INTRODUCTION

To Statistical Learning

Introduction to Statistical Learning

Support Vector Machines - Class 11

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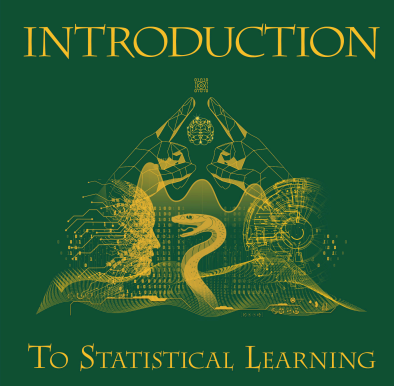
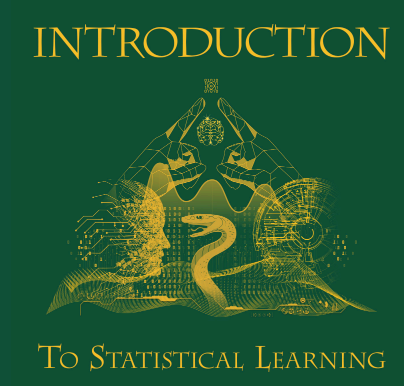
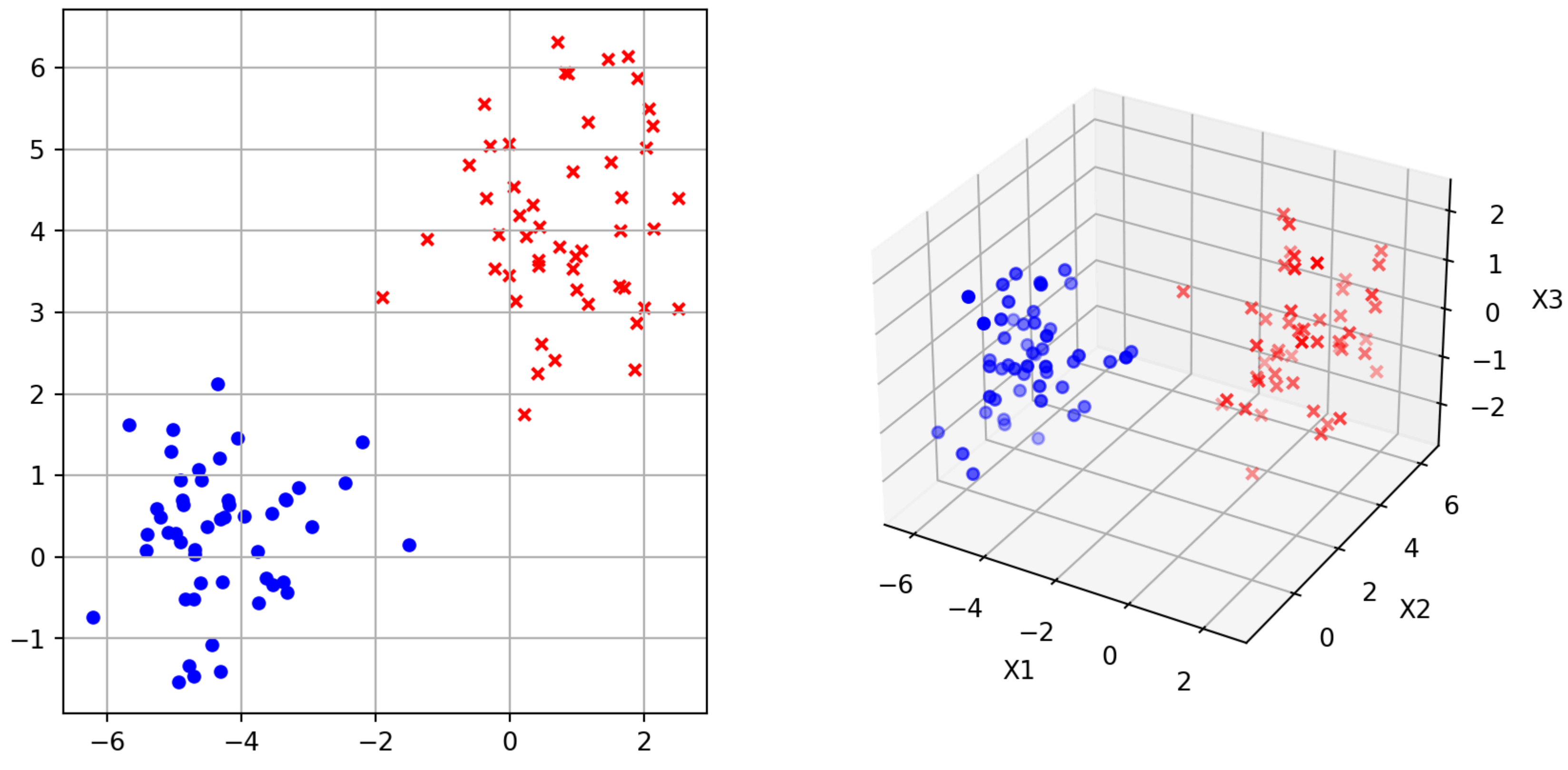


Maximum margin classifier



A big assumption

- Suppose $y \in \{-1, 1\}$
- Suppose the classes can be separated by a hyperplane, e.g. for data $T = \{(x_1, y_1), \ldots, (x_n, y_n)\}$:

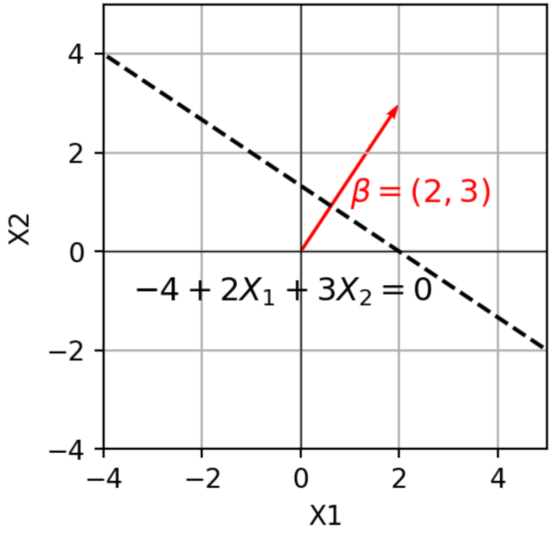


Separating hyperplanes (I)

- $\beta_0, \beta_1, \ldots, \beta_p$ define a p-dimensional plane for all points $x \in \mathbb{R}^p$ satisfying:

$$\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = \beta_0 + x^T \beta = 0$$

- We say $\beta^* = (\beta_1, \ldots, \beta_p)/\|\beta\|$ is normal to the hyperplane



> What would be a natural decision rule for separating $y \in \{-1, 1\}$?

Separating hyperplanes (II)

- In other words, a hyperplane is "separating" iff:

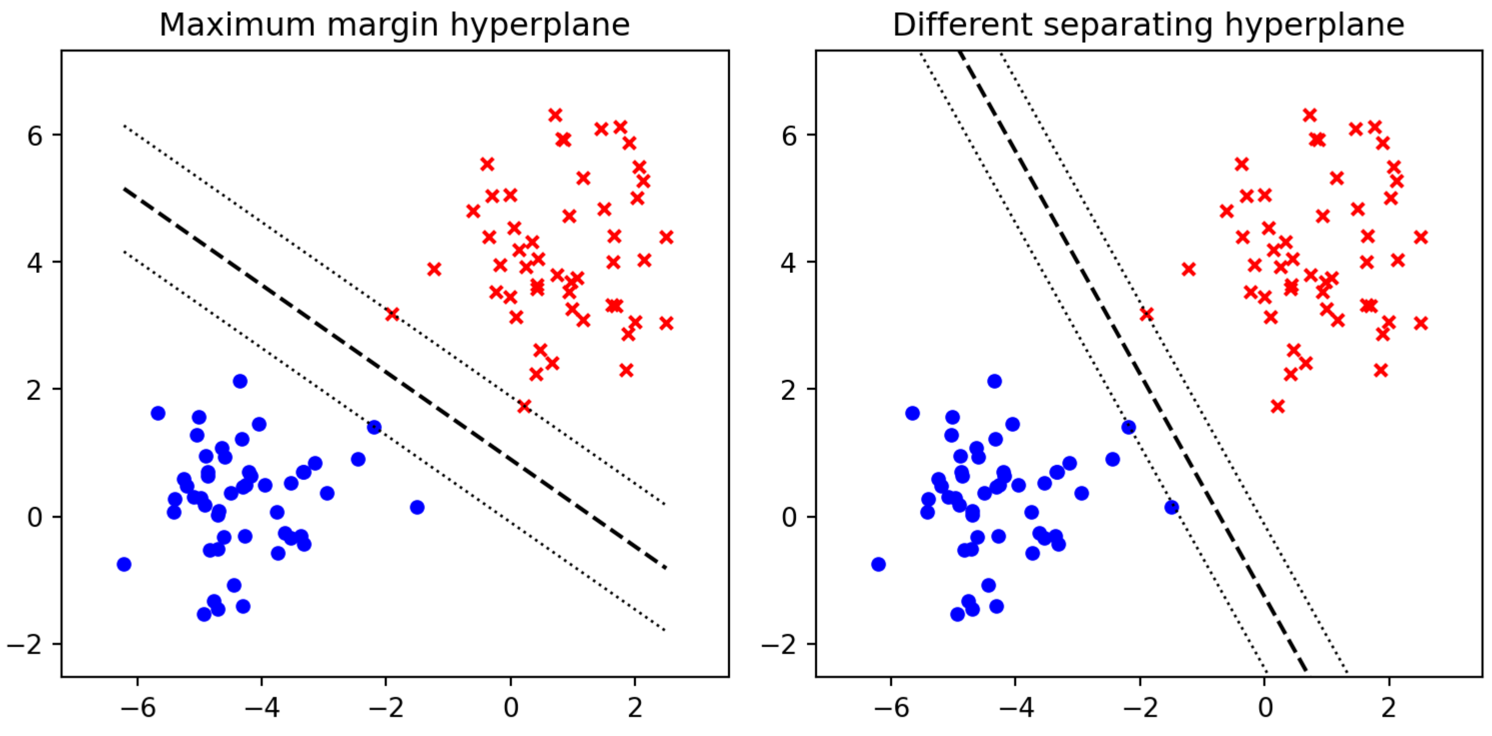
$$y_i \cdot (\beta_0 + x_i^T \beta) > 0 \quad \forall i$$

- And a natural decision rule for separating hyperplanes:

