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Lecture Support Vector Machines cont

PROF. LINDA SELLIE

SOME SLIDES FROM PROF. RANGAN



The "Kernel Trick"

• For some transformations, we can compute

$$K(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x})^T \Phi(\mathbf{x}')$$

- without transforming the features. Instead, we perform operations in the original feature space to compute the value of $K(\mathbf{x}, \mathbf{x}')$.
- In class, we will discuss two different types of transformations:
 - 1. Polynomial transformation
 - 2. RBF

SVM and feature transformation

Feature transformation

- Support vectors
- The kernel trick (polynomial and RBF)

Fundamental Insight

SVM's are typically implemented using the dual form. The kernel trick is especially efficient in the dual form. The dual form is outside the scope of the class.

We expressed w as a linear combination of the training examples!

$$\mathbf{w} = \sum_{i=1}^{N} \alpha^{(i)} y^{(i)} \Phi(\mathbf{x}^{(i)})$$

Keep track of a single variable per data point $\alpha^{(i)}$.

Predict for example **x**:
$$\hat{\mathbf{y}} = \text{sign}(\mathbf{w}^T \mathbf{x}) = \text{sign}\left(\left(\sum_{i=1}^N \alpha^{(i)} y^{(i)} \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x})\right) + w_0\right)$$

$$\mathbf{w} = \sum_{i=1}^N \alpha^{(i)} y^{(i)} \Phi(\mathbf{x}^{(i)})$$

SVM support vectors

The optimal w is a linear combination of the training examples whose $\alpha^{(i)} \neq 0$ (i.e. examples on the margin or inside the margin)

$$\mathbf{w} = \sum_{i=1}^{N} \alpha^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

$$\alpha^{(i)} = 0 \text{ if } y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) > 1$$
All points correctly classified outside the margin

These examples are called the support vectors

Example (with rounded numbers....)

$$\mathbf{w} = \sum_{i=1}^{N} \alpha^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

Given the set of training examples

$$((1,2.5), 1), ((0, 0.75), -1), ((1, 1), -1), ((2,2), 1), ((3,1), 1), ((2,3), 1), ...$$

$$\alpha^T = [0.9, 0, 1.4, 0, 0.5, 0, ..., 0]$$

What is w?

$$\mathbf{w} = \frac{0.9}{1} \begin{bmatrix} 1 \\ 2.5 \end{bmatrix} + \frac{1.4}{1} (-1) \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{0.5}{1} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{0.9}{1} \begin{bmatrix} 1 \\ 2.5 \end{bmatrix} + \frac{1.4}{1} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{0.5}{1} \begin{bmatrix} 3 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1.35 \end{bmatrix}$$

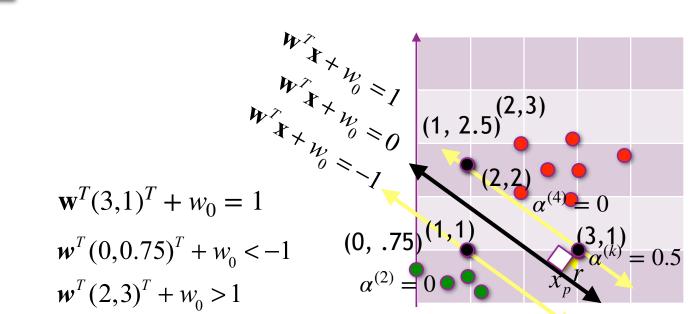
What is w_0 ?

No examples are inside the margin. Thus every support vector has a functional margin of one.

$$(1)\left(w_0 + \mathbf{w}^T \begin{bmatrix} 3\\1 \end{bmatrix}\right) = 1$$

$$w_0 + 4.35 = 1$$
$$w_0 = -3.35$$

Note... I rounded these numbers, so... (If I hadn't rounded $w_2 = 1.33, w_0 = -3.33$)



Prediction of $\begin{vmatrix} 1 \\ 0 \end{vmatrix}$

$$\mathbf{w} = \begin{bmatrix} 1 \\ 1.35 \end{bmatrix} = 0.9 \begin{bmatrix} 1 \\ 1.25 \end{bmatrix} + -1.4 \begin{bmatrix} 1 \\ 1 \end{bmatrix} + 0.5 \begin{bmatrix} 3 \\ 1 \end{bmatrix}, \ w_0 = -3.35$$

$$\operatorname{sign}\left(\mathbf{w}^{T} \begin{bmatrix} 1\\0 \end{bmatrix} + w_{0}\right) = \operatorname{sign}\left(\begin{bmatrix} 1\\1.35 \end{bmatrix}^{T} \begin{bmatrix} 1\\0 \end{bmatrix} - 3.35\right) = 1 - 3.35 = \operatorname{sign}(-2.25) = -1$$

