GENERAL ASSEMBLY

SUPPORT VECTOR MACHINES (SVM)

AGENDA

1. Introduction to SVMs
    1. Background understanding – Visualizing SVMs
    2. Background understanding – “A Little Math”
2. Linear SVMs
    1. Soft margin tuning
    2. Key points & comparison with Logistic Regression
3. Non-Linear Decision Boundaries
    1. Understanding non-linear decision boundaries
    2. Computational efficiency and “The Kernel Trick”
4. Non-Linear Kernel SVMs
    1. Review of popular Kernels
    2. Gaussian Kernel: Conceptualization and Tuning
    3. Wrap up and comparison with Logistic Regression

- What are Support Vector Machines (SVMs)?

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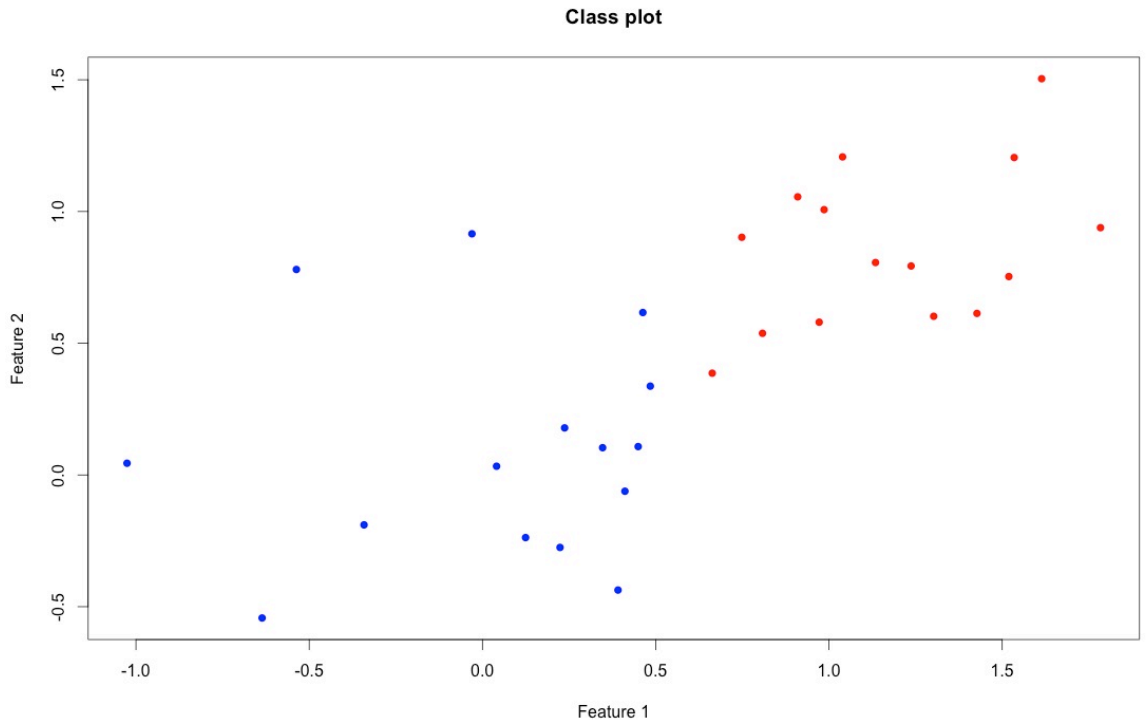
- An SVM separates data sets into (+) and (-) classes by "slicing" the feature space into 2 regions:
  1. A positive (+) region of the feature space, and
  2. A negative (-) region of the feature space.
- New data is then classified based on the region in which it lies.

- What does SVM classification look like?



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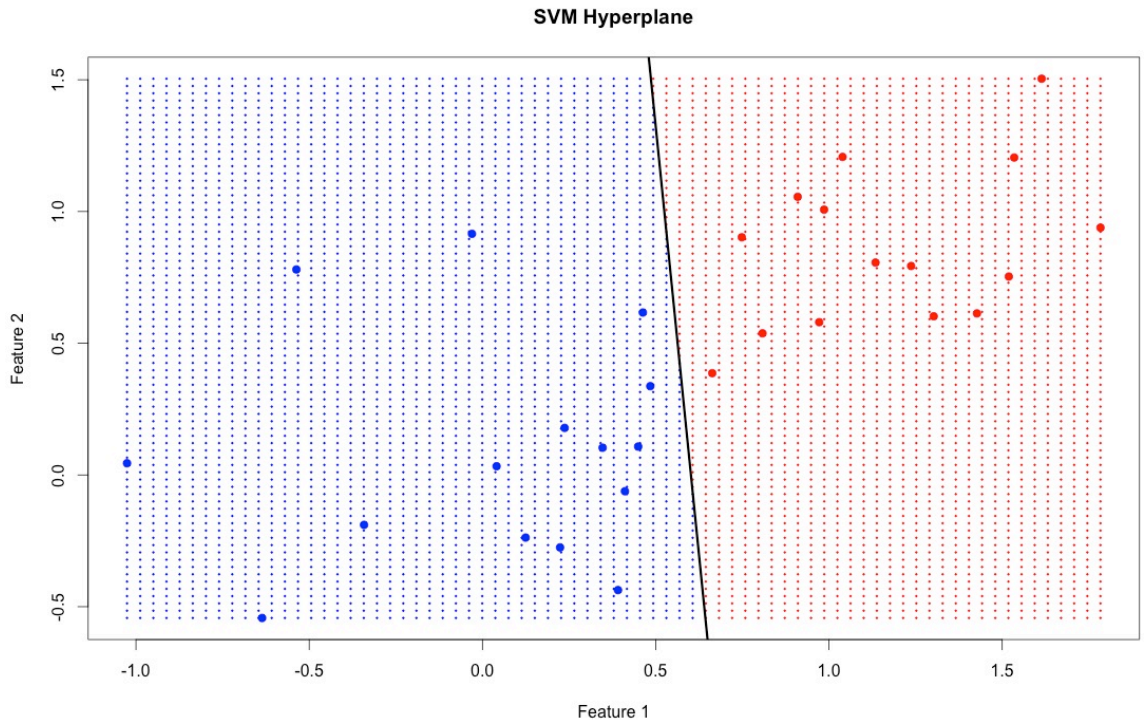
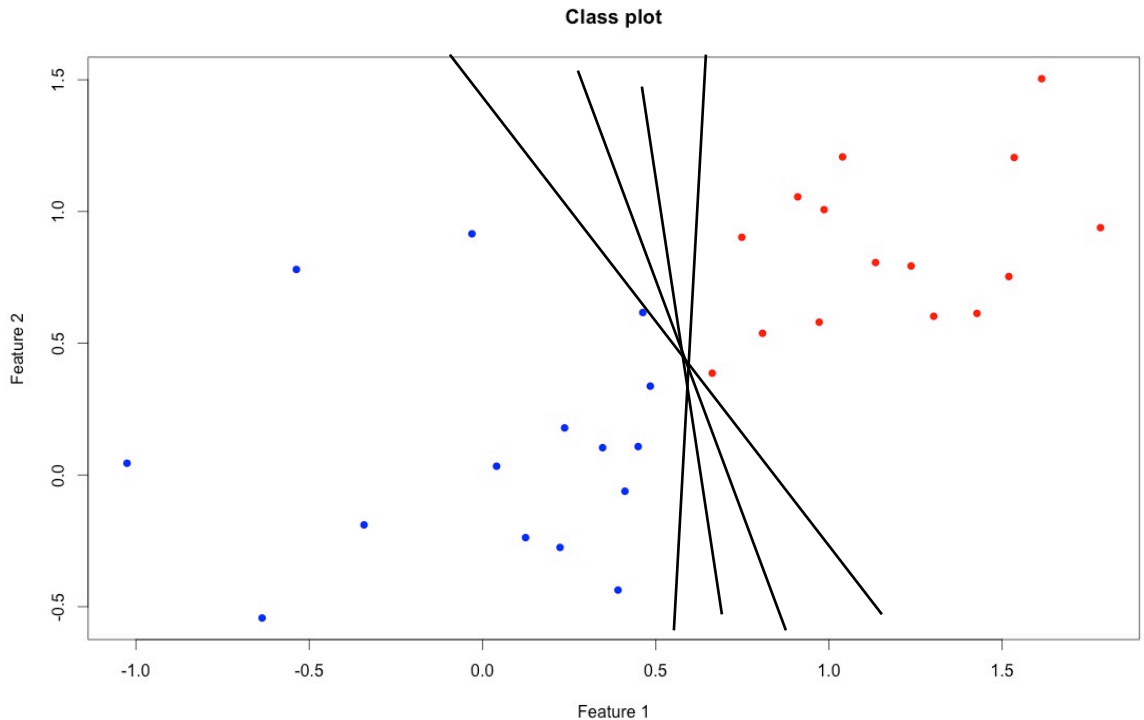


- When the data is “separable,” multiple boundary can be defined:



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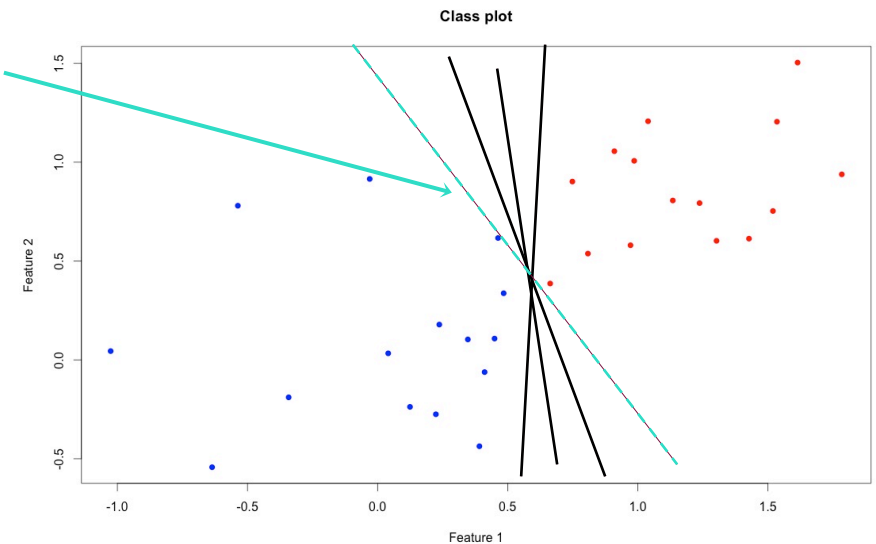
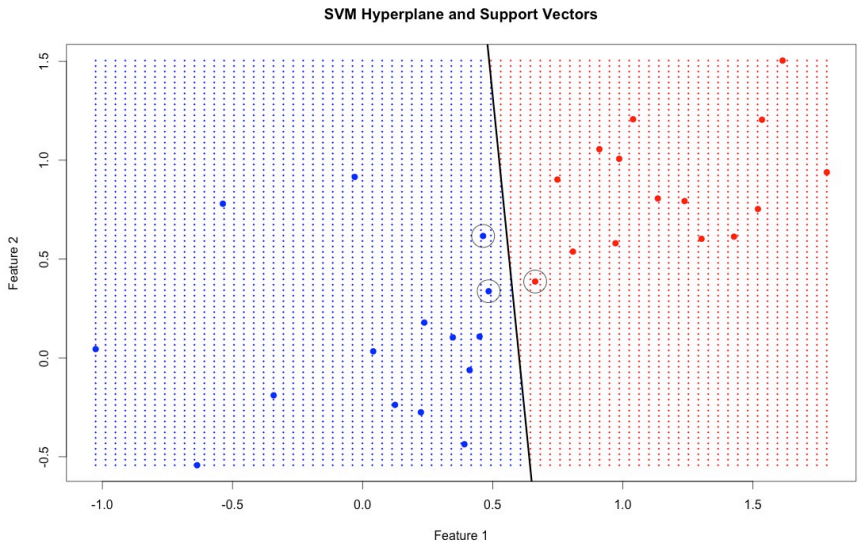
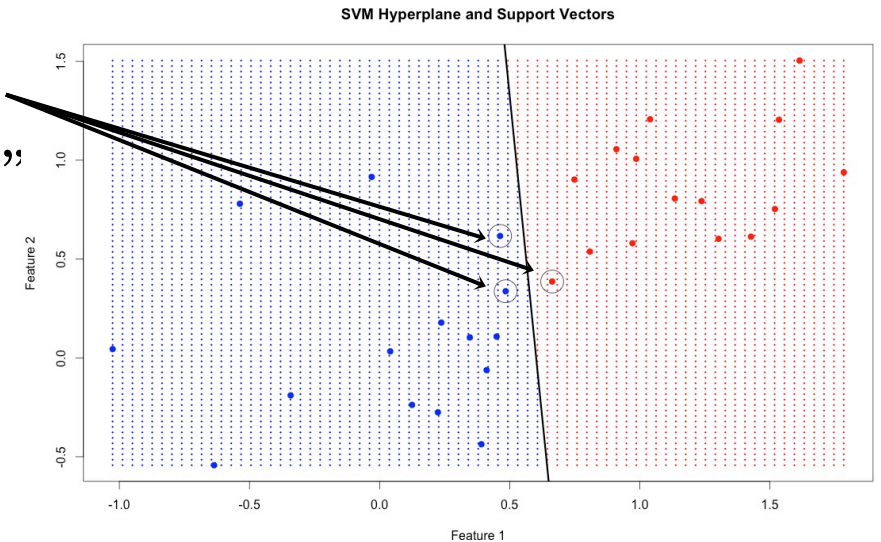
  - *Ceteris paribus*, separators that "cut too close" to potential **boundary points** run a risk of underperforming on new data…



