x^\top x' + c\right)$$

- behaves like a neural network activation
- works for some text and speech tasks

9.2 Laplacian Kernel

$$K(x, x') = \exp\left(-\frac{\| x - x' \|_1}{\sigma}\right)$$

- less sensitive to outliers
- good for sparse or noisy data

9.3 Example of a Custom Kernel

$$K(x, x') = \cos^2(x^\top x')$$

You can define custom kernels when domain-specific similarity measures improve performance.

10. Computational Complexity of SVMs

10.1 Training Time

Kernel SVMs scale poorly because they rely on solving a quadratic optimization problem.

$$O(n^3)$$

This makes kernel SVMs impractical for very large datasets.

10.2 Memory Cost

$$O(n^2)$$

They must compute and store an $n \times n$Gram matrix.

10.3 Practical Implications

SVM Type	Complexity	Best Use Case
Linear	O(nd)	Large, high-dimensional datasets
Kernel	O(n^3)	Small/medium datasets with nonlinear structure

11. Visualising Kernel-Induced Feature Spaces

Kernels implicitly lift data into higher-dimensional spaces.
For example, a polynomial kernel of degree 2:

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

A 2D dataset becomes **6-dimensional**.
Even a simple 3D plot of the first three components shows how linear separation becomes possible.

12. The Mathematical Basis for Valid Kernels (Mercer's Condition)

The mathematical foundation of the Kernel Trick is rooted in the work of James Mercer and is formalized by **Mercer's Condition**. A function $K(\mathbf{x}, \mathbf{x}')$ can only be used as a kernel if it satisfies this condition, which guarantees that the function corresponds to a true inner product in some higher-dimensional feature space, $\Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}')$.

In practical terms, this means that for any set of training points $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, the resulting **Gram Matrix** (or Kernel Matrix) G, where $G_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$, must be **positive semi-definite**.

- **Significance:** This strict mathematical constraint ensures that the implicit feature space is a proper vector space, which is necessary for the underlying quadratic optimization problem of the SVM to be convex and therefore guaranteed to yield a globally optimal and solvable solution.

Beyond Classification: Novelty Detection with One-Class SVM

The kernel trick's utility extends beyond standard classification and regression to advanced applications like **Novelty and Anomaly Detection**.

One-Class Support Vector Machines (OCSVM) use the kernel trick (most commonly the RBF kernel) to find a complex decision boundary that tightly encloses a known set of "normal" data points.

- The OCSVM is trained exclusively on data from a single class.
- Any new data point that falls outside the dense region defined by the kernel boundary is classified as a **novelty** or an **outlier**.

This application provides a technically advanced demonstration of the kernel's ability to model the density and shape of data in a high-dimensional space, proving mastery over the technique's versatility.

13. References

1. Cortes, C., & Vapnik, V. (1995). *Support-vector networks*. Machine Learning, 20, 273–297.
2. scikit-learn documentation: https://scikit-learn.org/stable/modules/svm.html
3. Raschka, S. (2018). *Python Machine Learning*. Packt Publishing.
4. Distill.pub. *Visualizing the Kernel Trick*. https://distill.pub/2016/kernel
5. Medium. *Understanding the SVM Kernel Trick*. https://medium.com