$$\hat{f}(x_0) = \text{sign}\left[\hat{\beta}_0 + x_0^T \hat{\beta}\right]$$

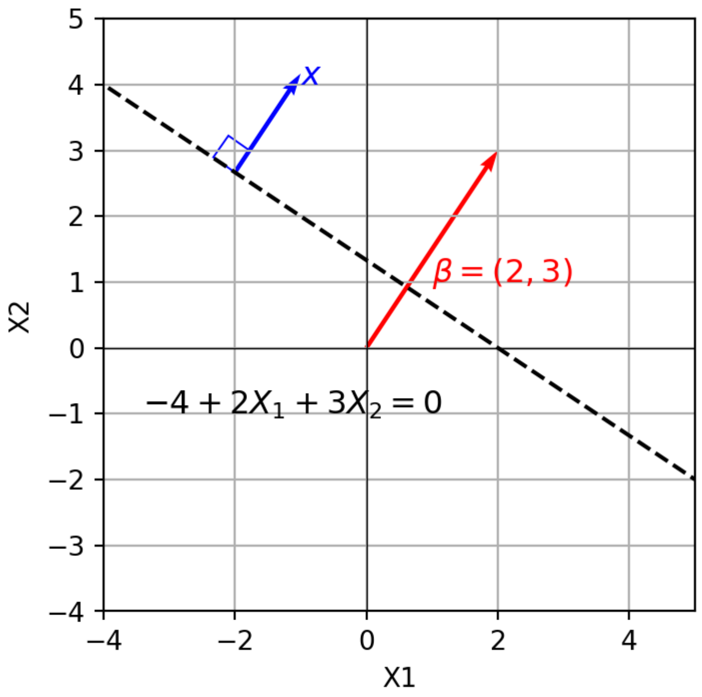
Maximum margin classifier

- Intuitively, we would like the hyperplane that is “fartherst” from points on both sides
- That is, the hyperplane that maximizes the margin:
  - the minimum distance of training points to the hyperplane



Maximum margin criterion

- So far we have:
  $\max_{\beta,\beta_0}$ "minimum distance" $\quad s.t.\ y_i(\beta_0 + x_i^T\beta) > 0 \quad \forall i$
- The distance between any point x to the hyperplane is: $\frac{|\beta_0+x^T\beta|}{\|\beta\|_2}$
  - because this distance is the length of a vector proportional to the normal β:



Maximum margin criterion

- So for any $M > 0$ a compact way of writing the criterion is:

$$\max_{\beta,\beta_0} M \quad s.t. \ \|\beta\| = 1 \text{ and } \quad y_i(\beta_0 + x_i^T\beta) \geq M \quad \forall i$$

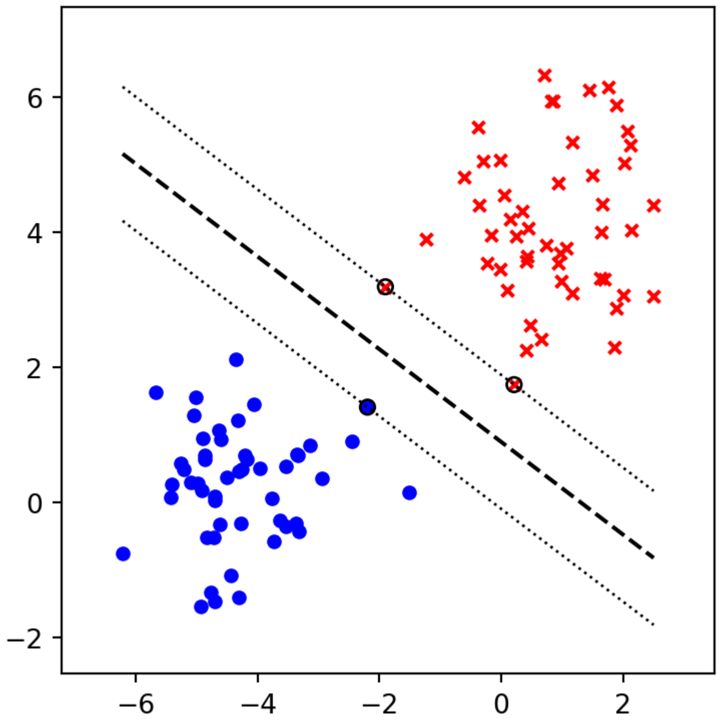
- All the points are at least a distance M from the decision boundary defined by β, β_0, and we seek β, β_0 that get the largest such M
- Equivalently if we insist on setting $\|\beta\| = 1/M$ we can write:

$$\min_{\beta,\beta_0} \|\beta\| \quad s.t. \ y_i(\beta_0 + x_i^T\beta) \geq 1 \quad \forall i$$

  - because $M = 1/\|\beta\|$ and maximizing M is minimizing $\|\beta\|$
- This is a convex optimization problem (quadratic criterion if we write $\|\beta\|^2$, linear inequality constraints), many efficient solvers exist

Support vectors

Back to the maximum margin classifier:



- The final classifier depends only on support vectors but was reached given all the training data
- Advantages/disadvantages to a classifier that only depends on few observations
- What would logistic regression do?
- What if there is no separable hyperplane?
- And as usual: this is very specific to binary classification, can we generalize?

Support vector classifier

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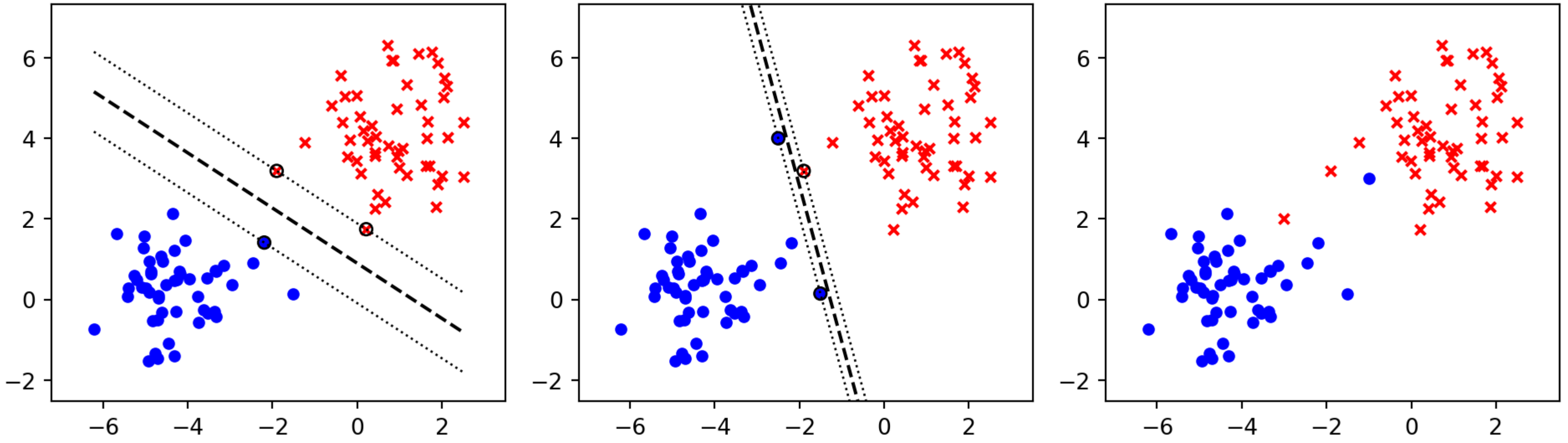
Not just the non-separable case



