Lecture 009

Support vector machines

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Admin

Today

- *Mini-survey* What are you missing?
- Results In-class competition
- Topic Support vector machines

Upcoming

Readings

- Today ISL Ch. 9
- Next 100ML Ch. 6

Project Project updates/questions?

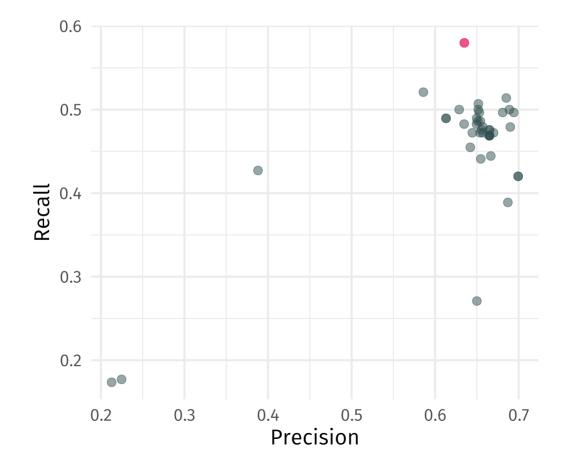
In-class competition Results

In-class competition

Submission +	Accuracy +	Precision ‡	Recall 	F1 \$
brad-bailey-simple-tree-model	0.791	0.665	0.469	0.550
coia_forest	0.789	0.657	0.472	0.549
coia_net	0.789	0.651	0.486	0.557
coia_tree	0.791	0.665	0.469	0.550
Craig_Submission	0.791	0.652	0.500	0.566
DNickles_cv_logistic_1_churn	0.802	0.689	0.500	0.579
DNickles_lasso_churn	0.793	0.699	0.420	0.525
DNickles_ridge_churn	0.793	0.699	0.420	0.525
Elliott_Eli_for	0.785	0.645	0.472	0.545
Elliott_Eli_net	0.789	0.650	0.490	0.558

In-class competition





Intro

Support vector machines (SVMs) are a *general class* of classifiers that essentially attempt to separate two classes of observations.

SVMs have been shown to perform well in a variety of settings, and are often considered one of the best "out of the box" classifiers. *ISL, p. 337*

The **support vector machine** generalizes a much simpler classifier—the **maximal margin classifier**.

The maximal margin classifier attempts to separate the **two classes** in our prediction space using **a single hyperplane**.

What's a hyperplane?

Consider a space with p dimensions.

A hyperplane is a p-1 dimensional subspace that is

- 1. **flat** (no curvature)
- 2. **affine** (may or may not pass through the origin)

Examples

- In p=2 dimensions, a hyperplane is a line.
- In p=3 dimensions, a hyperplane is a plane.
- In p = 1 dimensions, a hyperplane is a point.

Hyperplanes

We can define a hyperplane in p dimensions by constraining the linear combination of the p dimensions.[†]

For example, in two dimensions a hyperplane is defined by

$$eta_0+eta_1X_1+eta_2X_2=0$$

which is just the equation for a line.

Points $X = (X_1, X_2)$ that satisfy the equality *live* on the hyperplane.^{††}

† Plus some offset ("intercept")

†† Alternatively: The hyperplane is composed of such points.

Separating hyperplanes

More generally, in p dimensions, we defined a hyperplane by

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p = 0 \tag{A}$$

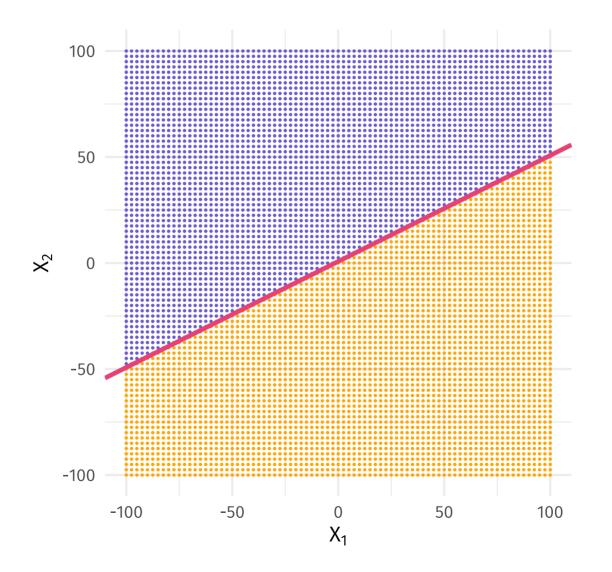
If $X = (X_1, X_2, \ldots, X_p)$ satisfies the equality, it is on the hyperplane.

Of course, not every point in the p dimensions will satisfy A.

- If $\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p > 0$, then X is **above** the hyperplane.
- If $\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p 0$, then X sits **below** the hyperplane.

The hyperplane separates the p-dimensional space into two "halves".

Ex: A **separating hyperplane** in two dimensions: $3 + 2X_1 - 4X_2 = 0$



Ex: A **separating hyperplane** in 3 dimensions: $3 + 2X_1 - 4X_2 + 2X_3 = 0$

• trace 0

Separating hyperplanes and classification

Idea: Separate two classes of outcomes in the p dimensions of our predictor space using a separating hyperplane.

To make a prediction for observation $(x^o,\,y^o)=(x_1^o,\,x_2^o,\,\ldots,\,x_p^o,\,y^o):$

We classify points that live "above" of the plane as one class, *i.e.*,

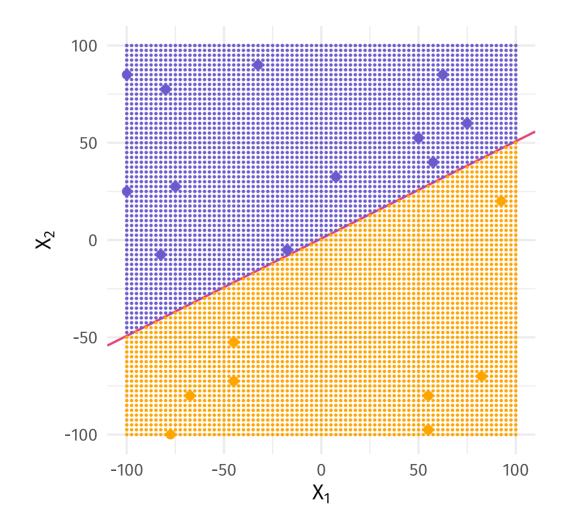
If
$$eta_0+eta_1x_1^o+\dots+eta_px_p^o>0$$
, then $\hat{y}^o=$ Class 1

We classify points "below" the plane as the other class, *i.e.*,

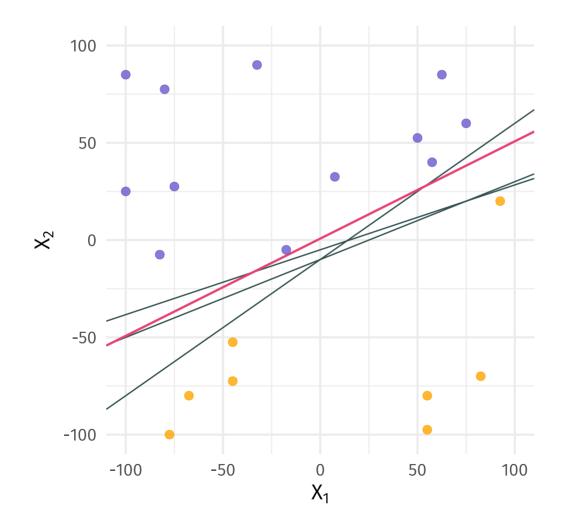
If $eta_0+eta_1x_1^o+\dots+eta_px_p^o<0$, then $\hat{y}^o=$ Class 2

Note This strategy assumes a separating hyperplane exists.

