Machine Learning in R

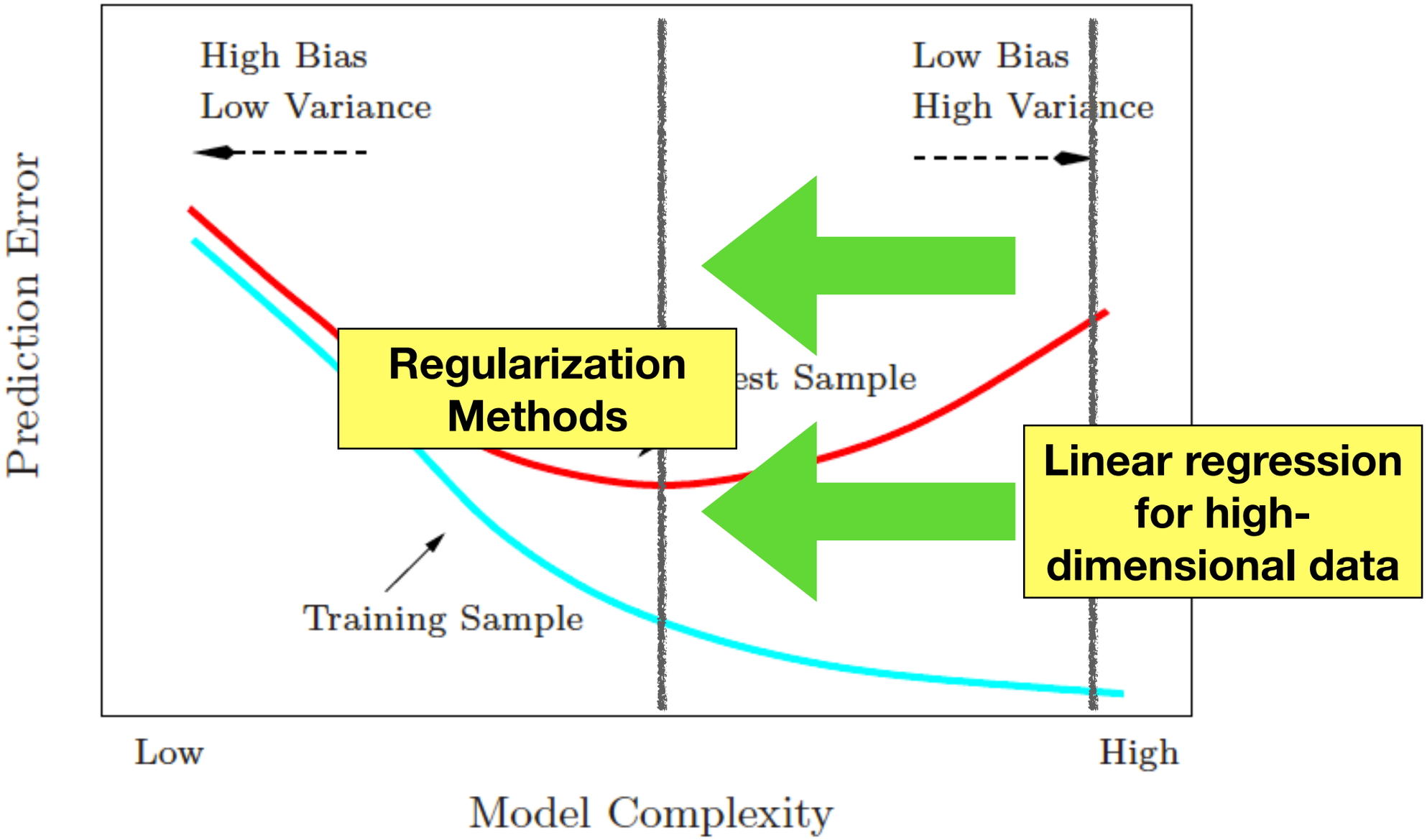
Lecture 4 – Support vector machines

Jean Feng – Epidemiology and Biostatistics

Last lecture

1. Model selection: Cross-validation
2. Low versus high-dimensional data
3. Regularization methods
    1. Ridge Regression
    2. Variable selection methods
        1. Variable subset selection
        2. Lasso
    3. Extensions

Recall: Regularization improves the bias-variance tradeoff



Recall: In penalized regression, we fit a model by minimizing the penalized empirical risk.

For example, ridge regression fits a model by solving:

$$\min_{\beta \in \mathbb{R}^p, \beta_0 \in \mathbb{R}} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \left(y_i - (x_i^\top \beta + \beta_0) \right)^2}_{\text{Mean squared error}} + \lambda \underbrace{\|\beta\|_2^2}_{\text{Penalty}}$$

We're going to see something like this pop up in today's lecture again!

Today's lecture

1. Maximum margin classifiers

2. Support vector classifiers

3. Support vector machines

4. SVMs as a penalization method

5. SVMs for multiple classes

Motivation

- ***Maximum margin classifier***, ***support vector classifier***, and ***support vector machine*** *(SVM)* are designed for binary classification tasks.

- Unlike logistic regression, there is no probability model for the data. Instead, SVMs are *geometrically motivated*.

- The idea is to generate ***decision boundaries*** that best separate the data.

Example dataset

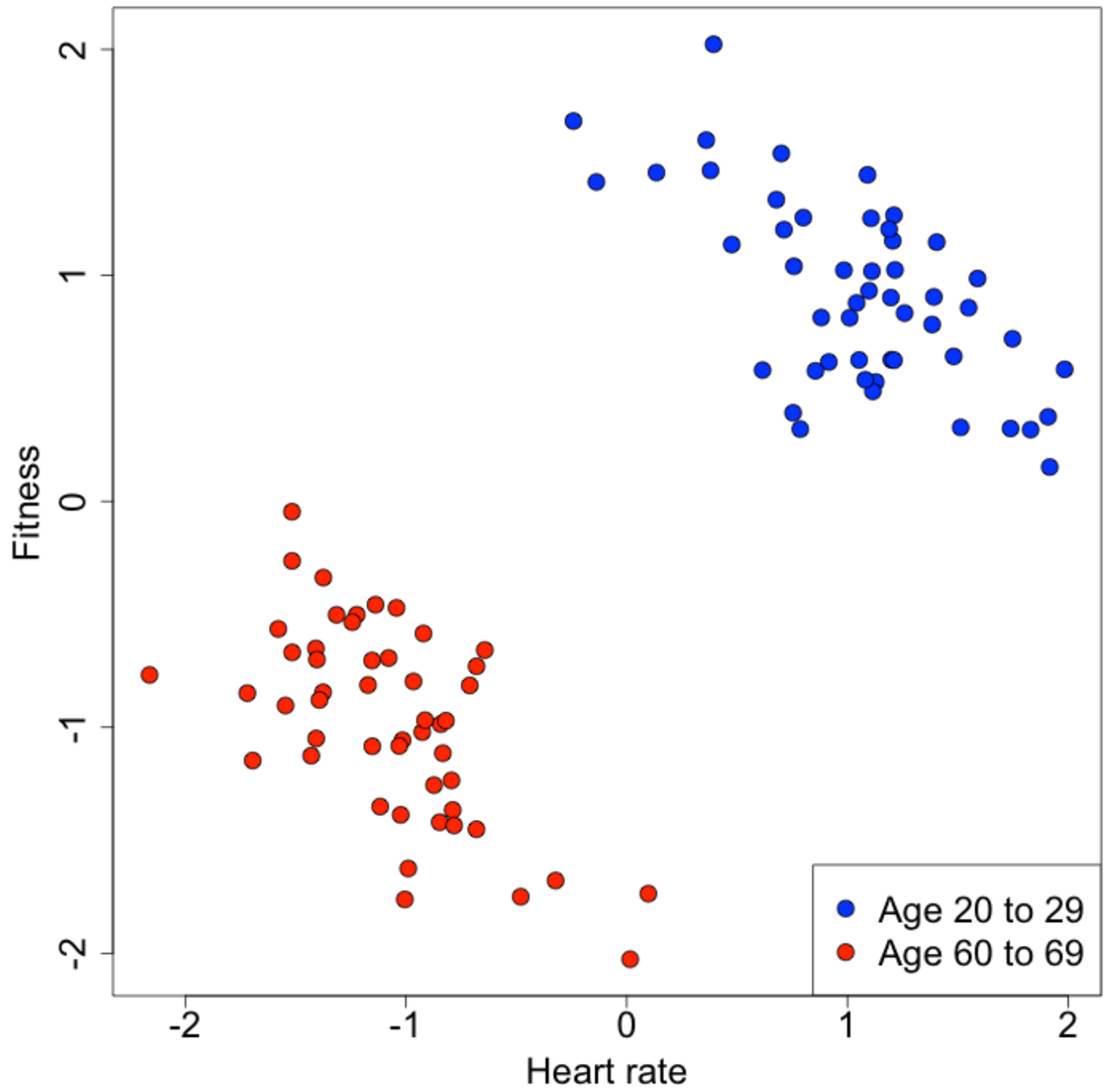
- Let's simulate data with the following measurements:
  - X_1 = normalized heart rate
  - X_2 = fitness measure
  - Y = age group
    - $Y = -1$ means the subject is 60-69 years old
    - $Y = 1$ means the subject is 20-29 years old

	HeartRate	Fitness	ageGrp
95	0.1518579	-2.51375243	-1
168	1.3867171	1.04422744	1
142	3.0515427	0.01138957	1
158	1.2044311	0.80480815	1
13	-0.3274814	-0.42026735	-1
164	1.6208782	1.64587715	1

Example dataset

- Constructing a decision rule that separates the two age groups is straightforward for this dataset.

- Draw a line to separate the groups.



A separating line

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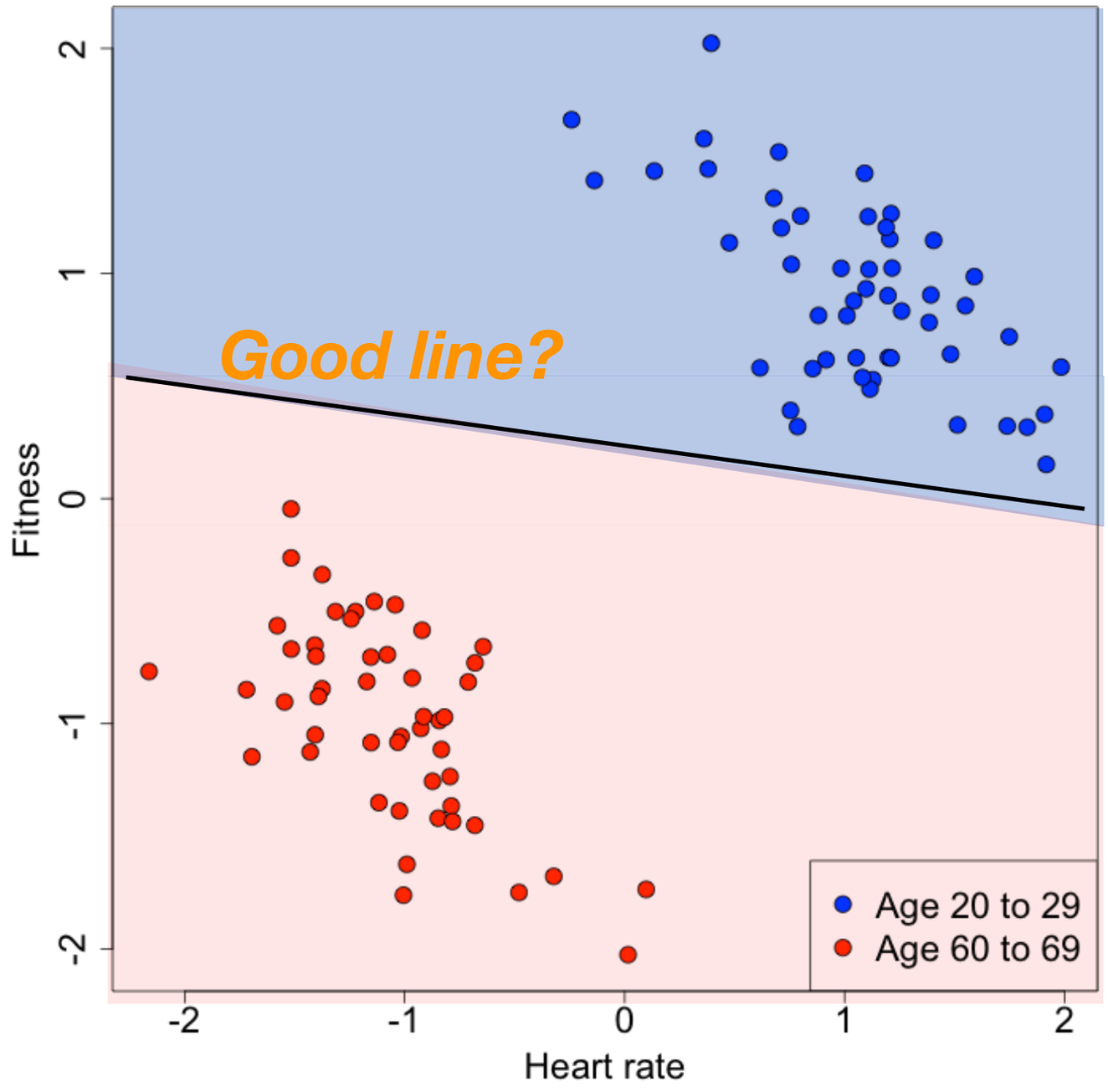

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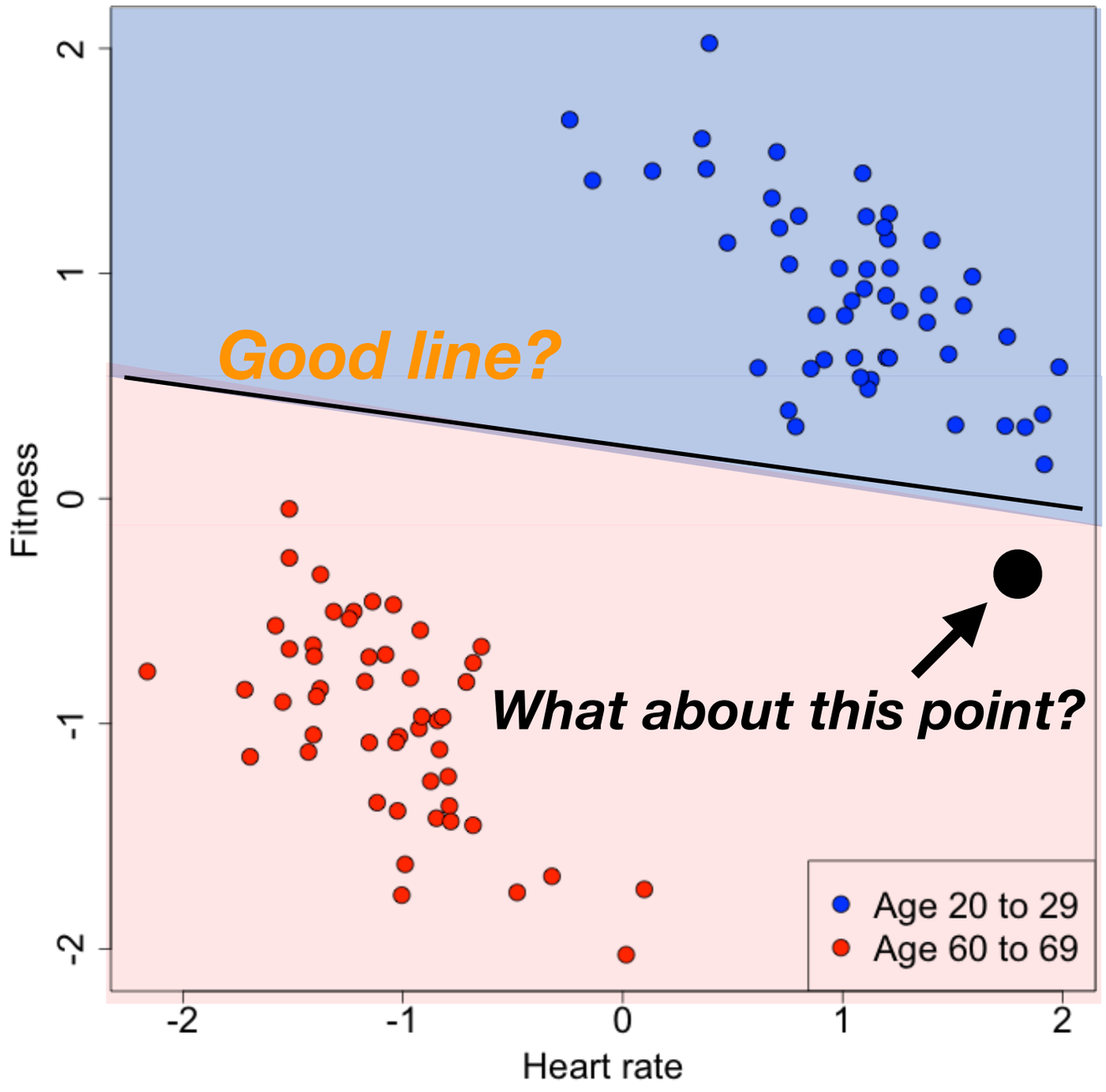

