

Support Vector Machine for Surrogate Modeling

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What is SVR?

- Support Vector Regression is the regression form of Support Vector Machines (SVMs). A kernel-based machine learning model that can approximate highly nonlinear functions. Works well even with small-to-medium datasets, making it ideal for engineering simulations.
- SVR can learn a mapping from design variables to simulation output.
- Used when dataset sizes are moderate (100–5000 samples).
- **Core Idea:** SVR fits a hyperplane (higher dim. "line") to the data while ensuring all errors are within a specified margin ϵ .

Finding the hyperplane

Objective: Find a function $f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + b$ that fits the data well, while minimizing the model complexity.

- **Optimization Problem:**

$$\min_{\mathbf{w}, b, \xi_i, \xi_i^*} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*)$$

- **Subject to Constraints:**

$$y_i - f(\mathbf{x}_i) \leq \epsilon + \xi_i$$

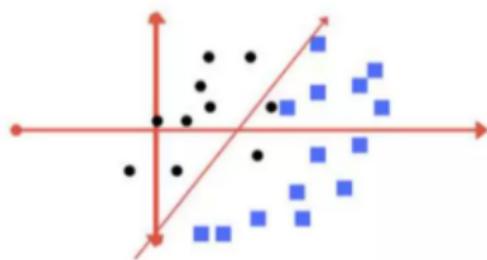
$$f(\mathbf{x}_i) - y_i \leq \epsilon + \xi_i^*$$

$$\xi_i, \xi_i^* \geq 0$$

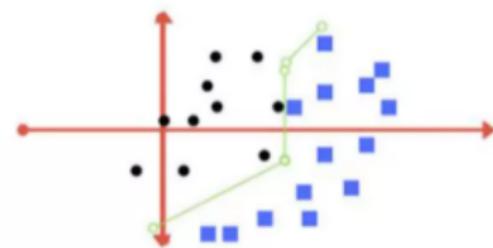
- **The Kernel Trick:** Allows operating in a high-dimensional feature space without explicitly computing the coordinates, handling non-linear relationships: $\mathbf{x} \cdot \mathbf{y} \rightarrow K(\mathbf{x}, \mathbf{y})$.

Key Hyper-parameters for SVR

- **Regularization Penalty (C):** Trade-off between model flatness and error tolerance.



low regularization value



high regularization value

- Low $C \rightarrow$ smoother model, more error tolerance
- High $C \rightarrow$ tighter fit, less error tolerance

Key Hyper-parameters for SVR

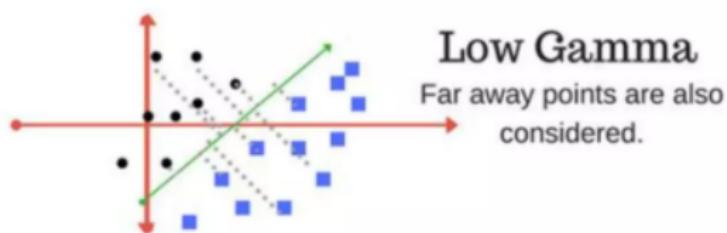
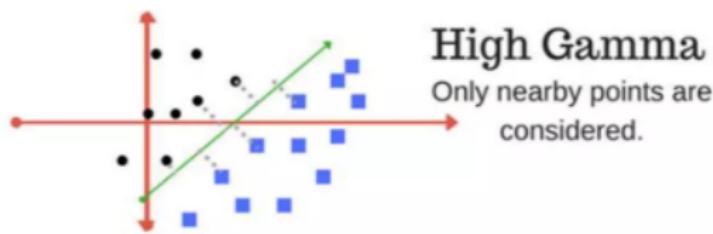
- **Kernel Choice:** Dependent upon the problem we are trying to solve – RBF should work for us.

$$K(\mathbf{X}_i, \mathbf{X}_j) = \begin{cases} \mathbf{X}_i \cdot \mathbf{X}_j & \text{Linear} \\ (\gamma \mathbf{X}_i \cdot \mathbf{X}_j + C)^d & \text{Polynomial} \\ \exp(-\gamma |\mathbf{X}_i - \mathbf{X}_j|^2) & \text{RBF} \\ \tanh(\gamma \mathbf{X}_i \cdot \mathbf{X}_j + C) & \text{Sigmoid} \end{cases}$$

- Allow SVR to approximate complex FEM response surfaces
- Control flexibility vs overfitting

Key Hyper-parameters for SVR

- **Kernel Coefficient (γ):** (specifically for RBF) Controls the influence of a single training example.



SVR as a Surrogate Model: Pros & Cons

Advantages

- **Robustness:** Insensitive to outliers due to the ϵ -tube.
- **High-Dimensional Data:** Works very well in high-dimensional spaces using the Kernel trick.
- **Efficiency:** The complexity is independent of the input space dimension.

Disadvantages

- **Computationally Expensive:** Training ($O(N^2)$ - $O(N^3)$) and hyperparameter optimization are expensive.
- **Lacks built-in uncertainty quantification** and is harder to interpret than simpler models.