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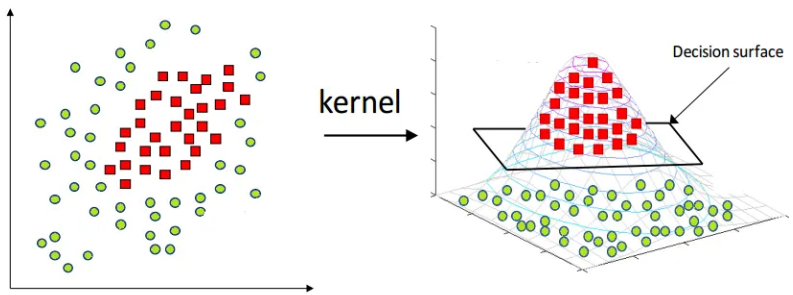
Kernel: Definition

- Consider a transformation $\Phi : \mathcal{X} \rightarrow \mathcal{Z}$
  - E.g., transform features in space $\mathcal{X}$ non-linearly into higher-dimensional space $\mathcal{Z}$
- **Kernel of transformation** Φ yields inner product of two points $\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}' \in \mathcal{X}$ in transformed space $\mathcal{Z}$

$$K_\Phi(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}') \triangleq \langle \Phi(\underline{\boldsymbol{x}}), \Phi(\underline{\boldsymbol{x}}') \rangle = \Phi(\underline{\boldsymbol{x}})^T \Phi(\underline{\boldsymbol{x}}') = \underline{\boldsymbol{z}}^T \underline{\boldsymbol{z}}'$$

- Why doing this?



Kernel: Expression From the Transform

- If you have an expression for Φ, compute a closed formula for the kernel
- E.g., if transformation is $\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^6$, it introduces interaction terms:

$$\underline{\boldsymbol{z}} = \Phi(\underline{\boldsymbol{x}}) = \Phi(x_1, x_2) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$$

- Kernel of Φ is:

$$\begin{aligned} K_\Phi(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}') &= (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)^T (1, x'_1, x'_2, x'^2_1, x'^2_2, x'_1 x'_2) \\ &= 1 + x_1 x'_1 + x_2 x'_2 + x_1^2 x'^2_1 + x_2^2 x'^2_2 + x_1 x_2 x'_1 x'_2 \end{aligned}$$

Gaussian Kernel

- Aka "exponential kernel" or "Radial Basis Function" (RBF) kernel
- A **Gaussian kernel** has the form:

$$K(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}') = \exp(-\gamma \|\underline{\boldsymbol{x}} - \underline{\boldsymbol{x}}'\|^2) = \exp(-\frac{\|\underline{\boldsymbol{x}} - \underline{\boldsymbol{x}}'\|^2}{\sigma^2})$$

- It can be shown to be an inner product in an infinite dimension $\mathcal{Z}$

Kernel as Way to Measure Similarity

- **Intuition**: The Gaussian kernel

$$K(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}') = \exp(-\gamma \|\underline{\boldsymbol{x}} - \underline{\boldsymbol{x}}'\|^2)$$

  measures "similarity" of point $\underline{\boldsymbol{x}}$ to point $\underline{\boldsymbol{x}}_i$:
  - $K(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}')$ is 1 when points are the same
  - Value is 0 when points are distant
  - Effect strength depends on γ
- Using kernels to compute features:
  - Kernels often rely on distance between vectors
    - E.g., euclidean norm $\|\underline{\boldsymbol{x}} - \underline{\boldsymbol{x}}'\|^2$
  - Need to scale features for similar effects among coordinates

Linear Kernel

- Consider the transformation Φ as the identity function $\Phi(\underline{\boldsymbol{x}}) = \underline{\boldsymbol{x}}$
- The kernel function is:

$$K_\Phi(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}') = \underline{\boldsymbol{x}}^T \underline{\boldsymbol{x}}'$$

  - A **linear kernel** means using no kernel
  - It is just a "pass-through"

Polynomial Kernel

- Given a point $\underline{\boldsymbol{x}} \in \mathbb{R}^n$, consider the function with two parameters k and d

$$K_\Phi(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}') = (k + \underline{\boldsymbol{x}}^T \underline{\boldsymbol{x}}')^d$$

- It is called **polynomial** since if you expand the dot product you get a polynomial
- It can be proved that this is always a kernel

Kernel: Identifying a Function as a Kernel

- **Problem**:
  - You have a certain function $K(\underline{x}, \underline{x}')$ and you want to show that $K(\cdot)$ is an inner product in the form for some function $\Phi(\cdot)$

$$K(\underline{x}, \underline{x}') = \Phi(\underline{x})^T \Phi(\underline{x}') \quad \forall \underline{x}, \underline{x}'$$

    for a certain Φ and $\mathcal{Z}$
- In theory, a given function $K(\underline{x}, \underline{x}')$ is a valid kernel iff:
  - It is a symmetric, and
  - Satisfies the Mercer's condition: the matrix $K(\underline{x}_i, \underline{x}_j)$ is definite semi-positive

