

ASSIGNMENT 3: CONSTRAINED OPTIMIZATION, SVMS



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SVMs for linear separability: The formal setup: Part 5: Abstract problem formulation

- **Original Problem:** For given linearly separable data set Z , $\mathbf{w} \in \mathbb{R}^d$ and $b \in \mathbb{R}$:

$$\text{Maximize} \quad \frac{2}{\|\mathbf{w}\|}$$

$$\text{subject to} \quad y_i(\mathbf{w} \cdot \mathbf{x}_i - b) - 1 \geq 0 \quad \text{for } i = 1, \dots, l.$$

- Equivalent: **Primal Problem:**

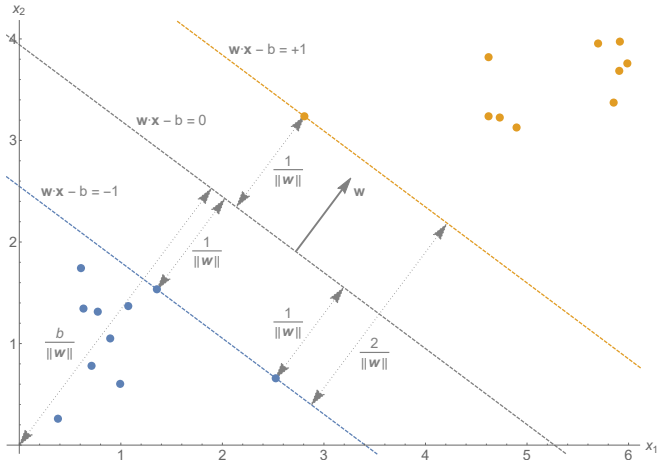
$$\text{Minimize} \quad \frac{1}{2} \|\mathbf{w}\|^2 = \frac{1}{2} \sum_{i=1}^d w_i^2$$

$$\text{subject to} \quad -(y_i(\mathbf{w} \cdot \mathbf{x}_i - b) - 1) \leq 0 \quad \text{for } i = 1, \dots, l.$$

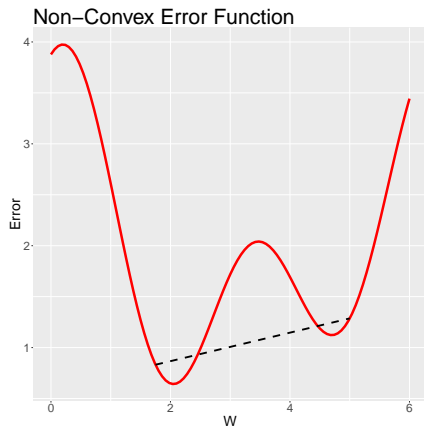
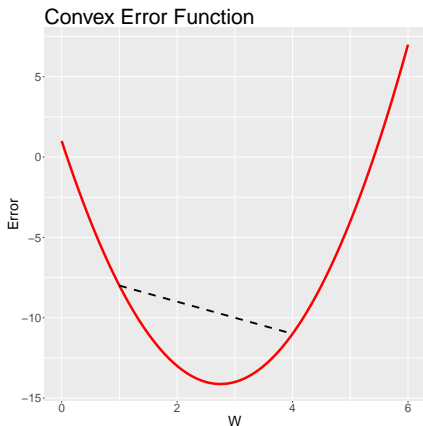
- \rightarrow Convex quadratic optimization problem with linear constraints. Next: recall basic mathematical tools.



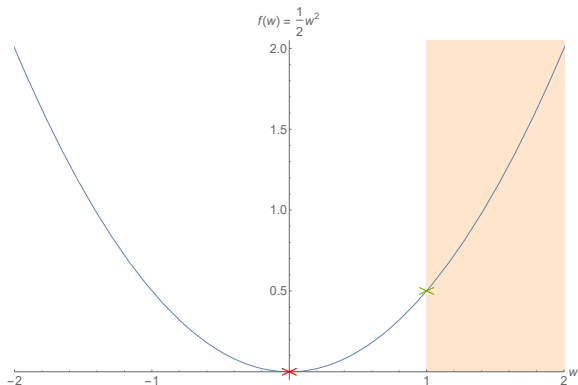
SVMs for linear separability: The formal setup: Part 3



