KSBi-BIML 2023

Bioinformatics & Machine Learning(BIML)
Workshop for Life Scientists, Data Scientists,
and Bioinformatians

생물정보학&머신러닝 워크샵(온라인)

SVM (Support Vector Machine)의 개념과 활용

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SBi 한국생명정보학회
Korean Society for Bioinformatics

본 강의 자료는 한국생명정보학회가 주관하는 BIML 2023 워크샵 온라인 수업을 목적으로 제작된 것으로 해당 목적 이외의 다른 용도로 사용할 수 없음을 분명하게 알립니다.

이를 다른 사람과 공유하거나 복제, 배포, 전송할 수 없으며 만약 이러한 사항을 위반할 경우 발생하는 **모든 법적 책임은 전적으로 불법 행위자 본인에게 있음을 경고**합니다.

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안녕하십니까?

한국생명정보학회가 개최하는 동계 교육 워크샵인 BIML-2023에 여러분을 초대합니다. 생명정보학 분야의 연구자들에게 최신 동향의 데이터 분석기술을 이론과 실습을 겸비해 전달하고자 도입한 전문 교육 프로그램인 BIML 워크샵은 2015년에 시작하여 올해로 9차를 맞이하게 되었습니다. 지난 2년간은 심각한 코로나 대유행으로 인해 아쉽게도 모든 강의가 온라인으로 진행되어 현장 강의에서만 가능한 강의자와 수강생 사이에 다양한 소통의 기회가 없음에 대한 아쉬움이 있었습니다. 다행히도 최근 사회적 거리두기 완화로 현장 강의가 가능해져 올해는 현장 강의를 재개함으로써 온라인과 현장 강의의 장점을 모두 갖춘 프로그램을 구성할 수 있게 되었습니다.

BIML 워크샵은 전통적으로 크게 인공지능과 생명정보분석 두 개의 분야로 구성되었습니다. 올해 AI 분야에서는 최근 생명정보 분석에서도 응용이 확대되고 있는 다양한 심층학습(Deep learning) 기법들에 대한 현장 강의가 진행될 예정이며, 관련하여 심층학습을 이용한 단백질구조예측, 유전체 분석, 신약개발에 대한 이론과 실습 강의가 함께 제공될 예정입니다. 또한 싱글셀오믹스 분석과 메타유전체분석 현장 강의는 많은 연구자의 연구 수월성 확보에 큰 도움을 줄 것으로 기대하고 있습니다. 이외에 다양한 생명정보학 분야에 대하여 30개 이상의 온라인 강좌가 개설되어 제공되며 온라인 강의의 한계를 극복하기 위해서 실시간 Q&A 세션 또한 마련했습니다. 특히 BIML은 각 분야 국내 최고 전문가들의 강의로 구성되어 해당 분야의 기초부터 최신 연구 동향까지 포함하는 수준 높은 내용의 강의가 될 것입니다.

이번 BIML-2023을 준비하기까지 너무나 많은 수고를 해주신 BIML-2023 운영위원회의 남진우, 우현구, 백대현, 정성원, 정인경, 장혜식, 박종은 교수님과 KOBIC 이병욱 박사님께 커다란 감사를 드립니다. 마지막으로 부족한 시간에도 불구하고 강의 부탁을 흔쾌히 허락하시고 훌륭한 현장 강의와 온라인 강의를 준비하시는데 노고를 아끼지 않으신 모든 연사분께 깊은 감사를 드립니다.

2023년 2월

한국생명정보학회장 이 인 석

강의개요

SVM (Support Vector Machine)의 개념과 활용

SVM은 분류 문제에 해결함에 있어 딥신경망, 그래디언트 부스팅과 함께 가장 좋은 성능을 보이는 감독 학습 기법으로, 기계학습의 아버지라 불리는 Vladmir Vapnik 교수님의 약 30년간의 기계학습 연구 끝에 탄생한 역작이다. SVM은 기본적으로 큰 마진 (large margin)을 갖는 선형 분류기를 학습하며, 커널 (kernel)이라는 매커니즘을 이용하여 원래의 데이터 공간 대신 소위 피처 공간 (feature space)에서 예측에 효과적인 선형 분류기를 학습할 수 있다. 이와 같이, 커널을 이용하는 SVM은 딥신경망과 마찬가지로 데이터의 새로운 표현형을 학습할 수 있기 때문에 비선형 결정 경계를 갖는 분류 문제 해결에 효과적이다.

SVM은 벡터 형 데이터 뿐만 아니라 시퀀스, 그래프 등의 구조를 갖는 데이터에 대해서도 커널을 정의함으로써 적용 가능하며, 다른 기계학습 기법에 비해 과적합 우려가 적으며, 특히 딥신경망 학습과 비교해서는 학습 문제가 볼록 최적화로 귀결되기 때문에 최적의 학습 파라미터를 찾기가 훨씬 용이하다는 장점을 지닌다. 특히, 후자의 사실은 분류기를 구성하는 학습 파라미터의 기여도를 통해 중요 인자를 추출함에 있어 큰 장점으로 작용할 수 있다.

본 강의에서는 SVM의 개념과 학습 최적화 문제, 듀얼 최적화 문제, 커널 SVM에 대해 이해하고, 이를 바탕으로 바이오 데이터를 활용한 문제 해결에 적용할 수 있는 역량을 함양한다.

* 교육생준비물:
  노트북 (메모리 8GB 이상, 디스크 여유공간 30GB 이상)
  구글 계정 생성
  Anaconda 다운로드 및 설치 (https://www.anaconda.com/)

* 강의 난이도: 초급

* 강의: 이상근 교수 (고려대학교 정보보호학과)

Curriculum Vitae

Speaker Name: Sangkyun Lee, Ph.D.

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Research Interest

Machine Learning, Secure AI, Collaborative Learning

Educational Experience

2003	B.S., Seoul National University
2005	M.S., Seoul National University
2011	Ph.D., University of Wisconsin-Madison, USA

Professional Experience

2011-2014	Post-doc researcher, Collaborative Research Center (SFB876), TU Dortmund University, Germany
2015-2017	Principal Investigator, Collaborative Research Center (SFB876), TU Dortmund University, Germany
2017-2019	Assistant Professor, Department of Computer Science, Hanyang University ERICA
2020-Current	Assistant Professor, Department of Cybersecurity, Korea University

Selected Publications (5 maximum)

