

Support Vector Machines

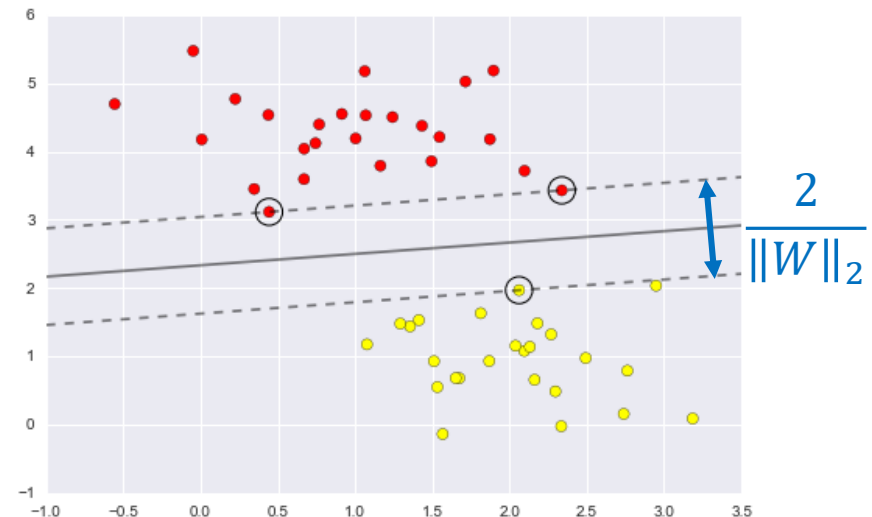
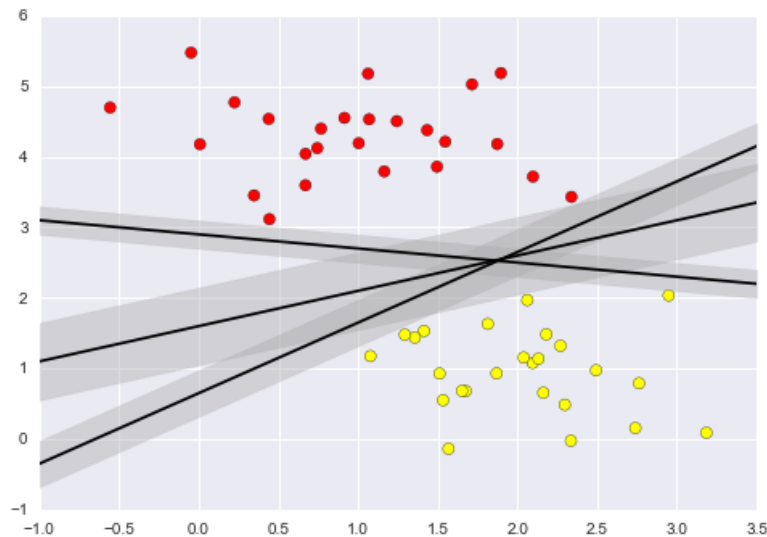
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Agenda

- Linear SVM
- Kernel SVM
- SVM in scikit-learn

Support Vector Machines

- Search for the boundary that separates classes with maximum margin
 - Linear SVM
 - C-SVM (SVM with soft margin)
 - Nonlinear SVM (SVM with kernel)



Linear SVM

- Search for $W^* = \operatorname{argmin}_W |W|_2^2$ s.t.
 - $WX_i + b \geq +1$ for $y_i = +1$
 - $WX_i + b \leq -1$ for $y_i = -1$
 - ➔ $y_i(WX_i + b) - 1 \geq 0$ combines the two conditions

- Loss function

$$L_p = \frac{1}{2} |W|_2^2 - \sum_{i=1}^l \alpha_i y_i (WX_i + b) + \sum_{i=1}^l \alpha_i$$

□ $\alpha_i \geq 0$'s are **Lagrange multipliers**

- Dual formulation

- Minimizing L_p subject to $\frac{\partial L_p}{\partial \alpha_i} = 0, \alpha_i \geq 0$
- Maximizing L_p subject to $\frac{\partial L_p}{\partial W} = 0, \frac{\partial L_p}{\partial b} = 0, \alpha_i \geq 0$