Interlude: constrained convex optimization: Part 1



Interlude: constrained convex optimization: Part 2



- Red: Global minimum
- Green: Constrained minimum under constraint $w > 1$

Interlude: constrained convex optimization: Part 3



- Assumptions: we have functions f and h_i ($i = 1, \dots, l$) from \mathbb{R}^d to \mathbb{R} with following requirements:
 1. Convex
 2. Continuously Differentiable
 3. Slater condition: there exists \mathbf{w}' with $h_i(\mathbf{w}') < 0$ for all $i = 1, \dots, l$.
- Primal Problem:

$$\begin{array}{ll} \text{Minimize} & f(\mathbf{w}) \\ \text{subject to} & h_i(\mathbf{w}) \leq 0 \quad \text{for } i = 1, \dots, l. \end{array}$$

- For simplicity: we don't deal with equality constraints here
- Next slide: strategy how to solve this problem



Interlude: constrained convex optimization: Part 4

■ Lagrange function:

$$L(\mathbf{w}; \alpha_1, \dots, \alpha_l) = f(\mathbf{w}) + \sum_{i=1}^l \alpha_i h_i(\mathbf{w})$$

$\alpha_1, \dots, \alpha_l$: Lagrange multipliers.

■ Dual Problem:

Maximize $\mathcal{L}(\alpha_1, \dots, \alpha_l) = \inf_{\mathbf{w}} L(\mathbf{w}; \alpha_1, \dots, \alpha_l)$ wrt. $\alpha_1, \dots, \alpha_l$

subject to $\alpha_i \geq 0$ for $i = 1, \dots, l$.

■ Karush-Kuhn-Tucker (KKT): \mathbf{w}^* solves primal problem \Leftrightarrow there exist non-negative Lagrange multipliers with:

1. $\mathcal{L}(\alpha_1, \dots, \alpha_l) = L(\mathbf{w}^*; \alpha_1, \dots, \alpha_l)$
2. $\alpha_1, \dots, \alpha_l$ solve dual problem, i.e. they maximize \mathcal{L} .
3. $\alpha_i h_i(\mathbf{w}^*) = 0$ for all $i = 1, \dots, l$.

Interlude: constrained convex optimization: Part 5



- Illustrative example (toy problem):

$$\begin{aligned} \text{Minimize} \quad & f(w_1, w_2) = (w_1 - 2)^2 + w_2^2 \\ \text{subject to} \quad & h_1(w_1, w_2) = -w_1 \leq 0 \\ & \text{and} \quad h_2(w_1, w_2) = w_1 - w_2 \leq 0. \end{aligned}$$

- Lagrange function:

$$L(w_1, w_2, \alpha_1, \alpha_2) = (w_1 - 2)^2 + w_2^2 - \alpha_1 w_1 + \alpha_2 (w_1 - w_2)$$

- To find $\inf_{(w_1, w_2)} L(w_1, w_2, \alpha_1, \alpha_2)$ for given (α_1, α_2) , consider:

$$\begin{aligned} \frac{\partial L}{\partial w_1}(w_1, w_2, \alpha_1, \alpha_2) &= 2w_1 - 4 - \alpha_1 + \alpha_2 \\ \frac{\partial L}{\partial w_2}(w_1, w_2, \alpha_1, \alpha_2) &= 2w_2 - \alpha_2 \end{aligned}$$

Interlude: constrained convex optimization: Part 6



- Setting the two derivatives to 0, we obtain $w_1^* = 2 + \frac{\alpha_1 - \alpha_2}{2}$ and $w_2^* = \frac{\alpha_2}{2}$. (This must be a minimum as L is convex and no maximum exists.)
- Furthermore:

$$\begin{aligned}\mathcal{L}(\alpha_1, \alpha_2) &= L(w_1^*, w_2^*, \alpha_1, \alpha_2) \\ &= -\frac{1}{4} (\alpha_1^2 + 8\alpha_1 - 2\alpha_1\alpha_2 - 8\alpha_2 + 2\alpha_2^2)\end{aligned}$$

