Lecture 9: Supervised learning

STAT598z: Intro. to computing for statistics

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Supervised learning

We are given training data $(X, Y) = \{(x_1, y_1), \cdots, (x_N, y_N)\}$

- X: independent variables, inputs, predictors, features
- Y: dependent variables, outputs, response

$x \in \mathbb{R}^P$ (usually)

- regression: $y \in \mathbb{R}$
- classification: $y \in \{0, 1\}$
- structured prediction: More complicated high-dimensional spaces with dependent components (e.g. the space of images or sentences)

We assume $y_i = f(x_i) + \varepsilon_i$

ε is noise (includes randomness and approximations)

- Independently and identically distributed (i.i.d.) according to some probability distrib. (e.g. Gaussian)

Given the training set (X, Y), we want to estimate f:

- to study the relation between x and y
- to make predictions of y's for unobserved x's

Good predictors can be hard to interpret

Parametric learning

Index functions f by a finite-dimensional parameter vector

E.g. linear regression

- Parameters are coefficients of a hyperplane
- Parameters have a clear interpretation
- Can be a bad approximation of reality

Linear regression

via the `lm` function in R

In [ ]:
```
DataIncm <- read.table('Data/Income2.csv',header=T,sep=',')
ggplot(DataIncm) + geom_point(aes(x=Education,y=Income))
```

In [ ]:
```
fit <- lm(Income ~ Education, DataIncm)
```

The first argument is a formula

- takes the form response ~ predictors
- response is a linear combination of predictors
- above we have just one predictor: $Education$
- $Income = \beta_1 \cdot Education + \beta_0 + \epsilon$

Second argument unnecessary if variables in formula exist in current environment

See documentation for other optional arguments

Can print `fit`:

In [ ]:
```
fit
```

This is not all the information in `fit` (why?)

- Try `typeof()`, `class()`, `str()`
- Try plotting it

In [ ]:
```
print.default(fit)
```

Observe fit contains the entire dataset!

Can disable with `model = FALSE` option

Can directly plot with ggplot :

In [ ]:
```
plt1 <- ggplot(DataIncm, aes(x=Education, y = Income)) +
          geom_point(size=2, color='blue') +
          theme(text=element_text(size=10))
```

In [ ]:
```
plt1 + geom_smooth(method='lm', se=FALSE, #Disable std. errors
                   color='magenta', size=2)
```

Can regress against Seniority

In [ ]:
```
fit <- lm(Income ~ Seniority, DataIncm)
```

Can regress against both Education and Seniority

In [ ]:
```
fit <- lm(Income ~ Education + Seniority, DataIncm)
```

- + does *not* mean input is sum of Educ. and Sen.

Rather: $Income = \beta_2 \cdot Seniority + \beta_1 \cdot Education + \beta_0 + \varepsilon$

For the former, use `I`:

```
fit <- lm(Income ~ I(Education + Seniority), DataIncm)
```

- $Income = \beta_1 \cdot (Seniority + Education) + \beta_0 + \varepsilon$

Prediction

In [ ]:
```
fit <- lm(Income ~ Education + Seniority, DataIncm)
```

How do we make predictions at a new set of locations? E.g. (15, 60) and (20, 160)?

In [ ]:
```
pred_locn <- data.frame(Education=c(15,20), Seniority= c(60,160))
predict.lm(fit, pred_locn)
```

In [ ]:

```
edu_pred <- 10:25
sen_pred <- seq(0,200,10)
pred <- data.frame(Education=rep(edu_pred, length(sen_pred)),
               Seniority=rep(sen_pred, each=length(edu_pred) ))
p_val <- predict.lm(fit, pred)
pred_full <- cbind(pred,p_val)
```

In [ ]:

```
plt <- ggplot(DataIncm, aes(x=Education, y=Seniority,
                          color=Income))+
    geom_tile(data=pred_full, aes(x=Education, y=Seniority,
                                  color=p_val, fill=p_val)) +
    geom_point(size=1) + theme(text=element_text(size=10)) +
    scale_color_continuous(low='blue', high='red') +
    scale_fill_continuous(low='blue', high='red') +
    geom_point(shape=1,size=1,color='black') +
      guides(fill=FALSE) # Remove legend for 'fill'
```

In [ ]:

```
plt
```

Specifying a model for `lm`

Symbol	Meaning	Example
+	Include variable	x + y
:	Interaction between vars	x + y + z + x:z + y:z
*	Variables and interactions	(x + y) * z
^	Vars and intrcns to some order	(x + y + z)^3
-	Delete variable	(x + y + z)^3 - x:y:z
poly	Polynomial terms	poly(x,3) + (x + y) * z
I	New combination of vars	I(x*y + z)
1	Intercept	x - 1

See documentation and http://ww2.coastal.edu/kingw/statistics/R-tutorials/formulae.html (http://ww2.coastal.edu/kingw/statistics/R-tutorials/formulae.html)

Generalized linear model

A linear model with Gaussian noise is often inappropriate. E.g.

