Elements of Machine Learning & Data Science

Winter semester 2025/26

Lecture 15 – Support Vector Machines II

15.12.2025

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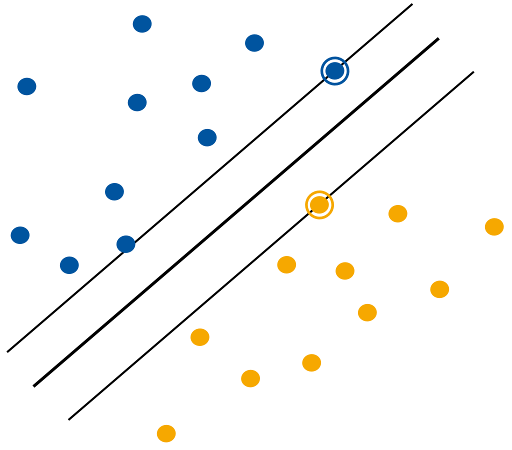
Machine Learning Topics

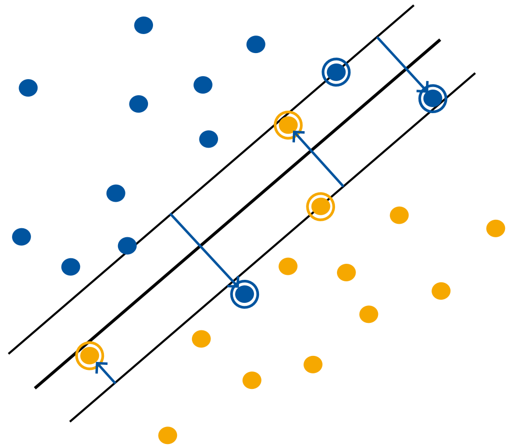
8. Introduction to ML
9. Probability Density Estimation
10. Linear Discriminants
11. Linear Regression
12. Logistic Regression
13. **Support Vector Machines**
14. Neural Network Basics



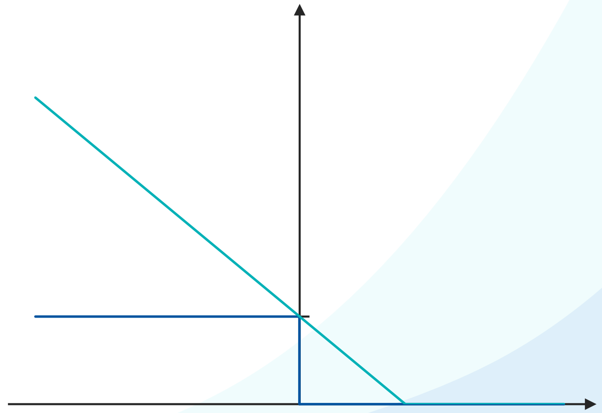
Maximum Margin Classification

$$L_p(\mathbf{w}, b, \mathbf{a})$$
$$L_d(\mathbf{a})$$

Primal & Dual Form



Soft-Margin SVM



Hinge Loss

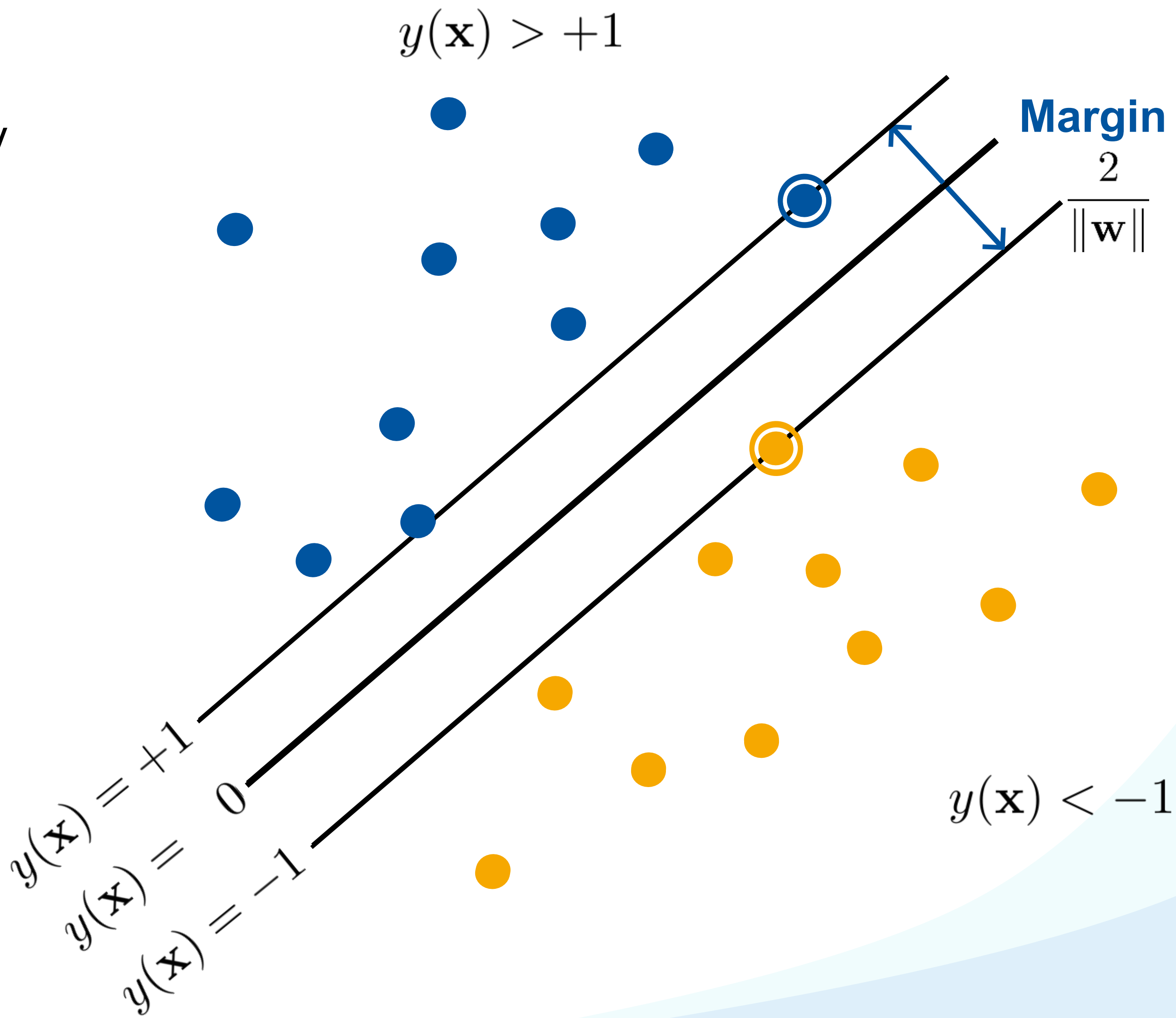
Recap: Maximum Margin Classification

- Intuitively, we want to choose the classifier which leaves maximal "safety room" for future data points.
- This classifier has the largest margin between positive and negative points.
- We can rescale $\mathbf{w}$ such that the distance of the points on the margin to the decision boundary is exactly 1.

$$t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) = 1$$

- If the data is linearly separable, then for all points, the following must hold:

$$t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \geq 1 \quad \forall n$$



- Optimization problem
  - Find the hyperplane with maximum margin by optimizing:

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

“Maximize the margin”

such that

$$t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \geq 1 \quad \forall n$$

“such that each point is on the correct side of the margin”

- This is a quadratic programming problem with linear constraints.

Recap: Primal SVM Formulation

- Recall the SVM objective:

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2, \quad \text{such that} \quad t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \geq 1 \quad \forall n$$

- We introduce positive Lagrange multipliers $a_n \geq 0$ and get the primal form of SVMs:

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left[t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) - 1\right]$$

Necessary and sufficient conditions:

$$a_n \geq 0$$
$$t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) - 1 \geq 0$$
$$a_n[t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) - 1] = 0$$

KKT conditions:

$$\lambda \geq 0$$
$$f(\mathbf{x}) \geq 0$$
$$\lambda f(\mathbf{x}) = 0$$

Recap: Dual Form of the SVM Objective

- We can equivalently reformulate the SVM to maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^{\mathsf{T}} \mathbf{x}_n)$$

under the conditions

$$a_n \geq 0 \quad \forall n$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