Support vectors classifier

- Let us relax our constraints:
  - Allow observations to be inside the margin
  - Or even on the wrong side of the hyperplane!
  - With a "budget" C for these violations (or penalty)

- We do this with the help of "slack variables": $\epsilon = (\epsilon_1, \ldots, \epsilon_n)$
- The new optimization problem:

$$\max_{\beta,\beta_0,\epsilon} M \quad s.t.\ \|\beta\| = 1, \quad y_i(\beta_0 + x_i^T \beta) \geq M(1 - \epsilon_i), \quad \epsilon_i \geq 0, \quad \sum_{i=1}^{n} \epsilon_i \leq C$$

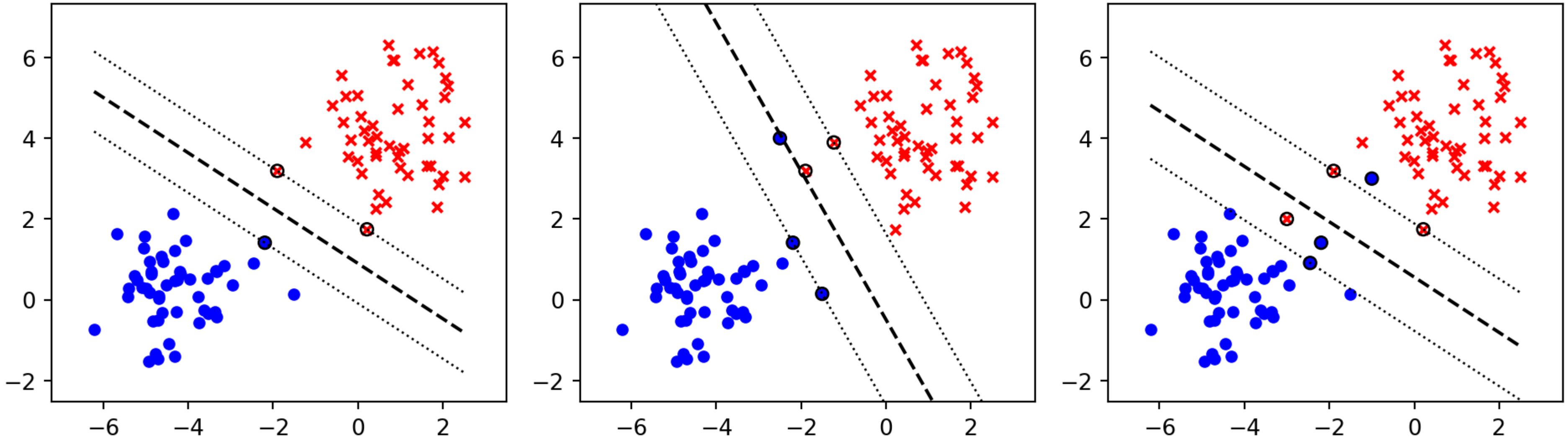
- The final prediction is still:

$$\hat{f}(x_0) = \text{sign}\left[\hat{\beta}_0 + x_0^T \hat{\beta}\right]$$

SVC: slack variables

$$\max_{\beta,\beta_0,\epsilon} M \quad s.t. \ \|\beta\| = 1, \quad y_i(\beta_0 + x_i^T\beta) \geq M(1-\epsilon_i), \quad \epsilon_i \geq 0, \quad \sum_{i=1}^n \epsilon_i \leq C$$

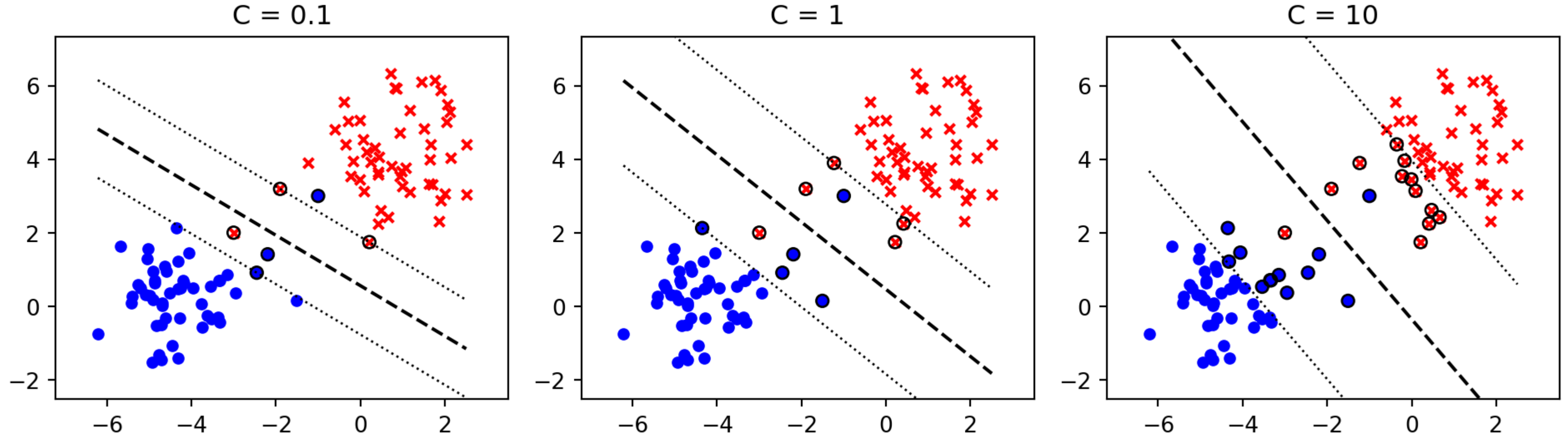
- ϵ_i is the amount by which observation x_i “violates” the margin:
  - If $\epsilon_i = 0$ then x_i is on the correct side of the margin
  - If $\epsilon_i > 0$ then x_i is on the wrong side of the margin
  - If $\epsilon_i > 1$ then x_i is on the wrong side of the hyperplane!



