Algorithmic Bias, Statistical Notions of Fairness, and the Seldonian Algorithm

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Abstract

The abstract should be a short summary of your thesis work. A paragraph is usually sufficient here.

Acknowledgments

Use this space to thank those who have helped you in the thesis process (professors, staff, friends, family, etc.). If you had special funding to conduct your thesis work, that should be acknowledged here as well.

Table of Contents

Abstract . . . . . **i**

Acknowledgments . . . . . **iii**

List of Tables . . . . . **v**

List of Figures . . . . . **vii**

Chapter 1: Introduction **1**

1.1 Algorithmic Bias 2

1.2 Statistical Definitions of Fairness 4

1.2.1 Group Fairness in Regression Settings 5

1.2.2 Group Fairness in Classification Settings 6

1.3 Fairness Conflicts 13

1.3.1 Fairness Conflicts in Regression 13

1.3.2 Fairness Conflicts in Classification 14

1.3.3 On Fairness Conflicts 16

Chapter 2: The Seldonian Algorithm **17**

2.1 The Standard Machine Learning Approach 17

2.1.1 Limitations of the Standard Approach 19

2.1.2 Potential Remedies 21

2.2 The Seldonian Framework 23

2.2.1 The Seldonian Optimization Problem 24

2.2.2 Quasi-Seldonian Algorithms 26
2.3 Toy Example: A Seldonian Regression Algorithm 26
2.4 Random Notes (Delete When Done): 27
Appendix A: Sufficiency v Separation Fairness Conflict Equation . . **29**
References **35**

List of Tables

List of Figures

1.1 COMPAS Prediction Fails Differently for Black v White Defendants . 3
1.2 An Example of Demographic Parity 8
1.3 A Confusion Matrix 10
1.4 An Example of Equality of Odds 12
2.1 Least Squares Fit on Synthetic Data Drawn from Different Distributions 20
2.2 Overview of the Seldonian Framework 25

Chapter 1 Introduction

The public and private sector are increasingly turning to data-driven methods to automate and to guide simple and complex decision-making. However, this trend raises an important question of bias. There is a lot of misinterpretation when it comes to the collection of data in many application areas, and there is a major concern for data-driven methods to further introduce and perpetuate discriminatory practices, or to otherwise be unfair because of the social and historical processes that operate to the disadvantage of certain groups.

For example, within healthcare, using mortality or readmission rates to measure hospital performance penalizes hospitals serving poor or non-White populations as those inherently have higher mortality and readmission rates due to confounding societal factors. Outside healthcare, credit-scoring algorithms predict outcomes based on income, which disadvantages low-income groups further perpetuating economic immobility. Policing algorithms result in increased scrutiny of Black neighborhoods because of the bias against Black people that is already present in the U.S. policing system, and hiring algorithms, which predict employment decisions, are affected by historical race and gender biases.

Yet, these algorithms are often regarded as ground truth and free of human limitations because they are based on mathematics, statistics, and computer science – otherwise regarded as objective disciplines. In theory, this should lead to greater fairness. However, left unregulated, these mathematical models privilege majority

groups and discriminate against minority groups because they often learn from inherently biased data. If the data used to train models contains bias, then the resulting algorithms will learn the bias and reflect it into their predictions. In many cases, this can be detrimental.

While there are widely-accepted, though sometimes disputed, societal notions of fairness, one key question emerges: are there any established statistical notions of fairness and bias? Is it possible to mathematically and statistically define algorithmic bias and unfairness, thereby paving a way for addressing the challenges they pose? And if so, are there ways leverage statistical tools to resolve such bias and unfairness? This thesis paper aims to explore and answer precisely these questions.

1.1 Algorithmic Bias

There are multiple different types and sources of bias in the realm of statistics. In particular, algorithmic bias arises when an algorithm's decisions are skewed towards a particular group of people, either positively or negatively (Mehrabi, Morstatter, Saxena, Lerman, & Galstyan, 2021). The danger with biased algorithmic outcomes is that they generate a feedback loop. Take, for example, a hiring algorithm that discriminates against female applicants for a specific job. In the long run, this can perpetuate, and even amplify, existing gender biases by further widening the gender-based class imbalance.

One such key example of algorithmic bias often cited in literature is regarding the broad use of the COMPAS – or the Correctional Offender Management Profiling for Alternative Sanctions – tool to predict a defendant's risk of recidivism (committing another crime) within two years. COMPAS is more likely to have higher false positive rates for African-American offenders than Caucasian offenders (Mehrabi et al., 2021).

Across the country, scores of similar assessments are given to judges, which injects bias into courts (Angwin, Larson, Mattu, & Kirchner, 2016).

COMPAS is based on data from 7000 people arrested in Broward County, Florida in 2013 and 2014 (Angwin et al., 2016). The response variable, recidivism, was encoded based on who was charged with new crimes over the next two years. Analyses on the predictive efficacy of the COMPAS algorithm found that the algorithm was 61% accurate for a full range of crimes, including misdemeanors, and only 20% of people forecasted to commit violent crimes actually went on to do so. While the overall accuracy rate for the full range of crimes is better than a coin flip, there exists room for enhancing the predictive performance, especially for a decision as critical as whether or not to grant a defendant bail or parole.

What's more concerning, however, is that when the effects of race, age, and gender are isolated and not included in the model, a statistical analysis showed that Black defendants were still 77% more likely to be predicted at higher risk of committing a future violent crime and 45% more likely to be predicted of committing a future crime of any kind, highlighting the role that proxies of race play into the predictions (Angwin et al., 2016). The table in Figure 1.1 highlights the performance discrepancy across race.

	WHITE	AFRICAN AMERICAN
Labeled Higher Risk, But Didn't Re-Offend	23.5%	44.9%
Labeled Lower Risk, Yet Did Re-Offend	47.7%	28.0%

Figure 1.1: Prediction Fails Differently for Black v White Defendants (Angwin et al., 2016)

Although the tool has 61% accuracy, Black defendants are almost twice as likely to be labeled as higher risk without re-offending than White defendants. It makes

the opposite mistake among White defendants. The reason for this is that classification models are trained to minimize average error, which fits majority populations (Chouldechova & Roth, 2018).

For example, different factors in society lead to different environmental and social experiences between Black people and White people. These factors, such as an offender's personal history, familial history, and residential neighborhood, are used in the COMPAS tool to predict recidivism. It would, thus, seem fair that the relationships between an offender's social experience and their likelihood of recidivism be calibrated differently for Black versus White offenders to account for this inherent difference. A classifier that does not take this into account will disproportionately affect one group negatively.

