



The curse of dimensionality

— Business problem: Prediction breast cancer in patients

Logistic regression

├ K nearest neighbors

Our conclusion
■



What is the curse of dimensionality and how we can show it with our dataset

The curse of dimensionality...



...refers to working with high-dimensional data which is due to large number of features



...occurs during analyzing the data to identify patterns and training the model



...is the model's decreasing performance with more features leaving all else constant as it becomes harder to generalize

We are aiming to show the curse in our dataset by...



... reducing and adding features into our models and observing model performances in each steps



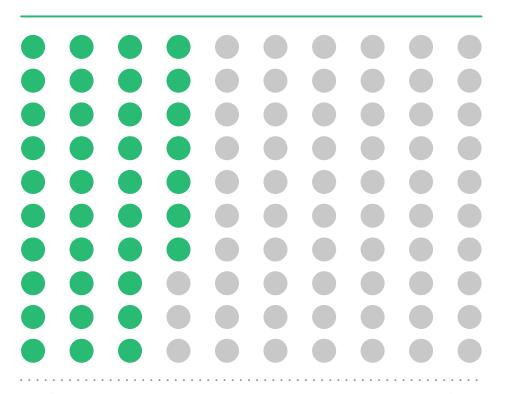
... showing that the model's ability to accurately predict the target is better with fewer than more features





Based on the breast cancer data, we try to predict the probability for breast cancer...

Breast Cancer data set



569 data points30 features1 target

...using two models

1 Logistic Regression

2 K nearest neighbors

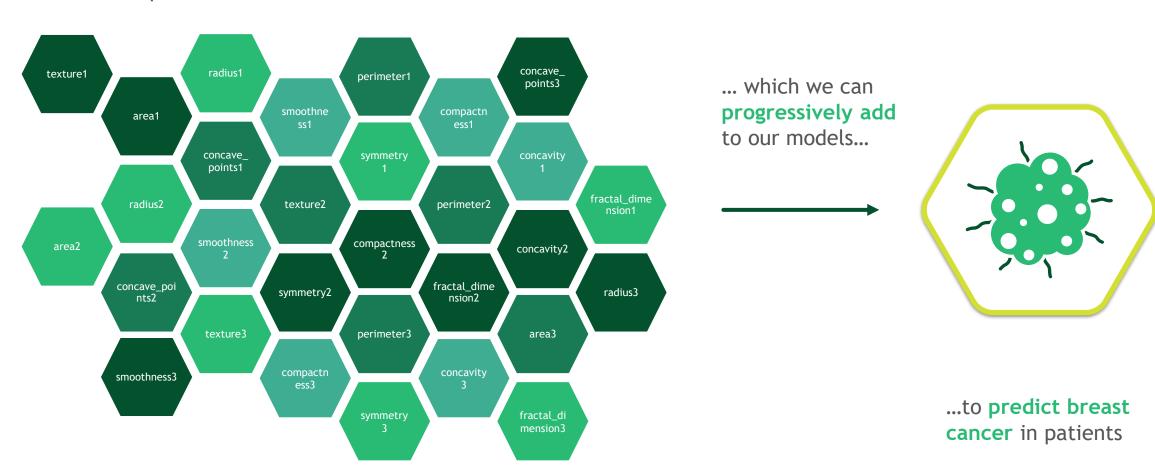
37% Breast Cancer patients

No Breast Cancer patients

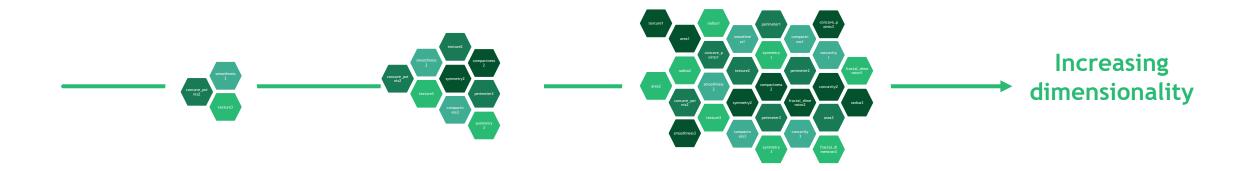


We have 30 features available to build our classification prediction models

Our dataset provides us with 30 features...