Kernel: Example of Identifying a Kernel

- Let's show that:

$$K(\underline{x}, \underline{x}') = (k + \underline{x}^T \underline{x}')^d$$

  is a **kernel** for any n, k, d

- According to the definition you need to show that there is always a transform Φ:

$$\Phi : \mathcal{X} = \mathbb{R}^n \to \mathcal{Z} = \mathbb{R}^q$$

  with $q \gg d$, such that $K_\Phi = (k + \underline{x}^T \underline{x}')^d$

- **Example**
  - $\mathcal{X} = \mathbb{R}^2$, $K(\underline{x}, \underline{x}') = (1 + \underline{x}^T \underline{x}')^2 = (1 + x_1 x_1' + x_2 x_2')^2$
  - Compute the full expression in terms of the coordinates:

$$K(\underline{x}, \underline{x}') = (1 + x_1^2 x'^2_1 + x_2^2 x'^2_2 + 2x_1 x_1' + 2x_2 x_2' + 2x_1 x_1' x_2 x_2')$$

  - Choose:
    - $\mathcal{Z} = \mathbb{R}^6$
    - $\Phi(x_1, x_2) = (1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2)$
  - This is a particular case of the polynomial kernel

A Kernel Is a Computational Shortcut

- In literature, the **kernel trick** is a **computational shortcut** for the dot product of transformed vectors
- Compare 2 ways to compute the inner product of transformed vectors for a polynomial kernel
  1. **Using definition**: compute images of vectors, then inner product in transformed space:

$$(1, x_1, x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2, ...)^T \cdot (1, x_1', ...)$$

     - Requires combinatorial powers and a large dot product
  2. **Kernel trick**: use kernel function for dot product in transformed space

$$(k + \underline{\boldsymbol{x}}^T \underline{\boldsymbol{x}}')^d$$

     - Requires inner product of small vectors, then power of a number
- Kernel trick is more computationally efficient for inner product computation

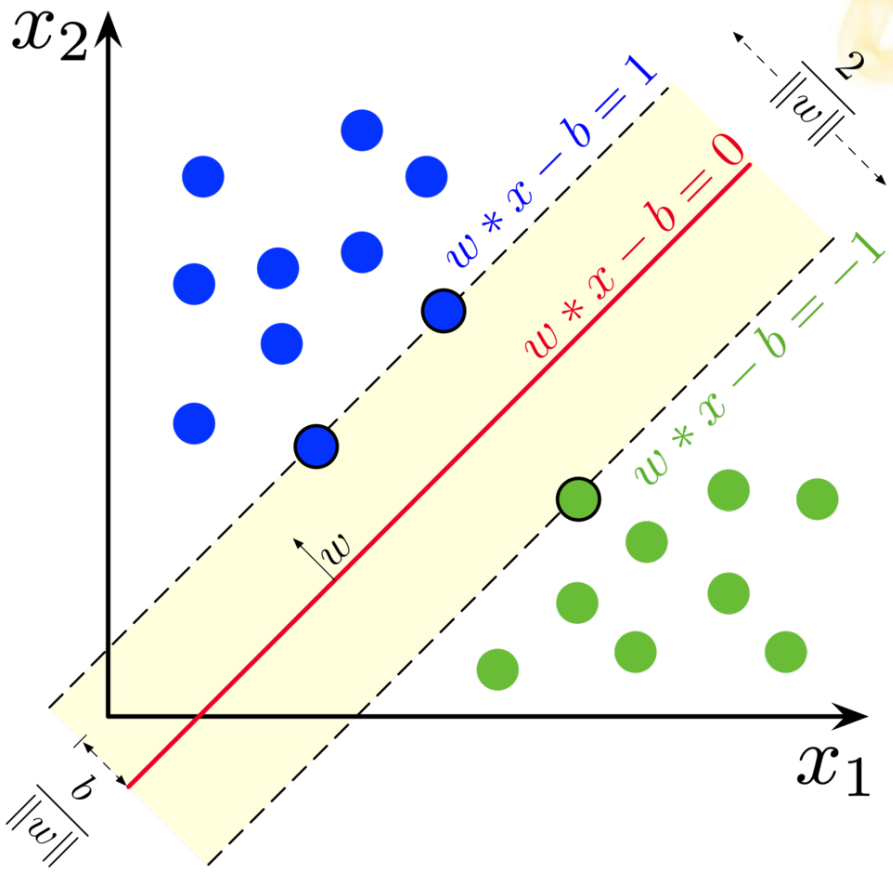
- ***Support Vector Machines (Optional)***
- Similarity-Based Models

Support Vector Machines (SVM)

- Arguably one of the most successful classification algorithm, together with neural networks and random forests
- **Idea**: find a separating hyperplane that maximizes the distance from the class points (aka "margin")
- **All the rage in 2005-2015**
  - Robust classifier handling outliers automatically
  - Strong theoretical justification of out-of-bound error
  - Strong link with VC dimension
  - Cool geometric interpretation
  - Solve a very complex optimization problem with some neat tricks
  - Works for both regression and classification
- SVM for classification:
  - Does not output probabilities (like logistic regression), but predicts directly the class
  - Has a notion of confidence, as distance from the margin

SVM Is a Large Margin Classifier

- Why **large margin** classifier is good?
- Given a linearly separable data set, the optimal separating line maximizes the margin:
  - More robust to noise
  - Large margin reduces VC dimension of hypothesis set