$$= \operatorname{sign}\left(\left(\frac{0.9}{1.25}\right) + \frac{1}{1.25}\right) + \frac{1.4}{1} + \frac{1}{1} + \frac{1$$

$$= \operatorname{sign}\left(\frac{0.9K\left(\begin{bmatrix}1\\1.25\end{bmatrix}, \begin{bmatrix}1\\0\end{bmatrix}\right) + -1.4K\left(\begin{bmatrix}1\\1\end{bmatrix}, \begin{bmatrix}1\\0\end{bmatrix}\right) + 0.5K\left(\begin{bmatrix}3\\1\end{bmatrix}, \begin{bmatrix}1\\0\end{bmatrix}\right) - 3.35\right)$$
Linear $K(\mathbf{x}^{(1)}, \mathbf{x})$ $K(\mathbf{x}^{(3)}, \mathbf{x})$ $K(\mathbf{x}^{(5)}, \mathbf{x})$

How did this save us any time?

Avoiding paying the time/space cost of feature transformation!

Key takeaway

If we can efficiently compute the inner product, we can *implicitly* work in high dimensional space

$$K(\mathbf{x}^{(i)}, \mathbf{x}) = \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x})$$

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SVM and feature transformation

- Feature transformation
- Support vectors
- Kernel trick (polynomial and RBF)

Standard Choices of Kernel functions

Dot product (no transformation):

$$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \mathbf{x}^{(i)T}\mathbf{x}^{(j)}$$

Polynomial kernels:

$$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = (1 + \mathbf{x}^{(i)T}\mathbf{x}^{(j)})^d$$

Radial basis function:

$$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \exp(-\gamma ||\mathbf{x}^{(i)} - \mathbf{x}^{(j)}||^2)$$

Polynomial transformation of degree exactly 2

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \Phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{bmatrix}$$

$$K(\mathbf{x}^T\mathbf{x}') = \Phi(\mathbf{x})^T \Phi(\mathbf{x}') = \begin{bmatrix} x_1^2 & x_2^2 & \sqrt{2}x_1x_2 \end{bmatrix} \begin{bmatrix} x_1'^2 \\ x_2'^2 \\ \sqrt{2}x_1'x_2' \end{bmatrix}$$

$$= x_1^2 \cdot x_1'^2 + x_2^2 \cdot x_2'^2 + \sqrt{2}x_1x_2 \cdot \sqrt{2}x_1'x_2' = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} x_1' \\ x_2' \end{bmatrix}^2 = (\mathbf{x}^T\mathbf{x}')^2$$

If
$$d = 200$$
, then $\tilde{d} = d + \frac{d(d-1)}{2} = 20100$

For 200 features, I only need to perform 201 multiplications (and 199 additions)

Polynomial kernel

$$\Phi_2(\mathbf{x})^T = [1, x_1, x_2, \dots, x_d, x_1^2, x_2^2, \dots, x_d^2, x_1x_2, \dots, x_{d-1}x_d]$$

$$\Phi_2(\mathbf{x})^T \Phi_2(\mathbf{x}')$$

If d=200 then in z-space we have a feature vector of size approx 20,000

Kernel Motivation

$$g(\mathbf{x}) = \operatorname{sign}\left(\sum_{i \in I} \alpha^{(i)} y^{(i)}(\mathbf{x}^{(i)T} \mathbf{x}) + w_0\right)$$

$$\mathbf{x} = [x_1, x_2]^T$$

$$\Phi_2: R^2 \to R^6$$

$$\Phi_2(\mathbf{x}) = [1, x_1, x_2, x_1 x_2, x_1^2, x_2^2]^T$$

$$\Phi_2(-0.75, -0.25) = (1, -0.75, -0.25, (-0.75) \cdot (-0.25), (-0.75)^2, (-0.25)^2)$$

$$\Phi_2(-1,1) = (1, -1, 1, -1 \cdot 1, (-1)^2, 1^2)$$

$$\Phi_2(\mathbf{x})^T \Phi_2(\mathbf{x}') = [1, x_1, x_2, x_1 x_2, x_1^2, x_2^2] \cdot [1, x_1', x_2', x_1' x_2', x_1'^2, x_2'^2]$$

$$\Phi_2(\mathbf{x})^T \Phi_2(\mathbf{x}') = 1 + x_1 x_1' + x_2 x_2' + x_1 x_2 x_1' x_2' + x_1^2 x_1'^2 + x_2^2 x_2'^2$$

$$\Phi_2(-0.75, -0.25) \cdot \Phi_2(-1,1) = 1 + 0.75 - 0.25 + 0.75 \cdot (-0.25) + (-0.75)^2 + (-0.25)^2$$

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Kernel motivation

$$g(\mathbf{x}) = \operatorname{sign}\left(\sum_{i \in I} \alpha^{(i)} y^{(i)}(\mathbf{x}^{(i)T} \mathbf{x}) + w_0\right)$$

