## All AlBridge

AlBridge Lecture 5

## Let's talk about the last lab!

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# What circumstances made the model fit better? worse? 

## Accuracy

"Why is it not enough?"


Progeria affects ~159 patients in the US we have a dataset of all American pediatric patients

Q: If my model predicts with 99.99\% accuracy, is it good enough?

Progeria affects $\sim 159$ patients in the US
we have a dataset of all American pediatric patients

## a proposed model: protein shape $\rightarrow$ Model $\rightarrow \begin{gathered}\text { no progeria } \\ \text { regardless }\end{gathered}$

Progeria affects $\sim 159$ patients in the US
we have a dataset of all American pediatric patients

## Accuracy , Precision, and Recall


"Selection space"

"Selection space"

Model selects positive and patient is positive


"Selection space"

Model selects positive and patient is positive

Model selects positive and patient is negative

"Selection space"

Model selects positive and patient is positive

Model selects positive and patient is negative

"Selection space"

Model selects negative and patient is negative

TRUE POSITIVE

TP: Model selects positive and patient is positive

## FALSE POSITIVE

FP: Model selects positive and patient is negative

"Selection space"

## FALSE NEGATIVE

FN: Model selects negative and patient is positive

## TRUE NEGATIVE

TN: Model selects negative and patient is negative


Overall ability of model

"Number of cases where we chose positive when patient is positive
and

Number of cases where we chose negative when patient is negative"

TP: Model selects positive and patient is positive

FP: Model selects positive and patient is negative


FN: Model selects negative and patient is positive

TN: Model selects negative and patient is negative

## Accuracy

Overall ability of model
"Number of cases where we chose positive when patient is positive"

## Precision

Accuracy of what we selected.
Or amount of selection that's actually correct.
"All selected positive by the model"

TP: Model selects positive and patient is positive

FP: Model selects positive and patient is negative

## Accuracy

Overall ability of model


TN: Model selects negative and patient is negative

"Selection space"


FN: Model selects negative and patient is positive

## Precision

Amount of selection
that's actually correct.
"Number of cases where we chose positive when patient is positive"

## Recall

Accuracy of what we should select.
Or amount of what needs to be selected that is selected

"All cases that the patients are positive"

TP: Model selects positive and patient is positive

FP: Model selects positive and patient is negative

## Precision

Amount of selection that's actually correct.

Accuracy
Overall ability of model

"Selection space"


FN: Model selects negative and patient is positive

TN: Model selects negative and patient is negative


Recall
Amount of what needs to be selected that is selected

## FALSE POSITIVE

## Accuracy

Overall ability of model

Precision
Amount of selection that's actually correct.