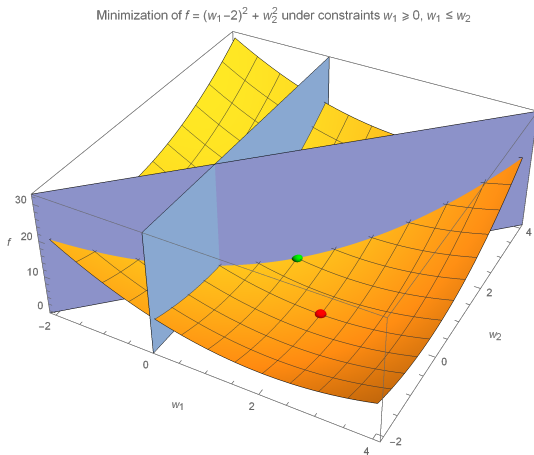
- Dual problem: maximize $\mathcal{L}(\alpha_1, \alpha_2)$ subject to $\alpha_1 \geq 0$ and $\alpha_2 \geq 0$. Yields $\alpha_1 = 0$ and $\alpha_2 = 2$ and thus $w_1^* = 1$ and $w_2^* = 1$. Can be deduced by KKT-conditions.
- In many practical situations: algorithms for solving dual problem exist, especially for SVMs (as we will see later). Here: argument for toy example using KKT conditions.

Interlude: constrained convex optimization: Part 7



- By the third KKT condition: $\alpha_1 h_1(w_1^*, w_2^*) = 0$.
- Assume $h_1(w_1^*, w_2^*) < 0$. Then $\alpha_1 = 0$. Now look at the second KKT-condition $\alpha_2 h_2(w_1^*, w_2^*) = 0$.
 - If $\alpha_2 = 0$: $h_2(w_1^*, w_2^*) = 2 > 0$ which contradicts constraint on h_2 \rightarrow can be ruled out.
 - If $h_2(w_1^*, w_2^*) = 0$ we can deduce $w_1^* = w_2^*$ and thus $\alpha_2 = 2$. (recall: $\alpha_1 = 0$). All the constraints are satisfied, thus we are done, since we have unique solution because of convexity. For sake of completeness, we will also provide arguments ruling out other possibilities:
- Assume $h_1(w_1^*, w_2^*) = 0$. Then $\alpha_2 = 4 + \alpha_1$.
 - If $\alpha_2 = 0$ then $\alpha_1 = -4 \rightarrow$ can be ruled out as $\alpha_i \geq 0$.
 - If $\alpha_2 \neq 0$ then $h_2(w_1^*, w_2^*) = 0$, which implies $\alpha_2 = \frac{\alpha_1}{2} + 2$, i.e. $4 + \alpha_1 = \frac{\alpha_1}{2} + 2$, i.e. $\alpha_1 = -4 \rightarrow$ can be ruled out again.
- Solution: $\alpha_1 = 0, \alpha_2 = 2$, yielding: $w_1^* = 1, w_2^* = 1$ and $f(w_1^*, w_2^*) = 2$.

Interlude: constrained convex optimization: Part 8



- Red: global minimum (not obeying the constraints)
- Green: solution for minimization under constraints



Back to linear SVMs: Part 1

- Associated Lagrange function is given as

$$\begin{aligned} L(\mathbf{w}, b; \alpha_1, \dots, \alpha_l) &= \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^l \alpha_i (y_i (\mathbf{w} \cdot \mathbf{x}_i - b) - 1) \\ &= \frac{1}{2} \|\mathbf{w}\|^2 - \mathbf{w} \cdot \sum_{i=1}^l \alpha_i y_i \mathbf{x}_i + b \sum_{i=1}^l \alpha_i y_i + \sum_{i=1}^l \alpha_i \end{aligned}$$

- Solving the dual problem enforces the conditions

$$\frac{\partial L}{\partial \mathbf{w}}(\mathbf{w}, b; \alpha_1, \dots, \alpha_l) = 0 \quad \frac{\partial L}{\partial b}(\mathbf{w}, b; \alpha_1, \dots, \alpha_l) = 0,$$

- This implies:

$$\mathbf{w}^* = \sum_{i=1}^l \alpha_i y_i \mathbf{x}_i \quad \sum_{i=1}^l \alpha_i y_i = 0$$

- Furthermore:

$$\mathcal{L}(\alpha_1, \dots, \alpha_l) = \sum_{i=1}^l \alpha_i - \frac{1}{2} \sum_{i=1}^l \sum_{j=1}^l \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j.$$

- Final solution: maximize \mathcal{L} with respect to α_i subject to $\alpha_i \geq 0$ (for all $i = 1, \dots, l$) and $\sum_{i=1}^l \alpha_i y_i = 0$.



