Lecture 10: Kernel Methods and Support Vector Machines

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WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

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A Brief History

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- **Key Papers:**
  - **1992 (Linearly Separable):** Boser, Guyon, and Vapnik introduce the optimal margin classifier.
    - Solution is a linear combination of “supporting patterns” (Support Vectors).
  - **1995 (Non-Separable):** Cortes and Vapnik extend the idea to non-separable data (the “Soft Margin”).
    - Introduces non-linear mapping to a high-dimension feature space.

Motivation: Reframing Classification Losses

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- Let's see how our loss functions change with this new y_n.

Motivation: Deriving the MSE Loss

- For Least Squares, let's assume bias e_0 is component 0. Define $\tilde{\mathbf{w}} = \frac{1}{2}(\mathbf{w} + e_0)$ (this is a one-to-one mapping).

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- The derivation becomes:

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4\sum_{n=1}^{N}(\tilde{y}_n - \mathbf{x}_n^\top \tilde{\mathbf{w}})^2 &= 4\sum_{n=1}^{N}(\frac{1}{2}(y_n + 1) - \frac{1}{2}\mathbf{x}_n^\top(\mathbf{w} + e_0))^2 \\
&= \sum_{n=1}^{N}((y_n + 1) - \mathbf{x}_n^\top(\mathbf{w} + e_0))^2 = \sum_{n=1}^{N}(y_n - \mathbf{x}_n^\top \mathbf{w})^2 \\
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- In step (a), we used $y_n^2 = 1$ (since $y_n \in \{\pm 1\}$).

- This gives the MSE loss in margin form:

$$
\text{MSE}(z, y) = (1 - yz)^2 \quad \text{where } z = \mathbf{x}_n^\top \mathbf{w}
$$

Motivation: Deriving the Logistic Loss

- For Logistic Regression, we can also rewrite the loss:

$$\sum_{n=1}^{N} \log(1 + e^{\mathbf{x}_n^\top \mathbf{w}}) - \tilde{y}_n \mathbf{x}_n^\top \mathbf{w} = \sum_{n=1}^{N} \log(1 + e^{-y_n \mathbf{x}_n^\top \mathbf{w}})$$

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- This is easily seen by checking the two cases:
  - $\tilde{y}_n = 1 \leftrightarrow y_n = 1$:

$$\begin{aligned} \log(1 + e^{\mathbf{w}^\top \mathbf{x}}) - \mathbf{w}^\top \mathbf{x} &= \log(e^{\mathbf{w}^\top \mathbf{x}}(e^{-\mathbf{w}^\top \mathbf{x}} + 1)) - \mathbf{w}^\top \mathbf{x} && (1) \\ &= \log(e^{\mathbf{w}^\top \mathbf{x}}) + \log(1 + e^{-\mathbf{w}^\top \mathbf{x}}) - \mathbf{w}^\top \mathbf{x} && (2) \\ &= \log(1 + e^{-\mathbf{w}^\top \mathbf{x}}) && (3) \end{aligned}$$

  - $\tilde{y}_n = 0 \leftrightarrow y_n = -1$:

$$\log(1 + e^{\mathbf{w}^\top \mathbf{x}}) - 0 = \log(1 + e^{-(-1)\mathbf{w}^\top \mathbf{x}}) \quad (4)$$

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$$= \log(e^{\mathbf{w}^\top \mathbf{x}}) + \log(1 + e^{-\mathbf{w}^\top \mathbf{x}}) - \mathbf{w}^\top \mathbf{x} \tag{2}$$

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- This gives the Logistic loss in margin form:

$$\text{LogisticLoss}(z, y) = \log(1 + \exp(-yz))$$

Motivation: The Hinge Loss (SVM)

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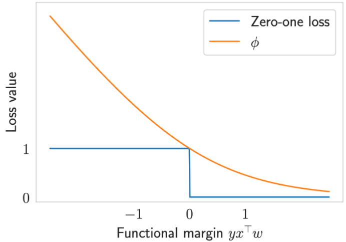
- ...and adding a regularization term.
- This leads directly to the SVM optimization problem we will study.

