

Statistical learning - Vinciotti (2022)

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Part I

Introduction

Chapter 1

General course information

1.1 Textbooks

- James et al (2021), Introduction to statistical learning in R, 2nd edition. (Book that is used as guideline for the course, but further concepts will be added during the lectures)
- Hastie et al (2001), Elements of statistical learning. (More advanced book for those who want to study the subject more in depth)

1.2 Assessment

- Three homework tasks during the course (Uploaded on moodle, two weeks of time for each, more practical and mainly focused on applying methods to some data. If done well they will add 2 points to the written exam score)
- Final written exam (More theoretical but still connected to the practical part, for instance by commenting on analysis output)

1.3 Topics

- Linear regression (Gauss, 1800) (Assumed to be already known from Statistical Learning 1)
- Linear discriminant analysis, LDA (Fisher, 1936) (Later extended to quadratic discriminant analysis, QDA)
- Logistic regression (1940s)
- Generalized linear models (Nelder and Wedderburn, 1972)
- Classification and regression trees (Breiman and Friedman, 1980s) (First introduction of computer intensive methods)
- Machine learning (1990s): support vector machines, neural networks/deep learning, unsupervised learning (clustering, PCA)
- Individual methods: theory, details, implementation ...

1.3. TOPICS

- General concept: model selection, inference, prediction ...

Part II

Statistical learning

Chapter 2

What is statistical learning?

2.1 Definition of statistical learning

In general, a statistical learning problem can be formalized as follows:

- Y : response/dependent/outcome variable
- $\underline{X} = (X_1, \dots, X_p)$: predictors/features/independent variables/covariates

We assume that there is a relationship between Y and \underline{X} , which can be written as:

$$Y = f(\underline{X}) + \varepsilon$$

Where:

- $f(\underline{X})$ is the deterministic (but unknown) function of the vector $\underline{X} = (X_1, \dots, X_p)$
- ε is the error (stochastic part), for which we assume the following properties:
 - $E[\varepsilon] = 0$ (Its expected value is zero)
 - $\varepsilon \perp \underline{X}$ (It is independent from \underline{X})

Therefore, the expression **statistical learning** encompasses different methods to estimate $f(\underline{X})$.

2.2 Why estimate f ?

There are two main reasons to estimate f , those two being **prediction** and **inference**.

2.2.1 Prediction

Predict Y when we only have observations about \underline{X} . Since $E[\varepsilon] = 0$, we usually take:

$$\hat{Y} = \hat{f}(\underline{X})$$

With \hat{f} being our estimate of f .

If this is the only reason to estimate f , then \hat{f} can be a black-box method (deep learning). The accuracy of \hat{Y} as a predictor of Y can be described in the following way:

$$\begin{aligned}
E[(Y - \hat{f}(\underline{X}))^2 | \underline{X} = \underline{x}] &= && \text{where } \hat{f} \text{ is a fixed known function} \\
&= E[(f(\underline{X}) + \varepsilon - \hat{f}(\underline{X}))^2] && \text{since } Y = f(\underline{X}) + \varepsilon \\
&= E[(f(\underline{X}) - \hat{f}(\underline{X})) + \varepsilon]^2 && \text{rearranging} \\
&= E[(f(\underline{X}) - \hat{f}(\underline{X}))^2 + \varepsilon^2 + 2\varepsilon(f(\underline{X}) - \hat{f}(\underline{X}))] && \text{solving the square} \\
&= E[(f(\underline{X}) - \hat{f}(\underline{X}))^2] + E[\varepsilon^2] + 2E[\varepsilon(f(\underline{X}) - \hat{f}(\underline{X}))] && \text{separating the expectations}
\end{aligned}$$

Furthermore, since we know that:

$$\begin{aligned}
Var(\varepsilon) &= E[(\varepsilon - E(\varepsilon))^2] && \text{formal definition of variance} \\
&= E[\varepsilon^2] - (E[\varepsilon])^2 && \text{definition generally used during calculation} \\
&= E[\varepsilon^2] && \text{since } E[\varepsilon] = 0
\end{aligned}$$