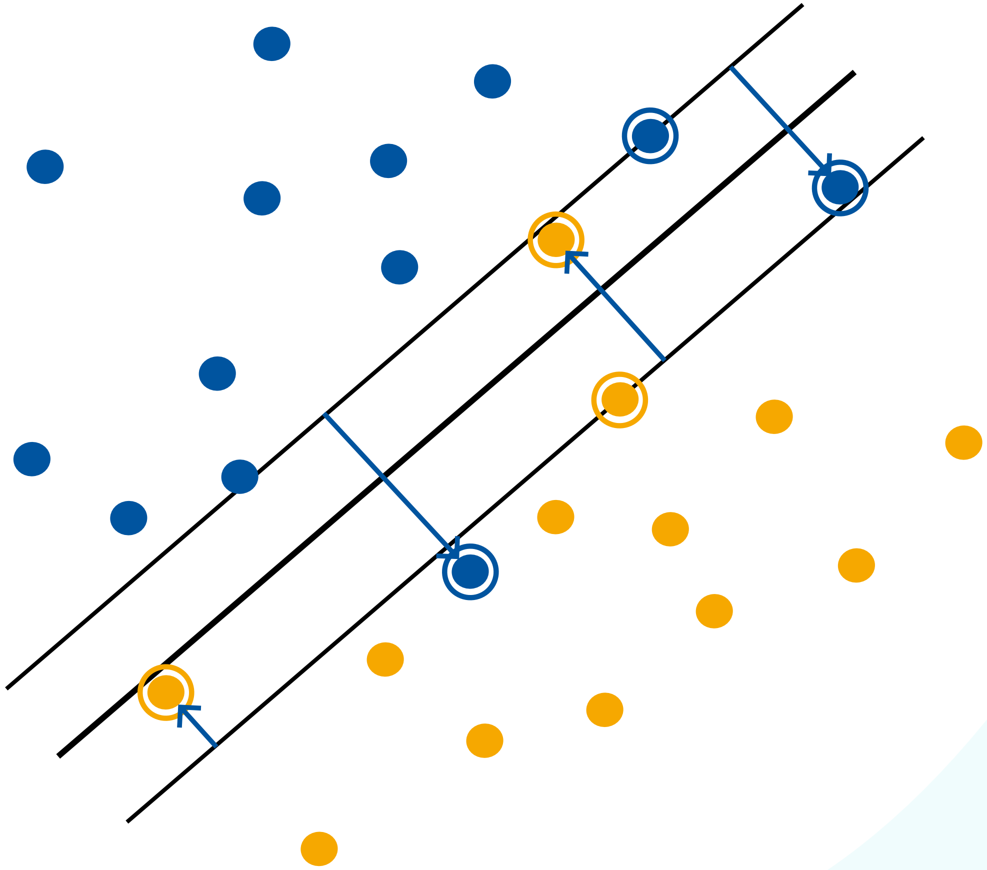
- We now have an optimization problem in N variables.

$\Rightarrow$ Complexity: $\mathcal{O}(N^3)$

For the derivation, please watch the video

Support Vector Machines

1. Maximum Margin Classification
2. Primal Formulation
3. Dual Formulation
4. **Soft-Margin SVMs**
5. Non-linear SVMs
6. Error Function Analysis

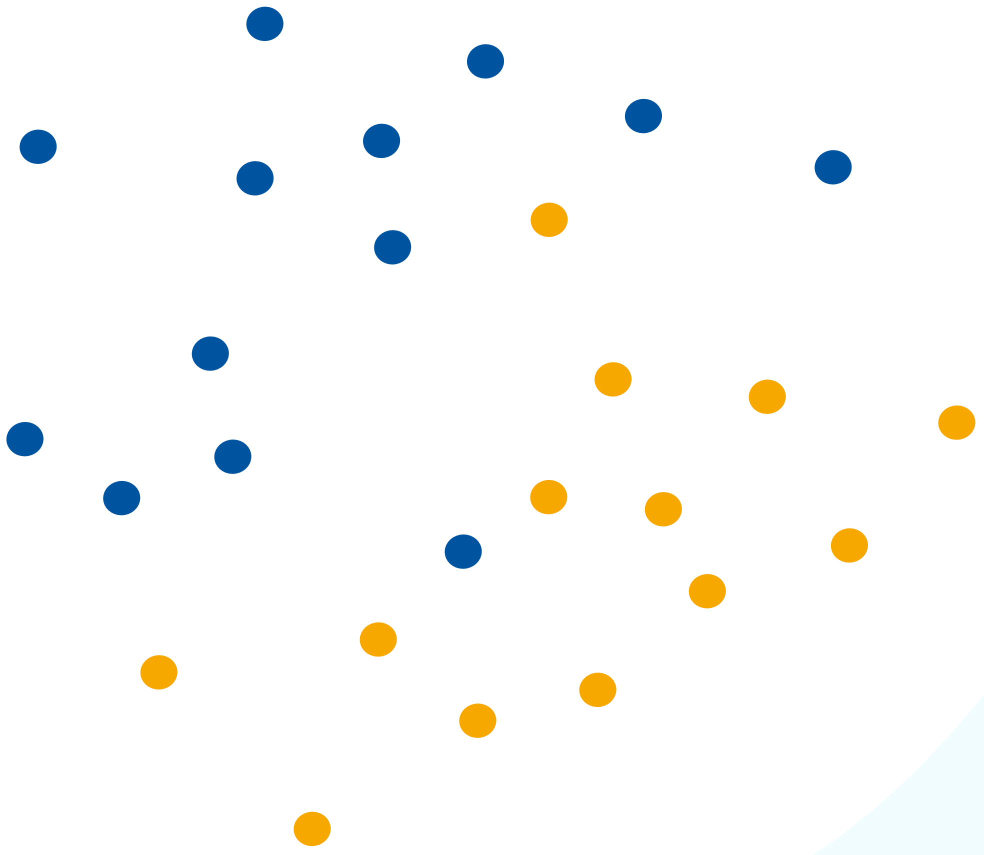


Soft-Margin SVM

- So far, we assumed linearly separable data.
  - Our current formulation has no solution if the data are not linearly separable!

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2,$$

such that $$t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \geq 1 \quad \forall n$$



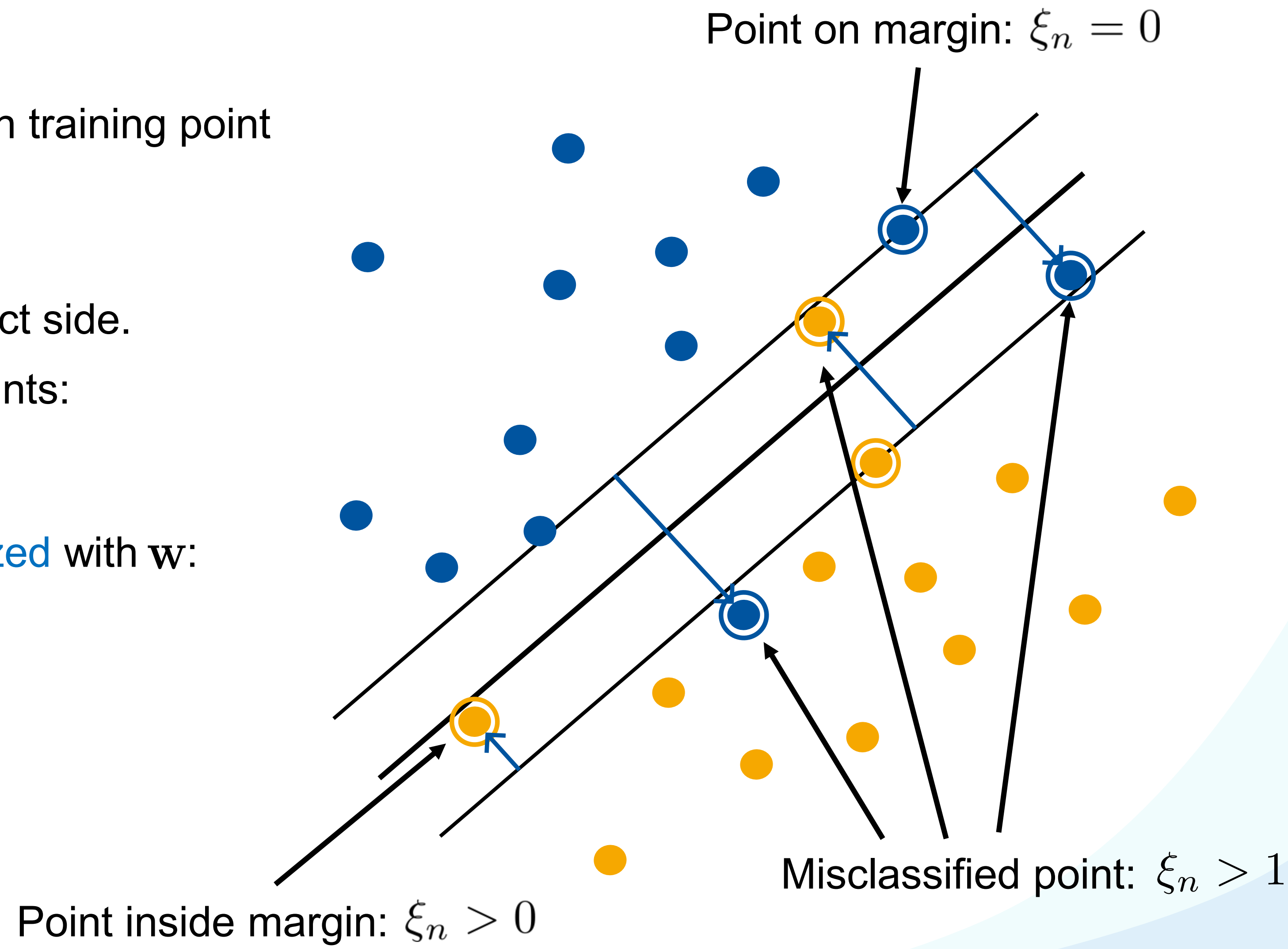
- Need to introduce tolerance to outlier data points.
  - The resulting model is called soft-margin SVM.

Recap: Soft-Margin SVM with Slack Variables

- Slack variables
  - One slack variable ξ_n for each training point
- Effect
  - $\xi_n = 0$ for points on the correct side.
  - Linear penalty for all other points:
    $\xi_n = |t_n - y(\mathbf{x}_n)|$
- Slack variables are jointly optimized with $\mathbf{w}$:

$$\min \frac{1}{2}\|\mathbf{w}\|^2 + C \sum_{n=1}^{N} \xi_n$$

where C is a tradeoff parameter.