But if we use a different (but similar) transformation:

$$\begin{split} \Phi(\mathbf{x}) &= [1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2]^T \\ \Phi(-0.75, -0.25) &= \left(1, \sqrt{2} \cdot (-0.75), \sqrt{2} \cdot (-0.25), \sqrt{2}(-0.75) \cdot (-0.25), (-0.75)^2, (-0.25)^2\right) \\ \Phi(-1,1) &= (1, -\sqrt{2}, \sqrt{2}, -\sqrt{2}, (-1)^2, 1^2) \\ K(\mathbf{x}, \mathbf{x}') &= \Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}') = 1 + 2x_1x_1' + 2x_2x_2' + 2x_1x_2x_1'x_2' + x_1^2x_1'^2 + x_2^2x_2'^2 \\ &= (1 + \mathbf{x} \cdot \mathbf{x}')^2 \\ K((-1,1), (-0.75, -0.25)) &= \frac{2.25}{(-0.25)} \\ &= (1 + (0.75 - 0.25))^2 \end{split}$$

So, instead of computing $\Phi(\mathbf{x})^T \Phi(\mathbf{x}')$, we compute $\mathbf{x} \cdot \mathbf{x}'$ in the original feature space, and then compute $(1 + \mathbf{x} \cdot \mathbf{x}')^2$

General form

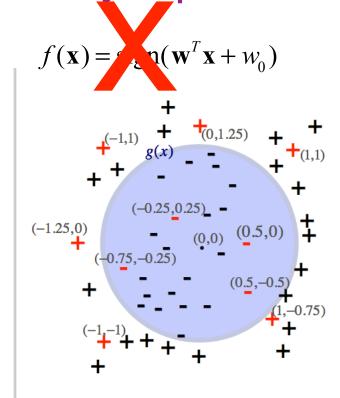
The polynomial kernel can be generalized to higher dimensions. A degree k polynomial is $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x} \cdot \mathbf{x}')^k$

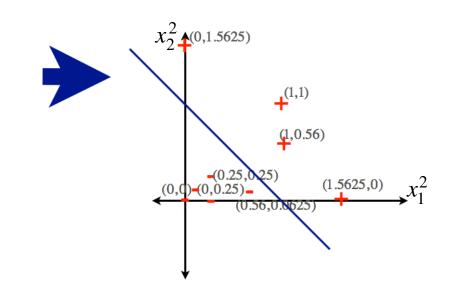
Example from the previous slide of $\Phi_2(\mathbf{x})$:

If d=200, then in z-space, we have a feature vector of size approx 20,000, but we do roughly the same amount of work to compute K(x,x') as if we hadn't transformed the features

Example

linearly separable?





If we transform the features using $\Phi(\mathbf{x}) = [1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2]^T$

$$\operatorname{sign}\left(\left(\sum_{i \in I} \alpha^{(i)} y^{(i)} \Phi(\mathbf{x}^{(i)})\right)^T \Phi(\mathbf{x}) + w_0\right) \qquad \Longrightarrow \qquad g(\mathbf{x}) = \operatorname{sign}\left(\sum_{i \in I} \alpha^{(i)} y^{(i)} K(\mathbf{x}^{(i)}, \mathbf{x}) + w_0\right) K(\mathbf{x}^{(i)}, \mathbf{x}) = (1 + \mathbf{x}^{(i)T} \mathbf{x})^2$$

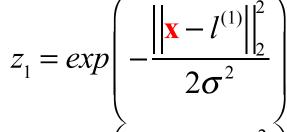
Radial Basis Function Kernel (RBF)



Another feature transformation idea

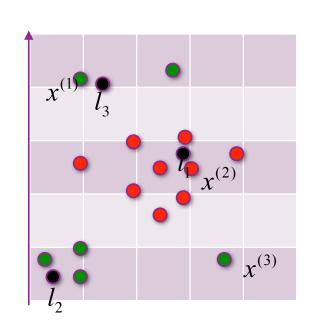
□Define new features, f_1 , f_2 , and f_3 for every example on how close it is to chosen "landmarks" $l^{(1)}$, $l^{(2)}$, and $l^{(3)}$

 \square For an example x we create new features z_1 , z_2 , z_3 :



$$z_{2} = exp\left(-\frac{\left|\left|\mathbf{x} - l^{(2)}\right|\right|_{2}^{2}}{2\sigma^{2}}\right)$$

$$z_{3} = exp\left(-\frac{\left|\left|\mathbf{x} - l^{(3)}\right|\right|_{2}^{2}}{2\sigma^{2}}\right)$$