The 0-1 Loss and Convex Relaxations

- The "ideal" loss for classification is the Zero-one loss:

$$L_{0-1}(\eta) = \mathbf{1}_{\eta<0} \quad \text{where } \eta = y\mathbf{x}^\top \mathbf{w}$$



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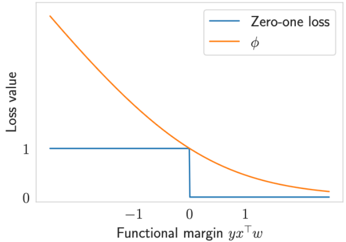

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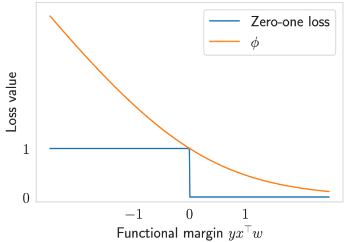

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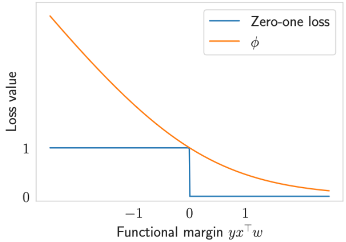
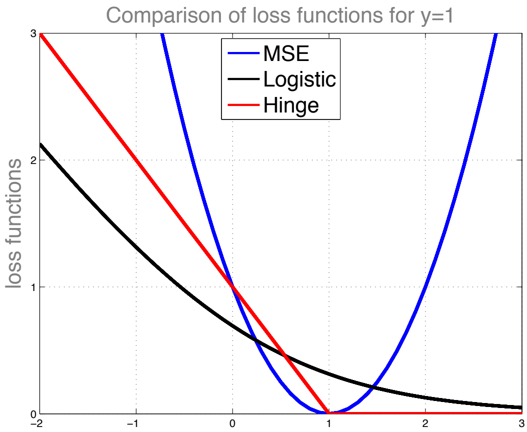
- **Solution:** We replace the 0-1 loss with a convex surrogate (an upper bound) that is easier to minimize.



Comparison of Loss Functions



- **MSE:** Penalizes all points, even correctly classified ones. Symmetric.

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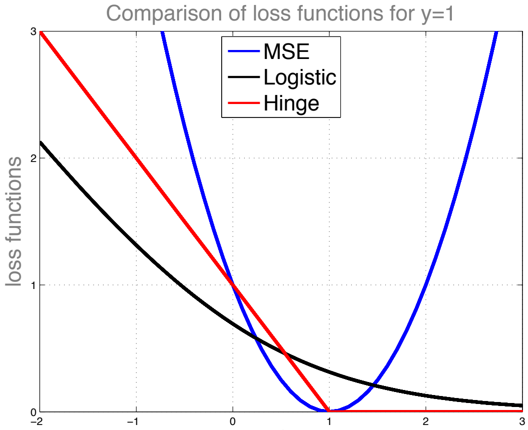

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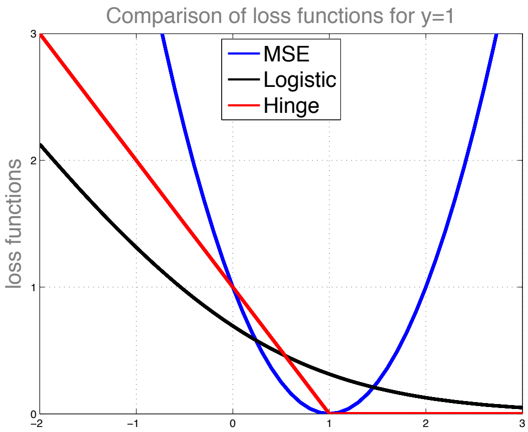

- **MSE:** Penalizes all points, even correctly classified ones. Symmetric.
- **Logistic:** Always incurs a cost, but it's asymmetric.
- **Hinge:** No cost if a point is "sufficiently far" on the correct side (i.e., $y_n \mathbf{x}_n^\top \mathbf{w} \geq 1$). Creates a margin.

Support Vector Machine Optimization Problem

SVMs solve the following optimization problem:

$$\min_{\mathbf{w}} \underbrace{\frac{1}{N}\sum_{n=1}^{N}\left[1 - y_n \mathbf{x}_n^\top \mathbf{w}\right]_+}_{\text{Hinge Loss (Empirical Risk)}} + \underbrace{\frac{\lambda}{2}\left\|\mathbf{w}\right\|^2}_{\text{Regularization}}$$

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- **Geometric Meaning:** Minimizing $\|\mathbf{w}\|^2$ is equivalent to **maximizing the margin**.
- λ is a hyperparameter that controls the trade-off:
  - **Small λ:** “Harder” margin. Focus on maximizing margin. Low bias, high variance.
  - **Large λ:** “Softer” margin. Focus on minimizing classification errors. High bias, low variance.