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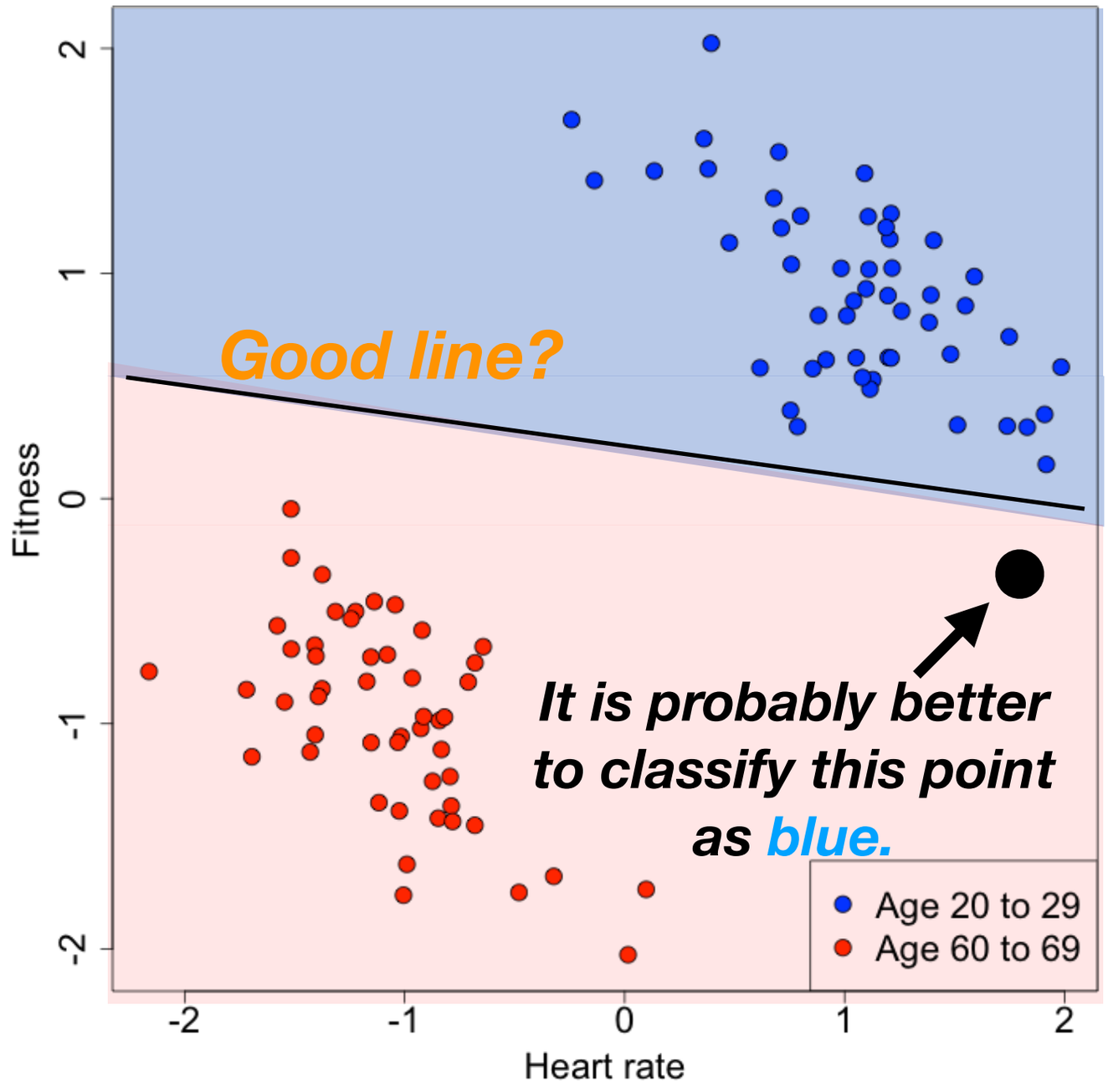
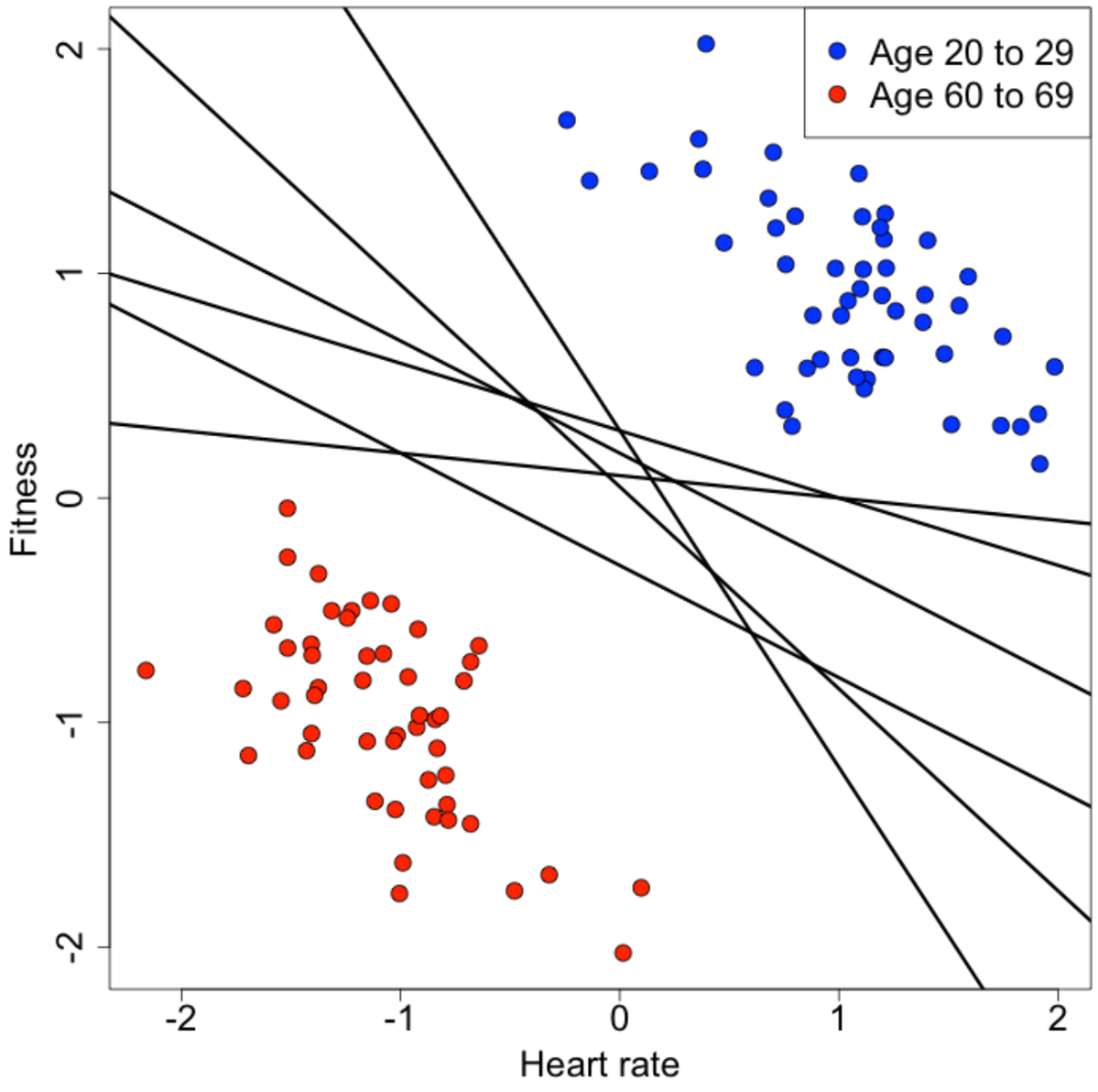


Many separating lines

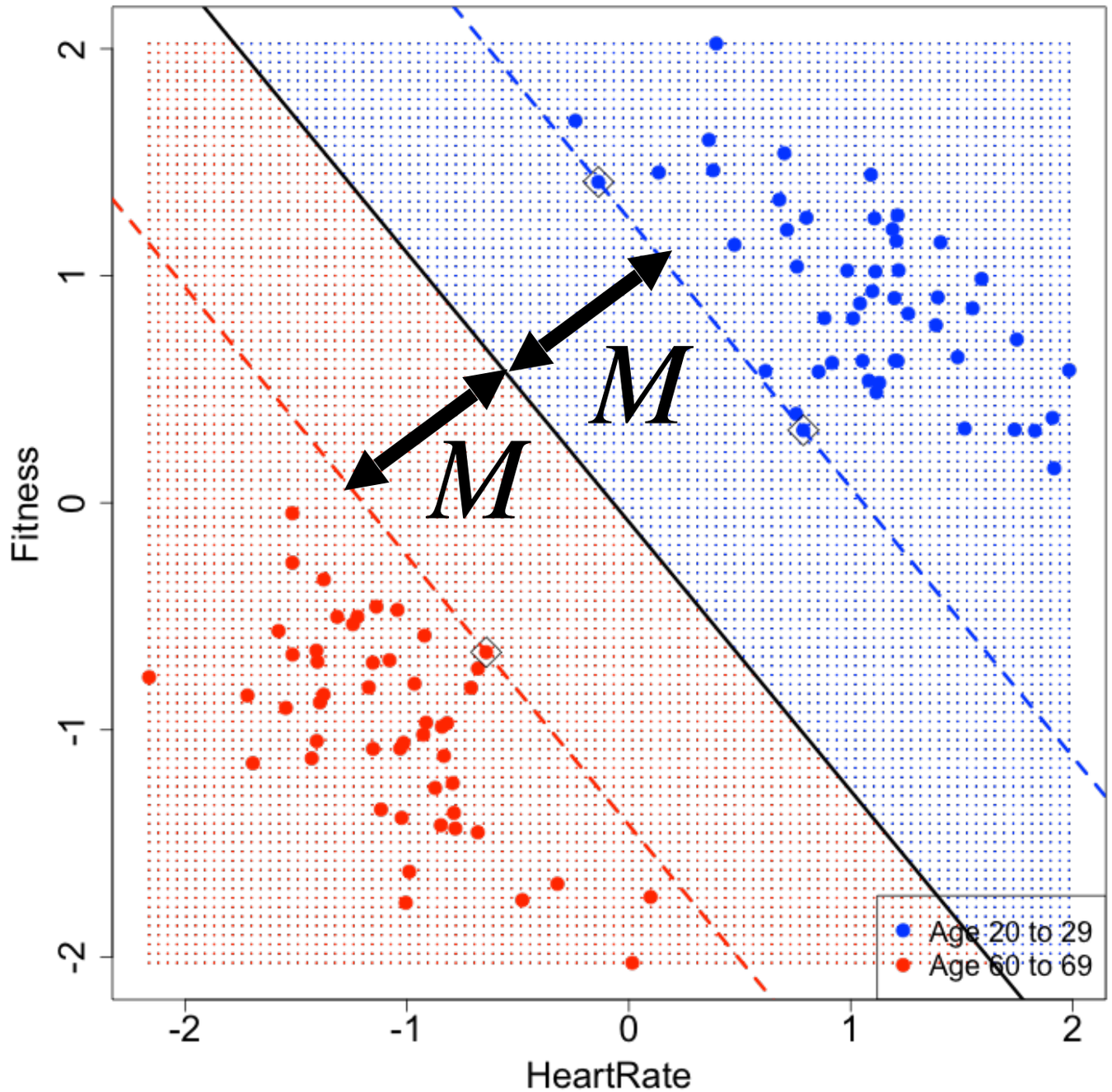
- There are actually many separating lines.
- Which one is the best one?



Maximum margin classifier

- The maximum margin classifier finds the separating line that is farthest away from any training points.

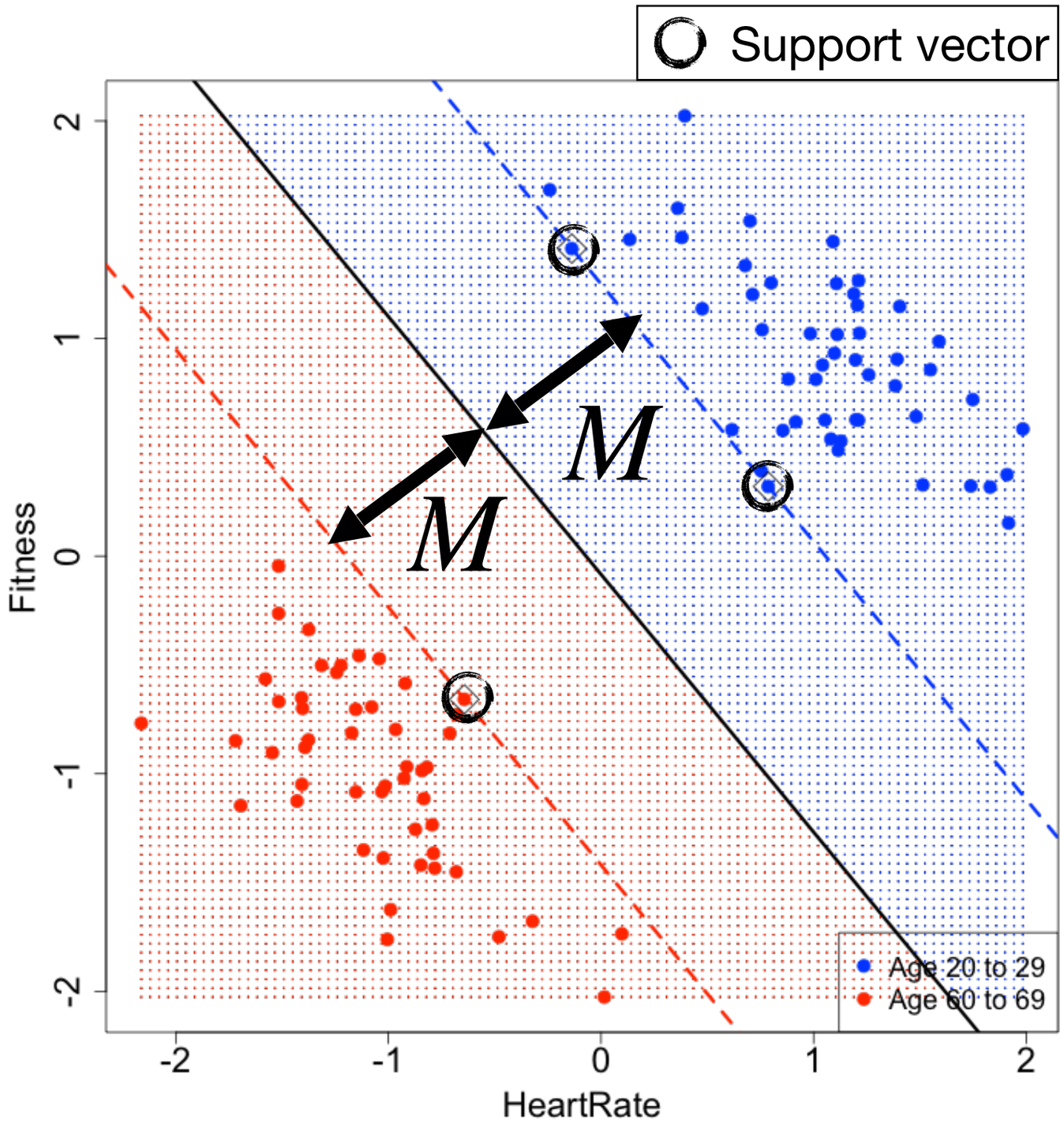
- The smallest distance between the decision boundary and training data is called the ***margin*** M.



Maximum margin classifier

- The points that are closest to the decision boundary determine the location and orientation of the decision boundary.

- These circled points are referred to as the ***support vectors***.



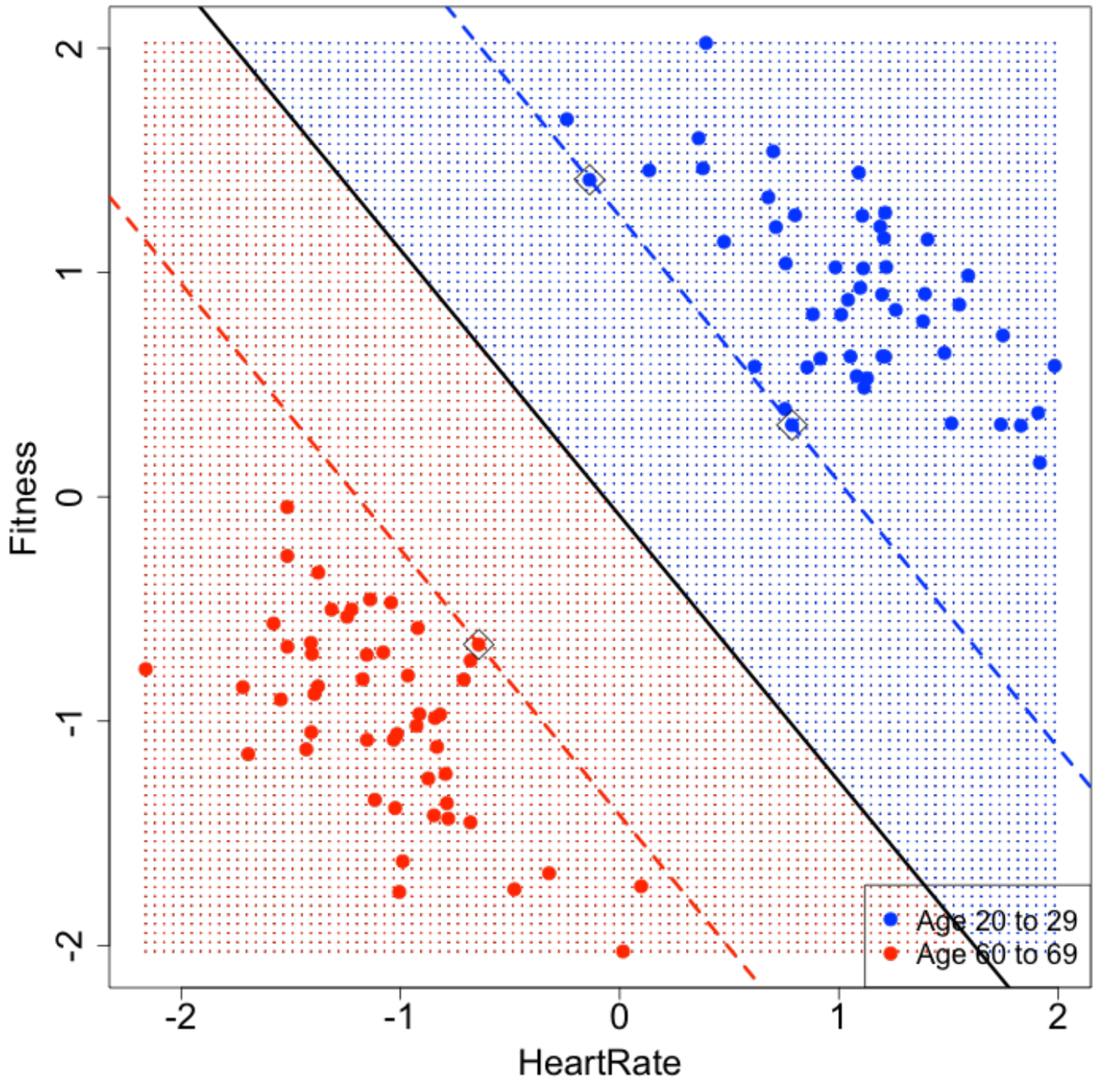
The decision function

- The maximum margin classifier fits a decision function of the form $f_{\beta_0,\beta}(x) = \beta_0 + \beta^\top x.$

- We can classify a new point x according to the sign of $f_{\beta_0,\beta}(x)$:

  - If $f_{\beta_0,\beta}(x)$ is positive, then predict class 1.