σ² is small, then lower bias and higher variance since the features taper off quicker

$$\Box \Phi(x^{(1)}) = (z_1, z_2, z_3) \text{approx } (0, 0, 1)$$

$$\Box \Phi(x^{(2)}) = (z_1, z_2, z_3)$$
approx (1, 0, 0)

☐The larger the sigma - the more weight is given to features far away from the landmark

This slide is adapted from: https://www.coursera.org/learn/machine-learning/lecture/YOMHn/kernels-i-https://en.wikipedia.org/wiki/Radial_basis_function_kernel

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Another feature transformation if o2 is large, then higher bias and low

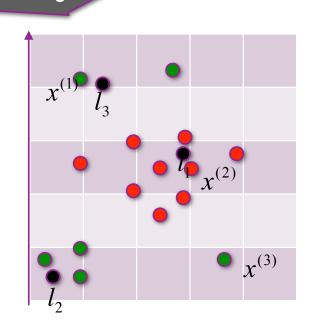
Define new features, f_1 , f_2 , and f_3 for every how close it is to chosen "landmarks" $l^{(1)}$

□ For an example x we create new feat square of the country is tance =:

$$z_1 = exp\left(-\frac{\left\|\mathbf{x} - l^{(1)}\right\|_2^2}{2\sigma^2}\right)$$

$$z_{2} = exp\left(-\frac{\left|\left|\mathbf{x} - l^{(2)}\right|\right|_{2}^{2}}{2\sigma^{2}}\right)$$

$$z_{3} = exp\left(-\frac{\left|\left|\mathbf{x} - l^{(3)}\right|\right|_{2}^{2}}{2\sigma^{2}}\right)$$



higher bias and lower variance since the features taper off slower. σ^2 is the radius of influence

$$\Box \Phi(x^{(1)}) = (z_1, z_2, z_3) \text{approx } (0, 0, 1)$$

$$\Box \Phi(x^{(2)}) = (z_1, z_2, z_3)$$
approx (1, 0, 0)

☐The larger the sigma - the more weight is given to features far away from the landmark

This slide is adapted from: https://www.coursera.org/learn/machine-learning/lecture/YOMHn/kernels-i-https://en.wikipedia.org/wiki/Radial_basis_function_kernel

Gausian-RBF Kernel

$$\Phi(\mathbf{x}) = exp\left(-\frac{(\mathbf{x})^2}{2\sigma^2}\right) \left(1, \sqrt{\frac{2^1}{1!}}(\mathbf{x})^1, \sqrt{\frac{2^2}{2!}}(\mathbf{x})^2, \sqrt{\frac{2^3}{3!}}(\mathbf{x})^3, \dots\right) \frac{infinite - dimensions}{transformation}$$

$$\left(\|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|^2\right) \left((\mathbf{x}^{(j)})^2\right) \left((\mathbf{x}^{(j)})^2\right)$$

The Taylor series expansion of ex $e^{x} = \sum_{k=1}^{\infty} x^{k}/k!$ see: http://

$$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = exp\left(-\frac{\left\|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\right\|_{2}^{2}}{2\sigma^{2}}\right) = exp\left(-\frac{(\mathbf{x}^{(i)})^{2}}{2\sigma^{2}}\right) exp\left(\frac{2\mathbf{x}^{(i)}\mathbf{x}^{(j)}}{2\sigma^{2}}\right) exp\left(-\frac{(\mathbf{x}^{(j)})^{2}}{2\sigma^{2}}\right) exp\left(-\frac{(\mathbf{$$

$$= \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x}^{(j)})$$

Gaussian Radial Basis Function

- For every example make a landmark: $l^{(1)} = \mathbf{x}^{(1)}, \ l^{(2)} = \mathbf{x}^{(2)}, \ ..., \ l^{(N)} = \mathbf{x}^{(N)}$
- ☐ Then for every x, we have created N new features z_1 , z_2 ,..., z_n :

$$K(\mathbf{x}^{(i)}, l^{(j)}) = z_j^{(i)} = exp\left(-\frac{\left\|\mathbf{x}^{(i)} - l^{(j)}\right\|_2^2}{2\sigma^2}\right) \qquad z =$$

☐The number of features is now N

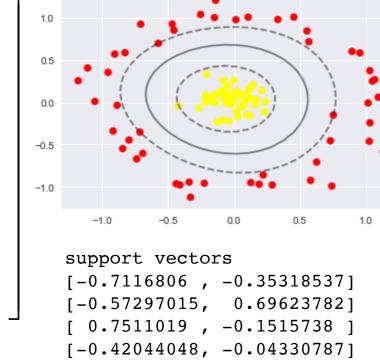
$$\exp(\left\|\mathbf{x} - l^{(1)}\right\|_{2}^{2} / 2\sigma^{2})$$