Geometric Preliminaries: Margins

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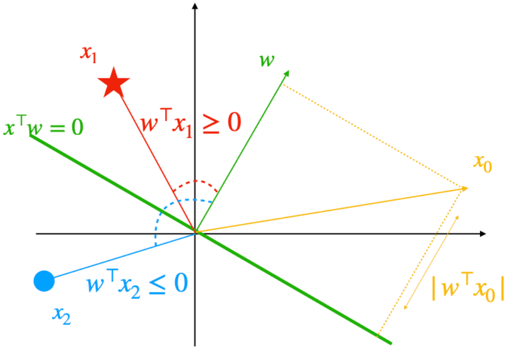

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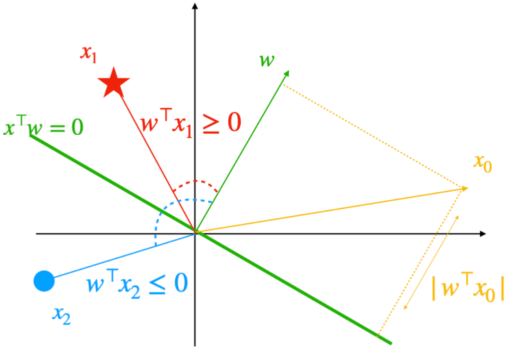

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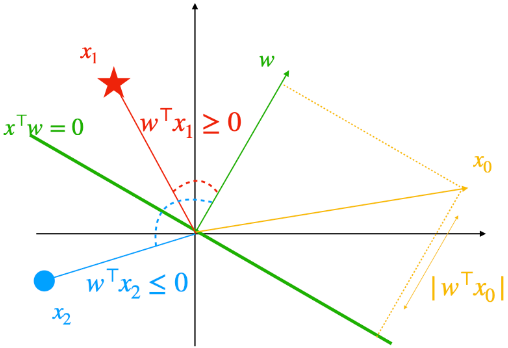

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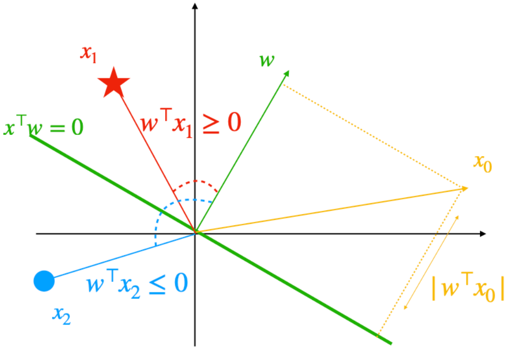
- The functional margin for a point $(\mathbf{x}_n, y_n)$ is $y_n(\mathbf{x}_n^\top \mathbf{w})$.
  - $g(\mathbf{x}_n) = y_n \iff$ functional margin is positive.



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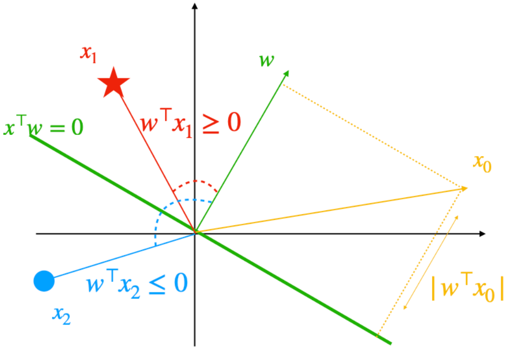
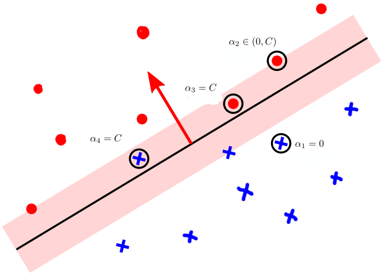
- The functional margin for a point $(\mathbf{x}_n, y_n)$ is $y_n(\mathbf{x}_n^\top \mathbf{w})$.
    - $g(\mathbf{x}_n) = y_n \iff$ functional margin is positive.
- We can rescale $\mathbf{w}$ without changing the hyperplane, but it changes the functional margin. The geometric margin is invariant.



Geometric Interpretation: The Margin



- The separating hyperplane is $\mathbf{x}^\top \mathbf{w} = 0$.