1. Data Quality Measures and Efficient Evaluation Algorithms for Large-Scale High-Dimensional Data, Hyeongmin Cho and Sangkyun Lee, Applied Sciences, 2021
2. Sparse Portfolio Selection via the sorted ℓ1 - Norm, Philipp J. Kremer*, Sangkyun Lee*, Małgorzata Bogdan, and Sandra Paterlini, Journal of Banking & Finance, 2020
3. Structure Learning of Gaussian Markov Random Fields with False Discovery Rate Control, Sangkyun Lee, Piotr Sobczyk and Malgorzata Bogdan, Symmetry, 2019
4. Compressed Learning of Deep Neural Networks for OpenCL-Capable Embedded Systems, Sangkyun Lee and Jeonghyun Lee, Applied Sciences, 2019
5. The mutational landscape of MYCN, Lin28b and ALKF1174L driven murine neuroblastoma mimics human disease, Bram De Wilde, Anneleen Beckers, Sven Lindner, Althoff Kristina, Katleen De Preter, Pauline Depuydt, Pieter Mestdagh, Tom Sante, Steve Lefever, Falk Hertwig, Zhiyu Peng, Le-ming Shi, Sangkyun Lee, Elien Vandermarliere, Lennart Martens, Björn Menten, Alexander Schramm, Matthias Fischer, Johannes Schulte, Jo Vandesompele and Frank Speleman, Oncotarget, 2017

KSBi-BIML

SVM (Support Vector Machine)의 개념과 활용

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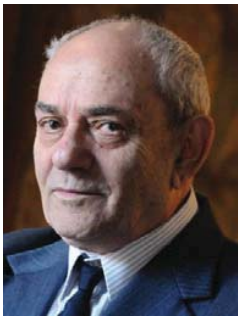
Agenda

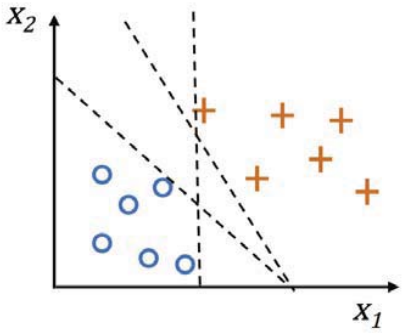
1. SVM의 개념
   - Two learning goals
     - Large margin classification
     - Good prediction: hinge loss
   - SVM Training
     - Optimization
   - Feature selection
   - Kernel의 활용

2. Python (Scikit-Learn)에서의 SVM

SVM (Support Vector Machine)

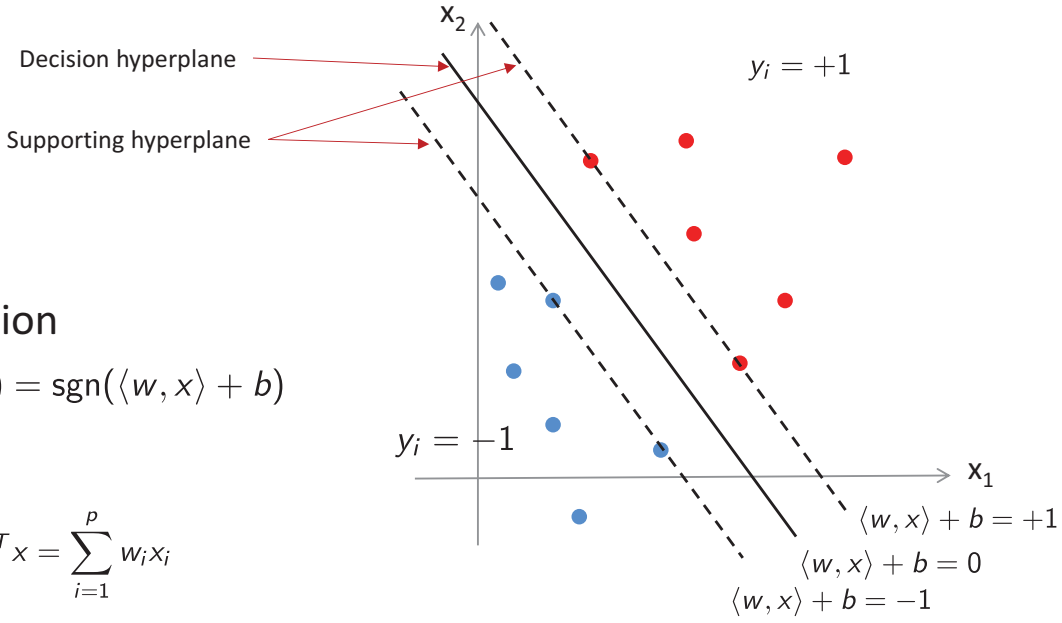


- A linear classifier, invented by V. Vapnik
  - V. Vapnik: the father of machine learning
  - Cortes, Corinna; Vapnik, Vladimir N., Support-vector net works, Machine Learning, 20 (3): 273–297 (1995)
  - The nature of statistical Learning Theory, Springer, 1999
- 'Margin' between two class point clouds
  - **Minimize prediction error**
  - **+ maximize the margin** at the same time
- SVM hardly overfits, under regular conditions
- SVM can use **kernels**



SVM

- Data
  - Input: $x \in \mathbb{R}^p$ ($x \in X$ in general)
  - Label: $y \in \{-1, +1\}$

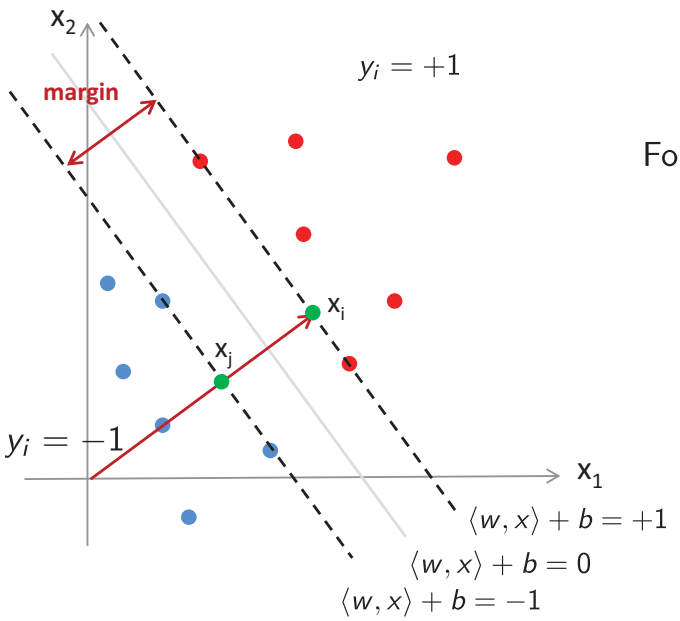


- Decision

$$f_w(x) = \text{sgn}(\langle w, x \rangle + b)$$

$$\langle w, x \rangle = w^T x = \sum_{i=1}^{p} w_i x_i$$

Margin of SVM



$$\langle w, x_i \rangle + b = +1$$
$$\langle w, x_j \rangle + b = -1$$
$$\Rightarrow \langle w, x_i - x_j \rangle = 2$$

