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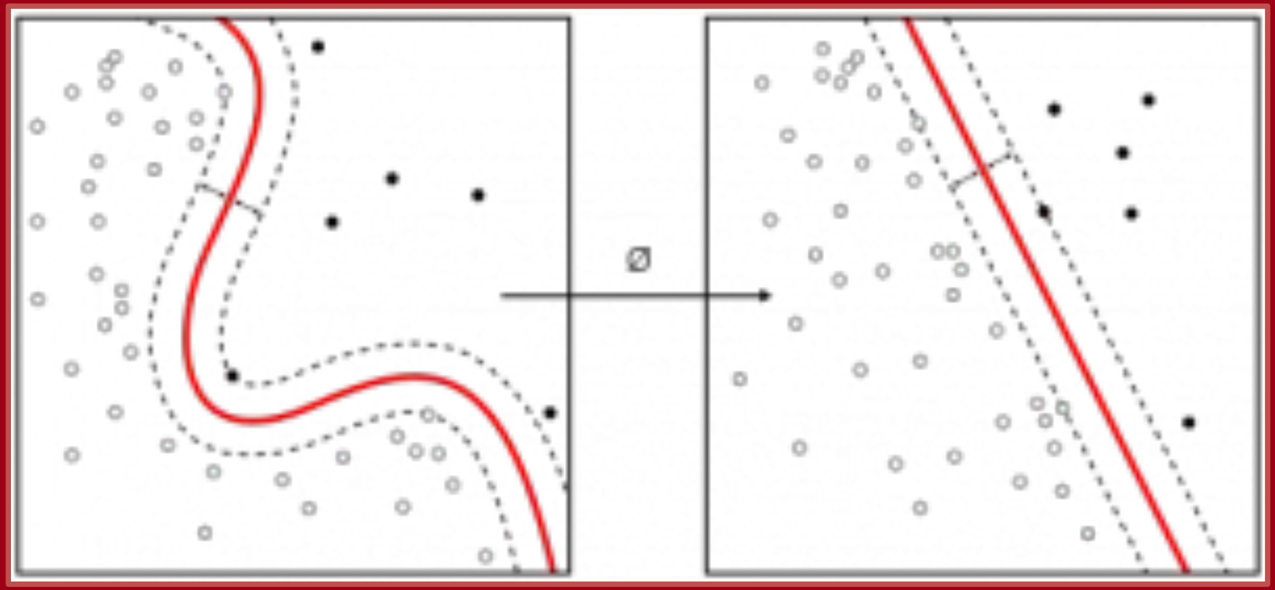

Kernel Methods

Machine Learning 2022-23
UML book chapter 16
Slides: F. Chiariotti, P. Zanuttigh, F. Vandin

Linear SVM: Key Limitation

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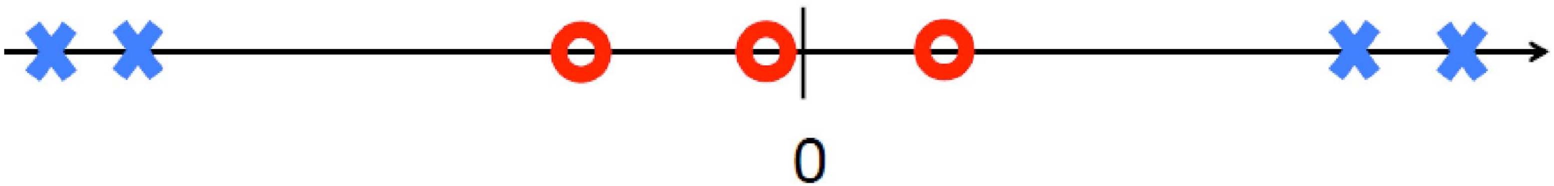
- SVM is a powerful algorithm, but still limited to linear models...
- … and linear models cannot always be used *(directly!)*

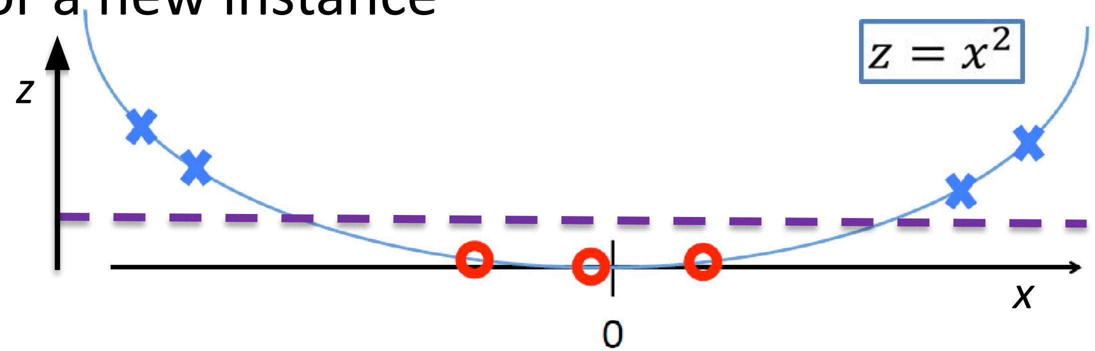
Example *(recall VC-dim of threshold is 1!)*



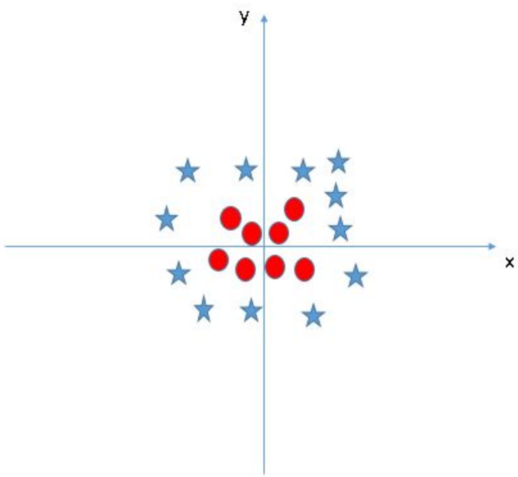
Idea:

- Apply a nonlinear transformation to each point in the training set
- Learn a linear predictor in the transformed space
- Make a prediction for a new instance

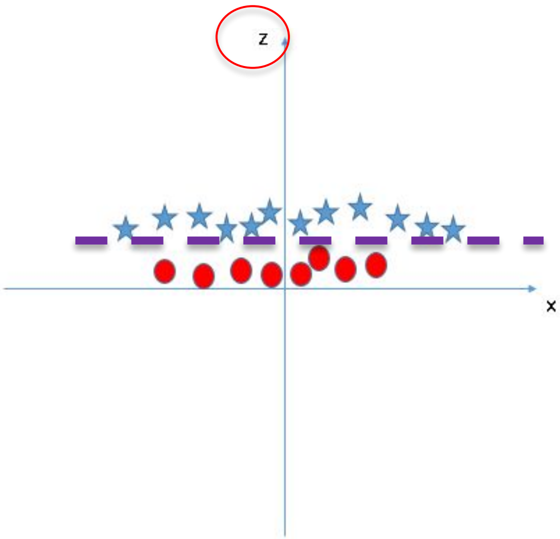
Example (*continued*)