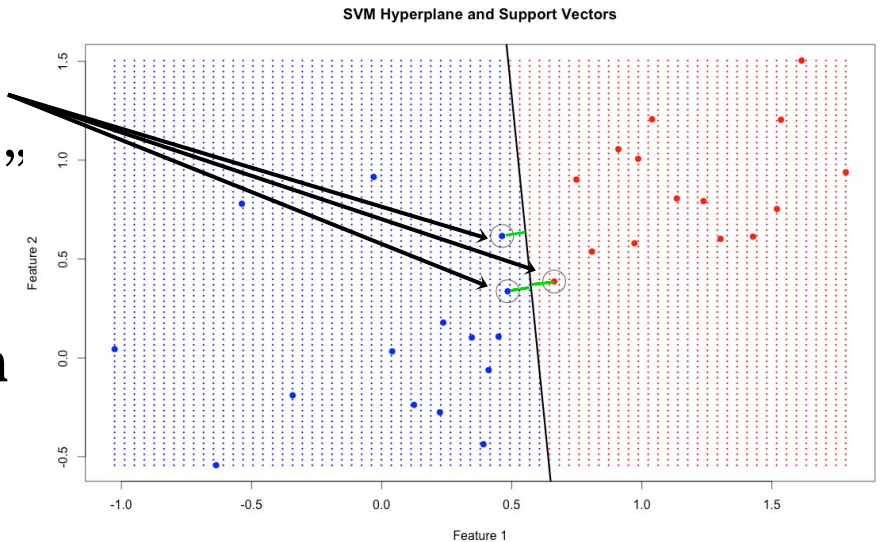
- When the data is "separable," multiple boundary can be defined:
  - *Ceteris paribus*, separators that "cut too close" to potential **boundary points** run a risk of underperforming on new data…
  - SVMs work by finding the boundary with an optimal chance of generalizing to new data, by avoiding these points.



- How is the the hyperplane detected?
  - The hyper-plane is defined by identifying the "*Support Vectors*."



- How is the the hyperplane detected?
  - The hyper-plane is defined by identifying the "***Support Vectors***."
  - And finding the boundary that *optimizes* the the distances from the set of support vectors to the hyperplane.



A LITTLE MATH...

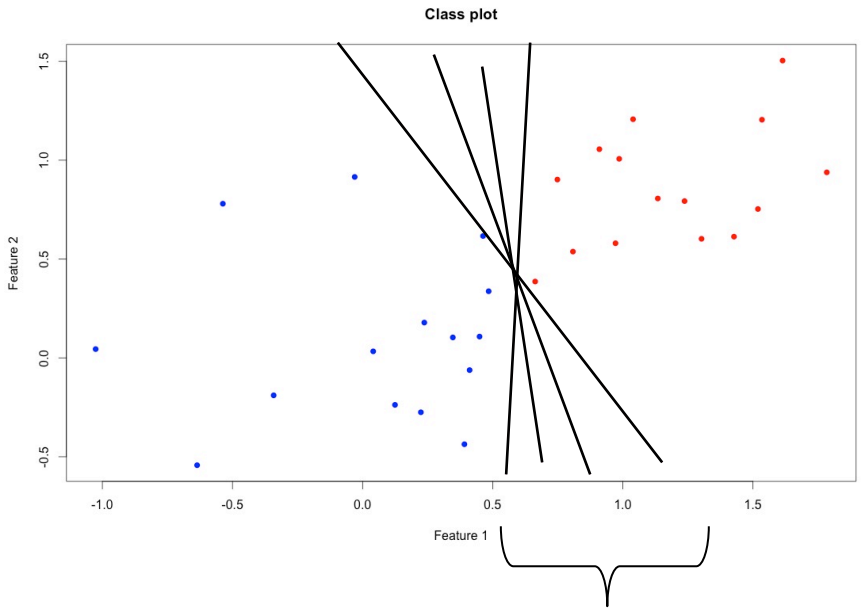
- How is the the hyperplane detected mathematically?
  - A hyperplane is defined as the set of all points $\boldsymbol{x}$ such that:

$$\sum_{i=1}^{n} x_i \beta_i = \beta_0$$

  - or

$$\sum_{i=0}^{n} x_i \beta_i = 0$$

where $x_0 := 1$



Hyperplanes defined by different choices of $\vec{\boldsymbol{\beta}}$

A LITTLE MATH…

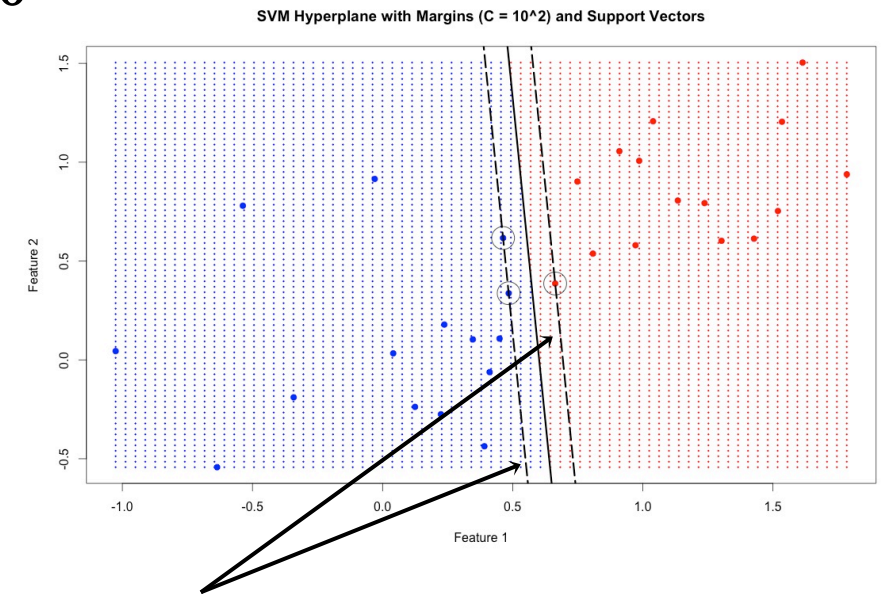
- SVM: find the line $\vec{\beta}$ values) *maximize the +/- separation (M).*
  - This is a "constrained optimizatio¬" problem:

$$\max_{\|\vec{\beta}\| \leq 1} M$$

Such that for all (x_j, y_j):

$$y_j \left(\sum_{i=0}^{n} x_{ji} \beta_i \right) \geq M$$

(where $y_j \epsilon \{1, -1\}$)

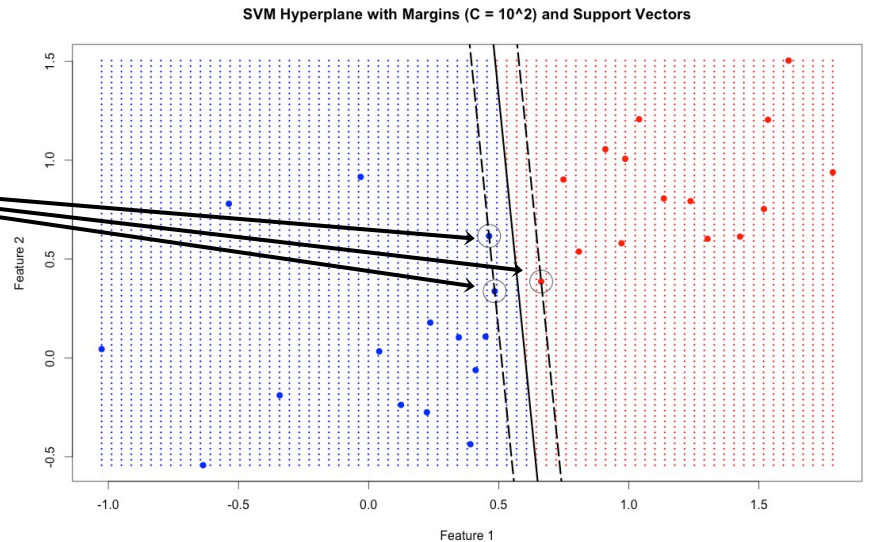


Margins of optimal distance *M* from all points.

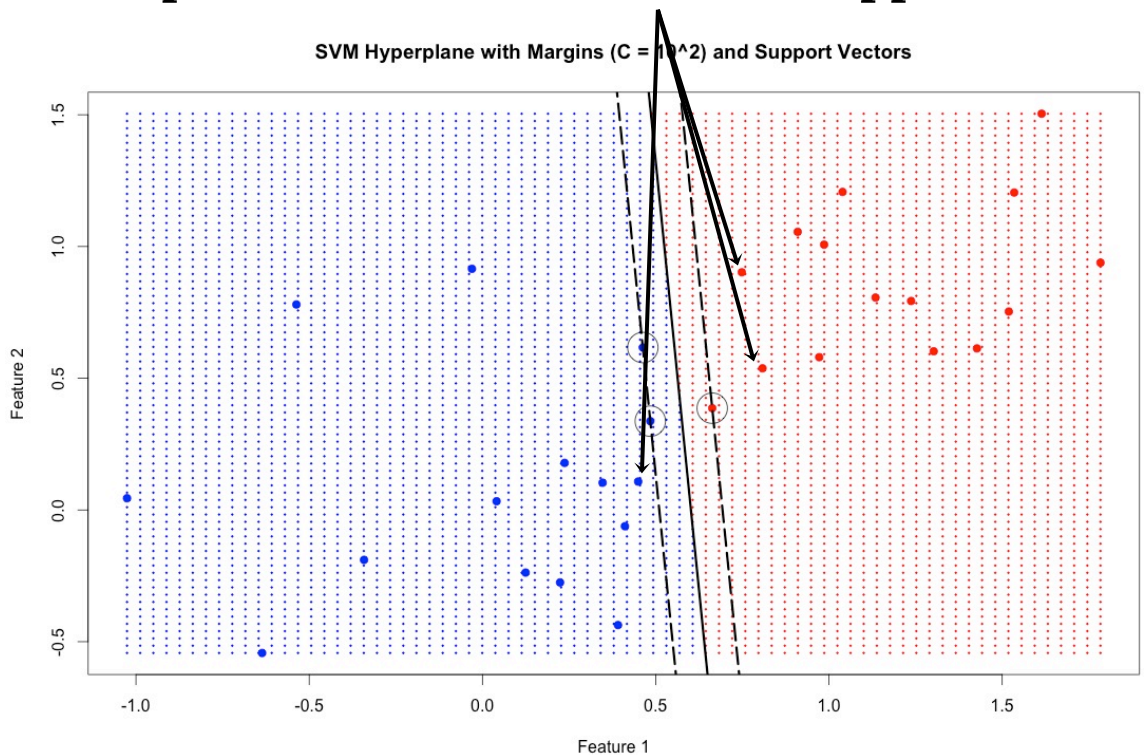
NOTE:

- The **maximized** margin M is based on it's distance from the "*Support Vectors*."