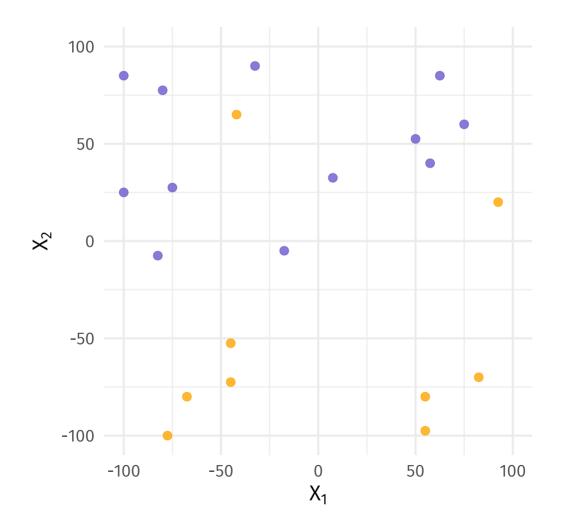
If a separating hyperplane exists, then it defines a binary classifier.



If a separating hyperplane exists, then many separating hyperplanes exist.



A a separating hyperplane may not exist.



Decisions

Summary A given hyperplane

$$eta_0+eta_1x_1+eta_2x_2+\cdots+eta_px_p=0$$

produces a decision boundary.

We can determine any point's (x^o) side of the boundary.

$$f(x^o)=eta_0+eta_1x_1^o+eta_2x_2^o+\dots+eta_px_p^o$$

We classify observationg x^o based upon whether $f(x^o)$ is positive/negative.

The magnitude of $f(x^o)$ tells us about our *confidence* in the classification.[†]

† Larger magnitudes are farther from the boundary.

Which separating hyperplane?

Q How do we choose between the possible hyperplanes?

A *One solution:* Choose the separating hyperplane that is "farthest" from the training data points—maximizing "separation."

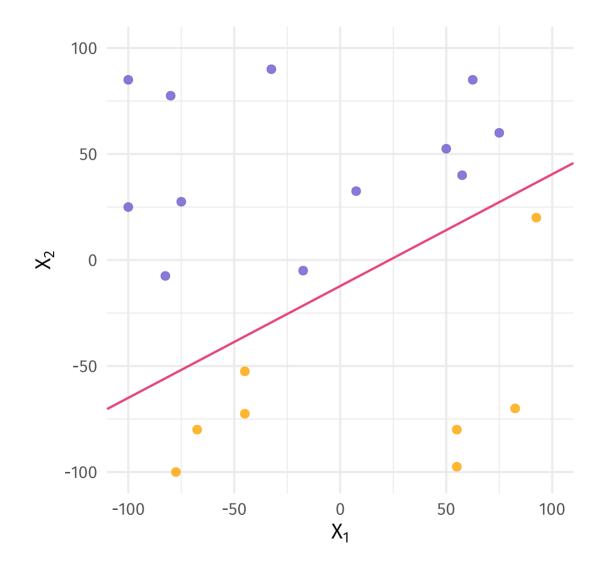
The maximal margin hyperplane[†] is the hyperplane that

- 1. **separates** the two classes of obsevations
- 2. **maximizes** the margin—the distance to the nearest observation^{††}

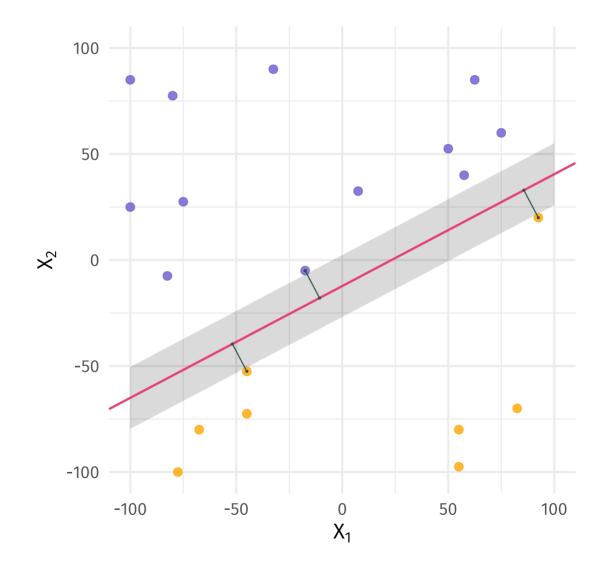
where *distance* is a point's perpendicular distance to the hyperplane.

+ AKA the optimal separating hyperplane++ Put differently: The smallest distance to a training observation.

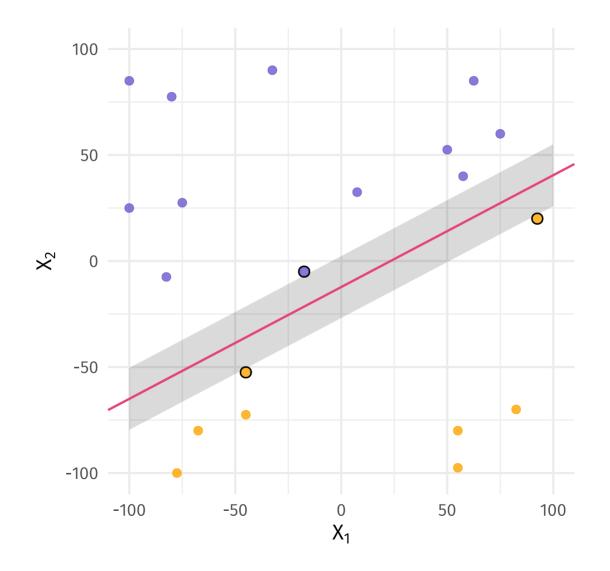
The maximal margin hyperplane...



...maximizes the **margin** between the hyperplane and training data...



...and is supported by three equidistant observations—the **support vectors**.



The maximal margin hyperplane

Formally, the **maximal margin hyperplane** solves the problem:

Maximize the margin M over the set of $\{\beta_0, \beta_1, \ldots, \beta_p, M\}$ such that

$$\sum_{j=1}^{p} \beta_j^2 = 1 \tag{1}$$

$$y_i\left(eta_0+eta_1x_{i1}+eta_2x_{i2}+\dots+eta_px_{ip}
ight)\geq M$$
 (2)

for all observations *i*.