Example



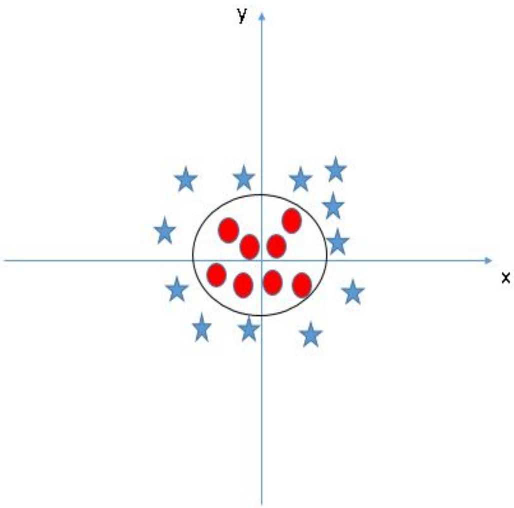
2 features *x,y* : find separating hyperplane ?



new feature *z*

$$z = x^2 + y^2$$

Now data is linearly separable!



The separating hyperplane corresponds to a circle in the original space !

Embeddings into Feature Spaces

Define a non-linear mapping ψ from the input space to a new (typically larger) space

1. Given a domain set $\mathcal{X}$ and a learning task, find a mapping to a new *feature space* $\mathcal{F}$ $\psi : \mathcal{X} \to \mathcal{F}$
   - $\mathcal{F}$ is usually $\mathbb{R}^n$ for some *n* but can be an arbitrary Hilbert space (*even of infinite size*)
2. Given a sequence of labeled examples $S = ((\boldsymbol{x_1}, y_1), \ldots, (\boldsymbol{x_m}, y_m))$ map them to $\hat{S} = ((\psi(\boldsymbol{x_1}), y_1), \ldots, (\psi(\boldsymbol{x_m}), y_m))$
3. Train a linear predictor *h* over $\hat{S}$
4. Predict the label of $\boldsymbol{x}$ as $h(\psi(\boldsymbol{x}))$

The Kernel Trick (1)

A good idea but…. there's a problem

☑ The learning over the new highly dimensional space makes halfspaces more expressive

☒ On the other side the computational complexity can become huge

- typically the new space has a much larger dimensionality

The solution: Kernel-based learning

- *Kernel*: inner product in the feature space
- Kernel function $K(x, x') =< \psi(x), \psi(x') >$
- $K()$ represent similarity of the samples in a space where the similarities are realized as inner products
- *Key Result*: machine learning algorithms for halfspaces can be carried out just on the basis of the values of the *kernel function* without explicitly representing the points in the feature space
- Sometimes we can compute $K(x, x')$ (faster) without computing $\psi(x)$ and $\psi(x')$

The Kernel Trick: Example (1)

Consider $\mathbf{x} \in \mathbb{R}^d$

Example with 2nd degree polynomial

$$\psi(\mathbf{x}) = (1, x_1, x_2, \ldots, x_d, x_1x_1, x_1x_2, x_1x_3, \ldots, x_dx_d)^T$$

The dimension of $\psi(\mathbf{x})$ is $1 + d + d^2$.

$$\langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle = 1 + \sum_{i=1}^{d} x_i x_i' + \sum_{i=1}^{d} \sum_{j=1}^{d} x_i x_j x_i' x_j' \qquad \boxed{\Theta(d^2)}$$

Note that

$$\sum_{i=1}^{d} \sum_{j=1}^{d} x_i x_j x_i' x_j' = \left(\sum_{i=1}^{d} x_i x_i' \right) \left(\sum_{j=1}^{d} x_j x_j' \right) = (\langle \mathbf{x}, \mathbf{x}' \rangle)^2$$

therefore

$$K_\psi(\mathbf{x}, \mathbf{x}') = \langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle = 1 + \langle \mathbf{x}, \mathbf{x}' \rangle + (\langle \mathbf{x}, \mathbf{x}' \rangle)^2 \qquad \boxed{\Theta(d)}$$

The Kernel Trick: Example (2)

We have:

$$\psi(\mathbf{x}) = (1, x_1, x_2, \dots, x_d, x_1x_1, x_1x_2, x_1x_3, \dots, x_dx_d)^T$$

$$K_\psi(\mathbf{x}, \mathbf{x}') = \langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle = 1 + \langle \mathbf{x}, \mathbf{x}' \rangle + (\langle \mathbf{x}, \mathbf{x}' \rangle)^2$$

Observation

Computing $\psi(\mathbf{x})$ requires $\Theta\left(d^2\right)$ time; computing $K_\psi(\mathbf{x}, \mathbf{x}')$ from the last formula requires $\Theta\left(d\right)$ time

When $K_\psi(\mathbf{x}, \mathbf{x}')$ is efficiently computable, we don't need to explicitly compute $\psi(\mathbf{x})$
$\Rightarrow$ *kernel trick*

Kernel Trick: Apply to SVM

SVM: the minimization in feature space can be rewritten as

$$\min_{\boldsymbol{w}}\left(f(<\boldsymbol{w},\psi(\boldsymbol{x_1})>,\ldots,<\boldsymbol{w},\psi(\boldsymbol{x_m})>) + R(\|\boldsymbol{w}\|) \right)$$

Where $f:\mathbb{R}^m \rightarrow \mathbb{R}$ is a generic function and $R:\mathbb{R}_+ \rightarrow \mathbb{R}$ is a monotonic not decreasing function

HARD-SVM (non-homogeneous): use

Hard-SVM: $(\boldsymbol{w}_0, b_0) = argmin_{(\boldsymbol{w},b)}\|\boldsymbol{w}\|^2$ *subject to* $\forall i$: $y_i(<\boldsymbol{w},\boldsymbol{x_i}> + b) \geq 1$

$$R(a) = a^2$$

$$f(a_1,\ldots,a_m) = \begin{cases} 0 & if\ \exists b: y_i(a_i + b) \geq 1\ \forall i \\ \infty & otherwise \end{cases}$$

SOFT-SVM (homogeneous): use

Soft-SVM: $\min_{\boldsymbol{w}}\left(\lambda\|\boldsymbol{w}\|^2 + L_S^{hinge}(\boldsymbol{w})\right)$

$$R(a) = \lambda a^2$$

$$f(a_1,\ldots,a_m) = \frac{1}{m}\sum_i \max\{0, 1 - y_i a_i\}$$

Representer Theorem

SVM: the minimization in feature space can be rewritten as

$$\min_{\boldsymbol{w}}(f(<\boldsymbol{w},\psi(\boldsymbol{x}_1)>,\dots,<\boldsymbol{w},\psi(\boldsymbol{x}_m)>)+R(\|\boldsymbol{w}\|))$$