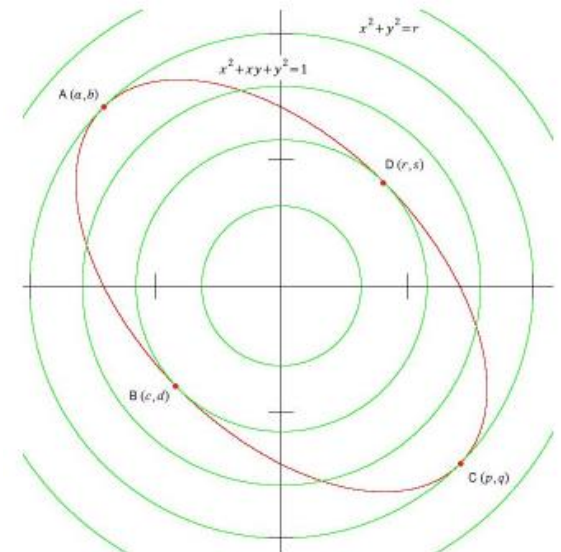
Lagrange Multiplier

- A strategy for finding the local maxima and minima of a function subject to equality constraints
 - Maximize $f(X) = f(x_1, \dots, x_n)$
 - Subject to $g_j(X) = g_j(x_1, \dots, x_n) = 0, 1 \leq j \leq m$
 - * Assume $f(\cdot)$ and $g_j(\cdot)$ are continuous and have 1st partial derivatives
- Lagrange function
 - $L(x_1, \dots, x_n, \lambda_1, \dots, \lambda_m) = f(x_1, \dots, x_n) - \sum_j \lambda_j g_j(x_1, \dots, x_n)$
 - λ_i 's are called **Lagrange multiplier**
- We can find local optimum X^* by jointly optimize $L(\cdot)$ w.r.t. X and all λ_j 's (assume $g_j'(\cdot) \neq 0$)

Lagrange Multiplier

Example)

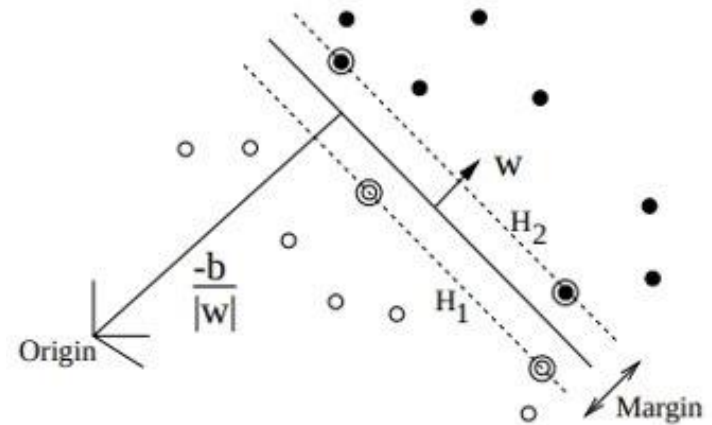
- Objective: $f(x, y) = x^2 + y^2$
- Subject to $g(x, y) = x^2 + xy + y^2 = 0$
- The optimum solution is found at the tangent points of the two curves.
- $\nabla f(x, y)$ and $\nabla g(x, y)$ are parallel
- $\nabla f(x, y) = \lambda \nabla g(x, y)$



Linear SVM

- Solution from $\frac{\partial L_p}{\partial W} = 0, \frac{\partial L_p}{\partial b} = 0$

- $W = \sum_{i=1}^l \alpha_i y_i X_i$
- $\sum_{i=1}^l \alpha_i y_i = 0$



- Substitute $\frac{\partial L_p}{\partial W} = 0, \frac{\partial L_p}{\partial b} = 0$ into L_p

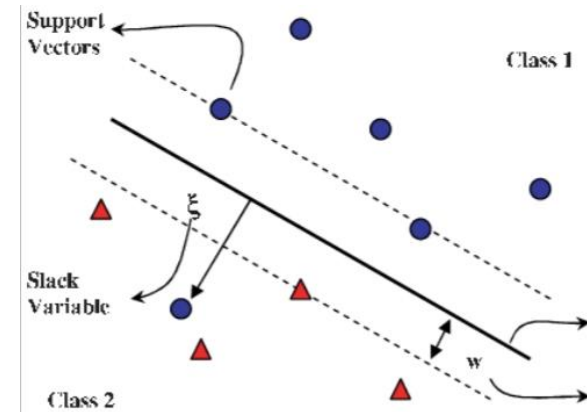
$$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j X_i \cdot X_j$$