$$\exp(\left\|\mathbf{x} - l^{(2)}\right\|_{2}^{2} / 2\sigma^{2})$$

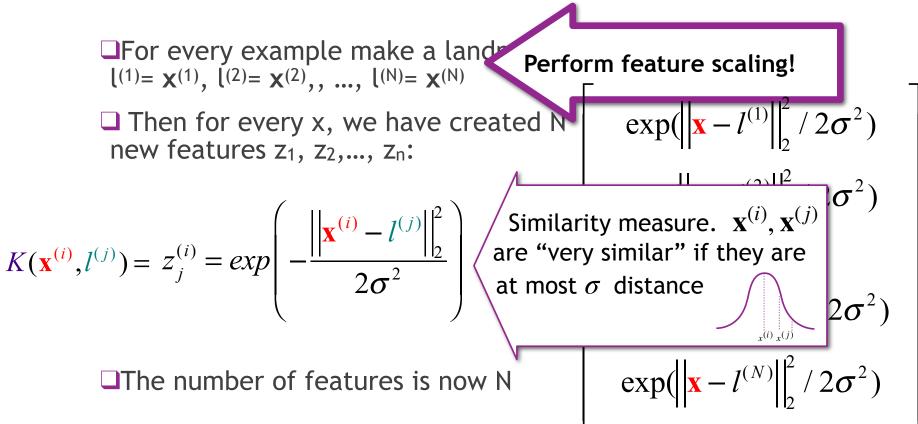
$$\vdots$$

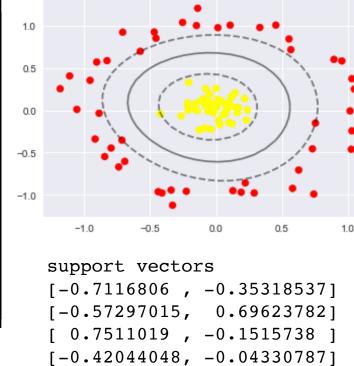
$$\exp(\left\|\mathbf{x} - l^{(N-1)}\right\|_{2}^{2} / 2\sigma^{2})$$