Back to linear SVMs: Part 2

■ Introduce

$$\begin{aligned}\mathbf{0} &= \overbrace{(0, \dots, 0)}^{l \text{ times}}^T, & \boldsymbol{\alpha} &= (\alpha_1, \dots, \alpha_l)^T, \\ \mathbf{1} &= \overbrace{(1, \dots, 1)}^{l \text{ times}}^T, & \mathbf{Q} &= (y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j)_{i=1, \dots, l}^{j=1, \dots, l},\end{aligned}$$

■ The dual problem can be written as follows:

$$\begin{aligned}\text{Minimize} \quad & -\mathcal{L} = \frac{1}{2} \boldsymbol{\alpha}^T \mathbf{Q} \boldsymbol{\alpha} - \mathbf{1}^T \boldsymbol{\alpha} \text{ wrt. } \boldsymbol{\alpha} \\ \text{subject to} \quad & \boldsymbol{\alpha} \geq \mathbf{0} \text{ and } \boldsymbol{\alpha}^T \mathbf{y} = 0.\end{aligned}$$

■ Easy observation: \mathbf{Q} is positive semi-definite.

■ \rightarrow convex quadratic optimization problem with linear constraints: only global minima: uniqueness if positive definite.



Back to linear SVMs: Part 3

- Once we solved the dual problem \rightarrow obtain $\alpha_1, \dots, \alpha_l$ which also solve primal problem. By the KKT-conditions:

$$\alpha_i (y_i (\mathbf{w} \cdot \mathbf{x}_i - b) - 1) = 0 \quad \text{for } i = 1, \dots, l.$$

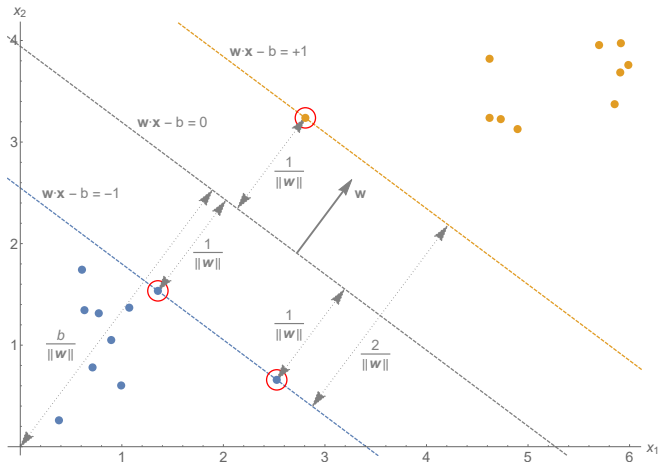
- Thus, for $i = 1, \dots, l$:

- ☐ either $\alpha_i = 0$
- ☐ or $y_i (\mathbf{w} \cdot \mathbf{x}_i - b) - 1 = 0$
- ☐ or both.

- Samples \mathbf{x}_i for which $\alpha_i > 0$ holds (i.e. $y_i (\mathbf{w} \cdot \mathbf{x}_i - b) - 1 = 0$) lie on the margin border and are called **support vectors** (encircled in red in next slide).



Back to linear SVMs: Part 4



Back to linear SVMs: Part 5

- Given Lagrange multipliers $\alpha_1, \dots, \alpha_l$ solving the primal problem, we can construct \mathbf{w} as noted above already:

$$\mathbf{w} = \sum_{i=1}^l \alpha_i y_i \mathbf{x}_i$$

- \rightarrow final classification function, i.e. the **linear Support Vector Machine (SVM)**, is given as

$$g(\mathbf{x}) = \text{sign}(\mathbf{w} \cdot \mathbf{x} - b) = \text{sign}\left(\underbrace{\sum_{i=1}^l \alpha_i y_i \mathbf{x}_i \cdot \mathbf{x}}_{\text{discriminant function } \bar{g}(\mathbf{x})} - b \right).$$



Back to linear SVMs: Part 6

- For arbitrary support vector \mathbf{x}_j (with $\alpha_j > 0$), the KKT condition implies $y_j(\mathbf{w} \cdot \mathbf{x}_j - b) = 1$, and thus

$$b = -y_j + \mathbf{w} \cdot \mathbf{x}_j = -y_j + \sum_{i=1}^l \alpha_i y_i \mathbf{x}_i \cdot \mathbf{x}_j$$

- Recommended: don't base the computation of b on only one support vector (for reasons of numerical precision), but compute a b value for each support vector and use the average finally.
- Under specific conditions: it may be useful to adjust b according to some other quality measure after training.



