LECTURE 32

Logistic Regression II

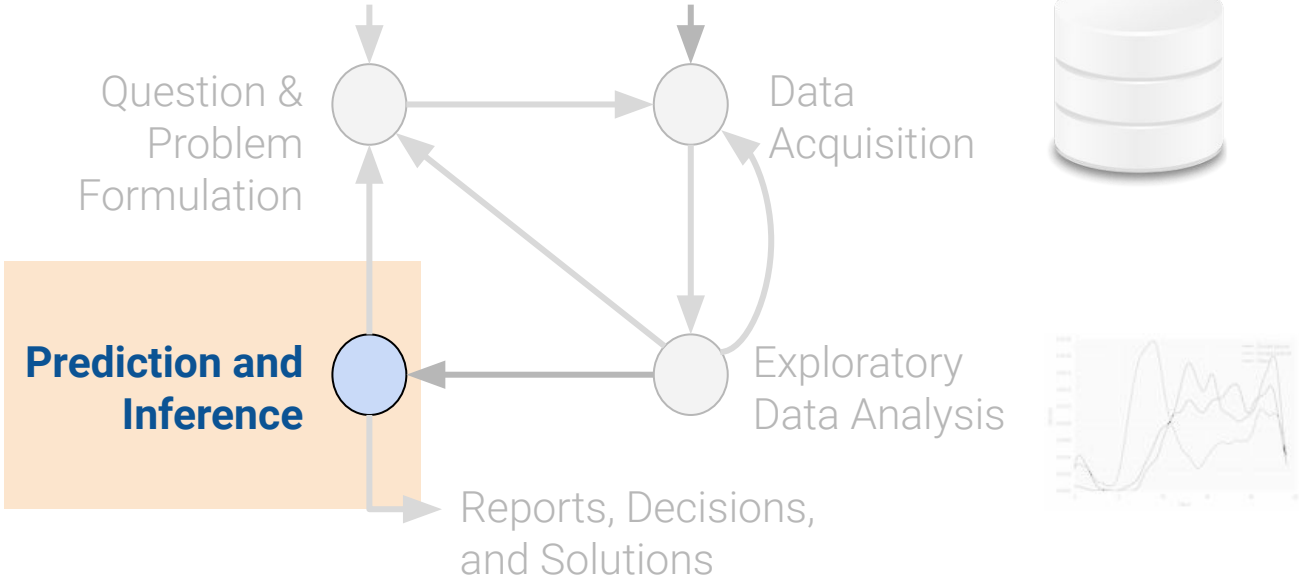
Model Performance.

CSCI 3022

Course Logistics: 14th and 15th Weeks At A Glance

Mon 4/22	Tues 4/23	Wed 4/24	Thurs 4/25	Fri 4/26	Sat.	Sun.
Attend & participate in class	TA NB Discussion 5pm-6pm via Zoom	Attend & participate in class	**Project Part 2 Due: 11:59pm MT No Late Submissions Accepted**	Attend & participate in class Quiz 8: Scope: L26-L29, HW 10, TA Discussion NB 12		
Mon 4/29	Tues 4/30	Wed 5/1	Thurs 5/2	Fri 5/3		Sunday 5/5
Attend & participate in class	TA NB Discussion 5pm-6pm via Zoom	**Last Day of Class: In-Class Review**				**FINAL: 1:30-4pm**

More Logistic Regression



(today)

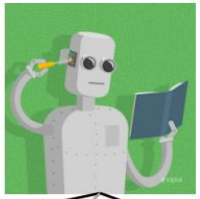
Logistic Regression I:
The Model
Cross-Entropy Loss
The Probabilistic View

Logistic Regression II:

Accuracy, Precision, Recall
Classification Thresholds

Taxonomy of Machine Learning

Taxonomy of Machine Learning



Labeled Data

Reward

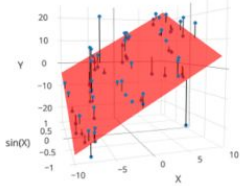
Unlabeled Data

Supervised Learning

Quantitative Response

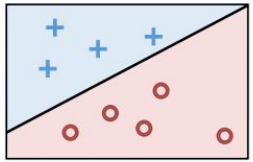
Categorical Response

Regression



OLS; linear regression w/regularization

Classification



k-nearest neighbors

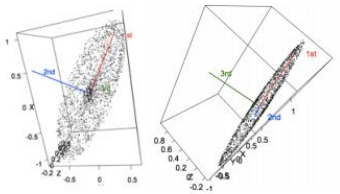
Logistic Regression

Reinforcement Learning

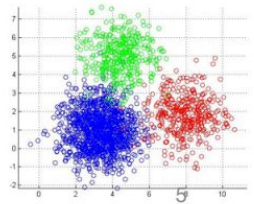
Alpha Go

Unsupervised Learning

Dimensionality Reduction



Clustering



Today's Roadmap

- Fitting Logistic Regression Models using Sklearn

Performance Metrics

- Accuracy
- Imbalanced Data, Precision, Recall
- ROC curves

Modeling Process

	Regression ($y \in \mathbb{R}$)	Classification ($y \in \{0, 1\}$)
1. Choose a model ✅	Linear Regression $\hat{y} = f_\theta(x) = x^T\theta$	Logistic Regression $\hat{P}_\theta(Y = 1\|x) = \frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\ldots+\theta_p x_p)}}$
2. Choose a loss function ✅	Squared Loss or Absolute Loss	Average Cross-Entropy Loss $: -\frac{1}{n}\sum_{i=1}^{n}\left(y_i \log\left(\frac{1}{1+e^{-x_i^T\theta}}\right) + (1-y_i)\log\left(1-\frac{1}{1+e^{-x_i^T\theta}}\right)\right.$
3. Fit the model	Sklearn & Regularization	Sklearn & Regularization
4. Evaluate model performance	R^2, Residuals, etc.	

Logistic Regression with sklearn

(documentation)

```
from sklearn.linear_model import LogisticRegression
model = LogisticRegression()
model.fit(X, Y)
```

Task/Model

Binary Classification ($y \in \{0, 1\}$)

$$\hat{P}_\theta(Y = 1|x) = \frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\ldots+\theta_p x_p)}}$$

Fit to objective function

Average Cross-Entropy Loss

$$: -\frac{1}{n}\sum_{i=1}^{n}\left(y_i \log\left(\frac{1}{1+e^{-x_i^T\theta}}\right) + (1-y_i)\log\left(1-\frac{1}{1+e^{-x_i^T\theta}}\right)\right)$$

+ regularization

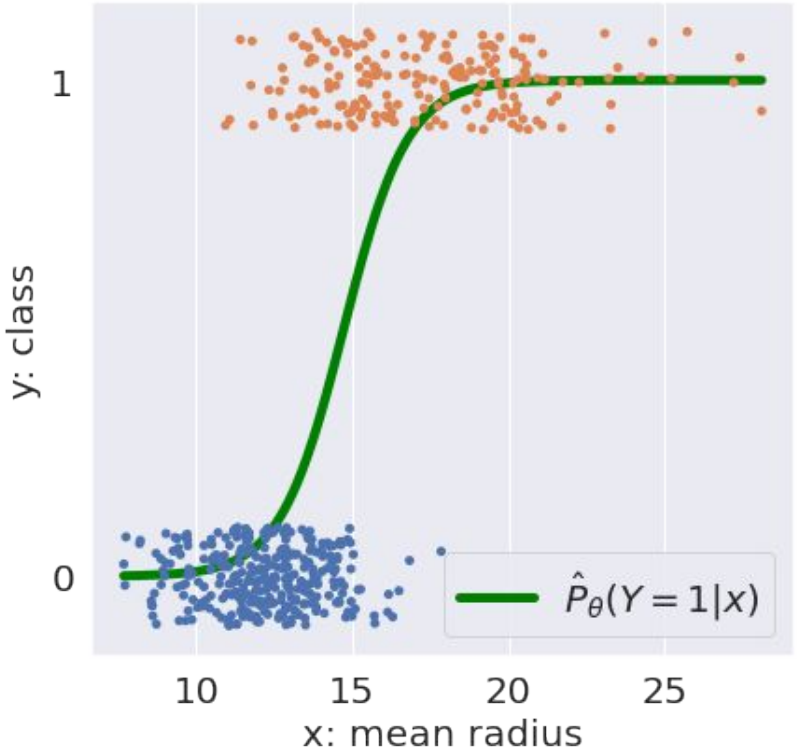
For logistic regression, sklearn applies regularization by default. See why in Appendix

Demo

Demo

Sklearn: Predict Probabilities

```
model.predict_proba(X) # probs for all classes
model.classes_         # array([0, 1])
```



Sklearn: Classification

```
model.predict_proba(X) # probs for all classes
model.classes_         # array([0, 1])
```

```
model.predict(X)         # predict 1 or 0
```

$$\hat{y} = \text{classify}(x) = \begin{cases} 1 & \hat{P}_\theta(Y = 1|x) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$

Equivalent "otherwise" condition: $\hat{P}_\theta(Y = 0|x) \geq 0.5$

Interpret: Given the input feature x:
If Y is more likely to be 1 than 0,
then predict $\hat{y} = 1$.
Else predict 0.

	X	Y	P(Y = 1 | x)	Y_hat
0	25.220	1	0.999965	1
1	13.480	1	0.226448	0
2	11.290	0	0.033174	0
3	12.860	0	0.137598	0
4	19.690	1	0.992236	1

Demo

Modeling Process

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3. Fit the model ✅	Sklearn & Regularization	Sklearn & Regularization
4. Evaluate model performance	R^2, Residuals, etc.	Let's do it!

Performance Metrics

Performance Metrics

- **Accuracy**
- **Imbalanced Data, Precision, Recall**

Adjusting the Classification Threshold

- A case study
- ROC curves

Classifier Accuracy

Now that we actually have our classifier, let's try and quantify how well it performs.

The most basic evaluation metric for a classifier is **accuracy**.

$$\text{accuracy} = \frac{\#\text{ of points classified correctly}}{\#\text{ points total}}$$

```
def accuracy(X, Y):
    return np.mean(model.predict(X) == Y)

accuracy(X, Y) # 0.8691
```

```
model.score(X, Y) # 0.8691
```

(sklearn documentation)

While widely used, the accuracy metric is **not so meaningful** when dealing with **class imbalance** in a dataset.

Pitfalls of Accuracy: A Case Study

Suppose we're trying to build a classifier to filter spam emails.

- Each email is **spam** (1) or **ham** (0).

Let's say we have 100 emails, of which only **5** are truly **spam**, and the remaining **95** are **ham**.