- Find α_i 's that maximize L_D .
 - X_i 's with $\alpha_i > 0$ are called **support vectors**
- Discriminant function: $W X_j + b = \sum_{i=1}^l \alpha_i y_i X_i \cdot X_j + b$

Linear SVM with Soft Margin (C-SVM)

- Allows **soft margin** for non-separable tasks

- $W^* = \operatorname{argmin}_W \left\{ \left[\frac{|W|^2}{2} + C(\sum_i \xi_i) \right] \right\}$ s.t.
 - $WX_i + b \geq +1 - \xi_i$ for $y_i = +1$
 - $WX_i + b \leq -1 + \xi_i$ for $y_i = -1$
- Equivalent to
 - $y_i(X_iW + b) - 1 + \xi_i \geq 0$



- Primal formulation

$$L_p = \frac{1}{2} |W|^2 + C \sum_i \xi_i - \sum_{i=1}^l \alpha_i \{y_i (X_i W + b) - 1 + \xi_i\} - \sum_i \mu_i \xi_i$$

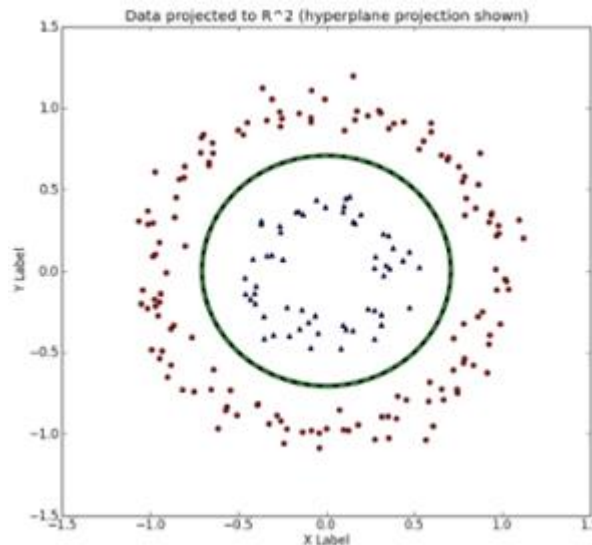
Agenda

- Linear SVM
- Kernel SVM
- SVM in scikit-learn

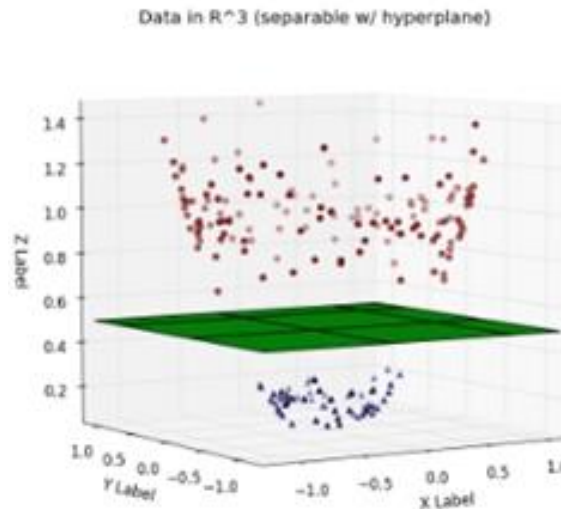
SVM with Kernel

■ Nonlinear SVM

- Transforms input feature to higher dimensional space using nonlinear kernel functions
- Samples are better separated in higher-dimensional space



(x, y)



$(x, y, x^2 + y^2)$

Nonlinear SVM

- Transform X to high dimension space through a nonlinear transform $\phi(\cdot)$

	Loss function	Discriminant function
Linear SVM	$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j X_i \cdot X_j$	$\begin{aligned} & WX + b \\ &= \sum_{i=1}^l \alpha_i y_i X_i \cdot X + b \end{aligned}$
Nonlinear SVM	$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \phi(X_i) \phi(X_j)$	$\begin{aligned} & W\phi(X) + b \\ &= \sum_i \alpha_i y_i \phi(X_i) \phi(X) + b \end{aligned}$

- It is hard to find appropriate high-dimensional transform $\phi(\cdot)$

Nonlinear SVM – Kernel Trick

- Replace $\phi(X_i)\phi(X_j)$ by $K(X_i, X_j)$
 - We don't need to know $\phi(\cdot)$
 - $K(X_i, X_j)$ eliminates computation in high-dimensional space.