(2) Ensures we separate (classify) observations correctly.

(1) allows us to interpret (2) as "distance from the hyperplane".

Fake constraints

Note that our first "constraint"

$$\sum_{j=1}^{p} \beta_{j}^{2} = 1$$
 (1)

does not actually constrain $-1 \leq \beta_j \leq 1$ (or the hyperplane).

If we can define a hyperplane by

$$eta_0+eta_1x_{i,1}+eta_2x_{i,2}+\dots+eta_px_{i,p}=0$$

then we can also rescale the same hyperplane with some constant k

$$k\left(eta_0+eta_1x_{i,1}+eta_2x_{i,2}+\dots+eta_px_{i,p}
ight)=0$$

The maximal margin classifier

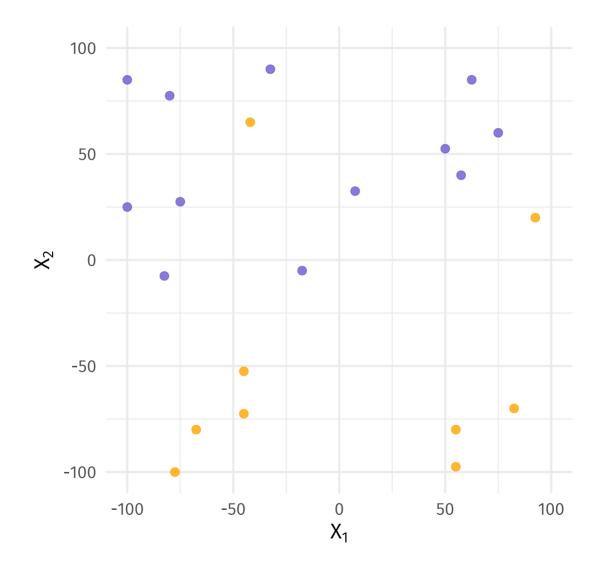
The maximal margin hyperplane produces the maximal margin classifier.

Notes

- 1. We are doing **binary classification**.
- 2. The decision boundary only uses the **support vectors**—very sensitive.
- 3. This classifier can struggle in **large dimensions** (big p).
- 4. A separating hyperplane does not always exist (**non-separable**).
- 5. Decision boundaries can be **nonlinear**.

Let's start by addressing non-separability...

Surely there's still a decent hyperplane-based classifier here, right?



Soft margins

When we cannot *perfectly* separate our classes, we can use **soft margins**, which are margins that "accept" some number of observations.

The idea: We will allow observations to be

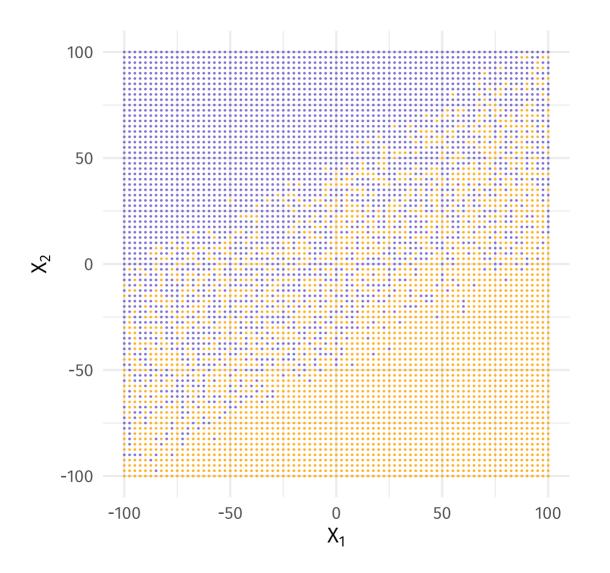
- 1. in the margin
- 2. on the wrong side of the hyperplane

but each will come with a price.

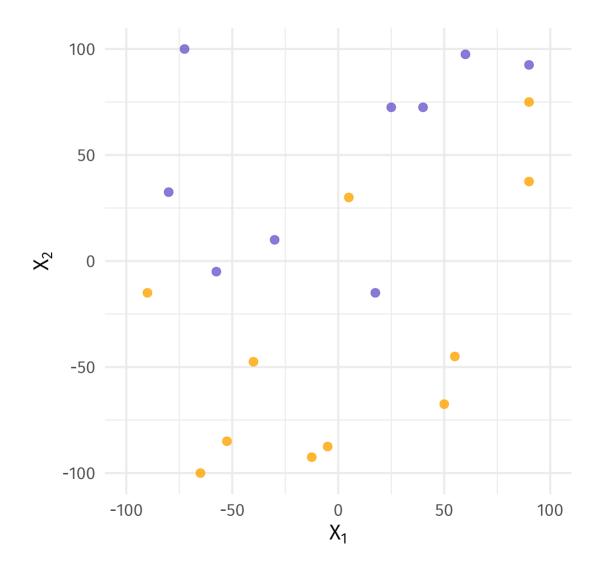
Using these *soft margins*, we create a hyperplane-based classifier called the **support vector classifier**.[†]

† Also called the *soft margin classifier*.

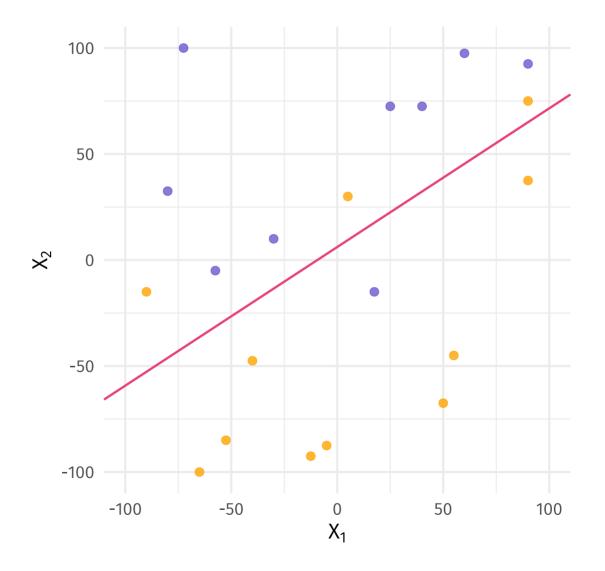
Our underlying population clearly does not have a separating hyperplane.