Your friend ("Friend 1"):

Classify every email as **ham** (0). $\hat{y} = \text{classify}_{\text{friend}}(x) = 0$

1. What is the accuracy of your friend's classifier?
2. Is accuracy a good metric of this classifier's performance?

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Your friend ("Friend 1"):

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$$\text{accuracy}_1 = \frac{95}{100} = 0.95$$

High accuracy…
…but we detected **none** ⚠️ of the spam!!!

Pitfalls of Accuracy: A Case Study

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$$\text{accuracy}_1 = \frac{95}{100} = 0.95$$

High accuracy…
…but we detected **none** ⚠️ of the spam!!!

Your other friend ("Friend 2"):

Classify every email as **spam** (1).

$$\text{accuracy}_2 = \frac{5}{100} = 0.05$$

Low ⚠️ accuracy…
…but we detected **all** of the spam!!!

Pitfalls of Accuracy: Class Imbalance

Suppose we're trying to build a classifier to filter spam emails.

- Each email is **spam** (1) or **ham** (0).

Let's say we have 100 emails, of which only **5** are truly **spam**, and the remaining **95** are **ham**.

Accuracy is not always a good metric for classification, particularly when your data have **class imbalance** (e.g., very few 1's compared to 0's).

Your friend ("Friend 1"):

Classify every email as **ham** (0).

$$\text{accuracy}_1 = \frac{95}{100} = 0.95$$

High accuracy…
…but we detected **none** ⚠️ of the spam!!!

Your other friend:

Classify every email as **spam** (1).

$$\text{accuracy}_2 = \frac{5}{100} = 0.05$$

Low ⚠️ accuracy…
…but we detected **all** of the spam!!!

Types of Classification Successes/Errors: The Confusion Matrix

- **True positives** and **true negatives** are when we correctly classify an observation as being positive or negative, respectively.
- **False positives** are "false alarms": we predicted 1, but the true class was 0.
- **False negatives** are "failed detections": we predicted 0, but the true class was 1.

Actual y \ Prediction $\hat{y}$	**0**	**1**
0	True **negative** (TN)	False **positive** (FP)
1	False **negative** (FN)	True **positive** (TP)

"**positive**" means a prediction of **1**.
"**negative**" means a prediction of **0**.

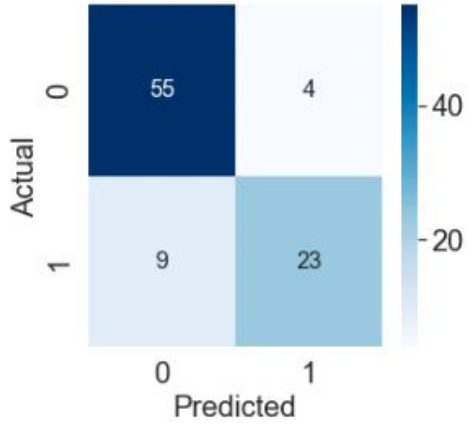
Types of Classification Successes/Errors: The Confusion Matrix

- **True positives** and **true negatives** are when we correctly classify an observation as being positive or negative, respectively.
- **False positives** are "false alarms": we predicted 1, but the true class was 0.
- **False negatives** are "failed detections": we predicted 0, but the true class was 1.

Actual y \ Prediction $\hat{y}$	**0**	**1**
0	True **negative** (TN)	False **positive** (FP)
1	False **negative** (FN)	True **positive** (TP)

A confusion matrix plots these four quantities for a particular classifier and dataset.

```
from sklearn.metrics import confusion_matrix
cm = confusion_matrix(Y_true, Y_pred)
```



Accuracy, Precision, and Recall

$$\text{accuracy} = \frac{TP + TN}{n}$$

What proportion of points did our classifier classify correctly?

Actual \ Prediction	**0**	**1**
0	TN	FP
1	FN	TP

Accuracy, Precision, and Recall

$$\text{accuracy} = \frac{TP + TN}{n}$$

What proportion of points did our classifier classify correctly?

		Prediction: 0	Prediction: 1
Actual	0	TN	FP
	1	FN	TP

Precision and recall are two commonly used metrics that, measure performance even in the presence of class imbalance.

$$\text{precision} = \frac{TP}{TP + FP}$$

Of all observations that were predicted to be 1, what proportion were actually 1?

- How **accurate** is our classifier **when it is positive**?
- Penalizes false positives.

Accuracy, Precision, and Recall

$$\text{accuracy} = \frac{TP + TN}{n}$$

What proportion of points did our classifier classify correctly?

		Prediction: 0	Prediction: 1
Actual	0	TN	FP
	1	FN	TP

Precision and **recall (aka true positive rate aka sensitivity)** are two commonly used metrics that,measure performance even in the presence of class imbalance.

$$\text{precision} = \frac{TP}{TP + FP}$$

Of all observations that were predicted to be 1, what proportion were actually 1?

- How accurate is our classifier when it is positive?
- Penalizes false positives.

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

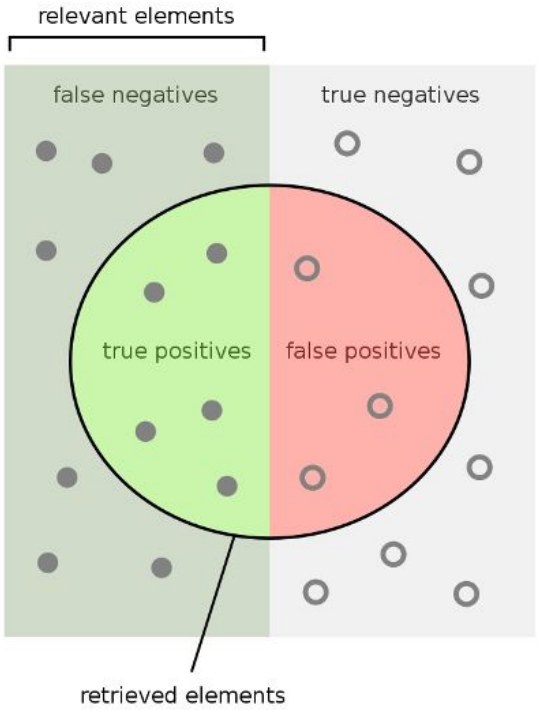
aka TPR (true positive rate)

Of all observations that were actually 1, what proportion did we predict to be 1? (Also known as sensitivity.)

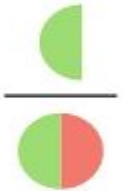
- How **sensitive** is our classifier to **positives**?
- Penalizes false negatives.

One of the Most Valuable Graphics on Wikipedia

(relevant elements means
true value of the data is 1)



How many retrieved items are relevant?



Precision =

$$\text{precision} = \frac{TP}{TP + FP}$$

How many relevant items are retrieved?

Recall =

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

(retrieved means you have predicted
the class to be 1)

[adapted from Wikipedia]

Back to the Spam

$$\text{accuracy} = \frac{TP + TN}{n}$$
$$\text{precision} = \frac{TP}{TP + FP}$$
$$\text{recall} = \frac{TP}{TP + FN}$$

Suppose we're trying to build a classifier to filter spam emails.

- Each email is **spam** (1) or **ham** (0).

Let's say we have 100 emails, of which only **5** are truly **spam**, and the remaining **95** are **ham**.

Your friend:

Classify every email as **ham** (0).

	0	**1**
0	TN: 95	FP: 0
1	FN: 5	TP: 0

$$\text{accuracy}_1 = \frac{95}{100} = 0.95$$

$$\text{precision}_1 = \frac{0}{0 + 0} = \text{undefined}$$

$$\text{recall}_1 = \frac{0}{0 + 5} = 0$$

Back to the Spam

$$\text{accuracy} = \frac{TP + TN}{n}$$
$$\text{precision} = \frac{TP}{TP + FP}$$
$$\text{recall} = \frac{TP}{TP + FN}$$

Suppose we're trying to build a classifier to filter spam emails.

- Each email is **spam** (1) or **ham** (0).

Let's say we have 100 emails, of which only **5** are truly **spam**, and the remaining **95** are **ham**.

Your friend:

Classify every email as **ham** (0).

$$\text{accuracy}_1 = \frac{95}{100} = 0.95$$

Never positive!

$$\text{precision}_1 = \frac{0}{0 + 0} = \text{undefined}$$

$$\text{recall}_1 = \frac{0}{0 + 5} = 0$$

Your other friend ("Friend 2"):

Classify every email as **spam** (1).

	0	1
0	TN: 0	FP: 95
1	FN: 0	TP: 5

$$\text{accuracy}_2 = \frac{5}{100} = 0.05$$

$$\text{precision}_2 = \frac{5}{5 + 95} = 0.05$$

Many false positives!

$$\text{recall}_2 = \frac{5}{5 + 0} = 1.0$$

No false negatives!

Precision vs. Recall

$$\text{precision} = \frac{TP}{TP + FP}$$

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

Precision penalizes false positives, and Recall penalizes false negatives.

We can achieve **100% recall** by making our classifier output "1", regardless of the input.

- Friend 2's "always predict spam" classifier.
- We would have no false negatives, but many false positives, and so our **precision would be low**.

This suggests that there is a **tradeoff** between precision and recall; they are often inversely related.

- Ideally, both would be near 100%, but that's unlikely to happen.

(see extra slides re: the precision-recall curve)

Which Performance Metric?

$$\text{accuracy} = \frac{TP + TN}{n}$$

$$\text{precision} = \frac{TP}{TP + FP}$$

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

For our tumor classifier, do you recommend we try to maximize: precision, recall, or accuracy?

How do we engineer classifiers to meet the performance goals of our problem?

Which Performance Metric?

$$\text{accuracy} = \frac{TP + TN}{n}$$

$$\text{precision} = \frac{TP}{TP + FP}$$

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

In many settings, there might be a higher cost to missing positive cases.
For our tumor classifier:

- We really don't want to miss any malignant tumors (avoid false negatives).
- We might be fine with classifying benign tumors as malignant (OK to have false positives), since pathologists could do further studies to verify all malignant tumors.
- This context would prioritize **recall**.

How do we engineer classifiers to meet the performance goals of our problem?