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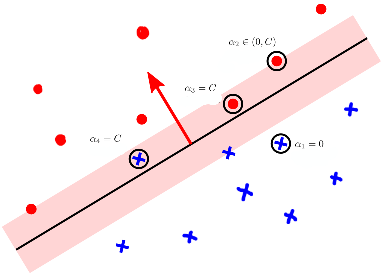

- The separating hyperplane is $\mathbf{x}^\top \mathbf{w} = 0$.
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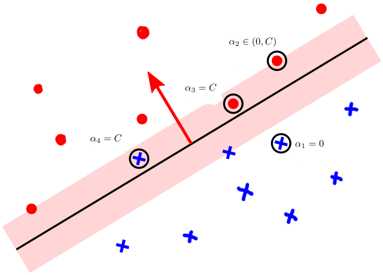

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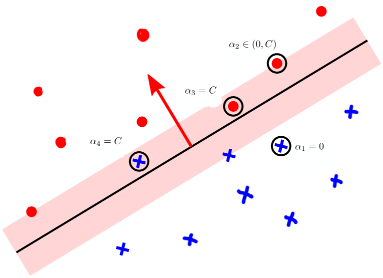

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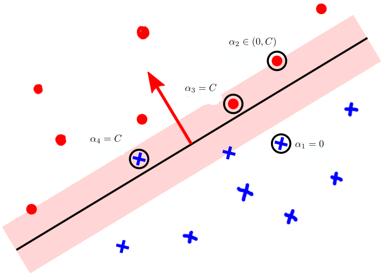

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- **Maximizing the margin** $\left(\frac{2}{\|\mathbf{w}\|}\right)$ is the same as **minimizing** $\|\mathbf{w}\|^2$.

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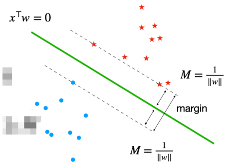
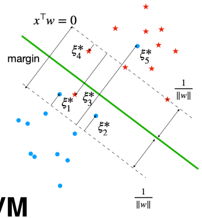
(III) Minimize $\|\mathbf{w}\|^2$ (Standard Form) Rescale $\mathbf{w}$ so the functional margin for the closest points is 1. Then minimize $\|\mathbf{w}\|^2$ (which maximizes geometric margin $1/\|\mathbf{w}\|$).

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|^2 \quad \text{s.t. } y_n(\mathbf{x}_n^\top \mathbf{w}) \geq 1, \forall n$$

From Hard-Margin to Soft-Margin SVM





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- Fails if data is not separable.

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- Allows for violations of the margin.
- Introduce positive “slack” variables $\xi_n \geq 0$.

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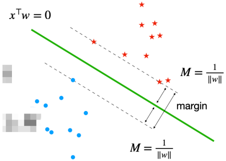

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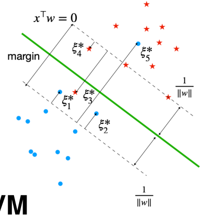

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The two formulations are equivalent. The optimal ξ_n is exactly the Hinge Loss:

$$\xi_n^* = \max(0, 1 - y_n \mathbf{x}_n^\top \mathbf{w}) = [1 - y_n \mathbf{x}_n^\top \mathbf{w}]_+$$

Optimization (Primal)

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- But this can be slow. An alternative, and very important, approach is to use duality.

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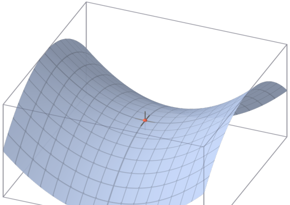
- For SVM, the domains are convex and G is convex in $\mathbf{w}$ and concave in $\boldsymbol{\alpha}$, so strong duality holds:



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- We can now rewrite the *entire* SVM problem:

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- This $G(\mathbf{w}, \boldsymbol{\alpha})$ is convex in $\mathbf{w}$ and concave (linear) in $\boldsymbol{\alpha}$.

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- **Crucial Insight:** The optimal weight vector $\mathbf{w}$ is a linear combination of the data points $\mathbf{x}_n$.