SVC: the C parameter

$$\max_{\beta,\beta_0,\epsilon} M \quad s.t.\ \|\beta\| = 1, \quad y_i(\beta_0 + x_i^T\beta) \geq M(1-\epsilon_i), \quad \epsilon_i \geq 0, \quad \sum_{i=1}^n \epsilon_i \leq C$$

- C is the amount by which the margin may be "violated":
  - If $C = 0$ then $\epsilon = \mathbf{0}$, back to maximum margin classifier
  - If $C > 0$ no more than C observations can be on the wrong side of the hyperplane



How to choose C? What is the relation between C and the bias-variance tradeoff?

SVC: equivalent forms

- As with maximum margin classifier, if we insist on setting $||\beta|| = 1/M$ we can write:

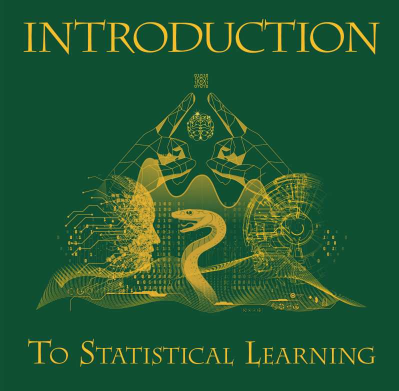
$$\min_{\beta,\beta_0,\epsilon} ||\beta|| \quad s.t. \; y_i(\beta_0 + x_i^T\beta) \geq 1 - \epsilon_i, \quad \epsilon_i \geq 0, \quad \sum_{i=1}^{n} \epsilon_i \leq C \quad \forall i$$

- In fact, it is more common to see the equivalent form:

$$\min_{\beta,\beta_0,\epsilon} \frac{1}{2}||\beta||^2 + C\sum_{i=1}^{n} \epsilon_i \quad s.t. \; y_i(\beta_0 + x_i^T\beta) \geq 1 - \epsilon_i, \quad \epsilon_i \geq 0 \quad \forall i$$

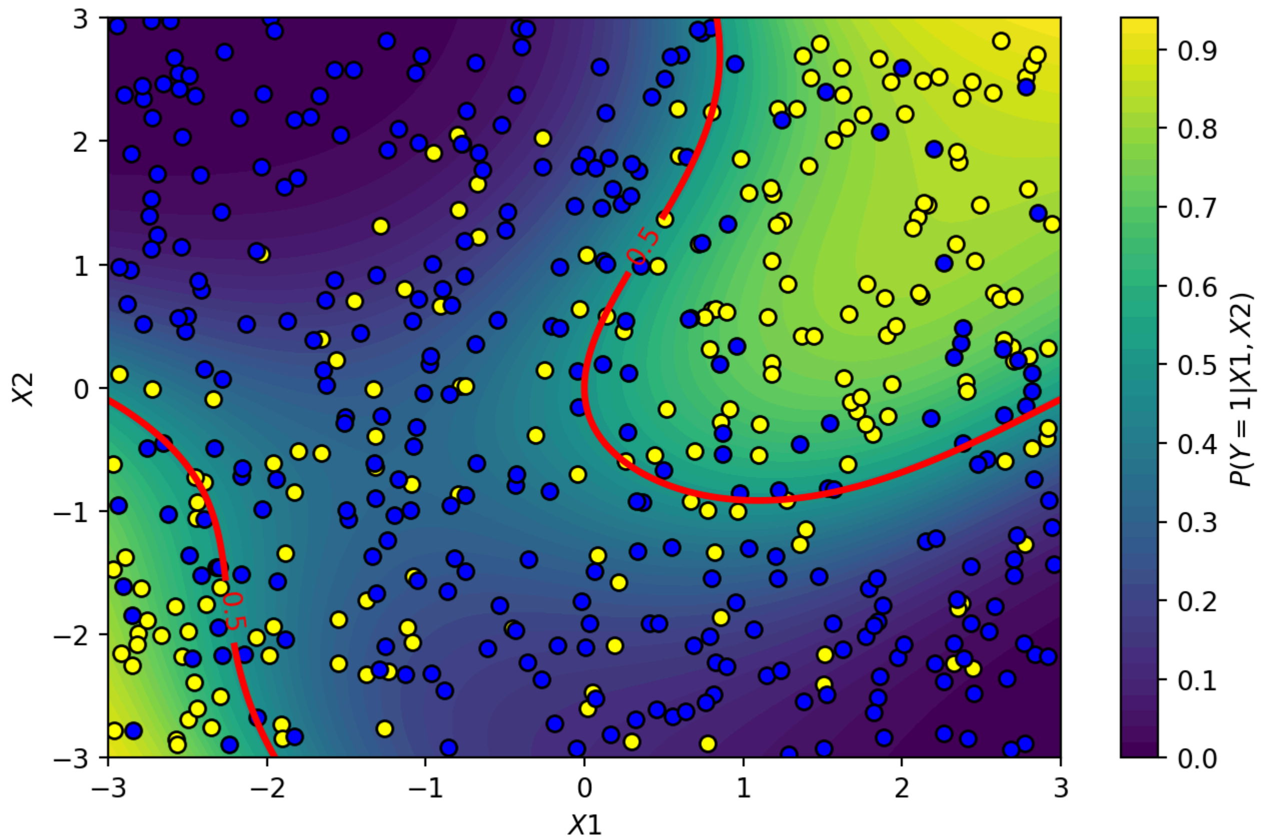
- In which case, notice the C hyperparameter is now a *penalty* (this is also more similar to how sklearn sees it)