For $x_i - x_j = t\frac{w}{\|w\|_2}$, $t \in \mathbb{R}$,

$$t = \frac{2}{\|w\|_2}$$

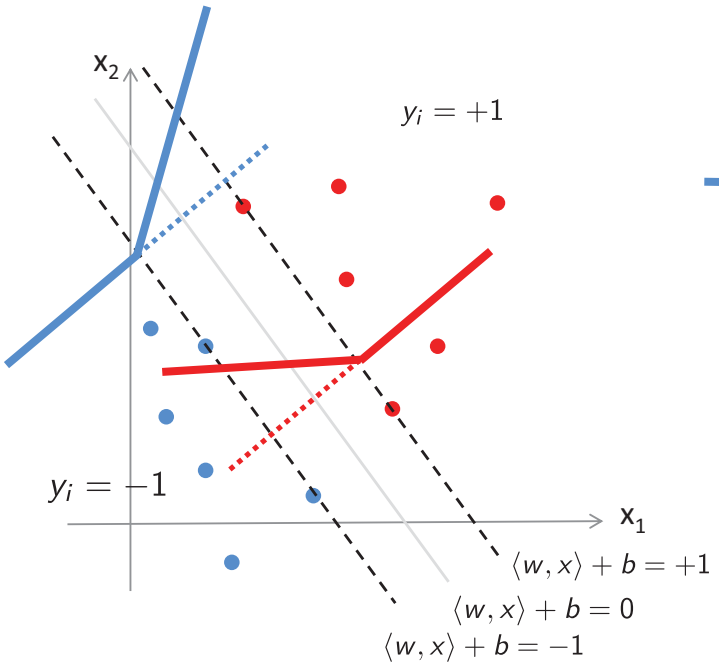
Learning Goal 1 (max. margin)

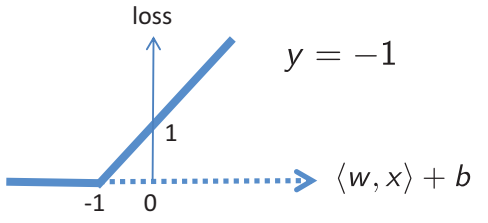
$$\min_w \ \frac{1}{2}\|w\|_2^2$$

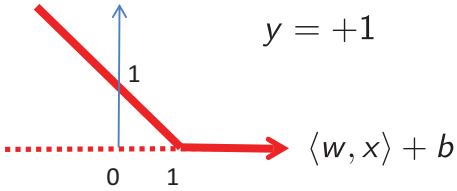
Learning Goal 2 (Min. Prediction Error)

- Avoid having data points within the margin (as much as possible)

➔ Design a loss function

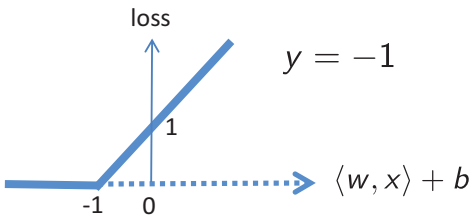


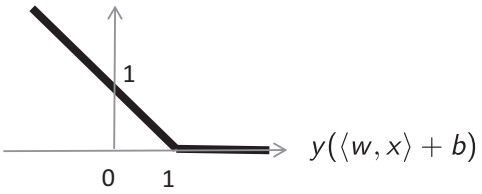




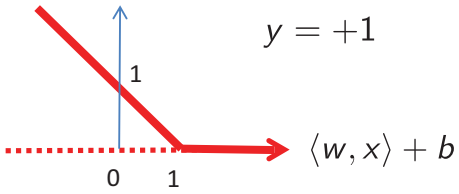
Learning Goal 2 (Min. Prediction Error)

- Hinge loss function





$$\max\{1 - y(\langle w, x \rangle + b), 0\}$$



Learning Goal 2 (min. pred error)

$$\min_{w,b} \sum_{i=1}^{n} \max\{1 - y_i(\langle w, x_i \rangle, b), 0\}$$

SVM Training Problem

$$\min_{w \in \mathbb{R}^p, b} \frac{1}{2}\|w\|_2^2 + C \sum_{i=1}^{n} \max\{1 - y_i(\langle w, x_i \rangle, b), 0\}$$

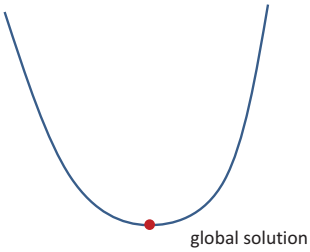
- n: number of observations (patients, etc)
- p: number of input features (genes, etc.)
- C > 0: a hyper-parameter for balancing the two learning goals

- This can be solved using SGD-type algorithms
  - Useful when n is huge
  - Pegasos solver [Shai Shalev-Shwartz et al., 2010]

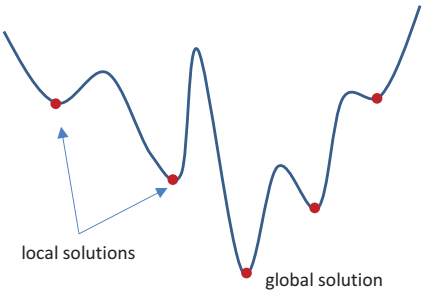
- However, it is convex optimization, where better alternatives exist
  - When n is in a modest range, non-SGD type algorithms will be better (n < 100,000)
    - Finds the global minimizer (important for feature selection)
  - Special solvers are available when p is large
  - When data points x is NOT in a vector form ➔ kernel trick is available

Convex vs. Non-convex Optimization

- ML methods
  - Based on convex optimization
    - Logistic regression, SVM, …
  - Based on non-convex optimization
    - Deep neural nets with nonlinear activations (DNN, CNN, RNN, …)
    - NMF
- Shape of loss functions



Convex



Non-convex

SVM Smooth Formulation

$$\min_{w\in\mathbb{R}^p, b\in\mathbb{R}} \ \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^{n} \max\{1 - y_i(\langle w, x_i\rangle, b), 0\}$$

➔

$$\min_{w\in\mathbb{R}^p, b\in\mathbb{R}, \xi\in\mathbb{R}^n} \ \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^{n} \xi_i$$
$$\text{subject to} \ \ \xi_i = \max\{1 - y_i(\langle w, x_i\rangle, b), 0\}, \ \ i = 1, \ldots, n$$

➔

$$\min_{w\in\mathbb{R}^p, b\in\mathbb{R}, \xi\in\mathbb{R}^n} \ \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^{n} \xi_i$$
$$\text{subject to} \ \ \xi_i \geq 1 - y_i(\langle w, x_i\rangle, b), \ \ i = 1, \ldots, n$$
$$\xi_i \geq 0, \ \ i = 1, \ldots, n$$

"The C-SVM"

C-SVM

$$\min_{w\in\mathbb{R}^p, b\in\mathbb{R}, \xi\in\mathbb{R}^n} \ \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^{n}\xi_i$$