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- This gives the final Dual Problem:

$$\max_{\boldsymbol{\alpha} \in [0,1]^N} \ \tfrac{1}{N} \boldsymbol{\alpha}^\top \mathbf{1} - \tfrac{1}{2\lambda N^2} \boldsymbol{\alpha}^\top \mathbf{Q} \boldsymbol{\alpha}$$

where $\mathbf{Q} = \mathbf{YKY} = \mathrm{diag}(\mathbf{y}) \mathbf{XX}^\top \mathrm{diag}(\mathbf{y})$

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The dual problem is often better:

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  - The problem complexity now depends on N (samples), not D (features).
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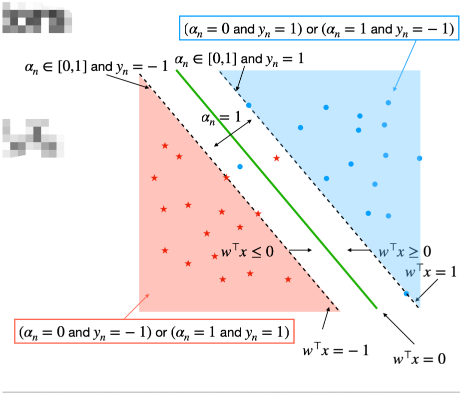
  - Most α_n will be 0.
  - The $\mathbf{w}$ vector ($\mathbf{w} = \frac{1}{\lambda N} \sum \alpha_n y_n \mathbf{x}_n$) only depends on the points $\mathbf{x}_n$ where $\alpha_n > 0$.
  - These points are the Support Vectors.

Interpretation: Support Vectors

From the KKT conditions (the optimality conditions for the dual):

- **Case 1: Point is outside margin.** $(\alpha_n = 0)$
  - $y_n \mathbf{x}_n^\top \mathbf{w} > 1$ (or $1 - y_n \mathbf{x}_n^\top \mathbf{w} < 0$).
  - The point is correctly classified with room to spare.
  - The Hinge Loss is 0.
  - This point has **no influence** on the decision boundary.



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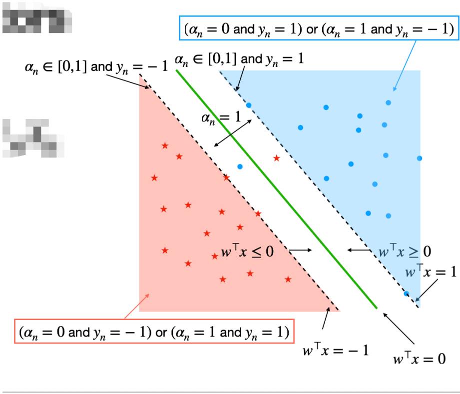
- **Case 2: Point is on the margin.** $(\alpha_n \in (0, 1])$
  - $y_n \mathbf{x}_n^\top \mathbf{w} = 1$ (or $1 - y_n \mathbf{x}_n^\top \mathbf{w} = 0$).
  - This is an Essential Support Vector. It lies exactly on the margin and holds the "street" in place.



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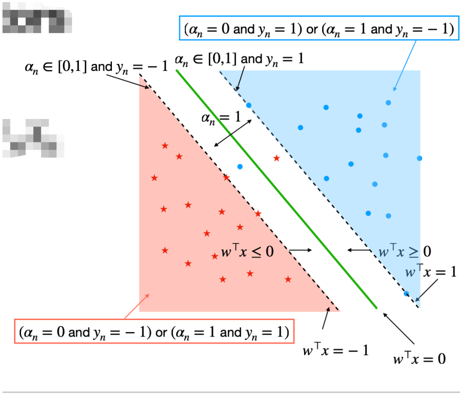
  - The point is correctly classified with room to spare.
  - The Hinge Loss is 0.
  - This point has **no influence** on the decision boundary.
- **Case 2: Point is on the margin.** ($\alpha_n \in (0, 1]$)
  - $y_n \mathbf{x}_n^\top \mathbf{w} = 1$ (or $1 - y_n \mathbf{x}_n^\top \mathbf{w} = 0$).
  - This is an Essential Support Vector. It lies exactly on the margin and holds the "street" in place.
- **Case 3: Point is inside margin or misclassified.** ($\alpha_n = 1$)
  - $y_n \mathbf{x}_n^\top \mathbf{w} < 1$ (or $1 - y_n \mathbf{x}_n^\top \mathbf{w} > 0$).
  - This is a Bound Support Vector. It is either inside the margin or on the wrong side of the hyperplane.