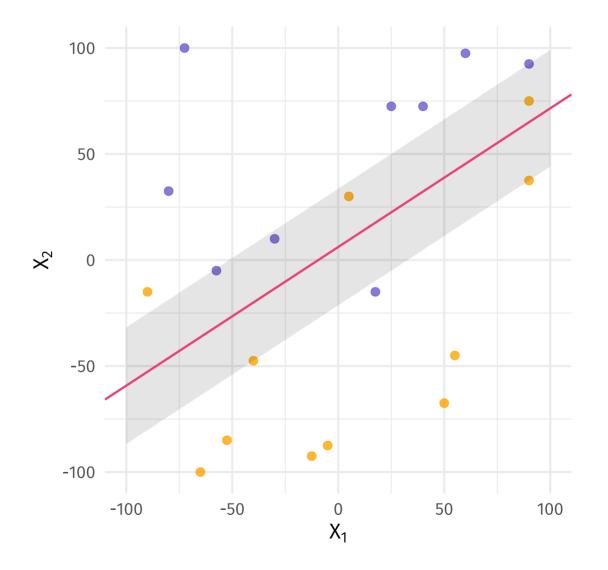
Our sample population also does not have a separating hyperplane.



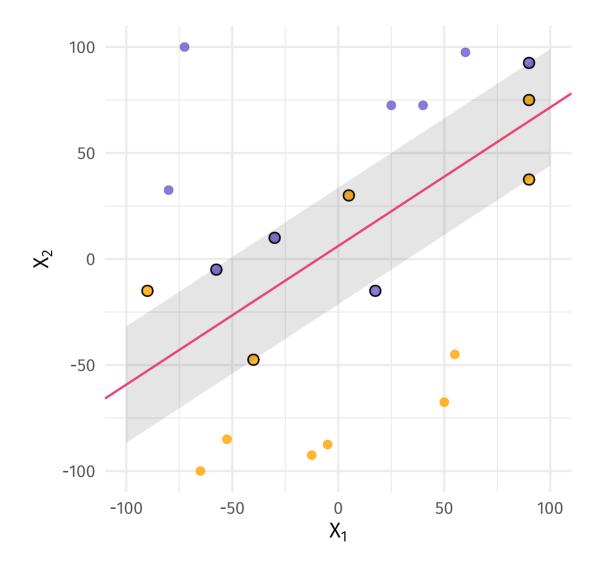
Our hyperplane



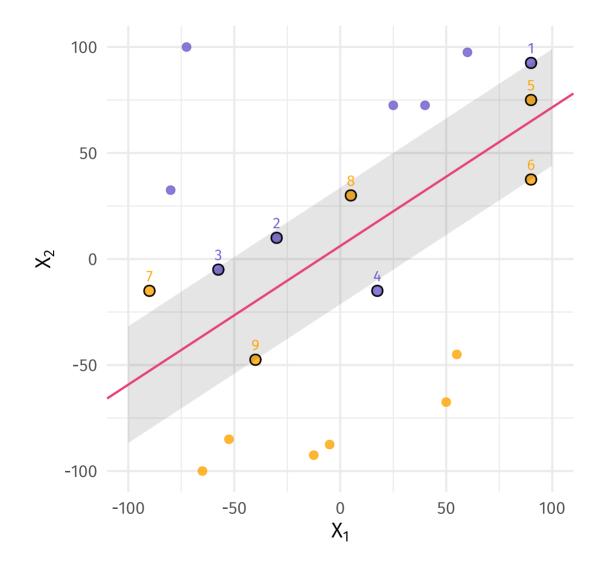
Our **hyperplane** with **soft margins**...



Our hyperplane with soft margins and support vectors.



Support vectors: on (i) the margin or (ii) on the wrong side of the margin.



Support vector classifier

The **support vector classifier** selects a hyperplane by solving the problem

Maximize the margin M over the set $\{\beta_0, \beta_1, \ldots, \beta_p, \epsilon_1, \ldots, \epsilon_n, M\}$ s.t.

$$\sum_{j=1}^{p} \beta_j^2 = 1 \tag{3}$$

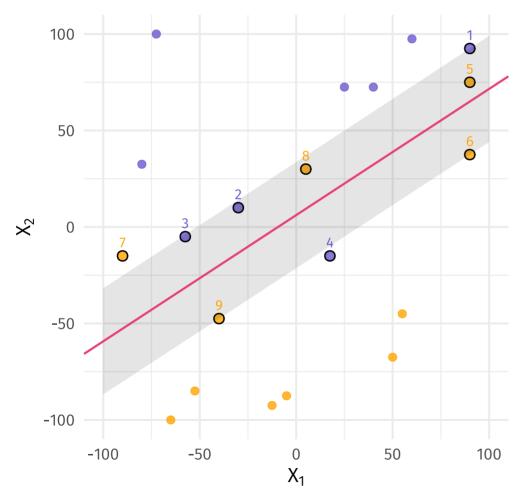
$$y_i \left(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}\right) \ge M \left(1 - \epsilon_i\right) \tag{4}$$

$$\epsilon_i \ge 0, \quad \sum_{i=1}^n \epsilon_i \le C$$
 (5)

The ϵ_i are slack variables that allow *i* to violate the margin or hyperplane. *C* gives is our budget for these violations. Let's consider constraints (4) and (5) work together...

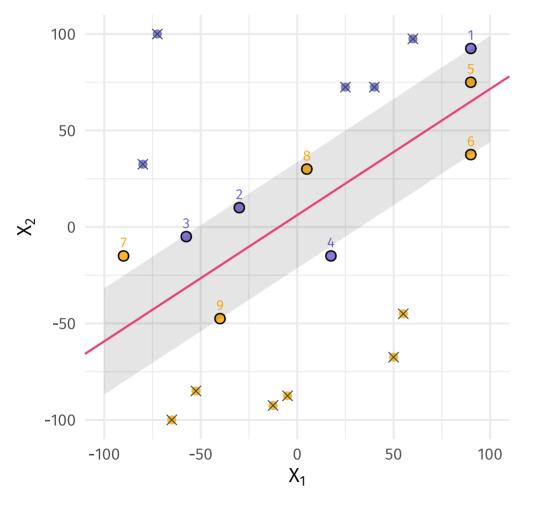
$$y_i \left(eta_0 + eta_1 x_{i1} + eta_2 x_{i2} + \dots + eta_p x_{ip}
ight) \ge M \left(1 - \epsilon_i
ight)$$
 (4) $\epsilon_i \ge 0, \quad \sum_{i=1}^n \epsilon_i \le C$ (5)

$y_i\left(eta_0+eta_1x_{i1}+eta_2x_{i2}+\dots+eta_px_{ip} ight)\geq M\left(1-\epsilon_i ight), \quad \epsilon_i\geq 0, \quad \sum_{i=1}^n\epsilon_i\leq C$



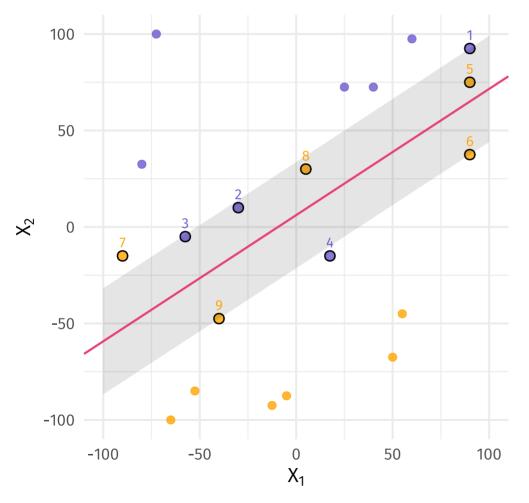
For $\epsilon_i=0$:

- $M\left(1-\epsilon_i\right)>0$
- Correct side of hyperplane
- Correct side of margin
 (or on margin)
- No cost (C)
- Distance $\geq M$
- Examples?