In the following, we will explore by progressively increasing the dimensionality



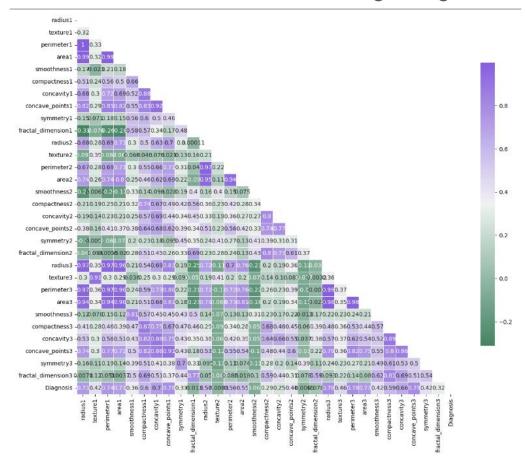
For both the logistic regression and KNN models

Please see on the following slide for the order

- 1. We are sorting our features in a meaningful order,
- 2. Then progressively adding the next best feature into our model.
- 3. As we have 30 features, we train and fit our models 30 times, each time with one more feature.
- 4. Progressively adding one features after another allows us to see the models' performance while increasing the number of features (= dimensions).

To order the features in a meaningful order to later progressively add them to the models, we look at their correlation to the target 'Diagnosis'

Correlation between 30 features and target 'Diagnosis'



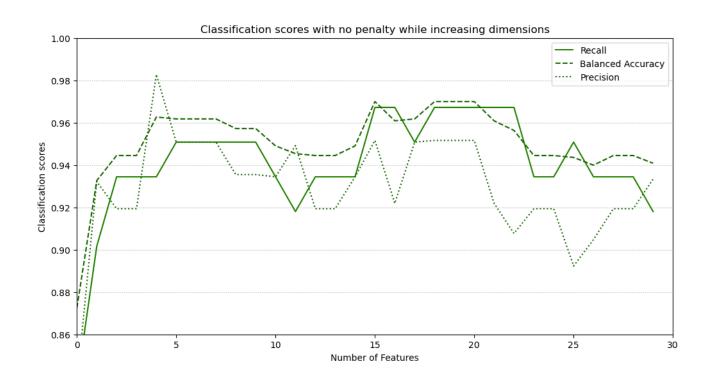
Features ordered according to their correlation

perimeter3 0.782914 symmetry3 0.41 concave_points1 0.776614 texture1 0.41 radius3 0.776454 concave_points2 0.40 perimeter1 0.742636 smoothness1 0.35 area3 0.733825 symmetry1 0.33 radius1 0.730029 fractal_dimension3 0.32 concavity1 0.696360 compactness2 0.29 concavity3 0.659610 fractal_dimension2 0.07 compactness1 0.596534 smoothness2 0.06 compactness3 0.590998 fractal_dimension1 0.01 radius2 0.567134 texture2 0.00	8560 0499 3872 2999 3730 7972 7016 2838 8303 6522
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We will pass the features one by one according to this order into our logistic regression and KNN models and observe their performance in prediction breast cancer in patients



The baseline logistic regression suffers the curse of dimensionality



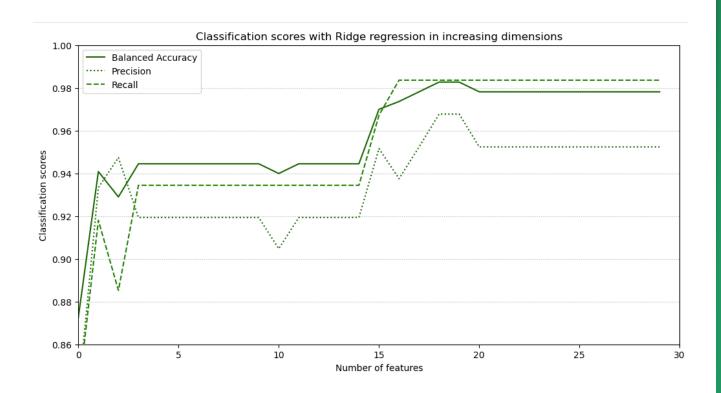
The baseline logistic regression model does not penalize the coefficients

While we pass more and more features into the model, the classification scores

- improve up until approx. 5 features
- decrease starting from approx. 20 features

Hence, after the 20th dimension we observe the model suffering from the curse of dimensionality