  - If $f_{\beta_0,\beta}(x)$ is negative, then predict class -1.



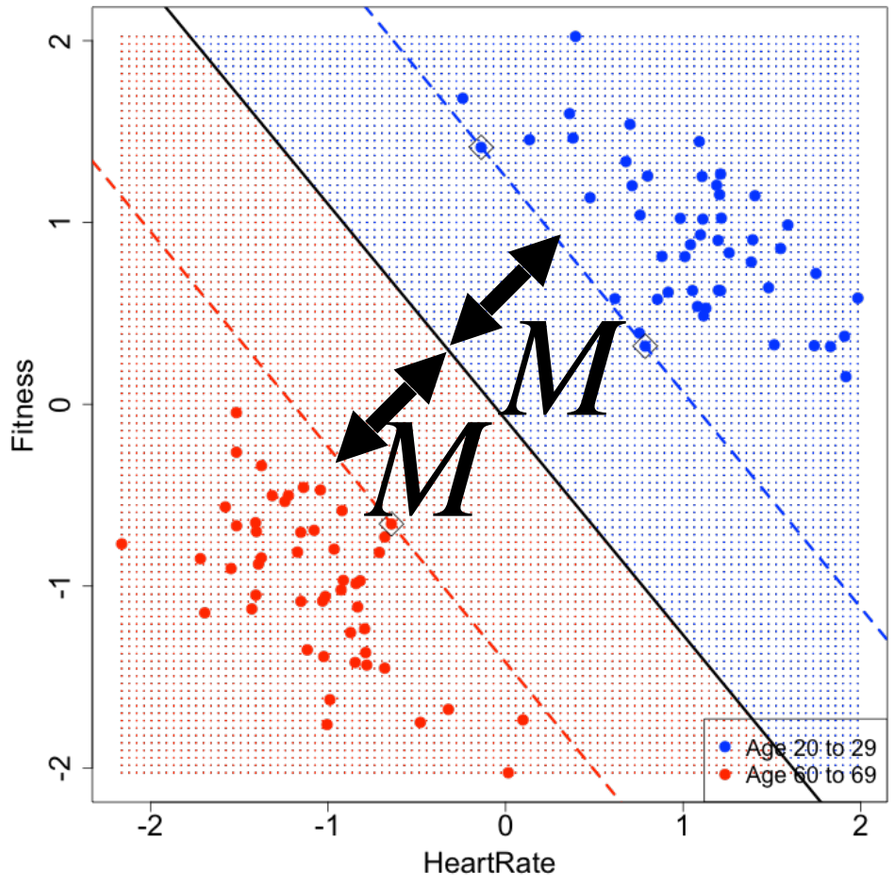
Fitting a decision function

For a training dataset $\{(x_i, y_i) : i = 1,...,n\}$, the maximum margin classifier fits the decision function by solving the following optimization problem:

$$\max_{\beta_0,\beta,M} M \quad \textit{(maximize the margin)}$$

such that $\|\beta\|_2^2 = 1$ and

$$\underbrace{y_i(\beta_0 + \beta^\top x_i)}_{\textit{Distance to the decision boundary}} \geq M \text{ for all } i = 1,...,n$$

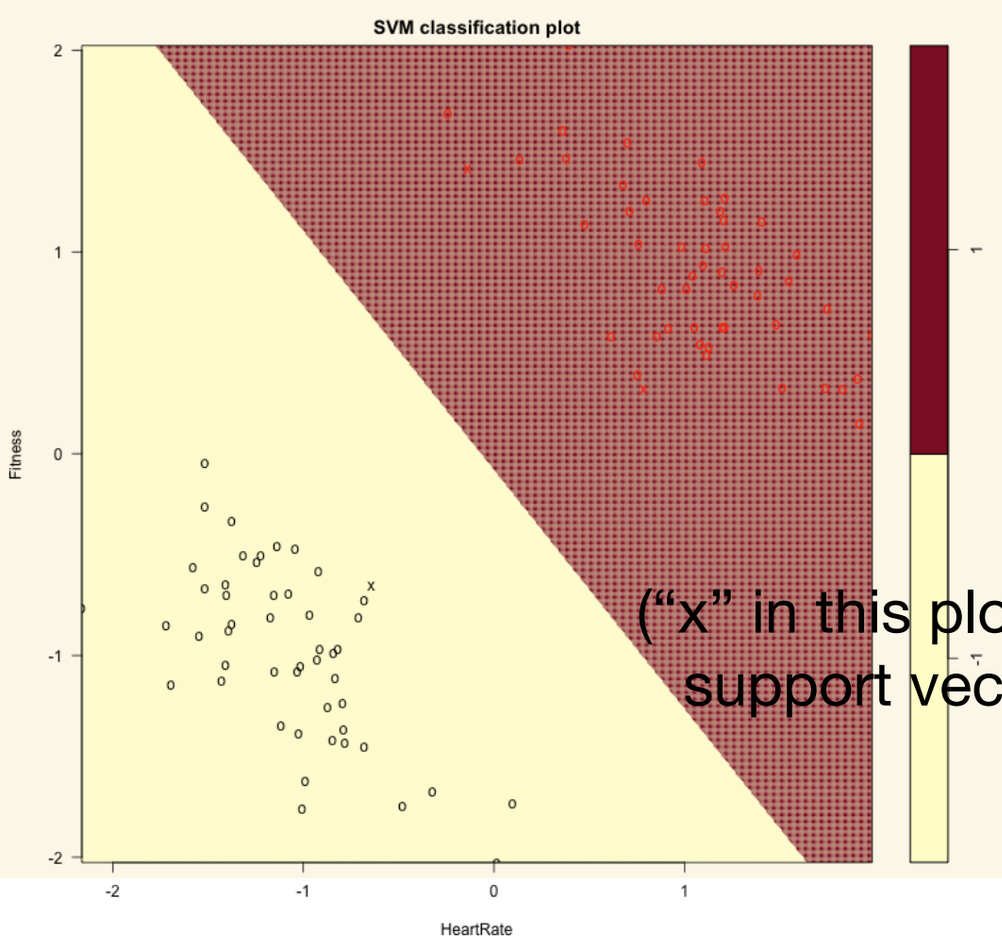


(Such that all points are correctly classified and are at least distance M away from the decision boundary)

Fitting a maximum margin classifier in R

```
> library(e1071)  ### library containing svm function
>
> svmFit <- svm(ageGrp ~ Fitness + HeartRate, data=dat, kernel="linear", cost=10, scale=FALSE)
> summary(svmFit)

Call:
svm(formula = ageGrp ~ Fitness + HeartRate, data = dat, kernel = "linear",
    cost = 10, scale = FALSE)

Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  linear
       cost:  10

Number of Support Vectors:  3

 ( 1 2 )


Number of Classes:  2

Levels:
 -1 1
```

```
> plot(svmFit, grid=500, data=dat)
```



("x" in this plot is a support vector)

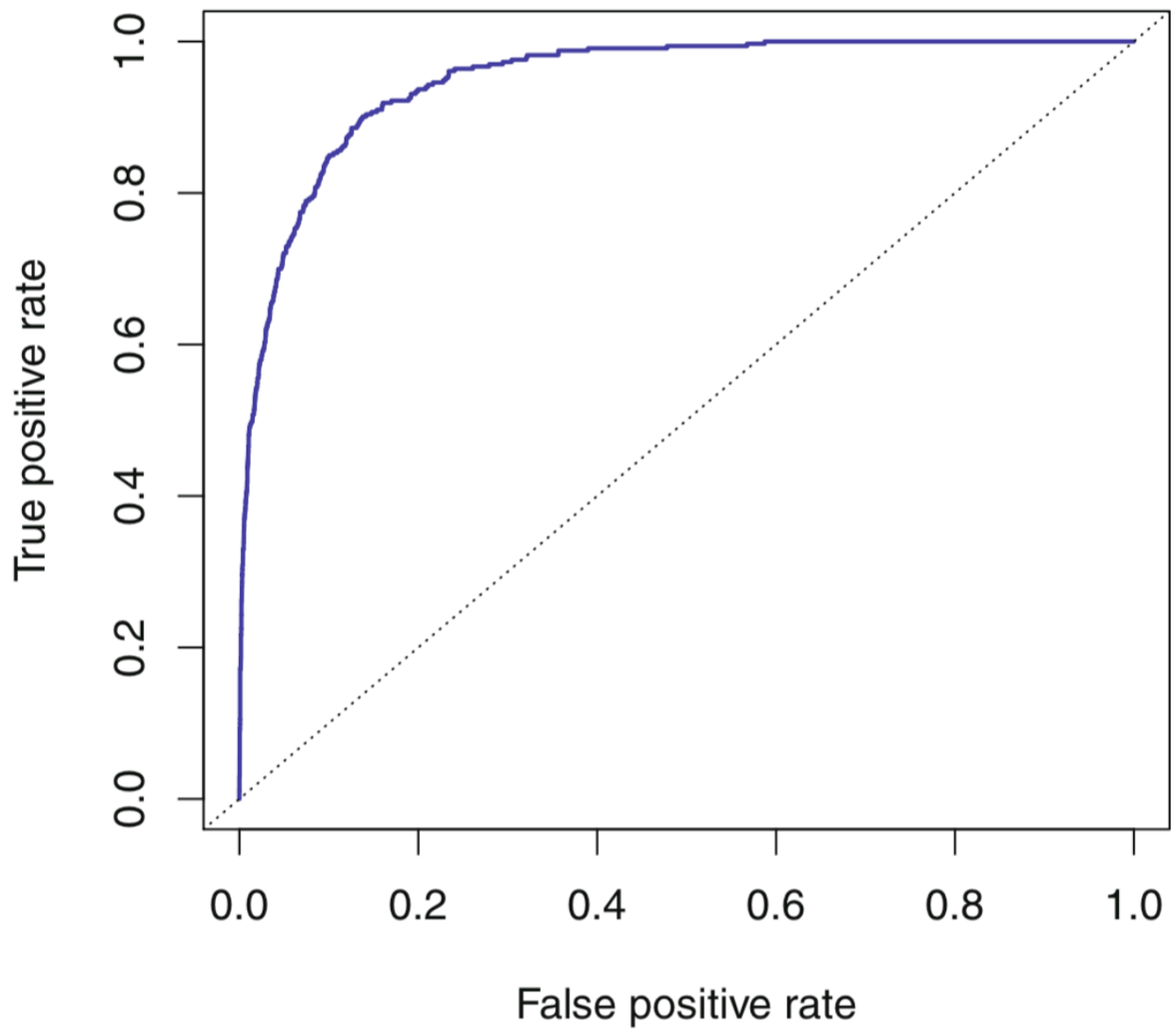
Quiz: ROC curves and SVMs

- **Q**: How would you make an ROC curve for a maximum margin classifier?

- **A**. You don't. The maximum margin classifier only outputs binary predictions.

- **B**. Threshold on the value of the decision function.

- **C**. Threshold on the distance to the decision boundary.



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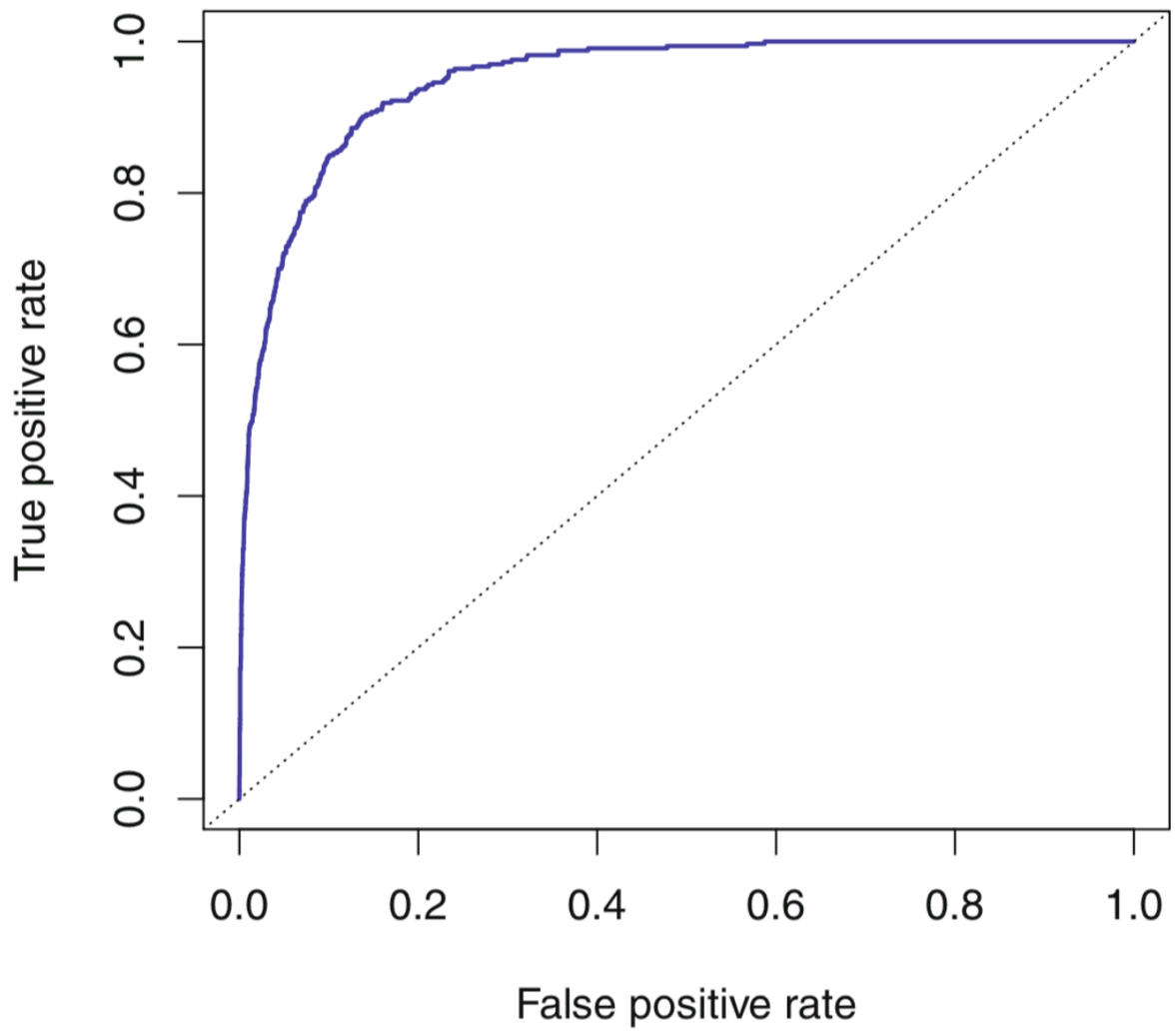
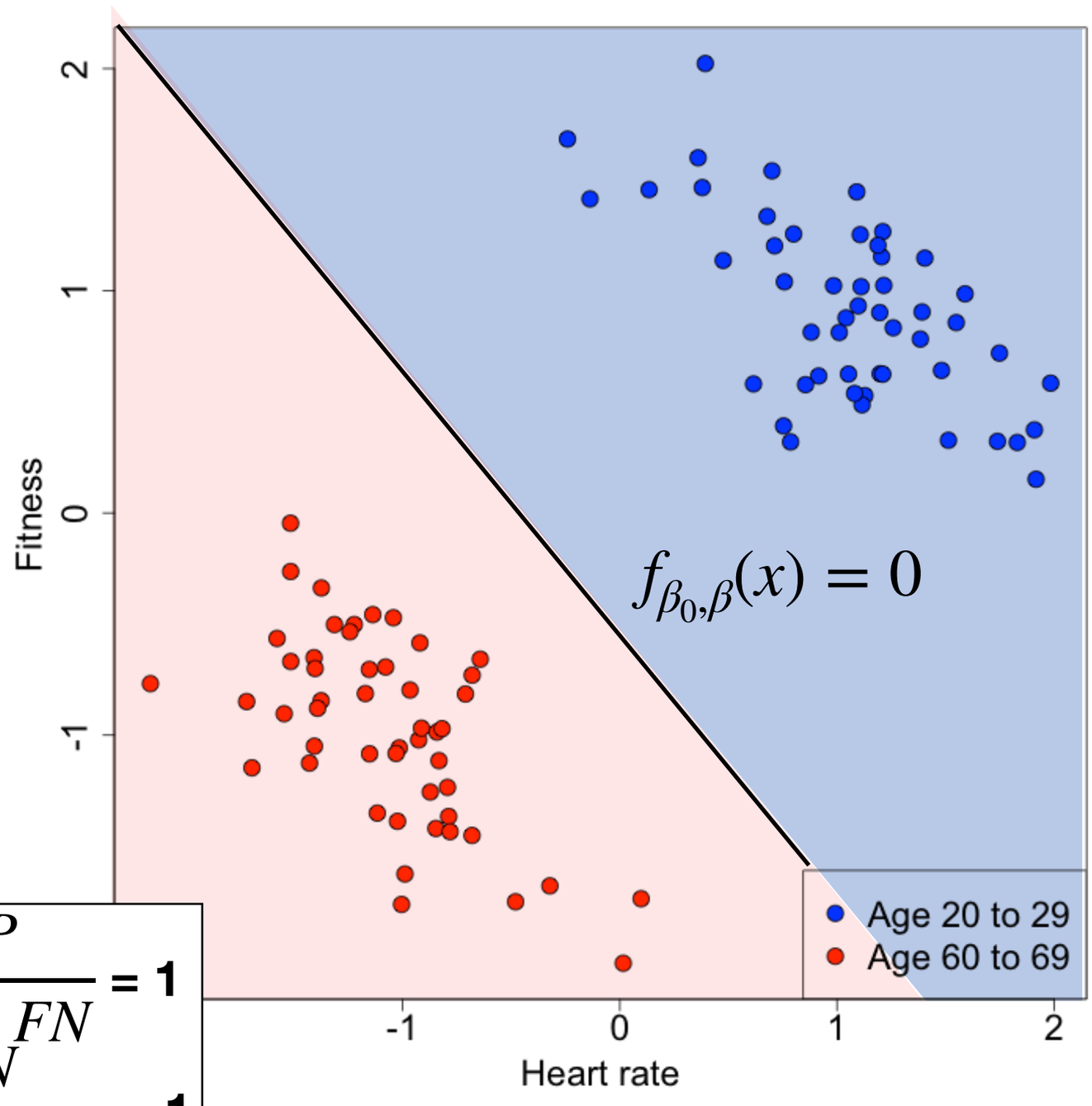