- response is always positive
- count valued response
- {0, 1} or binary-valued as in classification

A better model might be:

$response = g(\sum_{i=1}^{N} \beta_i \cdot predictor_i) + \varepsilon$

g is a ‘link’ function, ε is no longer Gaussian

Can fit in R with `glm()` (see documentation)

Nonparametric methods

No longer limit yourself to a parametric family of functions

Much more flexible

Often much better prediction

Complexity of f can grow with size of dataset

Often hard to interpret

k-nearest neighbors

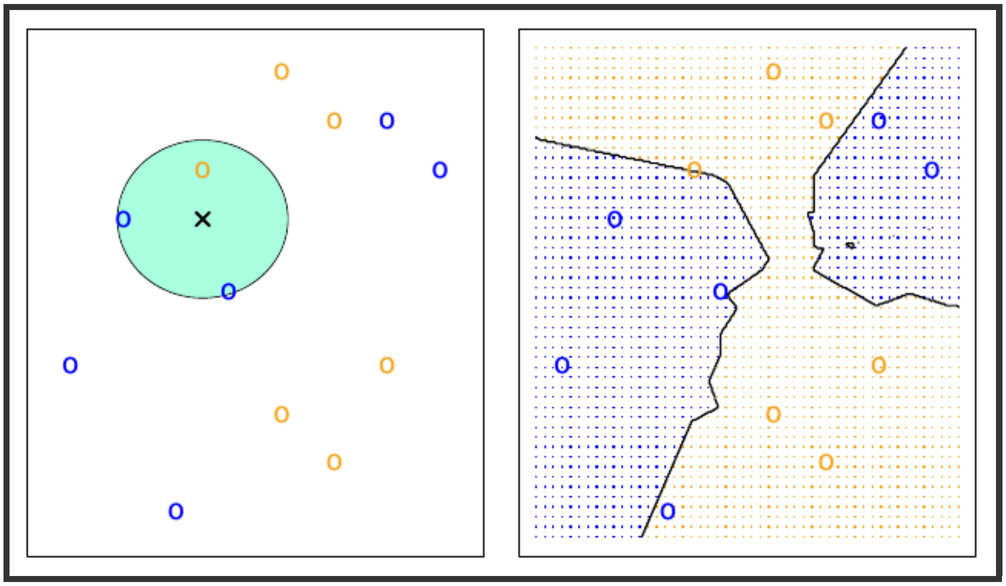
Given training data (X, Y)

Given a new x^* , what is the corresponding y^*?

Find the k-nearest neigbours of x^* . Then:

- **Classification**: Predicted y^* is the majority class-label of the neighbors
- **Regression**: Predicted y^* is the average of the y's of the neighbors

3-nearest neighbors



 (*An Introduction to Statistical Learning*, James, Witten, Hastie and Tibshirani)

Complexity of decision boundary grows with size of training set: ‘Nonparametric’