Regularizing with Ridge regression does reduce effect of the curse of dimensionality



Introducing Ridge regression into our baseline model penalizes coefficients

While we pass more and more features into the model, the classification scores

- keep improving until the 20th dimension
- and manages to retain classification scores beyond

Hence, when regularizing with Ridge regression, we do not observe the model suffering from the curse of dimensionality anymore We are choosing to look at Recall as we think this metric is most important for doctors

Definition of recall

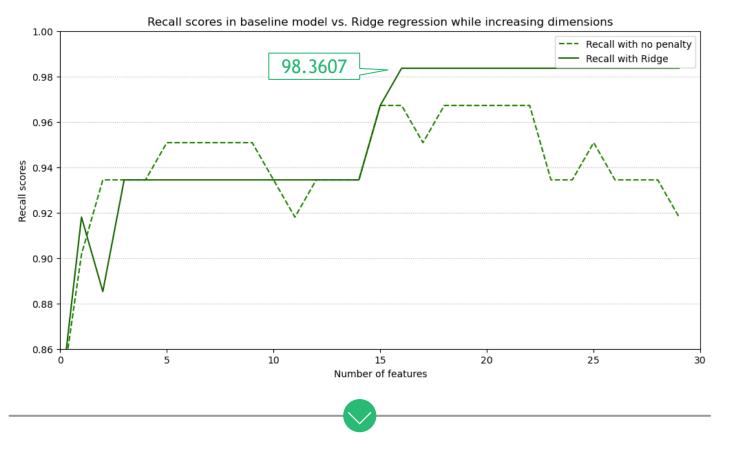
"Out of all the positive examples, how many are predicted as positive?"

$$recall = \frac{tp}{tp + fn}$$

For this business problem, we choose to primarily compare recall to minimize the number of patients who do have breast cancer, but it goes undetected

Hence, we prefer false positives over false negatives

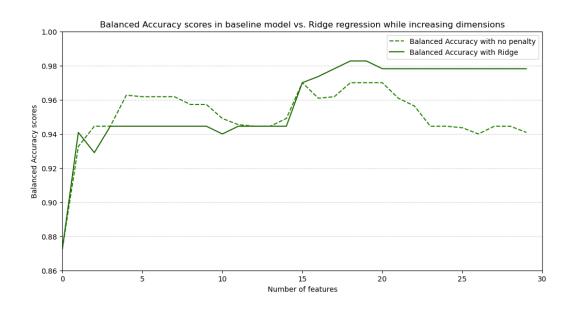
Comparing Recall from both models, we can more clearly see the success in addressing the curse of dimensionality



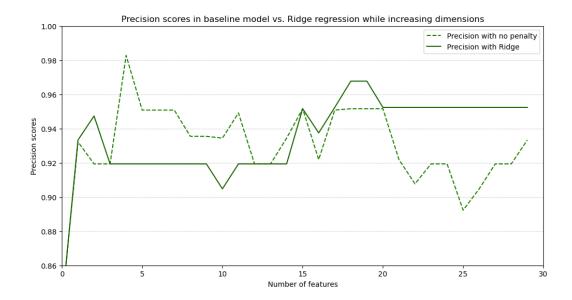
- Looking at Recall, the logistic regression which regularizes with **Ridge does** perform better than the logistic regression with no penalty on coefficients
- Starting from and **beyond the 15**th **dimension**, regularization does help the model to quite accurately predict whether a patient has breast cancer or not

We yield the same results from looking at Balanced Accuracy and Precision

Observing the curse of dimensionality with Balanced Accuracy starting from the 15th dimension



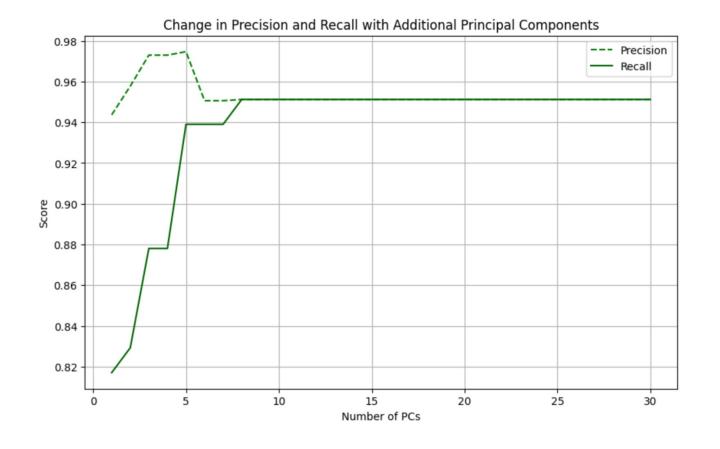
Looking at Precision, the curse of dimensionality starts around the 20th dimension