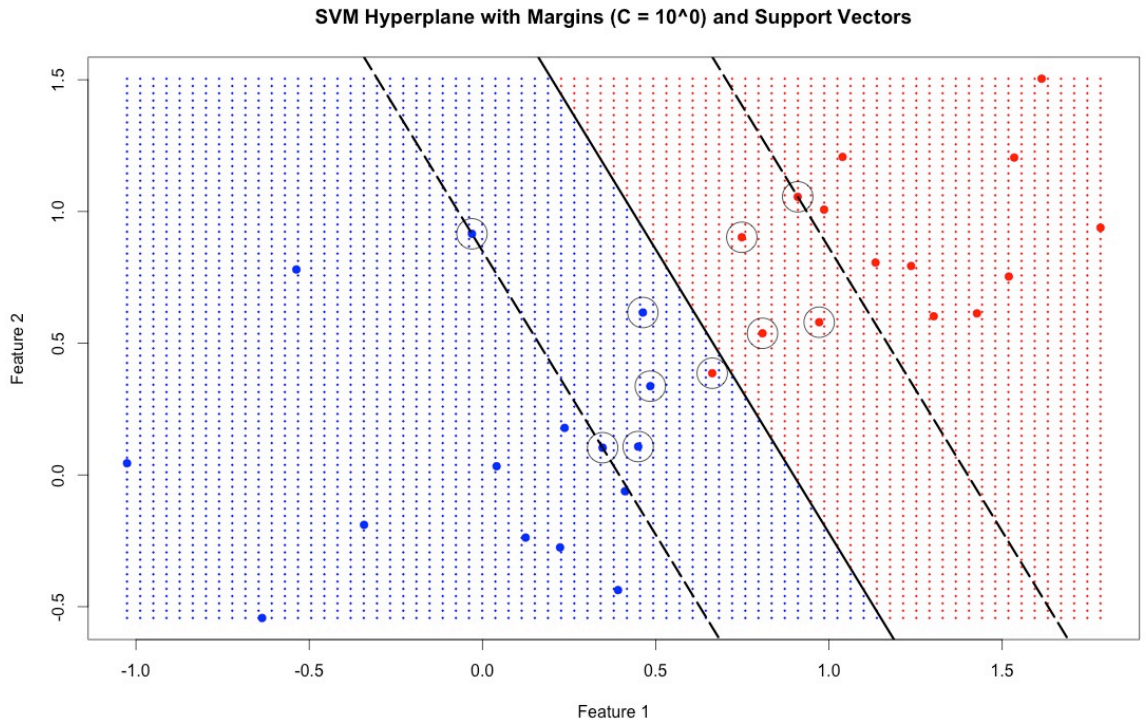
- However, in order to determine which points count as Support Vectors, the inequality must be taken over all data points.



- What about data points that were “almost” Support Vectors?



- SVMs allow for a *tuning parameter* (C) that "softens" the margins.



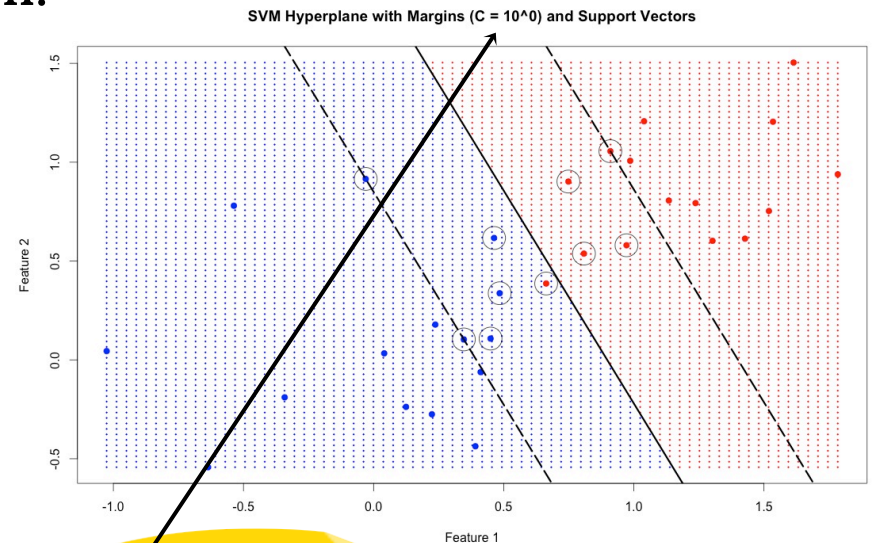
- Margins are softened, by adding error factors to the constraint equations:
  - Softened constrained optimization:

$$\max_{\|\vec{\beta}\| \leq 1} M$$

Such that for all $(\boldsymbol{x}_j, y_j)$:

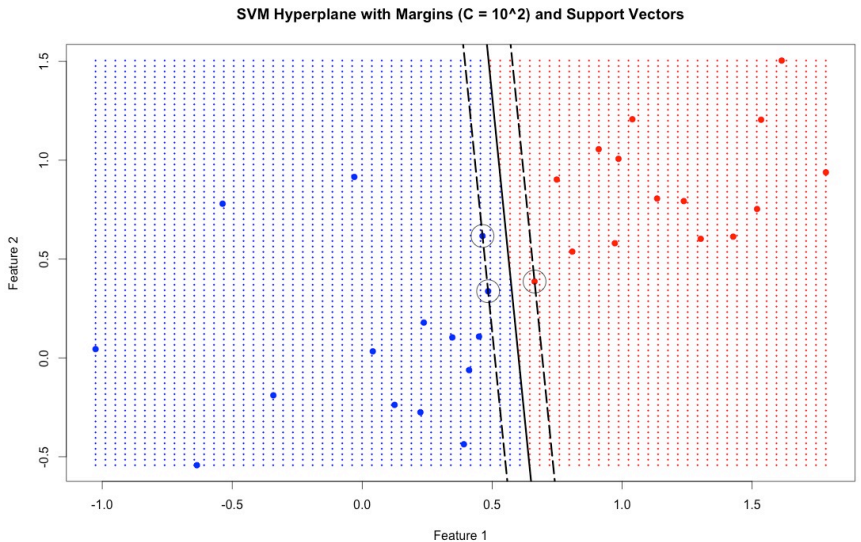
$$y_j \left(\sum_{i=0}^{n} x_{ji} \beta_i \right) \geq M(1 - \varepsilon_j)$$

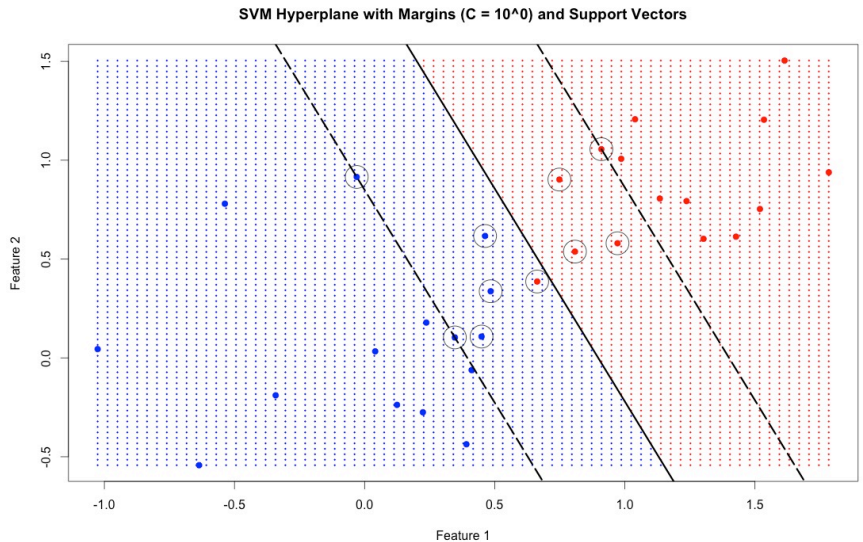
where the $\varepsilon_j \geq 0$ and $\sum \varepsilon_j \propto \frac{1}{C}$.



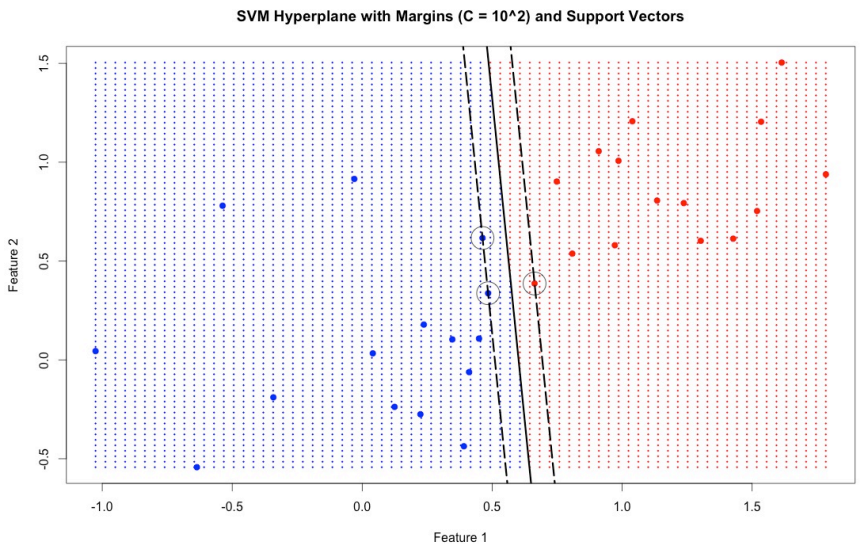
Note: The smaller the value of C the wider the margins become.

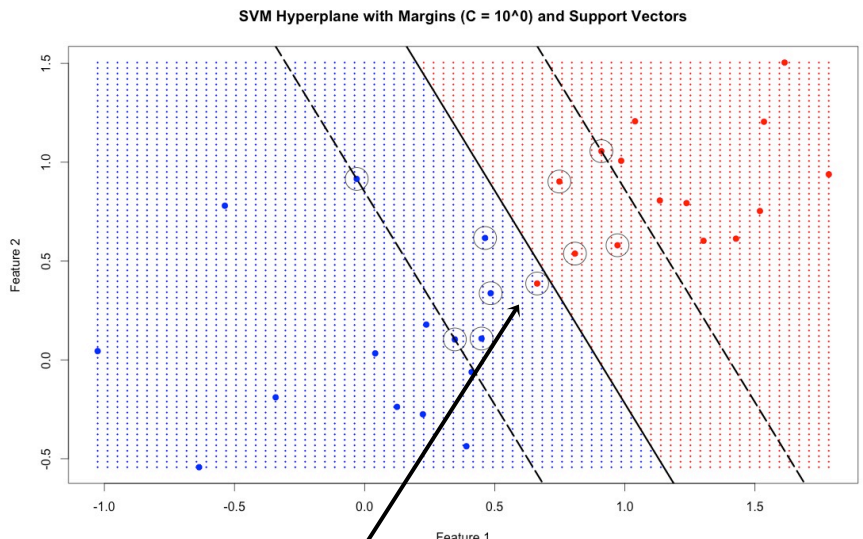
- Tuning the margins (C-value) affects the Hyperplane boundary.