C-SVMs: Non-linear separability: Part 1

- If positive and negative samples are **not** linearly separable, the constraints

$$y_i (\mathbf{w} \cdot \mathbf{x}_i - b) \geq 1 \quad (i = 1, \dots, l)$$

cannot be all fulfilled simultaneously.

- Introduce **non-negative slack variables** $\xi_i \geq 0$:

$$y_i (\mathbf{w} \cdot \mathbf{x}_i - b) \geq 1 - \xi_i \quad (i = 1, \dots, l)$$

- Require slack variables to be as small as possible. Are scaled by factor $C > 0$.
- The adapted primal problem (called **C-SVM**) is given as:

$$\begin{aligned} \text{Minimize} \quad & \frac{1}{2} \|\mathbf{w}\|_2^2 + C \sum_{i=1}^l \xi_i \\ \text{subject to} \quad & -(y_i (\mathbf{w} \cdot \mathbf{x}_i - b) - 1 + \xi_i) \leq 0 \\ \text{and} \quad & -\xi_i \leq 0 \end{aligned}$$

C-SVMs: Non-linear separability: Part 2

- Using the same techniques as for linear case (i.e. formulate dual problem and apply KKT-Theorem), the problem can be cast into the framework of convex quadratic optimization again.
- Classification function g also has similar structure, however, KKT-conditions are a bit more involved
- Overview of calculations: next slides.
- As meaning of C is not very intuitive: different variant called ν -SVM also exists (see later slides). KKT Theorem applies again.
- Connection to hinge loss: $L_h(y_i, \bar{g}(\mathbf{x}_i)) = \max(0, 1 - y_i \bar{g}(\mathbf{x}_i))$. In case of SVMs:
 - L_h is zero \Leftrightarrow data point lies on correct side of margin.
 - If not: loss value is proportional to distance from margin.



C-SVMs: Mathematical details: Part 1

- Again introduce $\alpha_1, \dots, \alpha_l$ and $\lambda_1, \dots, \lambda_l$. Then:

$$\begin{aligned} L(\mathbf{w}, b, \xi_1, \dots, \xi_l; \alpha_1, \dots, \alpha_l, \lambda_1, \dots, \lambda_l) \\ = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^l \xi_i - \sum_{i=1}^l \alpha_i (y_i (\mathbf{w} \cdot \mathbf{x}_i - b) - 1 + \xi_i) - \sum_{i=1}^l \lambda_i \xi_i \end{aligned}$$

- For dual problem: minimize L for \mathbf{w} , b and ξ_1, \dots, ξ_l .
- This enforces:

$$\begin{aligned} \frac{\partial L}{\partial \mathbf{w}}(\mathbf{w}, b, \xi_1, \dots, \xi_l; \alpha_1, \dots, \alpha_l, \lambda_1, \dots, \lambda_l) &= 0, \\ \frac{\partial L}{\partial b}(\mathbf{w}, b, \xi_1, \dots, \xi_l; \alpha_1, \dots, \alpha_l, \lambda_1, \dots, \lambda_l) &= 0, \\ \frac{\partial L}{\partial \xi_j}(\mathbf{w}, b, \xi_1, \dots, \xi_l; \alpha_1, \dots, \alpha_l, \lambda_1, \dots, \lambda_l) &= 0, \quad \text{for all } j = 1, \dots, l \end{aligned}$$

- Which implies (the first two conditions are the same as for linear SVMs):

$$\begin{aligned} \mathbf{w} &= \sum_{i=1}^l \alpha_i y_i \mathbf{x}_i, \\ \sum_{i=1}^l \alpha_i y_i &= 0, \\ C - \alpha_j - \lambda_j &= 0 \text{ for all } j = 1, \dots, l \end{aligned}$$