COMPAS is just one such algorithm. In the education sector, different factors lead to different SAT scores between majority and minority populations. It would, thus, seem fair that the relationship between SAT and college admissions be calibrated differently for each demographic group. However, if a group-blind classifier is trained, it cannot simultaneously fit both groups optimally and will fit the majority population as it's more important to overall error.

Can we modify these algorithms to be group-blind but also fair? In order to do so, fairness constraints that reduce, or even correct for, algorithmic bias during the modeling process must be set. However, one must first define fairness mathematically, statistically, and quantifiably.

1.2 Statistical Definitions of Fairness

Statistical notions of fairness can be defined at a group level or an individual level. *Group notions* fix a few demographic groups and assess the parity of some statisti-

cal measures across all the groups (Chouldechova & Roth, 2018). Note that group measures, on their own, do not guarantee fairness to individuals or structured subgroups within protected demographic groups, but rather, give guarantees to "average" numbers of protected groups. These notions are the focus of this thesis paper.

Individual notions, on the other hand, are assessed on specific pairs of individuals rather than averaged across groups (Chouldechova & Roth, 2018). In other words, similar individuals should be treated similarly along some defined similarity or inverse distance metrics. Counter-factual fairness, for example, relies on the intuition that a decision is fair towards an individual if it's the same in both the real world and a counter-factual world where the individual belongs to a different demographic group (Mehrabi et al., 2021). This can be impractical, relies on strong assumptions about the data, and approaches the realm of causality (Chouldechova & Roth, 2018). Moreover, there is a gap in literature with regard to individual notions of fairness.

Ultimately, group notions and individual notions are not in conflict per se. Instead, they are on the same spectrum of how much dependence is allowed between predictions and the sensitive attribute (Castelnovo et al., 2022). Subgroup fairness is an alternative notion that intends to obtain the best properties of both, for example, by picking a group fairness constraint and assessing whether it holds over a large collection of subgroups (Mehrabi et al., 2021). Group and individual fairness notions can be defined in both classification settings and regression settings, although most of the literature focuses on fairness within classification.

1.2.1 Group Fairness in Regression Settings

Fair regression is the quantitative notion of fairness of real-valued targets (Agarwal, Dudík, & Wu, 2019). Consider a general prediction setting where the training set consists of X, a feature vector with all the predictor variables, A, the levels of the

protected attribute/ demographic group, and Y, the real-valued continuous response variable. F is a set of possible prediction models, and the goal is to find $f \in F$ that is a good predictive model of Y given X and some fairness constraints. The accuracy of a prediction $f(X)$ / $\hat{Y}$ on Y is measured by the loss function $l(Y, f(X))$ or mean squared error (MSE). The goal is to minimize $l(Y, f(X))$, hence, maximizing accuracy.

Statistical parity refers to minimizing the expected loss function/ MSE such that the probability that each predicted $f(X)$/ $\hat{Y}$ is above a certain threshold z for each sensitive attribute is the same as the probability over the entire data set, given some margin ϵ_a that is dependent on the protected attribute (Agarwal et al., 2019):

$$\min_{f \in F} E[l(Y, f(X))] \text{ such that } \forall a \in A, z \in [0, 1] :$$

$$|P[f(X) \geq z | A = a] - P[f(X) \geq z]| \leq \epsilon_a.$$

This is akin to the classification setting where it may be desirable to have the probability of being in the positive class be above some certain threshold for each group as well as across the entire data set. A similar notion, known as *bounded loss*, requires that the MSE for each group is below some pre-specified level c_a that is dependent on the protected attribute (Agarwal et al., 2019):

$$\min_{f \in F} E[l(Y, f(X))] \text{ such that } \forall a \in A :$$

$$E[l(Y, f(X)) | A = a] \leq c_a.$$

1.2.2 Group Fairness in Classification Settings

Group notions of fairness in classification, at the core, refer to treating different groups equally. They aim to remedy or prevent disparate impact, which is a setting

where there is unintended disproportionate adverse impact on a particular group (Chouldechova, 2017). There are three broad notions of observational group fairness: independence, separation, and sufficiency (Castelnovo et al., 2022).

Independence

This fairness definition requires predictions, $\hat{Y}$, to be independent of any sensitive attribute, A, that is, $\hat{Y} \perp\!\!\!\perp A$ (Castelnovo et al., 2022). Thus, it relies only on the distribution of features and decisions, that is, A, X, and $\hat{Y}$, and focuses on the equality of the predictions themselves by satisfying the following equation:

$$P(\hat{Y} = 1|A = a) = P(\hat{Y} = 1|A = b),\ \forall a, b \in A,$$

where a, b are the two demographic groups in question.

This definition is also known as *demographic parity*, *statistical parity*, or generally, group fairness, and requires that all levels of the demographic group have the same positive prediction ratio (PPR) where PPR is the ratio of positive outcomes (Castelnovo et al., 2022). In other words, the likelihood of a positive outcome should be the same regardless of the demographic group.

In the COMPAS data set, independence would be satisfied if the probability of recidivism is the same for both Black and White defendants in the data set. That is, the probability that a Black defendant is predicted to recommit a crime within the next two years should be the same as the probability that a White defendant is predicted to recommit a crime.

The visual example in Figure 1.2 illustrates a toy scenario where independence is met (Durahly, 2023).

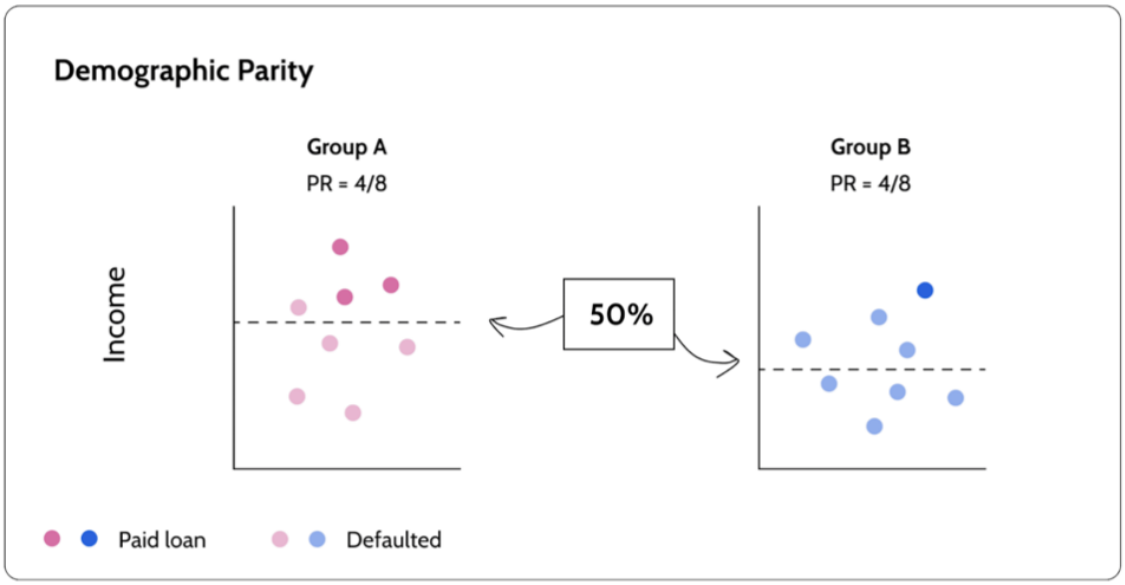


Figure 1.2: An Example of Demographic Parity (Durahly, 2023)

