Machine Learning (CE 40717)

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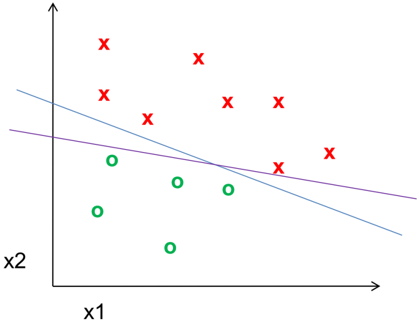
Support Vector Machines (SVMs)

- Developed in the 1990s by Vapnik and colleagues at Bell Labs, grounded in statistical learning theory.
- Remained one of the most widely used learning techniques until the resurgence of deep learning.
- Key aspects that make SVMs particularly interesting:
  - **Strong generalization capabilities**, including margin maximization and structural risk minimization.
  - Extension to non-linear classifiers through the use of **kernel functions**.
  - A **dual formulation** that reveals how linear classifiers can be interpreted as a weighted combination of training examples.
  - Optimization via **stochastic gradient descent (SGD)**, which is also widely used in training neural networks.

What is the Best Linear Classifier?

- **Logistic Regression**
  - Maximizes the expected likelihood of the label given the data.
  - Every training example contributes to the overall loss.
- **Support Vector Machine (SVM)**
  - Ensures that all examples are classified with at least a minimal level of confidence.
  - Bases its decision on a minimal subset of examples, known as **support vectors**.



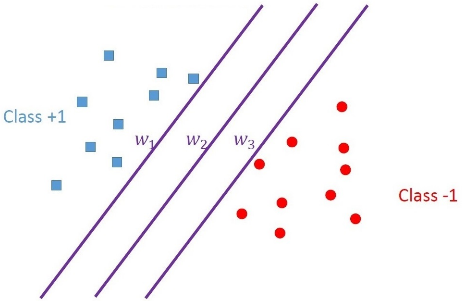
Multiple Optimal Solutions?

- Given training data $\{(\mathbf{x}_i, y_i) : 1 \leq i \leq n\}$ drawn i.i.d. from distribution D.
- Hypothesis:

$$y = \text{sign}(f_{\mathbf{w}}(\mathbf{x})) = \text{sign}(\mathbf{w}^\top \mathbf{x})$$

  - $y = +1$ if $\mathbf{w}^\top \mathbf{x} > 0$
  - $y = -1$ if $\mathbf{w}^\top \mathbf{x} < 0$

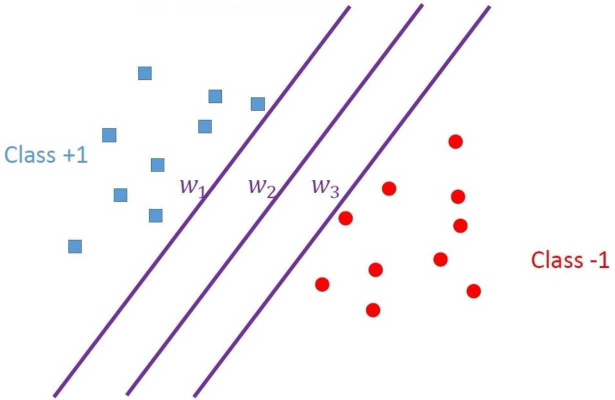
- Let's assume that we can optimize to find $\mathbf{w}$.



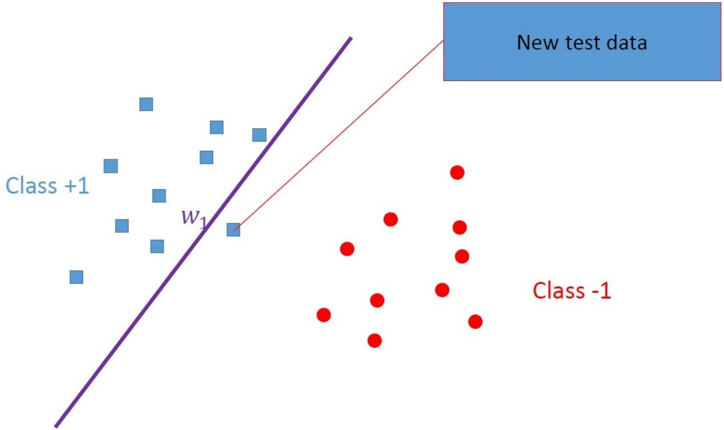
Same empirical loss,
different test/expected loss.

What Is a Better Linear Separation?

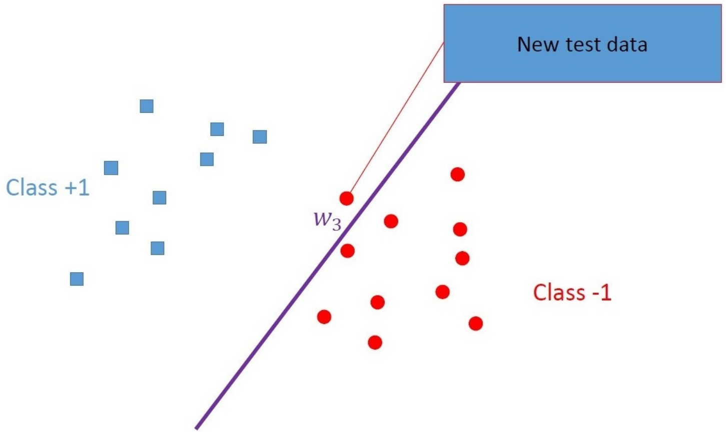
Which Separator Would You Choose?



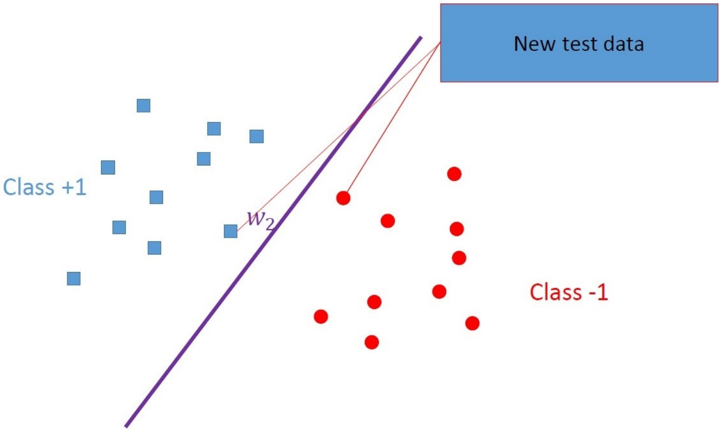
What Is a Better Linear Separation?



What Is a Better Linear Separation?