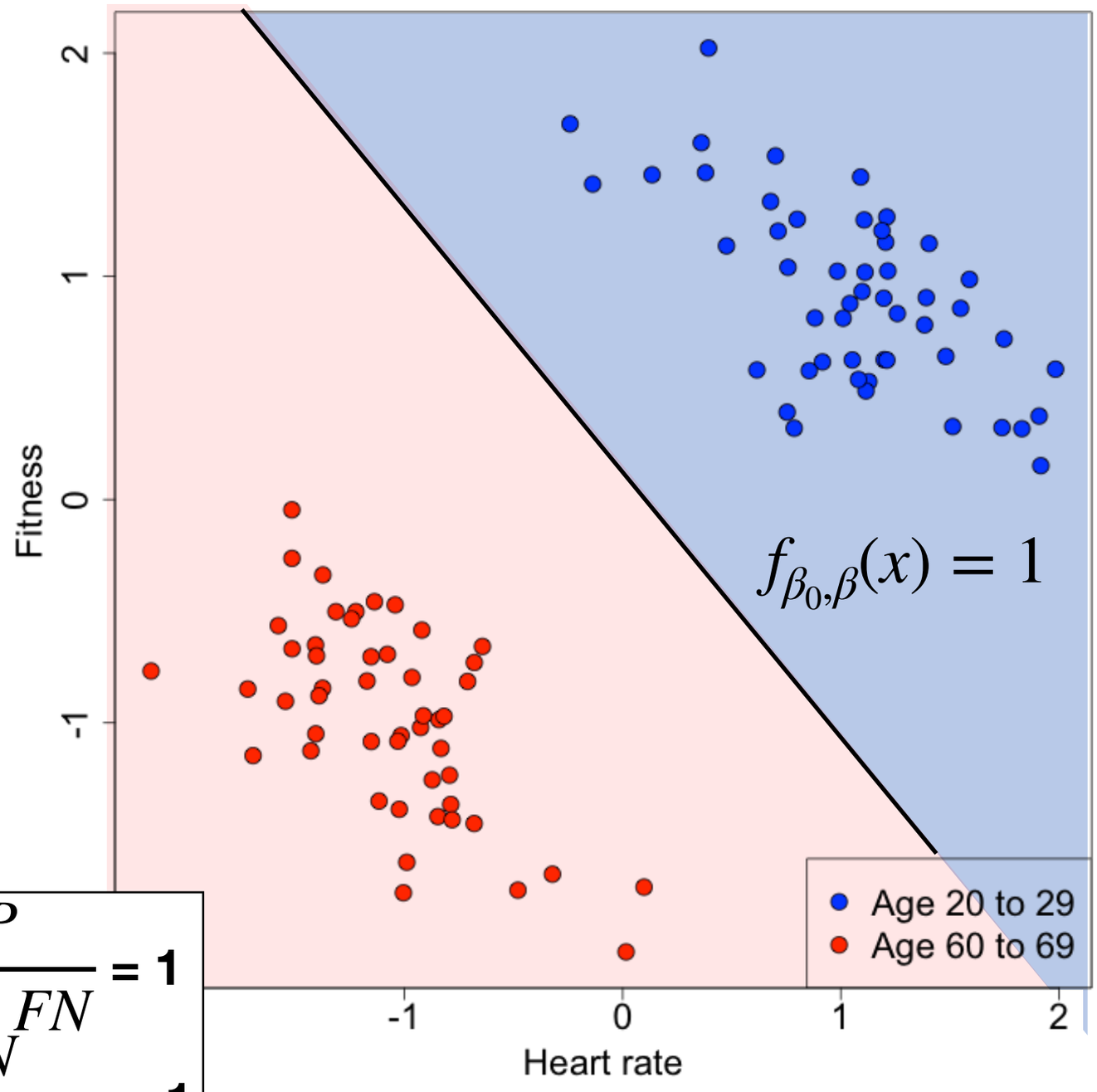
Thresholding on the decision function



$$\textbf{Sensitivity} = \frac{TP}{TP + FN} = 1$$

$$\textbf{Specificity} = \frac{TN}{TN + FP} = 1$$

Thresholding on the decision function



$$\textbf{Sensitivity} = \frac{TP}{TP + FN} = 1$$

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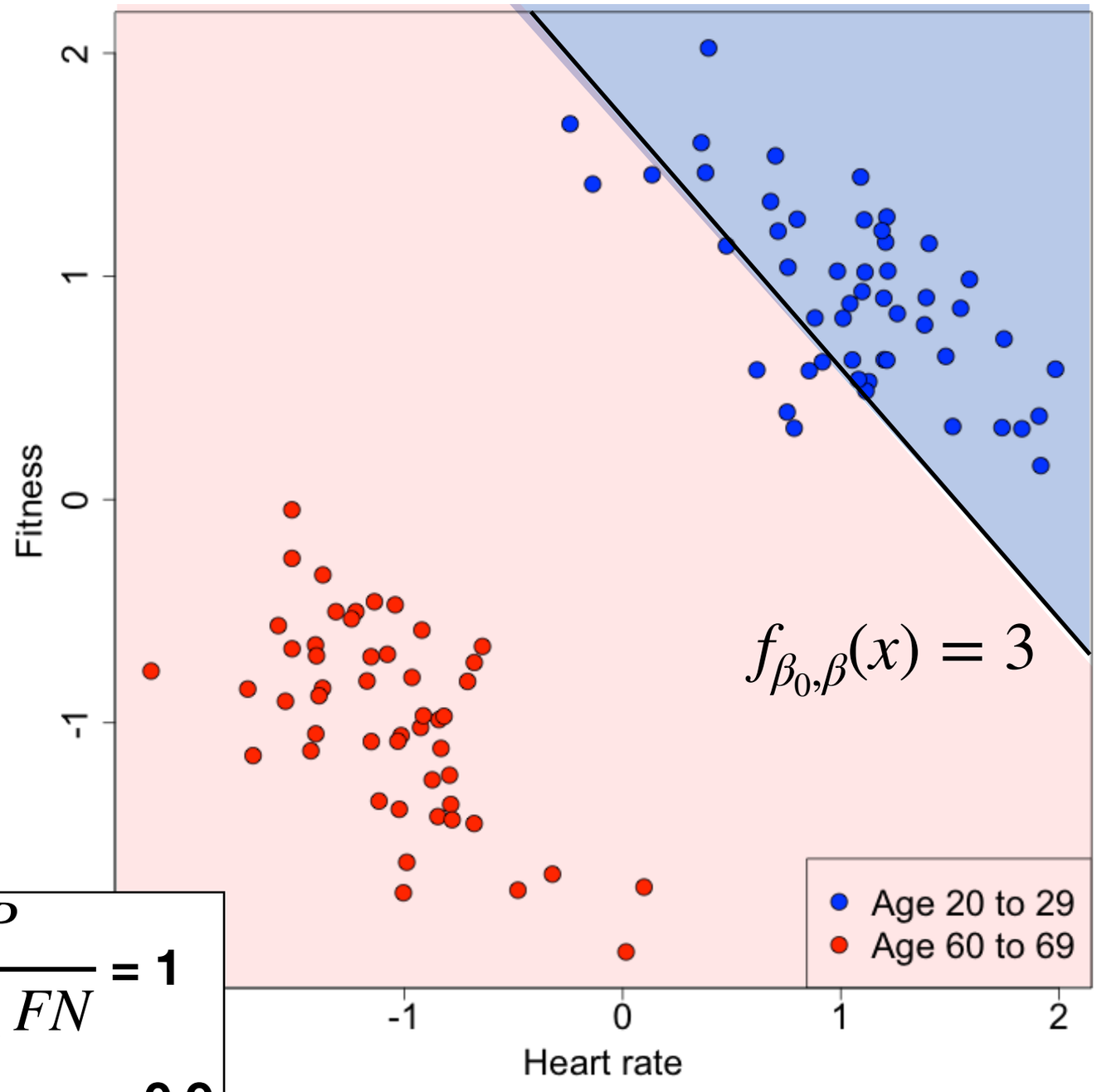
Thresholding on the decision function

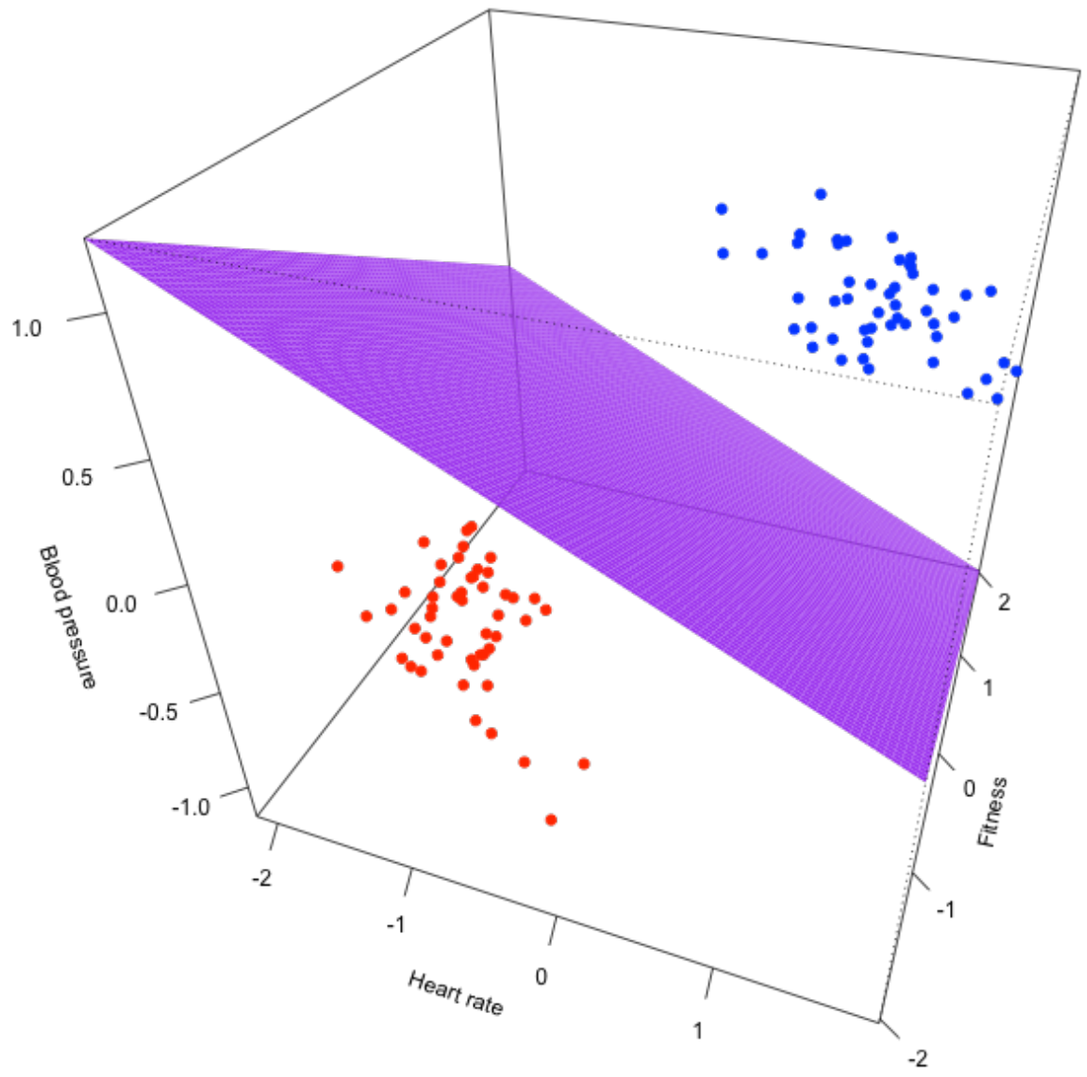


$$\textbf{Sensitivity} = \frac{TP}{TP + FN} = 1$$

$$\textbf{Specificity} = \frac{TN}{TN + FP} = 0.9$$

More than 2 predictors

- When there are p predictors where $p > 2$, we refer to the decision boundary as a ***hyperplane***. The hyperplane is a $(p - 1)$ dimensional plane.



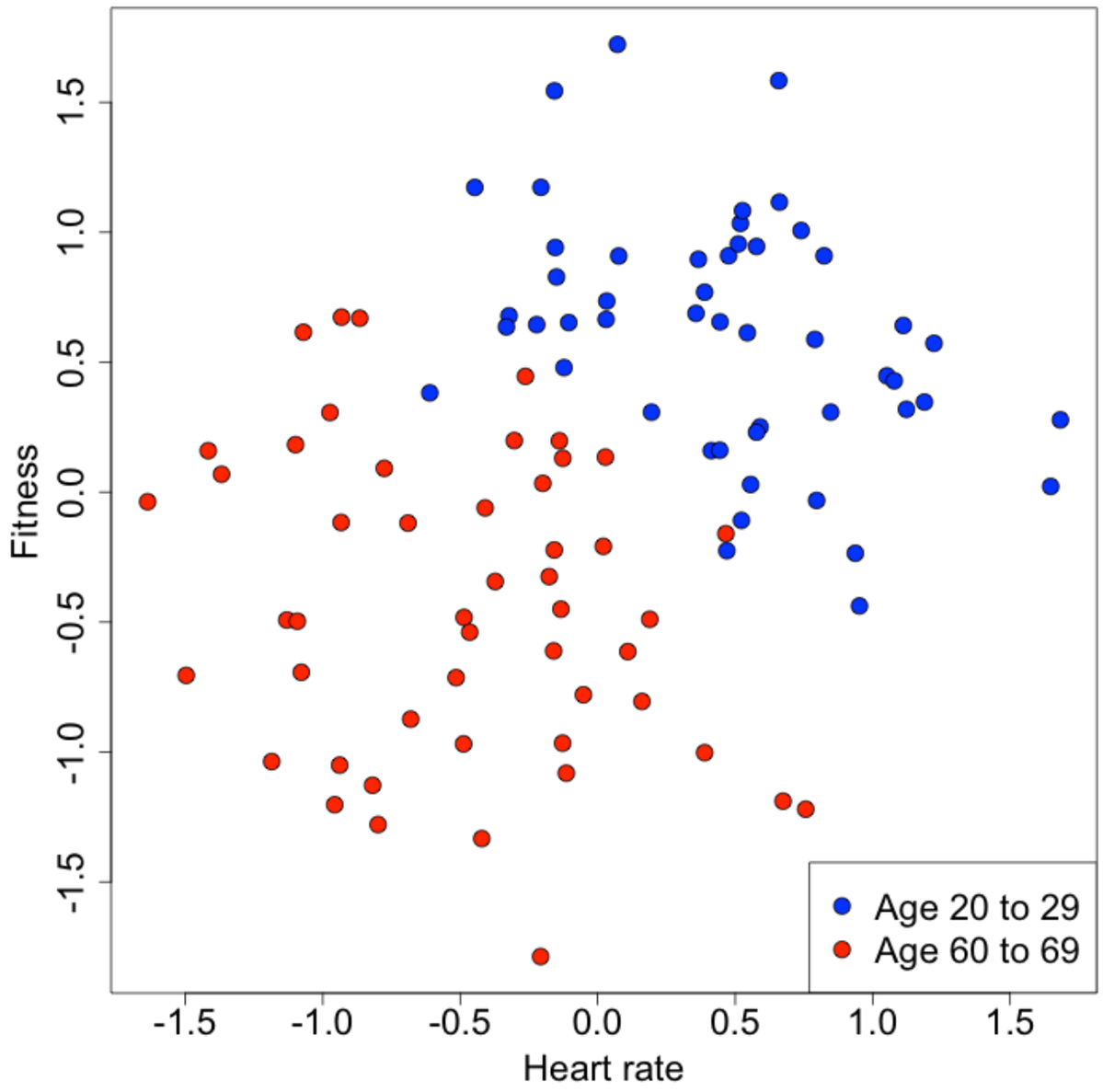
Today's lecture

1. Maximum margin classifiers
2. Support vector classifiers
3. Support vector machines
4. SVMs as a penalization method
5. SVMs for multiple classes

A more realistic dataset

- Let's simulate a more realistic dataset where the two age groups are harder to separate.