The dashed line represents the decision boundary. In both group A and group B, four out of the eight participants were predicted to repay a loan. The other half of the participants were predicted to default. Notice, however, that the class imbalance in this toy credit lending example results in a higher error rate within group B than group A.

A difference in demographic parity close to 0 or a ratio close to 1 by some defined margin is considered a fair solution (Castelnovo et al., 2022). To achieve demographic parity, the different demographic groups must be treated differently, which may seem contrary to societal pre-conceived notions of fairness. Therefore, demographic parity should be used when the primary objective is to enforce some form of equality between groups regardless of all other information and when the objectivity of the target variable, Y, is under question, perhaps because of historical biases. This, however, can unknowingly amplify biases if used in the wrong setting. For example, when imposing demographic parity on a hiring algorithm, if qualifications are different across a protected attribute, then less-qualified candidates may be hired. If these

candidates end up being low-performers, then this can perpetuate stereotypes about their demographic group.

In the above example of using a hiring algorithm with gender as the protected attribute, it may then seem fairer to require independence on gender only for men and women with the same rating or qualification, that is, $\hat{Y} \perp\!\!\!\perp A|R$. This is known as *conditional demographic parity* and requires that the following equation is satisfied (Castelnovo et al., 2022):

$$P(\hat{Y} = 1|A = a, R = r) = P(\hat{Y} = 1|A = b, R = r),\ \forall a, b \in A, \forall r.$$

This idea can be generalized more to condition on all attributes, that is, $\hat{Y} \perp\!\!\!\perp A|X$. As this is more generalized, however, it begins to satisfy individual fairness and can be achieved by a gender-blind model (Castelnovo et al., 2022). This type of individual fairness is also referred to as fairness through unawareness (FTU), which requires that any protected attributes, or their covariates, are not explicitly used in the decision-making process (Mehrabi et al., 2021). This definition of fairness requires that the following equation be satisfied (Castelnovo et al., 2022):

$$P(\hat{Y} = 1|A = a, X = x) = P(\hat{Y} = 1|A = b, X = x),\ \forall a, b \in A, \forall x \in X.$$

Separation

Independence does not make use of the true target Y and simply requires equality of predictions. However, as observed in Figure 1.2, this can lead to different error rates between different groups. In other words, the model is more accurate for one group than it is for another group. Separation precisely focuses on equality of the error rates

and is widely known as the *equality of odds* (Castelnovo et al., 2022). This definition requires the same type I and type II error rates, precisely, the same false positive rate (FPR) and false negative rate (FNR) across all demographic groups. FPR and FNR are defined by:

$$FPR = P(\hat{Y} = 1|Y = 0) = \frac{FP}{FP + TN}$$
$$FNR = P(\hat{Y} = 0|Y = 1) = \frac{FN}{TP + FN}$$

where FP refers to false positive predictions, TP refers to true positive predictions, FN refers to false negative predictions, and TN refers to true negative predictions. These metrics can be understood through a confusion matrix as in Figure 1.3 (Mohajon, 2021).

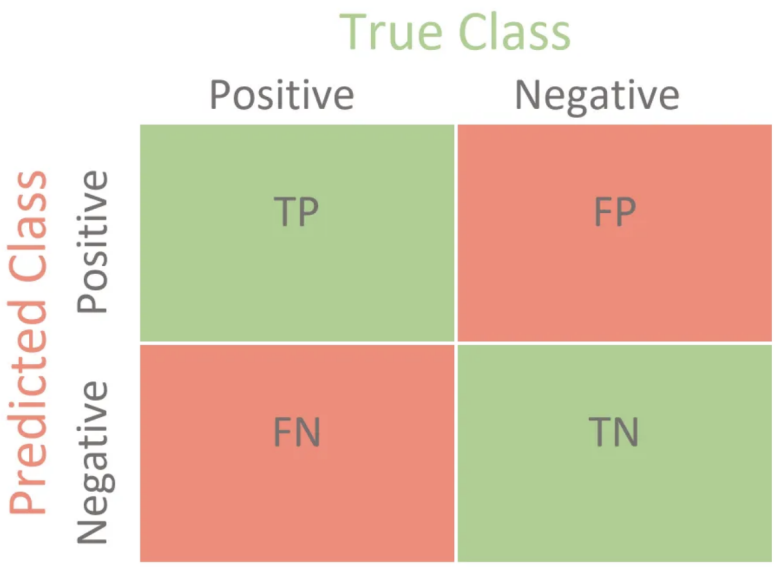


Figure 1.3: A Confusion Matrix (Mohajon, 2021)

In the COMPAS data set, separation would be satisfied if both Black defendants and White defendants had equal error rates. However, as observed in Figure 1.1,

Black defendants had an FPR of 45% while White defendants had an FPR of 24% – these refer to the percentage of times the algorithm predicted the defendants had recidivated when they hadn't. Similarly, Black defendants had an FNR of 28% while White defendants had an FNR of 48% – these refer to the percentage of times the algorithm predicted the defendants had not recommitted a crime when they had.

Separation requires independence of the predictions $\hat{Y}$ and the sensitive attribute A conditioned on the true value of the target variable Y, that is, $\hat{Y} \perp\!\!\!\perp A|Y$ (Castelnovo et al., 2022). In other terms, the following equation must be satisfied:

$$P(\hat{Y} = 1|A = a, Y = y) = P(\hat{Y} = 1|A = b, Y = y),\ \forall a, b \in A,\ y \in \{0, 1\},$$

where 0 is a negative outcome and 1 is a positive outcome. This is a reasonable fairness metric, as long as the objectivity of the target variable is trusted, as it ensures that the model optimizes performance for all groups, not just majority groups.