Recap: New Primal Formulation

- Minimize

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \underbrace{\sum_{n=1}^{N} a_n \left[t_n(y(\mathbf{x}_n) - 1 + \xi_n\right]}_{\substack{\text{Constraint} \\ t_n y(\mathbf{x}_n) \geq 1 - \xi_n}} - \underbrace{\sum_{n=1}^{N}\mu_n\xi_n}_{\substack{\text{Constraint} \\ \xi_n \geq 0}}$$

- KKT conditions

$$\begin{aligned} a_n &\geq 0 & \mu_n &\geq 0 \\ t_n y(\mathbf{x}_n) - 1 + \xi_n &\geq 0 & \xi_n &\geq 0 \\ a_n\left[t_n y(\mathbf{x}_n) - 1 + \xi_n\right] &= 0 & \mu_n\xi_n &= 0 \end{aligned}$$

Recap: New Dual Formulation

- Maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\mathbf{x}_m^{\mathsf{T}} \mathbf{x}_n)$$

- Under the side conditions

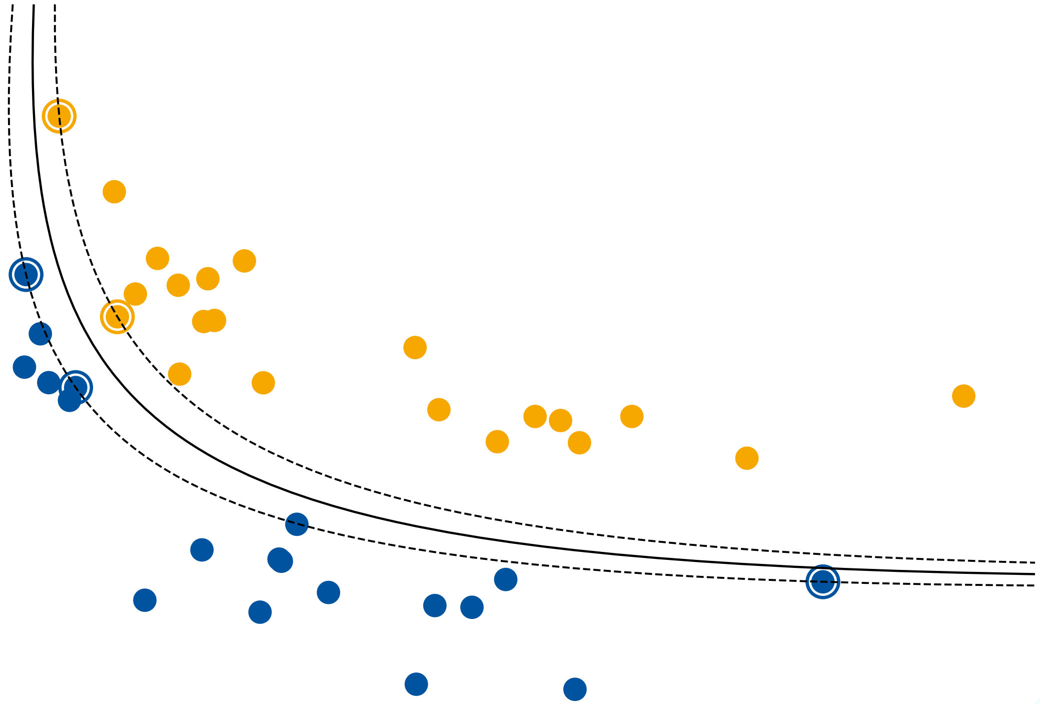
$$\boxed{0 \leq a_n \leq C \quad \forall n}$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

This is the only difference to before.

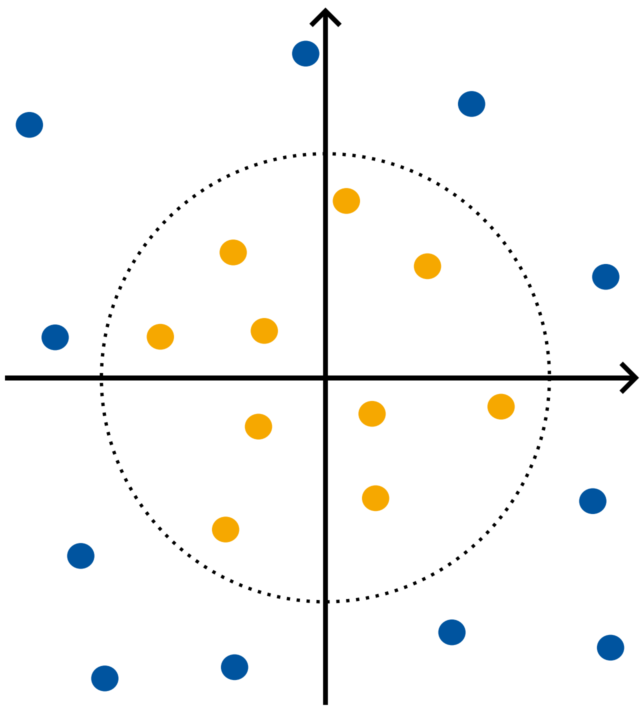
Support Vector Machines

1. Maximum Margin Classification
2. Primal Formulation
3. Dual Formulation
4. Soft-Margin SVMs
5. **Non-Linear SVMs**
6. Error Function Analysis



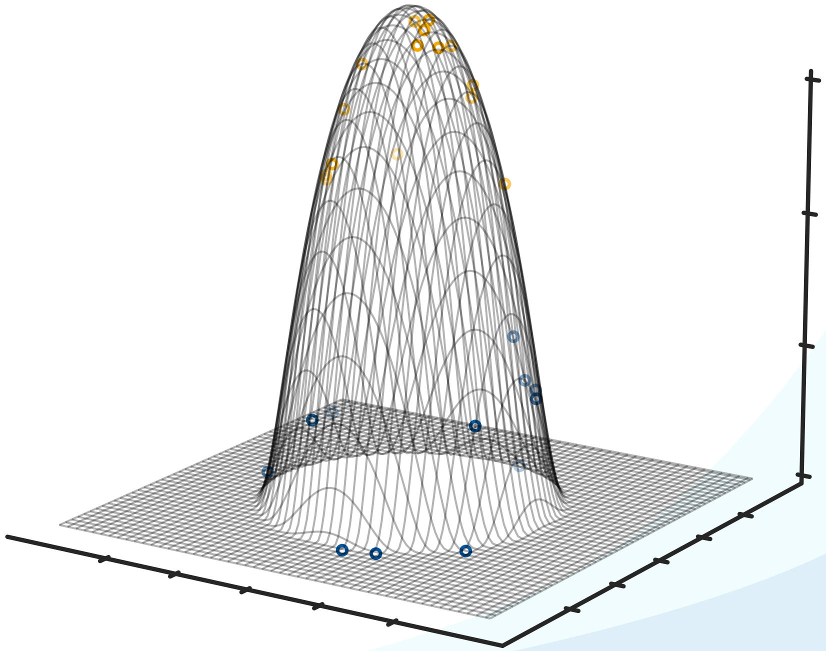
Non-Linear SVMs

- So far, we have only considered linear decision boundaries.
- We now combine non-linear basis functions with SVMs.



$$\phi : \mathbb{R}^D \to \mathbb{R}^M$$

$$M \gg D$$



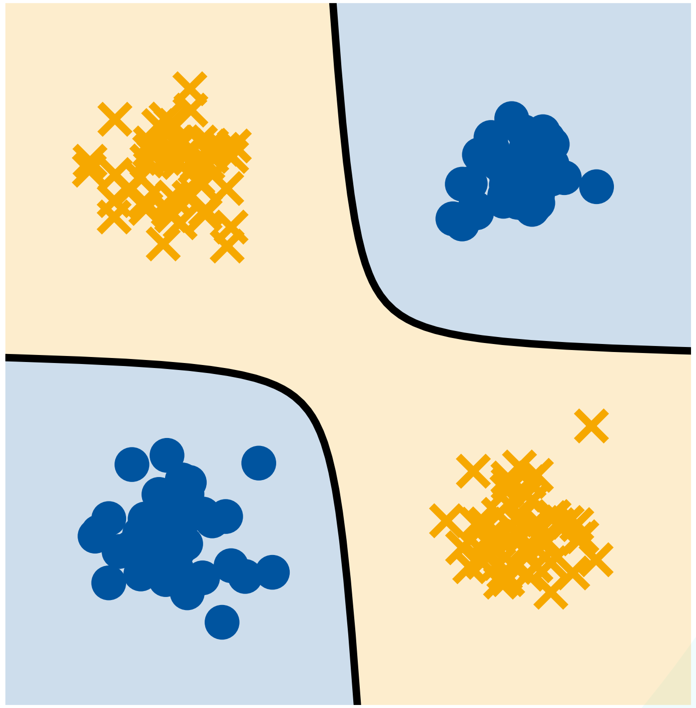
Feature Spaces

- We have already seen non-linear basis functions:
  - Apply a nonlinear transformation ϕ to the data points $\mathbf{x}_n$:
    $$\mathbf{x} \in \mathbb{R}^D, \quad \boldsymbol{\phi} : \mathbb{R}^D \rightarrow \mathbb{R}^M$$
  - Classify with a hyperplane in higher-dim. space $\mathbb{R}^M$:
    $$\mathbf{w}^\mathsf{T}\phi(\mathbf{x}) + b = 0$$

  $\Rightarrow$ Linear classifier in $\mathbb{R}^M$, nonlinear classifier in $\mathbb{R}^D$.

- Let us now apply this to SVMs…
  - We can train our SVM on the transformed features $\phi(\mathbf{x})$ to get non-linear decision boundaries.
  - Usually, $M \gg D$: evaluating $\mathbf{w}^\mathsf{T}\phi(\mathbf{x})$ can be quite expensive!