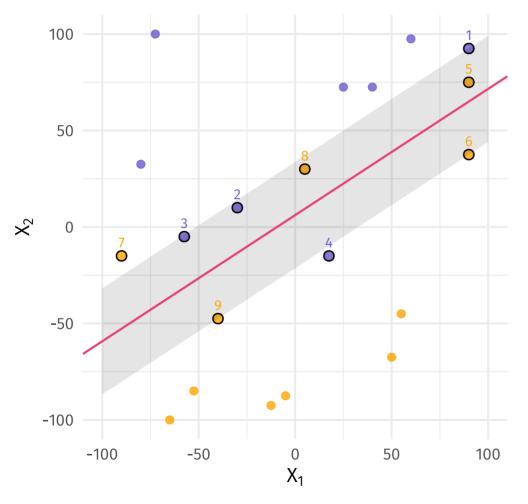
For $\epsilon_i = 0$:

- $M\left(1-\epsilon_i\right)>0$
- Correct side of hyperplane
- Correct side of margin
 (or on margin)
- No cost (C)
- Distance $\geq M$
- Correct side of margin: (×)
- On margin: 1, 6, 9



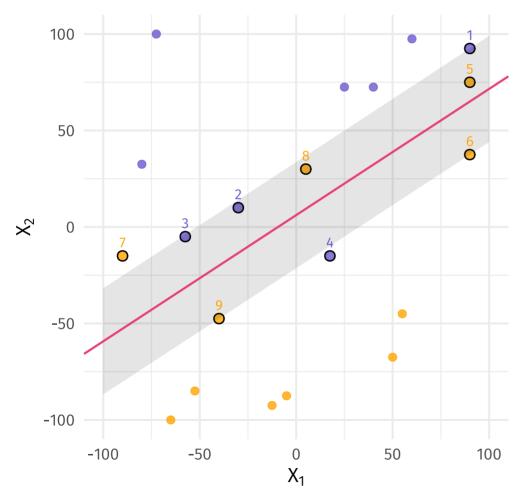
For $0 \leq \epsilon_i \leq 1$:

- $M\left(1-\epsilon_i\right)>0$
- Correct side of hyperplane
- Wrong side of the margin
 (violates margin)
- Pays cost ϵ_i
- Distance < M
- Examples?



For $0 \leq \epsilon_i \leq 1$:

- $M\left(1-\epsilon_i\right)>0$
- Correct side of hyperplane
- Wrong side of the margin
 (violates margin)
- Pays cost ϵ_i
- Distance < M
- Ex: 2, 3

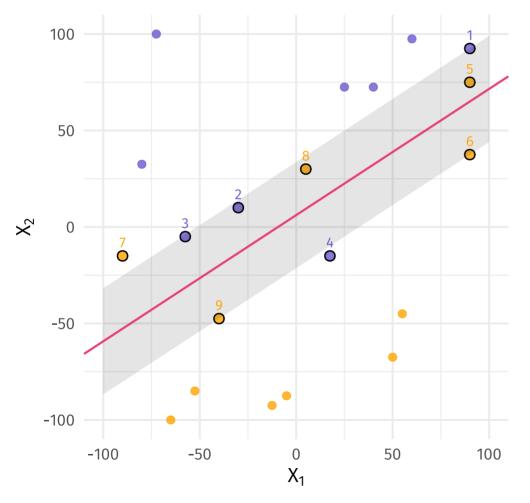


For $\epsilon_i \geq 1$:

- $M\left(1-\epsilon_i\right) < 0$
- Wrong side of hyperplane
- Pays cost ϵ_i

• Distance
$$\stackrel{\leq}{=} M$$

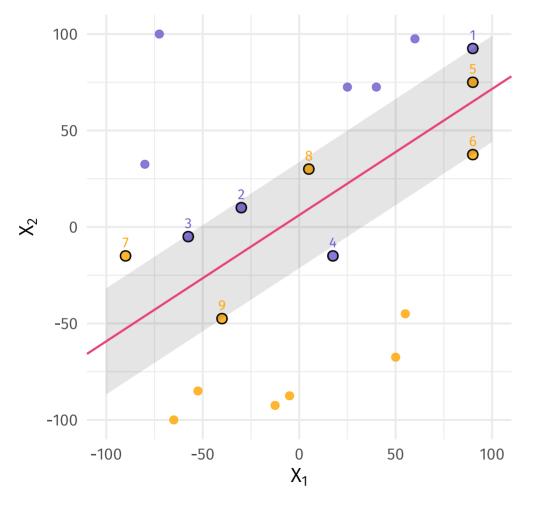
• Examples?



For $\epsilon_i \geq 1$:

- $M\left(1-\epsilon_{i}
 ight) < 0$
- Wrong side of hyperplane
- Pays cost ϵ_i
- Distance $\stackrel{\leq}{=} M$
- Ex: 4, 5, 7, 8

$$y_i\left(eta_0+eta_1x_{i1}+eta_2x_{i2}+\dots+eta_px_{ip}
ight)\geq M\left(1-\epsilon_i
ight), \quad \epsilon_i\geq 0, \quad \sum_{i=1}^n\epsilon_i\leq C$$



Support vectors

- On margin
- Violate margin
- Wrong side of hyperplane

determine the classifier.

Support vector classifier

The tuning parameter *C* determines how much *slack* we allow.

C is our budget for violating the margin—including observations on the wrong side of the hyperplane.

Case 1: C=0

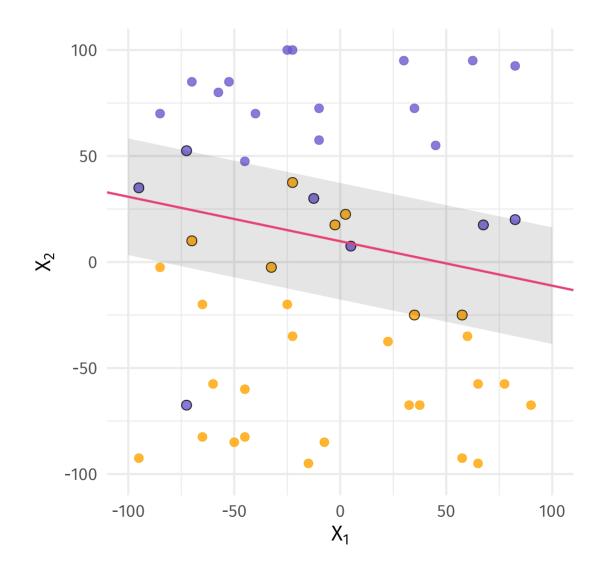
- We allow no violations.
- Maximal margin hyperplane.
- Trains on few obs.