The visual example in Figure 1.4 illustrates a toy scenario where separation is met (Castelnovo et al., 2022). The dashed line represents the decision boundary. Filled in circles represent positive predictions and empty circles represent negative predictions. The error rates are consistent between both men and women.

Figure 1.4: An Example of Equality of Odds (Castelnovo et al., 2022)

There are two relaxed versions of this measure depending on which outcome is most important to predict (Castelnovo et al., 2022):

i) *Predictive equality*: equality of false positive rates (FPR) across groups:

$$P(\hat{Y} = 1|A = a, Y = 0) = P(\hat{Y} = 1|A = b, Y = 0), \ \forall a, b \in A.$$

ii) *Equality of Opportunity*: equality of false negative rates (FNR) across groups:

$$P(\hat{Y} = 0|A = a, Y = 1) = P(\hat{Y} = 0|A = b, Y = 1), \ \forall a, b \in A.$$

Sufficiency

Finally, sufficiency takes the perspective of people that receive the same model prediction and requires parity among them regardless of sensitive features (Castelnovo et al., 2022). This is also knows as *predictive parity* and requires that the precision

be the same across sensitive groups, that is, $Y \perp\!\!\!\perp A|\hat{Y}$. In other words, the following equation must be satisfied:

$$P(Y = y|A = a, \hat{Y} = y) = P(Y = y|A = b, \hat{Y} = y),\ \forall a, b \in A,\ \text{for } y \in \{0, 1\}.$$

Simply put, the probability of a positive outcome given a positive prediction, and that of a negative outcome given a negative prediction, should be equal across all sensitive groups.

Consistent with this line of reasoning, many fairness metrics can be defined. This begs the fundamental question: can multiple definitions be simultaneously enforced?

1.3 Fairness Conflicts

Because of the way different fairness definitions are defined, it can be impossible to simultaneously enforce multiple definitions and unexpected behavior may result from a particular definition of fairness. This section highlights some conflicts that arise both in the regression and classification setting.

1.3.1 Fairness Conflicts in Regression

The UFRGS Entrance Exam and GPA Data contains entrance exam scores of students applying to the Federal University of Rio Grande do Sul in Brazil, along with the students' GPAs during their first three semesters at the university (Silva, 2019). Each student's score in nine different entrance exams is used to predict their GPA during their first 3 semesters of study at the university. Gender and race are the protected

attributes.

Taking gender as the protected attribute in a gender-blind model, independence, in this setting, would require that the average predictions be the same for each gender. That is,

$$E[\hat{Y}|G = Male] = E[\hat{Y}|G = Female].$$

This is violated if, on average, a model predicts a higher or lower GPA based on gender.

Separation, on the other hand, would require that the average error of predictions be the same for each gender. In defined notion,

$$E[\hat{Y} - Y|G = Male] = E[\hat{Y} - Y|G = Female].$$

This is violated if, on average, the model over-predicts for one gender but under-predicts for another gender or the model either over-predicts or under-predicts more or less for one gender.

However, a study found that because male and female applicants had different GPAs in the original data set, these two fairness definitions cannot be simultaneously satisfied (P. Thomas, 2020). A result in the Section 1.3.2 will explain this in a mathematically tractable way.

1.3.2 Fairness Conflicts in Classification

Define prevalence p as the probability of a positive outcome given the demographic group (Chouldechova, 2017). It directly relates to the class distribution of the outcome. $p \in (0, 1)$ and can be denoted by:

$$p_a = P(Y = 1|A = a).$$

Further define the positive predictive value (PPV) of a prediction as the probability of a positive outcome given a positive prediction (Chouldechova, 2017):

$$PPV(\hat{Y}|A = a) \equiv P(Y = 1|\hat{Y} = 1, A = a).$$

Similarly, the negative predictive value (NPV) of a prediction is the probability of a negative outcome given a negative prediction and can be denoted as:

$$NPV(\hat{Y}|A = a) \equiv P(Y = 0|\hat{Y} = 0, A = a).$$

Sufficiency would require equal PPV and equal NPV across the different demographic groups. Note that NPV and PPV can be computed from a confusion matrix (Figure 1.3) as shown below (Saeed, Alireza, Mohamed, & Ahmed, 2015):

$$PPV = \frac{TP}{TP + FP} \; ; \; NPV = \frac{TN}{TN + FN}.$$

Now, given values of the $PPV \in (0, 1)$ and $p \in (0, 1)$, it can be shown that (Chouldechova, 2017):

$$FPR = \frac{p}{1 - p}\frac{1 - PPV}{PPV}(1 - FNR).$$

Appendix A provides the details for the derivation of this equation. However, its direct implication is that if the prevalence differs between two groups, then it is impossible to satisfy sufficiency (equal PPV across all groups) and separation (equal FPR and FNR across all groups) simultaneously. For example, in the COMPAS data set, if recidivism rates differ between Black and White offenders, then an algorithm that guarantees

predictive parity/ equal precision for both Black and White offenders cannot also guarantee equality of odds. Indeed, the recidivism rate for Black defendants in the data is 51%, compared to 39% for White defendants, and hence, the disparate impact of the COMPAS tool as observed in Figure 1.1 (Chouldechova, 2017).

Figure 1.2 illustrates a similar conflict between independence and separation. Satisfying independence resulted in an imbalance of error rates between group A and group B because of the difference in the prevalence of loan repayment between both groups.

Unfortunately, the distribution of the outcome of interest often differs for different demographic groups, posing the all-important question: how can fairness be achieved in the face of this conflict?

1.3.3 On Fairness Conflicts

As observed, disparate impact can result from the use of a prediction tool that is perceived to be free from predictive bias. Just because an algorithm satisfies a particular definition of fairness doesn't infer that the algorithm is *fair* in every sense of that word. Balancing overall error rates alone is not enough as it does not produce models that are free from bias or that guarantee fairness at finer levels of granularity. This highlights the need for human value and domain expertise in defining fairness within the context of a particular problem before the fairness constraints can be set. Once that is done, Chapter 2 introduces a framework for setting these constraints.

Chapter 2 The Seldonian Algorithm

Chapter 1 introduced the problem of algorithmic bias, discussed existing statistical definitions of fairness both in regression and classification settings, and finally, highlighted fairness conflicts that can arise in certain settings. Of important note is that there are a plethora of fairness definitions that have been developed in statistical machine learning, many of which have been shown to be incompatible in ways similar to the illustration in Appendix A. In any effort to enforce fairness on machine learning models, a critical first step is to define what fairness means in the specific context (P. Thomas, 2020). This responsibility falls on domain experts, social scientists, and regulators. Once there is consensus on that, machine learning researchers can work to develop appropriate algorithms that enforce the chosen definition of fairness. The Seldonian framework, introduced in this chapter, offers one such way to place probabilistic fairness constraints on traditional algorithms. However, because Seldonian algorithms place constraints on traditional machine learning (ML) algorithms, an initial in-depth understanding of the standard approach is key. Section 2.1 discusses the typical ML approach before diving into the Seldonian framework later in Section 2.2.