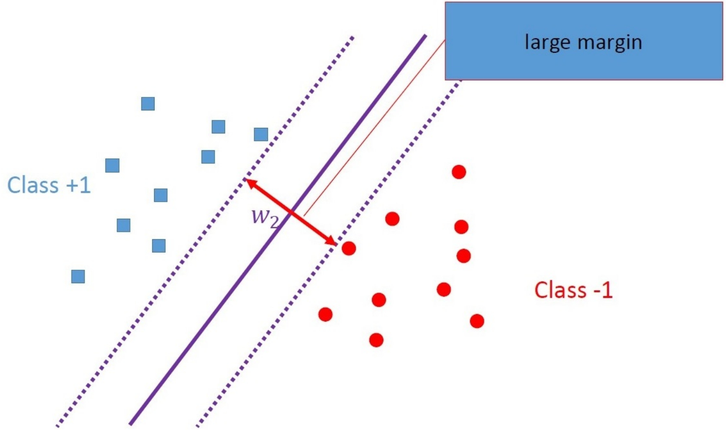


What Is a Better Linear Separation?

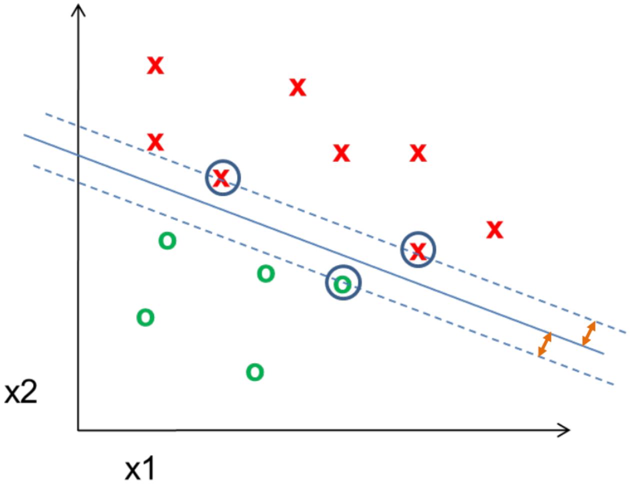


What Is a Better Linear Separation?

Larger margins lead to better generalization on unseen data.



SVM Terminology

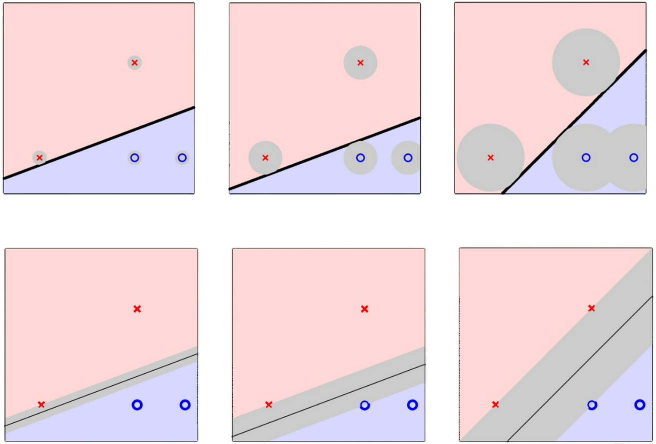


Margin: the smallest distance between any training observation and the hyperplane (orange double-headed arrow).

Support Vector: a training observation whose distance to the hyperplane is equal to the margin (circled).

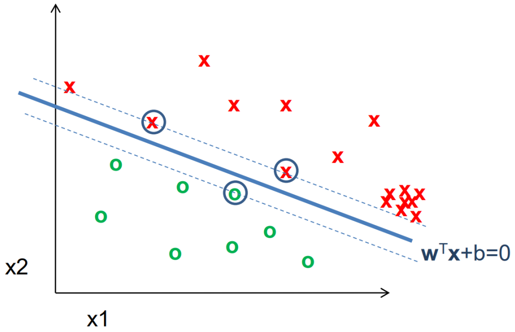
Fat Hyperplane

We refer to such hyperplanes as **fat hyperplanes.**



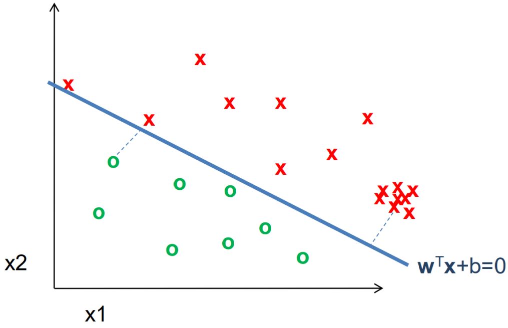
SVMs Minimize $\mathbf{w}^\top\mathbf{w}$ While Preserving a Margin of 1

Optimized SVM



The decision boundary depends only on the support vectors (circled).

Optimized Linear Logistic Regression



It minimizes the sum of the logistic error across all samples, so the boundary tends to lie farther from dense regions.

Why Is It Called a Support Vector?

- **Support**: the maximal-margin hyperplane depends only on these specific training observations.
- **Vector**: each point represents a vector in the p-dimensional feature space.

If the support vectors are perturbed, the maximal-margin hyperplane will change.

If other training observations are perturbed (provided they are not moved within the margin distance of the hyperplane), the maximal-margin hyperplane remains unaffected.

Finding $\mathbf{w}$ with a Large Margin

Let $\mathbf{x}_n$ be the nearest data point to the hyperplane:

$$\mathbf{w}^\top \mathbf{x} = 0.$$

How far is it? Two preliminary technicalities:

- **Normalize w:**

$$\left|\mathbf{w}^\top \mathbf{x}_n\right| = 1.$$

- **Separate the bias term** b:

$$\mathbf{w} = (w_1, \ldots, w_d)$$

apart from b.
The hyperplane can now be written as:

$$\mathbf{w}^\top \mathbf{x} + b = 0.$$

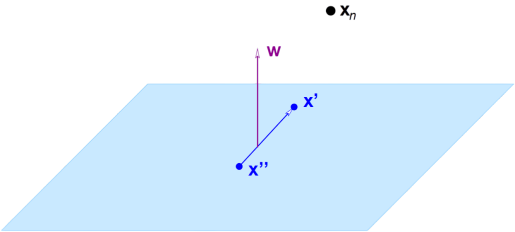
Computing the Distance

The distance between $\mathbf{x}_n$ and the hyperplane $\mathbf{w}^\top\mathbf{x} + b = 0$, where $\left|\mathbf{w}^\top\mathbf{x}_n + b\right| = 1$, is given as follows.

The vector $\mathbf{w}$ is *orthogonal* to the hyperplane in the feature space $\mathcal{X}$.