Recall
Amount of what needs to be selected that is selected

|  |  | Predicted condition |  | Sources: [6][7][8][9][10][11][12][13][14] view -talk - edit |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | Total population $=P+N$ | Positive (PP) | Negative (PN) | Informedness, bookmaker informedness (BM) $=$ TPR + TNR - 1 | Prevalence threshold (PT) $=\frac{\sqrt{T P R \times F P R}-F P R}{T P R-F P R}$ |
|  | Positive (P) | True positive (TP), hit | False negative (FN), type II error, miss, underestimation | True positive rate (TPR), recall, sensitivity (SEN), <br> probability of detection, hit rate, power $=\frac{T P}{P}=1-F N R$ | False negative rate (FNR), <br> miss rate $=\frac{F N}{P}=1-T P R$ |
|  | Negative ( N ) | False positive (FP), type I error, false alarm, overestimation | True negative (TN), correct rejection | False positive rate (FPR), probability of false alarm, fall-out $=\frac{F P}{N}=1-T N R$ | True negative rate (TNR), specificity (SPC), selectivity $=\frac{T N}{N}=1-F P R$ |
|  | Prevalence $=\frac{P}{P+N}$ | Positive predictive value (PPV), $\begin{gathered} \text { precision } \\ =\frac{\mathrm{TP}}{\mathrm{PP}}=1-\mathrm{FDR} \end{gathered}$ | False omission rate $\begin{gathered} \text { (FOR) } \\ =\frac{\mathrm{FN}}{\mathrm{PN}}=1-\mathrm{NPV} \end{gathered}$ | Positive likelihood ratio (LR+) $=\frac{\mathrm{TPR}}{\mathrm{FPR}}$ | Negative likelihood ratio (LR-) $=\frac{\mathrm{FNR}}{\mathrm{TNR}}$ |
|  | $\begin{gathered} \text { Accuracy (ACC) } \\ =\frac{T P+T N}{P+N} \end{gathered}$ | False discovery rate (FDR) $=\frac{F P}{P P}=1-P P V$ | Negative predictive $\begin{gathered} \text { value }(\mathrm{NPV})=\frac{T N}{P N} \\ =1-F O R \end{gathered}$ | $\begin{gathered} \text { Markedness (MK), deltaP }(\Delta \mathrm{p}) \\ \quad=\mathrm{PPV}+\mathrm{NPV}-1 \end{gathered}$ | Diagnostic odds ratio (DOR) $=\frac{\mathrm{LR}+}{\mathrm{LR}}$ |
|  | Balanced accuracy (BA) $=\frac{T P R+T N R}{2}$ | $=\frac{2 P P V \times T P R}{P P V+T P R}=\frac{2 T P}{2 T P+F P+F N}$ | $\begin{aligned} & \text { Fowlkes-Mallows } \\ & \text { index (FM) } \\ & =\sqrt{\mathrm{PPV} \times \mathrm{TPR}} \end{aligned}$ | Matthews correlation coefficient $\begin{aligned} & (\mathrm{MCC}) \\ & =\sqrt{\mathrm{TPR} \times \mathrm{TNR} \times \mathrm{PPV} \times \mathrm{NPV}} \\ & -\sqrt{\mathrm{FNR} \times F P R \times F O R \times F D R} \end{aligned}$ | Threat score (TS), critical success index (CSI), Jaccard $\text { index }=\frac{T P}{T P+F N+F P}$ |

## Accuracy

Overall ability of model


## Precision

Amount of selection that's actually correct.

$$
\frac{T P}{T P+F P}
$$

## Progeria affects $\mathbf{\sim 1 5 9}$ patients in the US

## Recall

Amount of what needs to be selected that is selected

## Model $\rightarrow \quad \begin{gathered}\text { no progeria } \\ \text { regardless }\end{gathered}$

## storytime!

## storytime!



## storytime!




## storytime!




## storytime!




## quantifying "threshold"

## ROC Curve!




## AUC area under [the ROC] curve

Q: how do you compare these points

False Positive

## Self-test



## Precision-recall AUC

Q: When do we really need it? Q: what would it look like?

Especially for unbalanced datasets
more data

## what makes models fit better

balanced data
normalized data
quality data
more data
balanced data
normalized data
quality data
more data
more data

more data

Quality on the $y$ axis
Acidity on the $x$ axis

more data

Quality on the $y$ axis
Acidity on the $x$ axis

more data

Quality on the $y$ axis
Acidity on the $x$ axis

more data

Quality on the $y$ axis
Acidity on the $x$ axis


## more data


more data


more data

## more

data
a
reminder...
that's linear(ish)*

more
data

more
data


## more

data

more
data

more
data

wait... this is a t-test!
more
data

more
data

more
data


## more

data


■ increased degrees-of-freedom increases the probability of the population equaling sample
more
data


E-inereased-degrees-of-freedom inereases the probability of the population equaling sample ■ more data, better line
balanced data normalized data

## balanced data

## Let's think about logistic functions!

## balanced data


in an ideal world
...but no

## balanced data



What happens when we fit this dataset entirely?
balanced data
Let's think about logistic functions!


## balanced data

Let's think about logistic functions!

balanced data normalized data

## normalized data

Acidity



## normalized data

Acidity


## normalized data

Acidity



## normalized data



■ normalized data, better generalization, faster convergence

??? how to fit a line

Champagne
??? how to fit a line

??? how to fit a line

## normalized data


??? how to fit a line

## normalized data



## normalized data



- ensure all features are internally normalized (same order of mag.)


Image credit: Passionned Group
more data
balanced data normalized data
quality data

## Missing Data

# Missing completely at random 

## Missing Data

Missing at random
Missing not at random

## Missing Data

Use mean/most often
regression
more data
balanced data
normalized data
let's clean some data!