A Deeper Look: KKT Conditions

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Either the constraint is active (the point is on/inside the margin),
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- This is the formal reason for the three cases:
  - **Case 1: Point is outside margin.**
    - $y_n \mathbf{x}_n^\top \mathbf{w} > 1$. The constraint is *inactive* (slack).
    - KKT conditions force $\implies \alpha_n = 0$.
  - **Case 2 & 3: Point is on or inside margin.**
    - $y_n \mathbf{x}_n^\top \mathbf{w} \leq 1$. The constraint is *active* (tight).
    - KKT conditions allow $\implies \alpha_n > 0$.
    - These are the Support Vectors.

Optimization: Coordinate Ascent

Goal: Maximize the dual $g(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2\lambda N^2}\boldsymbol{\alpha}^\top \mathbf{Q}\boldsymbol{\alpha}$ subject to $\alpha_n \in [0, 1]$.

Idea: Update one coordinate at a time, keeping others fixed.

initialize $\boldsymbol{\alpha}^{(0)} \in \mathbb{R}^N$ (e.g., all zeros)
for $t = 0$ to maxIter **do**
    sample a coordinate n randomly from $1 \dots N$.
    optimize g w.r.t. that single coordinate α_n (which is just a 1D quadratic problem).
$$u^\star \leftarrow \arg\max_{u \in \mathbb{R}} g\left(\alpha_1^{(t)}, \dots, \alpha_{n-1}^{(t)}, u, \alpha_{n+1}^{(t)}, \dots, \alpha_N^{(t)}\right)$$
    clip the result to respect the “box” constraint:
$$u^\star \leftarrow \min(1, \max(0, u^\star))$$
    update $\alpha_n^{(t+1)} \leftarrow u^\star$

Issues with SVM

- There is no obvious probabilistic interpretation (unlike Logistic Regression).
  - The output is a “score” $\mathbf{x}^\top \mathbf{w}$, not a probability $p(y = 1|\mathbf{x})$.
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  - (Though this can be mitigated with “Platt Scaling”).
- Extension to multi-class classification is non-trivial. Common approaches:
  - **One-vs-Rest (OvR):** Train K binary classifiers (class k vs. all others).
  - **One-vs-One (OvO):** Train $\frac{K(K-1)}{2}$ binary classifiers (class i vs. class j).

Table of Contents

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- Let's see if this property holds for other algorithms, like Ridge Regression.
- This will lead us to a powerful general idea: the Kernel Trick.
- This trick allows us to use highly complex, non-linear, and even infinite-dimensional feature maps *without* paying the computational cost.

Alternative Formulation of Ridge Regression

Recall the **primal** problem for Ridge Regression:

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \left\| \mathbf{y} - \mathbf{X}\mathbf{w} \right\|^2 + \frac{\lambda}{2} \left\| \mathbf{w} \right\|^2$$

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The solution $\mathbf{w}^\star \in \mathbb{R}^D$ is:

$$\mathbf{w}^\star = \frac{1}{N}\left(\frac{1}{N}\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_D\right)^{-1}\mathbf{X}^\top\mathbf{y}$$

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- But what if $D \gg N$? (e.g., 100 samples, 1,000,000 features)

Alternative Formulation (Dual)

We claim the solution can be written alternatively as:

$$\mathbf{w}^\star = \frac{1}{N}\mathbf{X}^\top \left(\frac{1}{N}\mathbf{X}\mathbf{X}^\top + \lambda \mathbf{I}_N\right)^{-1}\mathbf{y} \tag{5}$$

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This relies on the “push-through” matrix identity:

$$(\mathbf{PQ} + \mathbf{I}_N)^{-1}\mathbf{P} = \mathbf{P}(\mathbf{QP} + \mathbf{I}_M)^{-1}$$

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- This switches a $D \times D$ inverse for an $N \times N$ inverse.

The Representer Theorem

The alternative form $\mathbf{w}^{\star} = \mathbf{X}^{\top}\boldsymbol{\alpha}^{\star}$ is not a coincidence.

$$\text{Define } \boldsymbol{\alpha}^{\star} = \frac{1}{N}\left(\frac{1}{N}\mathbf{X}\mathbf{X}^{\top} + \lambda\mathbf{I}_N\right)^{-1}\mathbf{y}. \quad \text{Then } \mathbf{w}^{\star} = \mathbf{X}^{\top}\boldsymbol{\alpha}^{\star}.$$

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The Representer Theorem (General) For any loss function $\mathcal{L}_n$, the solution $\mathbf{w}^\star$ to:

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Proof (Intuition): Decompose $\mathbf{w} = \mathbf{w}_\parallel + \mathbf{w}_\perp$, where $\mathbf{w}_\parallel$ is in the span of $\mathbf{X}$ and $\mathbf{w}_\perp$ is orthogonal to it.