Consider two points $\mathbf{x}'$ and $\mathbf{x}''$ lying on the hyperplane:

$$\mathbf{w}^\top\mathbf{x}' + b = 0 \quad \text{and} \quad \mathbf{w}^\top\mathbf{x}'' + b = 0 \Longrightarrow \quad \mathbf{w}^\top(\mathbf{x}' - \mathbf{x}'') = 0.$$

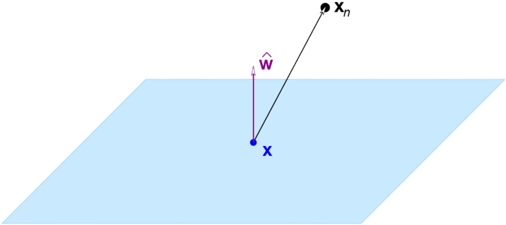


And the Distance Is ...

The distance between $\mathbf{x}_n$ and the hyperplane can be derived as follows. Take any point $\mathbf{x}$ lying on the hyperplane. The distance is the projection of the vector $(\mathbf{x}_n - \mathbf{x})$ onto $\mathbf{w}$:

$$\hat{\mathbf{w}} = \frac{\mathbf{w}}{\|\mathbf{w}\|} \quad \Longrightarrow \quad \text{distance} = |\hat{\mathbf{w}}^\top (\mathbf{x}_n - \mathbf{x})|.$$

$$\text{distance} = \frac{1}{\|\mathbf{w}\|}|\mathbf{w}^\top \mathbf{x}_n - \mathbf{w}^\top \mathbf{x}| = \frac{1}{\|\mathbf{w}\|}|\mathbf{w}^\top \mathbf{x}_n + b - \mathbf{w}^\top \mathbf{x} - b| = \frac{1}{\|\mathbf{w}\|}.$$



The Optimization Problem

$$\begin{array}{rl} \text{Maximize} & \frac{1}{\|\mathbf{w}\|} \\ \text{subject to} & \min_{n=1,2,\dots,N} |\mathbf{w}^\top \mathbf{x}_n + b| = 1. \end{array}$$

Note: $|\mathbf{w}^\top \mathbf{x}_n + b| = y_n(\mathbf{w}^\top \mathbf{x}_n + b)$

Equivalent Formulation

$$\begin{array}{rl} \text{Minimize} & \frac{1}{2}\mathbf{w}^\top \mathbf{w} \\ \text{subject to} & y_n(\mathbf{w}^\top \mathbf{x}_n + b) \geq 1, \quad \text{for } n = 1, 2, \dots, N. \\ & \mathbf{w} \in \mathbb{R}^d, \quad b \in \mathbb{R}. \end{array}$$

Next step: Introduce Lagrange multipliers. Since the constraints are inequalities, the **KKT conditions** apply.

Lagrangian Formulation

We define the Lagrangian function as:

$$\mathscr{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}^\top\mathbf{w} - \sum_{n=1}^{N} \alpha_n\big(y_n(\mathbf{w}^\top\mathbf{x}_n + b) - 1\big),$$

to be minimized with respect to $\mathbf{w}$ and b, and maximized with respect to each $\alpha_n \geq 0$.

Taking derivatives:

$$\nabla_{\mathbf{w}}\mathscr{L} = \mathbf{w} - \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n = 0,$$

$$\frac{\partial \mathscr{L}}{\partial b} = -\sum_{n=1}^{N} \alpha_n y_n = 0.$$

Substituting into the Lagrangian

Using the KKT optimality conditions:

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n, \qquad \sum_{n=1}^{N} \alpha_n y_n = 0,$$

we substitute these into the primal Lagrangian:

$$\mathscr{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}^\top \mathbf{w} - \left(\sum_{n=1}^{N} \alpha_n y_n \mathbf{w}^\top \mathbf{x}_n + \sum_{n=1}^{N} \alpha_n y_n b - \sum_{n=1}^{N} \alpha_n \right).$$

Now insert the optimal value of **w**:

$$\mathscr{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}^\top \mathbf{w} - \left(\mathbf{w}^\top \mathbf{w} + 0 - \sum_{n=1}^{N} \alpha_n \right).$$

Substituting into the Lagrangian

Simplifying:

$$\mathcal{L}(\boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}^\top\mathbf{w} - \mathbf{w}^\top\mathbf{w} + \sum_{n=1}^{N}\alpha_n.$$

Thus the dual becomes:

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\mathbf{w}^\top\mathbf{w}, \qquad \mathbf{w} = \sum_{n=1}^{N}\alpha_n y_n \mathbf{x}_n.$$

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}\alpha_n\alpha_m y_n y_m \mathbf{x}_n^\top\mathbf{x}_m.$$

The Solution: Quadratic Programming

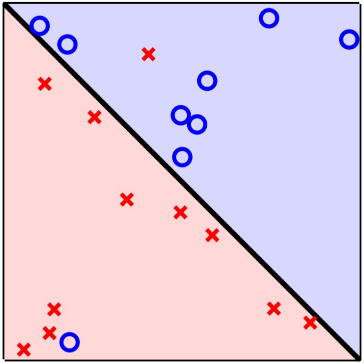
The dual optimization problem can be expressed as a standard quadratic program:

$$\min_{\boldsymbol{\alpha}} \ \frac{1}{2}\boldsymbol{\alpha}^\top \begin{bmatrix} y_1 y_1 \mathbf{x}_1^\top \mathbf{x}_1 & y_1 y_2 \mathbf{x}_1^\top \mathbf{x}_2 & \dots & y_1 y_N \mathbf{x}_1^\top \mathbf{x}_N \\ y_2 y_1 \mathbf{x}_2^\top \mathbf{x}_1 & y_2 y_2 \mathbf{x}_2^\top \mathbf{x}_2 & \dots & y_2 y_N \mathbf{x}_2^\top \mathbf{x}_N \\ \vdots & \vdots & \ddots & \vdots \\ y_N y_1 \mathbf{x}_N^\top \mathbf{x}_1 & y_N y_2 \mathbf{x}_N^\top \mathbf{x}_2 & \dots & y_N y_N \mathbf{x}_N^\top \mathbf{x}_N \end{bmatrix} \boldsymbol{\alpha} + (-\mathbf{1})^\top \boldsymbol{\alpha},$$

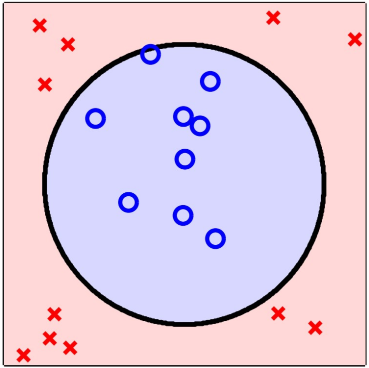
subject to

$$\mathbf{y}^\top \boldsymbol{\alpha} = 0, \quad \text{and} \quad \boldsymbol{\alpha} \geq \mathbf{0}.$$