$\mathbf{x} = (x_1, x_2)^\mathsf{T}$



$\phi(\mathbf{x}) = (x_1, x_2, x_1x_2, x_1^2, x_2^2)^\mathsf{T}$

The Kernel Trick

- On a closer look, $\phi(\mathbf{x})$ only appears in the form of dot products:

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m (\boldsymbol{\phi}(\mathbf{x}_m)^\mathsf{T} \boldsymbol{\phi}(\mathbf{x}_n))$$

$$\begin{aligned} y(\mathbf{x}) &= \mathbf{w}^\mathsf{T} \boldsymbol{\phi}(\mathbf{x}) + b \\ &= \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n)^\mathsf{T} \boldsymbol{\phi}(\mathbf{x}) + b \end{aligned}$$

$$\boxed{\mathbf{w} = \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n)}$$

The Kernel Trick

- On a closer look, $\phi(\mathbf{x})$ only appears in the form of dot products:

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m (\phi(\mathbf{x}_m)^\mathsf{T}\phi(\mathbf{x}_n))$$

$$y(\mathbf{x}) = \mathbf{w}^\mathsf{T}\phi(\mathbf{x}) + b$$

$$= \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n)^\mathsf{T}\phi(\mathbf{x}) + b$$

$$k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^\mathsf{T}\phi(\mathbf{y})$$

Define a kernel function $k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^\mathsf{T}\phi(\mathbf{y})$

$\Rightarrow$ *Use the kernel instead of the dot product.*

The Kernel Trick

- On a closer look, $\phi(\mathbf{x})$ only appears in the form of dot products:

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_m, \mathbf{x}_n)$$

$$\begin{aligned} y(\mathbf{x}) &= \mathbf{w}^{\mathsf{T}}\phi(\mathbf{x}) + b \\ &= \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b \end{aligned}$$

$$\boxed{k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{y})}$$

Define a kernel function $k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{y})$

$\Rightarrow$ *Use the kernel instead of the dot product.*

- $k(\cdot, \cdot)$ implicitly maps the data to some higher-dimensional space, without having to compute $\phi(\mathbf{x})$.

When Can We Apply the Kernel Trick?

- In order for this to work, $k(\cdot,\cdot)$ needs to define an implicit mapping.
- Formally
  - A function $k(\mathbf{x}_1,\mathbf{x}_2) : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$ is a kernel function, iff
    - There is a mapping $\phi(\mathbf{x}) : \mathbb{R}^D \to \mathcal{H}$ such that

$$k(\mathbf{x}_1,\mathbf{x}_2) = \phi(\mathbf{x}_1)^{\mathsf{T}}\phi(\mathbf{x}_2) \quad \forall \mathbf{x}_1,\mathbf{x}_2$$

- *When will this be the case?*

- When is a function $k(\mathbf{x}_1, \mathbf{x}_2)$ a valid kernel function? Two ways to check:

  1. Every Gram matrix K of k is symmetric positive definite:

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

A matrix M is positive definite if all eigenvalues of K are positive.

  - This is easy to verify for a given training set $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$.
  - Unfortunately, it has to hold for *every possible* such set.

$\Rightarrow$ *Very hard to prove in practice.*

- When is a function $k(\mathbf{x}_1, \mathbf{x}_2)$ a valid kernel function? Two ways to check:

  2. We can construct valid kernels from other valid kernels:
     - Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following combinations will also be valid

$$k(\mathbf{x}, \mathbf{x}') = c \cdot k_1(\mathbf{x}, \mathbf{x}')$$
$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}')$$
$$k(\mathbf{x}, \mathbf{x}') = polynomial(k_1(\mathbf{x}, \mathbf{x}')) \quad (with\ nonnegative\ coefficients)$$
$$k(\mathbf{x}, \mathbf{x}') = \exp(k_1(\mathbf{x}, \mathbf{x}'))$$
$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}')$$
$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}')$$
$$k(\mathbf{x}, \mathbf{x}') = k_3(\boldsymbol{\phi}(x), \boldsymbol{\phi}(x'))$$
$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^{\mathsf{T}} \mathbf{A} \mathbf{x}'$$

$\Rightarrow$ *Much easier to apply in practice.*

New SVM Formulation

- Maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_m, \mathbf{x}_n)$$

under the constraints $\quad 0 \leq a_n \leq C \quad \forall n$

$$\sum_{n=1}^{N} a_n t_n = 0$$

- Classify new data points using

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

Example: Polynomial Kernel

- We slightly adjust the polynomial basis function that we know:

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

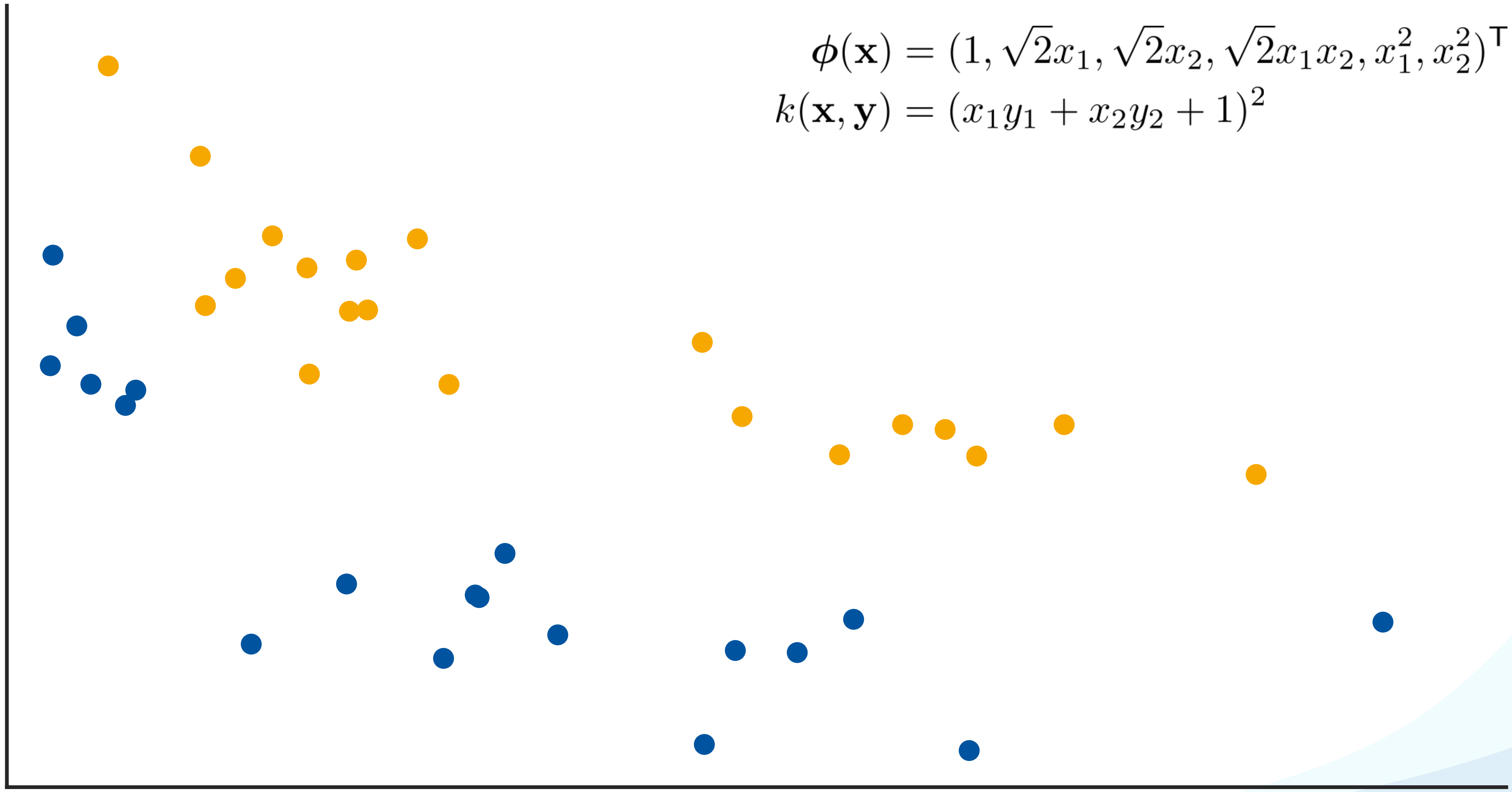
$$k(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^\top \mathbf{y} + 1)^2 = \phi(\mathbf{x})^\top \phi(\mathbf{y})$$

- In fact, $(\mathbf{x}^\top \mathbf{y} + 1)^p$ is the kernel function for a polynomial of degree p.