Representer Theorem:

Assume that ψ is a mapping from $\mathcal{X}$ to a Hilbert space.
Then, there exist a vector $\boldsymbol{\alpha}\in\mathbb{R}^m$ such that $\boldsymbol{w}=\sum_{i=1}^{m}\alpha_i\psi(\boldsymbol{x}_i)$ is an optimal solution of $\min_{\boldsymbol{w}}\left(f(<\boldsymbol{w},\psi(\boldsymbol{x}_1)>,\dots,<\boldsymbol{w},\psi(\boldsymbol{x}_m)>)+R(\|\boldsymbol{w}\|)\right)$

Consequence:

We can optimize the problem w.r.t. the coefficients α_i getting a problem that depends only on $K(\boldsymbol{x},\boldsymbol{x}')=<\psi(\boldsymbol{x}),\psi(\boldsymbol{x}')>$ without explicitly computing $\psi(\boldsymbol{x})$ or $\psi(\boldsymbol{x}')$

(recall "dual" SVM problem)

Representer Theorem: Demonstration

Representer Theorem:

- Assume that ψ is a mapping from $\mathcal{X}$ to a Hilbert space.
- Then, there exist a vector $\boldsymbol{\alpha} \in \mathbb{R}^m$ such that $\boldsymbol{w} = \sum_{i=1}^{m} \alpha_i \psi(\boldsymbol{x}_i)$ is an optimal solution of $\min_{\boldsymbol{w}} \left(f(< \boldsymbol{w}, \psi(\boldsymbol{x_1}) >, \dots, < \boldsymbol{w}, \psi(\boldsymbol{x_m}) >) + R(\|\boldsymbol{w}\|) \right)$ (*)

1. Let $\boldsymbol{w}^*$ be an optimal solution of (*) : recall that $\boldsymbol{w}^*$ belongs to an Hilbert space
2. We can decompose $\boldsymbol{w}^*$ in the part into the linear span of $\psi(\boldsymbol{x}_i)$ and what's outside, i.e.: $\boldsymbol{w}^* = \sum_{i=1}^{m} \alpha_i \psi(\boldsymbol{x}_i) + \boldsymbol{u}$ with $\langle \boldsymbol{u}, \psi(\boldsymbol{x}_i) \rangle = 0$ (**)
3. Set $\boldsymbol{w} = \boldsymbol{w}^* - \boldsymbol{u}$: $\|\boldsymbol{w}^*\|^2 = \|\boldsymbol{w}\|^2 + \|\boldsymbol{u}\|^2 \rightarrow \|\boldsymbol{w}\| \leq \|\boldsymbol{w}^*\|$
4. Since R is not decreasing $\mathrm{R}(\|\boldsymbol{w}\|) \leq R(\|\boldsymbol{w}^*\|)$
5. $\forall i: y_i \langle \boldsymbol{w}, \psi(\boldsymbol{x_i}) \rangle = y_i \langle \boldsymbol{w}^* - \boldsymbol{u}, \psi(\boldsymbol{x_i}) \rangle = y_i \langle \boldsymbol{w}^*, \psi(\boldsymbol{x_i}) \rangle$ (using $**$)
6. $f(y_1 \langle \boldsymbol{w}, \psi(\boldsymbol{x_1}) \rangle, \dots, y_m \langle \boldsymbol{w}, \psi(\boldsymbol{x_m}) \rangle) = f(y_1 \langle \boldsymbol{w}^*, \psi(\boldsymbol{x_1}) \rangle, \dots, y_m \langle \boldsymbol{w}^*, \psi(\boldsymbol{x_m}) \rangle)$
7. From 4. + 6. : the objective of (*) at **w** is $\leq$ than the objective at **w***: **w** is also an optimal solution and since $\boldsymbol{w} = \sum_{i=1}^{m} \alpha_i \psi(\boldsymbol{x}_i)$ we conclude the proof

Rewrite SVM model with Kernel Functions

Note that: (recall from Representer Theorem $w = \sum_{i=1}^{m} \alpha_i \psi(x_i)$)

$$\langle \boldsymbol{w}, \psi(\boldsymbol{x_i}) \rangle = \langle \sum_j \alpha_j \psi(\boldsymbol{x_j}), \psi(\boldsymbol{x_i}) \rangle = \sum_j \alpha_j \langle \psi(\boldsymbol{x_j}), \psi(\boldsymbol{x_i}) \rangle = \sum_j \alpha_j K(\boldsymbol{x_j}, \boldsymbol{x_i})$$

$$\|\boldsymbol{w}\|^2 = \langle \sum_j \alpha_j \psi(\boldsymbol{x_j}) \sum_j \alpha_j \psi(\boldsymbol{x_j}) \rangle = \sum_{i,j} \alpha_i \alpha_j \langle \psi(\boldsymbol{x_i}), \psi(\boldsymbol{x_j}) \rangle = \sum_{i,j} \alpha_i \alpha_j K(\boldsymbol{x_i}, \boldsymbol{x_j})$$

Rewrite objective function $\min_{\boldsymbol{w}} \left(f(<\boldsymbol{w}, \psi(\boldsymbol{x_1})>, \dots, <\boldsymbol{w}, \psi(\boldsymbol{x_m})>) + R(\|\boldsymbol{w}\|) \right)$ **as**

$$\min_{\boldsymbol{\alpha}} \left(f\left(\sum_j \alpha_j K(\boldsymbol{x_j}, \boldsymbol{x_1}), \dots, \sum_j \alpha_j K(\boldsymbol{x_j}, \boldsymbol{x_m}) \right) + R\left(\sqrt{\sum_{i,j} \alpha_i \alpha_j K(\boldsymbol{x_i}, \boldsymbol{x_j})} \right) \right)$$

Notice: only kernel function K() is used without explicit constructing feature space

For the SOFT-SVM: *using Gram matrix G* : $G_{i,j} = K(\boldsymbol{x_i}, \boldsymbol{x_j})$

$$\min_{\boldsymbol{\alpha}} \left(\lambda \boldsymbol{\alpha}^T G \boldsymbol{\alpha} + \frac{1}{m} \sum_{i=1}^{m} \max\{0, 1 - y_i (G\boldsymbol{\alpha})_i\} \right)$$

Polynomial Kernels (1)

n: dimensionality of input space
K: degree of polynomial

$$\boxed{K(\boldsymbol{x},\boldsymbol{x}') = (1+\langle \boldsymbol{x},\boldsymbol{x}'\rangle)^K}$$

- It is a Kernel function, i.e., $K(\boldsymbol{x},\boldsymbol{x}') = \langle \psi(\boldsymbol{x}), \psi(\boldsymbol{x}')\rangle$