Non-Separable Data

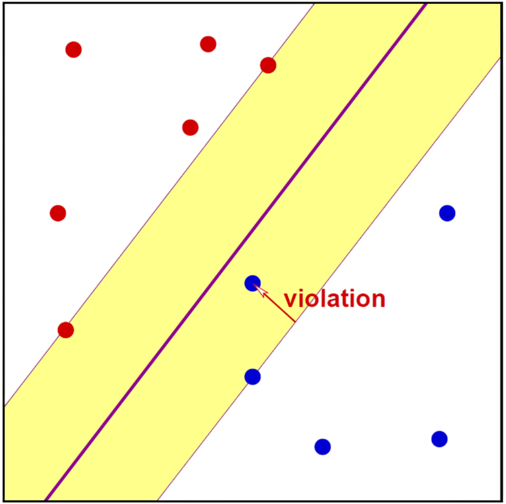


Allow Some Classification Error
(Tolerate error)



Apply a Nonlinear Transformation

Margin Violation



Introducing Slack Variables

Margin violation occurs when:

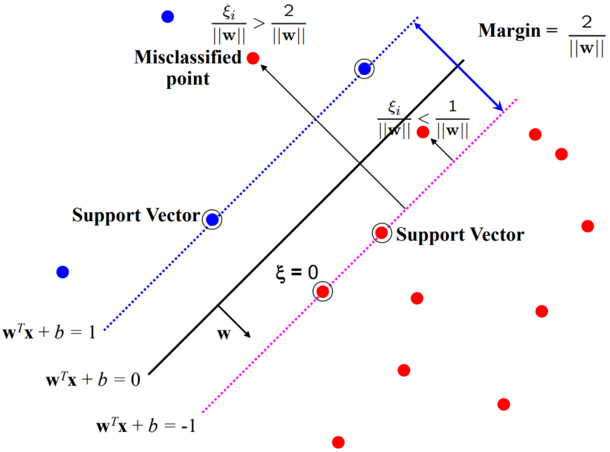
$$y_n(\mathbf{w}^\top \mathbf{x}_n + b) \geq 1$$

fails to hold.
To quantify this violation:

$$y_n(\mathbf{w}^\top \mathbf{x}_n + b) \geq 1 - \xi_n, \quad \xi_n \geq 0.$$

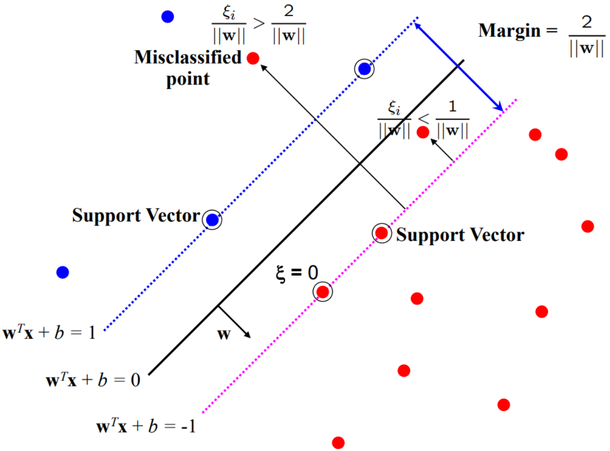
The total violation is:

$$\sum_{n=1}^{N} \xi_n.$$

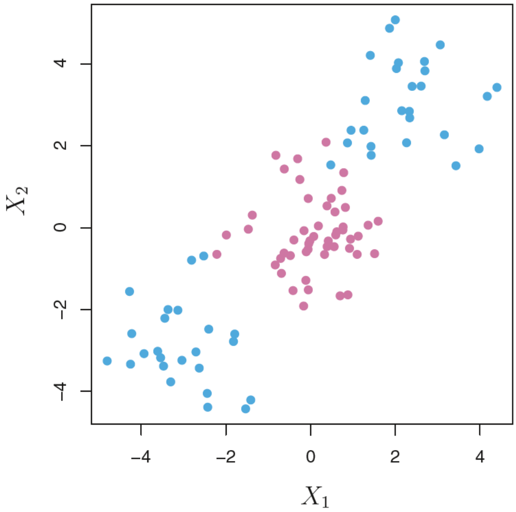


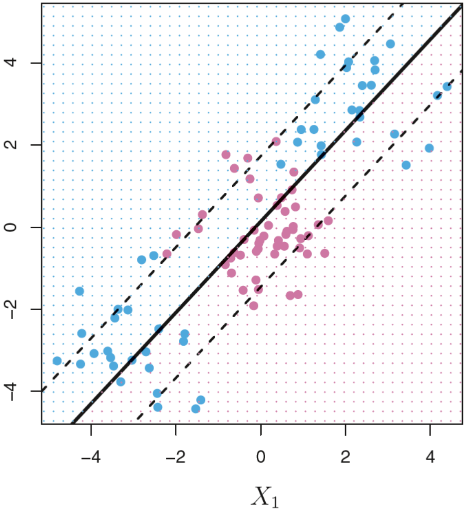
Introducing Slack Variables

- For $0 < \xi_n \leq 1$, the point lies between the margin and the correct side of the hyperplane. This is a **margin violation**.
- For $\xi_n > 1$, the point is **misclassified**.



Soft-Margin SVM





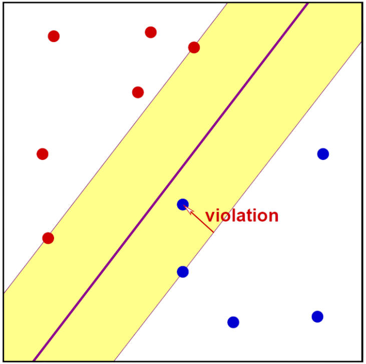
Soft-Margin SVM

$$\text{minimize}_{\mathbf{w},b,\boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^\top\mathbf{w} + C\sum_{n=1}^{N}\xi_n$$

$$\text{subject to:} \quad y_n(\mathbf{w}^\top\mathbf{x}_n + b) \geq 1 - \xi_n, \quad \text{for } n = 1,\ldots,N,$$

$$\xi_n \geq 0, \quad \text{for } n = 1,\ldots,N,$$

$$\mathbf{w} \in \mathbb{R}^d, \quad b \in \mathbb{R}, \quad \boldsymbol{\xi} \in \mathbb{R}^N.$$



Soft-Margin SVM

- Balances the **soft in-sample error**

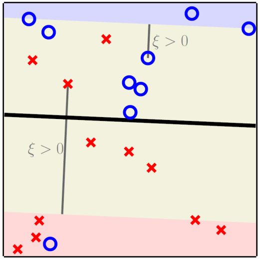
$$\sum_{n=1}^{N} \xi_n$$

against the **weight norm**

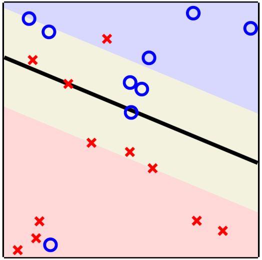
$$\frac{1}{2}\mathbf{w}^\top \mathbf{w}.$$

- Every constraint can be satisfied if ξ_n is sufficiently large.
- The parameter C is a **regularization term** that controls the trade-off:
    - Small C allows the constraints to be relaxed easily $\Rightarrow$ larger margin.
    - Large C enforces the constraints more strictly $\Rightarrow$ narrower margin.
    - $C = \infty$ enforces all constraints, resulting in a **hard-margin SVM**.
- The optimization problem remains **quadratic** and has a unique global minimum. Note that there is only one hyperparameter: C.