Case 2: C>0

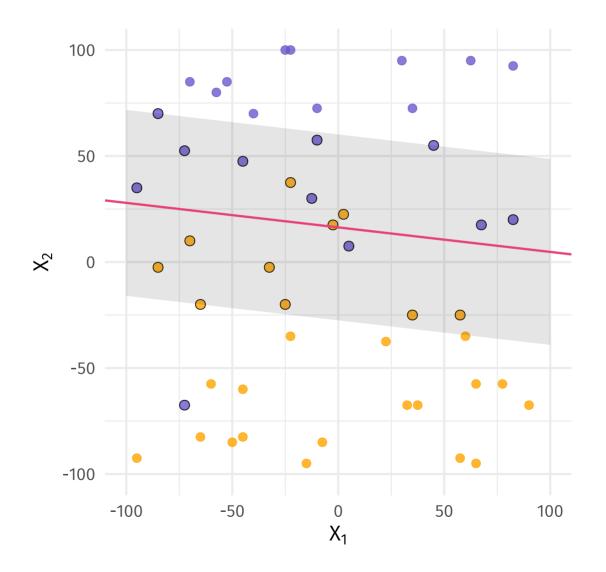
- $\leq C$ violations of hyperplane.
- Softens margins
- Larger C uses more obs.

We tune C via CV to balance low bias (low C) and low variance (high C).

Starting with a low budget (C).



Now for a high budget (C).



The support-vector classifier extends the maximal-margin classifier:

1. Allowing for **misclassification**

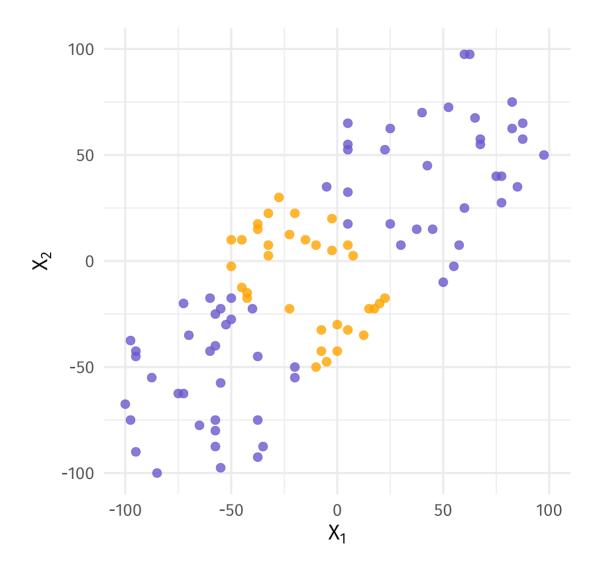
- Observations on the *wrong side of the hyperplane*.
- Situations where there is no separating hyperplane.

2. Permitting violations of the margin.

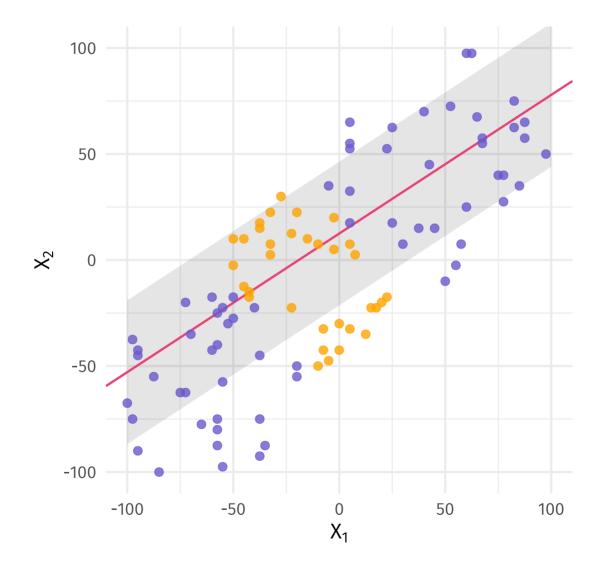
3. Typically using **more observations** to determine decision boundary.

However, we still are using a (single) linear boundary between our classes.

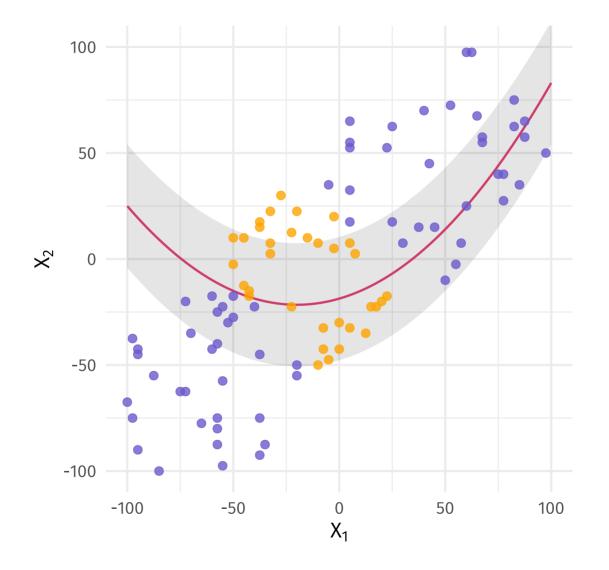
Ex: Some data



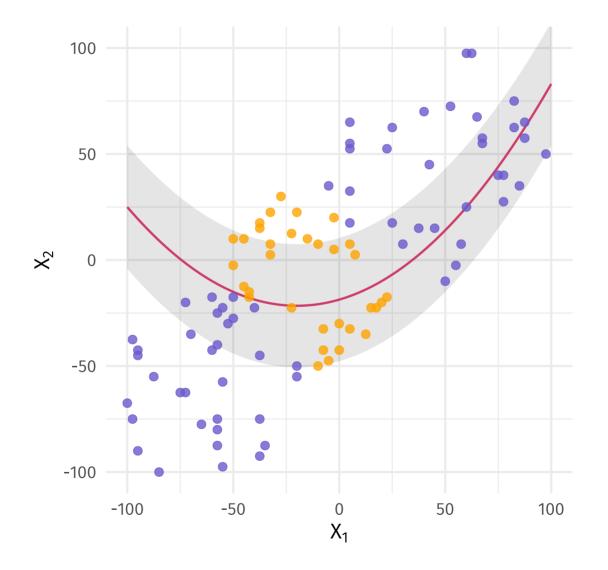
Ex: Some data don't really work with *linear* decision boundaries.



Ex: Some data may have *non-linear* decision boundaries.



Ex: We could probably do even better with more flexibility.



Flexibility

In the regression setting, we increase our model's flexiblity by adding polynomials in our predictors, e.g., $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i + \hat{\beta}_2 x_i^2 + \hat{\beta}_3 x_i^3$.