Adjusting the Classification Threshold

Performance Metrics

- Accuracy
- Imbalanced Data, Precision, Recall

Adjusting the Classification Threshold

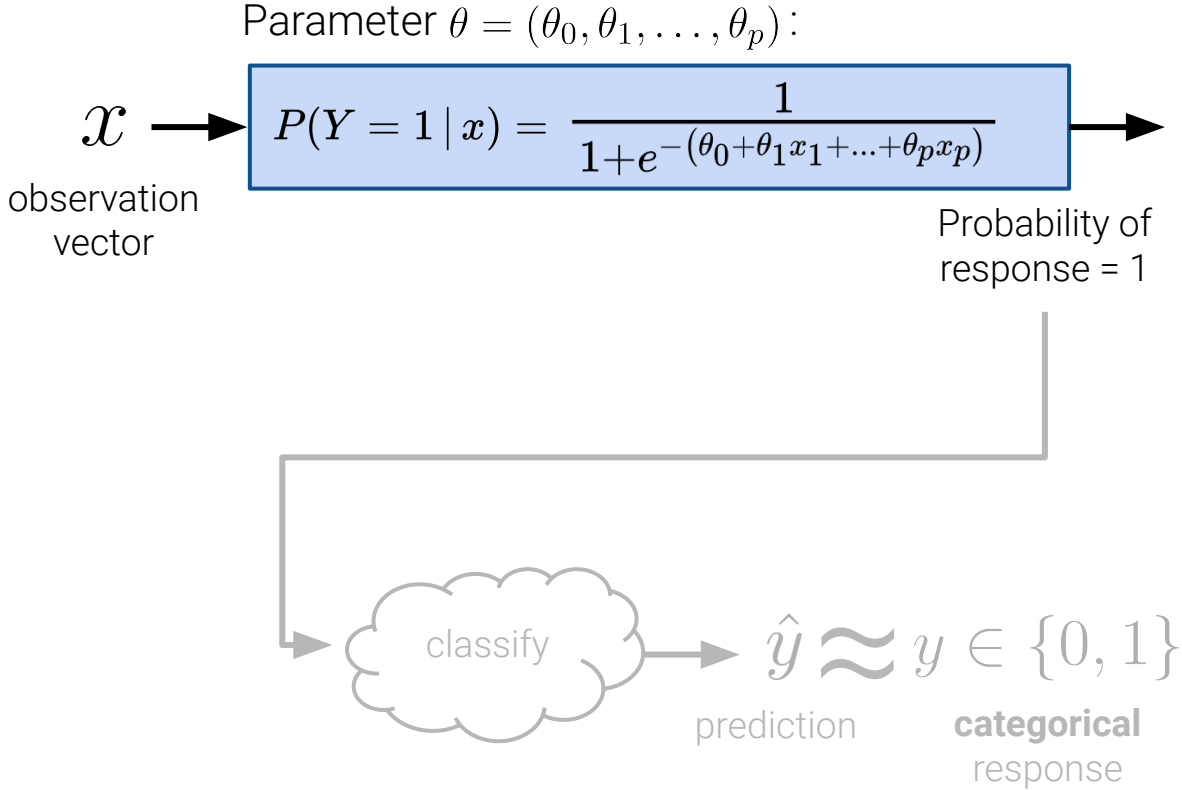
- **ROC curves, and AUC**

[

Engineering, Part 1: Deciding a Model

Feature Engineering:

What are the features x that generate great probabilities for prediction?



Engineering, Part 2: Deciding a Classification Threshold

Classification:

What is the best **classification threshold T** to choose that best fits our problem context?

Parameter $\theta = (\theta_0, \theta_1, \ldots, \theta_p)$:

x → observation vector

$$P(Y = 1 \mid x) = \frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\ldots+\theta_p x_p)}}$$

→ Probability of response = 1

$$\hat{y} = \text{classify}(x) = \begin{cases} 1 & \hat{P}_\theta(Y = 1|x) \geq T \\ 0 & \text{otherwise} \end{cases}$$

sklearn's model.predict() uses fixed 0.5

classify → $\hat{y} \approx y \in \{0, 1\}$

prediction

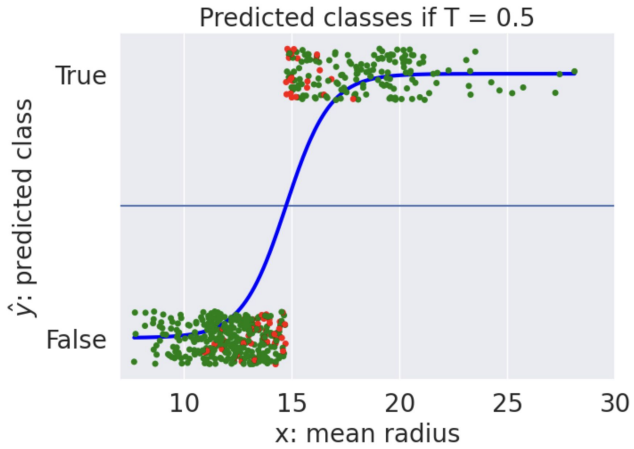
categorical response

Classification Threshold

$$\hat{y} = \text{classify}(x) = \begin{cases} 1 & \hat{P}_\theta(Y = 1|x) \geq T \\ 0 & \text{otherwise} \end{cases}$$

The default threshold in sklearn is T = 0.5.

	X	Y	P(Y = 1 | x)
0	25.220	1	0.999965
1	13.480	1	0.226448
2	11.290	0	0.033174
3	12.860	0	0.137598
4	19.690	1	0.992236
...	...	...	...
507	8.888	0	0.003257
508	11.640	0	0.046105
509	14.290	0	0.392796
510	13.980	1	0.323216
511	12.180	0	0.075786

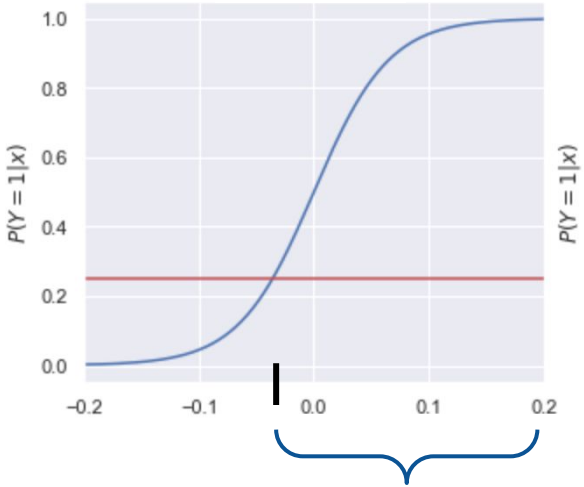


Classification Threshold

$$\hat{y} = \text{classify}(x) = \begin{cases} 1 & \hat{P}_\theta(Y = 1|x) \geq T \\ 0 & \text{otherwise} \end{cases}$$

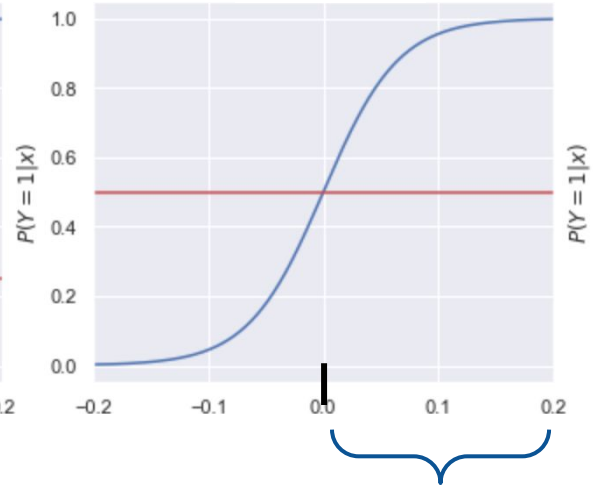
As we increase the threshold T, we “raise the standard” of how confident our classifier needs to be to predict 1 (i.e., “positive”).

T = 0.25

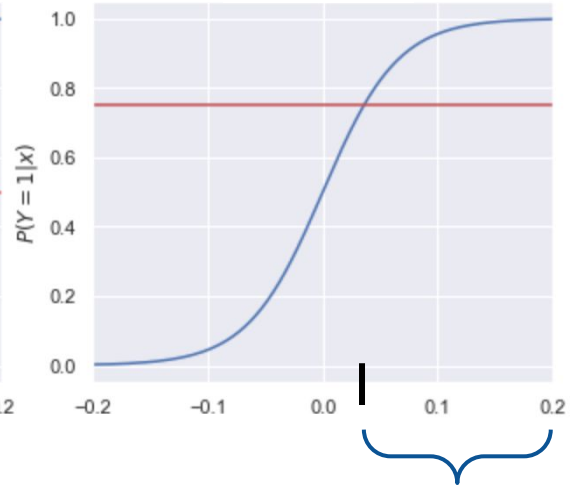


These x will all predict 1

T = 0.50



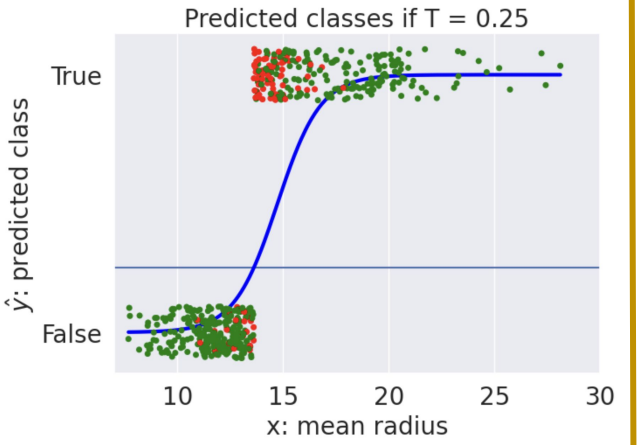
T = 0.75



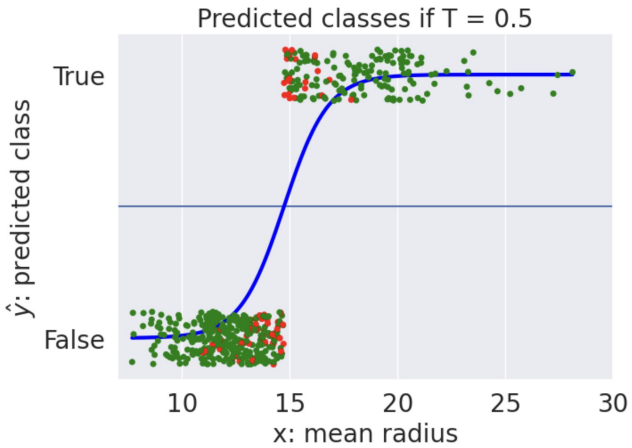
Fewer positives

Classification Threshold

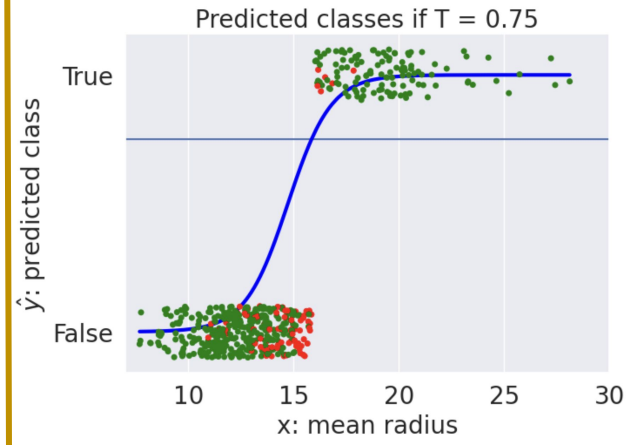
T = 0.25



T = 0.5



T = 0.75



Demo

See notebook for code snippets.