SVM: Notation and Conventions

- Assume that:
  1. Outputs are encoded as $y_i \in \{-1, 1\}$
  2. Pull out w_0 from $\underline{\boldsymbol{w}}$
     - The bias $w_0 = b$ plays a different role
     - $\underline{\boldsymbol{w}} = (w_1, ..., w_d)$ and there is no $x_0 = 1$
     - $\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}} + b = 0$ is the equation of the separating hyperplane
  3. $\underline{\boldsymbol{x}}_n$ is the closest point to the hyperplane
     - It can be multiple points from different classes
- Normalize $\underline{\boldsymbol{w}}$ and b to get a canonical representation of the hyperplane imposing $|\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_n + b| = 1$

SVM: Original Form of Problem

- The SVM problem is:

$$\begin{aligned} &\text{find } \underline{\boldsymbol{w}}, b \\ &\text{maximize } \frac{1}{\|\underline{\boldsymbol{w}}\|} && \text{(max margin)} \\ &\text{subject to } \min_{i=1,\ldots,n} |\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b| = 1 && \text{(hyperplane)} \end{aligned}$$

- This problem is not friendly to optimization since it has norm, min, and absolute value

Primal Form of SVM Problem

- You can rewrite it as:

$$\begin{aligned} &\text{find} && \underline{\boldsymbol{w}}, b \\ &\text{minimize} && \frac{1}{2}\underline{\boldsymbol{w}}^T\underline{\boldsymbol{w}} \\ &\text{subject to} && y_i(\underline{\boldsymbol{w}}^T\underline{\boldsymbol{x}}_i + b) \geq 1 \; \forall i = 1, ..., n \end{aligned}$$

- Note that under $\underline{\boldsymbol{w}}$ minimal and linear separable classes, it is guaranteed that for at least one $\underline{\boldsymbol{x}}_i$ in the second equation will be equal to 1 (as in the original problem)
  - In fact otherwise we could scale down $\underline{\boldsymbol{w}}$ and b (which does not change the plane) to use the slack, against the hypothesis of minimality of $\underline{\boldsymbol{w}}$

Dual (Lagrangian) Form of SVM Problem

minimize with respect to $\underline{\boldsymbol{\alpha}}$

$$\mathcal{L}(\underline{\boldsymbol{\alpha}}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j \underline{\boldsymbol{x}}_i^T \underline{\boldsymbol{x}}_j$$

subject to

$$\underline{\boldsymbol{\alpha}} \geq \underline{\mathbf{0}}, \sum_{i=1}^{N} \alpha_i y_i = 0$$

$$\underline{\boldsymbol{w}} = \sum_{i=1}^{N} \alpha_i y_i \underline{\boldsymbol{x}}_i$$

- The equation for $\underline{\boldsymbol{w}}$ is not a constraint, but it computes $\underline{\boldsymbol{w}}$ (the plane) given $\underline{\boldsymbol{\alpha}}$, while b is given by $\min|\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b| = 1$

Dual Form of SVM as QP Problem

- The dual form of SVM problem is a convex quadratic programming problem, in the form:

$$\begin{aligned} \text{minimize with respect to } \underline{\boldsymbol{\alpha}} \quad & \underline{\mathbf{1}}^T \underline{\boldsymbol{\alpha}} - \frac{1}{2} \underline{\boldsymbol{\alpha}}^T \underline{\underline{\boldsymbol{Q}}} \underline{\boldsymbol{\alpha}} \\ \text{subject to} \quad & \underline{\boldsymbol{\alpha}} \geq 0, \underline{\boldsymbol{y}}^T \underline{\boldsymbol{\alpha}} = 0 \end{aligned}$$

where:

- the matrix is $\underline{\underline{\boldsymbol{Q}}} = \{y_i y_j \underline{\boldsymbol{x}}_i^T \underline{\boldsymbol{x}}_j\}_{ij}$
- $\underline{\boldsymbol{\alpha}}$ is the column vector $(\alpha_1, \ldots, \alpha_N)$

Solving Dual Formulation of SVM Problem (1/2)

- **Solving convex problem** for α
  - Feeding this problem to a QP solver, you get the optimal vector $\underline{\boldsymbol{\alpha}}$
- **Compute hyperplane $\underline{\boldsymbol{w}}$**
  - From $\underline{\boldsymbol{\alpha}}$ recover the plane $\underline{\boldsymbol{w}}$ from the equation: $\underline{\boldsymbol{w}} = \sum_{i=1}^{N} \alpha_i y_i \underline{\boldsymbol{x}}_i$
  - Looking at the optimal α_i, you can observe that many of them are 0
  - This is because when you applied the Lagrange multipliers to the inequalities: $y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) \geq 1$, you got the KKT condition:

$$\alpha_i(y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) - 1) = 0$$

  - From these equations, either
    - $\alpha_i = 0$ and $\underline{\boldsymbol{x}}_i$ is an *interior point* since it has non-null distance from the plane (i.e., slack) from the plane; or
    - $\alpha_i \neq 0$ and the slack is 0, which implies that the $\underline{\boldsymbol{x}}_i$ point touches the margin, i.e., it is a *support vector*