2.1 The Standard Machine Learning Approach

When designing a machine learning algorithm, the first step is to mathematically define what the algorithm should do, in other words, the goal of the algorithm (P.

S. Thomas et al., 2019b). At an abstract level, this goal is identical for all machine learning problems: find a solution θ^*, within some feasible set Θ, that maximizes some objective function $f : \Theta \to \mathbf{R}$, where $\mathbf{R}$ is the set of real numbers. Precisely, the goal of the algorithm is to search for an optimal solution

$$\theta^* \in \arg\max_{\theta \in \Theta} f(\theta).$$

For example, let X and Y be dependent real-valued random variables in a regression setting with the goal of estimating Y given X. In this setting, Θ is the set of feasible functions that model the relationship between X and Y. Feasible functions are of the form $\theta(X) = \beta_0 + \beta_1 X = \hat{Y}$. Each function $\theta \in \Theta$ takes a real number as input and produces a real number as output; therefore, $\theta : \mathbf{R} \to \mathbf{R}$. A reasonable objective function would then be the negative mean squared error (MSE):

$$f(\theta) := -E[(\theta(X) - Y)^2].$$

In this case, minimizing MSE is equivalent to maximizing -MSE, defining the goal of the regression algorithm as finding the solution with the least average error. Note that the true value of $f(\theta)$ is unknown and can only be estimated from the data (P. S. Thomas et al., 2019a). For a sample with n observations, that is, (x_i, y_i) for $i = 1, 2, ..., n$, the objective function can be estimated by:

$$\hat{f(\theta)} = -\frac{1}{n}\sum_{i=1}^{n}(\theta(x_i) - y_i)^2.$$

However, defining objective functions in this way can sometimes lead to undesirable behavior as illustrated in Section 2.1.1.

2.1.1 Limitations of the Standard Approach

Consider a linear regression example to predict the qualifications of job applicants based on information on their resumes. Let G encode the gender of each applicant, with $G = 0$ if the applicant is female and $G = 1$ if the applicant is male. Let X encode a summary measure of an applicant's qualification based on information on their resume – a simple example would be a measure of how many job-relevant key words appear on their resume. Let Y encode their actual qualification for the job as determined by their observed performance.

If this linear regression estimator is designed to be used to filter which resumes submitted to a company will be forwarded for human review, it is worthwhile to ensure that the algorithm does not produce racist or sexist behavior. Drawing from definitions in Chapter 1.2, it might be less important to ensure that the algorithm, on average, has the same predictions for applicants of both genders because the distribution of qualifications may be different for both genders. However, of more concern is whether the algorithm, on average, predicts too high for one gender and too low for the other gender.

Suppose that the data has the following distribution: $Y \sim N(1, 1)$ if $G = 0$ and $Y \sim N(-1, 1)$ if $G = 1$, that is, Y is a normal variable $N(\mu, \sigma)$ with different means μ for different genders but with the same standard deviation σ for both genders. Further define $X \sim N(Y, 1)$, that is, an applicant's resume quality is equal to their true qualification plus some random noise. Figure 2.1 displays a scatterplot of 1000 such data points, 500 from each gender. The black solid line is the least squares fit on this data using a gender-blind model.

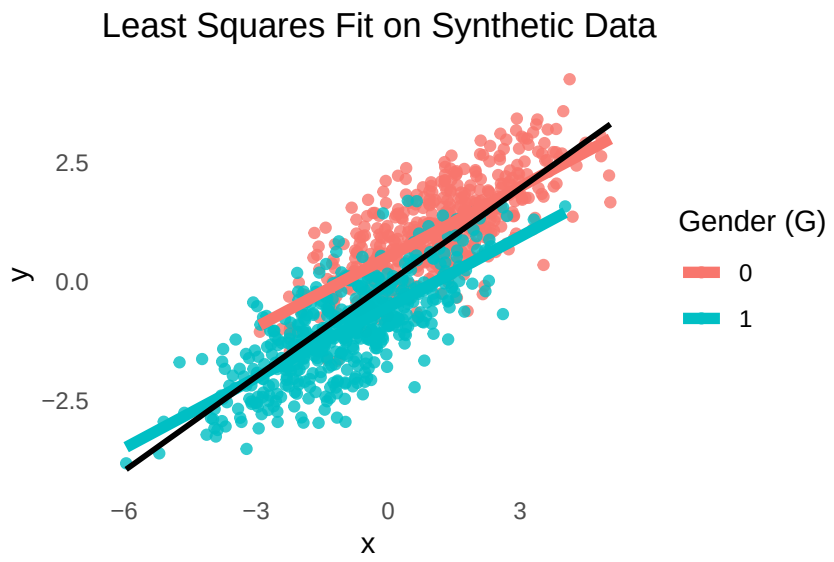


Figure 2.1: Least Squares Fit on Synthetic Data Drawn from Different Distributions

The least squares fit on Figure 2.1 is impartial to an observation's gender with an objective to make the most accurate predictions. While it may be expected that impartiality would produce fair results, observe that the linear model tends to over-predict if $G = 1$ and under-predict if $G = 0$, on the contrary, producing discriminatory behavior. In fact, by defining a discrimination statistic, $d(\theta)$, as defined below in line with the specified fairness definition, the discrimination statistic for the synthetic data set in Figure 2.1 can be shown to be -0.719, suggesting that the model predictions are in favor of $G = 1$:

$$d(\theta) = E[\hat{Y} - Y|G = 0] - E[\hat{Y} - Y|G = 1].$$

In crucial applications such as hiring, this is concerning and highlights how linear regression algorithms designed using the standard approach can result in predictions of applicant performance that systematically discriminate against a demographic group.

2.1.2 Potential Remedies

As illustrated in Section 2.1.1 above, machine learning algorithms that use the standard approach may produce undesirable behavior. In an attempt to remedy this problem, a number of approaches can be taken. One potential remedy is to identify the root cause of the undesirable behavior such as class imbalance in the training data, bias in the data set, the choice of linear estimator, the model's blindness to the demographic group, or insufficient data, to name a few (P. S. Thomas et al., 2019b). For instance, in the example set up in Section 2.1.1 and displayed in Figure 2.1, the root cause of the discriminatory behavior when using ordinary least squares linear regression was the fact that the objective function was designed to minimize MSE, which was at odds with minimizing the discrimination statistic. However, even though it might be possible to determine and correct the root cause of the undesirable behavior, doing so can be difficult, error-prone, and require extensive data analysis, rendering the central goal of machine learning algorithms, which are designed to automate and make decision-making processes simpler, obsolete.