Choosing an Accuracy Threshold

The choice of threshold T impacts classification performance.

- High T: Most predictions are 0. Lots of false negatives.
- Low T: Most predictions are 1. Lots of false positives.

Do we get max accuracy when T ≈ 0.5? Not always the case…

Best T ≈ 0.57 likely due to class imbalance. There are fewer malignant tumors and so we want to be more confident before classifying a tumor as malignant.

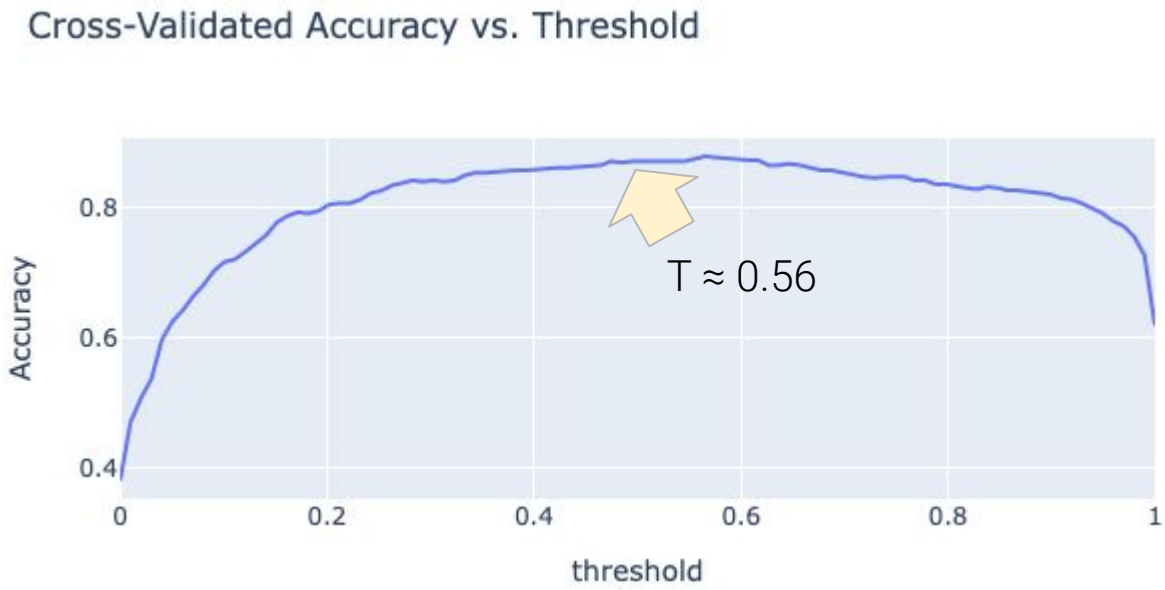
```
malignant
0          317
1          195
dtype: int64
```

Tune Thresholds with Cross Validation

The threshold should typically be tuned using cross validation.

For a threshold T:

$$\text{cross\_val\_acc} = (1/k)\left[\text{Model fit to train set 1, Acc on val set 1} + \ldots + \text{Model fit to train set k, Acc on val set k}\right]$$



Demo

See notebook for code snippets.
documentation

Choosing a Threshold According to Other Metrics?

The choice of threshold T impacts classification performance.

- High T: Most predictions are 0. Lots of false negatives.
- Low T: Most predictions are 1. Lots of false positives.

Could we choose a threshold T based on metrics that measure false positives/false negatives?

Yes! Two options:

- Precision-Recall Curve (PR Curve).
- “Receiver Operating Characteristic” Curve (**ROC Curve**).

Each of these visualizations have an associated performance metric: **AUC (Area Under Curve)**.

Demo

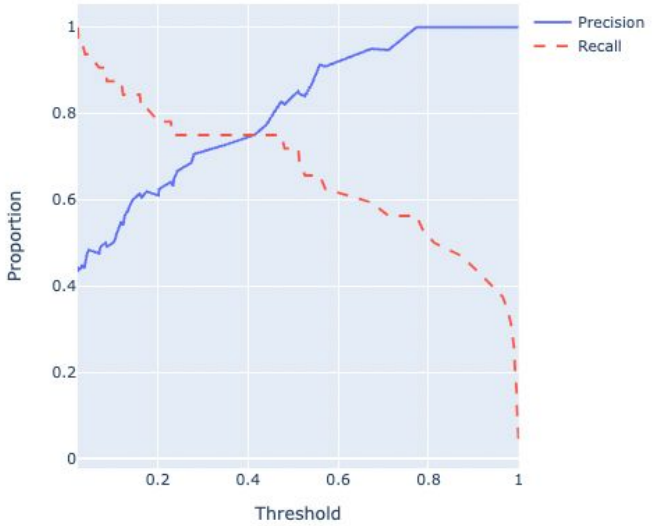
Demo

Demo: Precision vs Recall for our Tumor Classifier

The choice of threshold T impacts classification performance.

- High T: Most predictions are 0. Lots of false negatives.
- Low T: Most predictions are 1. Lots of false positives.

Could we choose a threshold T based on metrics that measure false positives/false negatives?



What about False Positives?

	Prediction	
	0	1
0	TN	FP
1	FN	TP

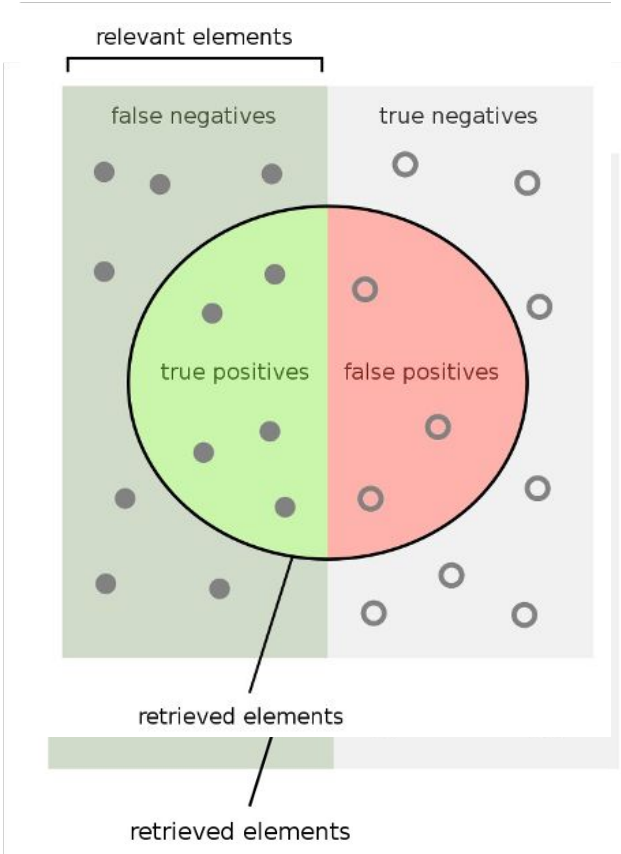
$$\text{FPR} = \frac{FP}{FP + TN}$$

False Positive Rate (FPR):
"What proportion of regular email did I mark as spam?
In statistics, also called specificity.

The ROC curve plots TPR (recall) vs FPR for different classification thresholds.

Demo

One of the Most Valuable Graphics on Wikipedia, Now With FPR



How many retrieved items are relevant?

Precision =

$$\text{precision} = \frac{TP}{TP + FP}$$

Want close to 1.0

How many relevant items are retrieved?

Recall =

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

TPR

Want close to 1.0

How many irrelevant items are retrieved?

FPR =

$$\text{FPR} = \frac{FP}{FP + TN}$$

Want close to 0.0

The ROC curve plots TPR vs FPR for different classification thresholds.

[adapted from Wikipedia]

Not the ROC Curve, but Useful to Start with

The choice of threshold T impacts classification performance.

- High T: Most predictions are 0. Lots of false negatives.
- Low T: Most predictions are 1. Lots of false positives.

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

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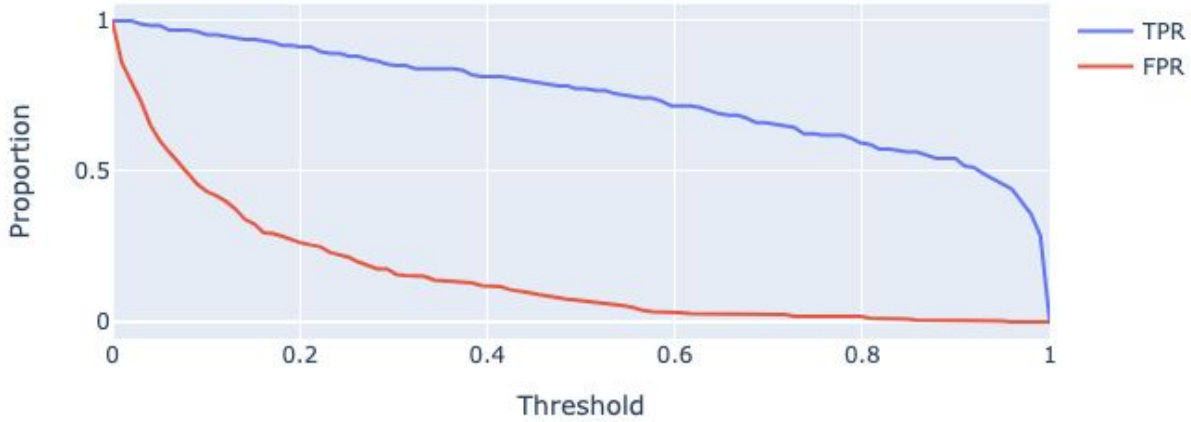


As we increase T, **both TPR** and FPR decrease.

- A decreased **TPR** is bad (detecting fewer positives).
- A decreased **FPR** is good (fewer false positives).

Demo

The ROC Curve

$$\text{TPR} = \frac{TP}{TP + FN}$$
$$\text{FPR} = \frac{FP}{FP + TN}$$

The ROC Curve plots this tradeoff.

- ROC stands for “Receiver Operating Characteristic.” [Wikipedia]
- We want high TPR, low FPR.

1. Which part of this curve corresponds to T = 0.9?
2. Which part of this curve corresponds to T = 0.1?

Demo

The ROC Curve

$$\text{TPR} = \frac{TP}{TP + FN}$$
$$\text{FPR} = \frac{FP}{FP + TN}$$

The ROC Curve plots this tradeoff.

- ROC stands for “Receiver Operating Characteristic.” [Wikipedia]
- We want high TPR, low FPR.