- The loss term $\mathcal{L}_n$ only depends on $\mathbf{x}_n^\top \mathbf{w} = \mathbf{x}_n^\top \mathbf{w}_\parallel$.
- The regularization term $\|\mathbf{w}\|^2 = \|\mathbf{w}_\parallel\|^2 + \|\mathbf{w}_\perp\|^2$.
- To minimize the cost, we must set $\mathbf{w}_\perp = 0$. Thus, $\mathbf{w}^\star = \mathbf{w}_\parallel^\star \in \text{span}(\mathbf{X})$.

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  So, $l(\mathbf{x}_n^\top \mathbf{w}^*, y_n) = l(\mathbf{x}_n^\top \mathbf{w}_\parallel, y_n)$.

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- **Conclusion:** The total cost for $\mathbf{w}_{||}$ is always less than or equal to the cost for $\mathbf{w}^*$.

Kernelized Ridge Regression

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- The dual problem only depends on the data through the kernel matrix $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$.

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The Kernel Matrix

- The dual formulations for SVM and Ridge Regression depend only on the $N \times N$ matrix $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$.
- This is called the Kernel Matrix or Gram Matrix.
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- This matrix is symmetric ($\mathbf{K} = \mathbf{K}^\top$) and positive semi-definite ($\mathbf{K} \geq 0$).

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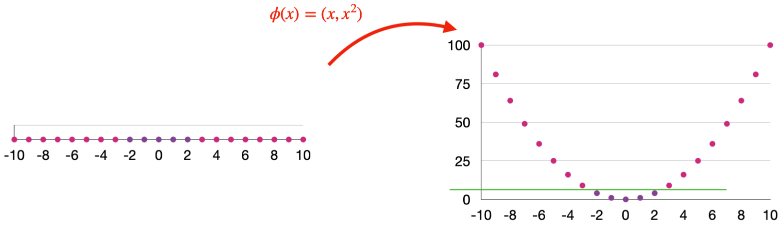
- **Example:** Data not linearly separable in 1D.



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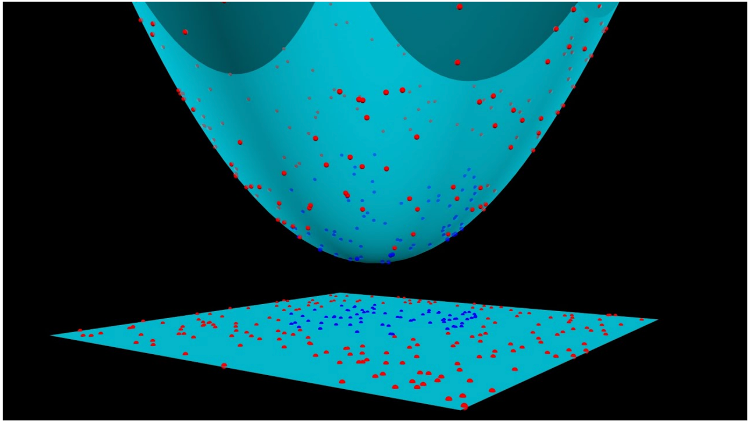
- This is too expensive, or impossible if $\tilde{D} = \infty$.

Usefulness of Feature Spaces

Data that is not linearly separable in 2D...



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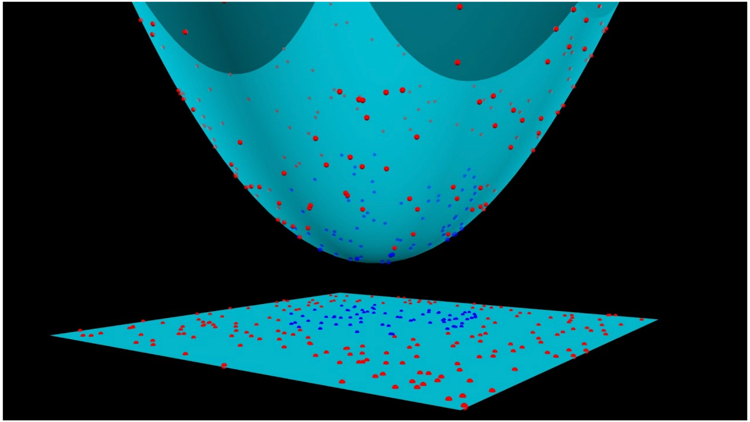

...can become linearly separable when mapped to a higher dimension (3D).