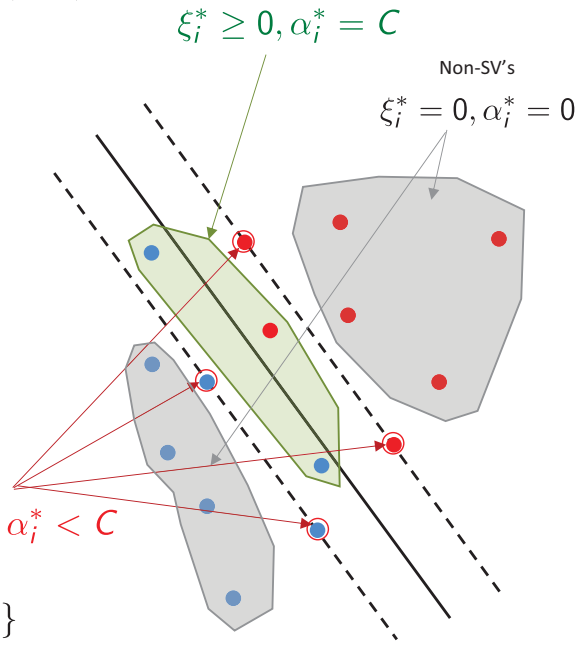
subject to $\xi_i \geq 1 - y_i(\langle w, x_i\rangle, b),\ i = 1,\ldots,n$

$\xi_i \geq 0,\ i = 1,\ldots,n$

KKT (Karush-Kuhn-Tucker) conditions: the conditions satisfied by the solution

Insights from the KKT conditions:

$$w^* = \sum_{i=1}^{n}\alpha_i^* x_i \qquad \text{dual variable} \quad 0 \leq \alpha_i^* \leq C$$



Support vector set: $\{i \in \{1,\ldots,n\} : \alpha_i^* > 0\}$

C-SVM

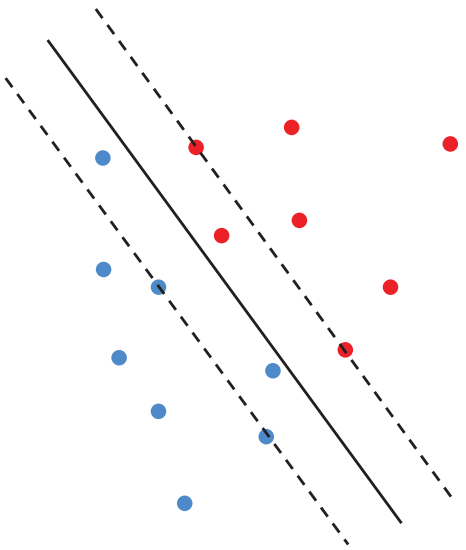
$$\min_{w\in\mathbb{R}^p, b\in\mathbb{R}, \xi\in\mathbb{R}^n} \ \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^{n}\xi_i$$

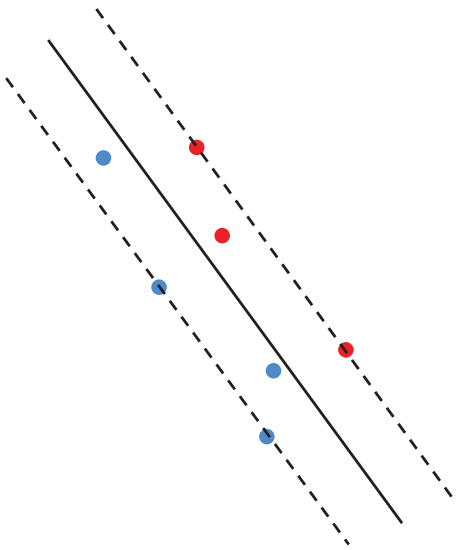
subject to $\xi_i \geq 1 - y_i(\langle w, x_i\rangle, b),\ i = 1,\ldots,n$

$\xi_i \geq 0,\ i = 1,\ldots,n$

$$w^* = \sum_{i\in SV}\alpha_i^* x_i$$

b* can be computed using only SV's

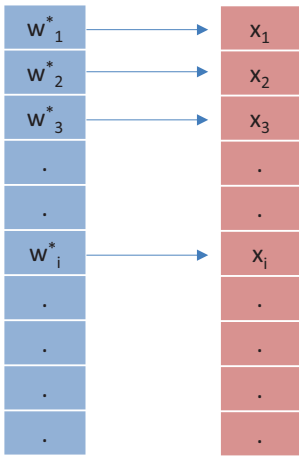


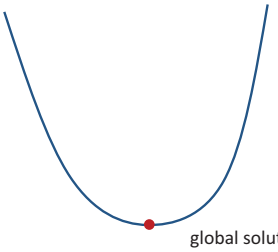


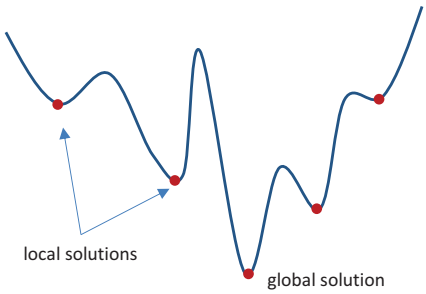
The same classifier will be obtained!

Feature Selection

- SVM decision function
  - $f_w(x) = \text{sgn}(\langle w^*, x \rangle + b^*)$
  - Each weight (coefficient) represents the contribution of each input feature to th e decision