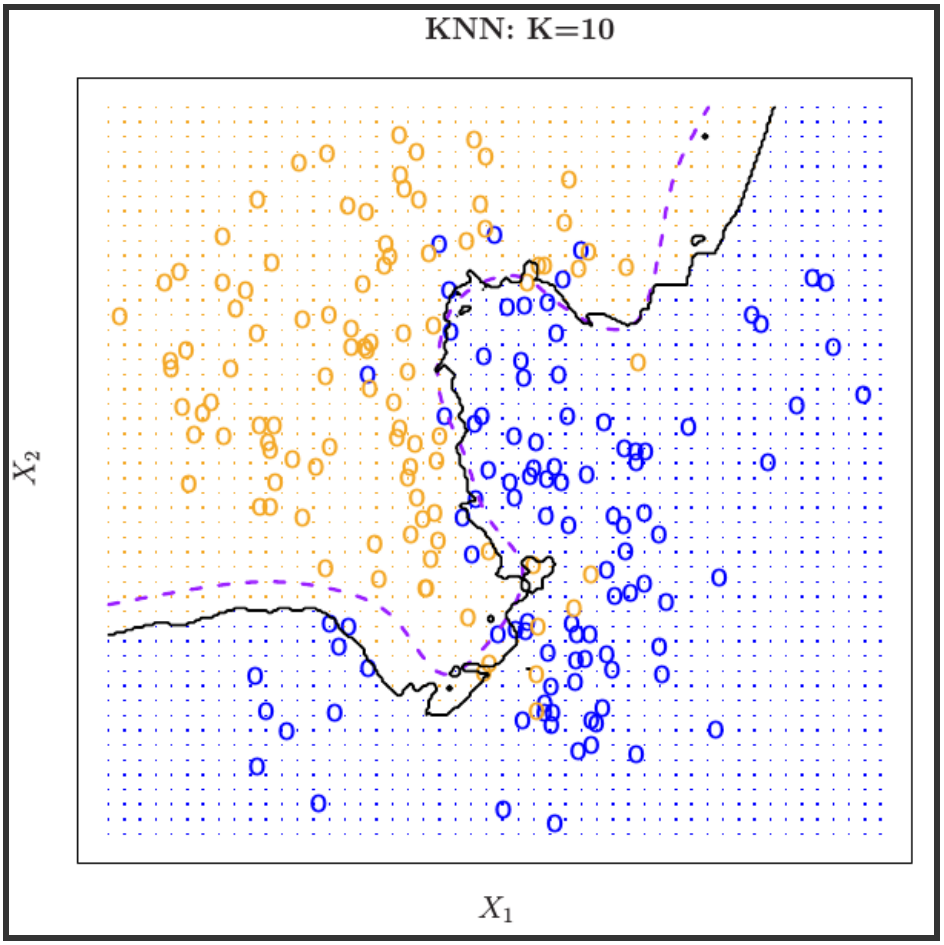
Pros:

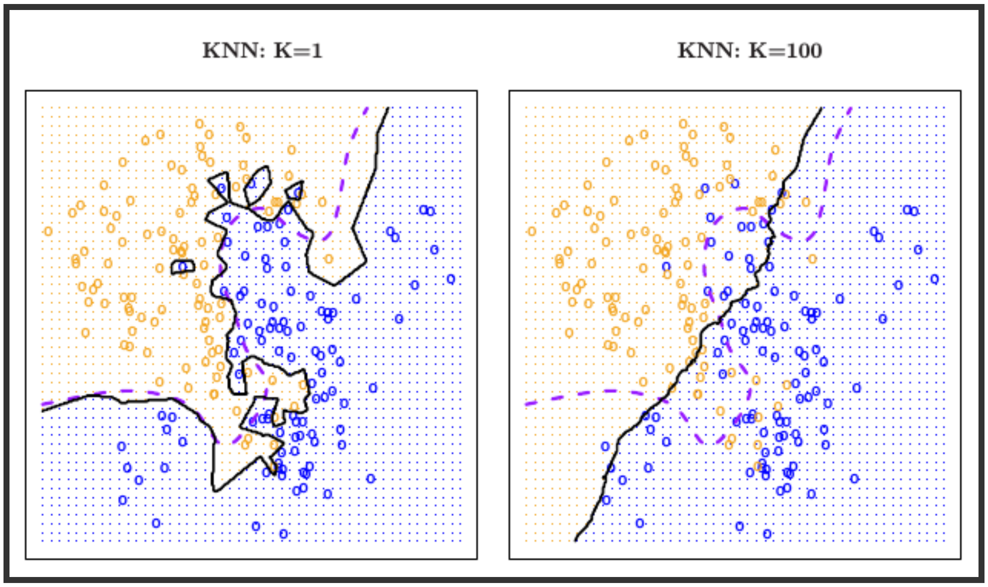
- Very intuitive computational algorithm.
- Very easy to ‘fit’ data (you don’t, you just store it)
- Tends to outperform more complicated models.
- Easy to develop more complicated extensions E.g. locally-adaptive kNN.
- Exists theory for such models.

Cons:

- Cost of prediction grows linearly with training set size (can be expensive for large datasets)
- Tends to break down in high-dimensional spaces.
- Exempler-based approaches are hard to interpret.

10-nearest neighbors





- What distance function do we use? Typically Euclidean.
- What k do we use? Typically 3, 5, 10

Usually chosen by cross-validation (more later)

Large k: smooth decision boundary

Small k: complex decision boundary (with local variations)

- k is a measure of model-complexity

How do we perform model selection?

Do we prefer simple or complex models?

Bias-variance trade-off

Overly simple models

- cause underfitting (or bias)
- ignore important aspects of training data

Overly complex models

- cause overfitting (or variance)
- can be overly sensitive to noise in training data

Complex models reduce training error, but generalize poorly.

Cross-validation

How do we estimate generalization ability? Create an unseen test dataset.

Cross-validation:

- Split your data into two sets, a training and test dataset.
- Fit all models on training set.
- Evaluate all models on test set.
- Pick best model.

Choosing k by cross-validation