Assuming that the problem is with the objective function and provided that detailed knowledge of the problem is available, hard constraints may be placed on the objective function, for example, requiring that MSE is minimized only on the set of solutions with a discrimination value $d(\theta)$ less than some value ϵ (P. S. Thomas et al., 2019b). Additionally, rather than placing hard constraints on the set of solutions, soft constraints that penalize undesirable behavior may also be placed on f, the objective function (Boyd & Vandenberghe, 2004). Although such penalty functions can be effective, they require a careful choice of the value of the parameter λ that places relative importance on the objective function and the constraint. For the linear regression example, the new objective function with a soft constraint would now be:

$$f(\theta) = -MSE(\theta) - \lambda d(\theta).$$

Observe that as λ increases, MSE increases and the discrimination statistic decreases. Cross-validation techniques can be employed to find optimal values for λ. Other remedies include maximizing multiple objective functions or allowing constraints on the probability that a solution with undesirable behavior will be returned, both of which may require detailed knowledge of the application problem and underlying distribution of the data (P. S. Thomas et al., 2019b).

In principle, there might be definitions of Θ or f that prevent the algorithm from converging on solutions that exhibit undesirable behavior (P. S. Thomas et al., 2019a). However, in practice and as explained, this might require extensive domain expertise and data analysis in order to properly balance the relative importance of the objective function and the constraints, which can be at odds with each other. These techniques may also require knowledge of the probability distribution from which the data is sampled, which is not always available and limits applications to parametric statistics.

A Seldonian algorithm, thus, addresses this problem precisely by allowing probabilistic constraints on undesirable behavior to be placed more easily without detailed knowledge of the specific problem or the distribution of the data, shifting the burden from the domain experts who use these tools to the experts in ML and statistics (P. S. Thomas et al., 2019a). It's named after Isaac Asimov's fictional character, Hari Seldon [1] (Asimov, 1994).

[1] In the fictional book, Hari Seldon was a resident of a fictional planet where he develops psychohistory, an algorithmic science that allows him to predict the future in probabilistic terms.

2.2 The Seldonian Framework

The first step of the Seldonian framework is to define mathematically the goal of the algorithm design (P. S. Thomas et al., 2019b). Define $\mathbf{D}$ as the set of all possible inputs (data sets) to the algorithm. Θ, as previously defined, is the set of all possible outputs (solutions) of the algorithm. Each solution is referred to as $\theta \in \Theta$. D is the data set (input) given to the algorithm and is the only random variable. Now, $a : \mathbf{D} \to \Theta$ is a machine learning algorithm which takes in a data set $D \in \mathbf{D}$ as an input and returns a solution $\theta \in \Theta$ as an output. $\mathbf{A}$ is the set of all possible machine learning algorithms. Synthesizing this, $f : \mathbf{A} \to \mathbf{R}$ is the objective function of the algorithm design, where $f(a) \in \mathbf{R}$ is a real-valued measure of the utility of the algorithm, such as the value of the objective function for the solution returned by this algorithm. This objective function is optimized – either minimized or maximized – to select a desired machine learning algorithm from the set $\mathbf{A}$.

Contrary to the standard ML approach, however, n behavioral constraints can then be specified (P. S. Thomas et al., 2019b). Specifically, $(g_i, \delta_i)_{i=1}^n$ can be defined as a set of n constraints, each of which contains a constraint function $g_i : \Theta \to \mathbf{R}$ and a desired confidence level δ_i. The constraint function takes in a solution returned from the chosen machine learning algorithm as an input and returns a real value encoding the "fairness" of the algorithm according to the fairness definition defined by the function. $(g_i, \delta_i)_{i=1}^n$ is defined such that:

- The i^{th} constraint function measures an undesirable behavior. Specifically, $\theta \in \Theta$ produces undesirable behavior if and only if $g_i(\theta) > 0$. This is to ensure that undesirable behavior is defined in a mathematically tractable way such as how the discrimination statistic $d(\theta)$ was defined in Section 2.1.1.

- The i^{th} confidence level specifies the maximum probability that an algorithm can return a solution θ where $g_i(\theta) > 0$. In other words, $1 - \delta_i$ specifies the minimum probability that desirable behavior ($g_i(\theta) \leq 0$) is met. Smaller values of δ_i are preferred.

In summary, a Seldonian algorithm ensures that for all $i \in \{1, 2, \ldots, n\}$:

$$P(g_i(a(D)) \leq 0) \geq 1 - \delta_i.$$

Section 2.2.1 goes into further detail about the Seldonian framework and how these probabilistic behavioral constraints are guaranteed.

2.2.1 The Seldonian Optimization Problem

As detailed, the Seldonian framework is different from current potential remedies of undesirable behavior because it defines a search over a possible set of algorithms with constraints, rather than over a possible set of solutions. This means that the constraints require that the probability that a machine learning algorithm returns an unsafe solution be bounded by some desired level of confidence, rather than the probability that a solution itself is unsafe. In summary, a Seldonian optimization problem (SOP) can be written as (P. S. Thomas et al., 2019a):

$$\arg\max_{a \in \mathbf{A}} f(a)$$

$$\text{s.t. } \forall\, i \in \{1, 2, \ldots, n\},\ P(g_i(a(D)) \leq 0) \geq 1 - \delta_i.$$

A Seldonian algorithm a, thus, returns, with high probability, a solution that guarantees desirable behavior. If one were to apply machine algorithm a to obtain

a solution from a large number of different data sets D drawn from the same distribution, then it would be expected that at most $100\delta_i\%$ solutions (models) would produce undesirable behavior.

Taking the previous regression example and turning it into a Seldonian optimization problem using the discrimination statistic in Section 2.1.1, f would still be an objective function like the MSE, Θ would still be the set of all possible linear models, and D would be the data set as described. There would be 1 behavioral constraint, $g_1(a(D)) = |d(a(D))| - \epsilon$, to guarantee with probability at least $1 - \delta_1$, that the absolute value of the discrimination statistic would be at most ϵ, where ϵ and δ_1 are chosen based on the specific application. Note that the user of the machine learning algorithm need not perform data analysis to determine whether $g_1(\theta) \leq 0$ for a particular solution $\theta \in \Theta$ returned. The burden is shifted to the computation algorithm to determine this with some desired level of probability.