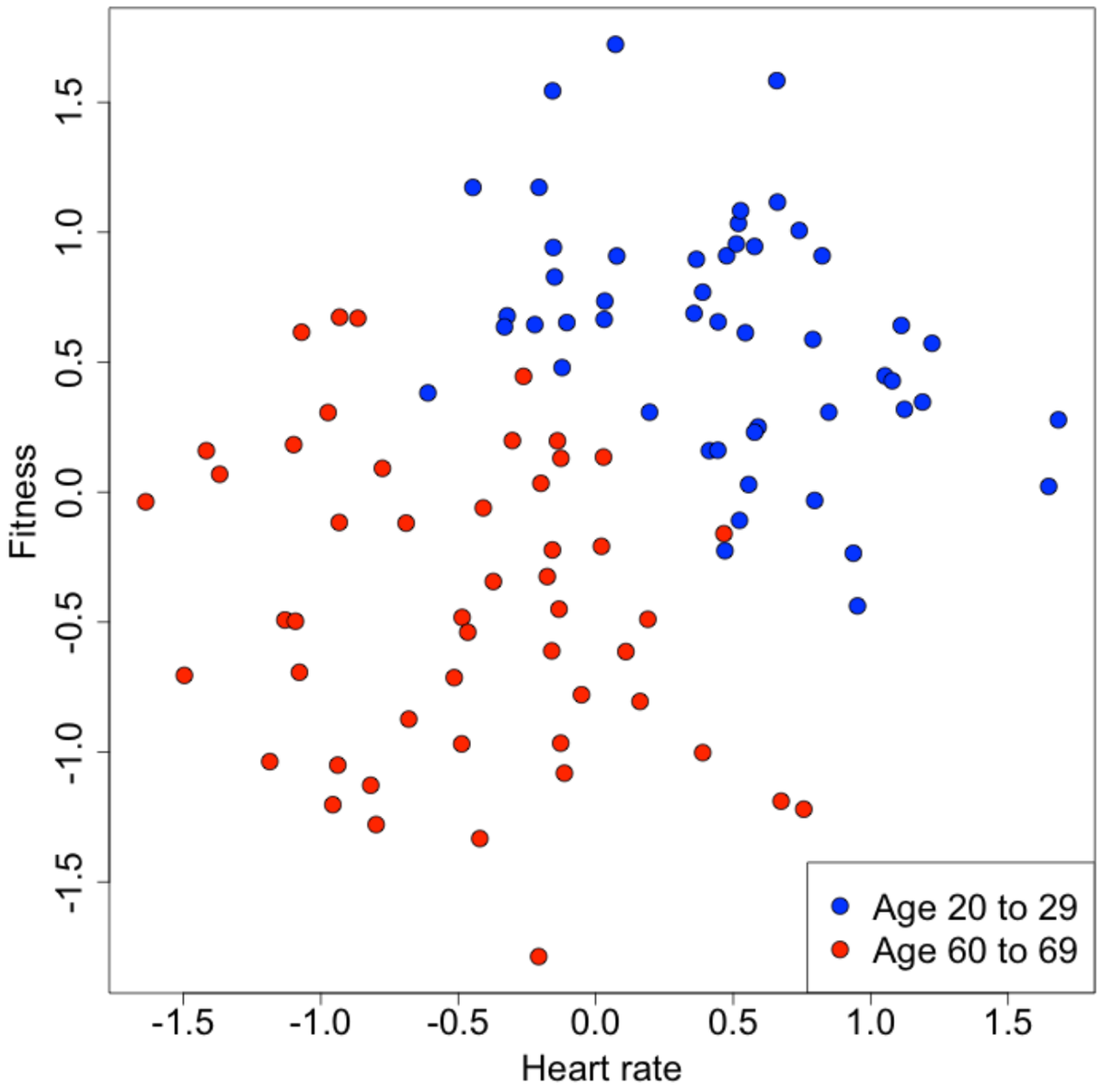
- What if there is no separating hyperplane?



What if there is no separating hyperplane?

- **Option 1**: Allow for misclassifications.
  - ***Support vector classifiers***

- **Option 2**: Draw a squiggly decision boundary between the two classes.
  - ***Support vector machines***



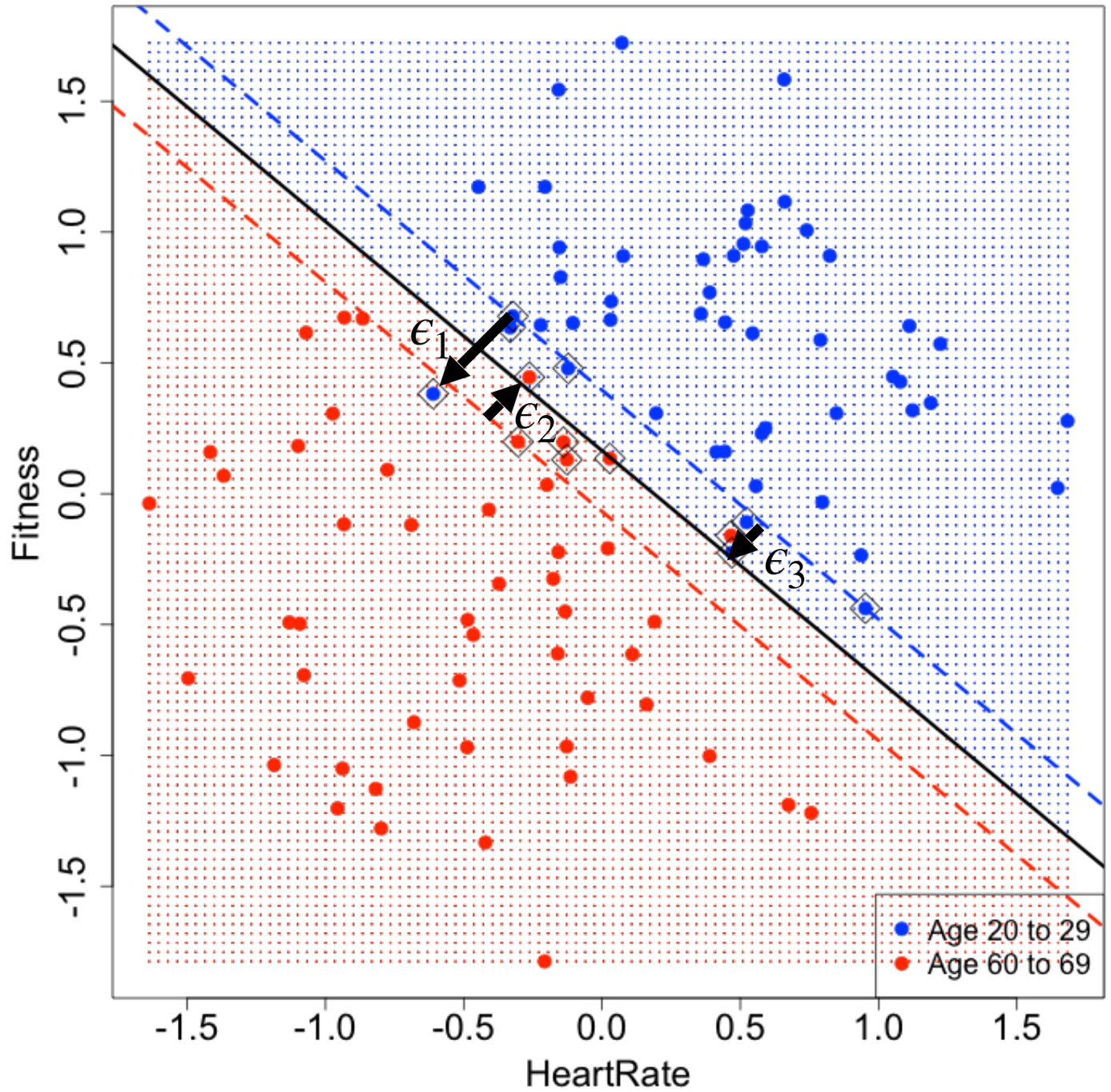
Support vector classifiers

(Also known as support vector machines with a linear kernel)

- Support vector classifiers allow for violations.

- The violation $\epsilon_i \geq 0$ for the i-th point measures how far the point is from the correct side of the margin boundary.

- ϵ_i is more commonly referred to as a ***slack variable***.



Support vector classifiers

For a training dataset $\{(x_i, y_i) : i = 1,...,n\}$, the support vector classifier finds a linear decision boundary that maximizes the margin M such that the **total allowed violation** is no more than some tuning parameter $C \geq 0$:

$$\max_{\beta_0,\beta,\epsilon,M} M$$ *(maximize the margin)*

such that $\|\beta\|_2^2 = 1$ and

$$\epsilon_i \geq 0 \text{ and } \sum_{i=1}^{n} \epsilon_i \leq C$$ *(constraint on the total violation)*

$$\underbrace{y_i(\beta_0 + \beta^\top x_i)}_{\text{Distance to the decision boundary}} \geq \underbrace{M(1 - \epsilon_i)}_{\text{A shrunken margin}} \text{ for all } i = 1,...,n$$

Maximum margin classifier

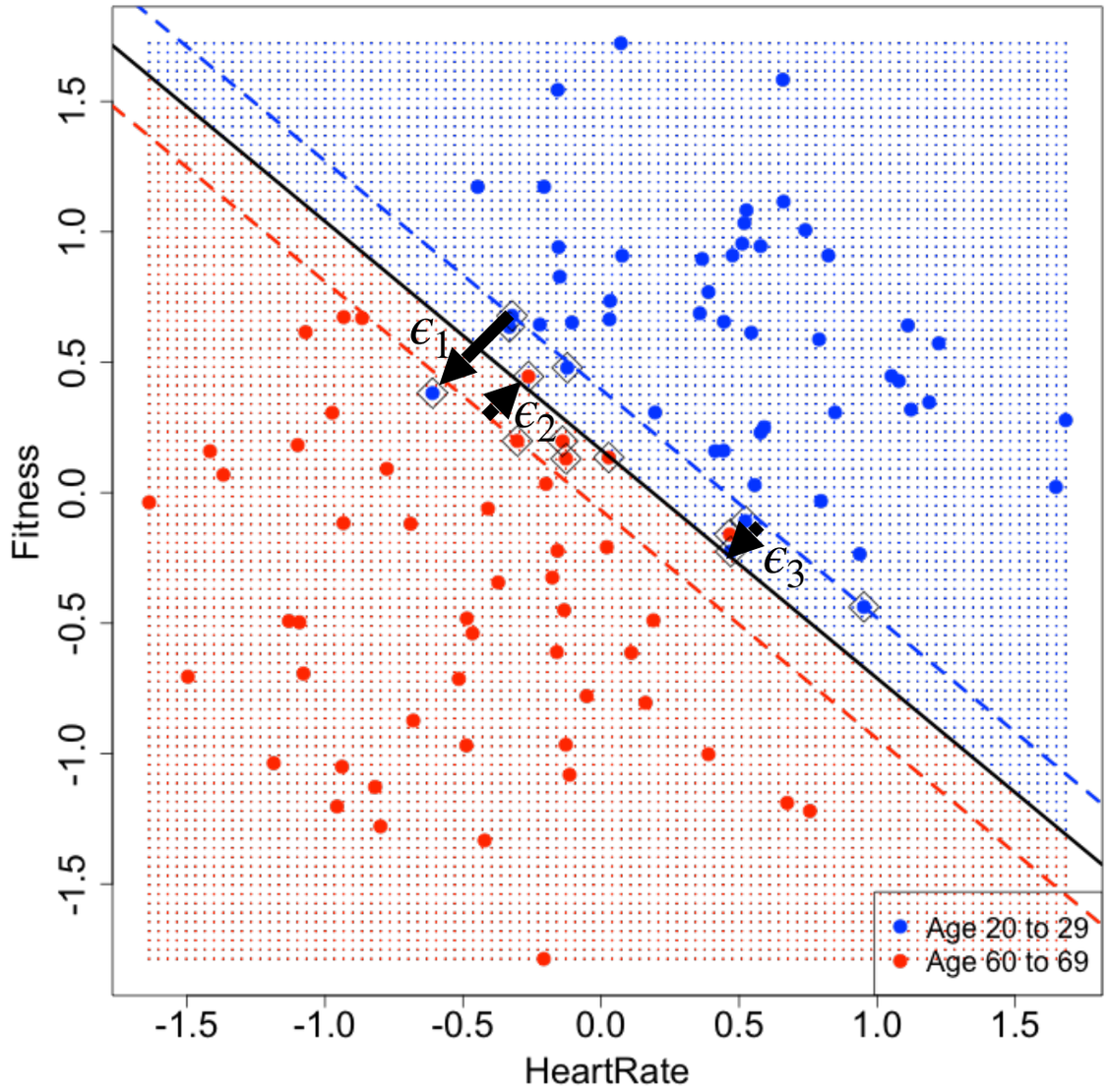
$$\max_{\beta_0,\beta,M} M$$

such that $\|\beta\|_2^2 = 1$ and

$$y_i(\beta_0 + \beta^\top x_i) \geq M \text{ for all } i$$

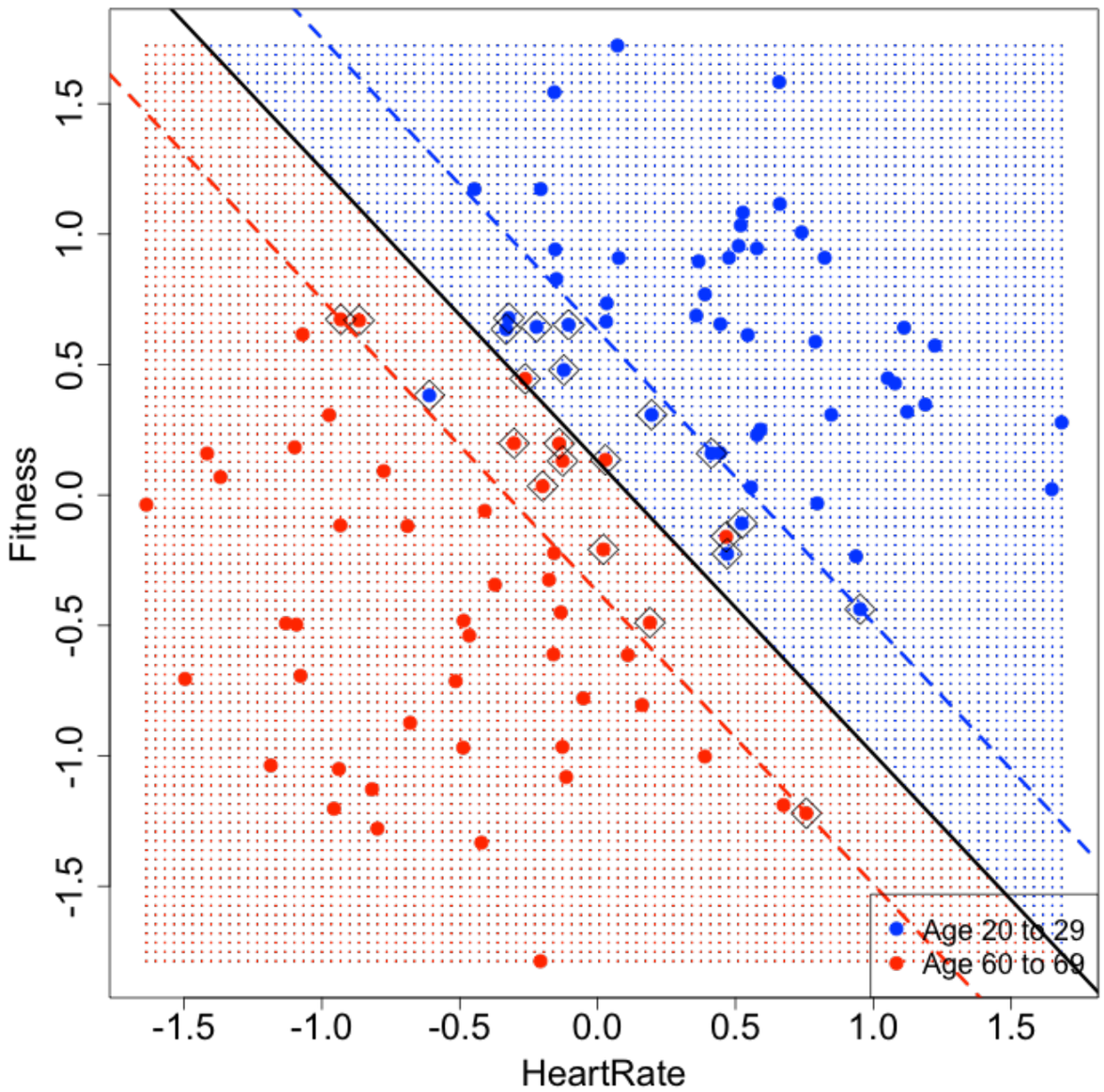
Support vector classifiers

- The value of slack variable ϵ_i indicates where the i-th observation is located:
  - $\epsilon_i = 0$ means the point is on the correct side of the margin boundary.
  - $0 < \epsilon_i \leq 1$ means the point is on the wrong side of the margin boundary but is on the correct side of the decision boundary.
  - $\epsilon_i > 1$ means the point is on the wrong side of the decision boundary.
- Support vectors = observations that determine the location/orientation of the decision boundaries, which includes points on the margin and points with $\epsilon_i > 0$