Demonstration (define $x_0 = x_0' = 1$):

$$K(\boldsymbol{x},\boldsymbol{x}') = (1+\langle \boldsymbol{x},\boldsymbol{x}'\rangle)^k = (1+\langle \boldsymbol{x},\boldsymbol{x}'\rangle)\dots(1+\langle \boldsymbol{x},\boldsymbol{x}'\rangle) =$$

$$\underbrace{\left(\sum_{j=0}^{n} x_j x_j'\right)\dots\left(\sum_{j=0}^{n} x_j x_j'\right)}_{\text{K-times}} = \sum_{J\in\{0,1,\dots,n\}^k} \prod_{i=1}^{k} x_{j_i} x'_{j_i} = \sum_{J\in\{0,1,\dots,n\}^k} \prod_{i=1}^{k} x_{j_i} \prod_{i=1}^{k} x'_{j_i}$$

By defining $\psi: \mathbb{R}^n \to \mathbb{R}^{(n+1)^k}$ such that for each $J \in \{0,1,\dots,n\}^k$ there is an element of ψ that equals $\prod_{i=1}^{k} x_{j_i}$, we obtain $K(\boldsymbol{x},\boldsymbol{x}') = \langle \psi(\boldsymbol{x}), \psi(\boldsymbol{x}')\rangle$

$J \in \{0,1,\dots,n\}^k$: select k elements from the 0,..,n set

Polynomial Kernels (2)

$$\boxed{K(\boldsymbol{x},\boldsymbol{x}') = (1 + \langle \boldsymbol{x},\boldsymbol{x}' \rangle)^K}$$

- It is a Kernel function, i.e., $K(\boldsymbol{x},\boldsymbol{x}') = \langle \psi(\boldsymbol{x}), \psi(\boldsymbol{x}') \rangle$
- $\psi\colon \mathbb{R}^n \rightarrow \mathbb{R}^{(n+1)k}$ contains all the monomials up to degree *k*
- Halfspace over ψ corresponds to a polynomial predictor of order *k* in the original space
- Complexity of computation is *O(n)* while the dimension of feature space is $O(n^k)$

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Gaussian Kernel (*Radial Basis Function*, RBF) (1)

$$K(\boldsymbol{x}, \boldsymbol{x}') = e^{-\frac{\left\|\boldsymbol{x}-\boldsymbol{x}'\right\|^2}{2\sigma^2}}$$

Recall:
$$\sum_{n=0}^{\infty} \frac{x^n}{n!} = e^x$$

- It is a Kernel function, i.e., $K(\boldsymbol{x}, \boldsymbol{x}') = \langle \psi(\boldsymbol{x}), \psi(\boldsymbol{x}') \rangle$

Demonstration (on 1D case $x \in \mathbb{R}$):

Consider the mapping $\psi(\mathrm{x})_{\mathrm{n}} = \frac{1}{\sqrt{n!}} \mathrm{e}^{-\frac{x^2}{2}} x^n$

$$\langle \psi(\boldsymbol{x}), \psi(\boldsymbol{x}') \rangle = \sum_{n=0}^{\infty} \left(\frac{1}{\sqrt{n!}} \mathrm{e}^{-\frac{x^2}{2}} x^n \right) \left(\frac{1}{\sqrt{n!}} \mathrm{e}^{-\frac{x'^2}{2}} x'^n \right) =$$

$$= \mathrm{e}^{-\frac{x^2+x'^2}{2}} \sum_{n=0}^{\infty} \left(\frac{(\mathrm{xx}')^{\mathrm{n}}}{n!} \right) = \mathrm{e}^{-\frac{x^2+x'^2}{2}} \mathrm{e}^{xx'} = \mathrm{e}^{-\frac{x^2+x'^2-2xx'}{2}} = \mathrm{e}^{-\frac{\left\|x-x'\right\|^2}{2}}$$

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Gaussian Kernel (*Radial Basis Function,* RBF) (2)

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

- It is a Kernel function, i.e., $K(\boldsymbol{x},\boldsymbol{x}') = \langle \psi(\boldsymbol{x}), \psi(\boldsymbol{x}') \rangle$
- The feature space is of infinite dimension
  - but computing the Kernel is simple and fast !
- Product is close to 0 if instances are far and close to 1 if they are close
- Parameter σ controls what we mean by "*close*"
- We can learn any polynomial predictor in the original space by using a Gaussian kernel
- VC-dimension is infinite (sample complexity depends on the margin in the feature space)

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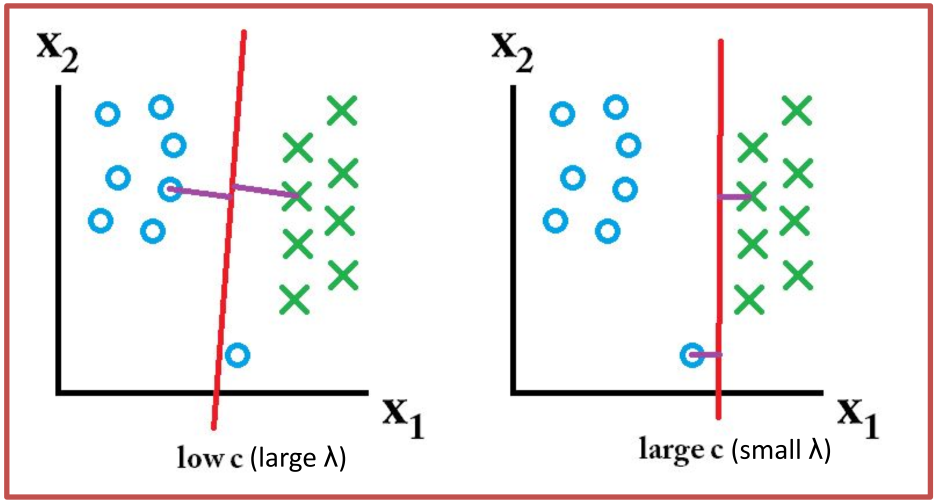
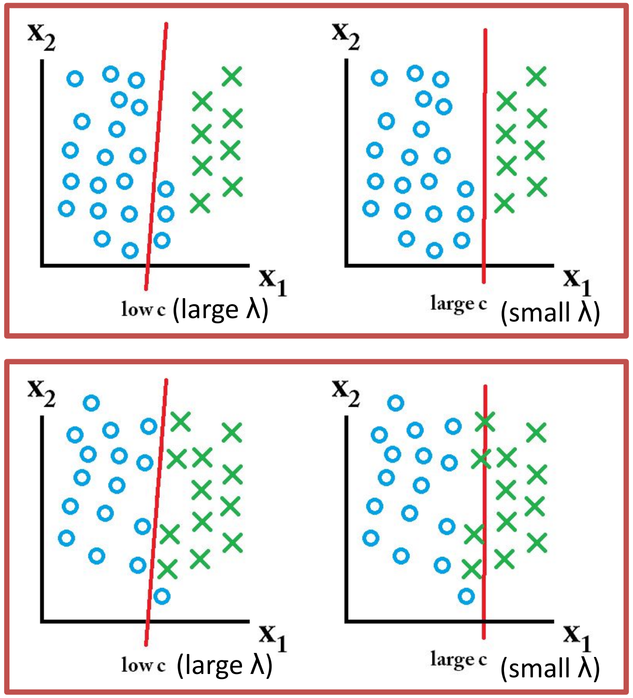
Practical SVM: The λ Parameter