Thus we get:

$$\begin{aligned}
E[(Y - \hat{f}(\underline{X}))^2 | \underline{X} = \underline{x}] &= \\
&= E[(f(\underline{X}) - \hat{f}(\underline{X}))^2] + Var(\varepsilon) + 2E[\varepsilon(f(\underline{X}) - \hat{f}(\underline{X}))] && \text{substituting } E[\varepsilon^2] = Var(\varepsilon) \\
&= (f(\underline{X}) - \hat{f}(\underline{X}))^2 + Var(\varepsilon) + 2(f(\underline{X}) - \hat{f}(\underline{X}))E[\varepsilon] && \text{since } f(\underline{X}) - \hat{f}(\underline{X}) \text{ is a constant} \\
&= (f(\underline{X}) - \hat{f}(\underline{X}))^2 + Var(\varepsilon) && \text{since } E[\varepsilon] = 0
\end{aligned}$$

With:

- $(f(\underline{X}) - \hat{f}(\underline{X}))^2$ being the **reducible error**. The model choice can increase or reduce this value, hence it is mostly controllable.
- $Var(\varepsilon)$ being the **irreducible error**. This value depends on the innate randomness present in the data, hence you can only try and minimize it by deciding which variables to use in your prediction (but it will never be zero otherwise you would have a deterministic situation).

2.2.2 Inference

Inference is used when you want to understand the relation between Y and \underline{X} (and not just be able to make predictions). Namely, inference answers questions such as:

- Which predictors/factors are most associated with the response?
- What is the relationship between Y and X_j ?

2.3 How to estimate f ?

Given some **training data** (\underline{x}_i, y_i) , $i = 1, \dots, n$, where $\underline{x}_i = (x_{i1}, \dots, x_{ip})^t$ is the vector of observations of unit i while y_i is the response for unit i , broadly speaking there are two types of methods to estimate f : **parametric methods** and **non-parametric methods**.

2.3.1 Parametric methods

In order to use parametric methods, we make an assumption about the functional form of $f(\underline{X})$, that assumption being that the form of the function depends on some parameters (which we can estimate). An example of parametric method is **linear regression**, which implies that $f(\underline{X})$ is in the form:

$$f(\underline{X}) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$$

Given this assumption, statistical learning becomes **fitting** (or training) the model on the data, which means estimating the parameters $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p$ such that:

$$\hat{f}(\underline{X}) = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \cdots + \hat{\beta}_p X_p$$

The main disadvantage of these methods is that they may be **too restrictive**.

Notice that linear models are linear in the parameters, not in the predictors, hence:

- $f(X_1) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_1^3 + \varepsilon$ (polynomial regression) is a linear model.
- $f(X_1) = \beta_0 X_1^{\beta_1}$ is not a linear model.

2.3.2 Non-parametric methods

Non-parametric methods do not make any explicit assumption on the function form of $f(\underline{X})$. These methods want to estimate f by getting as close as possible to the data, without being too *rough or wiggly* (basically **overfitting**).

2.3.3 Parametric vs non-parametric methods

Despite parametric methods being more restrictive than non-parametric ones, we might still choose to adopt the former for the sake of interpretability and generalizability outside of the training data.

2.4 Bias-variance trade-off

Assume you have some data pairs in the form (x_i, y_i) , $i = 1, \dots, n$; you can then define the estimate function $\hat{f}(x)$ as a linear model with up to $n - 1$ parameters (more parameters give the same result as $n - 1$ parameters) and an intercept value. You could thus use, for instance, the models:

| | |
|--------------------|---|
| 1 parameter | $f(x) = \beta_0 + \beta_1 x + \varepsilon$ |
| 2 parameters | $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon$ |
| \vdots | \vdots |
| $n - 1$ parameters | $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_{n-1} x^{n-1} + \varepsilon$ |

You could choose the model with the highest number of parameters; this model would explain all the variance of the training data ($R^2 = 1$) yet it would be very complex and perform badly with new data points. On the other hand a model with a lower number of parameters would explain less of the variance of the training data, yet it could perform better with new data points.