The PCA method is also successful in addressing the curse of dimensionality

Conducting the PCA method to address the curse of dimensionality,

- PCA contains information from all 30 columns
- we see that Precision and Recall scores stay constant at a high score of approx. 95 after the 8th principal component
- we interpret that it sufficient to extract the first 8 principal components to sufficiently capture the variation of the data



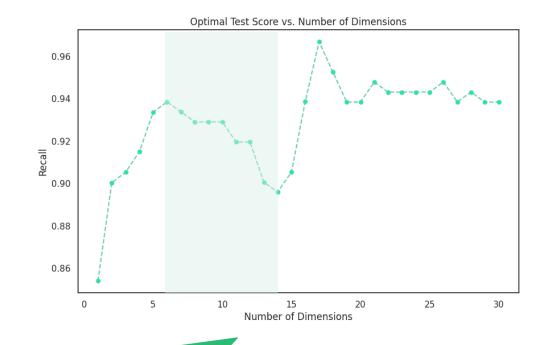


The baseline KNN model also suffers the curse of dimensionality

Best K values when dimensions are higher

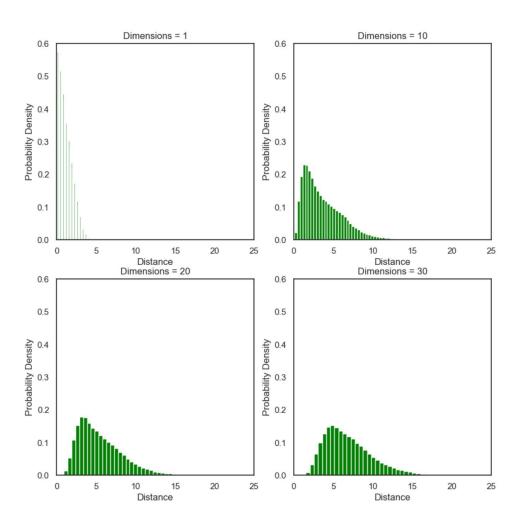
	Number	of	Dimensions	Best K	Recall Score
0			1	1	0.854042
1			2	1	0.900332
2			3	5	0.905316
3			4	13	0.914950
4			5	3	0.933666
5			6	3	0.938427
6			7	3	0.933776
7			8	3	0.929014
8			9	3	0.929014
9			10	5	0.929014
10			11	3	0.919491
11			12	3	0.919601
12			13	3	0.900664
13			14	3	0.895903
14			15	3	0.905316
15			16	1	0. 938538
16			17	1	0.966777
17			18	1	0.952602
18			19	3	0.938317
19			20	1	0.938427
20			21	1	0.947841
21			22	1	0.943079
22			23	1	0.943079
23			24	1	0.943079
24			25	1	0.943079
25			26	1	0.947841
26			27	1	0.938427
27			28	1	0.943079
28			29	3	0.938317
29			30	3	0.938427

Model performance under different dimensions



- Adding dimensions induces noisy and less informative data, leading to a temporary decrease in performance
- Correlation strength may not guarantee all features are equally relevant

In higher dimensions, the data points are located further apart from each other

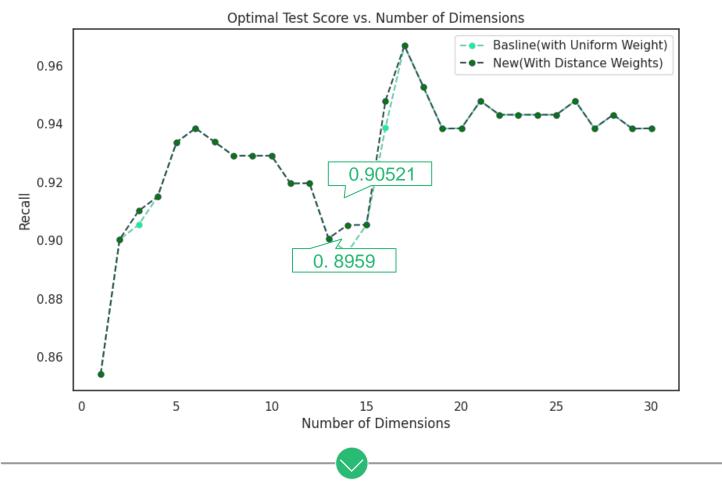


When calculating the distance between the data points to their neighbors

- we see that the distance between them increases as we move into higher dimensions.
- In one dimension, we see that most distances are very small (approx. 0)
- In 30th dimension, the mean of distances is around 5 and 6