Non-Separable Data and the Effect of C



$C = 1$



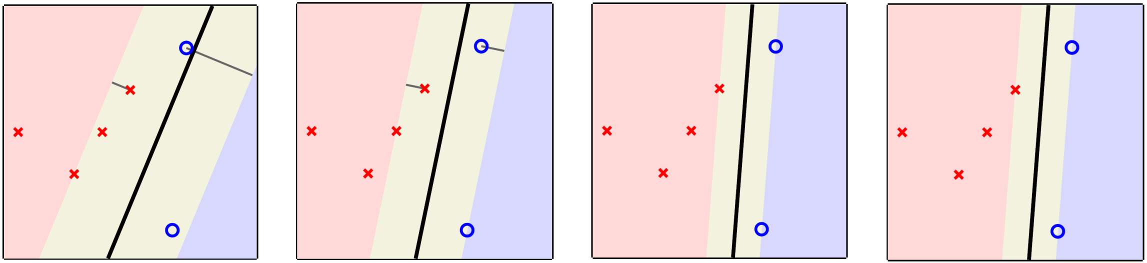
$C = 500$

$$\text{minimize}_{\mathbf{w}, b, \boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^\top \mathbf{w} + C \sum_{n=1}^{N} \xi_n$$

$$\text{subject to:} \quad y_n(\mathbf{w}^\top \mathbf{x}_n + b) \geq 1 - \xi_n, \quad \text{for } n = 1, \ldots, N,$$

$$\xi_n \geq 0, \quad \text{for } n = 1, \ldots, N.$$

Soft-Margin SVM with Separable Data



Small C — Medium C — Large C — Hard Margin

$$\text{minimize}_{\mathbf{w},b,\xi} \quad \frac{1}{2}\mathbf{w}^\top\mathbf{w} + C\sum_{n=1}^{N}\xi_n$$

$$\text{subject to:} \quad y_n(\mathbf{w}^\top\mathbf{x}_n + b) \geq 1 - \xi_n, \quad \text{for } n = 1,\ldots,N,$$

$$\xi_n \geq 0, \quad \text{for } n = 1,\ldots,N.$$

Choosing C Is Important

Lagrange Formulation for the Soft-Margin SVM

$$\mathscr{L}(\mathbf{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\mathbf{w}^\top\mathbf{w} + C\sum_{n=1}^{N}\xi_n - \sum_{n=1}^{N}\alpha_n\big(y_n(\mathbf{w}^\top\mathbf{x}_n + b) - 1 + \xi_n\big) - \sum_{n=1}^{N}\beta_n\xi_n$$

Minimize with respect to $\mathbf{w}$, b, and $\boldsymbol{\xi}$, and maximize with respect to each $\alpha_n \geq 0$ and $\beta_n \geq 0$.

$$\nabla_{\mathbf{w}}\mathscr{L} = \mathbf{w} - \sum_{n=1}^{N}\alpha_n y_n \mathbf{x}_n = 0$$

$$\frac{\partial \mathscr{L}}{\partial b} = -\sum_{n=1}^{N}\alpha_n y_n = 0$$

$$\frac{\partial \mathscr{L}}{\partial \xi_n} = C - \alpha_n - \beta_n = 0$$

Soft-Margin SVM: Dual Problem

$$\max_{\boldsymbol{\alpha}} \left(\sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{x}_n^\top \mathbf{x}_m \right)$$

Subject to:

$$\sum_{n=1}^{N} \alpha_n y_n = 0, \quad 0 \leq \alpha_n \leq C, \quad n = 1, \ldots, N.$$

After solving this quadratic optimization problem, the optimal weight vector is given by:

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n.$$

Non-Linearly Separable Data

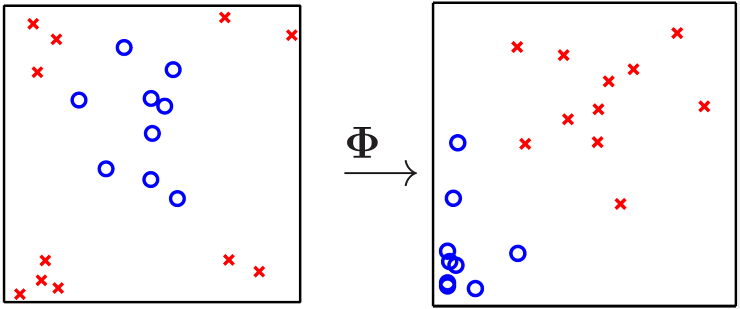
Noisy Data or Overlapping Classes

(as discussed earlier: soft margin)

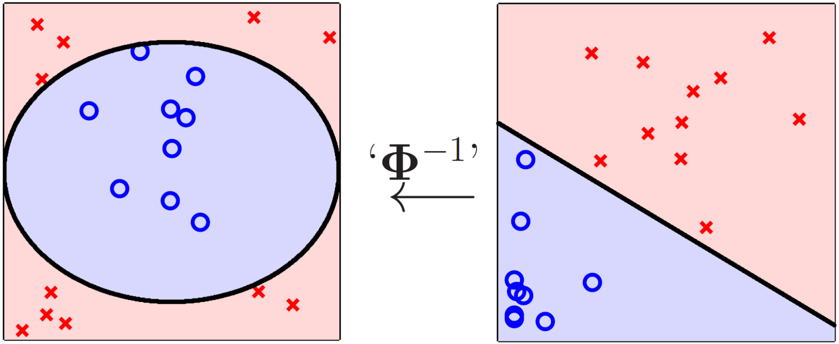
- Nearly linearly separable

Non-Linear Decision Surface

- Transform data into a new feature space



Mechanics of the Nonlinear Transform



Soft-Margin SVM in a Transformed Space: Primal Problem

- Primal problem:

$$\min_{\mathbf{w}, b, \boldsymbol{\xi}} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^{N} \xi_n$$

Subject to:

$$y_n \left(\mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}_n) + b \right) \geq 1 - \xi_n, \quad n = 1, \ldots, N,$$

$$\xi_n \geq 0, \quad n = 1, \ldots, N.$$

- $\mathbf{w} \in \mathbb{R}^m$: weight vector to be learned.
- If $m \gg d$ (i.e., the feature space is very high-dimensional), the model contains many more parameters to estimate.