$$\exp(\left\|\mathbf{x} - l^{(N)}\right\|_{2}^{2} / 2\sigma^{2})$$

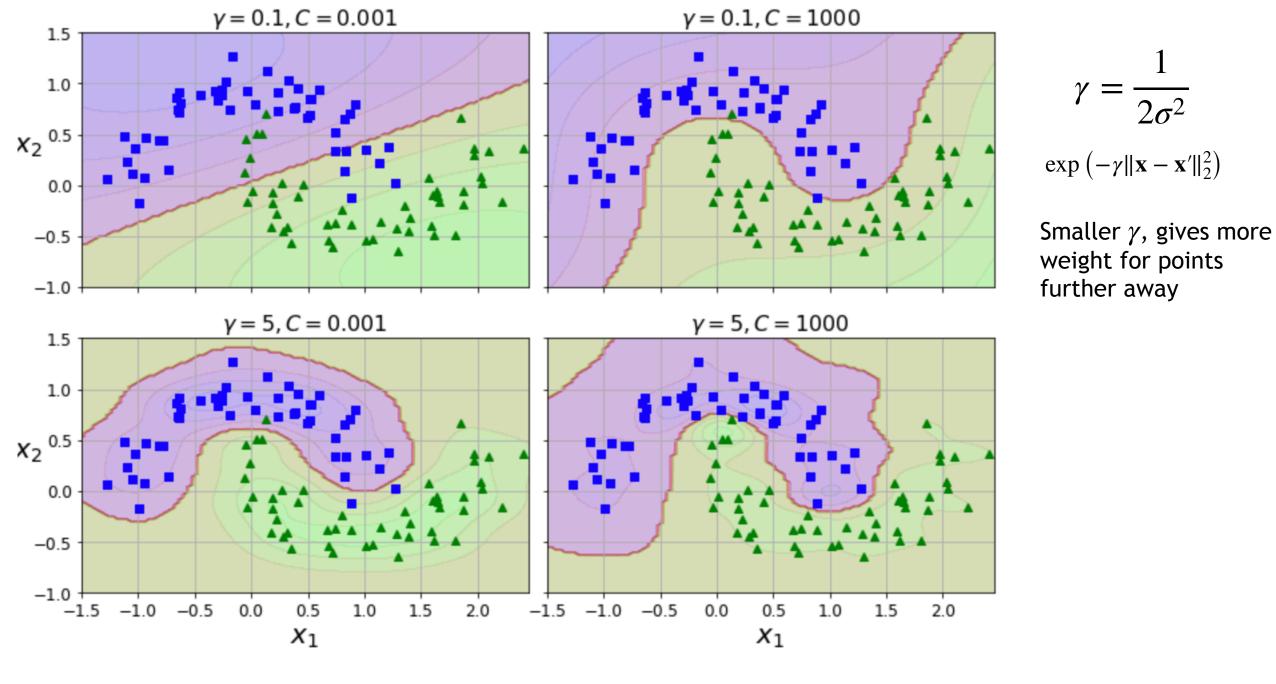


Gaussian Radial Basis Function



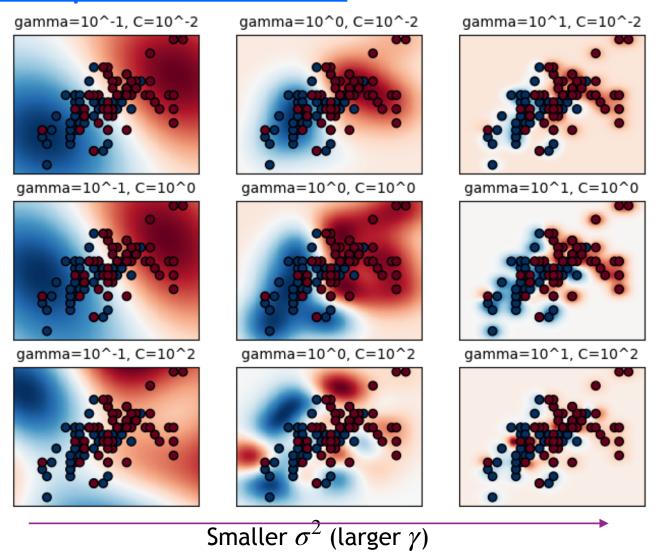


A great description is given at: https://www.coursera.org/learn/machine-learning/lecture/hxdcH/kernels-ii



Graph from Hands-On Machine Learning with Scikit-Learn, Keras & TensorFlow

Example from http://scikit-learn.org/stable/auto_examples/sym/plot_rbf_parameters.html



$$\gamma = 1/(2\sigma^2)$$

Larger C

"Intuitively, the gamma parameter defines how far the influence of a single training example reaches, with low values meaning 'far' and high values meaning 'close'."

SVMs

- Maximizes distance of training data to boundary (built in regularization)
- Generalizes to nonlinear decision boundaries (I.e. feature transformation)
- Performs well with high dimensional data

Sklearn

LinearSVC: optimizer for the primal particle of the particle

LinearSVC: optimizer for the primal problem

typically between $O(N^2 \times d)$ and $O(N^3 \times d)$

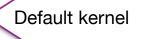
 $O(N \times d)$

From: https://scikit-learn.org/dev/modules/svm.html#svm-kernels

1.4.6. Kernel functions

The *kernel function* can be any of the following:

- linear: $\langle x, x' \rangle$.
- polynomial: $(\gamma \langle x, x' \rangle + r)^d$, where d is specified by parameter degree, r by coef0.
- rbf: $\exp(-\gamma \|x-x'\|^2)$, where γ is specified by parameter gamma, must be greater than 0.



• sigmoid $anh(\gamma\langle x,x'\rangle+r)$, where r is specified by coef0.

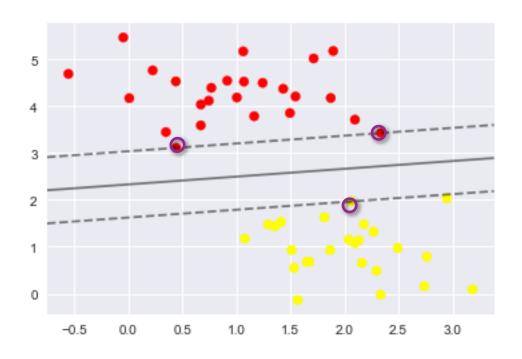
Different kernels are specified by the kernel parameter:

```
>>> linear_svc = svm.SVC(kernel='linear')
>>> linear_svc.kernel
'linear'
>>> rbf_svc = svm.SVC(kernel='rbf')
>>> rbf_svc.kernel
'rbf'
```

Using sklearn's support vector classifier to find the maximum margin on the training examples X

```
from sklearn.svm import SVC # "Support vector
model = SVC(kernel='linear', C=1E10)
model.fit(X, y)
By choosing the parameter C to be very large we assure no misclassification points
```

The classifier finds the optimal model for the training examples



We can observe what the support vectors are:

When using the SVM, we don't need to compute the coefficient vector.

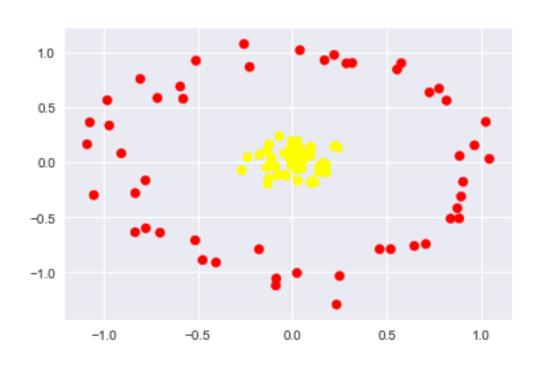
But, if we wanted to find it, how can we determine w?