The Kernel Trick: The "Shortcut"

The Kernel Trick: If we can find a kernel function $\kappa(\mathbf{x}, \mathbf{x}')$ that computes the inner product in the feature space *directly*, we never need to build $\phi(\mathbf{x})$.

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- We only need to compute the $N \times N$ kernel matrix $\mathbf{K}_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$.
- All “kernelized” algorithms (like SVM dual, Ridge dual) only need $\mathbf{K}$.
- We can work in an incredibly high-dimensional space, as long as we have an efficient $\kappa(\cdot, \cdot)$.

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- The kernel function is a huge computational shortcut!

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Building New Kernels from Old

If κ_1 and κ_2 are valid kernels, so are:

- **Positive Scaling:** $\kappa(\mathbf{x}, \mathbf{x}') = c\,\kappa_1(\mathbf{x}, \mathbf{x}')$ for $c \geq 0$.

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- **Function mapping:** $\kappa(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})f(\mathbf{x}')$ for any real-valued f.

Proofs for Building Kernels

- **Proof (Sum):** $\kappa(\mathbf{x}, \mathbf{x}') = \alpha\kappa_1(\mathbf{x}, \mathbf{x}') + \beta\kappa_2(\mathbf{x}, \mathbf{x}')$
  - We can define a new feature map $\phi(\mathbf{x})$ by concatenating the scaled original feature maps:
$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} \sqrt{\alpha}\boldsymbol{\phi}_1(\mathbf{x}) \\ \sqrt{\beta}\boldsymbol{\phi}_2(\mathbf{x}) \end{bmatrix} \in \mathbb{R}^{D_1+D_2}$$
  - The inner product is then:
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  - We define a new feature map $\phi(\mathbf{x})$ as the tensor (outer) product of the original features.
  - The new feature vector contains all possible products $(\phi_1(\mathbf{x}))_i(\phi_2(\mathbf{x}))_j$.
  - The inner product becomes:
$$\begin{aligned}
\phi(\mathbf{x})^\top\phi(\mathbf{x}') &= \sum_{i,j}(\phi_1(\mathbf{x}))_i(\phi_2(\mathbf{x}))_j(\phi_1(\mathbf{x}'))_i(\phi_2(\mathbf{x}'))_j \\
&= \left(\sum_i(\phi_1(\mathbf{x}))_i(\phi_1(\mathbf{x}'))_i\right)\left(\sum_j(\phi_2(\mathbf{x}))_j(\phi_2(\mathbf{x}'))_j\right) \\
&= \kappa_1(\mathbf{x}, \mathbf{x}')\kappa_2(\mathbf{x}, \mathbf{x}')
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2. The kernel matrix $\mathbf{K}$ is **positive semi-definite** for *any* set of points $\{\mathbf{x}_n\}_{n=1}^N$.

$$\mathbf{K}_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j) \Longrightarrow \mathbf{c}^\top \mathbf{K} \mathbf{c} \geq 0 \text{ for all } \mathbf{c} \in \mathbb{R}^N$$

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- This creates a non-linear model in the original input space, but one that is still linear (and convex) in a new, high-dimensional feature space.
- The Kernel Trick is that we can do this *without ever computing* the feature maps $\phi(\mathbf{x})$, which can be very high-dim or even infinite-dim.

Recap: Key Ideas

- Many algorithms (SVM, Ridge Regression, PCA) can be "kernelized" because their solutions can be written to depend only on inner products, $\mathbf{X}\mathbf{X}^\top$.
- This allows us to generalize a linear model by replacing the simple inner product $\mathbf{x}^\top\mathbf{x}'$ with a non-linear kernel function $\kappa(\mathbf{x}, \mathbf{x}')$.
- This creates a non-linear model in the original input space, but one that is still linear (and convex) in a new, high-dimensional feature space.
- The Kernel Trick is that we can do this *without ever computing* the feature maps $\phi(\mathbf{x})$, which can be very high-dim or even infinite-dim.
- To make a new prediction, we just need to compute the kernel (similarity) between the new point $\mathbf{x}$ and all the training points $\mathbf{x}_n$.