Soft-Margin SVM in a Transformed Space: Dual Problem

- Optimization problem:

$$\max_{\boldsymbol{\alpha}} \left\{ \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \boldsymbol{\phi}(\mathbf{x}_n)^\top \boldsymbol{\phi}(\mathbf{x}_m) \right\}$$

Subject to:

$$\sum_{n=1}^{N} \alpha_n y_n = 0, \quad 0 \le \alpha_n \le C, \quad n = 1, \ldots, N.$$

- Since only inner products $\boldsymbol{\phi}(\mathbf{x}_i)^\top \boldsymbol{\phi}(\mathbf{x}_j)$ appear, only the coefficients $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_N]$ need to be learned.
- It is not necessary to learn m parameters explicitly, unlike the primal problem.

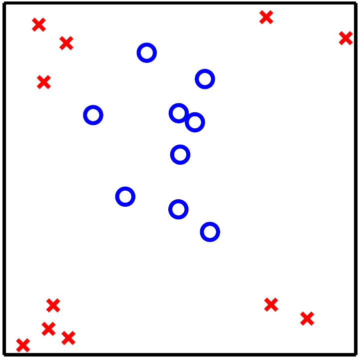
Classifying a New Data Point

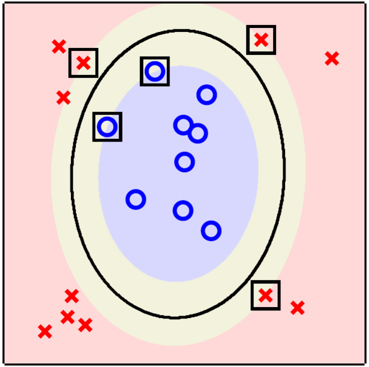
$$\hat{y} = \operatorname{sign}\left(b + \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x})\right)$$

$$\text{where } \mathbf{w} = \sum_{\alpha_n > 0} \alpha_n y_n \boldsymbol{\phi}(\mathbf{x}_n)$$

$$\text{and } b = y_s - \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}_s) \quad \text{for any support vector } s.$$

Non-Linearly Separable Data





Kernel SVM

- Learns a linear decision boundary in a high-dimensional feature space without explicitly computing the mapped data.

- Let

$$\boldsymbol{\phi}(\mathbf{x})^\top \boldsymbol{\phi}(\mathbf{x}') = K(\mathbf{x}, \mathbf{x}') \quad \text{(kernel function)}$$

- **Example:** for $\mathbf{x} = [x_1, x_2]$ and a second-order mapping $\boldsymbol{\phi}(\cdot)$:

$$\boldsymbol{\phi}(\mathbf{x}) = [\,1,\, x_1,\, x_2,\, x_1^2,\, x_2^2,\, x_1 x_2\,]$$

Then,

$$K(\mathbf{x}, \mathbf{x}') = 1 + x_1 x_1' + x_2 x_2' + x_1^2 x_1'^2 + x_2^2 x_2'^2 + x_1 x_2 x_1' x_2'$$

Kernel Trick

- Compute $K(\mathbf{x}, \mathbf{x}')$ directly, without explicitly transforming $\mathbf{x}$ and $\mathbf{x}'$.
- **Example:** consider

$$\begin{aligned} K(\mathbf{x}, \mathbf{x}') &= \left(1 + \mathbf{x}^\top \mathbf{x}'\right)^2 \\ &= \left(1 + x_1 x_1' + x_2 x_2'\right)^2 \\ &= 1 + 2x_1 x_1' + 2x_2 x_2' + x_1^2 x_1'^2 + x_2^2 x_2'^2 + 2x_1 x_2 x_1' x_2' \end{aligned}$$

This corresponds to an inner product in the feature space:

$$\boldsymbol{\phi}(\mathbf{x}) = [\,1,\ \sqrt{2}x_1,\ \sqrt{2}x_2,\ x_1^2,\ x_2^2,\ \sqrt{2}x_1 x_2\,]$$

$$\boldsymbol{\phi}(\mathbf{x}') = [\,1,\ \sqrt{2}x_1',\ \sqrt{2}x_2',\ x_1'^2,\ x_2'^2,\ \sqrt{2}x_1' x_2'\,]$$

Polynomial Kernel: Degree Two

- Instead of computing the explicit feature mapping, we use:

$$K(\mathbf{x}, \mathbf{x}') = \left(\mathbf{x}^\top \mathbf{x}' + 1\right)^2$$

which corresponds to an implicit feature mapping.

- For a d-dimensional input vector:

$$\mathbf{x} = [x_1, \ldots, x_d]^\top$$

- The corresponding feature mapping is:

$$\boldsymbol{\phi}(\mathbf{x}) = [1, \sqrt{2}x_1, \ldots, \sqrt{2}x_d, x_1^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_1x_d, \sqrt{2}x_2x_3, \ldots, \sqrt{2}x_{d-1}x_d]^\top$$

Polynomial Kernel

- This kernel can be generalized to a d-dimensional input vector with polynomial feature mappings of order M:

$$K(\mathbf{x},\mathbf{x}') = \left(1+\mathbf{x}^\top\mathbf{x}'\right)^M$$
$$= \left(1 + x_1x_1' + x_2x_2' + \cdots + x_dx_d'\right)^M$$

- **Example:** SVM decision boundary using a polynomial kernel:

$$b + \mathbf{w}^\top\boldsymbol{\phi}(\mathbf{x}) = 0$$
$$\Rightarrow b + \sum_{\alpha_i>0} \alpha_i y_i \boldsymbol{\phi}(\mathbf{x}_i)^\top \boldsymbol{\phi}(\mathbf{x}) = 0$$
$$\Rightarrow b + \sum_{\alpha_i>0} \alpha_i y_i K(\mathbf{x}_i,\mathbf{x}) = 0$$

$\Rightarrow b + \sum_{\alpha_i>0} \alpha_i y_i \left(1+\mathbf{x}_i^\top\mathbf{x}\right)^M = 0 \quad \Rightarrow$ Decision boundary is a polynomial of order M.

Why Kernel?

- Kernel functions K can be computed efficiently, with a cost proportional to the input dimensionality d instead of the (potentially much larger) feature space dimension m.