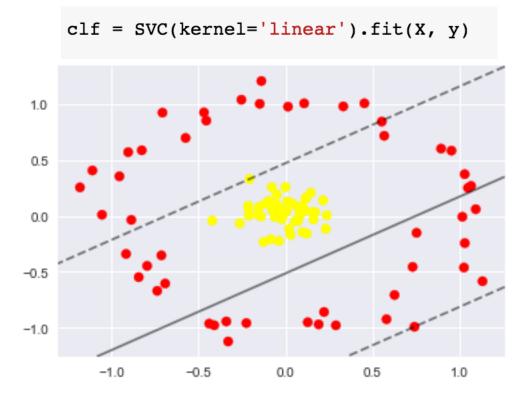
1) We could use the formula
$$\mathbf{w} = \sum_{i=1}^{N} \alpha^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

2) Or we retrieve the information from Sklearn if we are using a linear kernel: model.coef_

Suppose the data is not linearly separable

Lets try to fit it with a linear support vector machine (we will allow for some misclassification)...

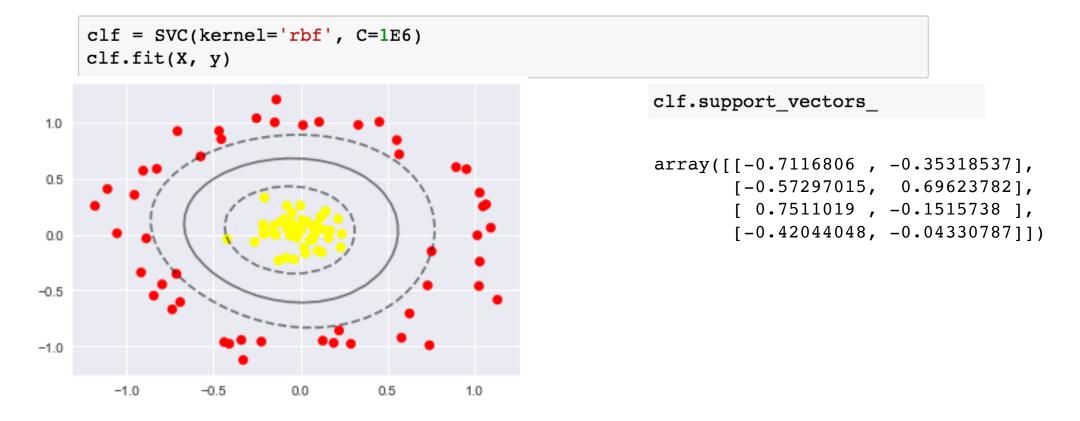




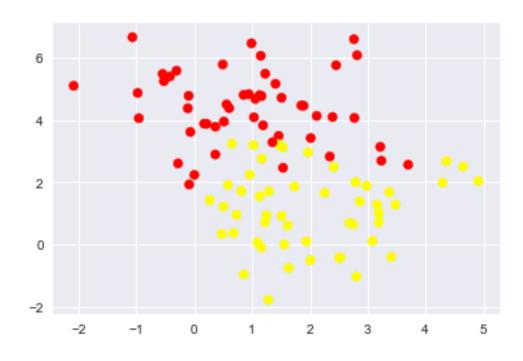
How can we find the right point to transform the points to become linearly separable?

Easiest answer is to compute the distance to every point in the data set! Problem? The number of features becomes N, the number of training examples

In sklearn, we can apply the radial basis function kernel (RBF kernel)



Another way to work with non separable data is to allowing for errors - Soft Margin SVM

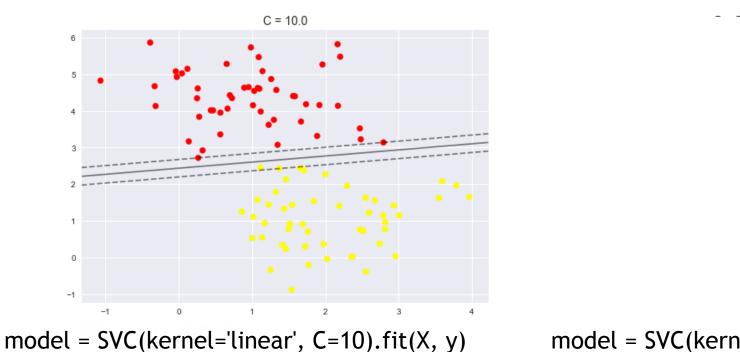


We create a soft- margin classifier by adding a cost to points that are not correctly classified and outside the margin