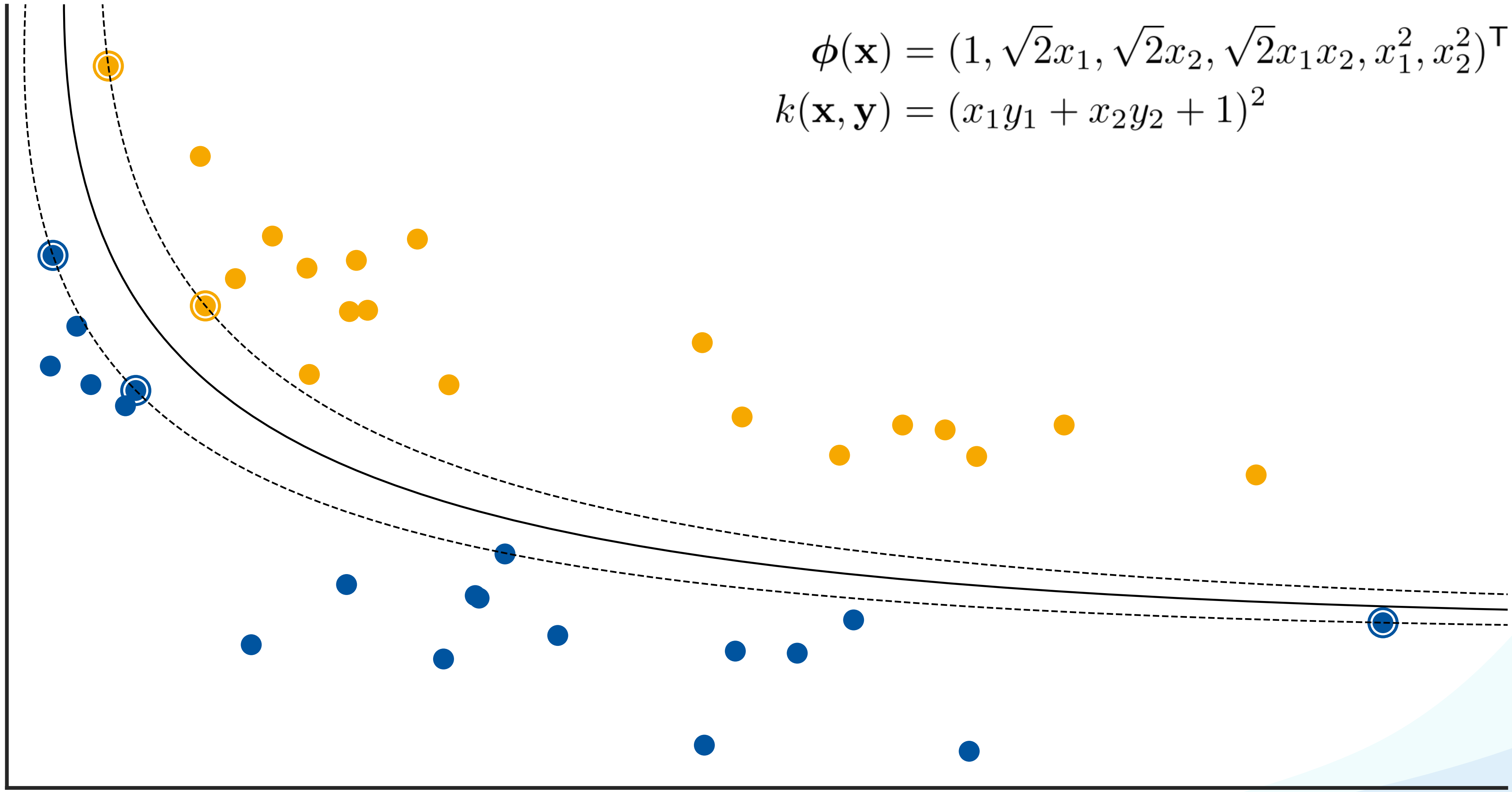
Example

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

$$k(\mathbf{x}, \mathbf{y}) = (x_1y_1 + x_2y_2 + 1)^2$$



Example



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

$$k(\mathbf{x}, \mathbf{y}) = (x_1y_1 + x_2y_2 + 1)^2$$

Advantages

- We can use high-dimensional or even infinite dimensional feature spaces
  - Since $\phi(\mathbf{x})$ is never computed explicitly.
- We can work with non-vector space data
  - We can define kernel functions for arbitrary data types!
  - Graphs, Sets, Sequences, Histograms, …
- Simple to use and work very well in most cases

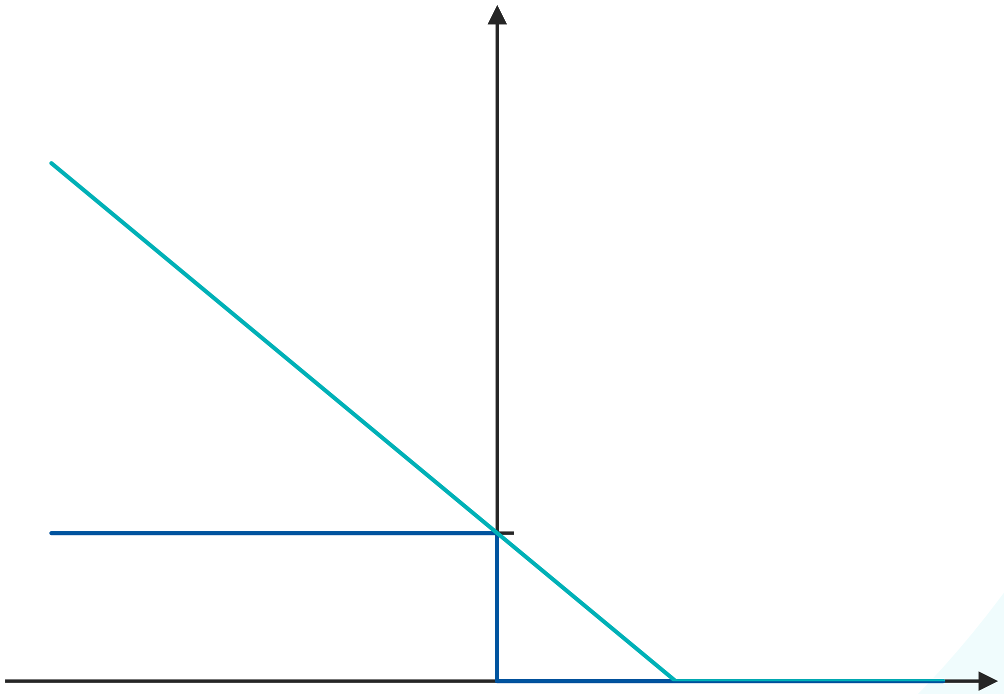
Limitations

- Which kernel to choose?
  - Model selection problem
- How to choose kernel parameters?
  - Hyperparameter optimization problem, usually solved by performing a grid search over the validation set
- Evaluation speed scales linearly with number of support vectors

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

Support Vector Machines

1. Maximum Margin Classification
2. Primal Formulation
3. Dual Formulation
4. Soft-Margin SVMs
5. Non-linear SVMs
6. **Error Function Analysis**



Error Function Analysis

- We know how to formulate and optimize an SVM as a convex optimization problem:

$$\underset{\mathbf{w},\, b,\, \xi_n \in \mathbb{R}^+}{\arg\min} \; \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

subject to the constraints

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n$$

Error Function Analysis

- We know how to formulate and optimize an SVM as a convex optimization problem:

$$\underset{\mathbf{w},\, b,\, \xi_n \in \mathbb{R}^+}{\arg\min} \; \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N} \xi_n$$

subject to the constraints

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n$$

But what error function does this correspond to?

- Integrate the constraints into the objective function:
  - Rewrite as $\xi_n \geq 1 - t_n y(\mathbf{x}_n)$
  - Thus, we obtain

$$\min_{\mathbf{w},\, b} E(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+$$