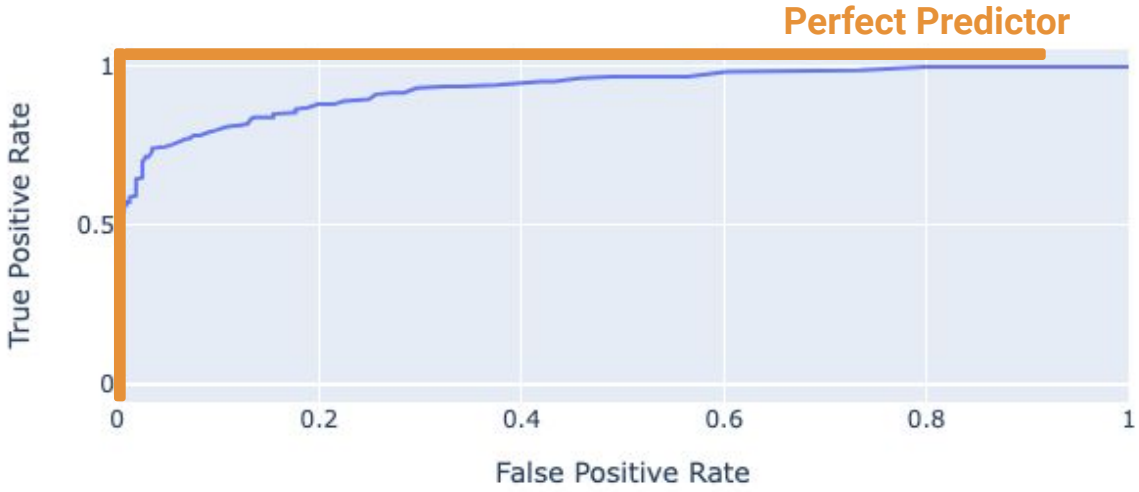
Demo

Demo

The Perfect Classifier

The “perfect” classifier is the one that has a TPR of 1, and FPR of 0.

- We want our logistic regression model to match that as well as possible.
- We want our ROC curve to be as close to the “top left” of this graph as possible.



Performance Metric: Area Under Curve (AUC)

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

$$\text{FPR} = \frac{FP}{FP + TN}$$

The “perfect” classifier is the one that has a TPR of 1, and FPR of 0.

- We want our model to match that as well as possible.
- We want our ROC curve to be as close to the “top left” of this graph as possible.

We can compute the **area under curve (AUC)** of our model.

- Different AUCs for both ROC curves and PR curves, but ROC is more common.
- Best possible AUC = 1. Terrible AUC = 0.5.
  - Random predictors have an AUC of around 0.5. Why?
- Your model’s AUC: somewhere between 0.5 and 1.

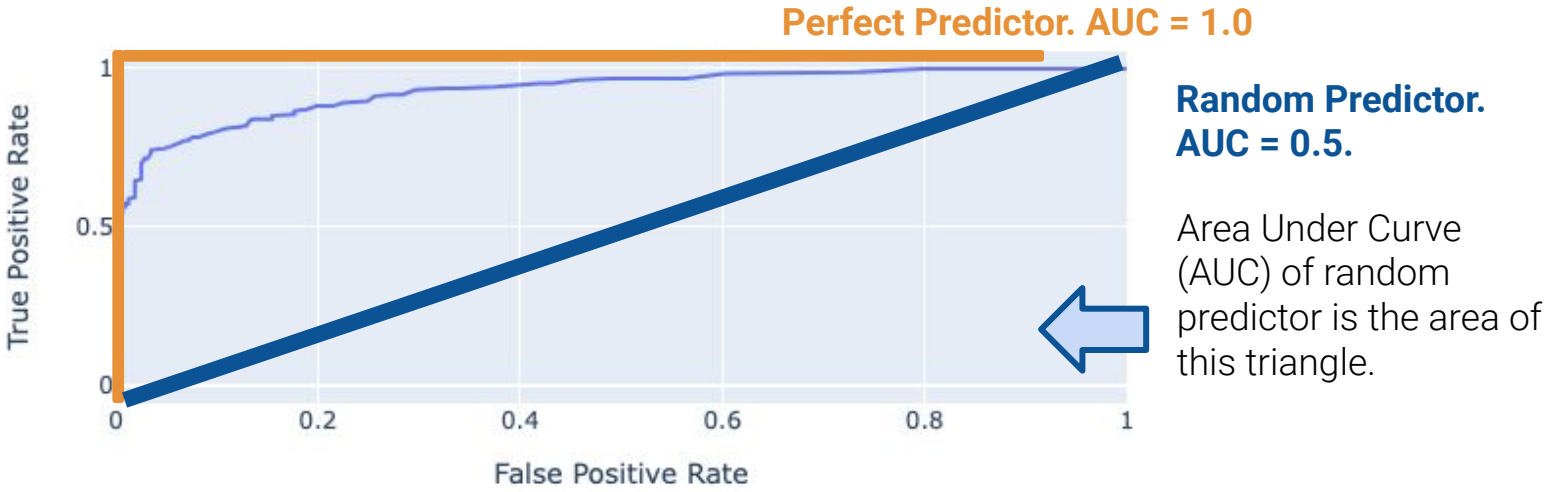
What is the “worst” AUC and why is it 0.5?

$$\text{TPR} = \frac{TP}{TP + FN}$$
$$\text{FPR} = \frac{FP}{FP + TN}$$

Best possible AUC = 1. Terrible AUC = 0.5.

- Random predictors have an AUC of around 0.5. (Why? - See Appendix!)

A **random predictor** randomly predicts P(Y = 1 | x) to be uniformly between 0 and 1.



Random Predictor. AUC = 0.5.

Area Under Curve (AUC) of random predictor is the area of this triangle.

Common techniques for evaluating classifiers

Numerical assessments:

- **Accuracy, precision, recall/TPR, FPR.**
- Area under curve (AUC), for ROC curves.

Visualizations:

- **Confusion matrices.**
- Precision/recall curves.
- ROC curves.

Terminology and derivations from a confusion matrix

condition positive (P)
the number of real positive cases in the data
condition negative (N)
the number of real negative cases in the data

true positive (TP)
eqv. with hit
true negative (TN)
eqv. with correct rejection
false positive (FP)
eqv. with false alarm, Type I error
false negative (FN)
eqv. with miss, Type II error

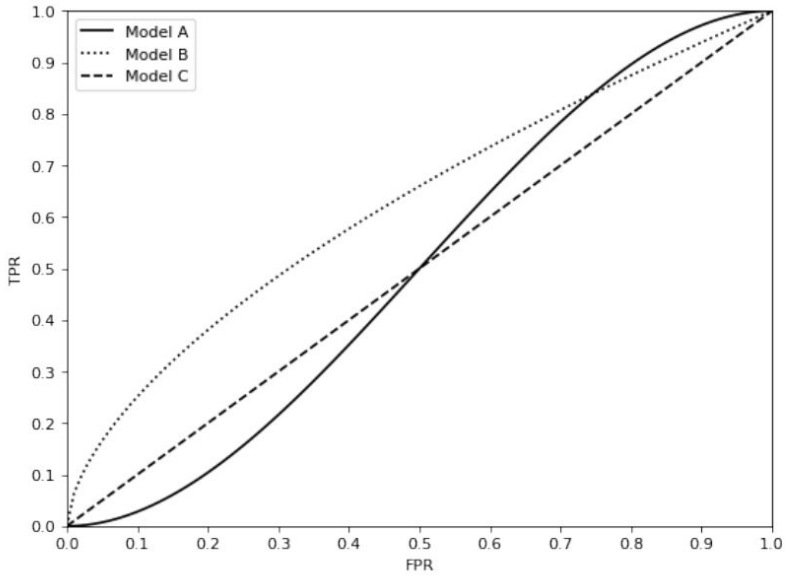
sensitivity, recall, hit rate, or true positive rate (TPR)
$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{P}} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} = 1 - \mathrm{FNR}$$
specificity, selectivity or true negative rate (TNR)
$$\mathrm{TNR} = \frac{\mathrm{TN}}{\mathrm{N}} = \frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FP}} = 1 - \mathrm{FPR}$$
precision or positive predictive value (PPV)
$$\mathrm{PPV} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}} = 1 - \mathrm{FDR}$$
negative predictive value (NPV)
$$\mathrm{NPV} = \frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FN}} = 1 - \mathrm{FOR}$$
miss rate or false negative rate (FNR)
$$\mathrm{FNR} = \frac{\mathrm{FN}}{\mathrm{P}} = \frac{\mathrm{FN}}{\mathrm{FN} + \mathrm{TP}} = 1 - \mathrm{TPR}$$
fall-out or false positive rate (FPR)
$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{N}} = \frac{\mathrm{FP}}{\mathrm{FP} + \mathrm{TN}} = 1 - \mathrm{TNR}$$
false discovery rate (FDR)
$$\mathrm{FDR} = \frac{\mathrm{FP}}{\mathrm{FP} + \mathrm{TP}} = 1 - \mathrm{PPV}$$
false omission rate (FOR)
$$\mathrm{FOR} = \frac{\mathrm{FN}}{\mathrm{FN} + \mathrm{TN}} = 1 - \mathrm{NPV}$$
Threat score (TS) or Critical Success Index (CSI)
$$\mathrm{TS} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN} + \mathrm{FP}}$$

accuracy (ACC)
$$\mathrm{ACC} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{P} + \mathrm{N}} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN}}$$
F1 score
is the harmonic mean of precision and sensitivity
$$\mathrm{F_1} = 2 \cdot \frac{\mathrm{PPV} \cdot \mathrm{TPR}}{\mathrm{PPV} + \mathrm{TPR}} = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$
Matthews correlation coefficient (MCC)
$$\mathrm{MCC} = \frac{\mathrm{TP} \times \mathrm{TN} - \mathrm{FP} \times \mathrm{FN}}{\sqrt{(\mathrm{TP} + \mathrm{FP})(\mathrm{TP} + \mathrm{FN})(\mathrm{TN} + \mathrm{FP})(\mathrm{TN} + \mathrm{FN})}}$$
Informedness or Bookmaker Informedness (BM)
$$\mathrm{BM} = \mathrm{TPR} + \mathrm{TNR} - 1$$
Markedness (MK)
$$\mathrm{MK} = \mathrm{PPV} + \mathrm{NPV} - 1$$

We're only scratching the surface here.

Comparing Classifiers: Practice!

Below are the ROC curves for 3 different models.



Suppose we fix the TPR to be 0.3.

(i) Which model would be most preferred?

- ◯ A. Model A
- ◯ B. Model B
- ◯ C. Model C
- ◯ D. Not enough information

(ii) Which model would be least preferred?