Training Set

$$\min_{\mathbf{w}} \left(\lambda \|\mathbf{w}\|^2 + L_S^{\text{hinge}}(\mathbf{w}) \right)$$



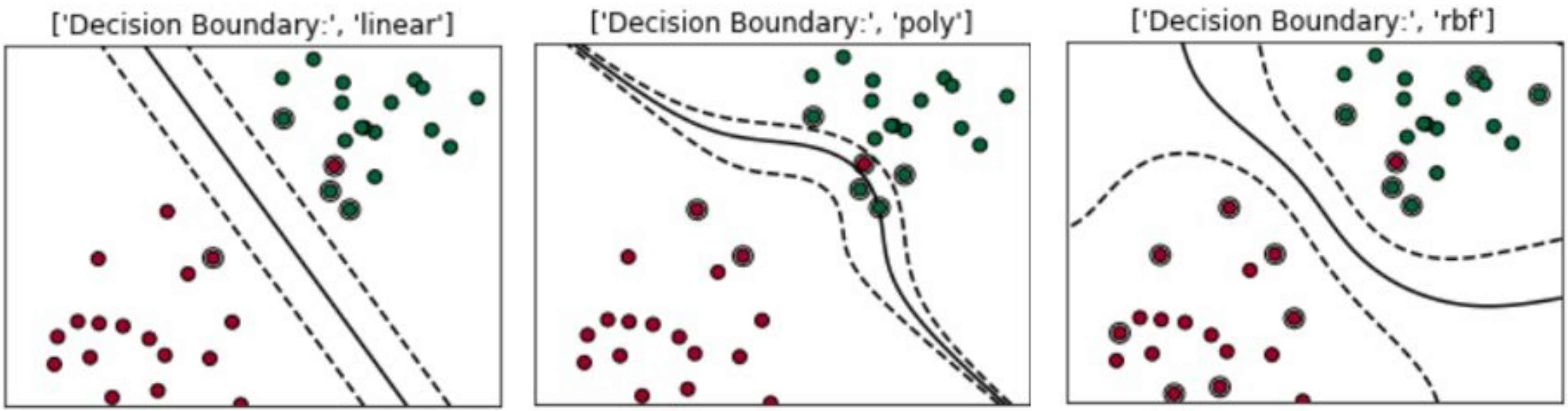
Examples on 2 different test sets

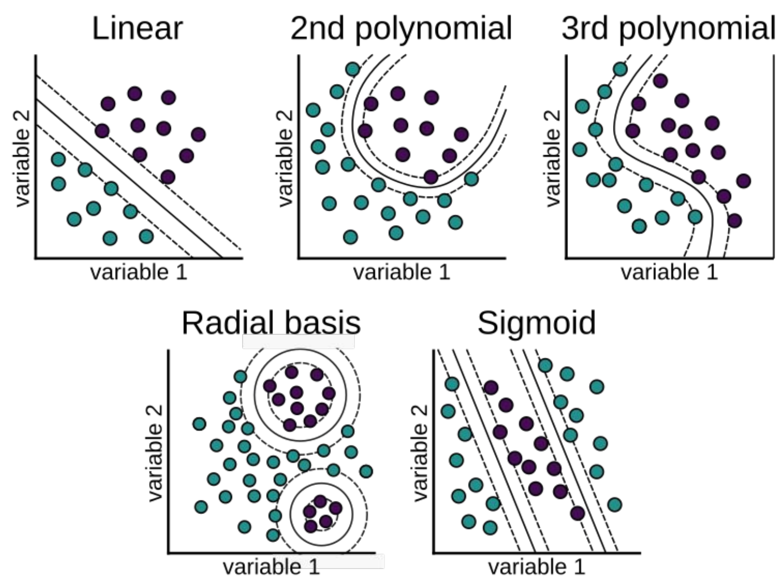
The parameter λ controls the trade-off between a solution with a large margin that makes some errors or one with a lower margin but with less errors

(the parameter C in *sklearn*, *libsvm* and other ML tools has the same role but weights the loss term, i.e., works in the opposite direction)