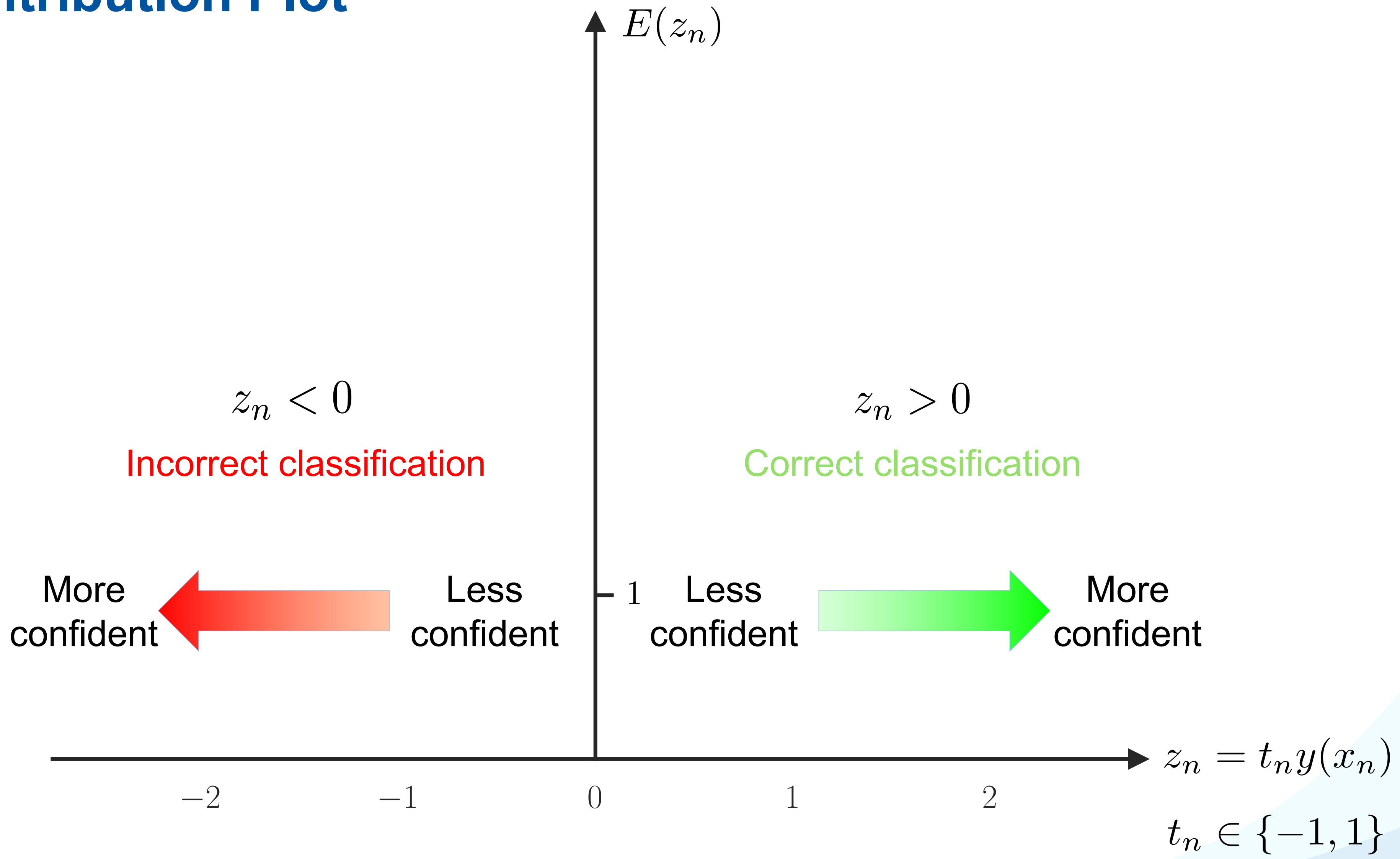
$$[x]_+ \equiv \max\{x, 0\}$$

The Hinge Loss

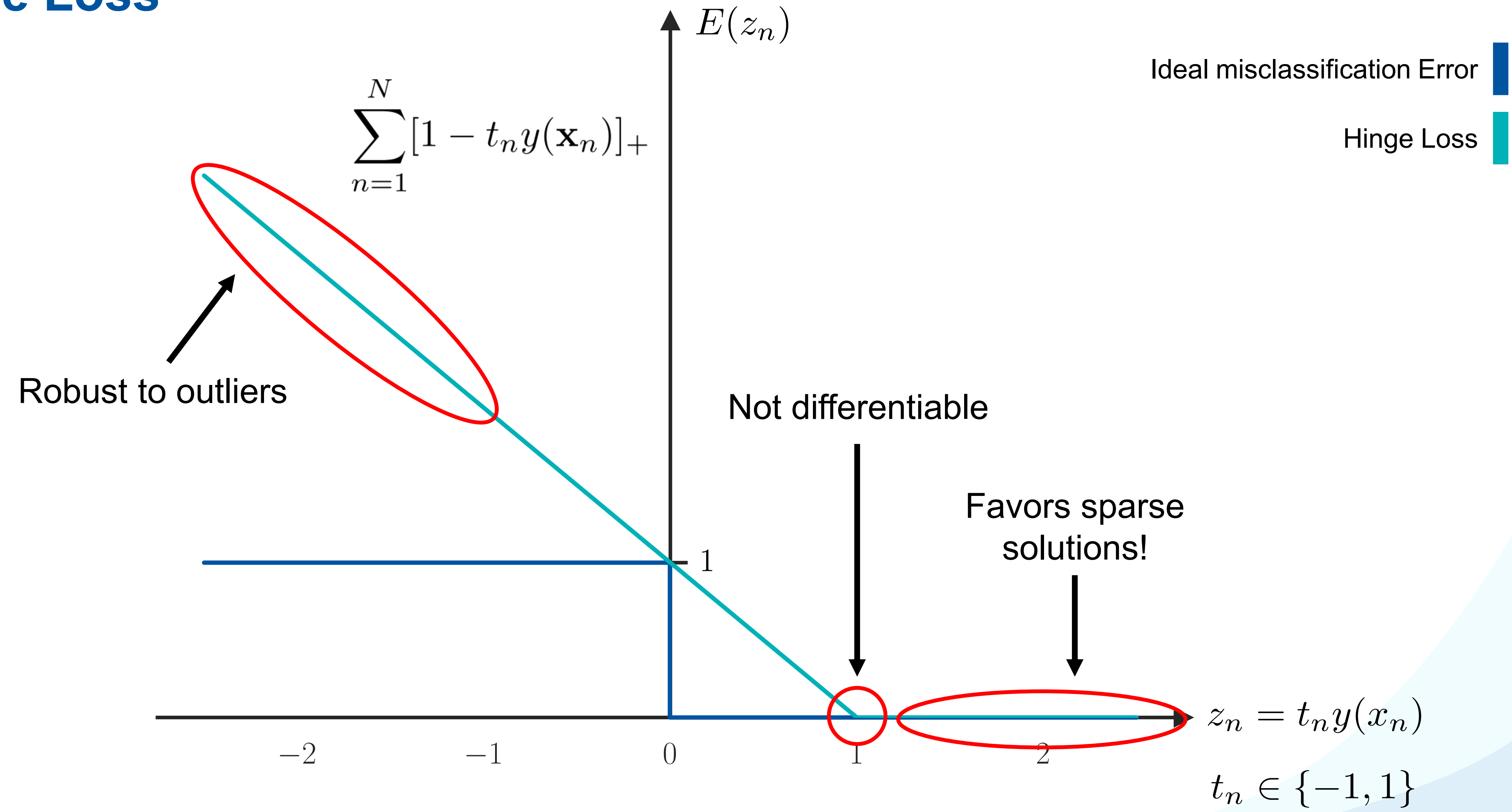
$$E(\mathbf{w}) = \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{\text{L}_2 \text{ regularization}} + C \underbrace{\sum_{n=1}^{N} [1 - t_n y(\mathbf{x}_n)]_+}_{\text{Hinge loss}}$$

- Regularization bounds parameter size.
- Hinge Loss enforces sparsity:
  - Only a subset of training data points actually influences the decision boundary.
  - Still, all input dimensions are used.
- This formulation corresponds to an unconstrained optimization of a non-differentiable function.
  - Very efficient: stochastic (sub-)gradient descent.