- **Example:** consider a second-order polynomial transformation:

$$\boldsymbol{\phi}(\mathbf{x}) = [1, x_1, \ldots, x_d, x_1^2, x_1 x_2, \ldots, x_d x_d]^\top, \quad m = 1 + d + d^2$$

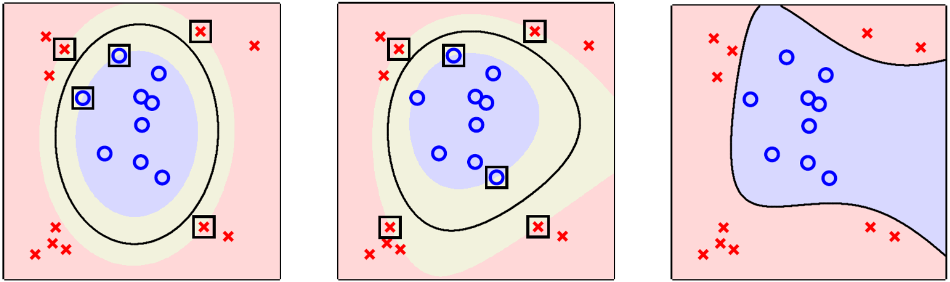
- Computing the inner product explicitly:

$$\boldsymbol{\phi}(\mathbf{x})^\top \boldsymbol{\phi}(\mathbf{x}') = 1 + \sum_{i=1}^{d} x_i x_i' + \sum_{i=1}^{d} \sum_{j=1}^{d} x_i x_j x_i' x_j' \quad O(m)$$

- Using the kernel trick instead:

$$\boldsymbol{\phi}(\mathbf{x})^\top \boldsymbol{\phi}(\mathbf{x}') = 1 + (\mathbf{x}^\top \mathbf{x}') + (\mathbf{x}^\top \mathbf{x}')^2 \quad O(d)$$

Nonlinear Transform and SVM



Φ_2+ SVM Φ_3+ SVM Φ_3+ pseudoinverse algorithm

- The mapping $\mathbf{\Phi}_3$ has almost twice as many parameters as $\mathbf{\Phi}_2$.
- The $\mathbf{\Phi}_3$-SVM does not exhibit significant overfitting compared to $\mathbf{\Phi}_3$-regression.
- The number of support vectors did not double.
- Higher-dimensional mappings are feasible as long as the number of support vectors remains small or the margin stays large.

Gaussian (RBF) Kernel

- If $K(\mathbf{x}, \mathbf{x}')$ represents an inner product in some transformed space of $\mathbf{x}$, it is a valid kernel.
- Gaussian or Radial Basis Function (RBF) kernel:

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

- For the one-dimensional case with $\gamma = 1$:

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

$$= \exp(-x^2)\exp(-x'^2)\exp(2xx')$$

$$= {\color{red}\exp(-x^2)}\,{\color{magenta}\exp(-x'^2)}\sum_{k=0}^{\infty}{\color{green}\frac{(2xx')^k}{k!}}$$

Some Common Kernel Functions

- Linear kernel:

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}'$$

- Polynomial kernel:

$$K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}' + 1)^M$$

- Gaussian (RBF) kernel:

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

- Sigmoid (tanh) kernel:

$$K(\mathbf{x}, \mathbf{x}') = \tanh(a\mathbf{x}^\top \mathbf{x}' + b)$$

Kernel Formulation of SVM

Optimization problem:

$$\max_{\boldsymbol{\alpha}} \left[\sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m K(\mathbf{x}_n, \mathbf{x}_m) \right]$$

$$\text{subject to:} \quad \sum_{n=1}^{N} \alpha_n y_n = 0, \quad 0 \le \alpha_n \le C, \quad n = 1, \ldots, N$$

Equivalent quadratic form:

$$\mathbf{Q} = \begin{bmatrix} y_1 y_1 K(\mathbf{x}_1, \mathbf{x}_1) & \cdots & y_1 y_N K(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ y_N y_1 K(\mathbf{x}_N, \mathbf{x}_1) & \cdots & y_N y_N K(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

Gaussian (RBF) Kernel

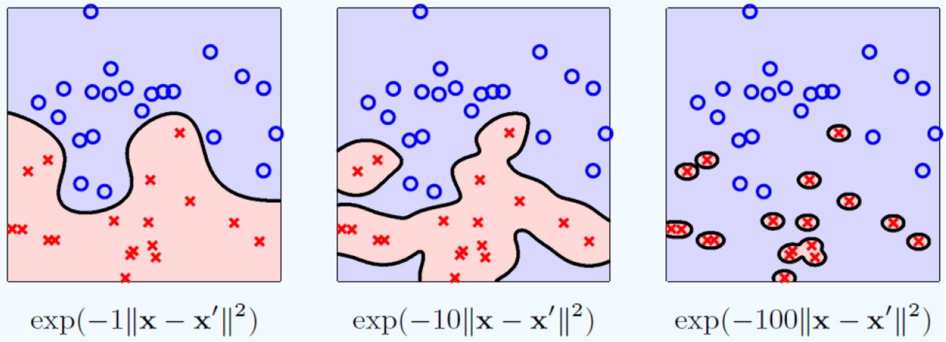
Example: SVM decision boundary with a Gaussian kernel

- Considers a Gaussian function centered around each training point:

$$b + \sum_{\alpha_i > 0} \alpha_i y^{(i)} \exp\left(-\gamma \|\mathbf{x} - \mathbf{x_i}\|^2\right) = 0$$

- An SVM with a Gaussian kernel can, in principle, classify *any* training set.
  - The training error becomes zero as $\sigma \to 0$.
    - In this case, all samples become support vectors — indicating potential **overfitting**.

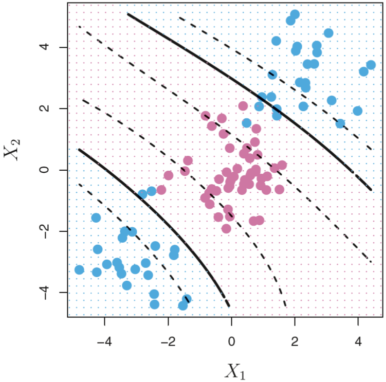
Hard-Margin Example



For a **narrow Gaussian** (i.e., small σ), even maintaining a large margin cannot prevent overfitting.

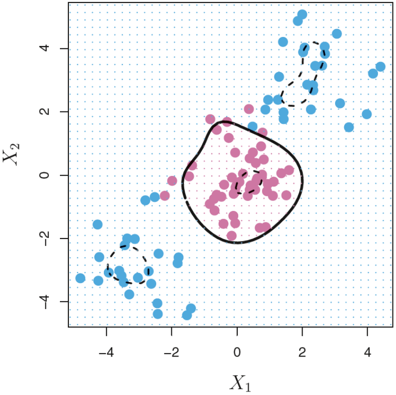
SVM with Polynomial and Gaussian Kernels

SVM with a Polynomial Kernel (degree 3)



$$K(\mathbf{x}_i, \mathbf{x}_i') = \left(1 + \sum_{j=1}^{p} x_{ij} x_{ij}'\right)^d$$

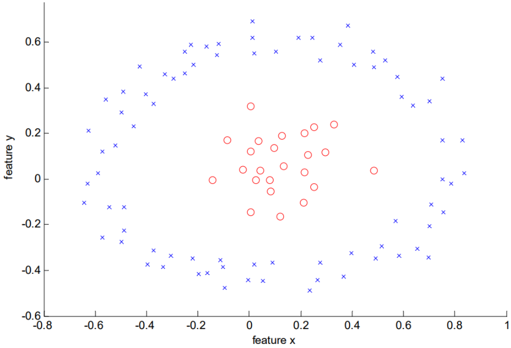
SVM with a Radial Kernel



$$K(\mathbf{x}_i, \mathbf{x}_i') = \exp\left(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{ij}')^2\right)$$