- ◯ A. Model A
- ◯ B. Model B
- ◯ C. Model C
- ◯ D. Not enough information

More Practice: Evaluating Logistic Regression Model

The table below shows a sample of validation data and predictions.

y_i	$\hat{P}(y = 1 \mid x_i)$
1	0.52
0	0.51
1	0.89
0	0.13
0	0.72
1	0.77

What is the largest range of classification thresholds that maximize accuracy while having no false positives on this sample of the validation set? Give your answer as an interval (be sure to indicate whether or not your interval endpoints are included).

Appendix: Linear separability and Regularization

Performance Metrics

- Accuracy
- Imbalanced Data, Precision, Recall

Adjusting the Classification Threshold

- A case study
- ROC curves, and AUC

[Extra] **Linear separability and Regularization**

[Extra] What is the “worst” AUC and why is it 0.5?

$$\text{TPR} = \frac{TP}{TP + FN}$$
$$\text{FPR} = \frac{FP}{FP + TN}$$

Best possible AUC = 1. Terrible AUC = 0.5.

- Random predictors have an AUC of around 0.5. Why?

A **random predictor** randomly predicts P(Y = 1 | x) to be uniformly between 0 and 1.

On average, if your dataset is size n_1+n_0 (with n_1 true class 1’s and n_0 true class 0’s):

If T = 0.5:

	0	1
0	TN = 0.5 n_0	FP = 0.5 n_0
1	FN = 0.5 n_1	TP = 0.5 n_1

FPR = 0.5 n_0/((0.5 + 0.5)n_0) = 0.5

TPR = 0.5 n_1/((0.5 + 0.5)n_1) = 0.5

Point on ROC curve is (0.5, 0.5).

If T = 0.8:

	0	1
0	TN = 0.8 n_0	FP = 0.2 n_0
1	FN = 0.8 n_1	TP = 0.2 n_1

FPR = 0.2 n_0/((0.2 + 0.8)n_0) = 0.2

TPR = 0.2 n_1/((0.2 + 0.8)n_1) = 0.2

Point on ROC curve is (0.2, 0.2).

If T = 0.3:

	0	1
0	TN = 0.3 n_0	FP = 0.7 n_0
1	FN = 0.3 n_1	TP = 0.7 n_1

FPR = 0.7 n_0/((0.7 + 0.3)n_0) = 0.7

TPR = 0.7 n_1/((0.7 + 0.3)n_1) = 0.7

Point on ROC curve is (0.7, 0.7).

Logistic Regression with sklearn

(documentation)

```
from sklearn.linear_model import LogisticRegression
model = LogisticRegression(fit_intercept=False)
model.fit(X, Y)
```

Task/Model

Binary Classification ($y \in \{0, 1\}$)

$$\hat{P}_\theta(Y = 1|x) = \sigma(x^T\theta)$$

Fit to objective function

Average Cross-Entropy Loss

$$-\frac{1}{n}\sum_{i=1}^{n}\left(y_i \log(\sigma(X_i^T\theta) + (1 - y_i)\log(1 - \sigma(X_i^T\theta))\right)$$

+ **regularization**

Why does sklearn always apply regularization?

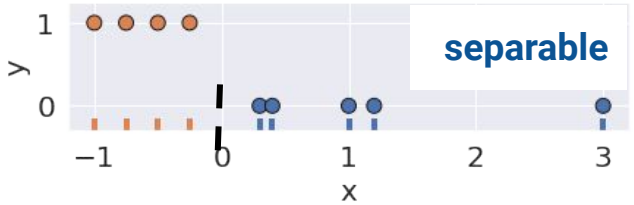
Demo

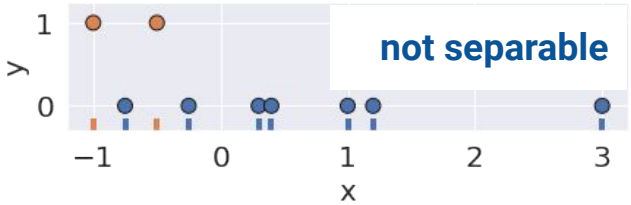
Linear Separability

A classification dataset is said to be **linearly separable** if there exists a hyperplane **among input features x** that separates the two classes y.

If there is one feature; the input feature is **1-D**.

- Class label is not a feature; it is output.
- Use rug plot to see separability.





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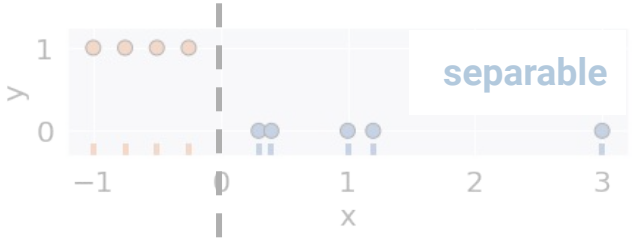
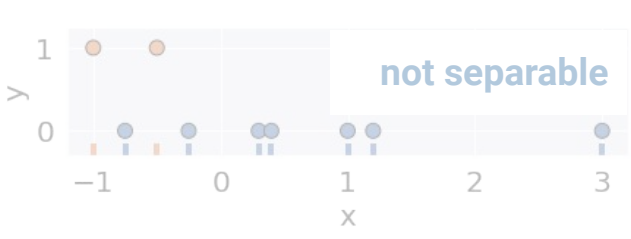
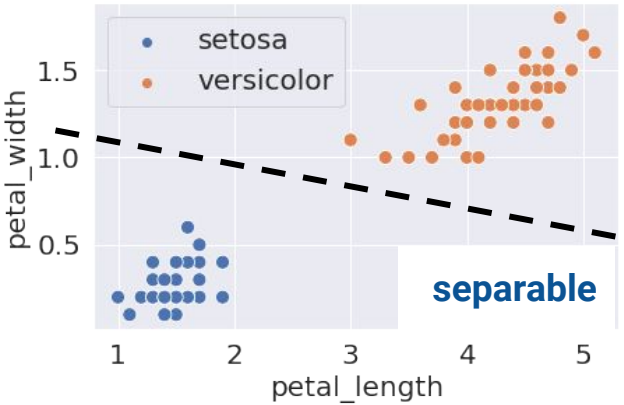
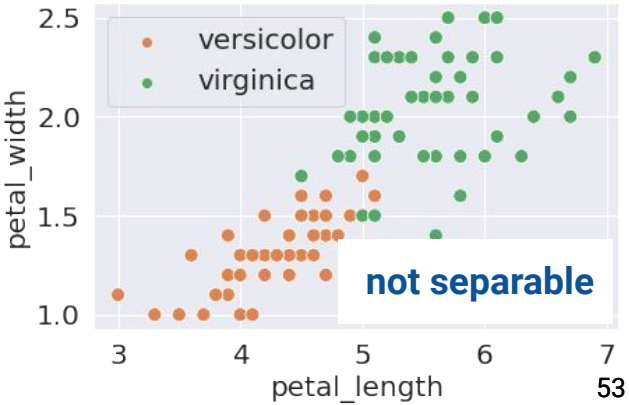




If there are two features, the input feature is **2-D**. Use scatter plot to see separability.





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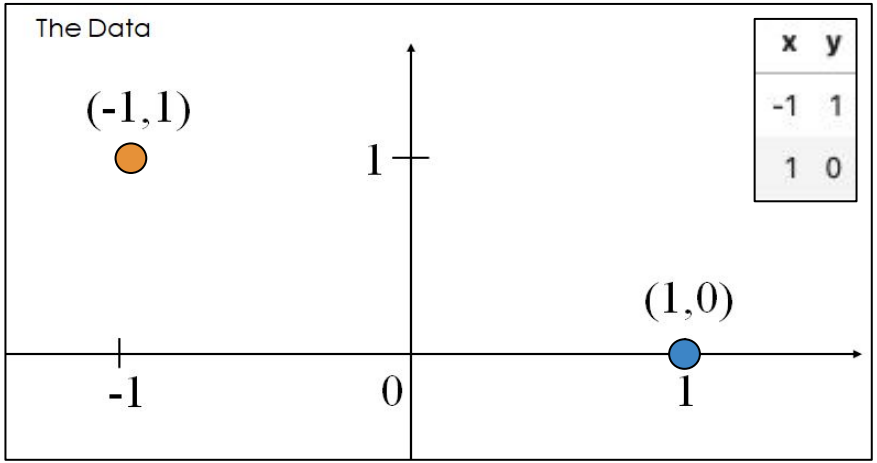
Decision Boundary Playground

Linearly Separability Creates Diverging Weights

Consider the simplified logistic regression model fit to the toy data:

$$\hat{P}_\theta(Y = 1|x) = \sigma(\theta x) = \frac{1}{1 + e^{-\theta x}}$$



What will be the optimal weight theta? Why?

A. $\hat{\theta} = -1$

B. $\hat{\theta} = 1$

C. $\hat{\theta} \to -\infty$

D. $\hat{\theta} \to \infty$

[Hint] The optimal theta should "push" probabilities in the direction of the true class:

- $\hat{P}_\theta(Y = 1|x = -1) = \frac{1}{1 + e^{\theta}} \quad \to 1$
- $\hat{P}_\theta(Y = 1|x = 1) = \frac{1}{1 + e^{-\theta}} \quad \to 0$

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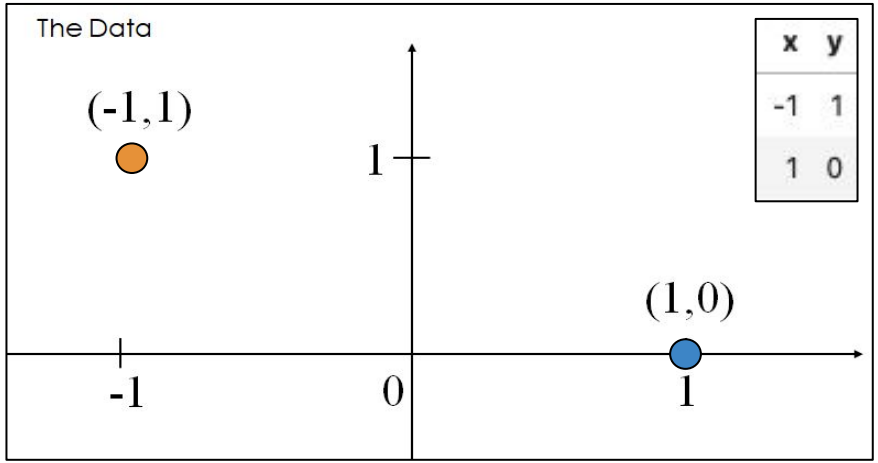

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happens as $\hat{\theta} \to -\infty$