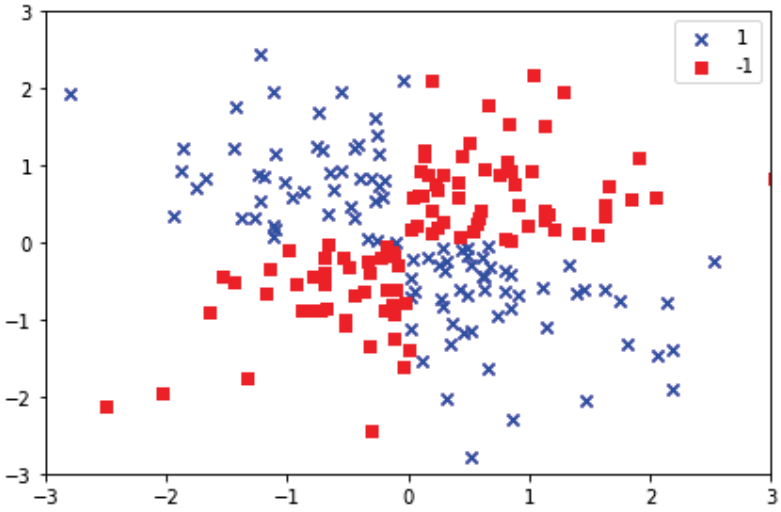




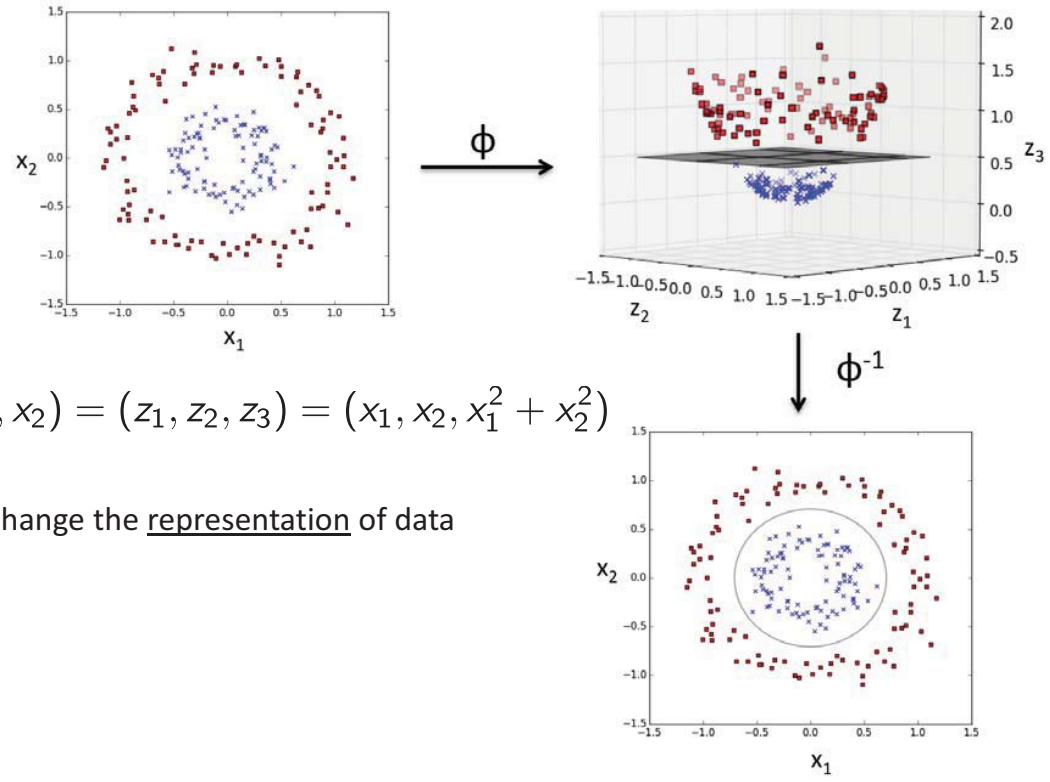


Nonlinear Classification Problems

- Data with XOR class pattern



Feature Map

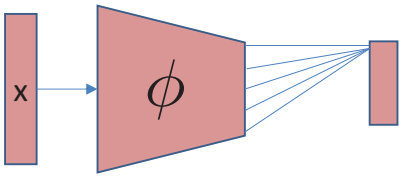


$$\phi(x_1, x_2) = (z_1, z_2, z_3) = (x_1, x_2, x_1^2 + x_2^2)$$

We change the representation of data

Representation Learning

Deep neural nets:

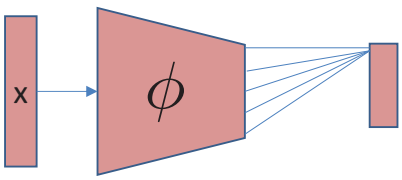


Network

$$\sigma\left(\sum_i w_i h_i + b\right)$$

Decision is a linear function of the final hidden outputs

SVM:



Feature map

$$\text{sgn}(\langle w_i, \phi(x) \rangle + b)$$

Decision is a linear function of the transformed input

Kernel Trick

- It is hard to design the feature map directly
- Instead, define the kernel:

$$k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle \qquad K \in \mathbb{R}^{n \times n}$$

Kernel (aka Gram) matrix

- Popular choices
  - Linear kernel $k(x_i, x_j) = \langle x_i, x_j \rangle$
  - Polynomial kernel $k(x_i, x_j) = (\langle x_i, x_j \rangle + 1)^d$
  - Gaussian (RBF: radial basis function) kernel $k(x_i, x_j) = \exp(-\gamma \|x_i - x_j\|_2^2)$
  - Sigmoid kernel $k(x_i, x_j) = \tanh(b\langle x_i, x_j \rangle + a)$

Supplementary Notes

https://github.com/sanglee/BIML2021

BIML21 SVM.ipynb ☆

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+ Code + Text

BIML 2021 (Introduction to SVM)

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Supplementary Notes

```
[ ] # A utility function to plot decision boundaries in 2D

    from matplotlib.colors import ListedColormap


    def plot_decision_regions(X, y, classifier, test_idx=None, resolution=0.02):

        # setup marker generator and color map
        markers = ('s', 'x', 'o', '^', 'v')
        colors = ('red', 'blue', 'lightgreen', 'gray', 'cyan')
        cmap = ListedColormap(colors[:len(np.unique(y))])

        # plot the decision surface
        x1_min, x1_max = X[:, 0].min() - 1, X[:, 0].max() + 1
        x2_min, x2_max = X[:, 1].min() - 1, X[:, 1].max() + 1
        xx1, xx2 = np.meshgrid(np.arange(x1_min, x1_max, resolution),
                               np.arange(x2_min, x2_max, resolution))
        Z = classifier.predict(np.array([xx1.ravel(), xx2.ravel()]).T)
        Z = Z.reshape(xx1.shape)
        plt.contourf(xx1, xx2, Z, alpha=0.4, cmap=cmap)
        plt.xlim(xx1.min(), xx1.max())
        plt.ylim(xx2.min(), xx2.max())

        for idx, cl in enumerate(np.unique(y)):
```

Loading the IRIS data

```
[ ] import pandas as pd

    df = pd.read_csv('https://archive.ics.uci.edu/ml/'
            'machine-learning-databases/iris/iris.data', names= ['Sepal Length', 'Sepal Width', 'Petal Length', 'Petal Width', 'Label'])
```

```
[ ] df.head()
```

	Sepal Length	Sepal Width	Petal Length	Petal Width	Label
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa

```
[ ]  # Prepare data matrix and labels

     import numpy as np
     from sklearn.preprocessing import LabelEncoder

     feat_idx = [2,3]
     feat_labels = df.columns[feat_idx]
     X = df.iloc[:, feat_idx].values
     y = df.iloc[:, 4].values
     enc_y = LabelEncoder()
     enc_y.fit(y)
     y = enc_y.transform(y)
     feature_names = df.columns.values[[2,3]]

     from sklearn.model_selection import train_test_split

     X_train, X_test, y_train, y_test = train_test_split(
         X, y, test_size=0.3, random_state=0)
     X_train, X_val, y_train, y_val = train_test_split(
         X_train, y_train, test_size=0.3, random_state=0)

     from sklearn.preprocessing import StandardScaler
     sc = StandardScaler()
     sc.fit(X_train)
     X_train_std = sc.transform(X_train)
     X_val_std = sc.transform(X_val)
     X_test_std = sc.transform(X_test)
```

Support Vector Machine (SVM)