images from stackexchange

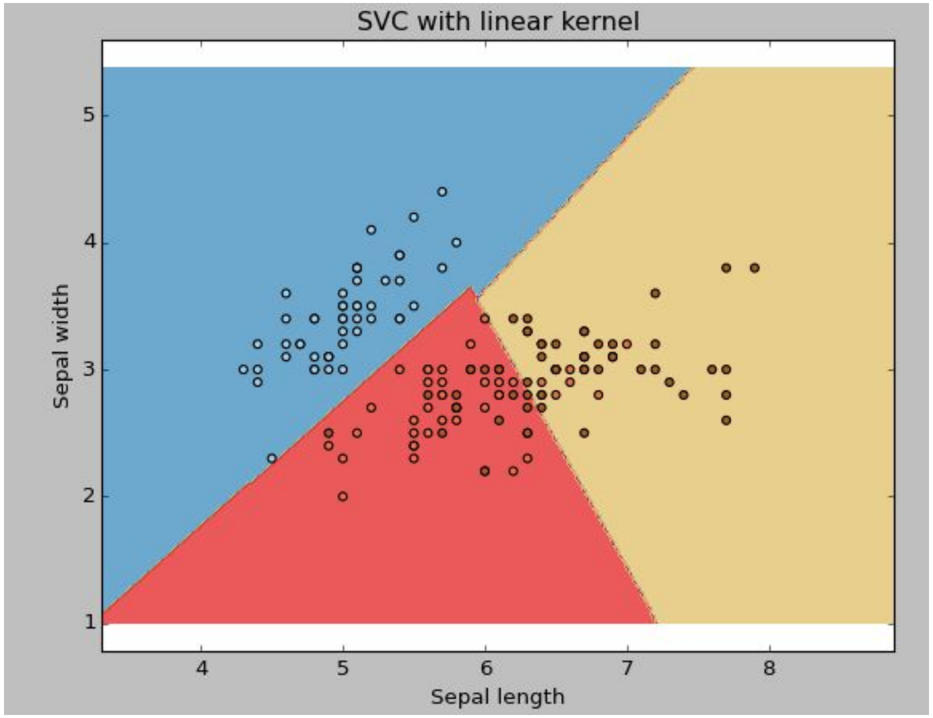
Practical SVM: Different Kernels

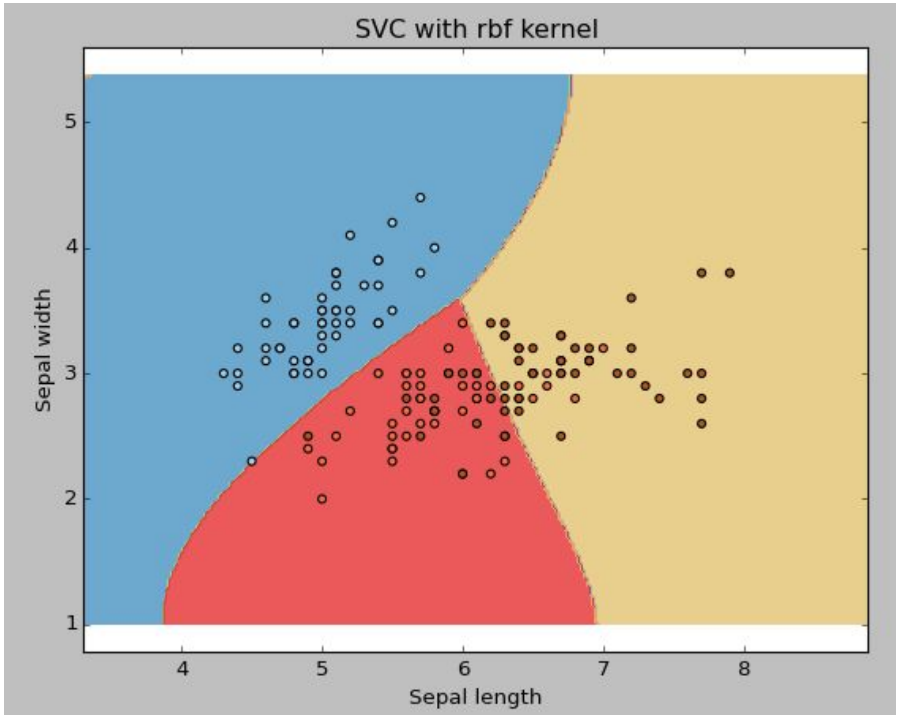




images from towardsdatascience and R-Bloggers

Practical SVM: Linear vs RBF Kernel





From: https://www.analyticsvidhya.com/blog/2017/09/understaing-support-vector-machine-example-code/

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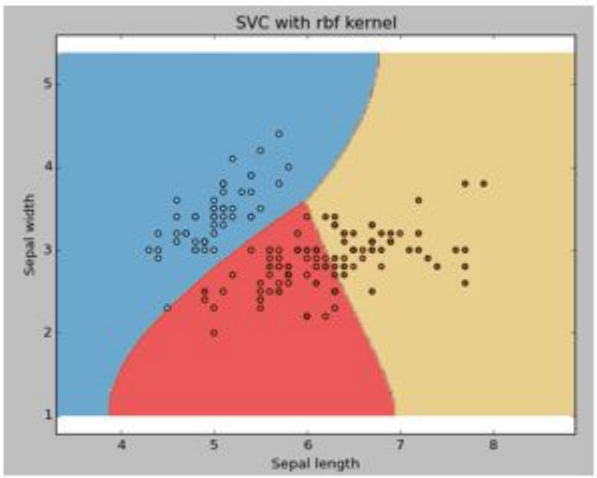
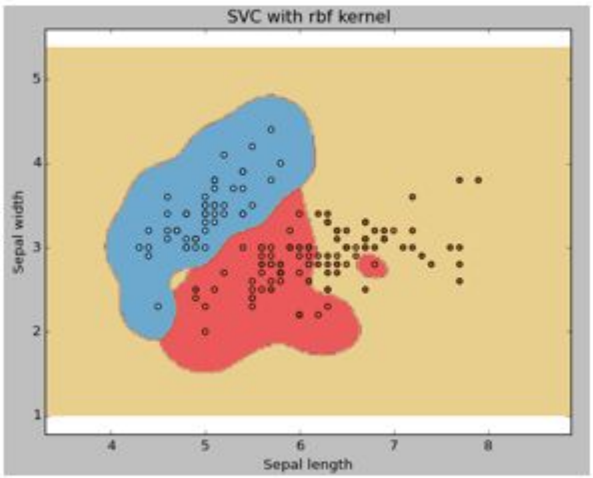
Practical SVM: Standard Deviation of RBF Kernel

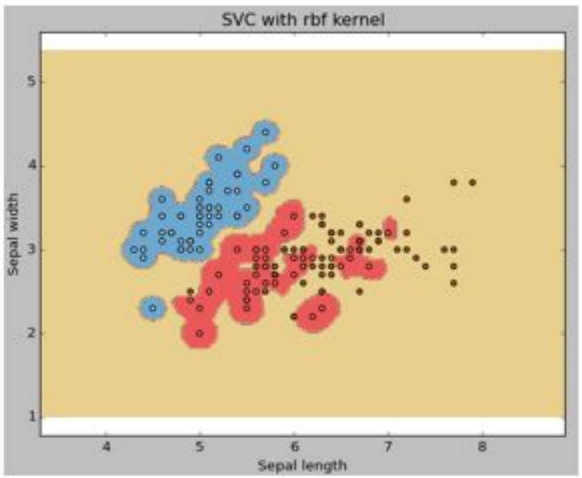
gamma =0 $(\sigma \rightarrow \infty)$



gamma =10 $(\sigma = 0.1)$



gamma =100 $(\sigma = 0.01)$



- The standard deviation σ of the Gaussian/RBF kernel controls the concept or "*close*" and "*far*" in the kernel function
- It corresponds to the trade-off between precisely fit the training set (with risk of overfitting) or finding a less accurate but more general solution
- The gamma parameter of *sklearn* correspond to the inverse of σ

Images from: https://www.analyticsvidhya.com/blog/2017/09/understaing-support-vector-machine-example-code/