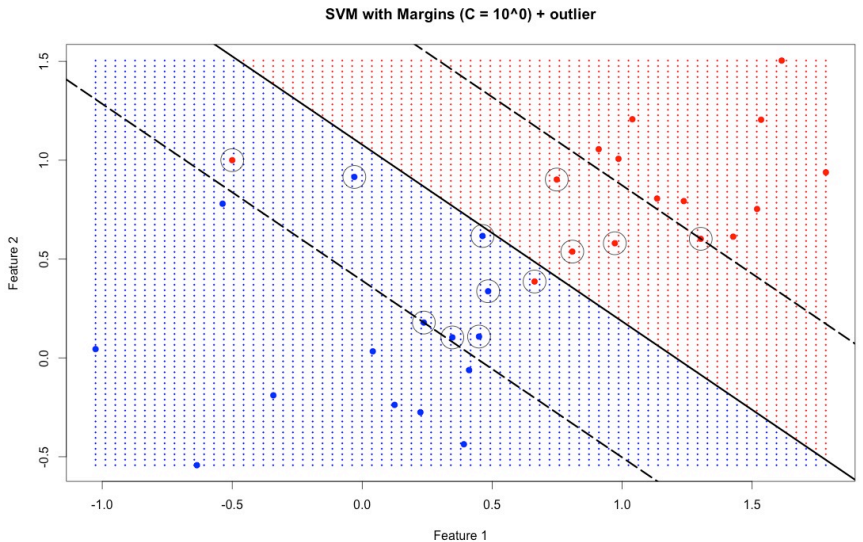
- Under-fitting C can lead to **Generalization Bias**

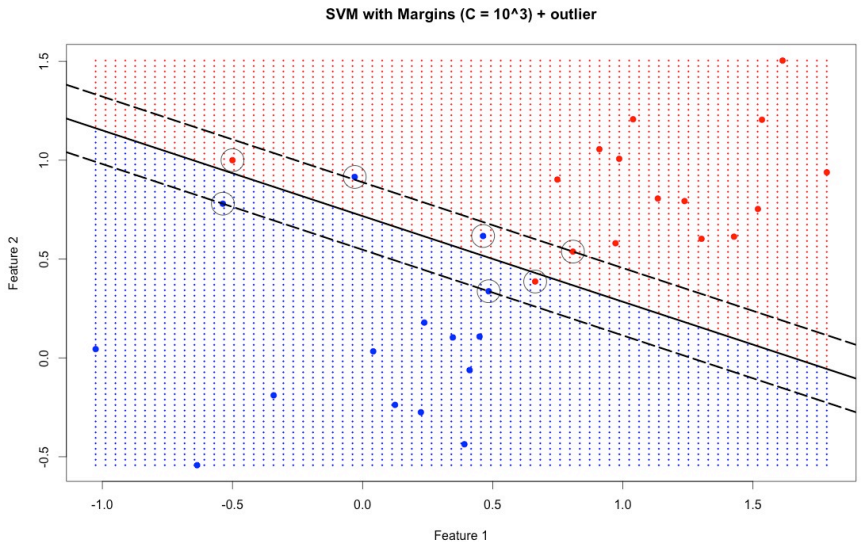




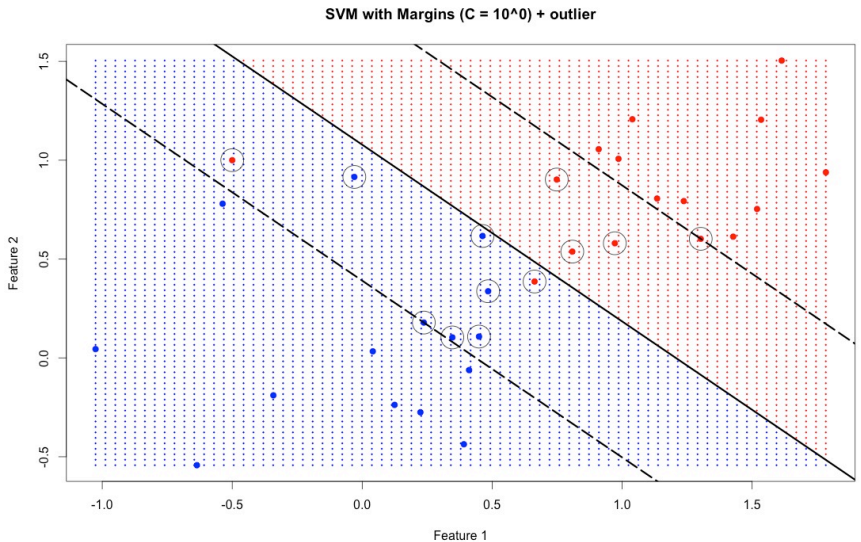
Margins that are too wide can cause miss-classification

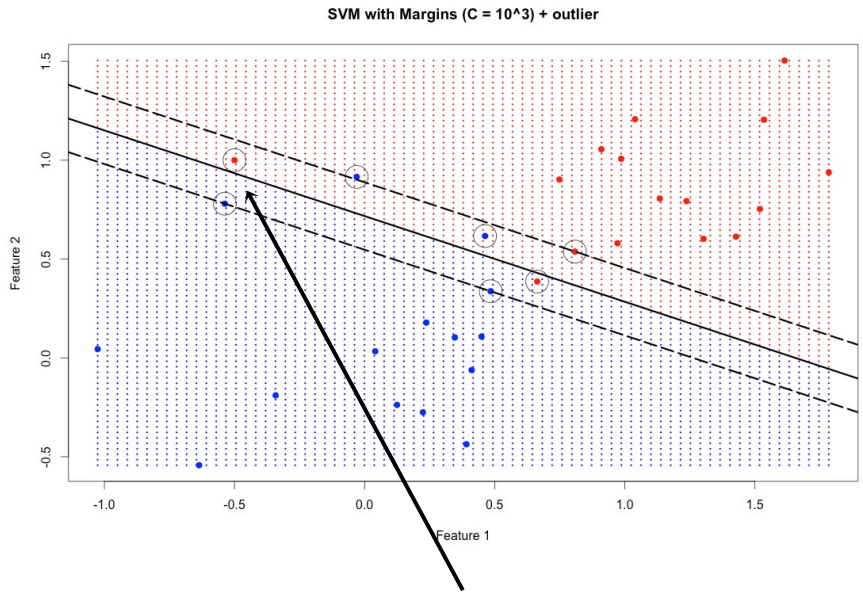
- Over-fitting C can lead to **Generalization Variance**





- Over-fitting C means **Generalization Variance**





Margins that are too narrow are over sensitive to training outliers

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    1. But non-SV data still plays a role in determining the SVs.

LINEAR SVM – KEY POINTS

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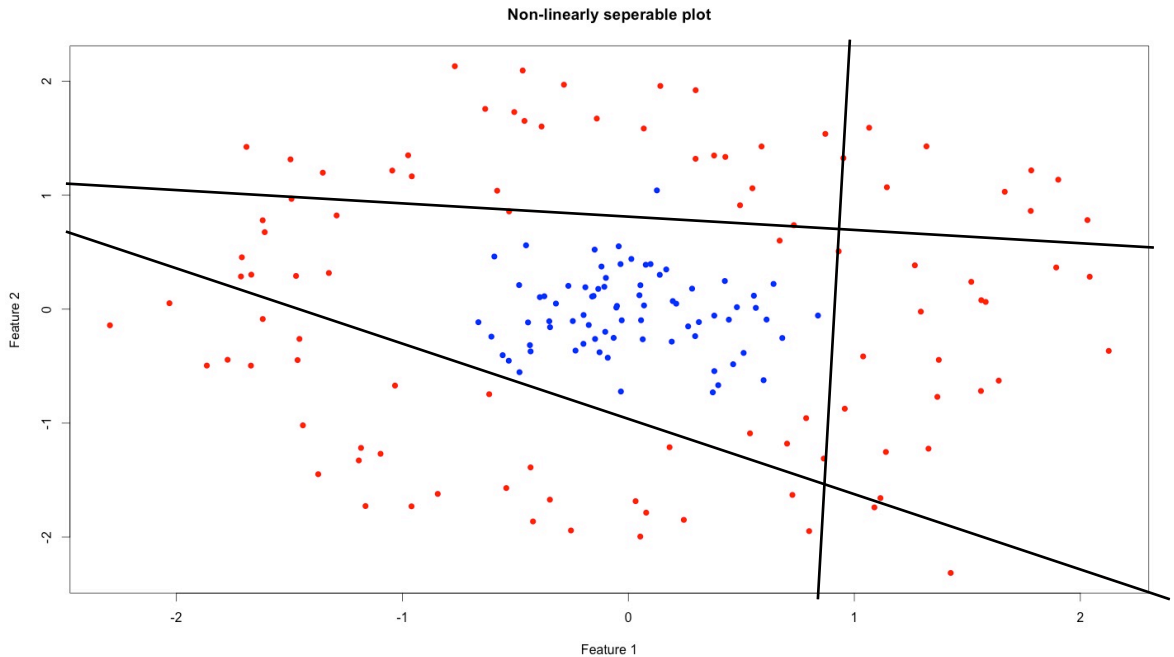
5. Linear SVMs are tuned by one parameter (C) to allow for "soft SV margins."
    1. Compare with lambda ($1/\lambda$) for Lasso or Ridge penalties in LR.
    2. Can be used for feature selection in the Linear SVM case.

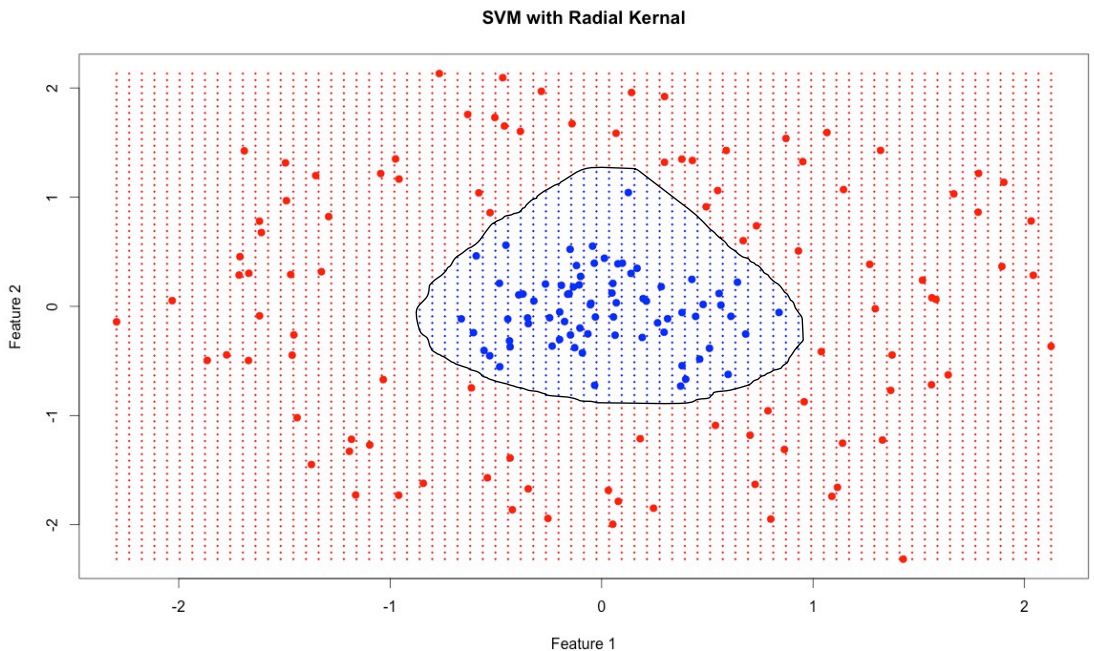
- What if the (+) and (-) data cannot be separated by a single hyperplane?