C-SVMs: Mathematical details: Part 2

- Equalities $C - \alpha_j - \lambda_j = 0$ imply $\lambda_j = C - \alpha_j$.
- Constraints $\lambda_j \geq 0$ imply that we must ensure $C - \alpha_j \geq 0$, hence $\alpha_j \leq C$ for all $j = 1, \dots, l$.
- Finally, we obtain the same objective function

$$\mathcal{L}(\alpha_1, \dots, \alpha_l) = \sum_{i=1}^l \alpha_i - \frac{1}{2} \sum_{i=1}^l \sum_{j=1}^l \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j.$$

- Solution: maximize \mathcal{L} with respect to α_i subject to $\alpha_i \geq 0$ (for all $i = 1, \dots, l$), $\sum_{i=1}^l \alpha_i y_i = 0$, and additional constraints $\alpha_i \leq C$ (for all $i = 1, \dots, l$).
- Dual problem:

$$\begin{array}{ll} \text{Minimize} & \frac{1}{2} \boldsymbol{\alpha}^T \mathbf{Q} \boldsymbol{\alpha} - \mathbf{1}^T \boldsymbol{\alpha} \\ \text{wrt.} & \boldsymbol{\alpha} \\ \text{subject to} & \boldsymbol{\alpha}^T \mathbf{y} = 0 \text{ and } \mathbf{0} \leq \boldsymbol{\alpha} \leq C \mathbf{1}. \end{array}$$



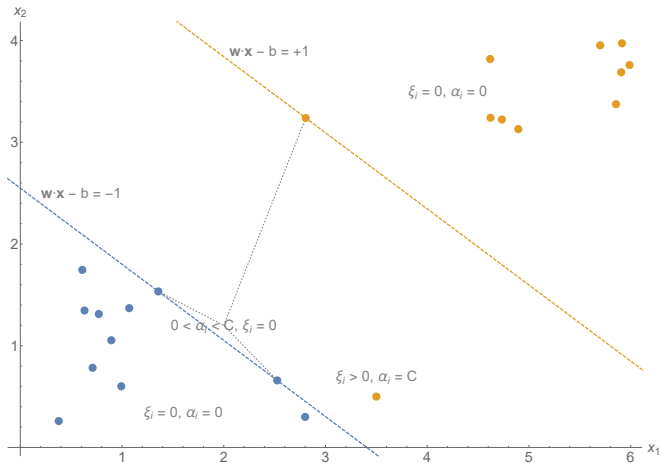
C-SVMs: Mathematical details: Part 3

- Analogously:

$$g(\mathbf{x}) = \text{sign}(\mathbf{w} \cdot \mathbf{x} - b) = \text{sign}\left(\sum_{i=1}^l \alpha_i y_i \mathbf{x}_i \cdot \mathbf{x} - b\right).$$

- Computation of b , however, requires a bit more caution.
- In non-separable case, the KKT-conditions tell us that $\alpha_i (y_i (\mathbf{w} \cdot \mathbf{x}_i - b) - 1 + \xi_i) = 0$ holds for all $i = 1, \dots, l$. If we choose an i such that $\alpha_i > 0$, we would need ξ_i to determine b .
- However, note that KKT conditions also imply (for the other set of constraints $\xi_i \geq 0$) that $\lambda_i \xi_i = (C - \alpha_i) \xi_i = 0$ holds for all $i = 1, \dots, l$.
- If we find j with $0 < \alpha_j < C$, we can infer $\xi_j = 0$ and thus $y_j (\mathbf{w} \cdot \mathbf{x}_j - b) - 1 = 0$, i.e. can use same method as before.
- Every $\alpha_j > 0$ corresponds to a support vector \mathbf{x}_j .

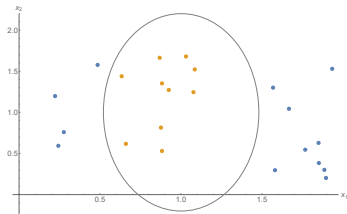
C-SVMs: Illustration



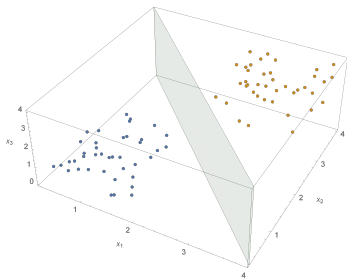


Nonlinear SVM: Part 1

- Linear separability is very restrictive.
- The **higher** the dimensionality, however, the **easier** linear separability can be achieved.