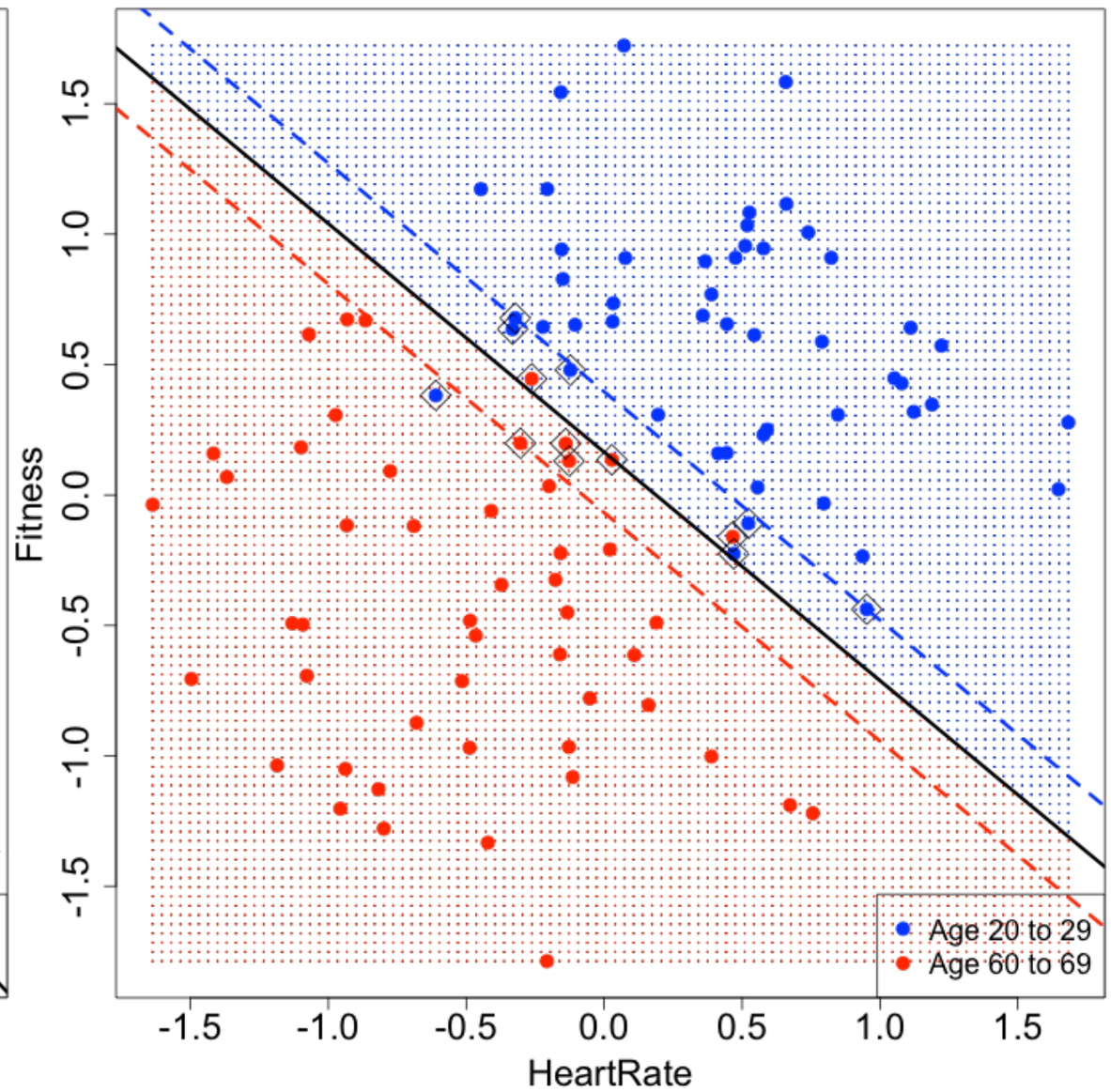


Different values of C

Allow for more violations (bigger C)

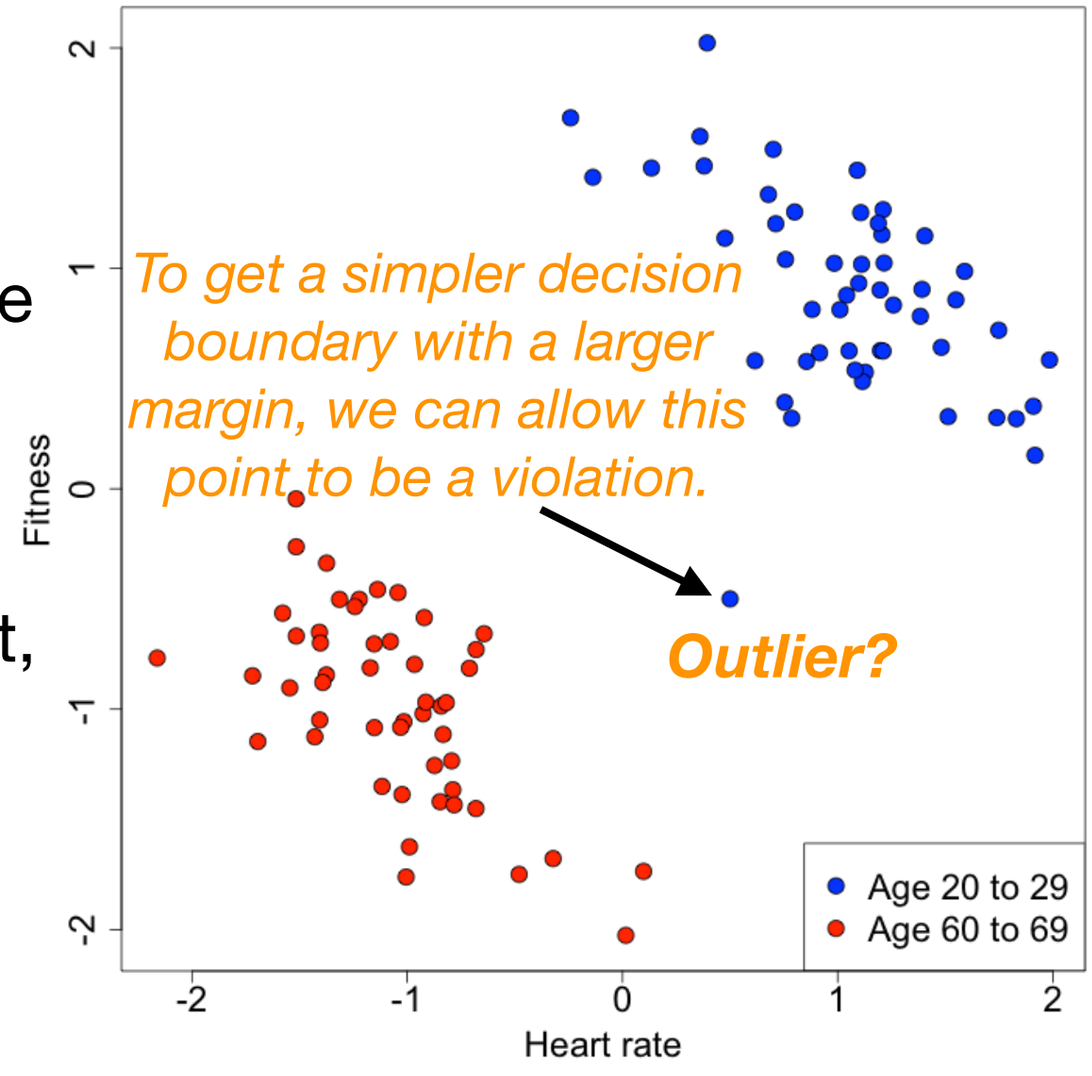


Allow for fewer violations (smaller C)



Support vector classifiers as a regularization method

- You can also view hyperparameter C as how much we want to regularize the decision boundary.
    - Bigger C means more regularization. As we allow for more violations, we can find "simpler" decision boundaries.
- Even for a perfectly separable dataset, you might still want to allow for violations (i.e. $C > 0$) because regularization can improve generalizability.



Fitting a support vector classifier in R

Same command, but now let's pay attention to the "cost" argument

```
> svmFit <- svm(ageGrp ~ Fitness + HeartRate, data=dat, kernel="linear", cost=10, scale=FALSE)
> summary(svmFit)

Call:
svm(formula = ageGrp ~ Fitness + HeartRate, data = dat, kernel = "linear",
    cost = 10, scale = FALSE)


Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  linear
       cost:  10

Number of Support Vectors:  3

 ( 1 2 )


Number of Classes:  2

Levels:
 -1 1
```

- `cost` in `svm` is the cost of violating, rather than the total violation hyperparameter C that we've been discussing.

- So higher `cost` in `svm` corresponds to smaller total allowed violation.

Cross-validation for support vector classifiers in R

- You can tune the value of the `cost` parameter using the `caret` package.

Support Vector Machines with Linear Kernel

```
method = 'svmLinear2'
```

Type: Regression, Classification

Tuning parameters:

- `cost` (Cost)

Required packages: `e1071`

http://topepo.github.io/caret/train-models-by-tag.html#support-vector-machines

```
train_control <- trainControl(method="cv", number=5)
cv_train <- train(
  ageGrp ~ Fitness + HeartRate,
  data = dat,
  method = "svmLinear2",
  trControl = train_control,
  tuneGrid = expand.grid(cost = exp(seq(-5, 5, length = 10)))
)
Support Vector Machines with Linear Kernel

100 samples
  2 predictor
  2 classes: '-1', '1'


No pre-processing
Resampling: Cross-Validated (5 fold)
Summary of sample sizes: 80, 80, 80, 80, 80
Resampling results across tuning parameters:

  cost          Accuracy  Kappa
  6.737947e-03  0.93      0.86
  2.046808e-02  0.95      0.90
  6.217652e-02  0.95      0.90
  1.888756e-01  0.95      0.90
  5.737534e-01  0.96      0.92
  1.742909e+00  0.96      0.92
  5.294490e+00  0.96      0.92
  1.608324e+01  0.95      0.90
  4.885657e+01  0.93      0.86
  1.484132e+02  0.93      0.86

Accuracy was used to select the optimal model using the largest value.
The final value used for the model was cost = 0.5737534.
```

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What if there is no separating hyperplane?

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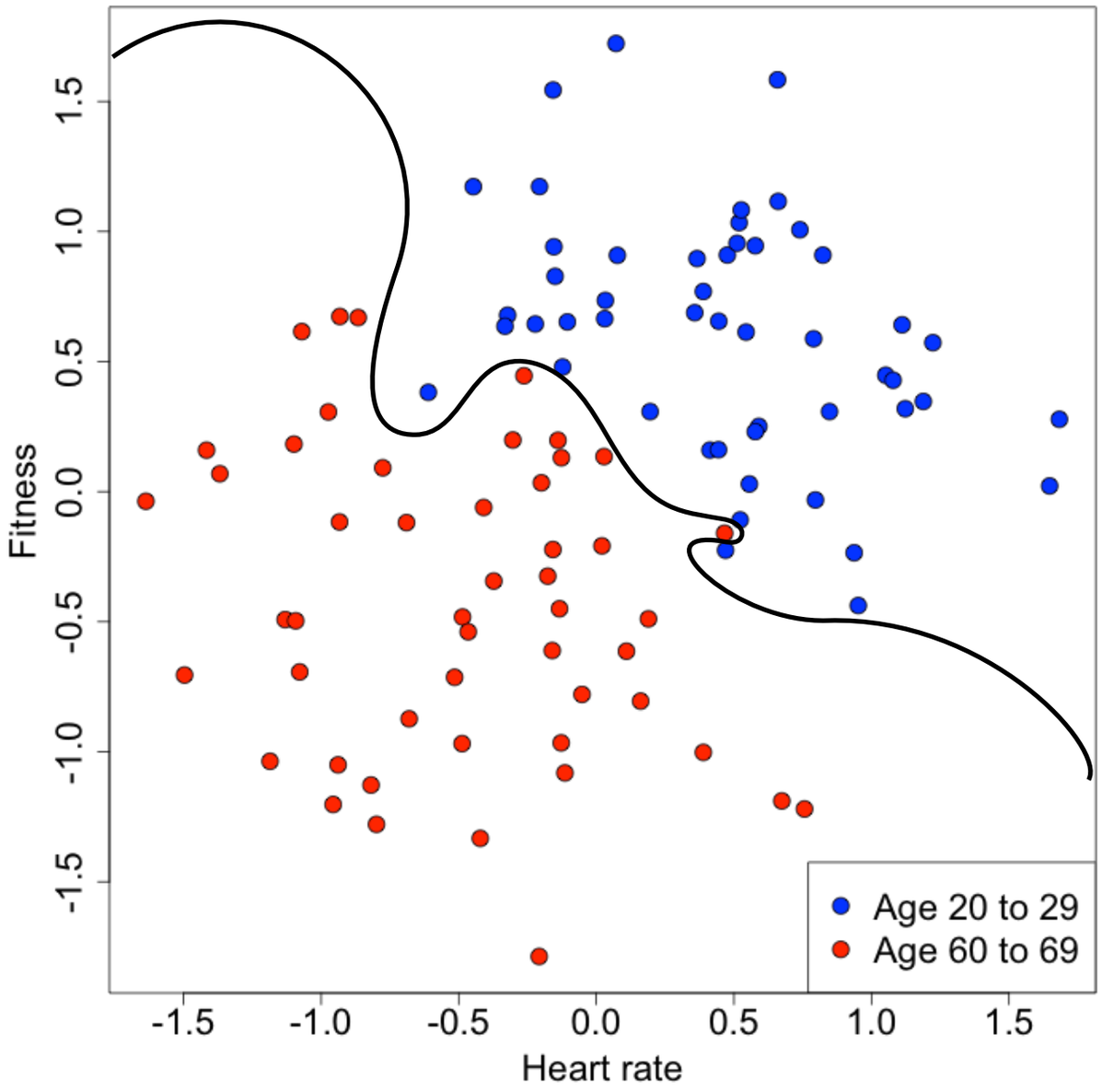
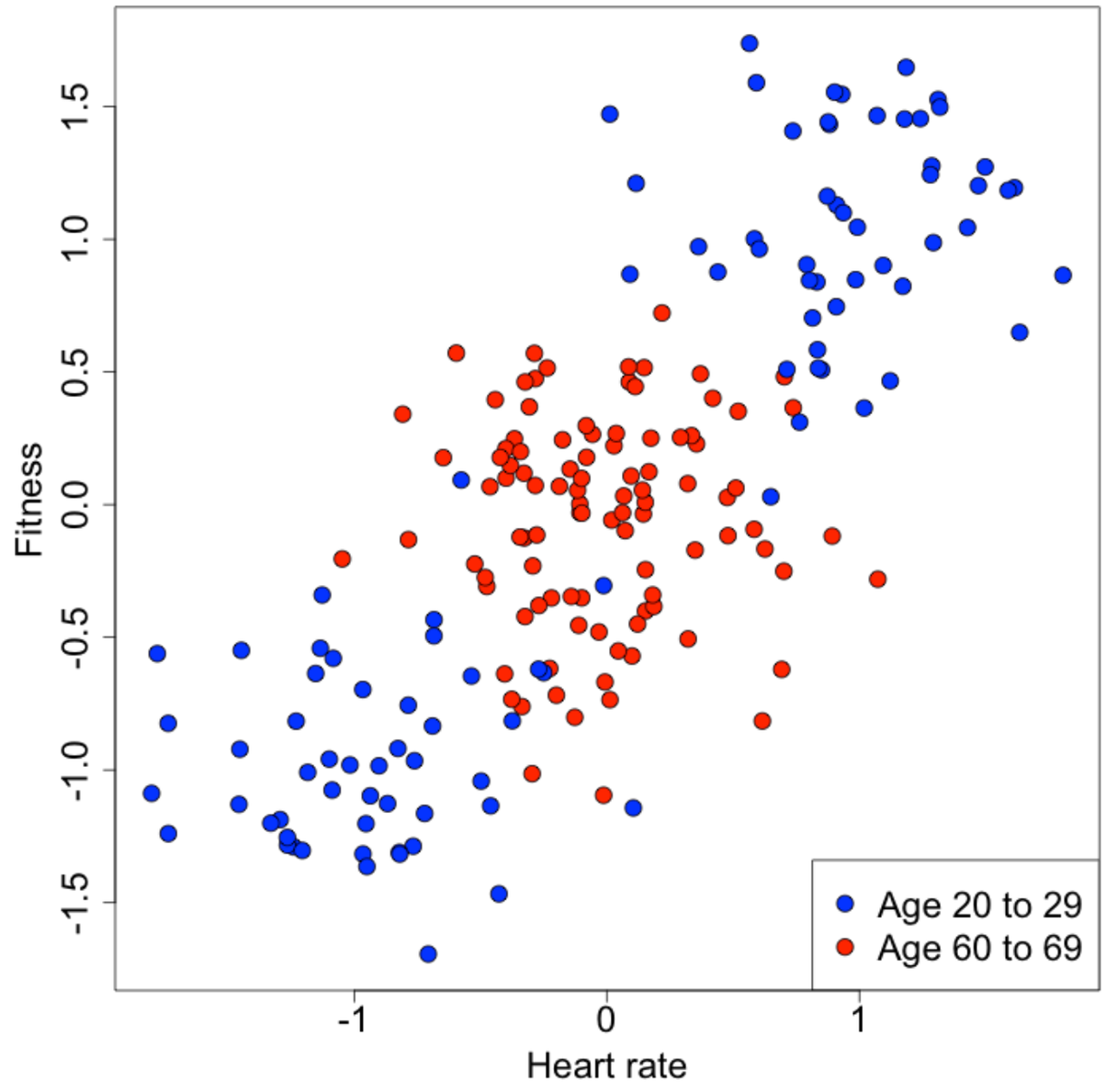


Warning: This decision boundary is probably not appropriate for this dataset

Example where a nonlinear decision boundary can help

- **Option 1**: Allow for misclassifications.
  - ***Support vector classifiers***

- **Option 2**: Draw a squiggly decision boundary between the two classes.
  - ***Support vector machines***