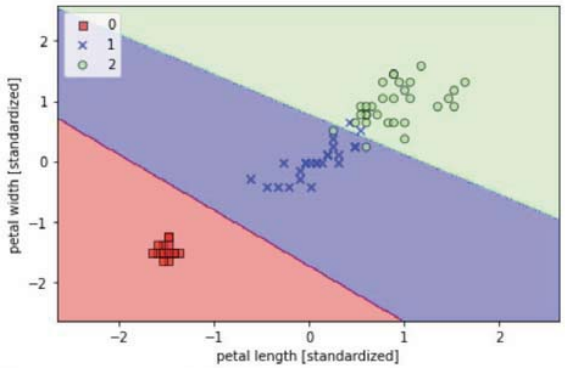
Multi-class Classification

```
[ ]  from sklearn.svm import SVC
     X = np.random.randn(4, 1)
     y = [1,2,3,4]

     svm = SVC(decision_function_shape='ovr', kernel='linear', C=10.0)
     svm.fit(X, y)

     dec = svm.decision_function([X[0,:]])
     print("No. of classifiers in OVR:", dec.shape[1])

     svm = SVC(decision_function_shape='ovo', kernel='linear', C=10.0)
     svm.fit(X, y)

     dec = svm.decision_function([X[0,:]])
     print("No. of classifiers in OVO:", dec.shape[1])
```

```
No. of classifiers in OVR: 4
No. of classifiers in OVO: 6
```

Linear SVM on IRIS dataset

```
[ ] from sklearn.svm import SVC
    import matplotlib.pyplot as plt
    from sklearn.metrics import accuracy_score

    svm = SVC(decision_function_shape='ovr', kernel='linear', C=10.0)

    svm.fit(X_train_std, y_train)          # standardization is recommended for numerical reasons here

    plot_decision_regions(X_train_std,
                          y_train,
                          classifier=svm)
    plt.xlabel('petal length [standardized]')
    plt.ylabel('petal width [standardized]')
    plt.legend(loc='upper left')
    plt.tight_layout()
    plt.show()

    print('Train accuracy: %f' % accuracy_score(svm.predict(X_train_std), y_train))
    print('Test accuracy: %f' % accuracy_score(svm.predict(X_test_std), y_test))
```




```
Train accuracy: 0.945205
Test accuracy: 0.977778
```

Feature Importance

- Linear models (logistic regression, linear SVM, perceptron, ...)
  - Prediction for an input $x^{(i)}$ is produced by $\hat{y}^{(i)} = f(w^T x^{(i)})$, where f is some function, e.g., to convert linear output to binary outcome.
  - $w^T x^{(i)} = \sum_{j=1}^{p} w_j x_j^{(i)}$
  - We call $w_1, w_2, \ldots, w_p$ as **coefficients**, **weights**, or **learning parameters**
  - In scikit-learn, `<model>.coef_` contains the coefficients
- Non-linear models (decision trees, random forest, nonlinear SVM, ...)
  - This type of models provides other ways to measure feature importance
    - DT, RF: `<model>.feature_importances_`
  - In some models, it is not easy to extract feature importance
    - Nonlinear SVM

```
[ ] print(svm.coef_)

    imporant_feat = pd.DataFrame(np.abs(svm.coef_))
    imporant_feat.columns = feat_labels
    imporant_feat
```

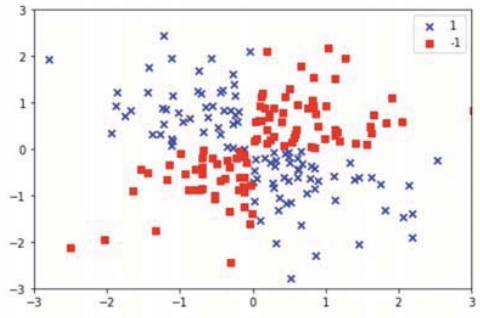
```
[[-1.06139348 -1.1489091 ]
 [-0.57330686 -0.57625103]
 [-2.65965384 -4.01574174]]
```

	Petal Length	Petal Width
0	1.061393	1.148909
1	0.573307	0.576251
2	2.659654	4.015742

Nonlinear Classification

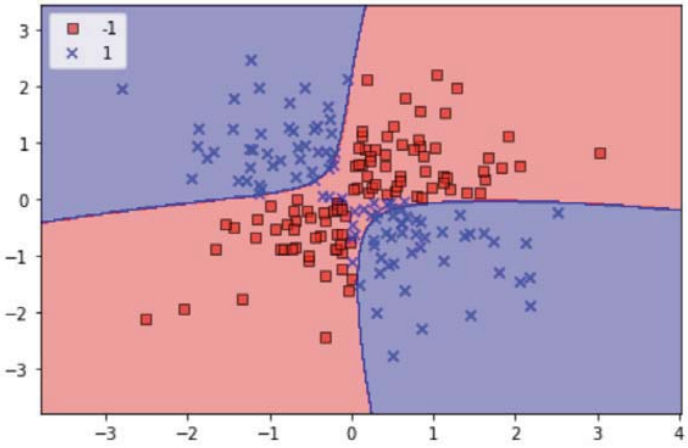
XOR Toy Data

```
[ ]  import matplotlib.pyplot as plt
     import numpy as np

     np.random.seed(1)
     X_xor = np.random.randn(200, 2)
     y_xor = np.logical_xor(X_xor[:, 0] > 0,
                            X_xor[:, 1] > 0)
     y_xor = np.where(y_xor, 1, -1)

     plt.scatter(X_xor[y_xor == 1, 0],
                 X_xor[y_xor == 1, 1],
                 c='b', marker='x',
                 label='1')
     plt.scatter(X_xor[y_xor == -1, 0],
                 X_xor[y_xor == -1, 1],
                 c='r',
                 marker='s',
                 label='-1')

     plt.xlim([-3, 3])
     plt.ylim([-3, 3])
     plt.legend(loc='best')
     plt.tight_layout()
     plt.show()
```



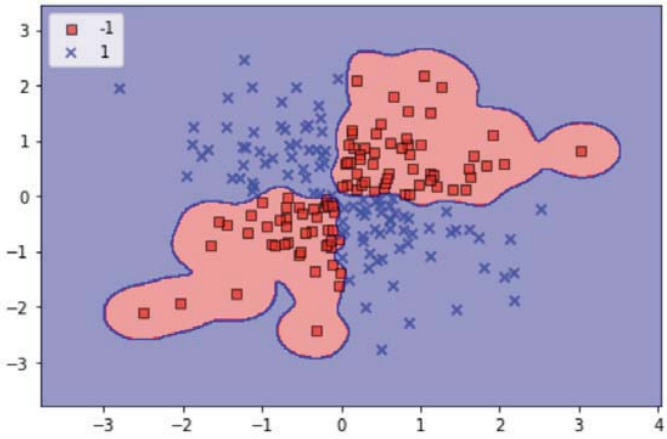
SVM on XOR data

```
#
# SVM on XOR data
#
svm = SVC(kernel='rbf', random_state=1, gamma=.1, C=10)
svm.fit(X_xor, y_xor)
plot_decision_regions(X_xor, y_xor,
                      classifier=svm)

plt.legend(loc='upper left')
plt.tight_layout()
plt.show()
```