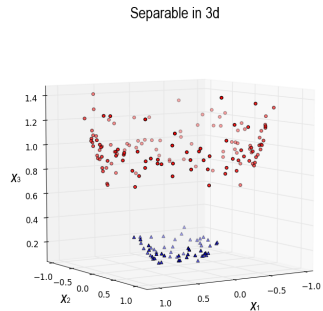
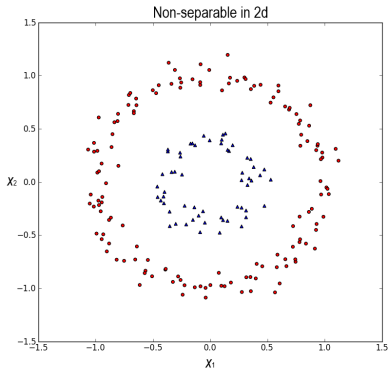


$$\begin{matrix} \xrightarrow{\Phi} \\ \xleftarrow{\Phi^{-1}} \end{matrix}$$





Nonlinear SVM: Part 2



- Left: (x_1, x_2) , data not linearly separable
- Right: $(x_1, x_2, x_3 = x_1^2 + x_2^2)$, data linearly separable



Nonlinear SVM: Part 3

- Basic idea of nonlinear SVMs: transform data into a higher-dimensional space such that problem hopefully becomes linearly separable there.
- More formal: choose a Hilbert space \mathcal{H} and a (nonlinear) mapping $\Phi : X \rightarrow \mathcal{H}$.
- Then try to apply linear method (presented in earlier slides) in the space \mathcal{H} .
- Problem: how to specify \mathcal{H} and Φ ?



Nonlinear SVM: Part 4

- Recall: In solving the dual problem and computing the final classification function: need **only scalar products of pairs of samples**. Therefore: **not** necessary to explicitly know \mathcal{H} and Φ .
- Only need $\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle_{\mathcal{H}}$ for all $\mathbf{x}_i, \mathbf{x}_j$ ($i, j = 1, \dots, l$).
- Required for computing the classification of a new sample \mathbf{x} : $\langle \Phi(\mathbf{x}), \Phi(\mathbf{x}_i) \rangle_{\mathcal{H}}$ for all $i = 1, \dots, l$.
- Suppose we are given a mapping $k : X \times X \rightarrow \mathbb{R}$ (the **kernel**) for which we know that there exists Hilbert space \mathcal{H} and mapping $\Phi : X \rightarrow \mathcal{H}$ such that $k(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathcal{H}}$ for all $\mathbf{x}, \mathbf{y} \in X$.

Nonlinear SVM: Part 5

- This is the case \Leftrightarrow (Aronszajn) k is **positive semi-definite** and **symmetric**, i.e.

1. $\sum_{i,j} c_i k(\mathbf{x}_i, \mathbf{x}_j) c_j \geq 0$
2. $k(\mathbf{x}_i, \mathbf{x}_j) = k(\mathbf{x}_j, \mathbf{x}_i)$

for $i, j = 1, \dots, l$, $c_i, c_j \in \mathbb{R}$, $\mathbf{x}_i, \mathbf{x}_j \in X$.

- Equivalent formulation: **Gram matrix**

$\mathbf{K} = (k_{ij})_{i=1, \dots, l}^{j=1, \dots, l} = (k(\mathbf{x}_i, \mathbf{x}_j))_{i=1, \dots, l}^{j=1, \dots, l}$ is positive semi-definite and symmetric.

- In practice: make an a priori choice of k using common sense and, if available, prior knowledge about problem: \rightarrow “**kernel trick**”.



Nonlinear SVM: Part 6

- Which kernels? \rightarrow Assume $X = \mathbb{R}^n$ and $k : X^2 \rightarrow \mathbb{R}$ continuous. The following statements are equivalent:

- ☐ k is a kernel
- ☐ For $(Af)(\mathbf{x}) = \int_X k(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}$ the inequality
$$\langle Af, f \rangle_{L^2(X)} = \int_{X^2} k(\mathbf{x}, \mathbf{y}) f(\mathbf{x}) f(\mathbf{y}) d\mathbf{x} d\mathbf{y} \geq 0.$$
holds for all square-integrable functions $f \in L^2(X)$.