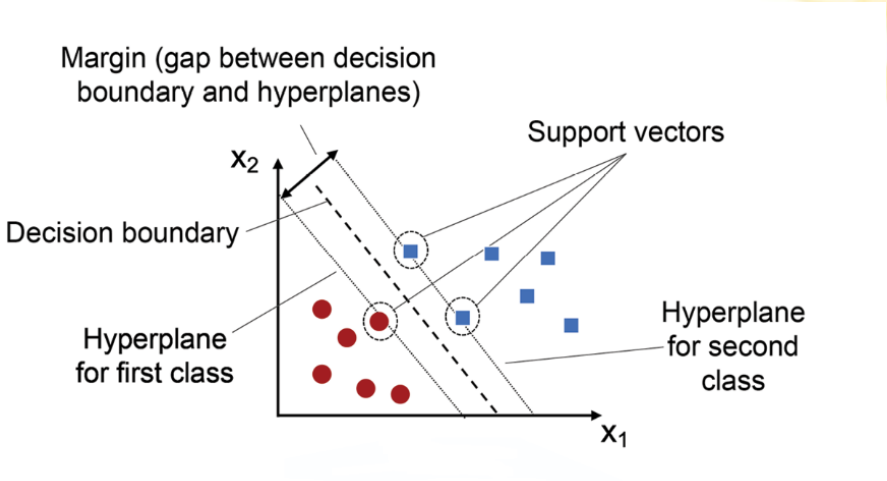
Solving Dual Formulation of SVM Problem (2/2)

- Thus the hyperplane is only function of the support vectors:

$$\underline{\boldsymbol{w}} = \sum_{i=1}^{N} \alpha_i y_i \underline{\boldsymbol{x}}_i = \sum_{\underline{\boldsymbol{x}}_i \in \mathrm{SV}} \alpha_i y_i \underline{\boldsymbol{x}}_i$$

since only for the support vectors $\alpha \neq 0$

  - The $\alpha_i \neq 0$ are the real degree of freedom



- **Compute** b
  - Once $\underline{\boldsymbol{w}}$ is known, you can use any support vector to compute b:

$$y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) = 1$$

Support Vectors and Degrees of Freedom for SVM

- The number of support vectors is related to the degrees of freedom of the model
- Because of the VC dimension, you have an in-sample quantity to bound the out-of-sample error:

$$E_{out} \leq E_{in} + c\frac{\text{num of SVs}}{N-1}$$

- You are "guaranteed" to not overfit

Non-Linear Transform for SVM

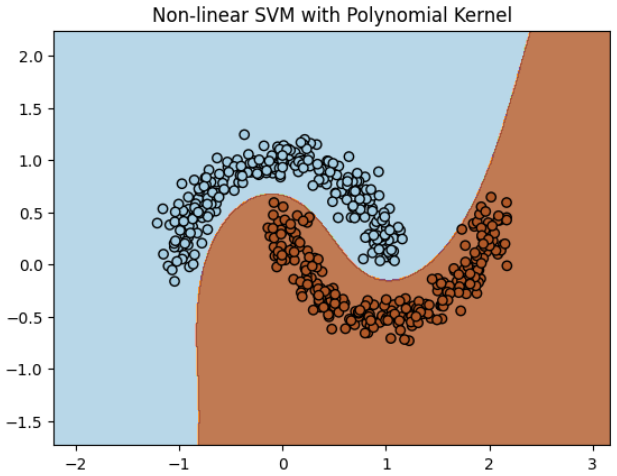
- $\Phi : \mathcal{X} \rightarrow \mathcal{Z}$ transforms $\underline{\boldsymbol{x}}_i$ into $\underline{\boldsymbol{z}}_i = \Phi(\underline{\boldsymbol{x}}_i) \in \mathbb{R}^{\tilde{d}}$ with $\tilde{d} > d$
- Transform vectors through Φ and apply SVM machinery
- Dual SVM formulation in $\mathcal{Z}$ space:

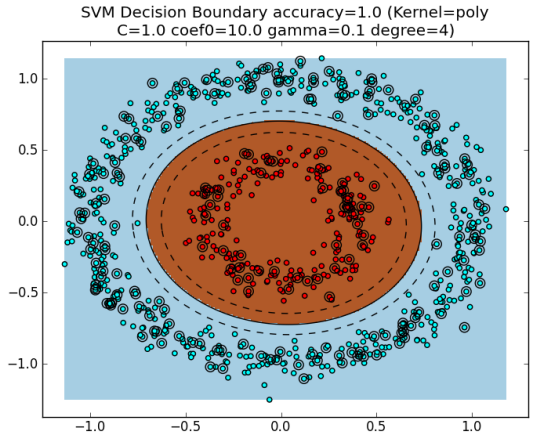
$$\mathcal{L}(\underline{\boldsymbol{\alpha}}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \underline{\boldsymbol{z}}_i^T \underline{\boldsymbol{z}}_j$$

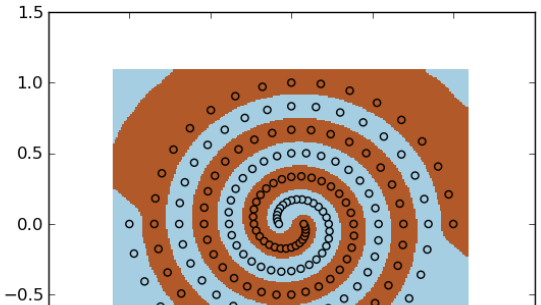
- Note:
  - Optimization problem has same number of unknowns as original space (number of points N)
  - Support vectors live in $\mathcal{Z}$: they have $\alpha = 0$. In $\mathcal{X}$, they are pre-images of support vectors
  - Decision boundary and margin can be represented in original space (not linear)

Non-Linear Transforms for SVM vs Others

- In SVM the non-linear transform does not change the number of unknowns and degrees of freedom of the model
- This is different from transforming the variables in a linear problem, since in that case the number of unknowns changes