NON-LINEAR SVM

- In these cases we use SVMs with a *Non-linear Kernal*

KEY TERM

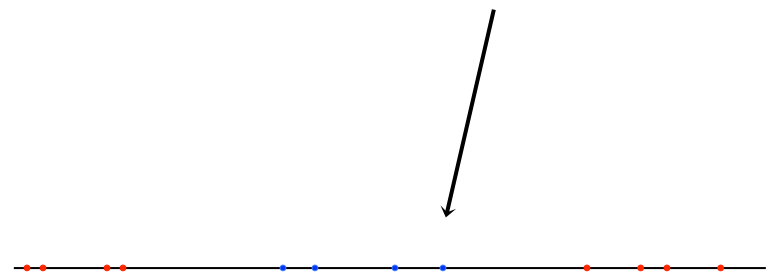


- What is the *Kernel Trick*?

Popular Interview Question!

  - Consider data distributed in 1D…

(+) and (-) data in a 1-d space



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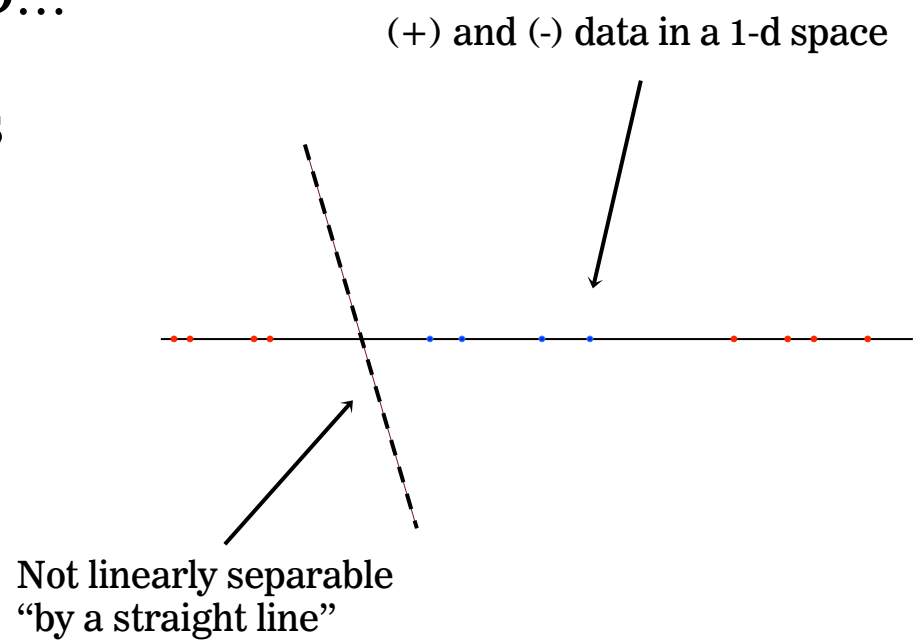
- Not separable using terms dependent on "linear" features
  e.g. $x_1,\ldots$



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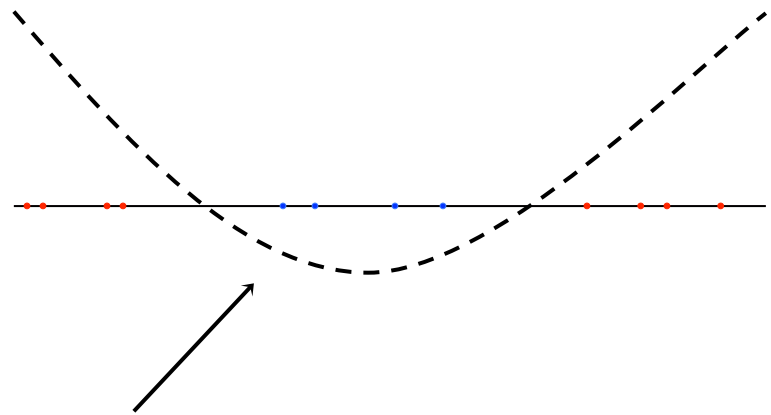
Popular Interview Question!

- Consider data distributed in 1D…
- Not separable using terms dependent on "linear" features
  e.g. x_1,…
- However, (+) and (-) points may still be separated by "non-linear" terms:
  e.g. x_1, x_1^2, x_1^3,…



Data is separable by a "parabolic dependency on x_1^2"

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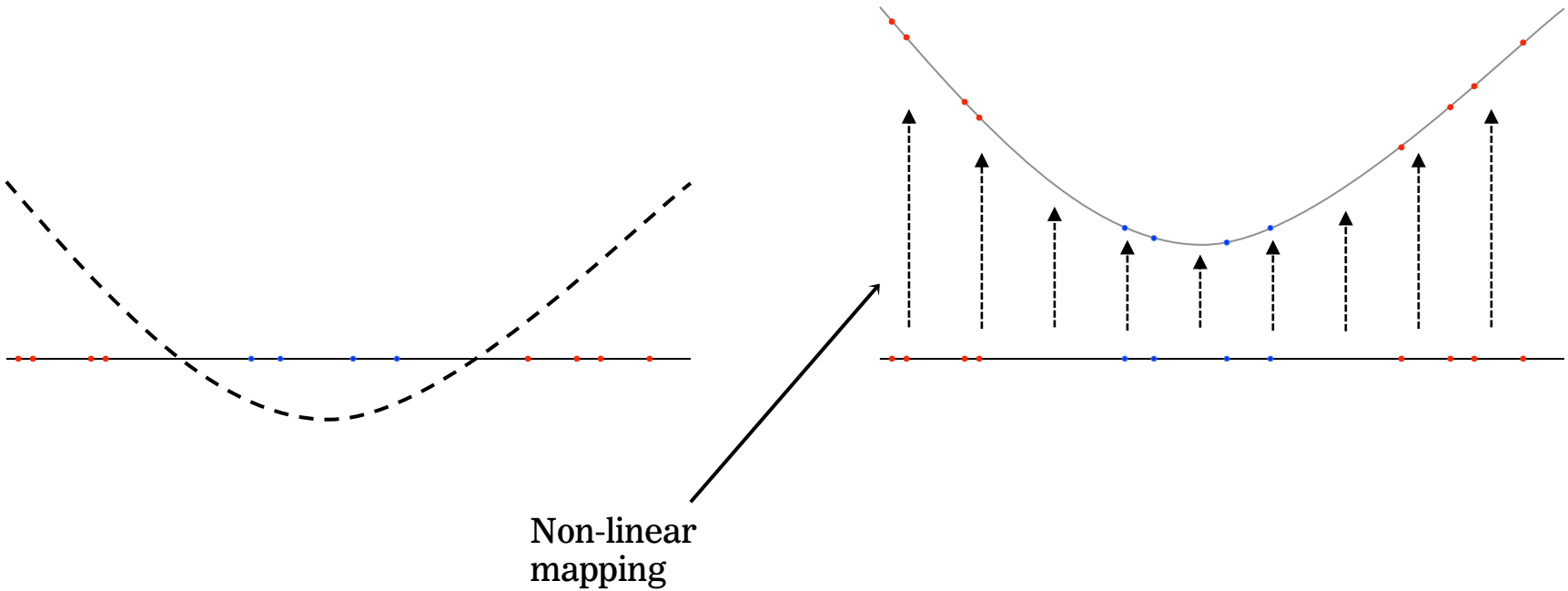

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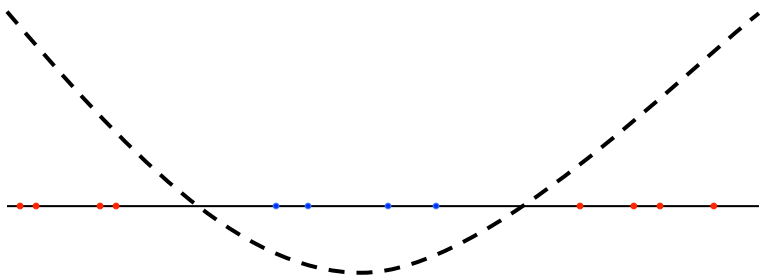
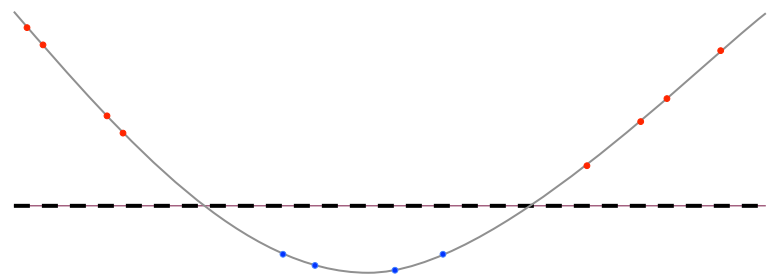


Non-linear separator defined for the original feature space



Linear separator defined for a *non-linearly related* new space

- What is the *Kernel Trick*?

Popular Interview Question!

Steps for non-linear separation:

- What is the ***Kernel Trick***?

Popular Interview Question!

Steps for non-linear separation:

- Step 1: Map the original dimensions $x_1, x_2, x_3, \ldots$ into a **higher dimensional** feature space $x_1^2, x_2^2, x_3^2, x_1x_2, x_1x_3, \ldots$
  - (New feature space not linearly dependent on the original space.)

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  - (New feature space not linearly dependent on the original space.)
- Step 2: Define a decision boundary in terms of the new higher dimensional feature space.
- Step 3: New data points can be defined by mapping to the new higher dimensional feature space and comparing with the high-D boundary

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Popular Interview Question!

Classifiers: Logistic Regression, Linear-SVM, Decision Trees*, …

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  - The count of features $|\{ x_1^2, x_2^2, x_3^2, x_1x_2, x_1x_3, \dots \}|$ in the high-D space can grow too quickly with the dimension of the base space .

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  - Significantly reduces the computational complexity.