Support vector machines (SVM)



The non-linear case

Recall the Bayes decision boundary example from our Bias-Variance discussion:



Unfortunately, “real data” looks more like this.

Adding polynomial terms?

- Similar to polynomial regression we could add quadratic terms:

$$\max_{\beta^1,\beta^2,\beta_0,\epsilon} M \quad s.t. \|\beta^1\|^2 + \|\beta^2\|^2 = 1, \quad y_i(\beta_0 + x_i^T \beta^1 + \left(x_i^2\right)^T \beta^2) \geq M(1-\epsilon_i)$$

$$\epsilon_i \geq 0, \quad \sum_{i=1}^{n} \epsilon_i \leq C$$

- What about cubic terms? What about interactions?
- Like in regression we could *expand* x_i to any feature mapping $h(x_i) : \mathbb{R}^p \to \mathbb{R}^q$ and continue as is
- But this becomes really high-dimensional, really fast.

The kernel trick (I)

- An amazing insight, after a lot of algebra, our solution can be written as:

$$f(x_0) = \text{sign}\left[\beta_0 + x_0^T\beta\right] = \text{sign}\left[\beta_0 + \sum_{i=1}^{n} \alpha_i \langle x_i, x_0\rangle\right]$$

- where:
  - $\langle x_i, x_0\rangle$ is the inner product $x_i^T x_0 = \sum_{j=1}^{p} x_{ij}x_{0j}$
  - $\alpha_i, \ldots, \alpha_n$ are n parameters for n observations,
    - but $\alpha_i > 0$ only for support vectors, otherwise $\alpha_i = 0$
- So for any $h(x_i)$, the solution can be written in terms of inner products only:

$$f(x_0) = \text{sign}\left[\beta_0 + h(x_0)^T\beta\right] = \text{sign}\left[\beta_0 + \sum_{i=1}^{n} \alpha_i \langle h(x_i), h(x_0)\rangle\right]$$

The kernel trick (II)

- Now suppose $x_i = (x_{i1}, x_{i2})$ and $h : \mathbb{R}^2 \to \mathbb{R}^6$ is:

$$h(x_i) = (1, \sqrt{2}x_{i1}, \sqrt{2}x_{i2}, x_{i1}^2, x_{i2}^2, \sqrt{2}x_{i1}x_{i2})$$

- Amazingly, the inner product with any point x_0 is quite compact:

$$\langle h(x_i), h(x_0) \rangle = \begin{pmatrix} 1 & \sqrt{2}x_{i1} & \sqrt{2}x_{i2} & x_{i1}^2 & x_{i2}^2 & \sqrt{2}x_{i1}x_{i2} \end{pmatrix} \begin{pmatrix} 1 \\ \sqrt{2}x_{01} \\ \sqrt{2}x_{02} \\ x_{01}^2 \\ x_{02}^2 \\ \sqrt{2}x_{01}x_{02} \end{pmatrix} =$$

$$= (1 + x_i^T x_0)^2$$

> Why is that helpful?

The kernel trick (III)

- Let this be a kernel function:

$$\langle h(x_i), h(x_0)\rangle = (1 + x_i^T x_0)^2 = K(x_i, x_0)$$

- Back to our solution:

$$f(x_0) = \text{sign}\left[\beta_0 + \sum_{i=1}^{n} \alpha_i \langle h(x_i), h(x_0)\rangle\right] = \text{sign}\left[\beta_0 + \sum_{i=1}^{n} \alpha_i K(x_i, x_0)\right]$$

- The **kernel trick**:
  - Forget about specifying $h(x_i) : \mathbb{R}^p \to \mathbb{R}^q$!
  - Focus on specifying kernel functions $K(x_i, x_j) : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$
  - That is, flexible similarity functions between feature vectors