Practical SVM: Grid Search Example

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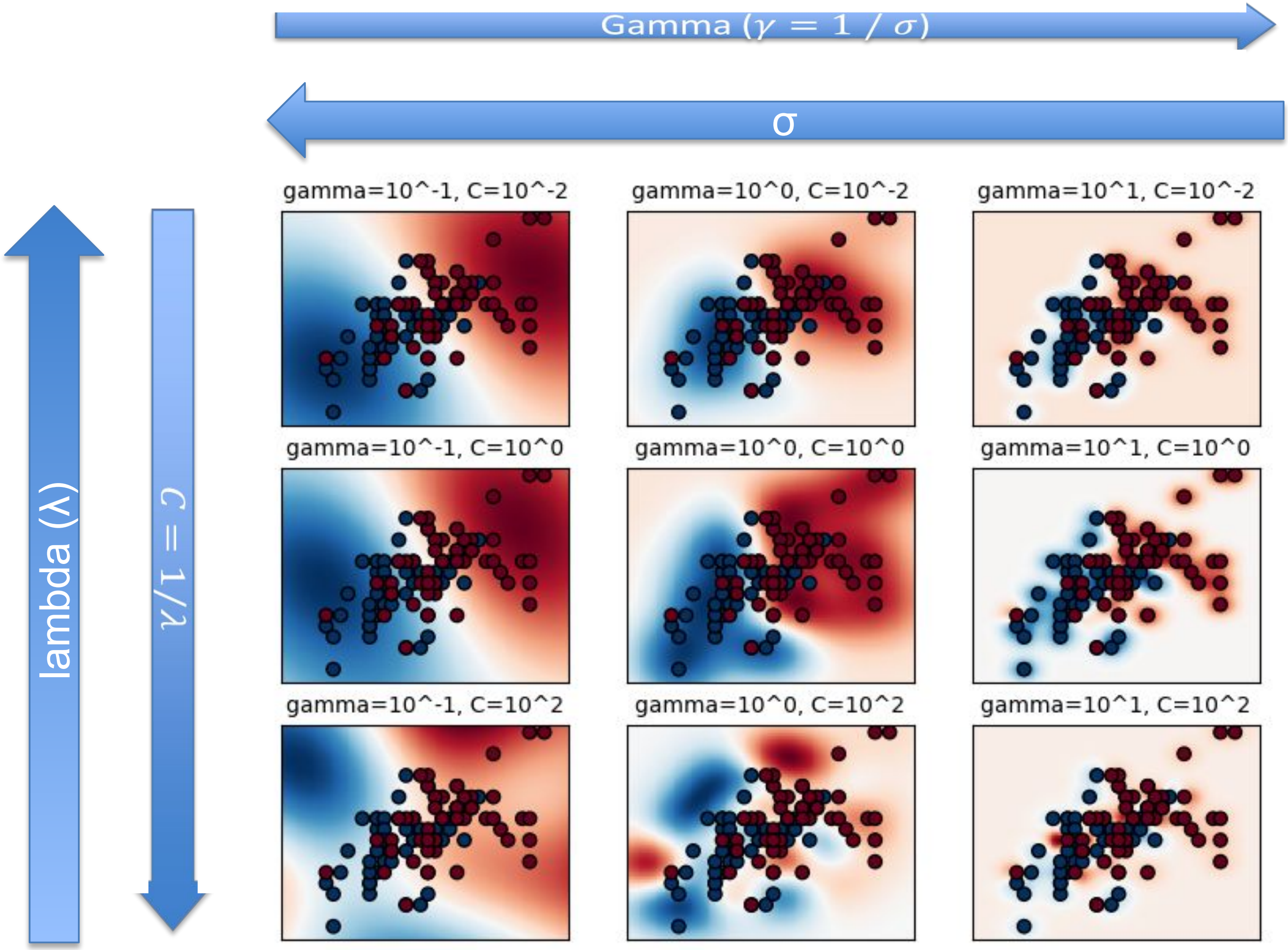


images from sklearn documentation

Exercise

Assume we have the dataset in the table ($x_i \in \mathbb{R}^2$) and by solving the SVM for classification we get the corresponding α coefficients (recall that $\boldsymbol{w} = \sum_i \alpha_i \boldsymbol{x_i}$ while in the dual optimization $\boldsymbol{w} = \sum_i \alpha_i^* y_i \boldsymbol{x}_i$):

i				
1	[0.2 -1.4]	-1	0	0
2	[-2.1 1.7]	1	0	0
3	[0.9 1]	1	0.5	0.5
4	[-1 -3.1]	-1	0	0
5	[-0.2 -1]	-1	-0.25	0.25
6	[-0.2 1.3]	1	0	0
7	[2.0 -1]	-1	-0.25	0.25
8	[0.5 2.1]	1	0	0

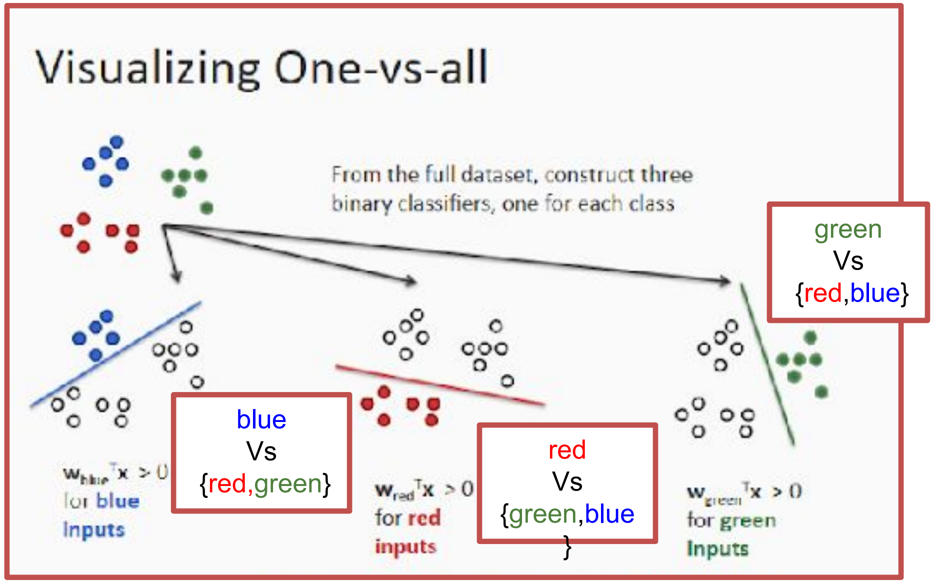
Answer to the following:

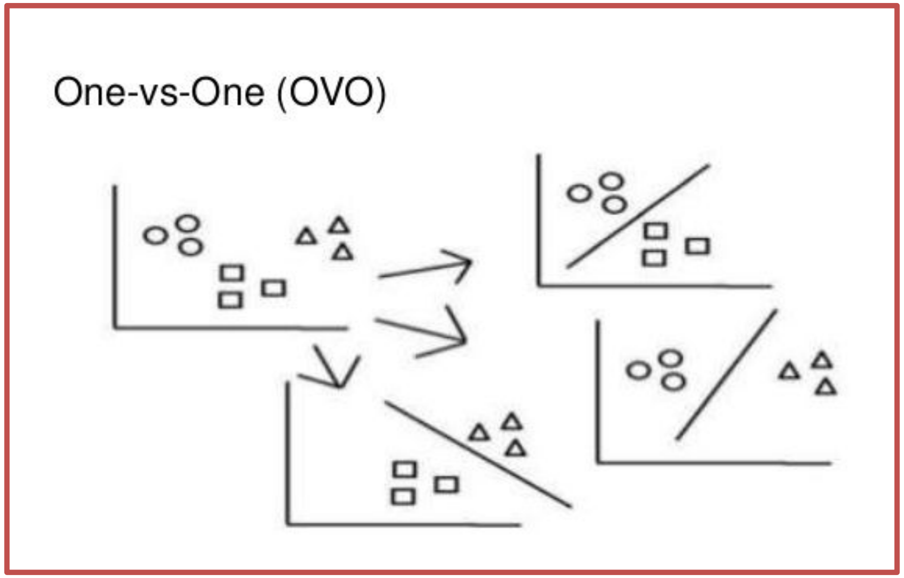
(A) Which are the support vectors?