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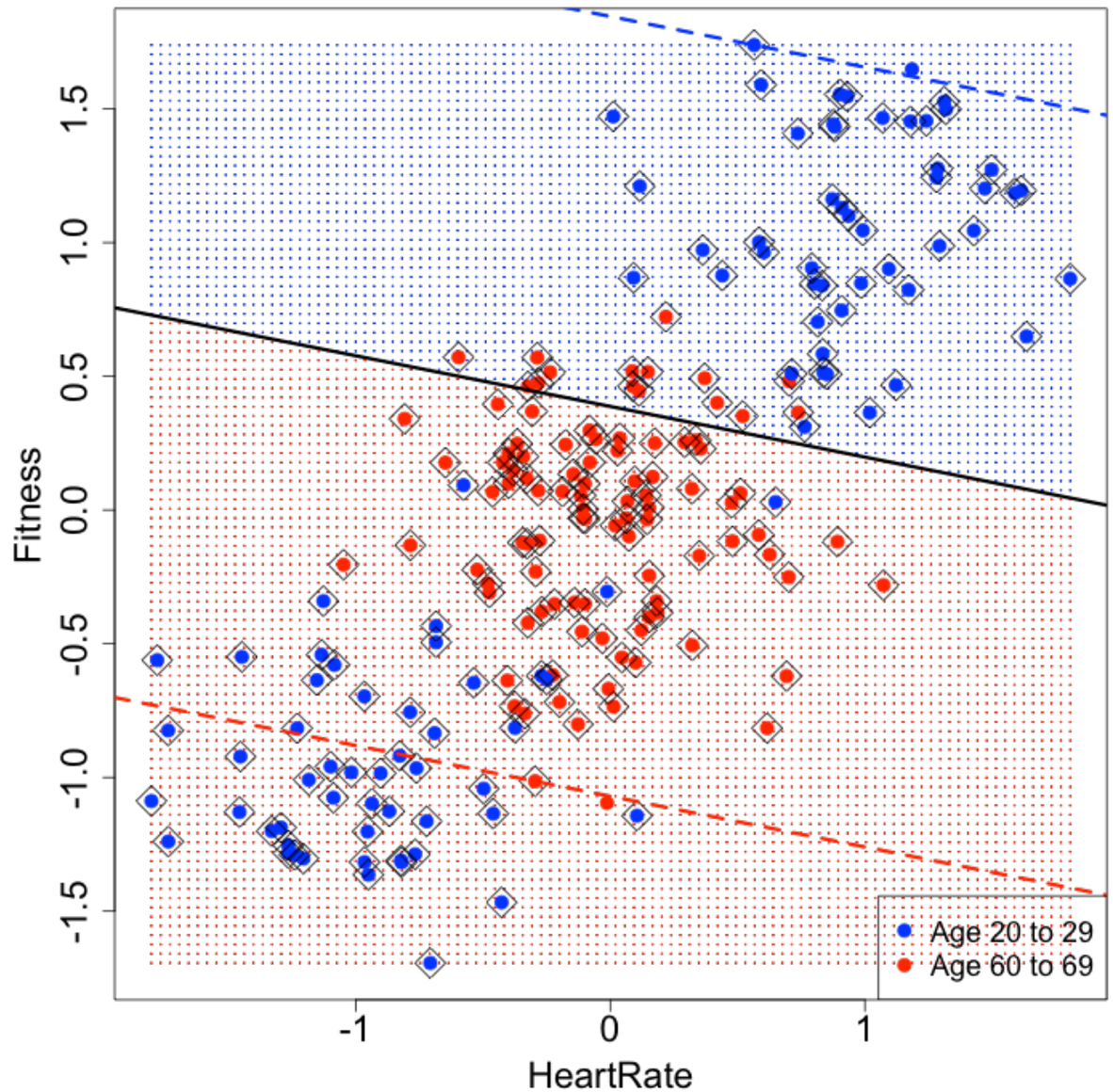

Example where a nonlinear decision boundary can help

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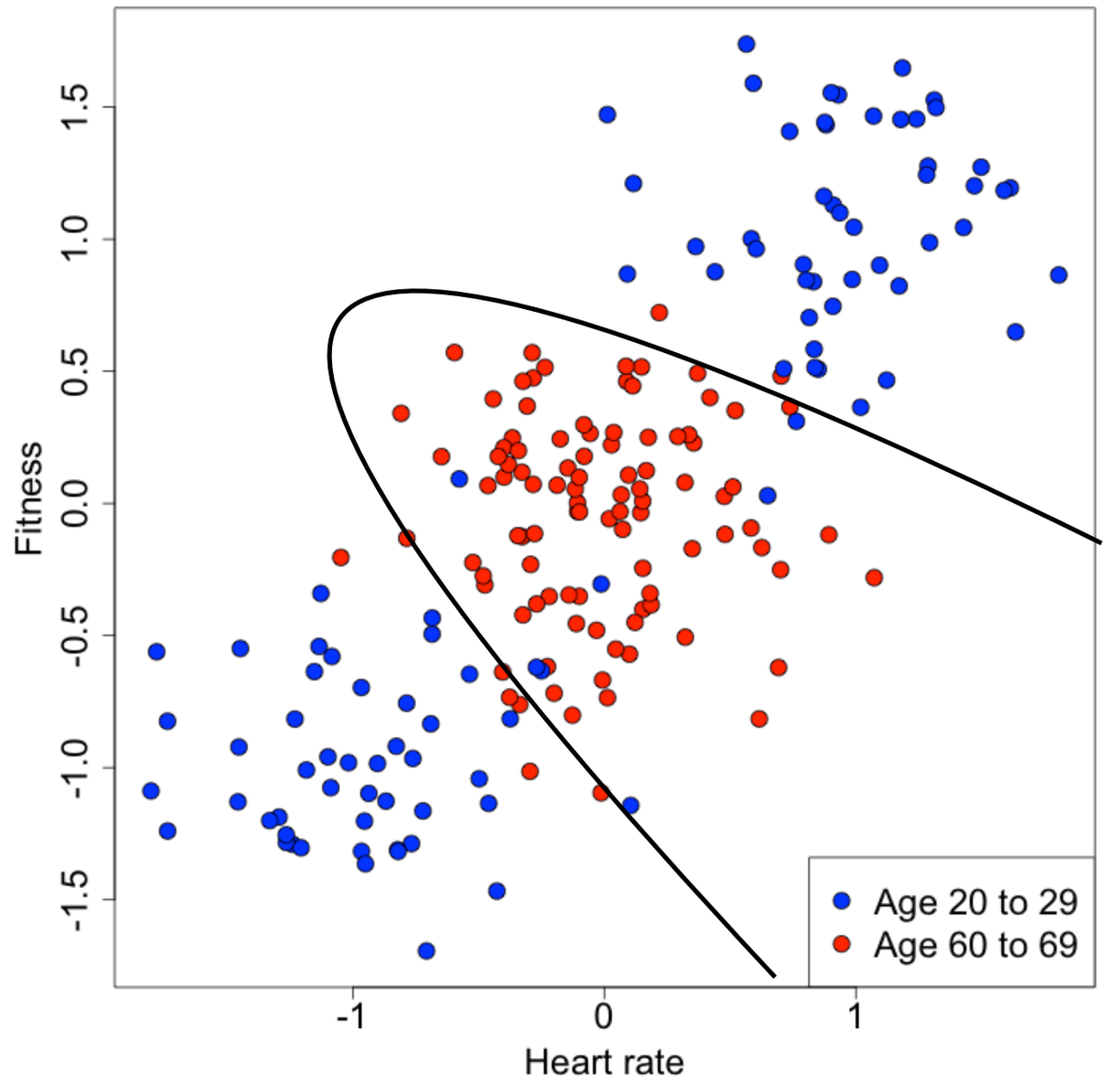


Suppose we had two variables (X_1, X_2). Which of these methods fits a quadratic decision boundary?

- **A**: Fit a support vector classifier on an augmented set of variables: $(X_1, X_2, X_1X_2, X_1^2, X_2^2)$

  This fits a quadratic decision boundary and accounts for interactions

- **B**: Fit a support vector classifier on an augmented set of variables: (X_1, X_2, X_1^2, X_2^2)

  This fits a quadratic decision boundary, but doesn't allow for interactions

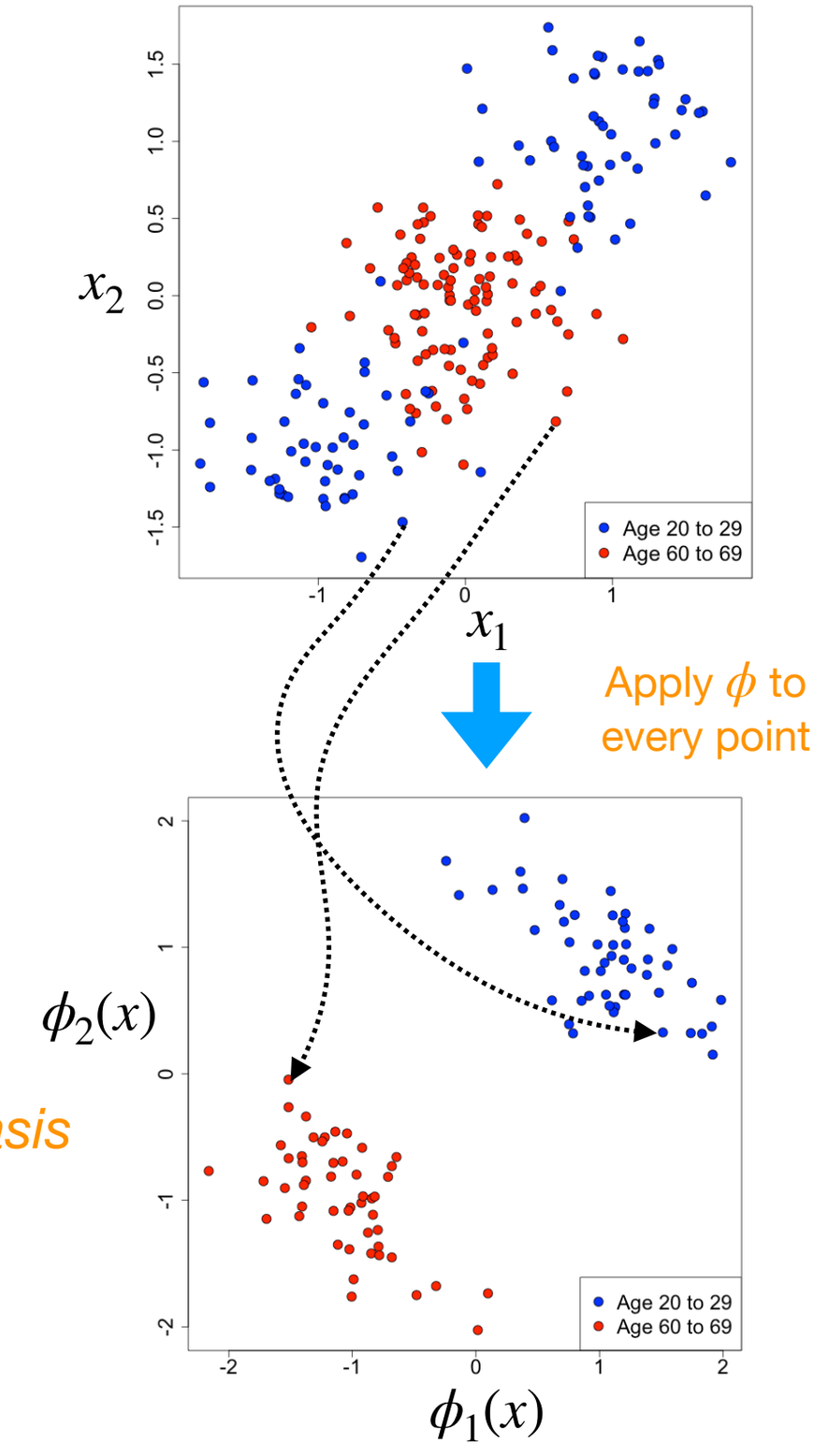
- **C**: Fit a support vector classifier for the variables: (X_1, X_2)

  This fits a linear decision boundary.

Recall: Polynomial regression

- Remember that we can fit non-linear models using linear regression by expanding terms. For example:
  - $(x_1) \rightarrow (x_1, x_1^2, x_1^3)$
  - $(x_1, x_2) \rightarrow (x_1, x_1^2, x_2, x_2^2, x_1 x_2)$
- More generally, we can perform a **basis expansion**. That is, we create a new feature set using a sequence of basis functions $\{\phi_1, \cdots, \phi_k\}$ as follows:
  - $x \rightarrow (\phi_1(x), \phi_2(x), \cdots, \phi_k(x))$

Polynomial basis
Spline basis
Radial basis
…



Fitting a non-linear decision boundary

- We can fit a non-linear decision boundary by applying a basis expansion and before fitting a support vector classifier.

- The decision function will have the form

$$f_{\beta_0,\beta}(x) = \beta_0 + \sum_{j=1}^{k} \beta_j \phi_j(x).$$

- However, this procedure can be very computationally expensive if k is very big and impossible to run if we want to consider $k = \infty$.

Support vector machines

- Support vector machines extend support vector classifiers to fit non-linear decision boundaries.

- SVMs use the "***Kernel Trick***" to efficiently estimate a nonlinear decision boundary when k is very large.

The Kernel Trick

It turns out that…

<u>Support vector classifier</u>

$$\max_{\beta_0,\beta,M,\epsilon} M$$

such that $\|\beta\|_2^2 = 1, \epsilon_i \geq 0\,, \sum_{i=1}^{n} \epsilon_i \leq C$

$y_i(\beta_0 + \beta^\top x_i) \geq M(1-\epsilon_i)$ for all i

must have a solution of the form:

$$f_{\beta_0,\alpha}(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle$$

where $\langle x, z \rangle = \sum_{j=1}^{p} x_j z_j$.

Inner product with the i-th training observation

<u>Support vector machine</u>

$$\max_{\beta_0,\beta,M,\epsilon} M$$

such that $\|\beta\|_2^2 = 1, \epsilon_i \geq 0\,, \sum_{i=1}^{n} \epsilon_i \leq C$

$y_i(\beta_0 + \beta^\top \phi(x_i)) \geq M(1-\epsilon_i)$ for all i

must have a solution of the form:

$$f_{\beta_0,\alpha}(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle \phi(x), \phi(x_i) \rangle.$$

Inner product with the i-th (transformed) training observation

The Kernel Trick

Support vector machine

$$\max_{\beta_0,\beta,M,\epsilon} M$$

such that $\|\beta\|_2^2 = 1, \epsilon_i \geq 0\ , \sum_{i=1}^{n} \epsilon_i \leq C$

$y_i(\beta_0 + \beta^\top \phi(x_i)) \geq M(1 - \epsilon_i)$ for all i

must have a solution of the form:

$$f_{\beta_0,\alpha}(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle \phi(x), \phi(x_i) \rangle.$$

Inner product with the i-th (transformed) training observation

- To solve this optimization problem, all we need to compute are the inner products. We don't need to actually compute $\phi(x)$.
- For special sequences of basis functions ϕ, the ***inner product*** can be computed very efficiently using a so-called "***Kernel function***": $K(x, x') = \langle \phi(x), \phi(x') \rangle$
- d-order Polynomial Kernel:

$$K(x, x') = \left(r + \sum_{j=1}^{p} x_i x'_j\right)^d$$

- Radial Basis Kernel:

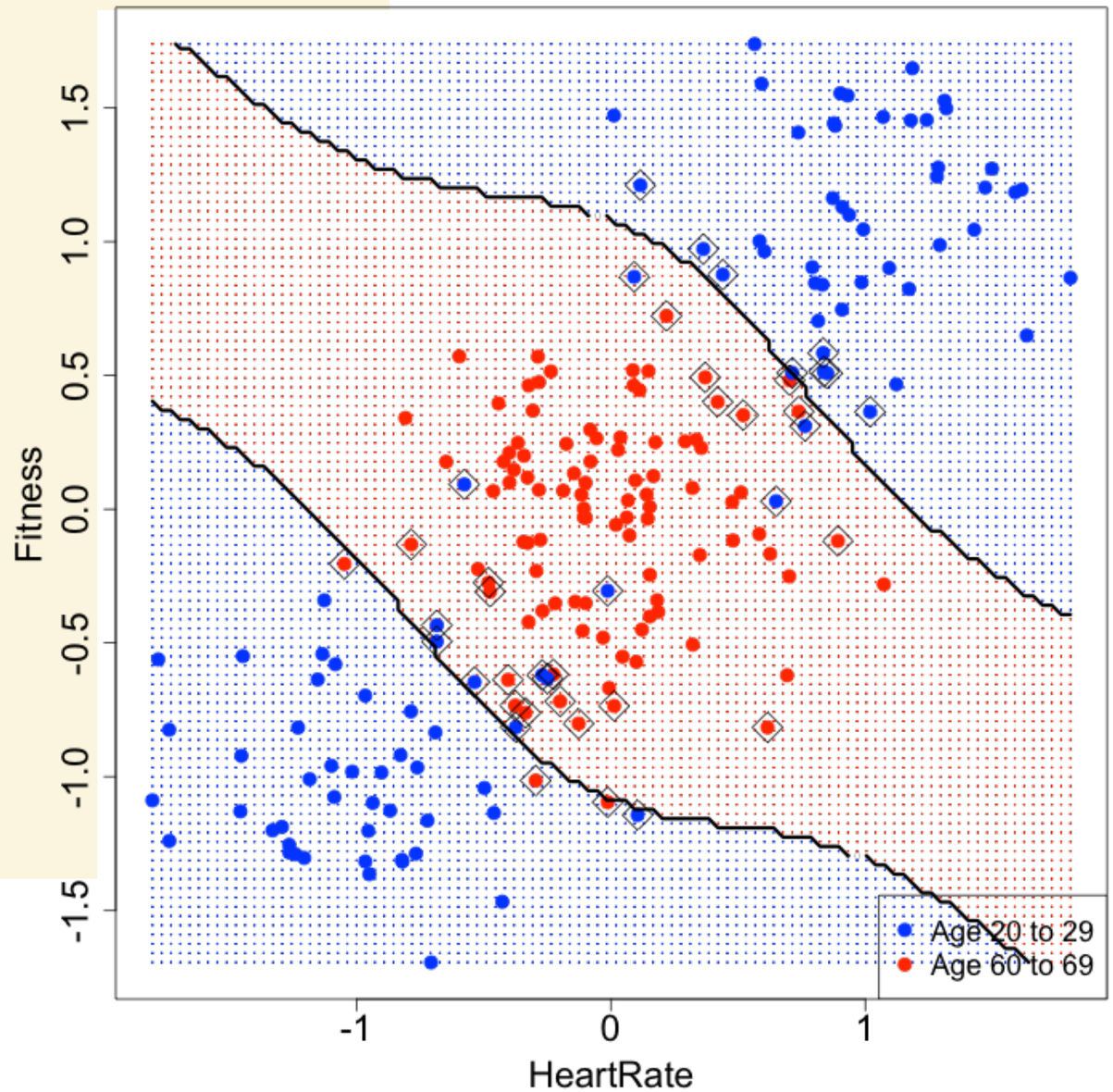
$$K(x, x') = \exp\left(-\gamma \left\| x - x' \right\|_2^2\right)$$

(In fact, $k = \infty$ for the radial basis kernel!)

Example: polynomial kernel

- Fit an SVM using a polynomial kernel with $d = 4$ and cost = 10.