SVM in Higher Dimensional Space

- **Pros**
  - You don't pay the price in terms of complexity of optimization problem
    - Number of unknowns is still N (different than a linear problem)
  - You don't pay the price in terms of increased generalization bounds
    - Number of support vectors is $\leq N$
    - This is because each hypothesis h can be complex but the cardinality of the hypothesis set $\mathcal{H}$ is the same
- **Cons**
  - You pay a price to compute $\Phi(\underline{x}_i)^T \Phi(\underline{x}_j)$, since Φ could be very complex
    - The kernel trick will remove this extra complexity by doing $\Phi(\underline{x}_i)^T \Phi(\underline{x}_j) = K_\Phi(\underline{x}_i, \underline{x}_j)$

Non-Linear Transform in SVM vs Kernel Trick

- The trivial approach is:
  - Transform vectors with $\Phi(\cdot)$
  - Apply all SVM machinery to the transformed vectors
  - **Cons**: Φ might be very complex, e.g., potentially exponential number of terms
- You can express the SVM problem formulation and the prediction in terms of a kernel

$$K_\Phi(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}') = \Phi(\underline{\boldsymbol{x}})^T \Phi(\underline{\boldsymbol{x}}') = \underline{\boldsymbol{z}}^T \underline{\boldsymbol{z}}'$$

  - You only need the kernel $K_\Phi(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}')$ of the transformation $\Phi(\cdot)$ and not $\Phi(\cdot)$ itself

SVM in Terms of Kernel: Optimization Step

- When you build the QP formulation for the Lagrangian to compute the α we can use $K_\Phi(\underline{\boldsymbol{x}}_i, \underline{\boldsymbol{x}}_j)$ instead of $\underline{\boldsymbol{z}}_i^T \underline{\boldsymbol{z}}_j$

$$\mathcal{L}(\underline{\boldsymbol{\alpha}}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \alpha_n \alpha_m K_\Phi(\underline{\boldsymbol{x}}_n, \underline{\boldsymbol{x}}_m)$$

- $\underline{\boldsymbol{z}}_n$ does not appear in the constraints

$$\underline{\boldsymbol{\alpha}} \geq \underline{\mathbf{0}}, \underline{\boldsymbol{\alpha}}^T \underline{\boldsymbol{y}} = 0$$

SVM in Terms of Kernel: Prediction Step

- You need only inner products to compute a prediction for a given $\underline{z}$
- In fact to make predictions, you replace the expression of $\underline{\tilde{w}} = \sum_{i:\alpha_i>0} \alpha_i y_i \underline{z}_i$ in $h(\underline{x}) = \text{sign}(\underline{w}^T \Phi(\underline{x}) + b)$, yielding:

$$h(\underline{x}) = \text{sign}\Big(\sum_{i:\alpha_i>0} \alpha_i y_i K_\Phi(\underline{x}_i, \underline{x}) + b\Big)$$

where b is given by $y_i(\underline{w}^T \underline{z}_i + b) = 1$ for any support vector $\underline{x}_m$ and thus

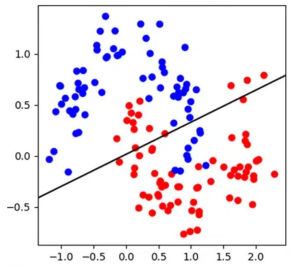
$$b = \frac{1}{y_m} - \sum_{i:\alpha_i>0} \alpha_i y_i K_\Phi(\underline{x}_i, \underline{x}_m)$$

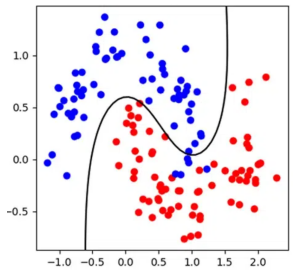
Implications of Kernel Trick in SVM

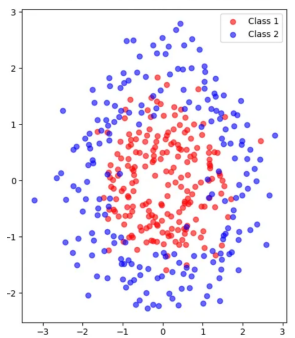
- The "kernel trick" is a computational shortcut:
  - Use the kernel of the transformation instead of the transformation itself
- To use SVMs, compute inner products between transformed vectors $\underline{\boldsymbol{z}}$
- The kernel trick implies:
  - No need to compute $\Phi()$
    - Use the kernel K_Φ, not the transformation Φ
  - No need to know Φ
    - With function K_Φ as an inner product, use SVM machinery without knowing $\mathcal{Z}$ space or transformation Φ
  - Φ can be impossible to compute
    - K_Φ can correspond to a transformation Φ to an infinite dimensional space (e.g., Gaussian kernel)

Non-Linearly Separable SVM Problem

- In general there are different types of **non-linearly separable data sets**
- **Slightly non-separable**
  - Few points crossing the boundary
  - $\Longrightarrow$ use soft margin SVMs
- **Seriously non-separable**
  - E.g., the class inside the circle
  - $\Longrightarrow$ use non-linear kernels