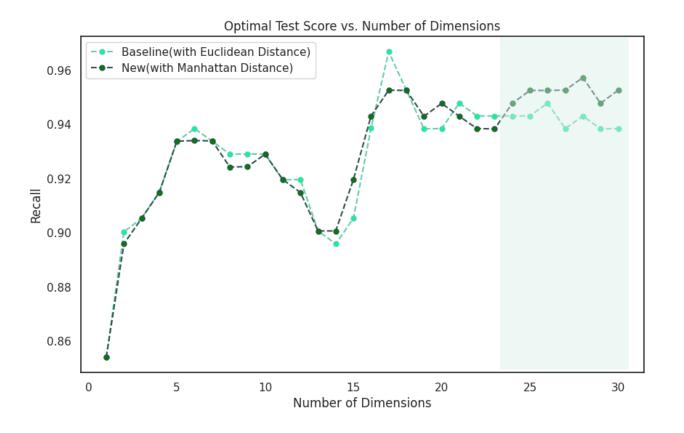
As the distance between data points increases in higher dimensions, it will become more difficult for the KNN model to find the nearest neighbor

To address the curse of dimensionality, we change the weight function from uniform to distance which slightly improves Recall

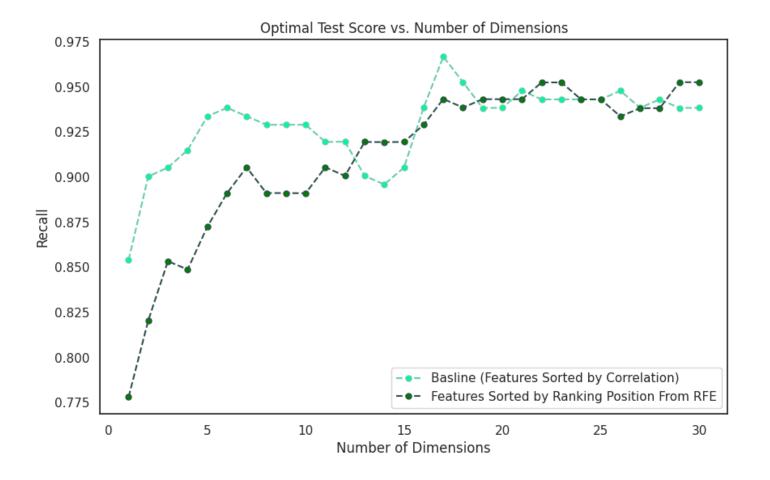


- At first, all points in each neighborhood were weighted equally as the weights are uniform
- With the distance weight function, closer neighbors of a data point will have a greater influence than neighbors further away, hence improving the prediction performance
- This can solely enhance few of the test scores

Manhattan distance yields higher Recall than Euclidean distance when the dimension increases



Sorting features by ranking with Recursive Feature Elimination (REF) effectively mitigates the curse of dimensionality



- All the features are ranked with recursive feature elimination using Logistic Regression as the estimator
- This method identifies the most important features effectively, which enables the recall score to keep increasing even in higher dimensions
- On the other hand, ordering features by their correlation strength to the target introduces noise probably because only linearity is assumed



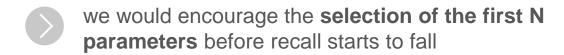
To predict breast cancer, we conclude that it is better to use logistic regression rather than KNN because ...

Comparing logistic regression with KNN

logistic regression performs better for most N features

logistic regression is more flexible as regularization is an option, which cannot be conducted for KNN

When feature selection is possible



- LASSO regularization was thus not utilized, as we acknowledge that in some scenarios:
 - dimensional reduction may not be a possibility
 - feature selection may have already been done
 - certain features may have to be included due to domain specific knowledge