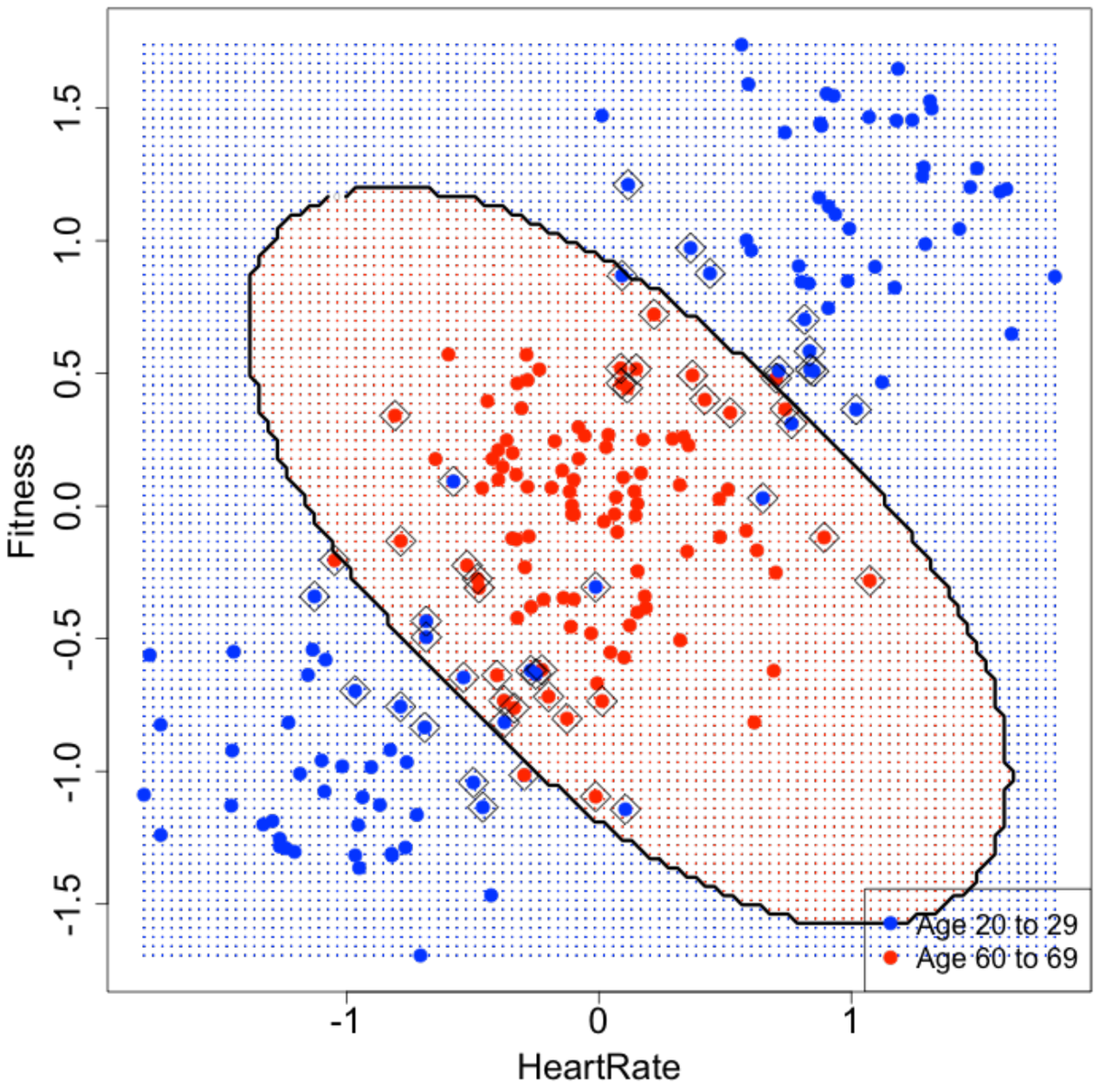
```
> svmFitSVM <- svm(ageGrp ~ Fitness + HeartRate, data=dat, kernel="polynomial",
 degree=4, cost=10, scale=FALSE)
> summary(svmFitSVM)

Call:
svm(formula = ageGrp ~ Fitness + HeartRate, data = dat, kernel = "polynomial",
    degree = 4, cost = 10, scale = FALSE)


Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  polynomial
       cost:  10
     degree:  4
     coef.0:  0

Number of Support Vectors:  41

 ( 21 20 )


Number of Classes:  2

Levels:
 -1 1
```



Example: Radial basis kernel

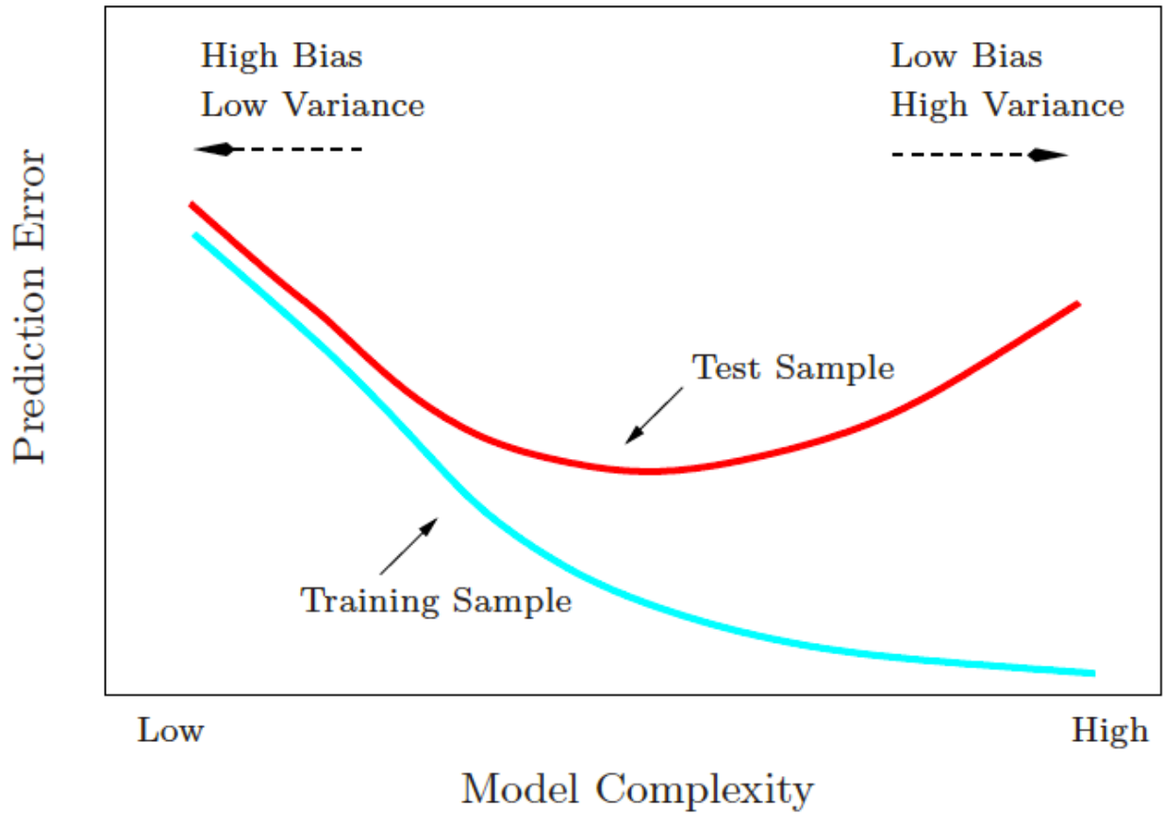
- Fit an SVM using a radial basis kernel with $\gamma = 0.1$ and cost=10.

```
> svmFit_radial <- svm(ageGrp ~ Fitness + HeartRate, data=dat, kernel="radial",
  gamma=0.15, cost=10, scale=FALSE)
```



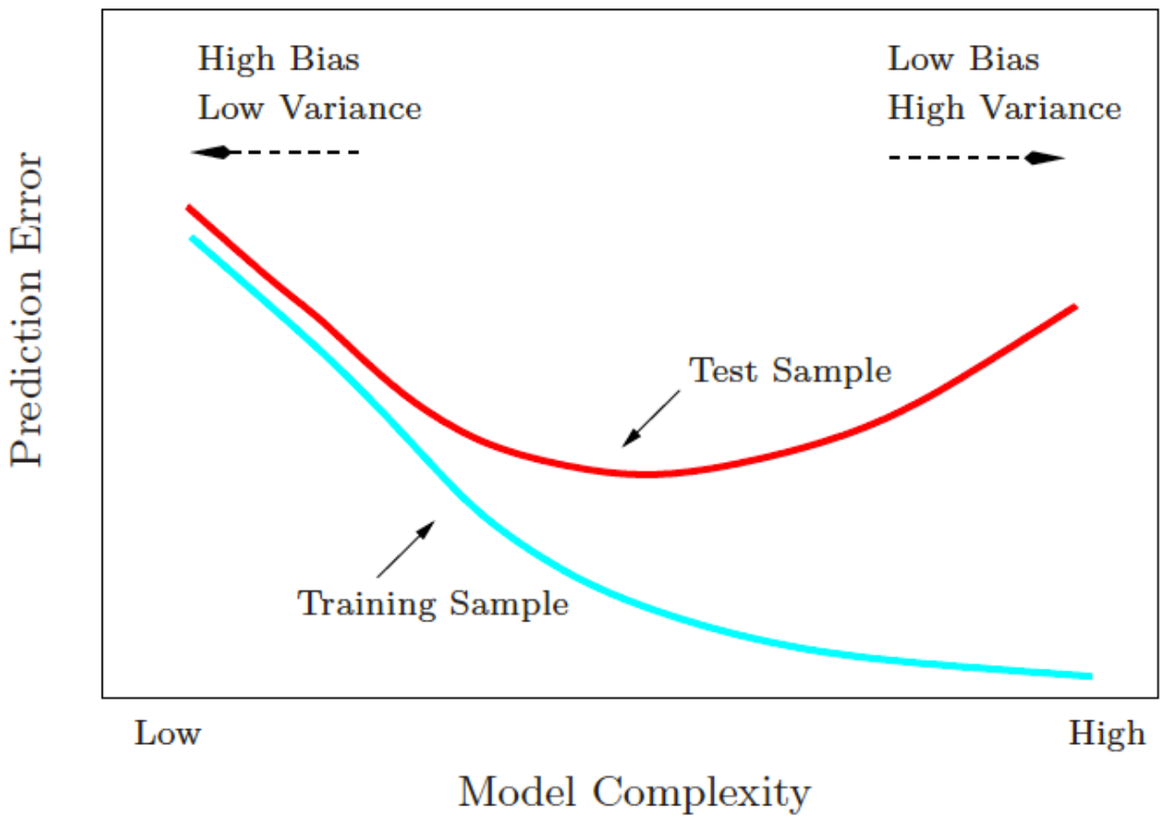
$$K(x, x') = \exp\left(-\gamma \parallel x - x' \parallel_2^2\right)$$

Q: In terms of the bias-variance tradeoff, how would you rank an SVM with a linear kernel versus an SVM with a non-linear kernel?



- **A**: SVM with a linear kernel has lower model complexity.
- **B**: SVM with a non-linear kernel has lower model complexity.

Q: In terms of the bias-variance tradeoff, how would you rank an SVM with a linear kernel versus an SVM with a non-linear kernel?



- **A**: SVM with a linear kernel has lower model complexity.

- **B**: SVM with a non-linear kernel has lower model complexity.

Estimating a non-linear decision boundary accurately generally requires more observations and is particularly difficult in high-dimensional settings where $p \gg n$.

How should I choose between using a linear versus non-linear kernel?

- **A**: Hard to tell. Use cross-validation.
    - Good choice!
- **B**: If the true decision boundary is non-linear, use a non-linear kernel.
    - A non-linear kernel is most effective when 1) *you have lots of observations relative to the number of features* and 2) the boundary is truly non-linear.
- **C**: If the number of observations is small, it will be impossible to accurately estimate a non-linear decision boundary.
    - Estimating a non-linear decision boundary accurately generally requires more observations and is particularly difficult in high-dimensional settings where $p \gg n$.

Today's lecture

1. Maximum margin classifiers

2. Support vector classifiers

3. Support vector machines

4. SVMs as a penalization method

5. SVMs for multiple classes

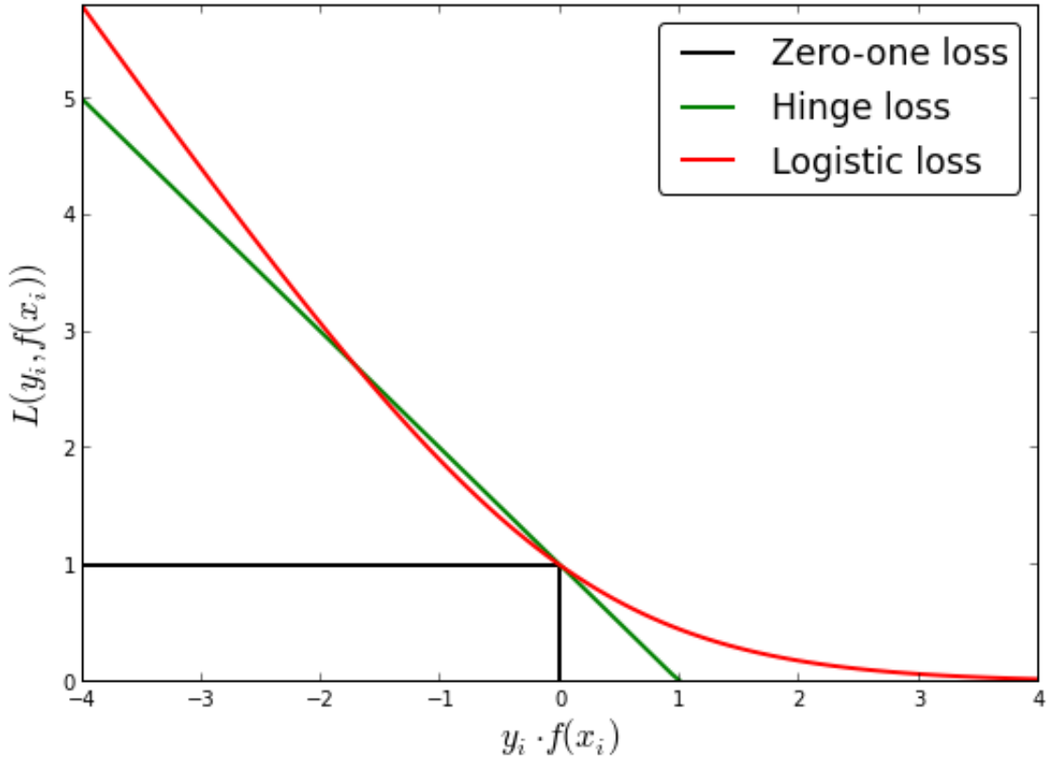
SVMs as a penalized regression method

Support vector classifier (SVC)

$$\max_{\beta_0,\beta,M,\epsilon} M$$

such that $\|\beta\|_2^2 = 1, \epsilon_i \geq 0\,, \sum_{i=1}^{n} \epsilon_i \leq C$

$y_i(\beta_0 + \beta^\top x_i) \geq M(1-\epsilon_i)$ for all i



The same thing (SVC)

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, f_\beta(x_i)\right) + \lambda\|\beta\|^2$$

with hinge loss:

$\ell(y, f(x)) = \max(0, 1 - f(x)y)$

Logistic regression with a ridge penalty

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, f_\beta(x_i)\right) + \lambda\|\beta\|^2$$

with logistic loss

$\ell(y, f(x)) = \log(1 + \exp(-f(x)y))$

Solving the more general penalized regression problem…

Support vector classifier

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, f_\beta(x_i)\right) + \lambda \|\beta\|^2$$

with hinge loss:

$$\ell(y, f(x)) = \max(0, 1 - f(x)y)$$

Logistic regression with a ridge penalty

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, f_\beta(x_i)\right) + \lambda \|\beta\|^2$$

with logistic loss

$$\ell(y, f(x)) = \log(1 + \exp(-f(x)y))$$

Introduce non-linearities using basis functions $\{\phi_1, \ldots, \phi_k\}$

Support vector ***machine***

$$\min_{\beta_0, \alpha} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, \beta_0 + \sum_{j=1}^{k} \alpha_j \phi_j(x_i)\right) + \lambda \|\alpha\|^2$$

with hinge loss:

$$\ell(y, f(x)) = \max(0, 1 - f(x)y)$$

Logistic regression with a ridge penalty

$$\min_{\beta_0, \alpha} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, \beta_0 + \sum_{j=1}^{k} \alpha_j \phi_j(x_i)\right) + \lambda \|\alpha\|^2$$

with logistic loss

$$\ell(y, f(x)) = \log(1 + \exp(-f(x)y))$$

We can use the ***kernel trick*** *with* $K(x, x') = \langle \phi(x), \phi(x') \rangle$ *to solve* ***both*** *of these optimization problems efficiently*

Is the Kernel Trick unique to SVMs?

- **No**. Both SVMs and logistic regression can be written as minimizers of a penalized empirical loss. Both can be combined with the Kernel Trick to fit non-linear decision boundaries.

- For historical reasons, non-linear kernels are much more common in the context of SVMs.

In high dimensions…

- In SVMs, the tuning parameter C controls the amount of flexibility of the classifier.

- Because SVMs can be written as ridge regression but with a hinge loss, tuning C is similar to tuning the penalty parameter in ridge regression. The SVM decision rule involves all p variables.

- You can fit a sparse SVM by replacing the ridge penalty with a lasso penalty; this yields a decision rule involving only a subset of the features.

- People used to claim that SVMs overcome the "curse of dimensionality". This is not true!

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Multiple classes

- The separating hyperplane idea in SVMs does not lend itself naturally to more than 2 classes. Still, there are some extensions that are quite popular:

  - **One-versus-One** (OVO): Construct an SVM for every pair of classes. For a test observation, predict the class that won the most pairwise competitions.

  - **One-versus-All** (OVA): Fit K SVMs, where each SVM predicts a class vs. the rest. For a test observation, predict the class with the largest decision function.

Summary

- Pros:
    - SVMs are very good off-the-shelf binary classifiers. They have won many machine learning competitions.
    - SVMs are computationally efficient.
- Cons:
    - When non-linear decision boundaries are used, they are not easily interpretable.
    - It doesn't output probabilities for each class.

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