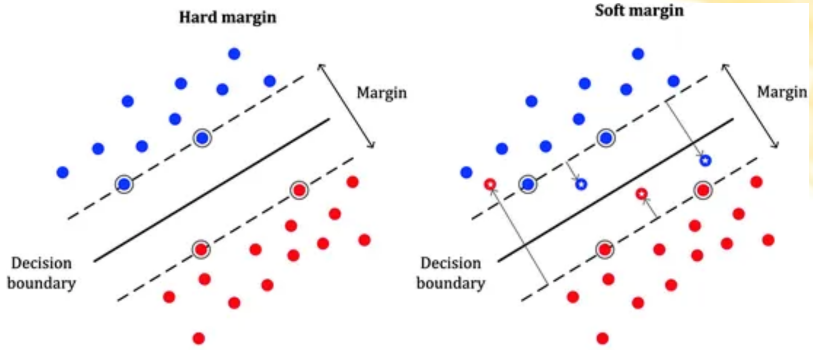


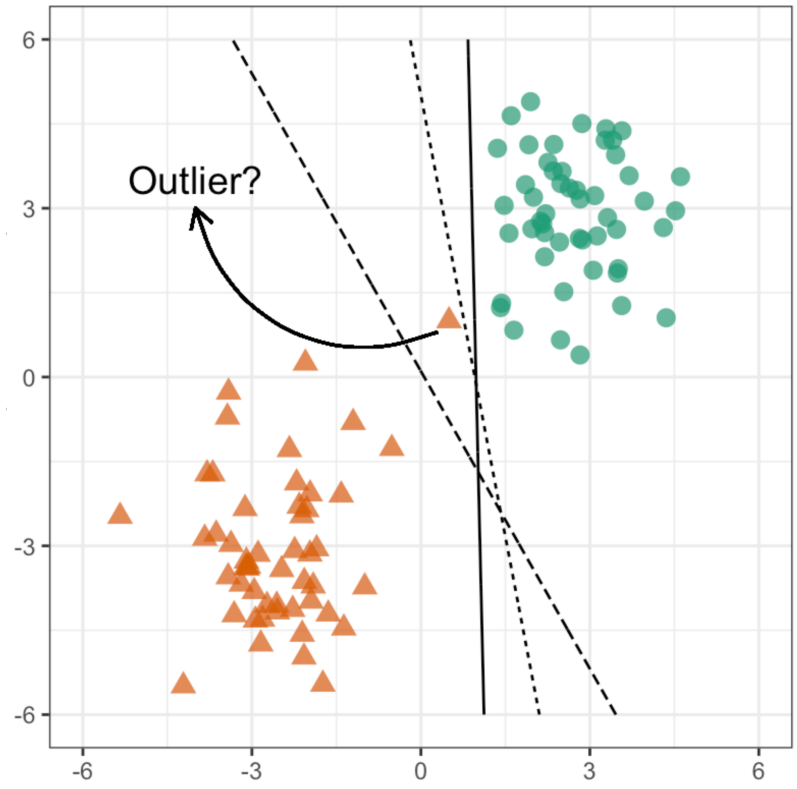


- In practice, both issues are present
  - Combine soft margin SVM and non-linear kernel transforms

Soft-Margin SVM: Advantages

- Even with linearly separable data, improve E_{out} using soft margin SVM at the cost of worse E_{in}
  - Trade-off between in-sample and out-of-sample performance
- E.g., outliers force a smaller margin
  - Ignoring outliers could increase margin
- Large C parameter in SVM requires minimizing error, trading off large margin for correct classification





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Primal Formulation for Soft Margin SVM

- You want to introduce an error measure based on the margin violation for each point, so instead of the constraint:

$$y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) \geq 1 \text{ (hard margin)}$$

- You can use:

$$y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) \geq 1 - \xi_i, \text{ where } \xi_i \geq 0 \text{ (soft margin)}$$

- The cumulative margin violation is $C \sum_{i=1}^{N} \xi_i$
- The soft margin SVM optimization (primal form) is:

$$\text{find } \underline{\boldsymbol{w}}, b, \underline{\boldsymbol{\xi}}$$

$$\text{minimize} \quad \frac{1}{2} \underline{\boldsymbol{w}}^T \underline{\boldsymbol{w}} + C \sum_{i=1}^{N} \xi_i$$

$$\text{subject to} \quad y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) \geq 1 - \xi_i \; \forall i$$