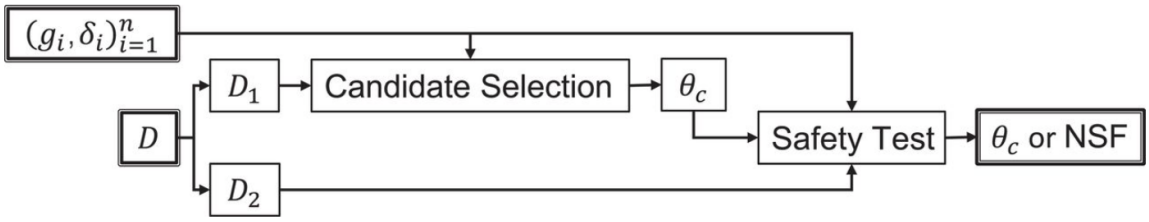


Figure 2.2: Overview of the Seldonian Framework (P. S. Thomas et al., 2019a)

Figure 2.2 illustrates how this is achieved at a high level. A Seldonian algorithm takes in n behavioral constraints $(g_i, \delta_i)_{i=1}^n$ and a data set D as the inputs and returns either a solution (model) θ or NSF, which means "No Solution Found". That is, no algorithm was found that returned a model which satisfied the behavioral constraints with the desired probability. First, the data D is partitioned into 2 sets D_1 and D_2 that essentially serve as train and test sets, respectively. D_1 is then passed through

the candidate selection mechanism, which performs a search over algorithms to settle on a candidate solution θ_c. θ_c is selected not only so that it optimizes the primary objective function f, but also so that it is predicted to pass the subsequent safety test. D_2 is then passed through the safety test to check whether θ_c indeed satisfies the n behavioral constraints with the desired confidence for each, that is $P(g_i(\theta_c) \leq 0) \geq 1 - \delta_i$ for each constraint $i \in \{1, 2, \ldots, n\}$. If so, θ_c is returned as the desired solution, and otherwise, NSF (P. S. Thomas et al., 2019a).

Note that finding exact confidence intervals may be impractical and require large amounts of data. Quasi-Seldonian algorithms, thus, are an extension of this idea that rely on standard statistical tools to transform sample statistics computed from D into approximate bounds on the probability of undesirable behavior (P. S. Thomas et al., 2019a). Section 2.2.2 discusses the statistical framework employed to achieve this.

2.2.2 Quasi-Seldonian Algorithms

https://aisafety.cs.umass.edu/tutorial3.html

Introduce quasi-seldonian algorithms to show how we would actually compute and execute this. Good place to talk about some of the key steps/ functions defined in the section above in mathematical detail.

Finish by Monday :)

2.3 Toy Example: A Seldonian Regression Algorithm

Walk through key parts of the jupyter notebook

Finish by Tuesday evening :)

2.4 Random Notes (Delete When Done):

Submit on Wednesday/ Thursday!

Need another source for this section?

Change colors on image.

Assign equations labels in Chapter 1 & 2 like below?

Review notes to fill in missing pieces.

$$d(\theta) = E[\hat{Y} - Y|G = 0] - E[\hat{Y} - Y|G = 1]. \tag{2.1}$$

Appendix A Sufficiency v Separation Fairness Conflict Equation

Recall from Chapter 1 that (Castelnovo et al., 2022):

$$PPV = P(Y = 1|\hat{Y} = 1),$$

$$FPR = P(\hat{Y} = 1|Y = 0),$$

$$FNR = P(\hat{Y} = 0|Y = 1),$$

$$p = P(Y = 1).$$

Using Bayes' rule,

$$PPV = P(Y = 1|\hat{Y} = 1) = \frac{P(\hat{Y} = 1|Y = 1)P(Y = 1)}{P(\hat{Y} = 1|Y = 1)P(Y = 1) + P(\hat{Y} = 1|Y = 0)P(Y = 0)}$$

$$\Rightarrow PPV = \frac{P(\hat{Y} = 1|Y = 1)p}{P(\hat{Y} = 1|Y = 1)p + P(\hat{Y} = 1|Y = 0)(1 - p)}$$

$$\Rightarrow PPV = \frac{(1 - FNR)p}{(1 - FNR)p + FPR(1 - p)}$$

$$\Rightarrow (1 - FNR)p + FPR(1 - p) = \frac{(1 - FNR)p}{PPV}$$

$$\Rightarrow FPR(1 - p) = \frac{(1 - FNR)p}{PPV} - (1 - FNR)p$$

$$\Rightarrow FPR = \frac{(1 - FNR)p}{PPV(1 - p)} - \frac{(1 - FNR)p}{(1 - p)}$$

$$\Rightarrow FPR = \frac{p}{1 - p}\left[\frac{(1 - FNR)}{PPV} - (1 - FNR)\right]$$

$$\Rightarrow FPR = \frac{p}{1 - p}\left[\frac{(1 - FNR) - PPV(1 - FNR)}{PPV}\right]$$

$$\Rightarrow FPR = \frac{p}{1 - p}\left[\frac{(1 - FNR)(1 - PPV)}{PPV}\right]$$

$$\Rightarrow FPR = \frac{p}{1 - p}\frac{1 - PPV}{PPV}(1 - FNR)\blacksquare.$$

A similar equation can be derived relating $NPV = P(Y = 0|\hat{Y} = 0)$ and both FPR and FNR.

Additionally, in conventional statistics notation, the sensitivity of a prediction tool can be defined as $P(\hat{Y} = 1|Y = 1) = 1 - FNR$ and its specificity can be defined as $P(\hat{Y} = 0|Y = 0) = 1 - FPR$. Given a prevalence p, sensitivity s_e, and specificity s_p, then:

$$PPV = \frac{s_e p}{s_e p + (1 - s_p)(1 - p)}.$$

Similarly, it can shown that:

$$NPV = \frac{s_p(1 - p)}{(1 - s_e)p + s_p(1 - p)}.$$

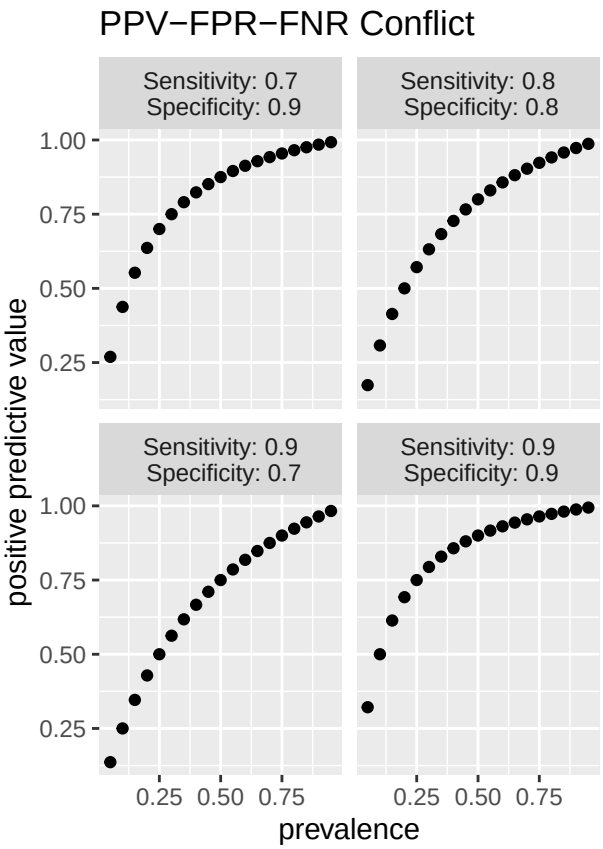
The code chunk below fixes arbitrary sensitivity (1 - FNR) and specificity (1 - FPR) values to illustrate through the proceeding plots that as prevalence varies, then

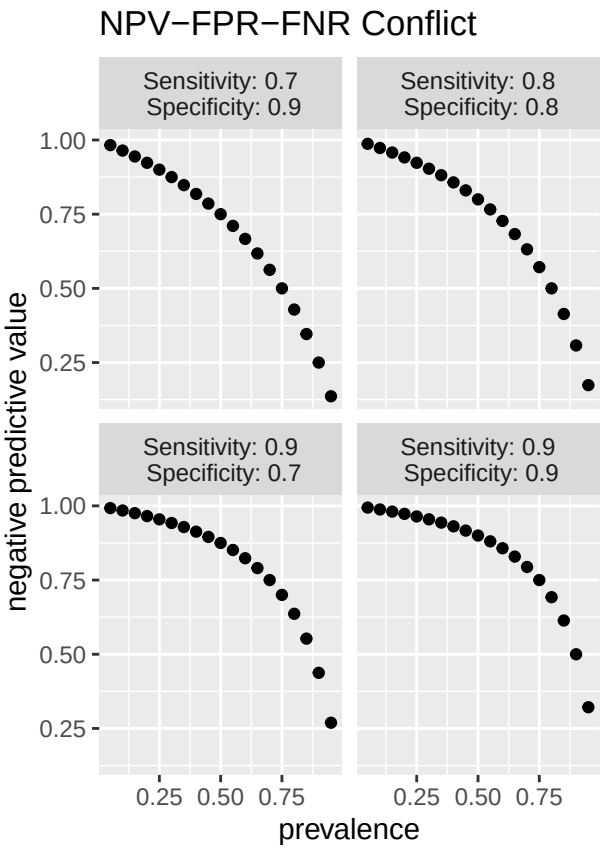
PPV/ NPV varies and cannot be equal as long as sensitivity and specificity are held constant, hence a conflict.

```
library(dplyr)
library(ggplot2)
library(gridExtra)
```

```
ppv <- function(p, sens, spec){
  ppv <- (sens*p)/((sens*p) + ((1-spec)*(1-p)))
  return(ppv)
}

npv <- function(p, sens, spec){
  npv <- (spec*(1-p))/(((1-sens)*p) + (spec*(1-p)))
  return(npv)
}

dat_8080 <- data.frame(prevalence = seq(0.05,0.95,0.05)
                       , sens=0.80
                       , spec=0.80
                       , ppv = ppv(p=seq(0.05,0.95,0.05),
                                   sens=0.80,
                                   spec=0.80)
                       , npv = npv(p=seq(0.05,0.95,0.05),
                                   sens=0.80,
                                   spec=0.80))

dat_9090 <- data.frame(prevalence = seq(0.05,0.95,0.05)
                       , sens=0.90
                       , spec=0.90
                       , ppv = ppv(p=seq(0.05,0.95,0.05),
                                   sens=0.90,
                                   spec=0.90)
                       , npv = npv(p=seq(0.05,0.95,0.05),
                                   sens=0.90,
                                   spec=0.90))

dat_9070 <- data.frame(prevalence = seq(0.05,0.95,0.05)
                       , sens=0.90
                       , spec=0.70
```

```
                        , ppv = ppv(p=seq(0.05,0.95,0.05),
                                    sens=0.90,
                                    spec=0.70)
                        , npv = npv(p=seq(0.05,0.95,0.05),
                                    sens=0.90,
                                    spec=0.70))

dat_7090 <- data.frame(prevalence = seq(0.05,0.95,0.05)
                        , sens=0.70
                        , spec=0.90
                        , ppv = ppv(p=seq(0.05,0.95,0.05),
                                    sens=0.70,
                                    spec=0.90)
                        , npv = npv(p=seq(0.05,0.95,0.05),
                                    sens=0.70,
                                    spec=0.90))

dat_all <- bind_rows(dat_8080, dat_7090, dat_9070, dat_9090) |>
  mutate(sens_spec = paste0("Sensitivity: ", sens,
                            "\n Specificity: ", spec)
         , fpr = 1 - spec
         , fnr = 1 - sens)

g1 <- ggplot(dat_all, aes(x=prevalence, y=ppv)) +
        geom_point() +
        labs(x="prevalence", y="positive predictive value",
             title = "PPV-FPR-FNR Conflict") +
        facet_wrap(~sens_spec)

g2 <- ggplot(dat_all, aes(x=prevalence, y=npv)) +
        geom_point() +
        labs(x="prevalence", y="negative predictive value",
             title = "NPV-FPR-FNR Conflict") +
        facet_wrap(~sens_spec)

grid.arrange(g1,g2, nrow=1, ncol=2)
```


PPV−FPR−FNR Conflict
Sensitivity: 0.7
Specificity: 0.9
Sensitivity: 0.8
Specificity: 0.8
Sensitivity: 0.9
Specificity: 0.7
Sensitivity: 0.9
Specificity: 0.9
positive predictive value
1.00
0.75
0.50
0.25
0.25 0.50 0.75
prevalence


NPV−FPR−FNR Conflict
Sensitivity: 0.7
Specificity: 0.9
Sensitivity: 0.8
Specificity: 0.8
Sensitivity: 0.9
Specificity: 0.7
Sensitivity: 0.9
Specificity: 0.9
negative predictive value
1.00
0.75
0.50
0.25
0.25 0.50 0.75
prevalence

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