	Loss function	Discriminant function
Linear SVM	$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j X_i \cdot X_j$	$WX + b = \sum_{i=1}^l \alpha_i y_i X_i \cdot X + b$
Nonlinear SVM	$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \phi(X_i) \phi(X_j)$	$W\phi(X) + b = \sum_i \alpha_i y_i \phi(X_i) \phi(X) + b$
Nonlinear SVM (kernel)	$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j K(X_i, X_j)$	$W\phi(X) + b = \sum_i \alpha_i y_i K(X_i, X) + b$

Popular Kernels for SVM

- Polynomial kernel

$$k(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j + 1)^d$$

- Gaussian kernel

$$k(x, y) = \exp\left(-\frac{\|x - y\|^2}{2\sigma^2}\right)$$

- RBF kernel

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\gamma\|\mathbf{x}_i - \mathbf{x}_j\|^2)$$

SVM in scikit-learn



- SVM classifiers in scikit-learn

- SVC
- NuSVC (ν – *SVC*)
- LinearSVC

- Example

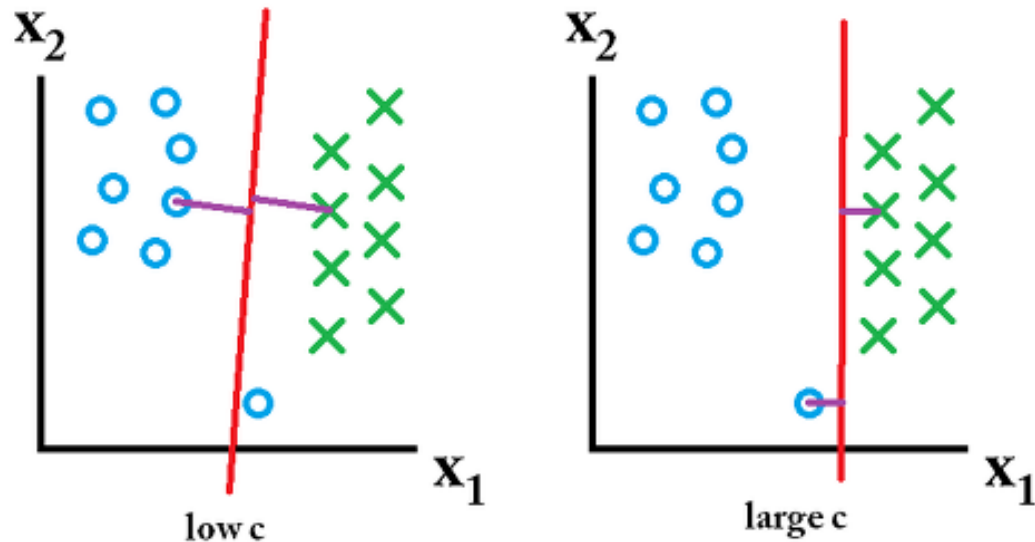
```
from sklearn import svm          # import
X = [[0, 0], [1, 1]]           # input data
y = [0, 1]                      # target label
clf = svm.SVC(gamma='scale')    # create SVC
clf.fit(X, y)                   # train
clf.predict([[2., 2.]])         # predict
```