2.4. BIAS-VARIANCE TRADE-OFF

Keeping in mind that Y is random and that \hat{f} is a random variable estimated from the data, when using the general formula to determine how well a model performs at generic \underline{X} , we notice:

$$\begin{aligned}
 E[(Y - \hat{f}(\underline{X}))^2 | \underline{X} = \underline{x}] &= \\
 &= E[(f(\underline{X}) + \varepsilon - \hat{f}(\underline{X}))^2] && \text{since } Y = f(\underline{X}) + \varepsilon \\
 &= E[(f(\underline{X}) + \varepsilon - \hat{f}(\underline{X}) + E[\hat{f}(\underline{X})] - E[\hat{f}(\underline{X})])^2] && \text{since } E[\hat{f}(\underline{X})] - E[\hat{f}(\underline{X})] = 0 \\
 &= E[(f(\underline{X}) - E[\hat{f}(\underline{X})] + \varepsilon + (E[\hat{f}(\underline{X})] - \hat{f}(\underline{X})))^2] && \text{grouping} \\
 &= E[(f(\underline{X}) - E[\hat{f}(\underline{X})])^2] + E[\varepsilon^2] + E[(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))^2] + \\
 &\quad + 2E[(f(\underline{X}) - E[\hat{f}(\underline{X})])\varepsilon] + \\
 &\quad + 2E[(f(\underline{X}) - E[\hat{f}(\underline{X})])(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))] + && \text{solving the square and} \\
 &\quad + 2E[(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))\varepsilon] && \text{dividing the expectations}
 \end{aligned}$$

But notice that:

$$\begin{aligned}
 E[(f(\underline{X}) - E[\hat{f}(\underline{X})])\varepsilon] &= E[\varepsilon](f(\underline{X}) - E[\hat{f}(\underline{X})]) && \text{since } f(\underline{X}) - E[\hat{f}(\underline{X})] \text{ is constant} \\
 &= 0 && \text{since } E[\varepsilon] = 0
 \end{aligned}$$

$$\begin{aligned}
 E[(f(\underline{X}) - E[\hat{f}(\underline{X})])(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))] &= \\
 &= (f(\underline{X}) - E[\hat{f}(\underline{X})])E[E[\hat{f}(\underline{X})] - \hat{f}(\underline{X})] && \text{since } f(\underline{X}) - E[\hat{f}(\underline{X})] \text{ is constant} \\
 &= (f(\underline{X}) - E[\hat{f}(\underline{X})])E[\hat{f}(\underline{X}) - \hat{f}(\underline{X})] && \text{since } \hat{f}(\underline{X}) \text{ is a constant} \\
 &= (f(\underline{X}) - E[\hat{f}(\underline{X})])E[0] \\
 &= 0
 \end{aligned}$$

$$\begin{aligned}
 E[(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))\varepsilon] &= E[\varepsilon]E[E[\hat{f}(\underline{X})] - \hat{f}(\underline{X})] && \text{since } \varepsilon \perp \underline{X} \implies E[\varepsilon \underline{X}] = E[\varepsilon]E[\underline{X}] \\
 &= 0 && \text{since } E[\varepsilon] = 0
 \end{aligned}$$

Therefore we can simplify as:

$$\begin{aligned}
 E[(Y - \hat{f}(\underline{X}))^2 | \underline{X} = \underline{x}] &= E[(f(\underline{X}) - E[\hat{f}(\underline{X})])^2] && + E[\varepsilon^2] && + E[(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))^2] \\
 &= f(\underline{X}) - E[\hat{f}(\underline{X})]^2 && + Var(\varepsilon) && + Var(\hat{f}(\underline{X}))
 \end{aligned}$$

Where:

- $f(\underline{X}) - E[\hat{f}(\underline{X})]^2$ is the bias
- $Var(\varepsilon)$ is the irreducible error
- $Var(\hat{f}(\underline{X}))$ is the variance of the model

Bias is basically the error of the estimated model due to the training data. If an estimated model performs well on the training data but it does not perform well on new data, the estimated model has high bias. If an estimated model performs well on multiple data sets, the estimated model has low bias. High bias means that an estimated model is far from the real model.