We can apply a very similar idea to our support vector classifier.

Previously: Train the classifier on X_1, X_2, \ldots, X_p .

Idea: Train the classifier on $X_1, X_1^2, X_2, X_2^2, \ldots, X_p, X_p^2$ (and so on).

The new classifier has a linear decision boundary in the expanded space.

The boundary is going to be **nonlinear** within the original space.

Introducing

The **support vector machine** runs with this idea of expanded flexiblity.

(Why stop at quadratic functions—or polynomials?)

Support vector machines **train a support vector classifier** on **expanded feature[†] spaces** that result from applying **kernels** to the original features.

Dot products

It turns out that solving the support vector classifier only involves the **dot product** of our observations.

The **dot product** of two vectors is defined as

$$\langle a,b
angle=a_1b_1+a_2b_2+\dots+a_pb_p=\sum_{i=1}^pa_ib_i$$

Ex: The dot product of a = (1,2) and b = (3,4) is $\langle a, b \rangle = 1 \times 3 + 2 \times 4 = 11$.

Dot products are often pitched as a measure of two vectors' similarity.

Dot products and the SVC

We can write the linear support vector classifier as

$$f(x)=eta_0+\sum_{i=1}^nlpha_i\langle x,x_i
angle$$

and we fit the $(n) \alpha_i$ and β_0 with the training observations' dot products.[†]

As you might guess, $lpha_i
eq 0$ only for support-vector obsevations.

† The actually fitting is beyond what we're doing today.

Generalizing

Recall: Linear support vector classifier $f(x)=eta_0+\sum_{i=1}^nlpha_i\langle x,x_i
angle$

Support vector machines generalize this linear classifier by simply replacing $\langle x, x_i \rangle$ with (non-linear) kernel functions[†] $K(x_i, x_{i'})$.

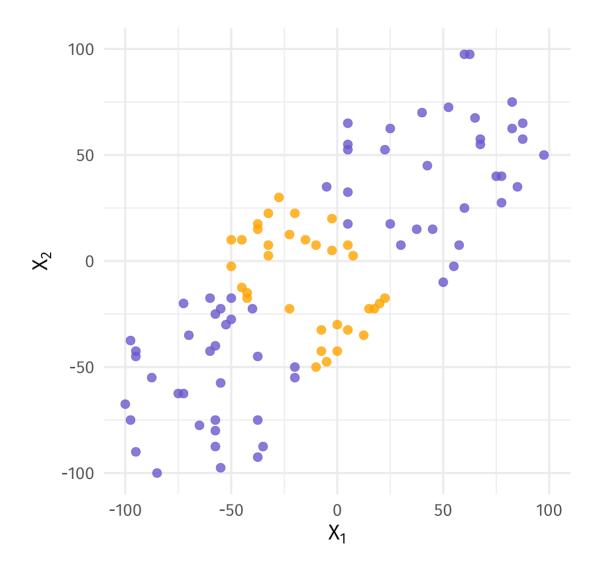
These magical **kernel functions** are various ways to measure similarity between observations.

- Linear kernel: $K(x_i,x_{i'})=\sum_{i=1}^p x_{i,j}x_{i',j}$ (back to SVC)
- Polynomial kernel: $K(x_i,x_{i'}) = \left(1+\sum_{i=1}^p x_{i,j}x_{i',j}
 ight)^2$

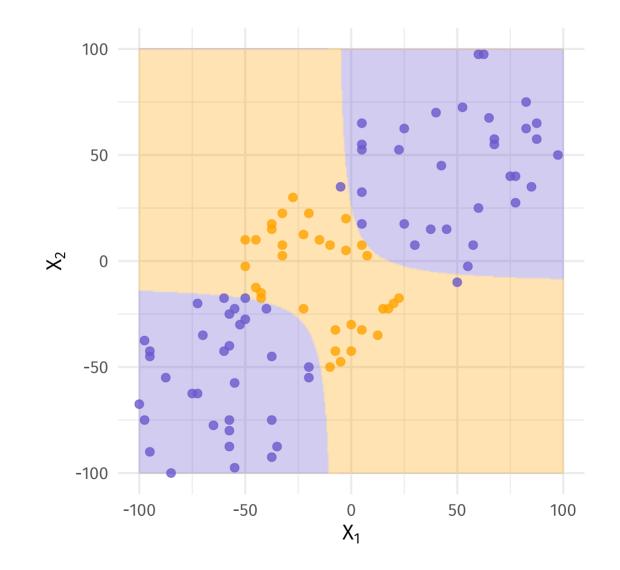
$$ullet$$
 Radial kernel: $K(x_i,x_{i'})=\exp\Bigl(-\gamma\sum_{j=1}^pig(x_{i,j}-x_{i',j}ig)^2\Bigr)$

† Or just kernels.

Our example data.

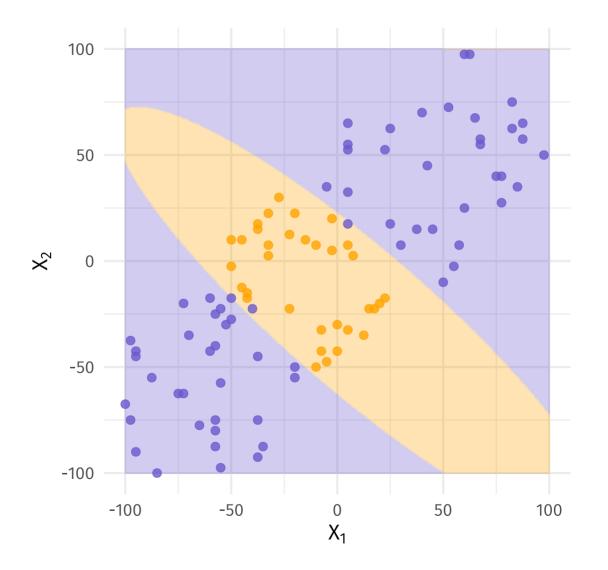


With a linear kernel *plus* and interaction between X_1 and X_2 .⁺



t Exciting!!

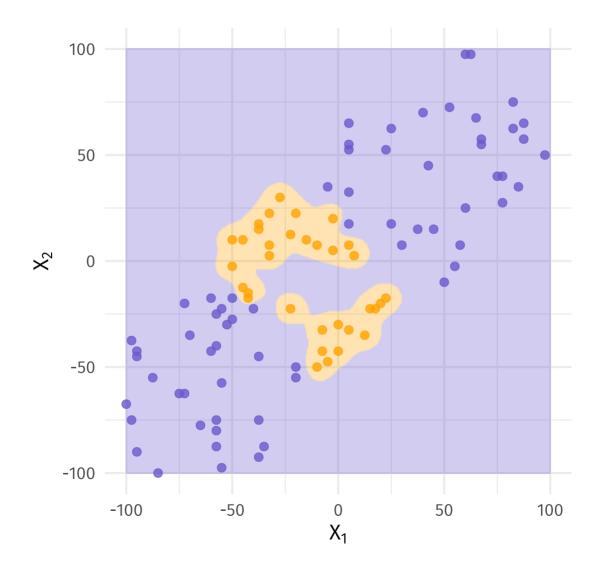
Polynomial kernel (of degree 2).