- Reference

- <https://scikit-learn.org/stable/modules/svm.html>

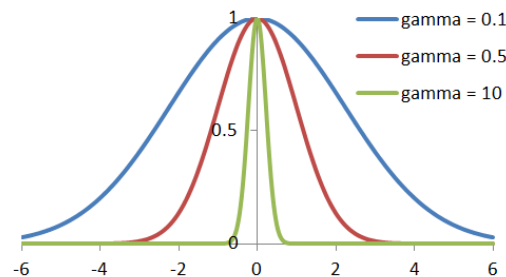
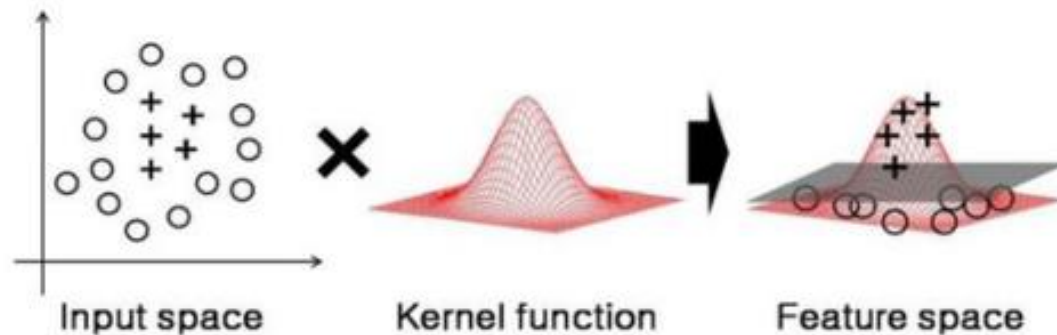
SVM Hyper-Parameters

- Penalty parameter C of the error term (default: 1)
 - Too small C : underfitting
 - Too high C : overfitting



SVM Hyper-Parameters

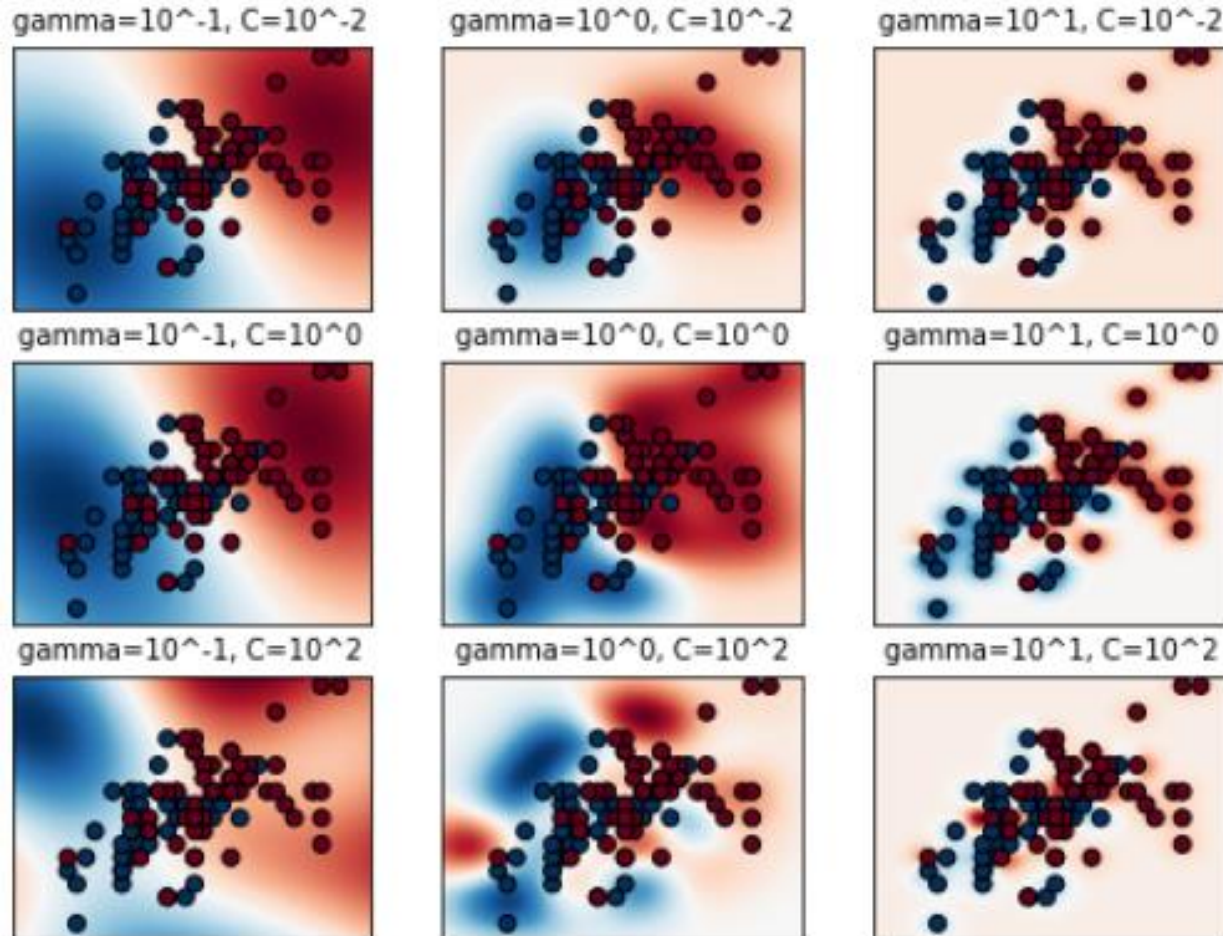
- Kernel coefficient **gamma** for 'rbf', 'poly' and 'sigmoid'.
 - Too small: underfitting
 - Too large: overfitting