In order to minimize the expected error, we need to achieve low bias and low variance. In practice, one needs to find a good trade-off between bias and variance, since reducing one often involves increasing the other. In general:

- A **simple model** has high bias (it is far from the real model) and low variance (when fitting using different training data you get similar estimated parameters).
- A **complex model** has low bias and high variance.

Both in parametric and non-parametric methods, you generally have at least one **tuning parameter**, which is a parameter that can be tweaked (for instance the degree of the polynomial) in order to choose the balance between bias and variance.

Chapter 3

Statistical decision theory

3.1 Definition of statistical decision theory

Statistical decision theory is a set of quantitative methods for reaching optimal decisions for well posed problems. Statistical decision theory applies to supervised learning, while it does not apply to unsupervised learning. For most of the course we will focus on supervised learning.

3.2 Supervised learning

Supervised learning is a set of methods whose objective is, given the observations (\underline{x}_i, y_i) with $i = 1, \dots, n$, to find a rule \hat{f} that allows us to predict Y from \underline{X} , meaning that $\hat{Y} = \hat{f}(\underline{X})$. $\hat{f}(\underline{X})$ is thus an approximation of the true rule $f(\underline{X})$. Finding \hat{f} corresponds to training (or fitting) a model using labelled data pairs (both predictors and response values are known).

Broadly, there are two main types of methods of supervised learning:

- **Regression methods**, in which the response Y is quantitative (numerical). In this case \hat{f} is called **regression function**.
- **Classification methods**, in which the response Y is qualitative (categorical). In this case \hat{f} is called **classifier**.

The predictors (\underline{X}) can take any form, numerical or categorical. In general there are no assumptions on the form of the predictors (but not always).

To evaluate a model you use **loss functions**, which are functions used to penalize the differences between Y and $f(\underline{X})$. Many loss functions can be used; the choice of a specific loss function determines which function is considered to be the true rule $f(\underline{X})$.

3.3 Regression setting

In a regression setting, the loss function which is generally used is the **squared error loss function**, which is defined as

$$L(Y, f(\underline{X})) = (Y - f(\underline{X}))^2$$

3.3. REGRESSION SETTING

When using this loss function, the criterion for choosing the model becomes finding f such that it minimizes the **expected prediction error** (EPE), which is the expected value of the squared error loss function:

$$\begin{aligned} \text{EPE}(f) &= E_{Y,\underline{X}}[(Y - f(\underline{X}))^2] \\ &= \iint (y - f(\underline{x}))^2 g_{Y,\underline{X}}(y, \underline{x}) dy d\underline{x} \quad \text{if } Y \text{ is continuous} \end{aligned}$$

This error is an expectation since you usually do not know the distribution of Y and \underline{X} . If Y is continuous you can rewrite this expectation as the double integral times the joint density function g .

Theorem 1 (Minimum of the expected prediction error). *$\text{EPE}(f) = E_{Y,\underline{X}}[(Y - f(\underline{X}))^2]$ has a **minimum** when $f(\underline{x}) = E[Y|\underline{X} = \underline{x}]$. $f(\underline{x})$ is called regression function.*

Proof. (Sketch of the proof) By definition we know that

$$\text{EPE}(f) = E_{Y,\underline{X}}[(Y - f(\underline{X}))^2]$$

Then, since the law of iterated expectations states that $E[X] = E[E[X|Y]]$ (analogously to profile likelihood, you fix one variable and variate the other), we get

$$E_{Y,\underline{X}}[(Y - f(\underline{X}))^2] = E_{\underline{X}}[E_{Y|\underline{X}}[(Y - f(\underline{X}))^2]|\underline{X}]$$

If we then consider a specific value of \underline{X} , meaning $\underline{X} = \underline{x}$, the inner expectation becomes

$$E[(Y - f(\underline{x}))^2 | \underline{X} = \underline{x}]$$

But since \underline{x} is fixed, $f(\underline{x})$ is a constant, hence this expectation can be written as a function in some parameter a

$$g(a) = E_Y[(Y - a)^2]$$

Then we want to find the (constant) value of a that minimizes $g(a)$

$$\begin{aligned} g(a) &= E_Y[(Y - a)^2] \\ &= E[Y^2 - 2aY + a^2] && \text{compute the square} \\ &= E[Y^2] - 2aE[Y] + E[a^2] && \text{separate expectations} \\ &= E[Y^2] - 2aE[Y] + a^2 && \text{pull out } a^2 \text{ since constant} \end{aligned}$$