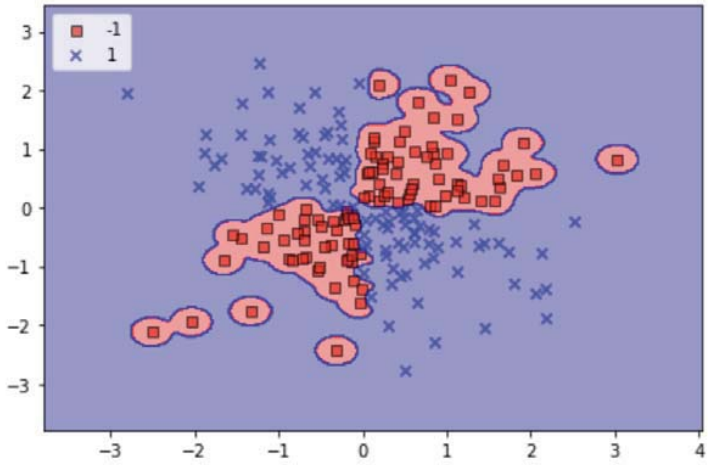
SVM on XOR data

```
[9]  #
     # SVM on XOR data
     #
     svm = SVC(kernel='rbf', random_state=1, gamma=10, C=10)
     svm.fit(X_xor, y_xor)
     plot_decision_regions(X_xor, y_xor,
                           classifier=svm)

     plt.legend(loc='upper left')
     plt.tight_layout()
     plt.show()
```



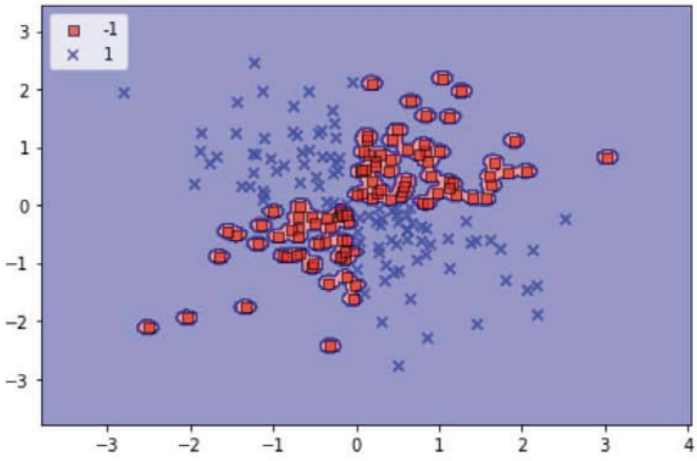
SVM on XOR data

```
[10] #
     # SVM on XOR data
     #
     svm = SVC(kernel='rbf', random_state=1, gamma=50, C=10)
     svm.fit(X_xor, y_xor)
     plot_decision_regions(X_xor, y_xor,
                           classifier=svm)

     plt.legend(loc='upper left')
     plt.tight_layout()
     plt.show()
```



SVM on XOR data

```
[13] #
     # SVM on XOR data
     #
     svm = SVC(kernel='rbf', random_state=1, gamma=250, C=10)
     svm.fit(X_xor, y_xor)
     plot_decision_regions(X_xor, y_xor,
                           classifier=svm)

     plt.legend(loc='upper left')
     plt.tight_layout()
     plt.show()
```



Support Vectors

```
[ ] print(svm.n_support_)
    svm.support_
```

```
[46 46]
array([  6,   8,   9,  13,  17,  20,  23,  24,  36,  40,  41,  42,  44,
        45,  47,  58,  60,  65,  69,  70,  72,  73,  78,  92,  93, 109,
       111, 113, 114, 115, 117, 120, 121, 125, 132, 133, 141, 142, 143,
       145, 147, 160, 166, 173, 190, 193,   4,  14,  18,  22,  25,  27,
        31,  32,  38,  43,  48,  52,  54,  77,  79,  81,  82,  86,  87,
        89,  94, 100, 108, 123, 127, 129, 130, 131, 134, 139, 144, 146,
       153, 158, 161, 164, 171, 172, 176, 178, 182, 185, 186, 192, 196,
       199], dtype=int32)
```

```
[ ] #svm.support_vectors_
```

```
[ ] # shape: n_classes-1, n_SV
    svm.dual_coef_.shape
```

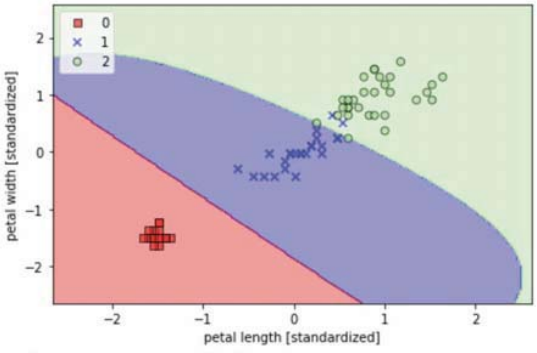
```
(1, 92)
```

```
[ ]  svm.dual_coef_
```

```
array([[-10.        , -10.        , -10.        , -10.        ,
        -10.        , -10.        ,  -7.99986544, -10.        ,
        -10.        , -10.        , -10.        , -10.        ,
        -10.        ,  -6.20496694, -10.        , -10.        ,
        -10.        , -10.        , -10.        , -10.        ,
        -10.        , -10.        , -10.        , -10.        ,
        -10.        , -10.        , -10.        , -10.        ,
        -10.        , -10.        , -10.        ,  -1.56513305,
        -10.        , -10.        , -10.        , -10.        ,
        -10.        , -10.        , -10.        , -10.        ,
        -10.        , -10.        , -10.        , -10.        ,
        -10.        , -10.        ,  10.        ,  10.        ,
         10.        ,  10.        ,  10.        ,  10.        ,
         10.        ,  10.        ,  10.        ,  10.        ,
         10.        ,  10.        ,  10.        ,  10.        ,
         10.        ,  10.        ,  10.        ,   1.23159626,
         10.        ,  10.        ,  10.        ,  10.        ,
         10.        ,  10.        ,   9.95761928,  10.        ,
         10.        ,  10.        ,  10.        ,  10.        ,
         10.        ,  10.        ,  10.        ,  10.        ,
         10.        ,  10.        ,  10.        ,  10.        ,
         10.        ,  10.        ,  10.        ,  10.        ,
          4.58074989,  10.        ,  10.        ,  10.        ]])
```

SVM on IRIS data

```
[ ]
from sklearn.svm import SVC

svm = SVC(kernel='rbf', gamma=0.2, C=1.0)  # gamma=100.0, C=1.0
svm.fit(X_train_std, y_train)

plot_decision_regions(X_train_std, y_train, classifier=svm)
plt.xlabel('petal length [standardized]')
plt.ylabel('petal width [standardized]')
plt.legend(loc='upper left')
plt.tight_layout()
plt.show()

print('Train accuracy: %f' % accuracy_score(svm.predict(X_train_std), y_train))
print('Test accuracy: %f' % accuracy_score(svm.predict(X_test_std), y_test))
```




```
Train accuracy: 0.945205
Test accuracy: 0.977778
```