(B) Draw a schematic picture reporting the data points (approximately) and the optimal separating hyperplane, and mark the support vectors.

(C) Would it be possible, by moving only two data points, to obtain the SAME separating hyperplane with only 2 support vectors? Draw the modified configuration (approximately)

Multi-class Classification





- Classify each class vs the union of all the others
- For each sample select the class with highest classification score, i.e. $\text{argmax} < \boldsymbol{w_i}, \boldsymbol{x} >$
- Requires $n_{classes}$ comparisons

- Classify each class vs each other class
- For each sample select the class that has "won" the largest number of classifications
- Requires $\frac{n_{classes}(n_{classes}-1)}{2}$ comparisons
- Used by *sklearn*

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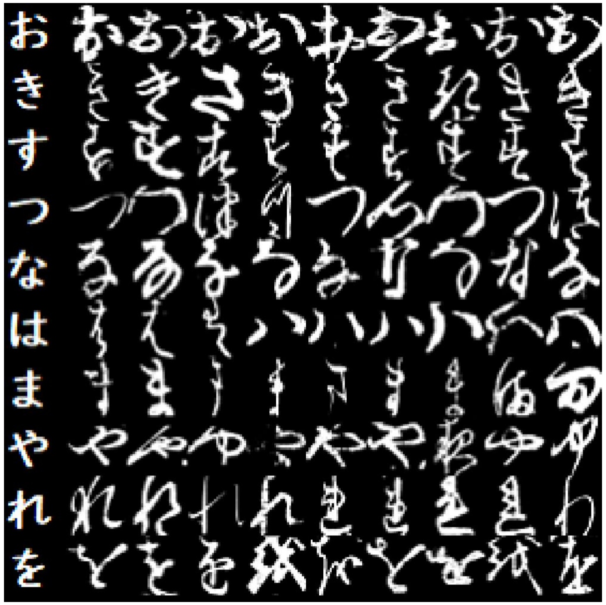
LAB2: Classification with SVM

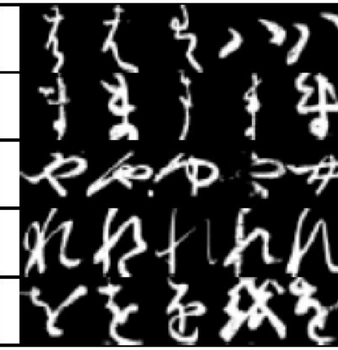


- Classify ancient cursive Japanese (Kuzushiji)writing
- Use Support Vector Machines (SVM)

Notebook released on 16/11
Lab 2 on 23/11
Delivery on 2/12

The KMNIST Dataset

Hiragana	Unicode	Samples	Sample Images
お (o)	U+304A	7000	
き (ki)	U+304D	7000	
す (su)	U+3059	7000	
つ (tsu)	U+3064	7000	
な (na)	U+306A	7000	

Hiragana	Unicode	Samples	Sample Images
は (ha)	U+306F	7000	
ま (ma)	U+307E	7000	
や (ya)	U+3084	7000	
れ (re)	U+308C	7000	
を (wo)	U+3092	7000	

- 10 classes corresponding to 10 different characters
- 70’000 samples (7’000 for each class)
- Divided into 60’000 for training and 10’000 for testing
- Recent deep learning schemes can reach an accuracy of 99%
- Expect an accuracy around 80% for a «baseline» SVM classification

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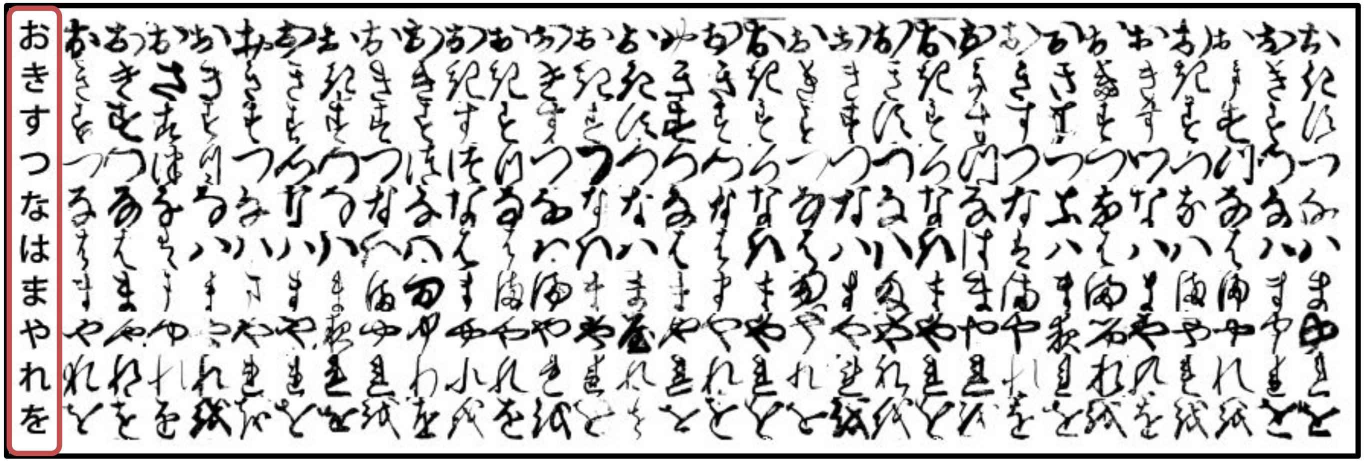
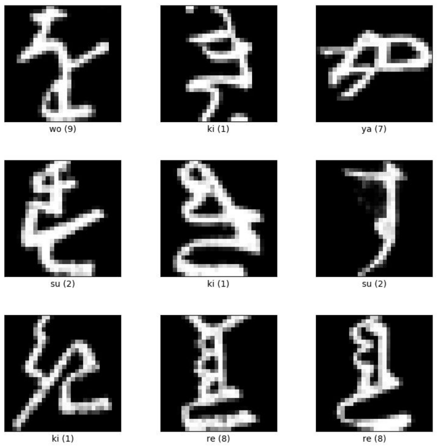
LAB2: Classification of Kuzushiji characters with SVM





- Classify images of characters
- Use Support Vector Machines (SVM)
- Dataset of small pictures of characters: multi-class classification problem
- Use Support Vector Machines
- Try different Kernels
- Estimate parameters with cross validation
- Visualize the results with confusion matrices