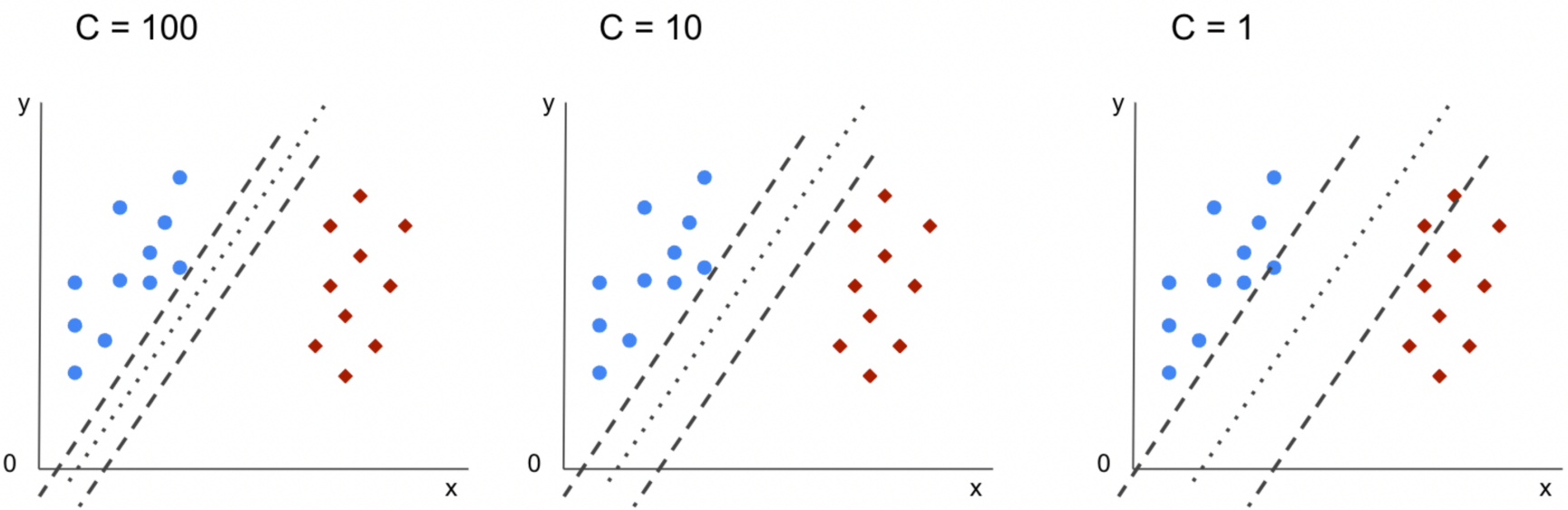
$$\xi_i \geq 0$$

Classes of Support Vectors for Soft Margin SVM

- There are 3 classes of points:
  - **Margin support vectors**: they are exactly on the margin and define it
    - In primal form: $y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) = 1 \iff \xi_i = 0$
    - In dual form: $0 < \alpha_i < C$
  - **Non-margin support vectors**: they are inside the margin and classified correctly or not
    - In primal form: $y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) < 1 \iff \xi_i > 0$
    - In dual form: $\alpha_i = C$
  - **Non-support vectors**, i.e., interior points:
    - In primal form: $y_i(\underline{\boldsymbol{w}}^T \underline{\boldsymbol{x}}_i + b) > 1$
    - In dual form: $\alpha_i = 0$

Intuition for C in SVM

- C represents how much penalty you incur for passing the margin
  - If C is large, then SVM will try to fit all the points to avoid being penalized
    - Lower bias / higher variance
    - $C \to \infty$ which yields hard-margin SVM
  - If C is small, then you allow margin violations
    - Higher bias / lower variance
- From another point of view $C \propto \frac{1}{\lambda}$, so large C means small λ and thus small regularization
  - C is chosen through cross validation, like any regularization parameter



Multi-Class Classification for SVM

- Often SVM packages have built-in multi-class classification
- Otherwise use the one-vs-all method:
  - Train K SVMs distinguishing each class from the rest using one-hot encoding
    - Get SVM parameters $(\underline{\boldsymbol{w}}_1, b_1), ..., (\underline{\boldsymbol{w}}_K, b_k)$
  - For a new example $\underline{\boldsymbol{x}}$ compute $\underline{\boldsymbol{w}}_i^T \underline{\boldsymbol{x}} + b_i$ for all the models
  - Pick the model that gives the largest positive value
    - I.e., more confident about its class vs the rest of the classes

- Support Vector Machines (Optional)
- ***Similarity-Based Models***

Similarity-Based Models: Intuition

- **Idea**: the model evaluated in one point $h(\underline{\boldsymbol{x}})$ is affected by:
  - Other data points in the training set $(\underline{\boldsymbol{x}}_n, y_n) \in \mathcal{D}$
  - The effect is based on the distance $d(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}_n) = \|\underline{\boldsymbol{x}} - \underline{\boldsymbol{x}}_n\|$
- The model is the sum of the effect of each point in the training set, scaled down by the distance
  - The model is a superposition of effects

$$h(\underline{\boldsymbol{x}}) = \sum_i \text{ effect of } h(\underline{\boldsymbol{x}}_i) \text{ scaled by } d(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}_i)$$

- This approach allows to define complex decision boundaries

Similarity-Based Models: Gaussian Kernels

- Consider a Gaussian kernel with a "landmark" point $\underline{\boldsymbol{x}}_i$ and a similarity distance defined as:

$$K(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}_i) = \exp(-\frac{\|\underline{\boldsymbol{x}} - \underline{\boldsymbol{x}}_i\|^2}{2\sigma^2})$$

- E.g., the hypothesis model has the form:

$$h(\underline{\boldsymbol{x}}) = \sum_{i=1}^{3} y_i K(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}_i) = y_1 K(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}_1) + y_2 K(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}_2) + y_3 K(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}_3)$$

  - The response is weighting the responses $y_i = \{0, 1\}$ through the similarity of $\underline{\boldsymbol{x}}$ from the landmark points
  - This can be seen by plotting $h(\underline{\boldsymbol{x}})$ on a plane

Radial Basis Function Model

- Aka RBF
- The model form for **regression** is:

$$h(\underline{\boldsymbol{x}}) = \sum_{i=1}^{N} w_i \exp(-\gamma \|\underline{\boldsymbol{x}} - \underline{\boldsymbol{x}}_i\|^2)$$

  where:

  - If γ is small, the exponential falls off slowly, and multiple training points affect a point between them
  - If γ is large, there are spikes centered in the training points and nothing outside