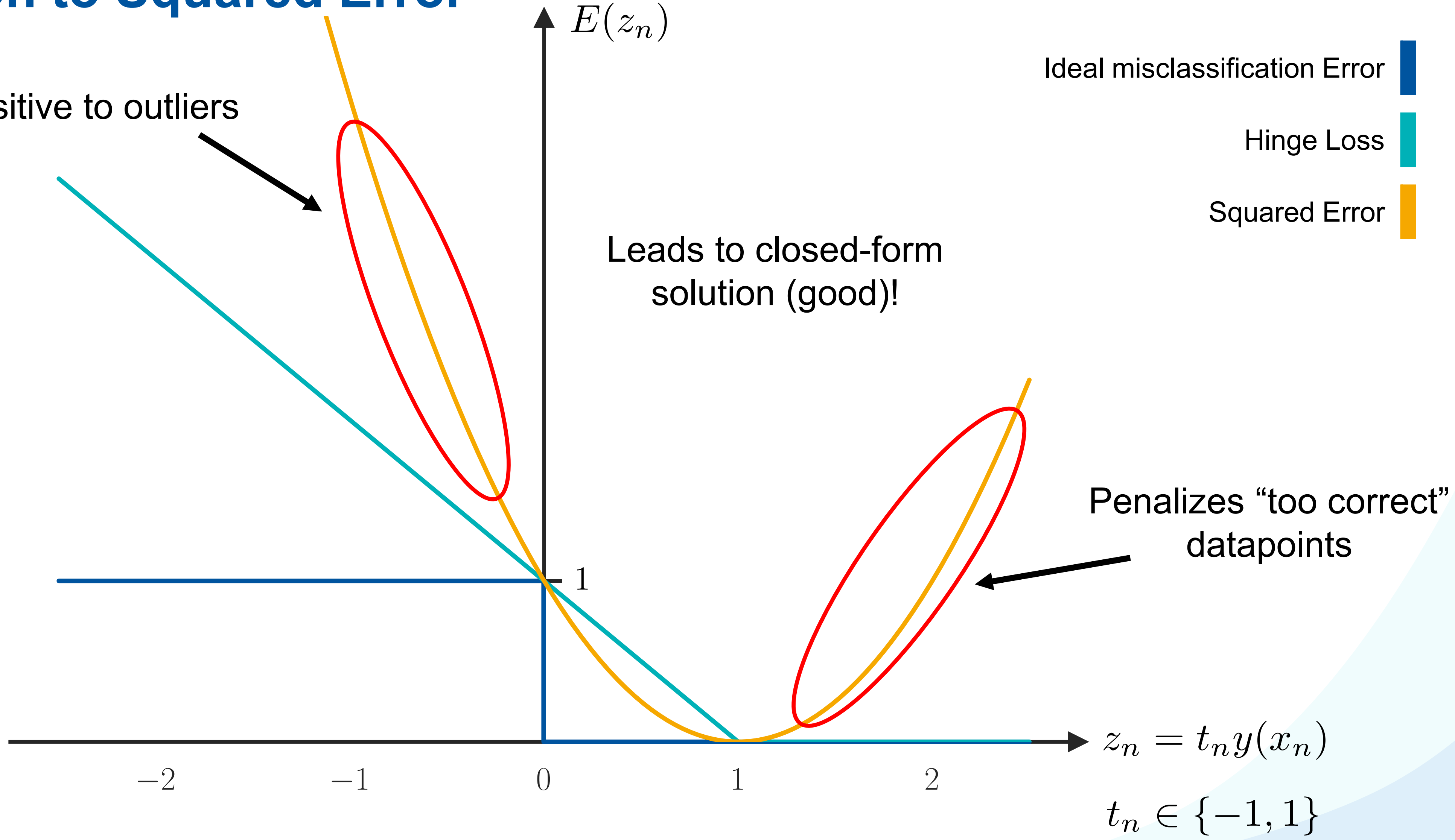
Error Contribution Plot



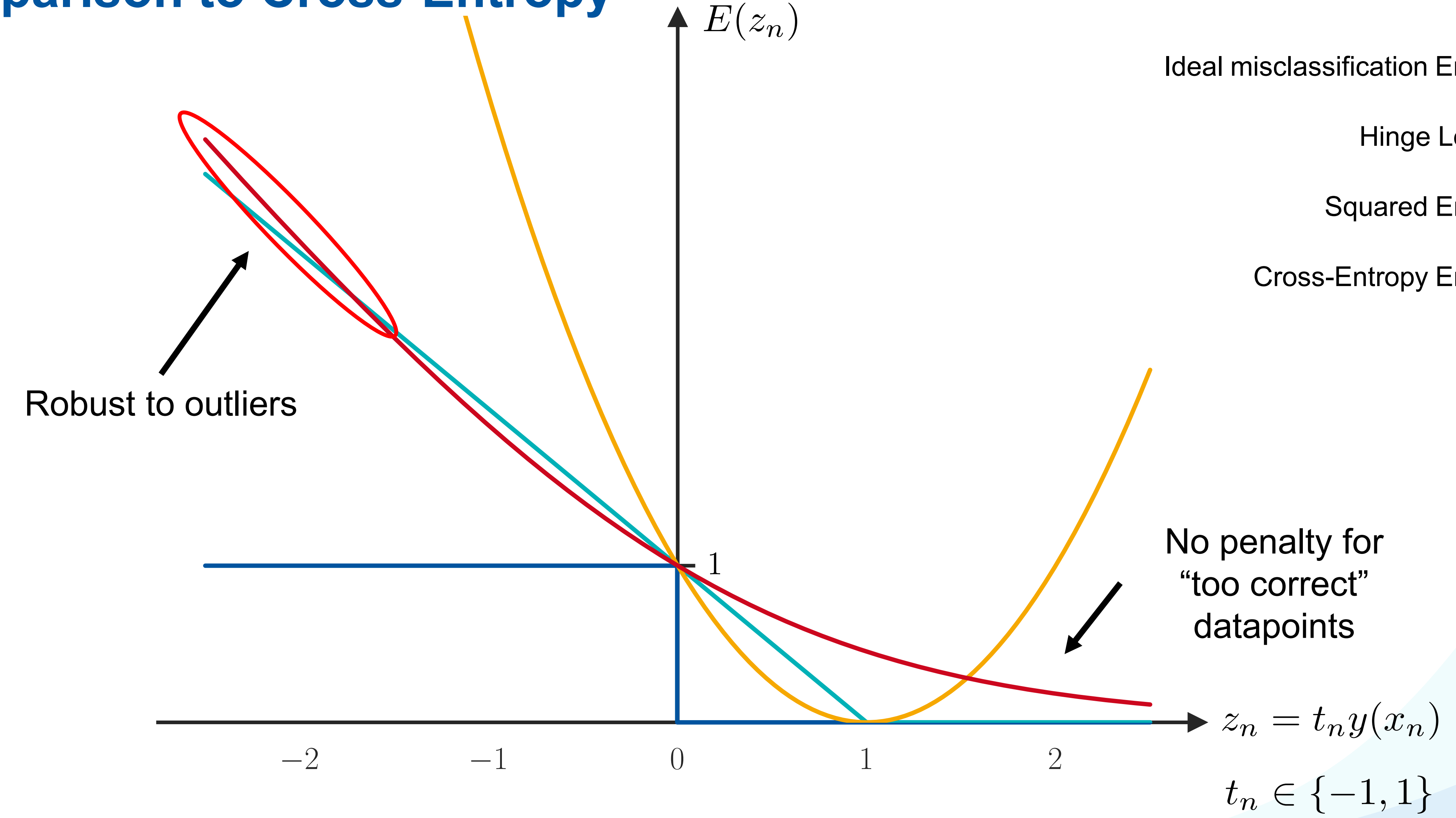
Hinge Loss


$E(z_n)$
Ideal misclassification Error
Hinge Loss
$\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+$
Robust to outliers
Not differentiable
Favors sparse solutions!
1
-2
-1
0
1
2
$z_n = t_n y(x_n)$
$t_n \in \{-1, 1\}$

Comparison to Squared Error



Comparison to Cross-Entropy



Discussion: Hinge Loss

Advantages

- Favors sparse solutions that only depend on a subset of training data points.
- Robust to outliers (only a linear penalty for misclassified points).
- Convex function, unique minimum exists.

Limitations

- Not differentiable (cannot minimize this loss using standard gradient descent, but need to use subgradient descent).

Support Vector Machines

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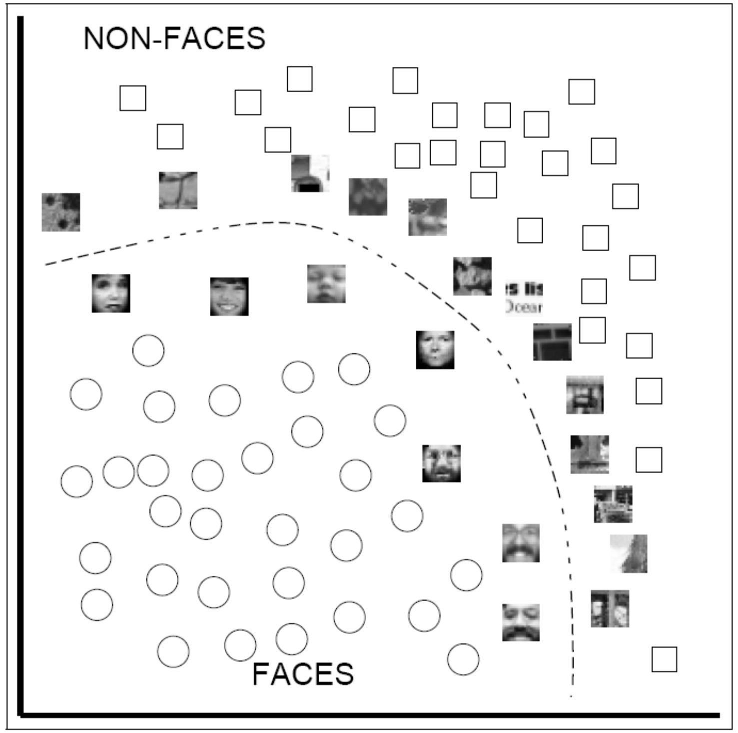
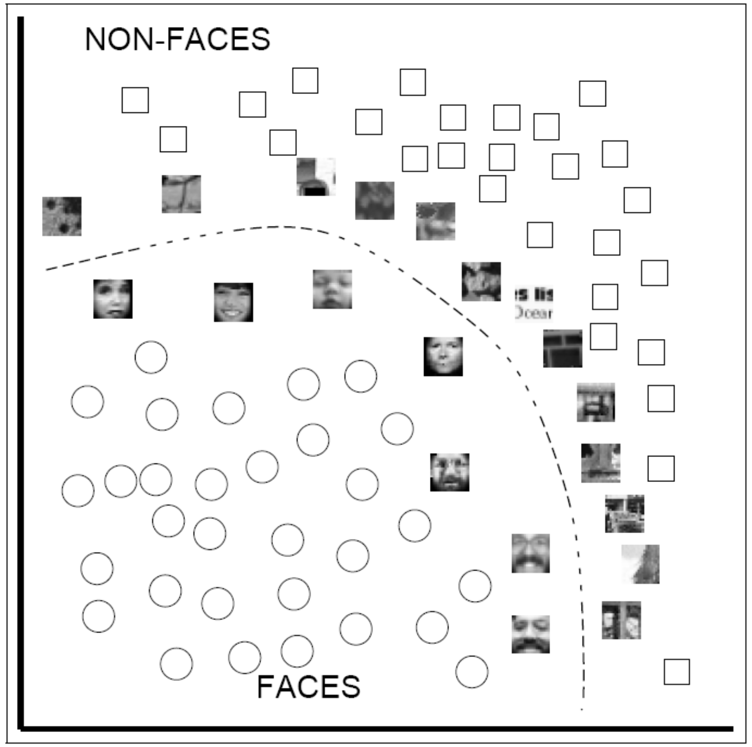
3. Dual Formulation
4. Soft-Margin SVMs
5. Non-linear SVMs
6. Error Function Analysis
7. **Applications**



Interpretation of Support Vectors

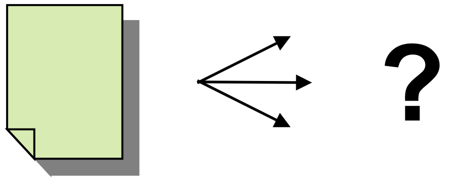
- Let's consider an image classification problem:
  - E.g., *faces* vs. *non-faces*

- The support vectors chosen by the SVM correspond to the hardest examples
  - The real faces closest to non-faces
  - The non-faces closest to real faces
- *We can visualize those support vectors again as images to get some insights into what the SVM reacts to…*

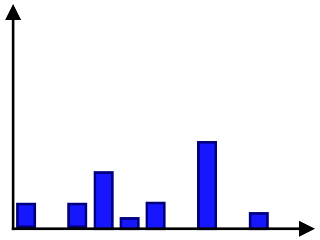


Example Application: Text Classification

- Problem:
  - Classify a document in a number of categories



- Representation:
  - “Bag-of-words” approach
  - Histogram of word counts (on learned dictionary)
    - Very high-dimensional feature space (~10.000 dimensions)
    - Few irrelevant features