scikit-learning **gamma** options

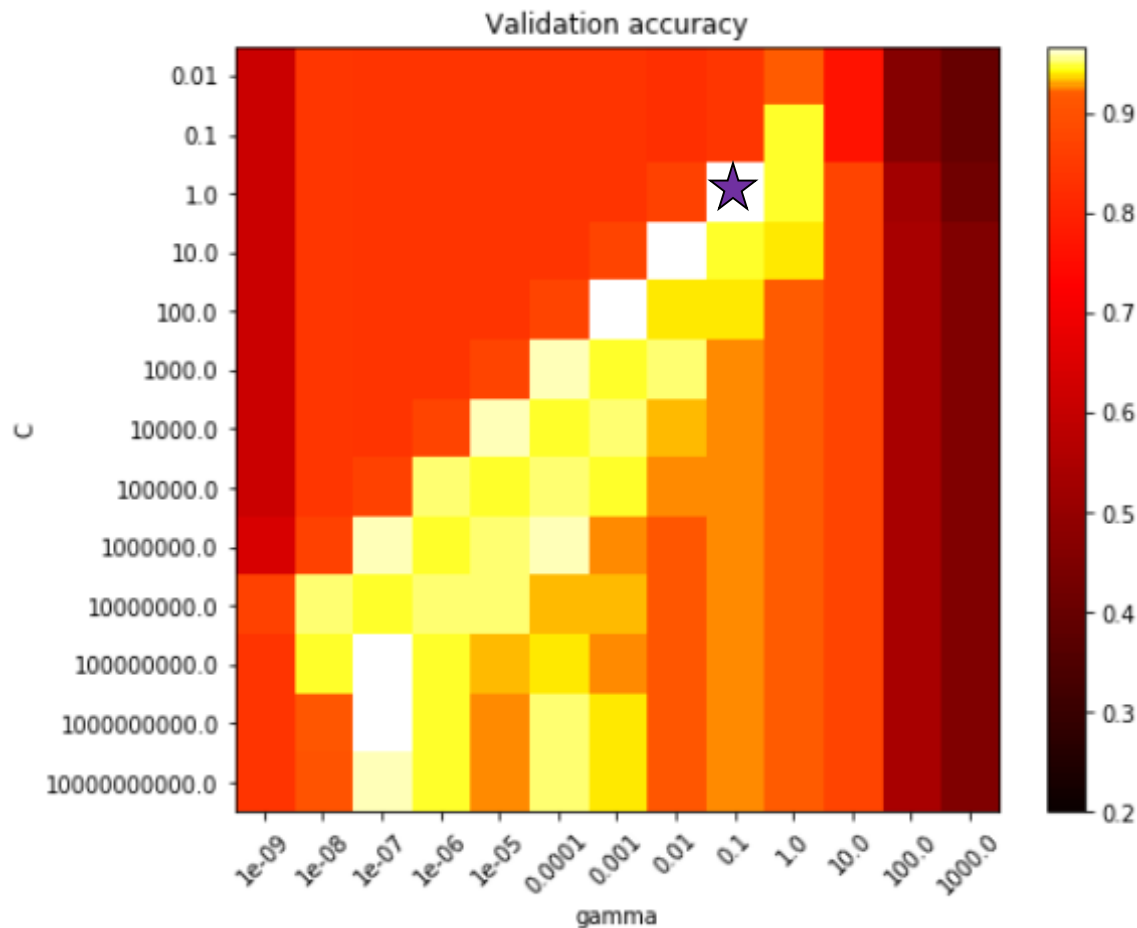
- 'auto': $1/n_{\text{features}}$
- 'scale': $1/(n_{\text{feature}} * X.\text{var}())$
 $X.\text{var}()$: variance of X