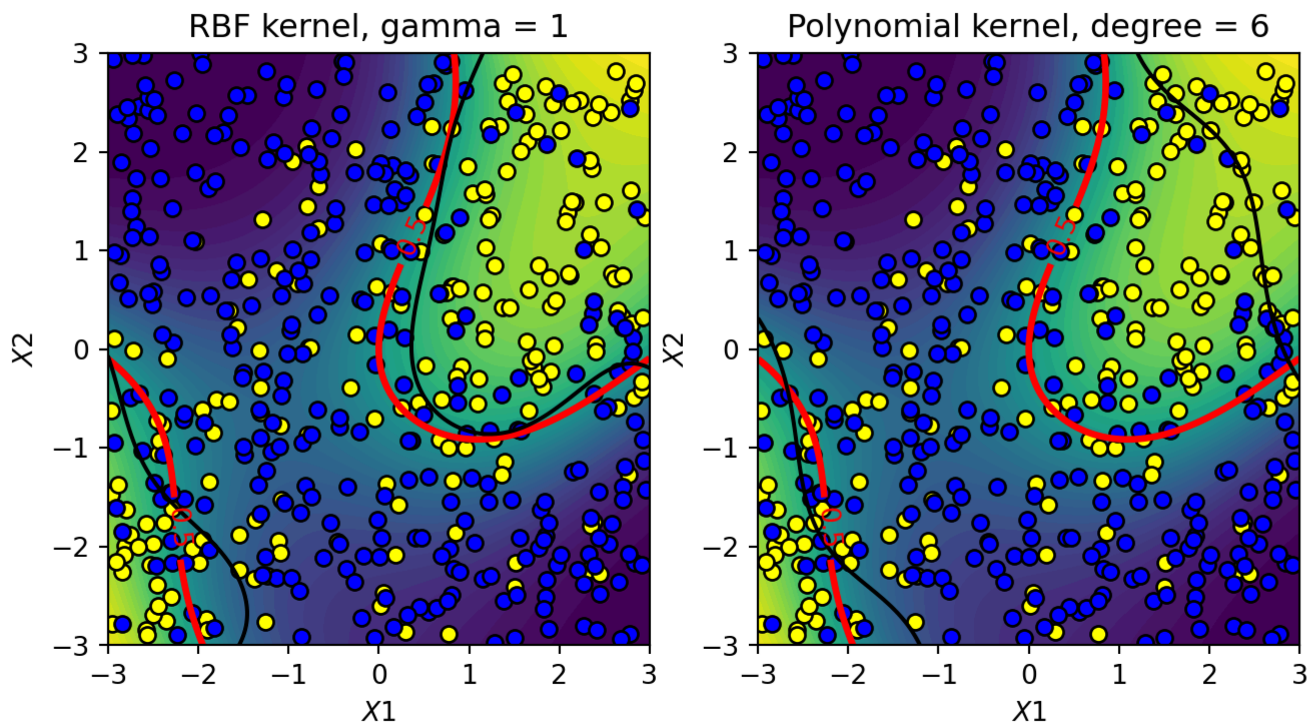
Common kernels

kernel	$K(x_i, x_j)$	comment
Linear	$\langle x_i, x_j \rangle$	SVC!
Polynomial	$(1 + \langle x_i, x_j \rangle)^d$	For $p = 2, d = 2$ we got $h(x)$
Gaussian/SE/RBF	$\exp\left(-\gamma \|\|x_i - x_j\|\|^2\right)$	infinite feature mapping space!
Sigmoid	$\tanh(\kappa_1 \langle x_i, x_j \rangle + \kappa_2)$	

- Each of these *implicitly* uses some mapping $h(x)$, but always: $K(x_i, x_j) = \langle h(x_i), h(x_j) \rangle$
- On entire training set need to compute: $K_{n \times n}$ (kernel matrix) where $K_{ij} = K(x_i, x_j) = \langle h(x_i), h(x_j) \rangle$

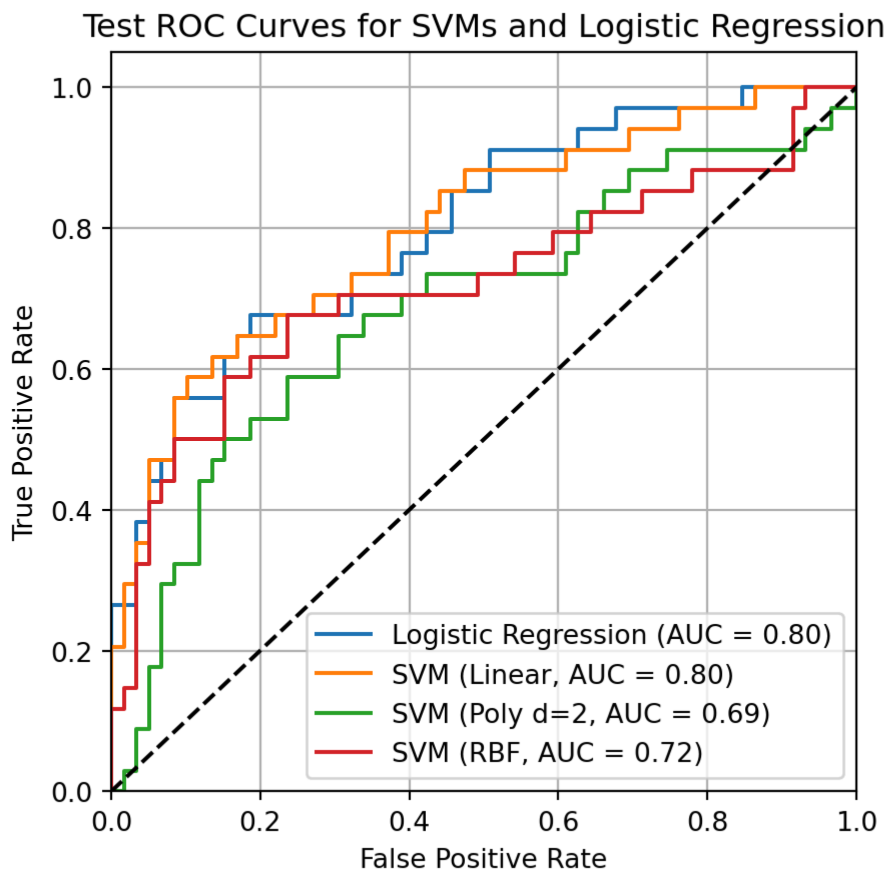
> ⓘ Can any $K(x_i, x_j) : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ function use as a kernel?

Support vector machines (SVM)



Notice this might add a few hyperparameters, including the kernel itself!

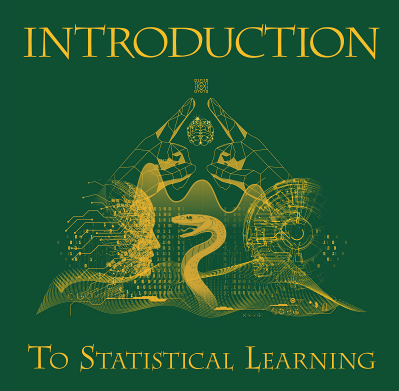
Example: SAHeart data



Notice to compute ROC SVM needs to output a probability or score.