And now for the radial kernel!



Very small γ forces radial kernel to be *even more* local.



More generalizing

So why make a big deal of kernels? Anyone can transform variables.

While anyone can transform variables, you cannot transform variables to cover all spaces that our kernels cover.

For example, the feature space of the radial kernel is infinite dimensional.[†]



† And implicit

In R

As you probably guessed, caret offers *many* SVM options.

Two common popular R packages: kernlab and e1071.

caret offers linear, polynomial, and radial kernels for both packages.

You can also find more kernels in the actual packages (or other packages).

```
# Set a seed
set.seed(12345)
# Tune linear SVM
svm lin = train(
  above fac \sim x1 + x2 + x1:x2,
  data = nonlin dt,
 method = "svmLinear",
  scaled = T.
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = data.frame(
    C = 10^{seq}(-3, 2, by = 0.5)
# Predict
predict(svm_linear, newdata = test_dt)
```

• Interactions!

```
# Set a seed
set.seed(12345)
# Tune linear SVM
svm lin = train(
  above fac \sim x1 + x2 + x1:x2,
  data = nonlin dt,
 method = "svmLinear",
  scaled = T.
  trControl = trainControl(
   method = "cv",
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  ).
  tuneGrid = data.frame(
    C = 10^{seq}(-3, 2, by = 0.5)
# Predict
predict(svm_linear, newdata = test_dt)
```

- Interactions!
- Method: "svmLinear" (kernlab)

```
# Set a seed
set.seed(12345)
# Tune linear SVM
svm lin = train(
  above fac \sim x1 + x2 + x1:x2,
  data = nonlin dt,
 method = "svmLinear",
  scaled = T.
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = data.frame(
    C = 10^{seq}(-3, 2, by = 0.5)
  )
# Predict
predict(svm_linear, newdata = test_dt)
```

- Interactions!
- Method: "svmLinear" (kernlab)
- One tuning param: cost

```
# Set a seed
set.seed(12345)
# Tune polynomial SVM
svm poly = train(
  above fac \sim x1 + x2,
  data = nonlin dt,
 method = "svmPoly",
  scaled = T.
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = expand.grid(
    degree = 2:4,
    scale = 1,
    C = 10^{seq(-2, 1, by = 0.5)}
# Predict
predict(svm poly, newdata = test dt)
```

• Method: "svmPoly" (kernlab)

```
# Set a seed
set.seed(12345)
# Tune polynomial SVM
svm poly = train(
  above fac \sim x1 + x2,
  data = nonlin dt,
 method = "svmPoly",
  scaled = T.
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = expand.grid(
    degree = 2:4,
    scale = 1,
    C = 10^{seq}(-2, 1, by = 0.5)
# Predict
predict(svm poly, newdata = test dt)
```

- Method: "svmPoly" (kernlab)
- Scale (and center) variables?

```
# Set a seed
set.seed(12345)
# Tune polynomial SVM
svm polv = train(
  above fac \sim x1 + x2,
  data = nonlin dt,
 method = "svmPoly",
  scaled = T,
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = expand.grid(
    degree = 2:4,
    scale = 1,
    C = 10^{seq(-2, 1, by = 0.5)}
# Predict
predict(svm poly, newdata = test dt)
```

- Method: "svmPoly" (kernlab)
- Scale (and center) variables?
- Tuning parameters:
 - Polynomial degree

```
# Set a seed
set.seed(12345)
# Tune polynomial SVM
svm polv = train(
  above fac \sim x1 + x2,
  data = nonlin dt,
 method = "svmPoly",
  scaled = T.
  trControl = trainControl(
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- Method: "svmPoly" (kernlab)
- Scale (and center) variables?
- Tuning parameters:
 - Polynomial degree
 - \circ scale dotproduct in $K(\cdot)$

```
# Set a seed
set.seed(12345)
# Tune polynomial SVM
svm polv = train(
  above fac \sim x1 + x2,
  data = nonlin dt,
 method = "svmPoly",
  scaled = T,
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = expand.grid(
    degree = 2:4,
    scale = 1,
    C = 10^{seq(-2, 1, by = 0.5)}
# Predict
predict(svm poly, newdata = test dt)
```

- Method: "svmPoly" (kernlab)
- Scale (and center) variables?
- Tuning parameters:
 - Polynomial degree
 - \circ scale dotproduct in $K(\cdot)$
 - cost (c)

```
# Set a seed
set.seed(12345)
# Tune radial
svm radial = train(
  above fac \sim x1 + x2,
  data = nonlin dt,
 method = "svmRadial",
  scaled = T.
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = expand.grid(
    sigma = c(0.1, 1, 5, 10, 20),
    C = 10^{seq}(-2, 1, by = 1)
# Predict
predict(svm_radial, newdata = test_dt)
```

• Method: "svmRadial"

```
# Set a seed
set.seed(12345)
# Tune radial
svm radial = train(
  above fac \sim x1 + x2,
  data = nonlin dt,
 method = "svmRadial",
  scaled = T.
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = expand.grid(
    sigma = c(0.1, 1, 5, 10, 20),
    C = 10^{seq}(-2, 1, by = 1)
# Predict
predict(svm radial, newdata = test dt)
```

- Method: "svmRadial"
- Scale (and center) variables?

```
# Set a seed
set.seed(12345)
# Tune radial
svm radial = train(
  above fac \sim x1 + x2,
  data = nonlin dt,
 method = "svmRadial",
  scaled = T.
  trControl = trainControl(
   method = "cv",
    number = 5
  ).
  tuneGrid = expand.grid(
    sigma = c(0.1, 1, 5, 10, 20),
    C = 10^{seq(-2, 1, by = 1)}
# Predict
predict(svm radial, newdata = test dt)
```

- Method: "svmRadial"
- Scale (and center) variables?
- Tuning parameters (CV)
 - sigma: radial param.
 - C:cost

Note: Costs have units. You often want to center/scale your variables.

Multi-class classification

You will commonly see SVMs applied in settings with K>2 classes.

What can we do? We have options!

One-versus-one classification

- Compares each *pair* of classes, one pair at a time.
- Final prediction comes from the most-common pairwise prediction.

One-versus-all classification

- Fits *K* unique SVMs—one for each class: *k* vs. not *k*.
- Predicts the class for which $f_k(x)$ is largest.

SVM

More material

Visualizing decision boundaries

- From scikit-learn
- From sub-subroutine

The kernlab paper (describes kernel parameters)

A Practical Guide to Support Vector Classification

Coming up: A nice neural-net video

Sources

These notes draw upon

• An Introduction to Statistical Learning (ISL)

James, Witten, Hastie, and Tibshirani

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