The primal objective function:

$$\min_{\substack{w_0, \mathbf{w}, \{\xi^{(i)}\}_{i=1}^N \\ \text{subject to } \mathbf{y}^{(i)}(w_0 + \mathbf{w}^T \mathbf{x}^{(i)}) \ge 1 - \xi^{(i)} \text{ for all } i = 1, ..., \mathbf{N} \quad \xi^{(i)} \ge 0}$$

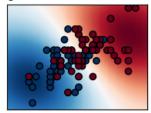
The tuning parameter C softens (C smaller) or hardens (C larger)



model = SVC(kernel='linear', C=0.1).fit(X, y)

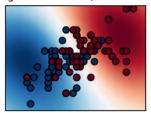
SVC

gamma=10^-1, C=10^-2

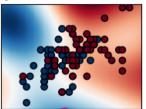


Underfitting for small C

gamma=10^-1, C=10^0



gamma=10^-1, C=10^2



Under-fitting for Small gamma from sklearn.svm import <u>SVC</u>

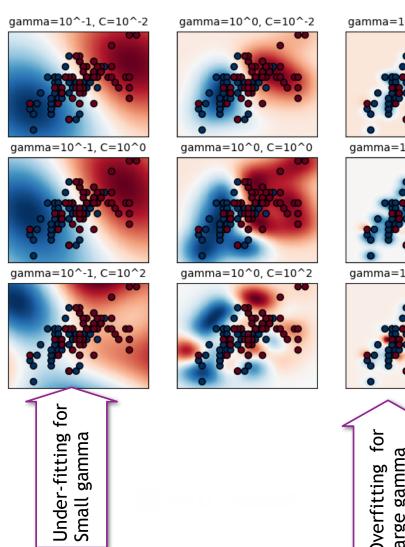
```
C_2d_range = [1e-2, 1, 1e2]
gamma_2d_range = [1e-1, 1, 1e1]
classifiers = []
for C in C_2d_range:
    for gamma in gamma_2d_range:
        clf = SVC(C=C, gamma=gamma)
        clf.fit(X_2d, y_2d)
        classifiers.append((C, gamma, clf))
```

"Intuitively, the gamma parameter defines how far the influence of a single training example reaches, with low values meaning 'far' and high values meaning 'close'."

"The C parameter trades off correct classification of training examples against maximization of the decision function's margin"

The radius of the RBF kernel alone acts as a good structural regularizer.

SVC



```
gamma=10^1, C=10^-2

gamma=10^1, C=10^0

gamma=10^1, C=10^2
```

```
C_2d_range = [1e-2, 1, 1e2]
gamma_2d_range = [1e-1, 1, 1e1]
classifiers = []
for C in C_2d_range:
    for gamma in gamma_2d_range:
        clf = SVC(C=C, gamma=gamma)
        clf.fit(X_2d, y_2d)
        classifiers.append((C, gamma, clf))
```

"Intuitively, the gamma parameter defines how far the influence of a single training example reaches, with low values meaning 'far' and high values meaning 'close'."

from sklearn.svm import <u>SVC</u>

"The C parameter trades off correct classification of training examples against maximization of the decision function's margin"

The radius of the RBF kernel alone acts as a good structural regularizer.

Ack!!! There are too many parameters to tune

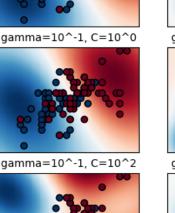


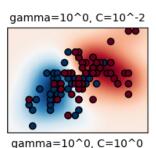
sklearn's RandomizedSearchCV and GridSearchCV are classes for parameter tuning that methodically builds and evaluates different combinations of parameters as a grid

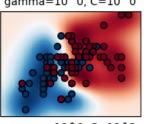
GridSearchCV

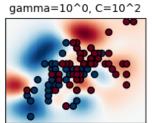


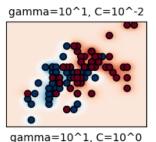
```
gamma=10^-1, C=10^-2
gamma=10^-1, C=10^0
```

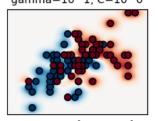


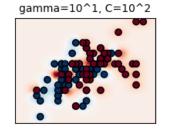












```
from sklearn.svm import SVC
from sklearn.model_selection import StratifiedShuffleSplit
from sklearn.model_selection import GridSearchCV

# Train classifiers
#
# For an initial search, a logarithmic grid with basis
# 10 is often helpful. Using a basis of 2, a finer
# tuning can be achieved but at a much higher cost.
```

```
C_range = np.logspace(-2, 10, 13)
gamma_range = np.logspace(-9, 3, 13)
param_grid = dict(gamma=gamma_range, C=C_range)
cv = StratifiedShuffleSplit(n_splits=5, test_size=0.2, random_state=42)
grid = GridSearchCV(SVC(), param_grid=param_grid, cv=cv)
grid.fit(X, y)
```