- For **classification** use a similar approach to "linear regression for classification"

  - Fit a regression model:

$$s(\underline{\boldsymbol{x}}) = \sum_{i=1}^{N} w_i \exp(-\gamma \|\underline{\boldsymbol{x}} - \underline{\boldsymbol{x}}_i\|^2)$$

  - Take the sign to make predictions:

$$h(\boldsymbol{x}) = \text{sign}(s(\boldsymbol{x}))$$

RBF: Block Diagram

- One can represent graphically an RBF model
  - The (fixed by learning) params, one for each training point
  - The weights depending on the distance of the input to the examples
  - The weighted params are summed together

RBF: Reducing Model VC Dimension

- Some variants for RBF:
  - Add a bias term
  - Use different γ_i for each point, i.e., different influence of different points
  - Then the number of degrees of freedom increases even more
- In RBF there are many parameters:
  - There are as many parameters $\underline{\boldsymbol{w}}$ as data points N (e.g., $N = 10^9$)
  - One parameter w_i per training point (e.g., N can be 10^6)
  - Cons: negative consequences on generalization error
- To reduce number of parameters
  - Pick $K \ll N$ centers $\underline{\boldsymbol{\mu}}_1, ..., \underline{\boldsymbol{\mu}}_K$ instead of $\underline{\boldsymbol{x}}_1, ..., \underline{\boldsymbol{x}}_N$
    - We can use k-means clustering to find the centers
    - Note: this doesn't burn the training set since this is unsupervised learning and we don't use the labels
  - Same as RBF model using the distances from the centers of the clusters:

$$h(\underline{\boldsymbol{x}}) = \sum_{i=1}^{K} w_i \exp(-\gamma \|\underline{\boldsymbol{x}} - \underline{\boldsymbol{\mu}}_i\|^2)$$

- Still a lot of parameters because:
  - K (scalar) weights w_k
  - K reference points $\underline{\boldsymbol{\mu}}_k$ (d-dimensional vectors)

RBF: Learning Models

- We want to learn w_i, γ, with fixed centers $\underline{\boldsymbol{\mu}}_i$, for an RBF model:

$$h(\underline{\boldsymbol{x}}) = \sum_{i=1}^{K} w_i \exp(-\gamma \|\underline{\boldsymbol{x}} - \underline{\boldsymbol{\mu}}_i\|^2)$$

- **Minimize:**

$$E_{in} = \sum_i (h_{\underline{\boldsymbol{w}},\gamma}(\underline{\boldsymbol{x}}_i) - y_i)^2 = f(\underline{\boldsymbol{w}}, \gamma)$$

  - Use an iterative approach (e.g., EM, coordinate descent)

Learning RBF Models

- Use iterative approach (similar to EM algorithm):
  - Fix γ, solve for $\underline{\boldsymbol{w}}$ (using one-step learning)
  - Fix $\underline{\boldsymbol{w}}$, solve for γ (with gradient descent)
- **Step 1**
  - Assume that γ is known and fixed
  - Learn $\underline{\boldsymbol{w}}$
- We can impose perfect interpolation:

$$E_{in} = \frac{1}{n}\sum(h(\underline{\boldsymbol{x}}_i) - y_i)^2 = 0$$

and get the problem:

$$h(\underline{\boldsymbol{x}}_j) = \sum_i w_i \exp(-\gamma\|\underline{\boldsymbol{x}}_i - \underline{\boldsymbol{x}}_j\|^2) = \sum_i w_i \phi_{i,j} = \underline{\phi}_j^T \underline{\boldsymbol{w}} = y_i$$

  - We have N equations (one per point) and N unknowns $\underline{\boldsymbol{w}}$
  - $\underline{\underline{\boldsymbol{\Phi}}}$ is known since it is function of the data set and γ
- The problem in matrix form is like: $\underline{\underline{\boldsymbol{\Phi}}} \cdot \underline{\boldsymbol{w}} = \underline{\boldsymbol{y}}$

Learning RBF Models

- The problem in matrix form is like

$$\underline{\underline{\mathbf{\Phi}}} \cdot \underline{\boldsymbol{w}} = \underline{\boldsymbol{y}}$$

  - If $\underline{\underline{\mathbf{\Phi}}}$ is invertible, then $\underline{\boldsymbol{w}} = \underline{\underline{\mathbf{\Phi}}}^{-1}\underline{\boldsymbol{y}}$
    - We have the desired values on the training points and the exponential interpolates in the other points
  - If $\underline{\underline{\mathbf{\Phi}}}$ is not invertible, optimize the problem in a least square sense:

$$\text{argmin}_{\underline{\boldsymbol{w}}} E_{in} = \sum_i (h(\underline{\boldsymbol{x}}_j) - y_i)^2$$

    - Compute the pseudo-inverse (assuming $\underline{\underline{\mathbf{\Phi}}}^T\underline{\underline{\mathbf{\Phi}}}$ is invertible)
    - Assign the weights as:

$$\underline{\boldsymbol{w}} = (\underline{\underline{\mathbf{\Phi}}}^T\underline{\underline{\mathbf{\Phi}}})^{-1}\underline{\underline{\mathbf{\Phi}}}^T\underline{\boldsymbol{y}}$$

- **Step 2**
  - Assume that $\underline{\boldsymbol{w}}$ is known and fixed
  - Learn γ