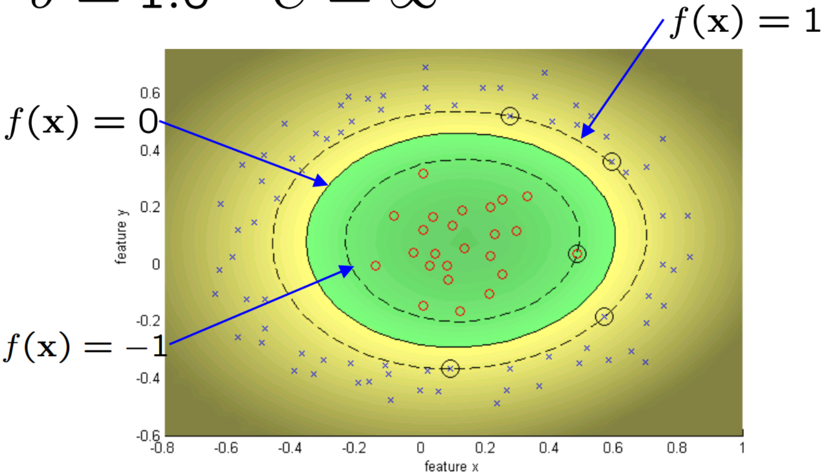
SVM with a Gaussian (RBF) Kernel: Example

$$f(\mathbf{x}) = w_0 + \sum_{\alpha_i>0} \alpha_i y^{(i)} \exp\left(-\gamma \|\mathbf{x}-\mathbf{x}^{(i)}\|^2\right)$$



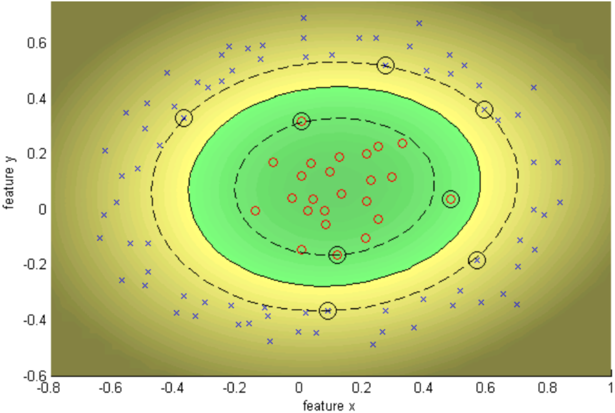
SVM Gaussian kernel: Example

$\sigma = 1.0 \quad C = \infty$



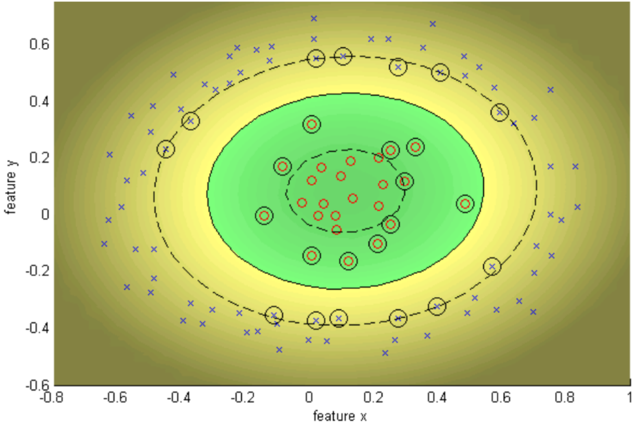
SVM Gaussian Kernel: Example

$$\sigma = 1.0 \quad C = 100$$



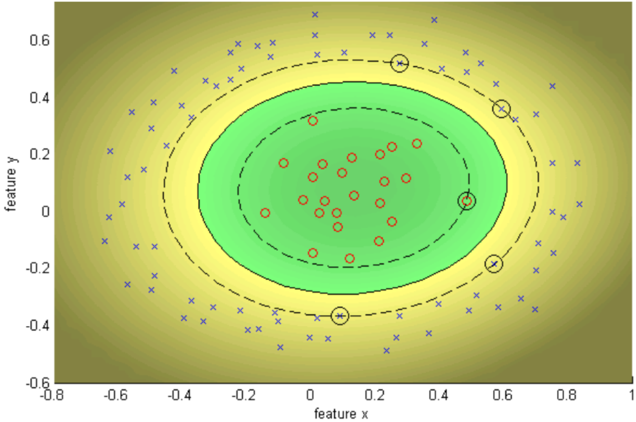
SVM Gaussian Kernel: Example

$\sigma = 1.0 \quad C = 10$



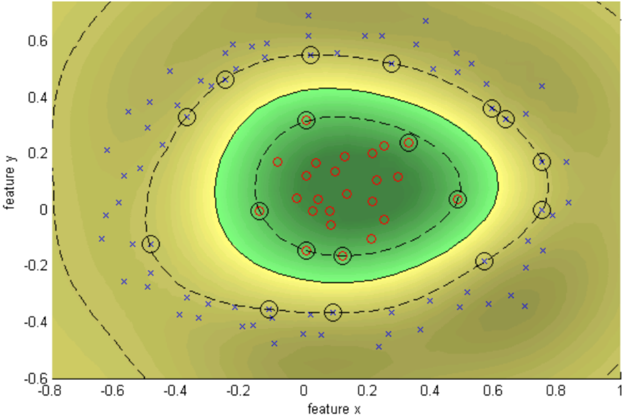
SVM Gaussian Kernel: Example

$$\sigma = 1.0 \qquad C = \infty$$



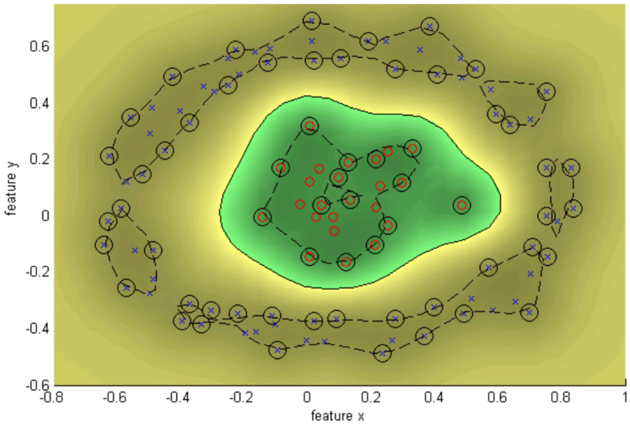
SVM Gaussian Kernel: Example

$$\sigma = 0.25 \quad C = \infty$$



SVM Gaussian Kernel: Example

$$\sigma = 0.1 \qquad C = \infty$$



Contributions

- **This slide has been prepared thanks to:**
  - Mahdi Aghaei