Support Vectors

```
print(svm.n_support_)
svm.support_
```

```
[13 24 23]
array([ 3, 12, 21, 24, 29, 30, 33, 35, 36, 48, 50, 54, 60,  4,  6,  8, 15,
       19, 20, 22, 23, 34, 37, 41, 42, 44, 47, 49, 55, 61, 62, 63, 64, 65,
       66, 69, 70,  1,  2, 10, 11, 13, 14, 16, 17, 18, 26, 27, 31, 32, 38,
       39, 43, 51, 56, 59, 67, 68, 71, 72], dtype=int32)
```

```
svm.support_vectors_
```

```
array([[-1.36607872, -1.50714415],
       [-1.42392312, -1.50714415],
       [-1.53961192, -1.37297156],
       [-1.48176752, -1.23879897],
       [-1.48176752, -1.50714415],
       [-1.53961192, -1.50714415],
       [-1.42392312, -1.50714415],
       [-1.53961192, -1.50714415],
       [-1.42392312, -1.50714415],
       [-1.48176752, -1.23879897],
       [-1.48176752, -1.37297156],
       [-1.59745632, -1.37297156],
       [-1.48176752, -1.50714415],
       [ 0.08003129, -0.03124567],
       [-0.20919071, -0.43376344],
       [ 0.3114089 , -0.03124567],
       [ 0.25356449,  0.3712721 ],
       [-0.09350191, -0.29959085],
       [ 0.4270977 ,  0.63961727],
       [-0.32487951, -0.43376344],
       [ 0.25356449,  0.23709951],
       [-0.03565751, -0.03124567],
```

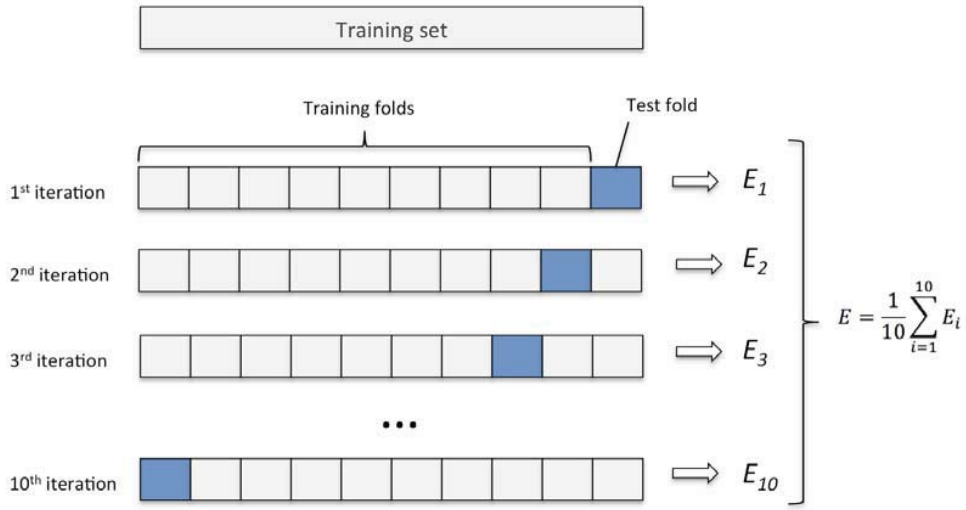
```
# shape: n_classes-1, n_SV
svm.dual_coef_.shape
```

```
(2, 60)
```

```
svm.dual_coef_
```

```
array([[ 1.        ,  1.        ,  1.        ,  1.        ,  1.        ,
         1.        ,  1.        ,  1.        ,  1.        ,  1.        ,
         1.        ,  1.        ,  1.        , -1.        , -1.        ,
        -0.        , -0.        , -1.        , -0.        , -1.        ,
        -0.        , -1.        , -1.        , -1.        , -0.        ,
        -1.        , -1.        , -0.        , -1.        , -0.        ,
        -1.        , -0.        , -1.        , -0.        , -1.        ,
        -0.        , -0.        , -0.        , -0.38609855, -0.        ,
        -0.        , -0.        , -0.        , -0.        , -0.        ,
        -0.        , -0.        , -1.        , -1.        , -1.        ,
        -1.        , -0.        , -0.        , -0.        , -0.        ,
        -1.        , -1.        , -0.        , -0.        , -0.        ],
       [ 1.        ,  0.        ,  1.        ,  1.        ,  0.        ,
         0.        ,  0.38609855,  0.        ,  1.        ,  1.        ,
         1.        ,  0.        ,  0.        ,  1.        ,  1.        ,
         1.        ,  1.        ,  1.        ,  1.        ,  1.        ,
         1.        ,  1.        ,  0.        ,  1.        ,  1.        ,
         1.        ,  1.        ,  1.        ,  1.        ,  1.        ,
         0.20659426,  1.        ,  1.        ,  1.        ,  1.        ,
         1.        ,  1.        , -1.        , -1.        , -1.        ,
        -0.20659426, -1.        , -1.        , -1.        , -1.        ,
        -1.        , -1.        , -1.        , -1.        , -1.        ,
        -1.        , -1.        , -1.        , -1.        , -1.        ,
        -1.        , -1.        , -1.        , -1.        , -1.        ]])
```

K-Fold Cross Valiation (CV)



K-Fold Cross Valiation (CV)

```
[ ] from sklearn.model_selection import cross_val_score

    C_grid = [0.1, 1, 10]
    cv_err = []

    for c in C_grid:
        scores = cross_val_score(estimator=SVC(C=c),
                                 X=X_train,
                                 y=y_train,
                                 cv=5,
                                 scoring='accuracy',
                                 n_jobs=-1)  # no. cpu cores to use. -1 all cores
        print('C = %f' % c)
        print('CV accuracy scores:\n %s' % scores)
        print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores), np.std(scores)))
        print('-----------------------------------------------------------------------')
        cv_err.append(np.mean(scores))

    best_idx = np.argmax(cv_err)
    print(best_idx)
    best_C = C_grid[best_idx]

    print('Best C due to CV: %f' % best_C)
```

```
C = 0.100000
CV accuracy scores:
 [1.         0.93333333 0.93333333 0.86666667 1.        ]
CV accuracy: 0.947 +/- 0.050
-----------------------------------------------------------------------
C = 1.000000
CV accuracy scores:
 [1.         0.93333333 0.93333333 0.86666667 1.        ]
CV accuracy: 0.947 +/- 0.050
-----------------------------------------------------------------------
C = 10.000000
CV accuracy scores:
 [1.         0.93333333 0.86666667 0.86666667 1.        ]
CV accuracy: 0.933 +/- 0.060
-----------------------------------------------------------------------
0
Best C due to CV: 0.100000
```