Linearly Separability Creates Diverging Weights

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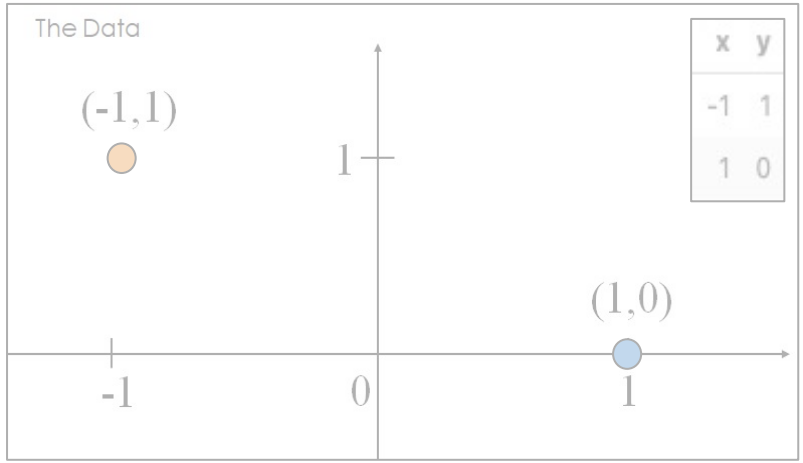

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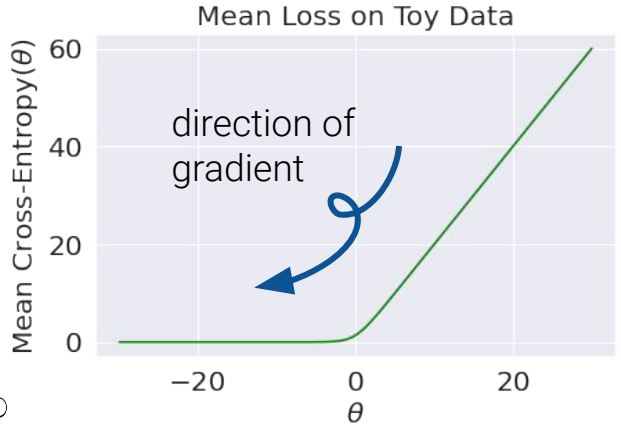


(Impossible to see, but) plateau is slightly tilted downwards.

Loss approaches 0 as theta decreases.

Linearly Separability Creates Diverging Weights

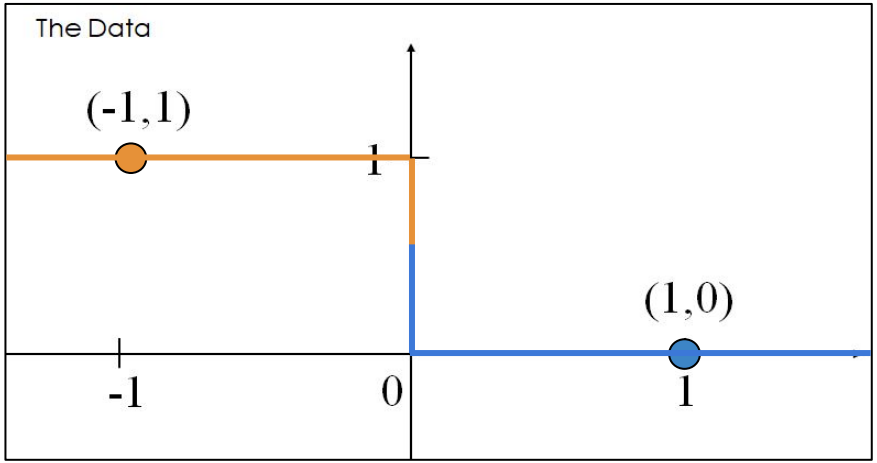
Consider the simplified logistic regression model fit to the toy data:

$\hat{\theta} \to -\infty$:

$$\hat{P}_\theta(Y = 1|x = -1) = \frac{1}{1 + e^{\theta}} \to 1$$

$$\hat{P}_\theta(Y = 1|x = 1) = \frac{1}{1 + e^{-\theta}} \to 0$$

$$\hat{P}_\theta(Y = 1|x) = \sigma(\theta x) \to \begin{cases} 1 & \text{if } x < 0 \\ 0 & \text{if } x \geq 0 \end{cases}$$



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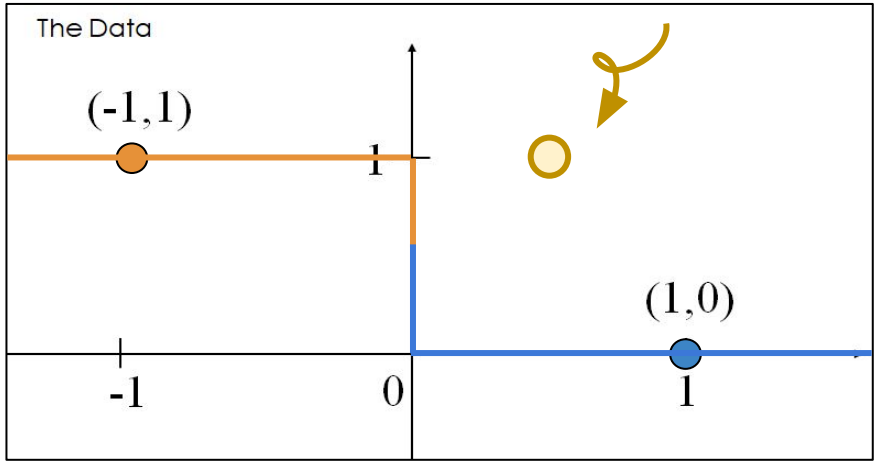


This model is **overconfident**.

- Consider a new point (0.5, **1**).
- The model incorrectly says **p = 0**, so it predicts **0**.

$$-\left(y \log(p) + (1 - y) \log(1 - p)\right)$$

$$\to 1 \log(0)$$

Loss is infinite.

Divergent weights (i.e., $|\theta| \to \infty$) occur with **linearly separable** data.

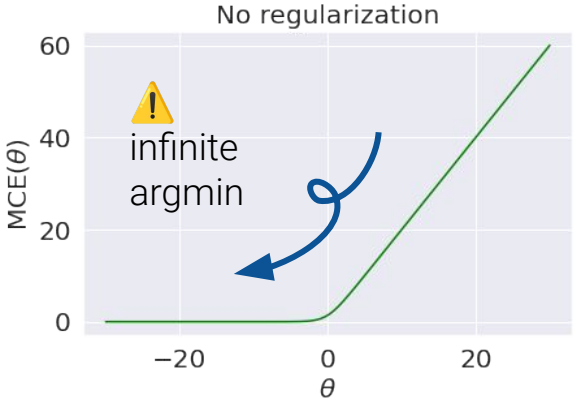
"Overconfidence" is a particularly dangerous version of overfitting.

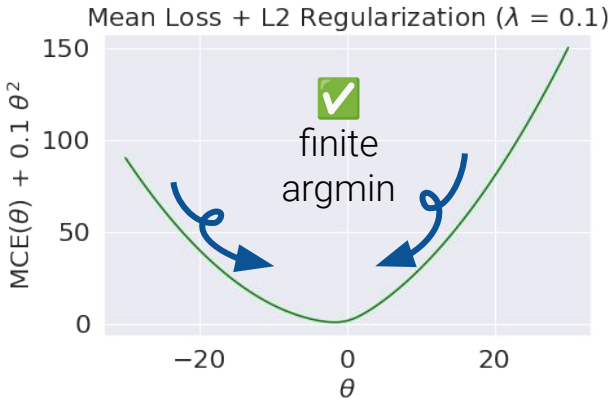
Regularized Logistic Regression

To avoid large weights (particularly on linearly separable data), use **regularization**.

- As with linear regression, standardize features first.

$$\underset{\theta}{\operatorname{argmin}} -\frac{1}{n}\sum_{i=1}^{n}\left(y_i \log(\sigma(X_i^T\theta) + (1-y_i)\log(1-\sigma(X_i^T\theta))\right) + \lambda\sum_{j=1}^{d}\theta_j^2$$






```
# sklearn defaults
model = LogisticRegression(
          penalty='l2', C=1.0, …)
model.fit()
```

Regularization hyperparameter C is the inverse of λ. C = 1 / λ.

Set C big for minimal regularization, e.g., `C=300.0`.

Reference slides. Out of scope.

[Extra] Precision-Recall Curves

Linear separability and Regularization

Performance Metrics

- Accuracy
- Imbalanced Data, Precision, Recall

Adjusting the Classification Threshold

- A case study
- ROC curves, and AUC

[Extra] PR curves

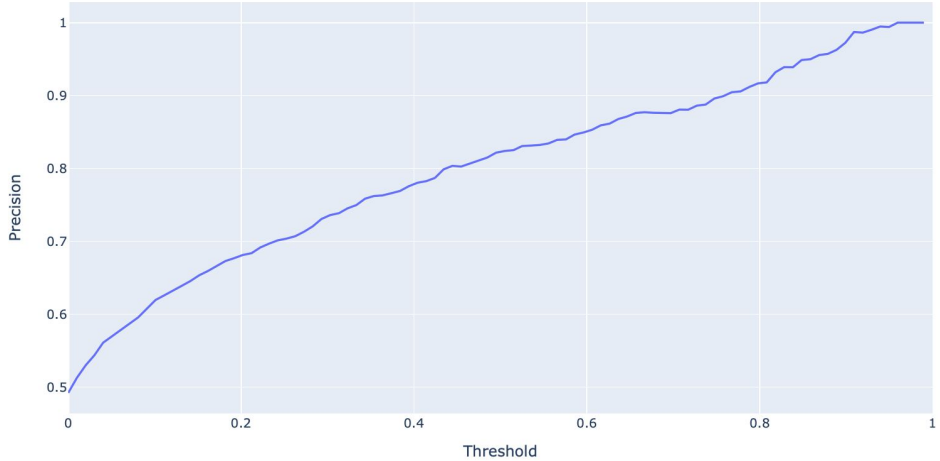
Precision vs. Threshold

As we increase our threshold, we have fewer and fewer false positives.

- Thus, precision tends to increase.

$$\text{Precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}$$
$$= \frac{\text{True Positives}}{\text{Predicted True}}$$

It is *possible* for precision to decrease slightly with an increased threshold. Why?