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- With SVM's, non-linear Kernels allow us to skip directly mapping to the high-D space for classification,
  - Significantly reduces the computational complexity.
- That's why it is called the "Kernal Trick"

A LITTLE MORE MATH…

- How does the ***Kernel Trick*** avoid high-D computation?
  - Recall SVMs are a "constrained optimization" problem:

$$\max_{\|\vec{\beta}\| \leq 1} M$$

Such that for all $(\boldsymbol{x}_j, y_j)$:

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  - Convex optimization in the "dual form":

$$\max_{\vec{\alpha}} 2 \sum_i \alpha_i + \sum_{i,j} \alpha_i \alpha_j y_i y_j \left(\sum_k x_{jk} x_{ik} \right)$$

  - In vector form:

$$\max_{\vec{\alpha}} 2 \|\vec{\alpha}\|_1 + \sum_{i,j} \alpha_i \alpha_j y_i y_j \langle \vec{x}_j, \vec{x}_i \rangle$$

- How does the ***Kernel Trick*** avoid high-D computation?
  - By replacing the inner product with a non-linear Kerne $K\left(\vec{x}_j, \vec{x}_i\right)$…
    - The decision boundary generated can be non-linear
    - Avoids direct calculations in the higher dimensional features space $x_1^2, x_2^2, x_3^2, x_1x_2, x_1x_3, \ldots$, significantly saving on memory and computation cost.

$$\max_{\vec{\alpha}} 2\|\vec{\alpha}\|_1 + \sum_{i,j} \alpha_i \alpha_j y_i y_j \underbrace{\langle \vec{x}_j, \vec{x}_i \rangle}$$

Euclidian "Inner product," a ***linear*** kernal

$$\max_{\vec{\alpha}} 2\|\vec{\alpha}\|_1 + \sum_{i,j} \alpha_i \alpha_j y_i y_j \underbrace{K\left(\vec{x}_j, \vec{x}_i\right)}$$

Non-linear Kernal

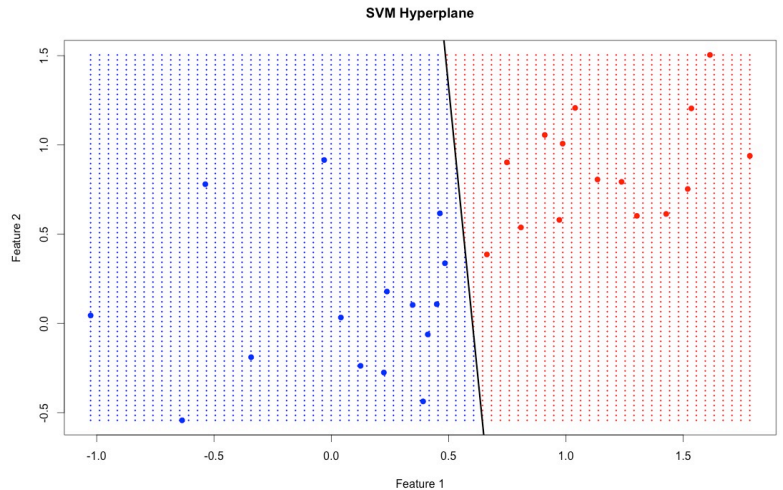
- Popular SVM Kernels:
  - Linear Kernel:

$$K\left(\vec{x}_j, \vec{x}_i\right) = \langle \vec{x}_j, \vec{x}_i \rangle + c$$

- Popular SVM Kernels:
  - Linear Kernel:

$$K\left(\vec{x}_j, \vec{x}_i\right) = \langle \vec{x}_j, \vec{x}_i \rangle + c$$

Linearly separable data



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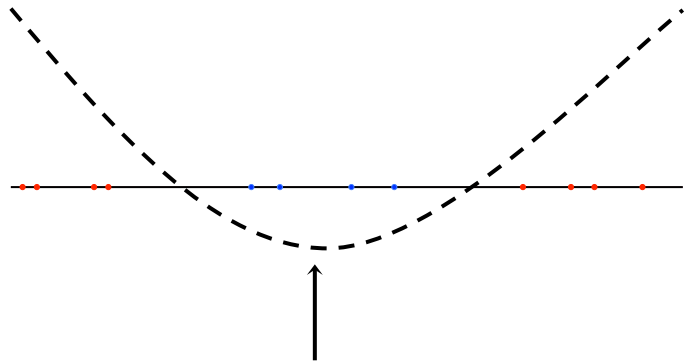
Data separable by a decision boundary with a ***finite*** d



parabolic decision boundary (d=2)

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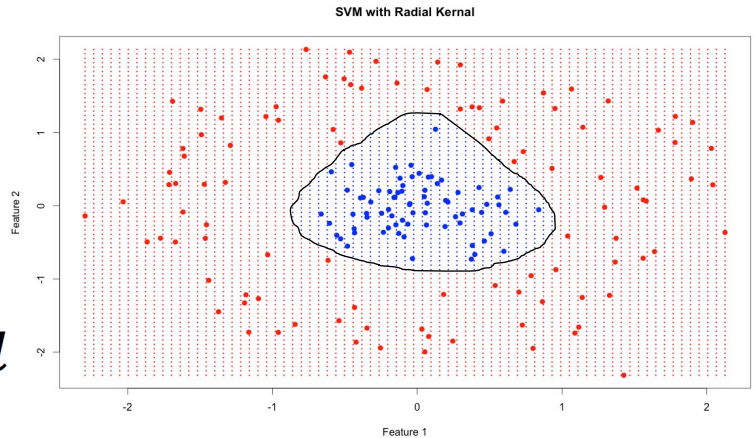

Data separable by a decision boundary with possibly unbounded degrees of freedom.

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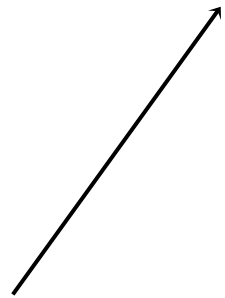


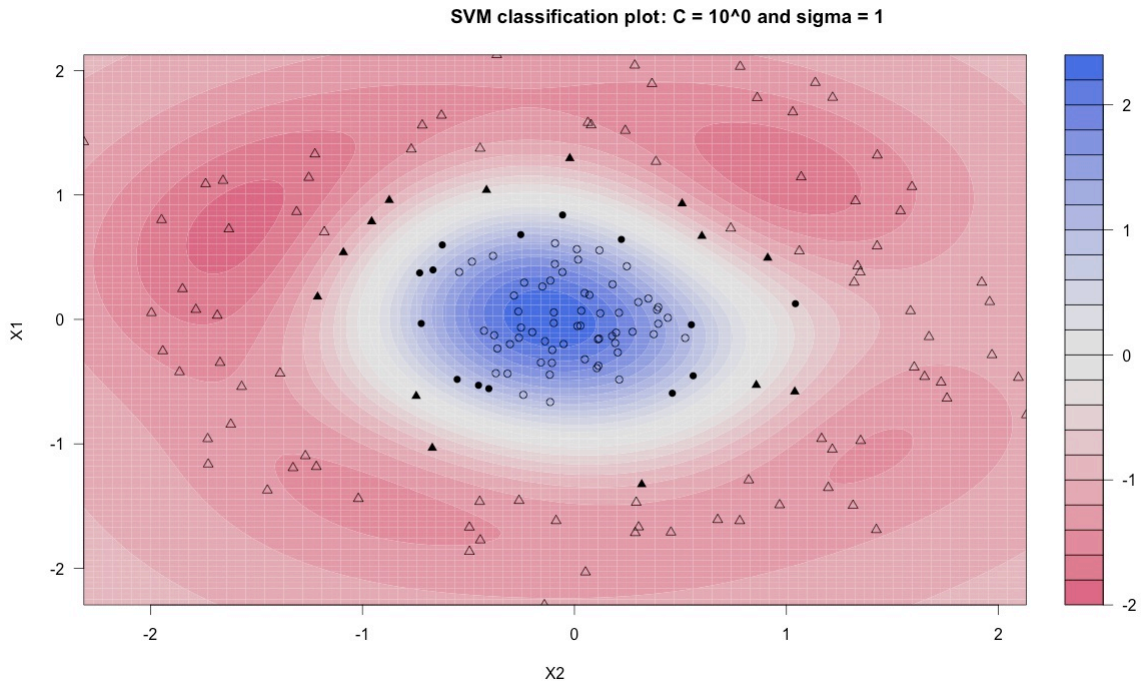
CODING NOTE (Python):
In SciKit Learn the SVM classifier:

```
sklearn.svm.SVC()
```

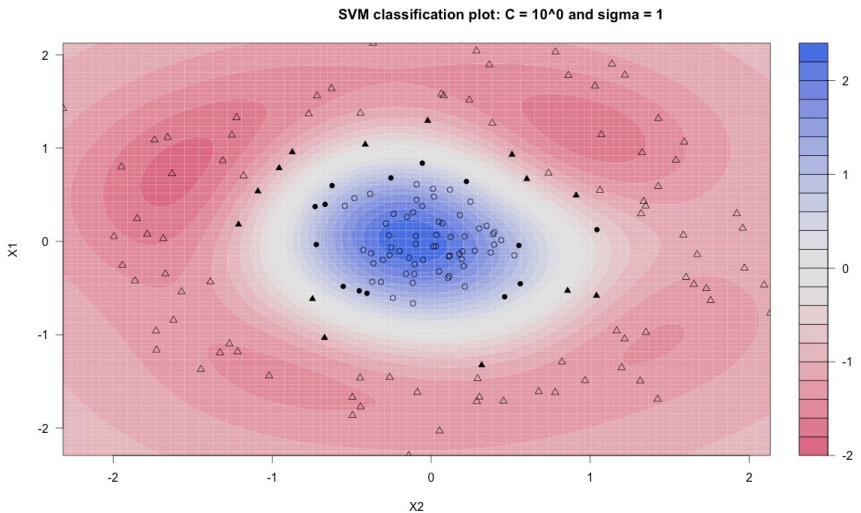
Tunes the "gamma" parameter defined by:

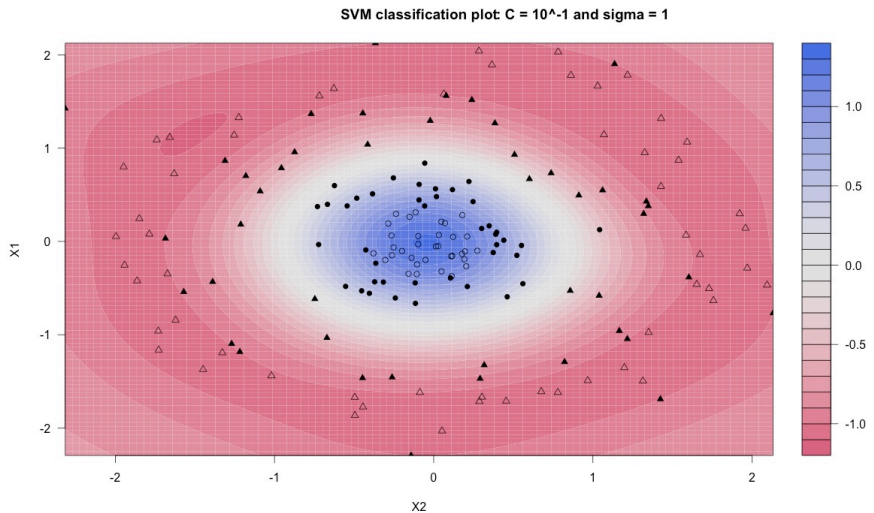
$$\gamma := 1/(2\sigma^2)$$

- Gaussian Kernel tuning example:



- Under-fitting C can lead to **Generalization Bias**





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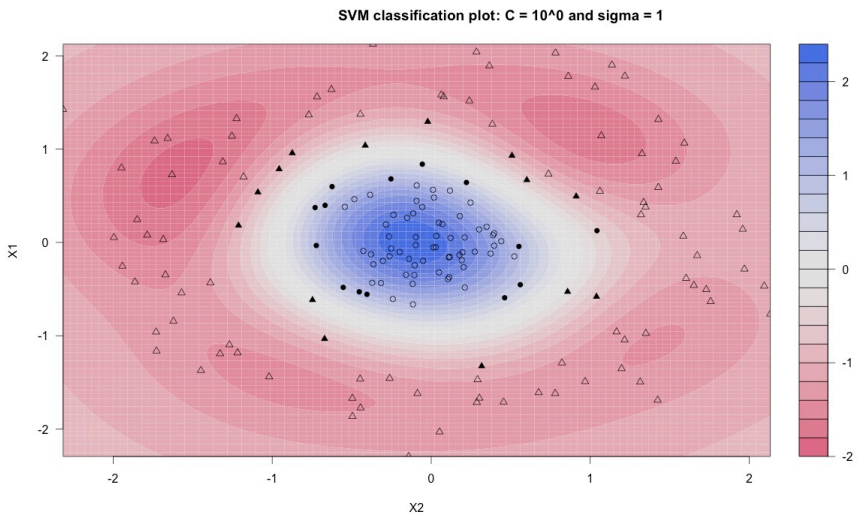
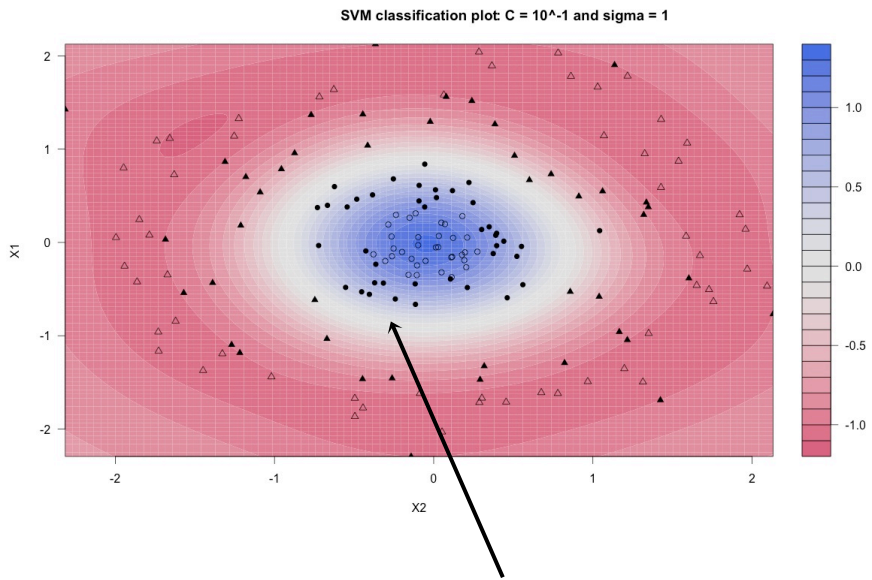
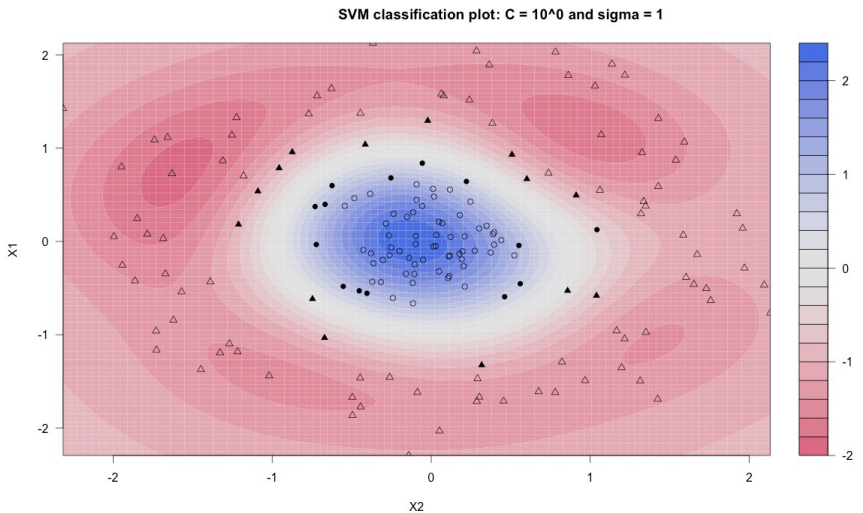


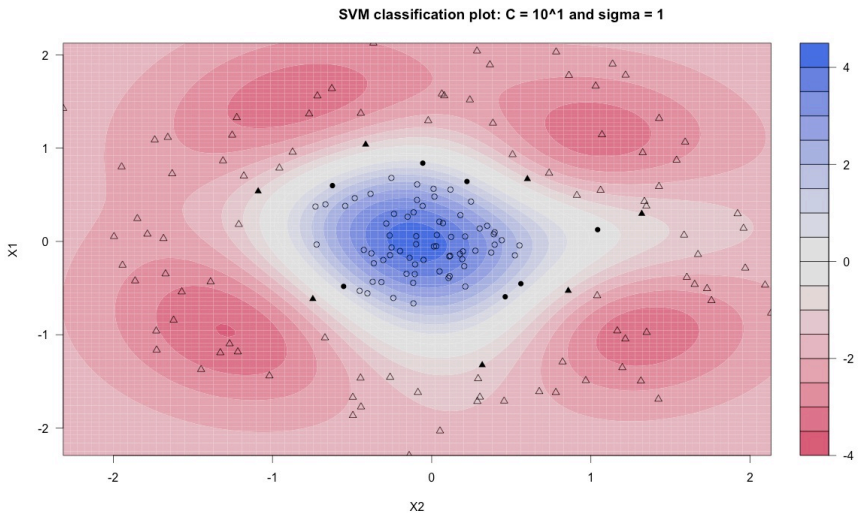


Lower C value means wider margins
so *more* support vectors

GAUSSIAN-KERNEL TUNING

- Over-fitting C can lead to **Generalization Variance**





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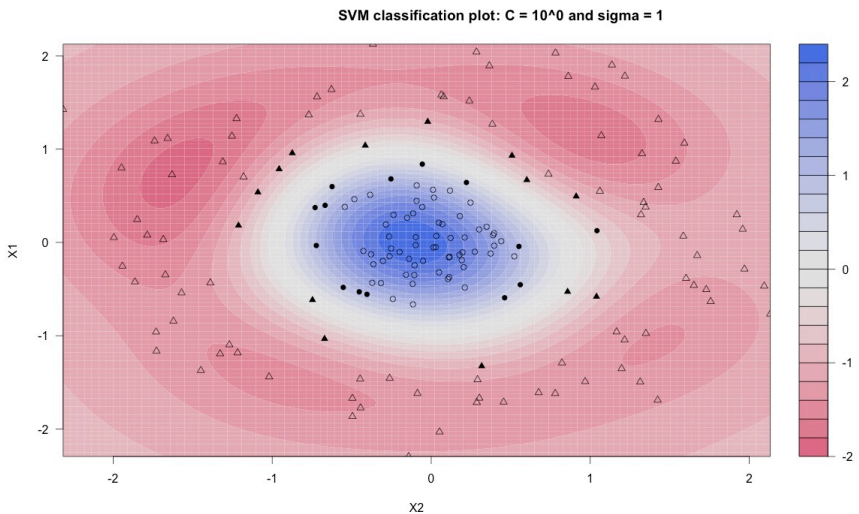
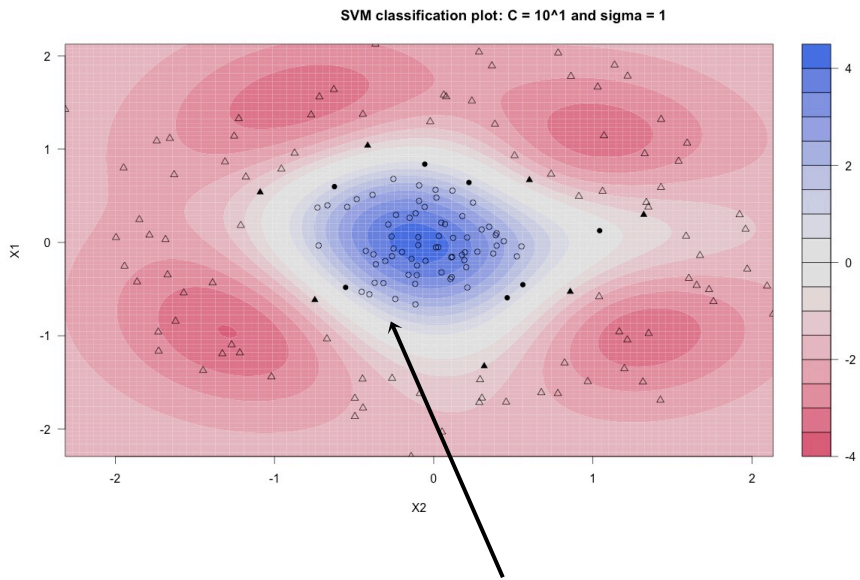
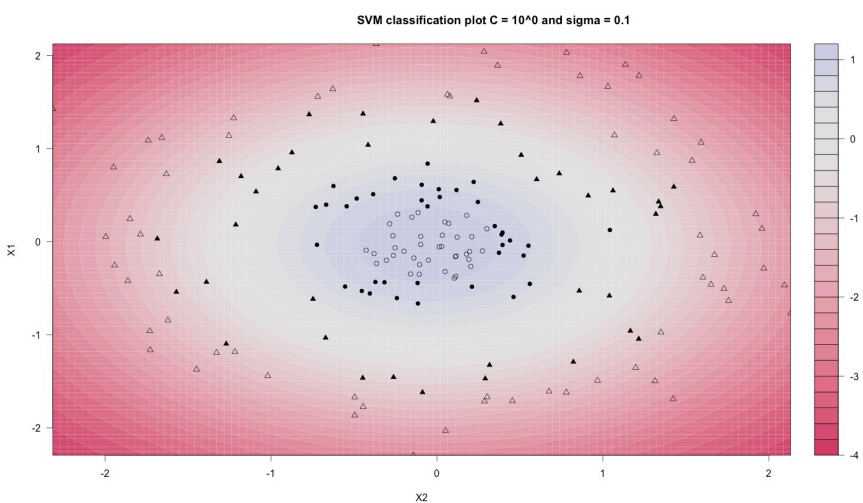
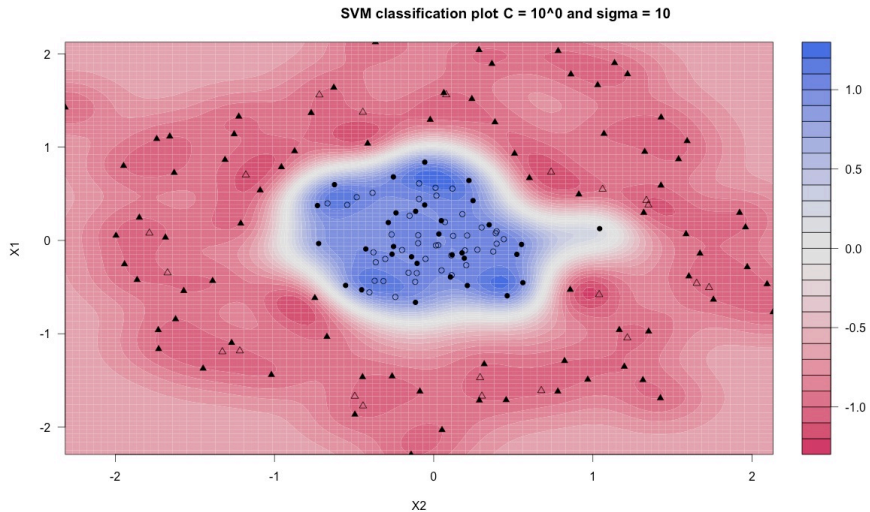




GAUSSIAN-KERNEL TUNING

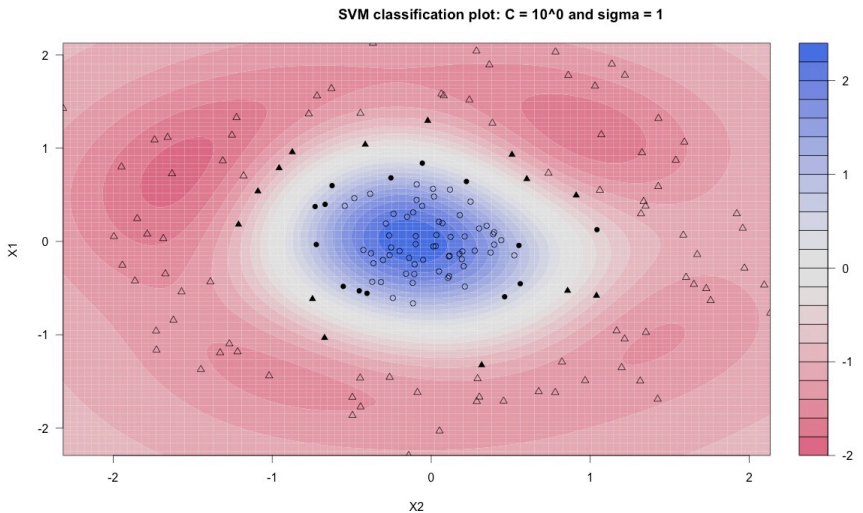
- Tuning sigma (σ) controls the "narrowness" of each point's effect