This is out of scope, but you could think of the distance of an observation to the hyperplane as a type of confidence.

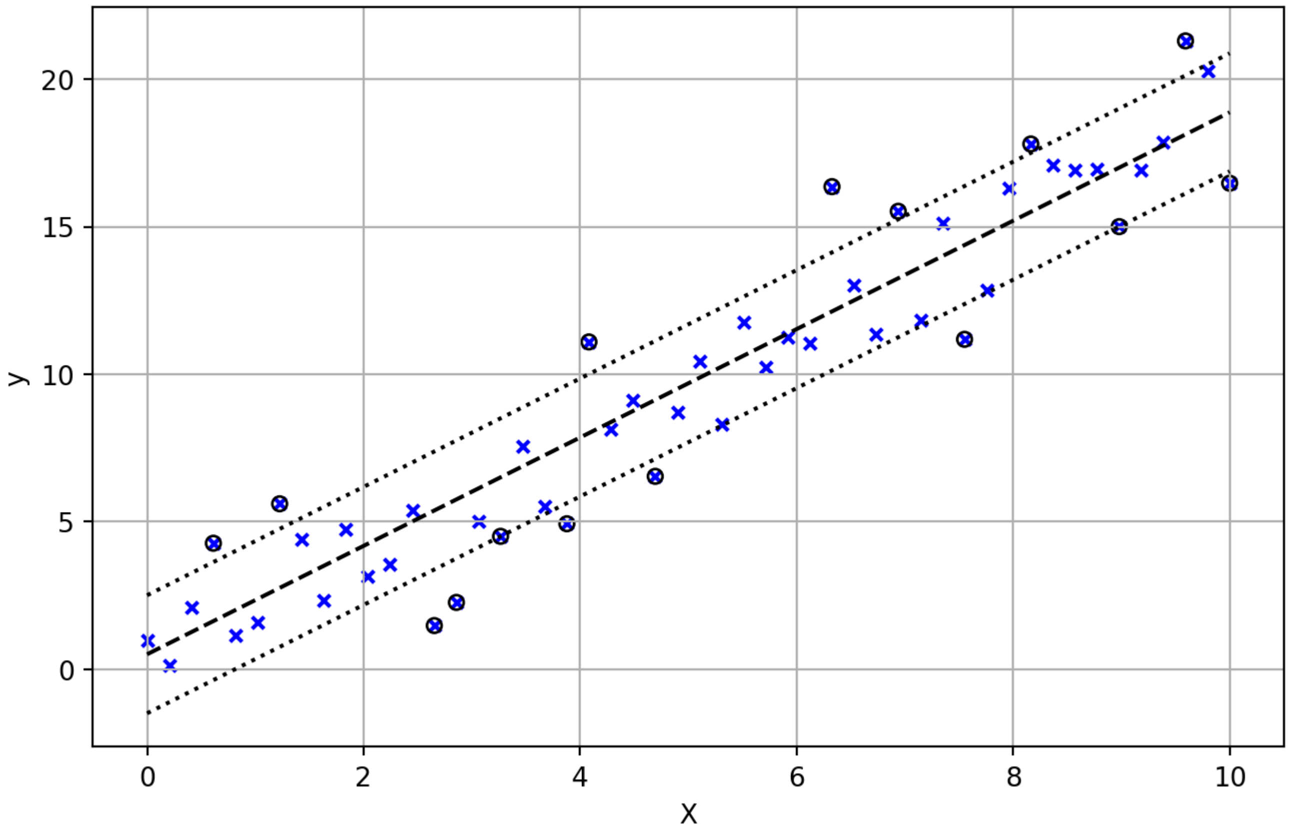
SVM extensions



SVM for K classes

- One-versus-one (OVO):
  - Run all $\binom{K}{2}$ pairwise models: class k vs. class k'
  - Assign x_0 to class k to which it was most frequently assigned to
- One-versus-rest (OVR):
  - Run all K models: class k (+1) vs. remaining $K - 1$ classes (-1)
  - Assign x_0 to class k in which it gets the highest distance (confidence) from hyperplane $\beta_{0k} + x_0^T \hat{\beta}_k$

Support vector regression (SVR)



What would be the support vectors for SVR?

SVR Criterion

- From maximum margin classifier:
  $\max_{\beta,\beta_0} M \quad s.t. \ \|\beta\| = 1 \text{ and } \quad y_i(\beta_0 + x_i^T\beta) \geq M \quad \forall i$
- To "maximum margin regressor" (not really a thing):
  $\max_{\beta,\beta_0} M \quad s.t. \ \|\beta\| = 1 \text{ and } \quad |y_i - (\beta_0 + x_i^T\beta)| \leq M \quad \forall i$
- From SVC:
  $\max_{\beta,\beta_0,\epsilon} M \quad s.t. \ \|\beta\| = 1, \quad y_i(\beta_0 + x_i^T\beta) \geq M(1-\epsilon_i), \quad \epsilon_i \geq 0, \quad \sum_{i=1}^n \epsilon_i \leq C$
- To SVR:
  $\max_{\beta,\beta_0,\epsilon} M \quad s.t. \ \|\beta\| = 1, \quad |y_i - (\beta_0 + x_i^T\beta)| \leq M + \epsilon_i, \quad \epsilon_i \geq 0, \ \sum_{i=1}^n \epsilon_i \leq C$
- Though this is more common:

$$\min_{\beta,\beta_0,\epsilon} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^n \epsilon_i \quad s.t. \ |y_i - (\beta_0 + x_i^T\beta)| \leq M + \epsilon_i, \ \epsilon_i \geq 0$$

- And of course SVR can be kernelized as well