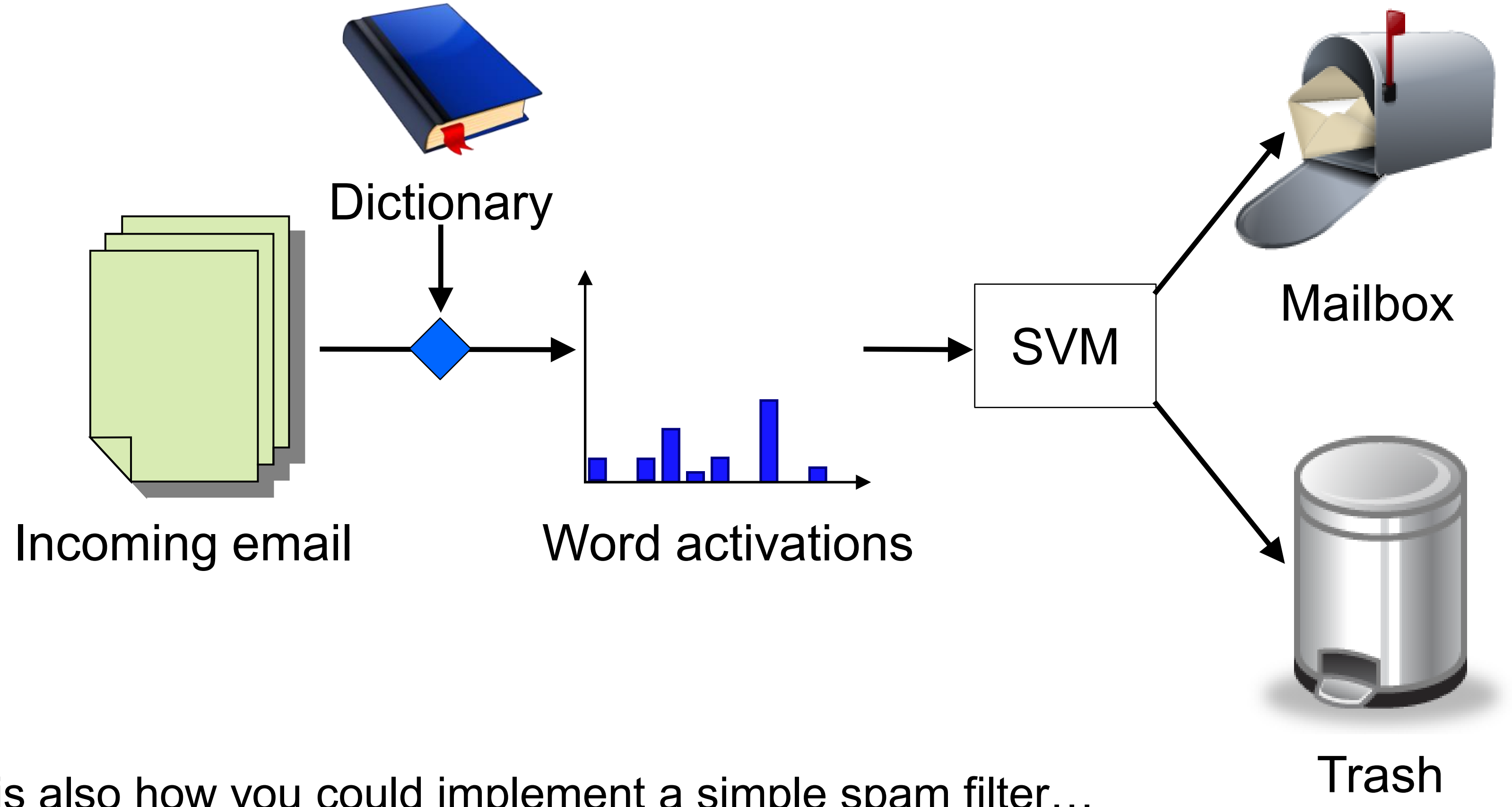
- This was one of the first applications of SVMs
  - T. Joachims (1997)

Example Application: Text Classification

					SVM (poly) degree $d =$					SVM (rbf) width $\gamma =$			
	Bayes	Rocchio	C4.5	k-NN	1	2	3	4	5	0.6	0.8	1.0	1.2
earn	95.9	96.1	96.1	97.3	98.2	98.4	**98.5**	98.4	98.3	**98.5**	98.5	98.4	98.3
acq	91.5	92.1	85.3	92.0	92.6	94.6	**95.2**	95.2	95.3	95.0	95.3	95.3	**95.4**
money-fx	62.9	67.6	69.4	78.2	66.9	72.5	75.4	74.9	**76.2**	74.0	75.4	**76.3**	75.9
grain	72.5	79.5	89.1	82.2	91.3	93.1	**92.4**	91.3	89.9	**93.1**	91.9	91.9	90.6
crude	81.0	81.5	75.5	85.7	86.0	87.3	88.6	**88.9**	87.8	**88.9**	89.0	88.9	88.2
trade	50.0	77.4	59.2	77.4	69.2	75.5	76.6	77.3	**77.1**	76.9	78.0	**77.8**	76.8
interest	58.0	72.5	49.1	74.0	69.8	63.3	67.9	73.1	**76.2**	74.4	75.0	**76.2**	76.1
ship	78.7	83.1	80.9	79.2	82.0	85.4	86.0	**86.5**	86.0	**85.4**	86.5	87.6	87.1
wheat	60.6	79.4	85.5	76.6	83.1	84.5	85.2	**85.9**	83.8	**85.2**	85.9	85.9	85.9
corn	47.3	62.2	87.7	77.9	86.0	86.5	85.3	**85.7**	83.9	**85.1**	85.7	85.7	84.5
microavg.	**72.0**	**79.9**	**79.4**	**82.3**	84.2	85.1	85.9	86.2	85.9	86.4	86.5	86.3	86.2
					combined: **86.0**					combined: **86.4**			

- Results by T. Joachims (1997)

Example Application: Text Classification

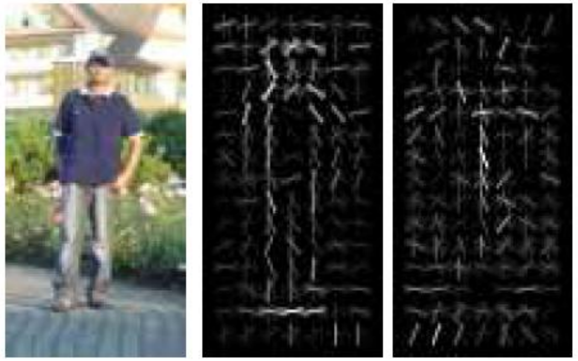


- This is also how you could implement a simple spam filter…

Example Application: Visual Object Detection

Sliding-Window Approach

- Densely scan an image with a sliding window
- Object detection by per-window classification
  - E.g., use a histogram of gradients (HOG) feature representation
  - Train a linear SVM for *object* vs. *non-object* classification.

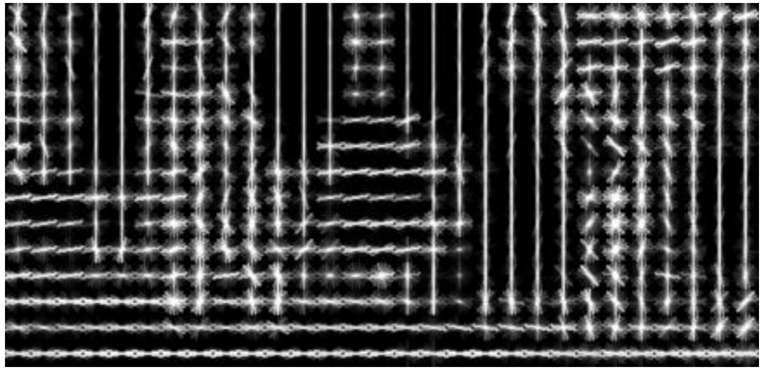


Example Application: Pedestrian Detection with SVMs

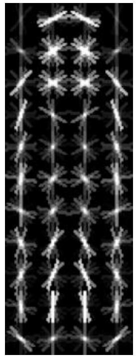
- Train a pedestrian template using a linear SVM
- At test time, convolve feature map with learned template $\mathbf{w}$
  - Linear SVM classification function ⇔ convolution with "template" $\mathbf{w}$

$$y(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

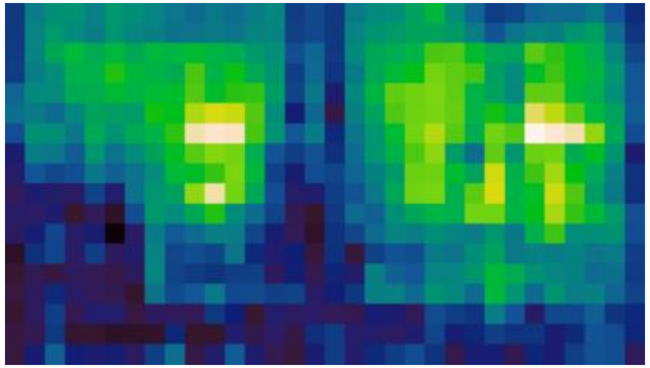
HOG feature map
$\mathbf{x}$



Template
$\mathbf{w}$



Detector response map
$y(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + \mathrm{b}$



N. Dalal, B. Triggs, Histograms of Oriented Gradients for Human Detection, CVPR 2005

Example Application: Pedestrian Detection with SVMs

N. Dalal, B. Triggs, Histograms of Oriented Gradients for Human Detection, CVPR 2005

References and Further Reading

- More information about SVMs is available in Chapter 7.1 of Bishop's book.

Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006