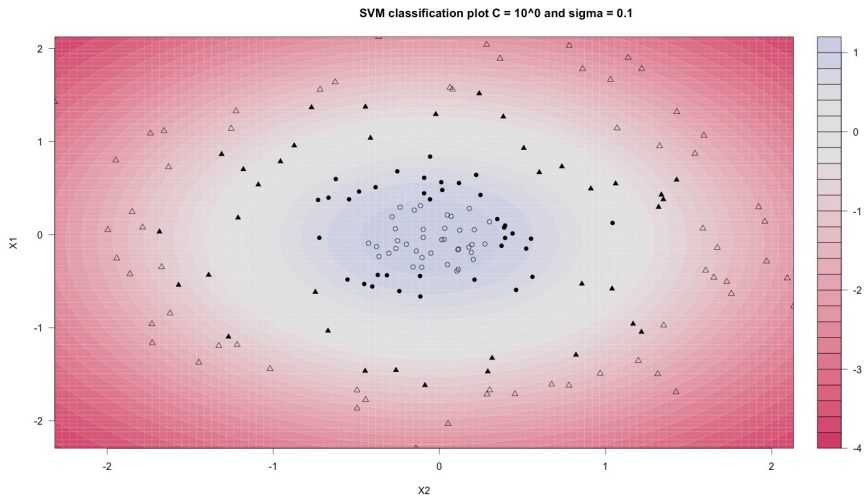




GAUSSIAN-KERNEL TUNING

- Small σ (large γ) can lead to **Generalization Bias** (under-fitting)





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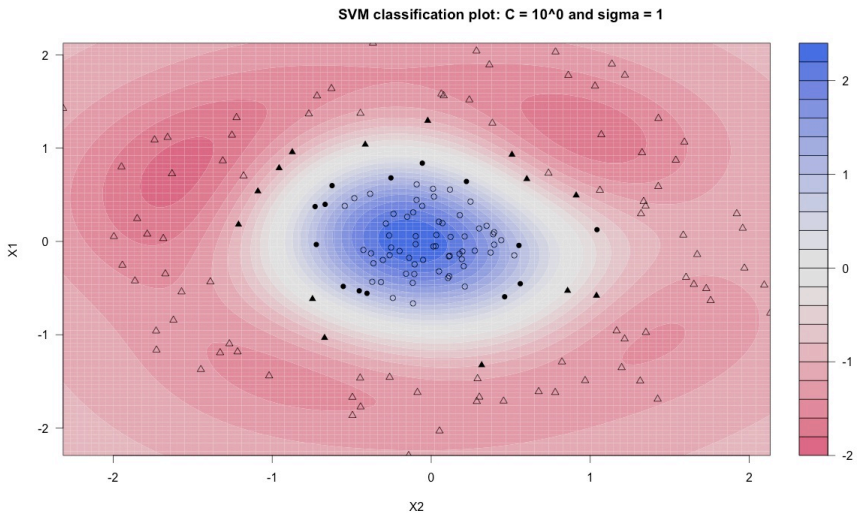
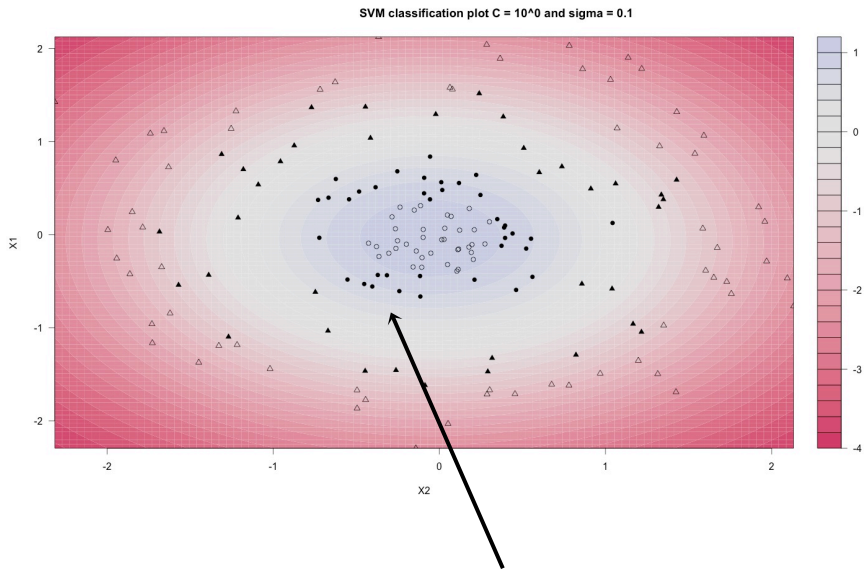
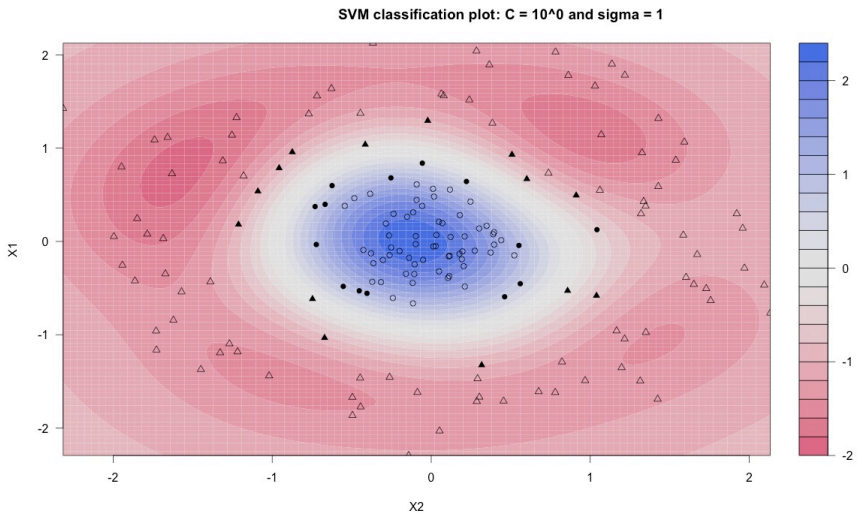
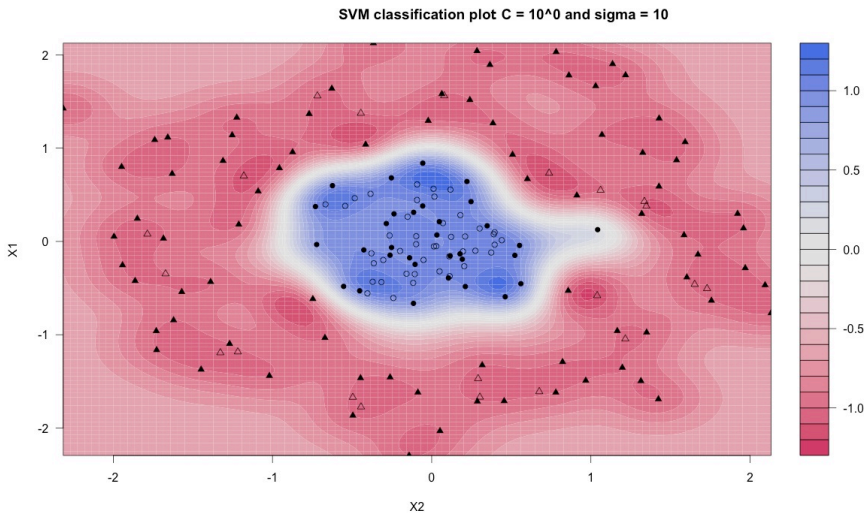




Lower σ value means the influence of each point is more dispersed.

- Large σ (small γ) can lead to **Generalization Variance** (over-fitting)





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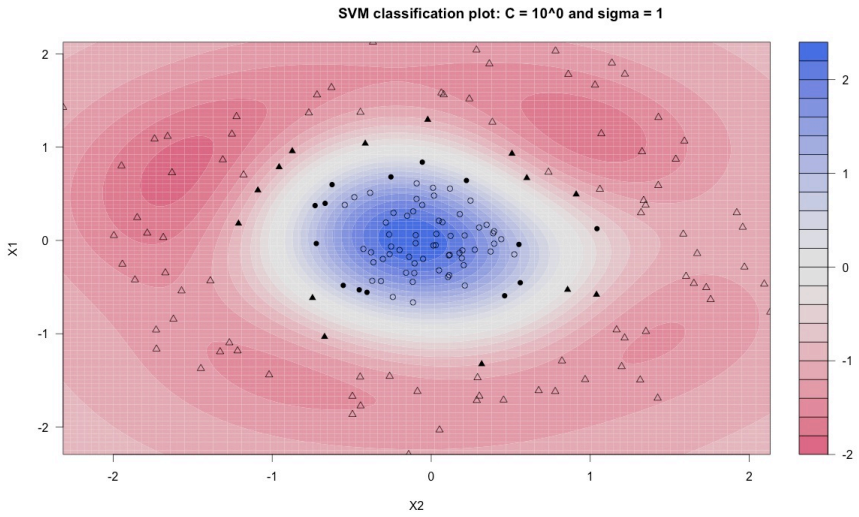

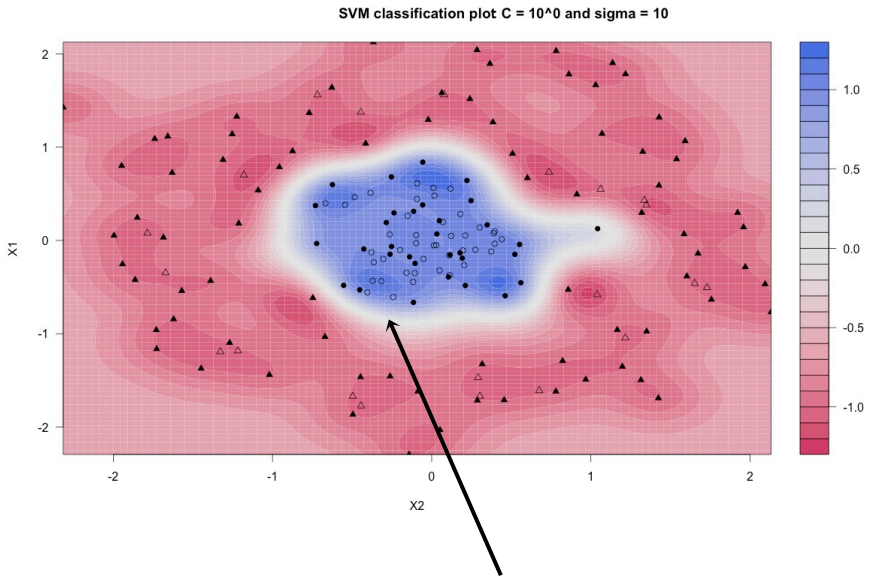

Higher σ value means higher "peaks" generated by individual points.

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3. The *kernel trick* allows SVMs to have non-linear decision boundaries without paying the high computation cost of an explosively high-D feature space.
4. Linear SVMs are tuned by two parameters C and σ:
    1. C is used to tune the "soft margins" for determining Support Vectors.
        1. C *cannot* be used be used for feature selection with non-linear kernels.
    2. σ (or γ) is used to tune how disperse the effect of individual data points are in influencing the decision boundaries.

Q&A