Then, setting the derivative to zero we get

$$\frac{dg}{da} = -2E[Y] + 2a \stackrel{!}{=} 0 \implies \hat{a} = E[Y]$$

If you then plug \hat{a} into $g(a) = E_Y[(Y - a)^2]$

$$g(\hat{a}) = E_Y[(Y - E[Y])^2]$$

which is the variance

So $f(\underline{x}) = E[Y|\underline{X} = \underline{x}]$ is the function that minimizes the EPE. □

3.4. CLASSIFICATION SETTING

This is not the only choice

$$L(Y|f(\underline{X})) = |Y - f(\underline{X})|$$

$f(\underline{x}) =$ median of Y given \underline{x} LAD regression (least absolute deviation) Robust statistics (median is more robust to outliers)

We will choose the squared error loss and this motivates how the methods are developed. For example: Linear regression:

$$Y|\underline{X} = \underline{x} \sim N(\underline{x}^t \underline{\beta}, \sigma^2)$$

Way to express linear regression focussing on conditional mean

$$E[Y|\underline{X} = \underline{x}] = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$

(parametric)

K nearest neighbour (non-parametric approach for regression)

K nearest neighbour

$$\hat{f}(\underline{x}) = \text{Average } (y_i | \underline{x}_i \in N_K(\underline{x}))$$

Sample mean, neighbourhood of k points closest to \underline{x}

It makes two approximations: Using sample mean to approximate population mean Uses a neighbourhood of \underline{x} rather than only \underline{x}

Works well if a lot of data and p (number of predictors is small)

This simple approach inspired the development of more sophisticated kernel methods.

3.4 Classification setting

Response Y is categorical, with K categories. A classifier is deciding which class to assign to a new observation \underline{x} . Our \hat{Y} in this case is the predicted class.

0 – 1 LOSS The loss function basically penalizes choosing wrong

$$L(Y, \hat{Y}(\underline{X})) =$$

True class predicted class In this case every mistake counts as 1

Leading to the criterion: find \hat{y} that minimizes Expected 0-1 loss

$$E[L(Y, \hat{Y}(\underline{X}))]$$

Main question: what function of \underline{X} minimizes the expected 0-1 loss

Let us concentrate on one \underline{x} : (inner part of the expectation)

$$E[L(Y, \hat{Y}(\underline{X}))] = \sum_{k=1}^K L(k, \hat{Y}(\underline{x})) p(k|\underline{x})$$

Considering the binary case, if the classifier predicts \underline{x} to class 0 ($\hat{y} = 0$),

$$\begin{aligned} E[L(Y, 0)] &= L(0, 0)p(0|\underline{x}) + L(1, 0)p(1|\underline{x}) \\ &= 0 \cdot p(0|\underline{x}) + 1 \cdot p(1|\underline{x}) \\ &= p(1|\underline{x}) \end{aligned}$$

3.4. CLASSIFICATION SETTING

If the classifier predicts \underline{x} to class 1 ($\hat{y} = 1$),

$$\begin{aligned} E[L(Y, 1)] &= L(0, 1)p(0|\underline{x}) + L(1, 1)p(1|\underline{x}) \\ &= 1 \cdot p(0|\underline{x}) + 0 \cdot p(1|\underline{x}) \\ &= p(0|\underline{x}) \end{aligned}$$

Predicting \underline{x} to the class that minimizes the expected loss results in: classifying \underline{x} to class 1 if

$$p(1|\underline{x}) > p(0|\underline{x})$$

Since $p(0|\underline{x}) = 1 - p(1|\underline{x})$, we have that

$$p(1|\underline{x}) > 1 - p(1|\underline{x}) \implies 2p(1|\underline{x}) > 1 \implies p(1|\underline{x}) > 0.5$$