SVM Hyper-Parameters



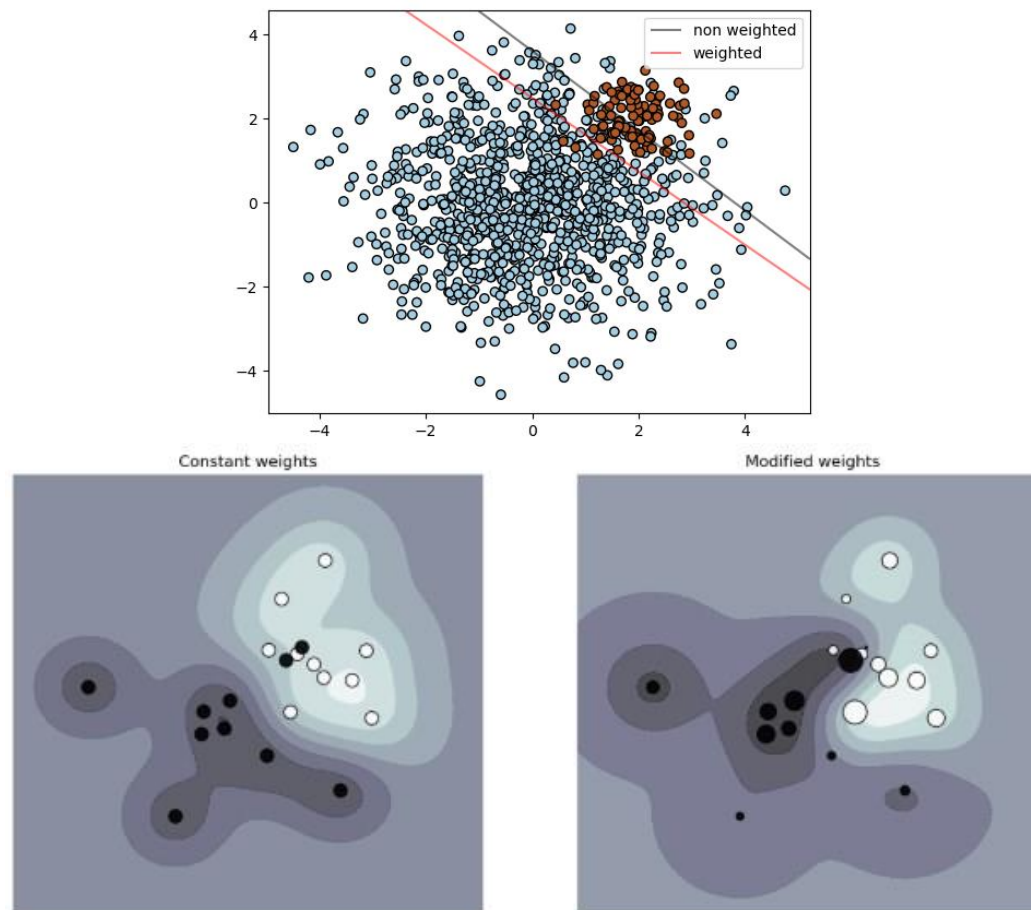
SVM Hyper-Parameters

■ C – gamma grid



Handling Unbalanced Datasets

- Assign heavier weights to the class with less sample



References



■ Handling unbalanced data

- <https://machinelearningmastery.com/tactics-to-combat-imbalanced-classes-in-your-machine-learning-dataset/>
- https://shiring.github.io/machine_learning/2017/04/02/unbalanced
- <https://www.datascience.com/blog/imbalanced-data>

■ Support Vector Regression

- https://www.saedsayad.com/support_vector_machine_regression.htm



Thank you
for your attention!