- **Mercer's Theorem:** If in addition the diagonal $k(x, x)$ is integrable:

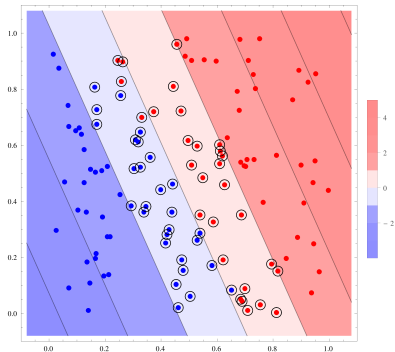
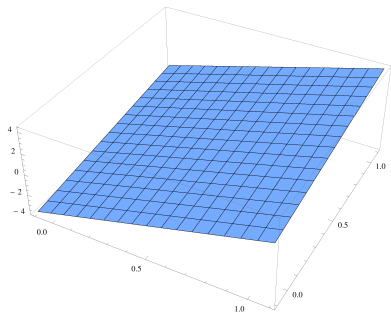
- ☐ There are sequences $(\varphi_m)_{m \in \mathbb{N}}$ of continuous eigenfunctions and positive eigenvalues $(\sigma_m)_{m \in \mathbb{N}}$ of A .
- ☐ $k(\mathbf{x}, \mathbf{y}) = \sum_{m \geq 1} \sigma_m \varphi_m(\mathbf{x}) \varphi_m(\mathbf{y})$ and sum converges uniformly on compact sets of X^2 .

- More details with proofs: e.g. [these notes](#), chapter 3.5.

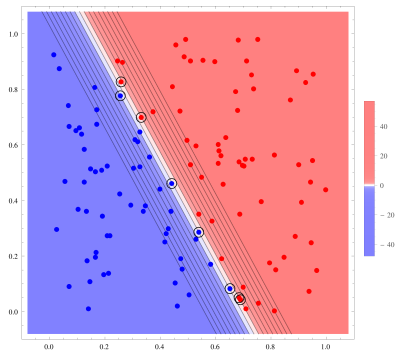
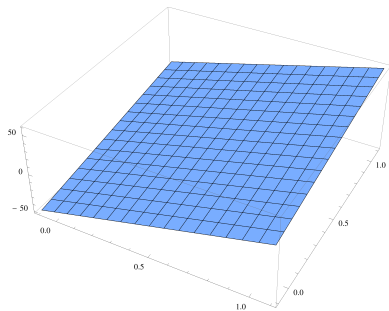
- Standard kernels (" \cdot " here denotes Euclidean inner product):

1. Linear: $k(\mathbf{x}, \mathbf{y}) = \mathbf{x} \cdot \mathbf{y}$
2. Polynomial: $k(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y} + \beta)^\alpha$
3. Gaussian / RBF: $k(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{x} - \mathbf{y}\|^2\right)$
4. Sigmoid: $k(\mathbf{x}, \mathbf{y}) = \tanh(\alpha \mathbf{x} \cdot \mathbf{y} + \beta)$

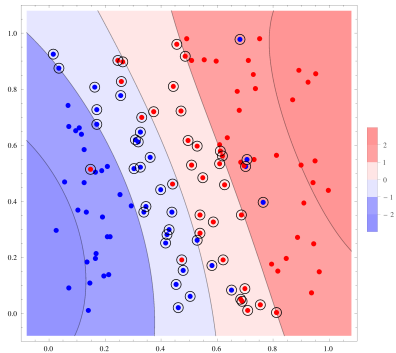
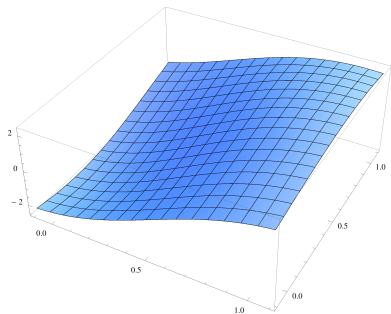
C-SVM Illustration Part 1: $C = 1$, Kernel = linear



C-SVM Illustration Part 2: $C = 1000$, Kernel = linear



C-SVM Illustration Part 3: $C = 1$, Kernel = RBF, $\frac{1}{2\sigma^2} = 1$



C-SVM Illustration Part 4: $C = 1000$, Kernel = RBF, $\frac{1}{2\sigma^2} = 100$