In general (k classes), the 0-1 loss is minimized by the following rule: Bayes classifier Assign \underline{x} to class

$$j = \operatorname{argmax}_{i \in \text{classes}} p(Y = i | X = \underline{x})$$

(assign \underline{x} to the class with the highest probability) Just tells us how to set the problem, but then the single method has to make us estimate the probabilities. Bayes classifier is optimal in 0-1 loss

Try with $k = 3$ and classes 0,1,2

In the binary case:

$$\text{assign } \underline{x} \text{ to class } \begin{cases} 1 & \text{if } p(1|\underline{x}) > 0.5 \\ 0 & \text{if } p(1|\underline{x}) < 0.5 \end{cases}$$

$p(1|\underline{x}) = 0.5$ Bayes decision boundary

Bayes error rate

$$\text{BER} = 1 - E_{\underline{X}}(\max_j p(j|\underline{x}))$$

Probability of committing an error

$$\text{perfect separation} \implies \max_j p(j|\underline{x}) = 1 \implies \text{BER} = 0$$

$$\text{BER} > 0$$

(irreducible error)

There is a more general loss function: Misclassification loss (binary example)

$$L(Y, \hat{Y}(\underline{x})) =$$

Misclassification errors are not equal C_0 is the misclassification cost of misclassifying a class 0 to 1 C_1 is the misclassification cost of misclassifying a class 1 to 0 Often the errors are not equal (credit risk, medical context) Often there are unbalanced classes (rare disease, but if you do not penalize enough "Diseased" you get a classifier which has high accuracy but just tells that everyone is healthy)

If we repeat the same procedure with this

$$E[L(Y, 0)] = c_1 p(1|\underline{x})$$

$$E[L(Y, 1)] = c_0 p(0|\underline{x})$$

So assign \underline{x} to the class 1 if

$$c_1 p(1|\underline{x}) > c_0 p(0|\underline{x})$$

Since

$$\begin{aligned} p(0|\underline{x}) &= 1 - p(1|\underline{x}) \\ c_1 p(1|\underline{x}) &> c_0 - c_0 p(1|\underline{x}) \\ p(1|\underline{x}) &> \frac{c_0}{c_0 + c_1} \end{aligned}$$

New threshold that takes into account different errors.

3.5 Model accuracy

In practice, we would use our chosen method to estimate $f(\underline{x}) = E[Y|X = \underline{x}]$ in a regression or $p(1|\underline{x})$ in a classification from training data (\underline{x}_i, y_i) , $i = 1, \dots, n$

Accuracy is typically measured on test data

$$(\underline{x}_i^{(t)}, y_i^{(t)}), i = 1, \dots, m$$

in a regression setting, using MSE

$$\text{MSE} = \frac{1}{m} \sum_{i=1}^m (y_i^{(t)} - \hat{f}(\underline{x}_i^{(t)}))^2$$

In classification estimate and plug in formula Confusion matrix

$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

sensitivity

$$\begin{aligned} \text{FPR} &= \frac{\text{FP}}{\text{TN} + \text{FP}} \\ &= 1 - \frac{\text{TN}}{\text{TN} + \text{FP}} \end{aligned}$$

1 - specificity

$$\text{ERROR RATE} = \frac{\text{FP} + \text{FN}}{m}$$

These above only work if you assume a 1-0 loss, no if different

If costs are unequal, you still count misclassifications but multiply by weight

$$\text{Misclassification cost} = \frac{c_0 \text{FP} + c_1 \text{FN}}{m}$$

Since precise costs are difficult to say, better to plot Receiver Operating Characteristic (ROC) curve Basically you change all possible values of the threshold from zero to one; extrema will be wrong but some value in the middle would be fine, thus you remake the confusion matrix with the new cutoff FPR vs TPR for all possible thresholds $t \in [0, 1]$ Best possible case would be top left corner (deterministic) so you want the highest curve you can Diagonal worst case (would be the same as tossing a coin) Area under the curve is called AUC (the higher the better, best 0.5, worst 0) If lines cross you decide based on which area you are interested in