Recall vs. threshold

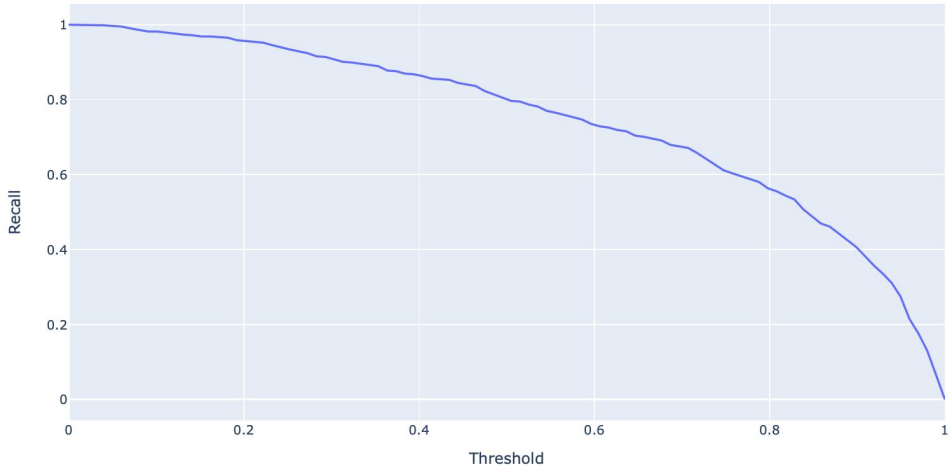
As we increase our threshold, we have more and more false negatives.

- Thus, recall tends to decrease.

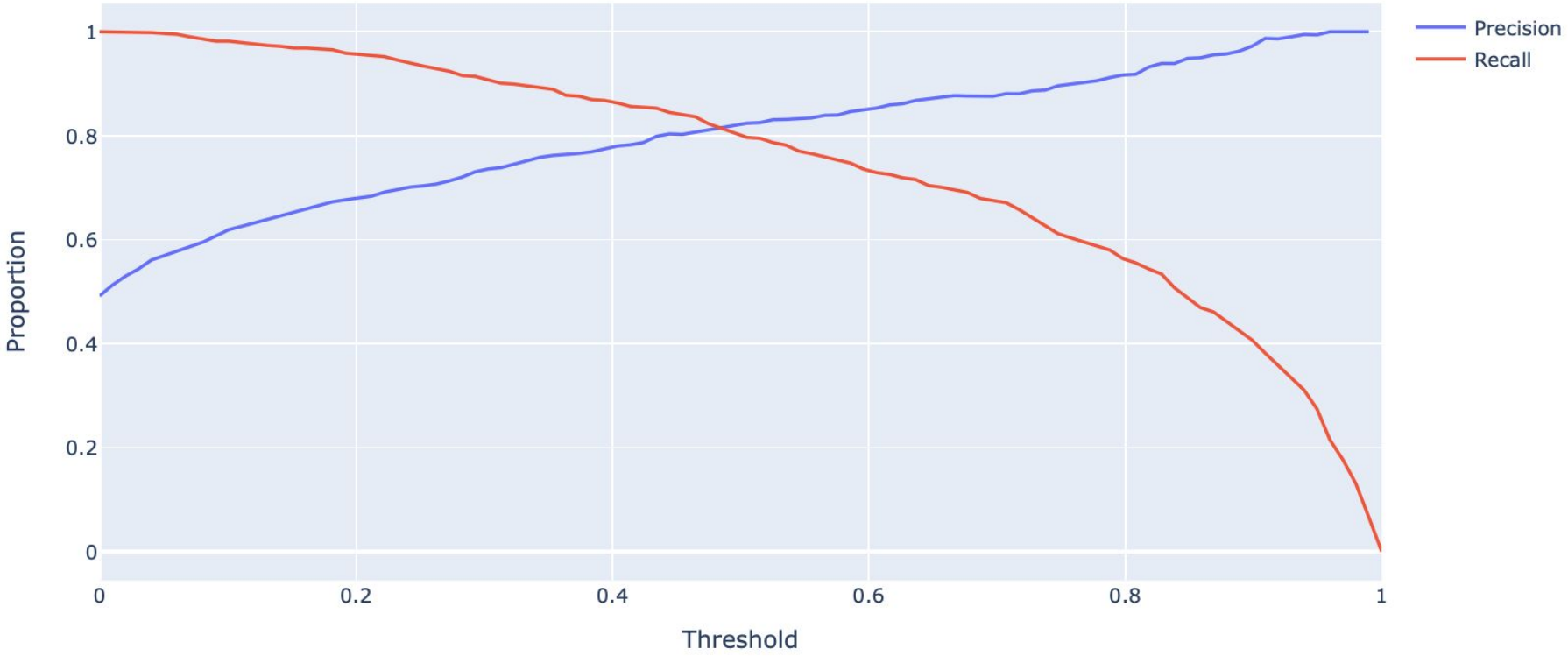
$$\text{Recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

$$= \frac{\text{True Positives}}{\text{Actually True}}$$

Recall strictly decreases as we increase our threshold. Why?



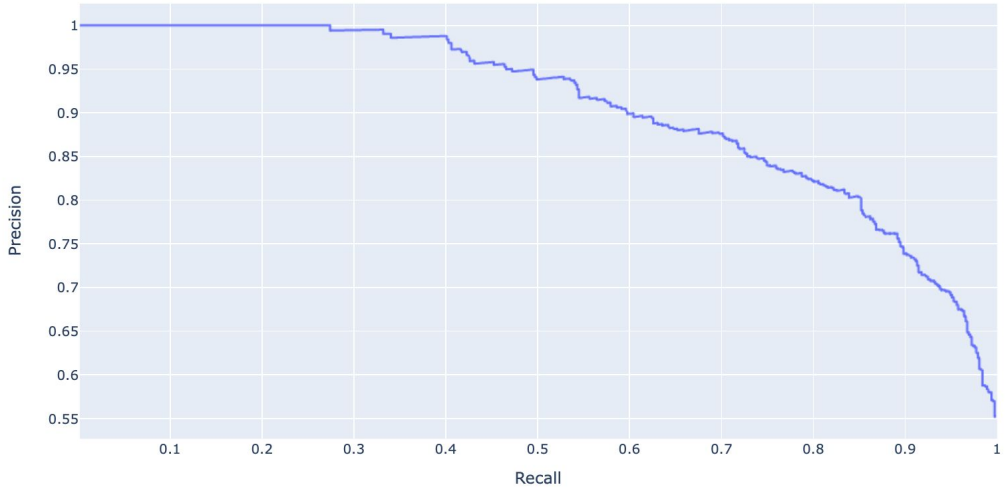
Precision and Recall vs. Threshold



Precision-recall curves

We can also plot precision vs. recall, for all possible thresholds.

1. Which part of this curve corresponds to T = 0.9?
2. Which part of this curve corresponds to T = 0.1?

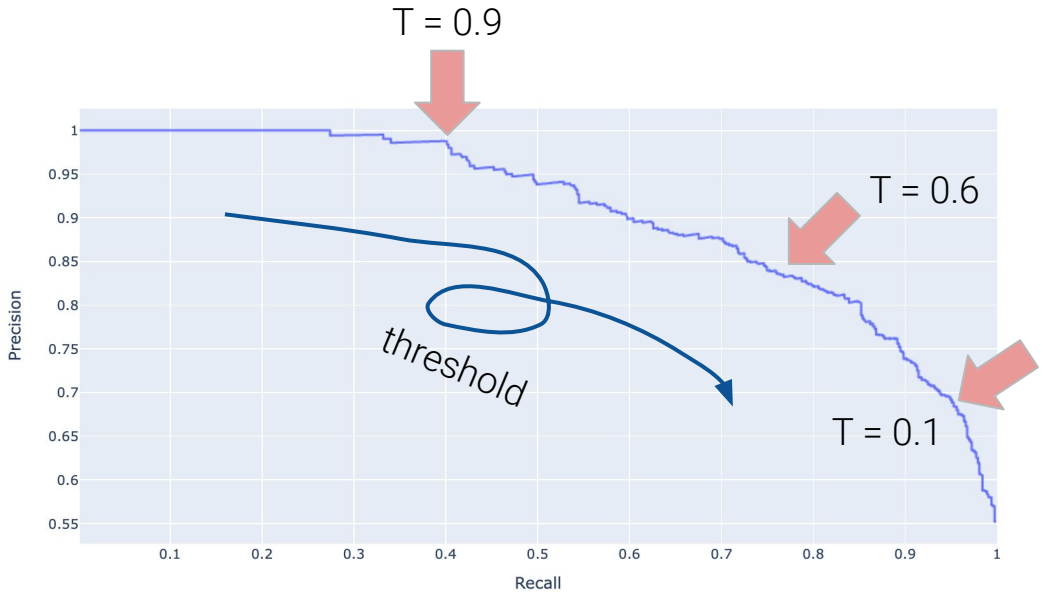


Precision-recall curves

We can also plot precision vs. recall, for all possible thresholds.

Answer:

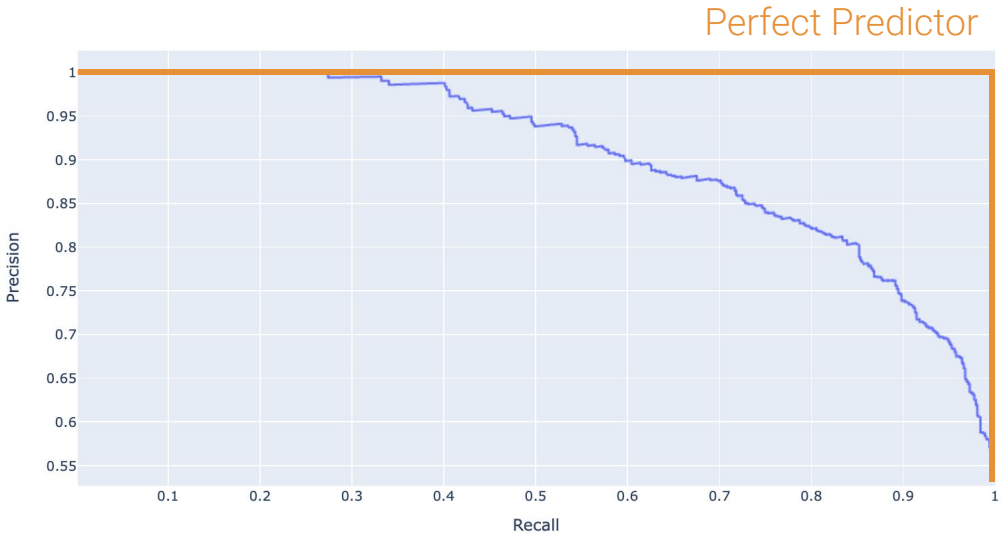
- Threshold decreases from the top left to the bottom right.
- In the notebook, there's an interactive version of this plot.



Precision-recall curves

The “perfect classifier” is one with precision of 1 and recall of 1.

- We want our PR curve to be as close to the “top right” of this graph as possible.
- One way to compare our model is to compute its **area under curve (AUC)**.
  - The area under the “optimal PR curve” is 1.
  - More commonly, we look at the area under ROC curve.



LECTURE 24

Logistic Regression II

Content credit: Acknowledgments