Measuring regressor and classifier errors

Quantifying model performance

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Regressor losses/metrics

Common regressor loss funcs / metrics

- Mean squared error
  Range 0..∞, units(y)^2, symmetric
  e.g., y=90 vs 95 = 5^2 = 25

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- Mean absolute value
  Range 0..∞, units(y), symmetric
  e.g., y=90 vs 95 = 5

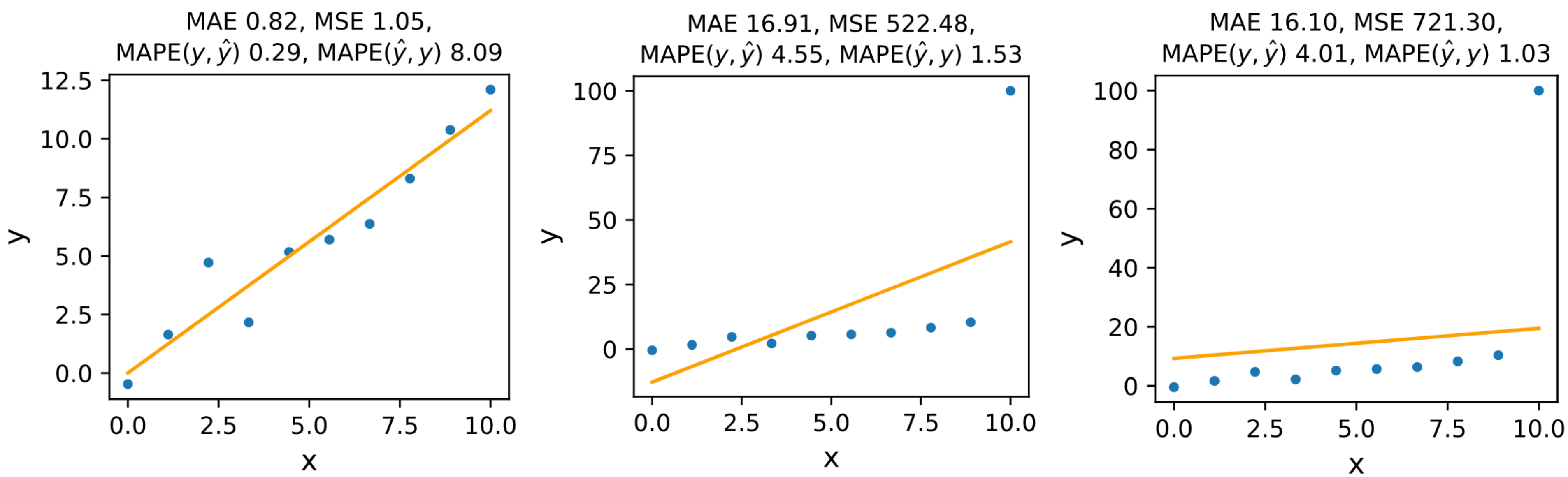
$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

- Mean absolute percentage error
  Range 0..∞, unitless, **asymmetric**
  undefined if y=0; e.g., y=90 vs 95 = 5/90=0.0555

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right|$$

(For moment, think of symmetry as metric(y, $\hat{y}$)=metric($\hat{y}$, y))

MAE, MSE, MAPE example



MSE incorrectly makes last model look horrible and worse than 2nd model due to outlier.
MAE isn't perfect either as it thinks 2nd and 3rd models are about the same.
Note MAPE asymmetry!

R^2

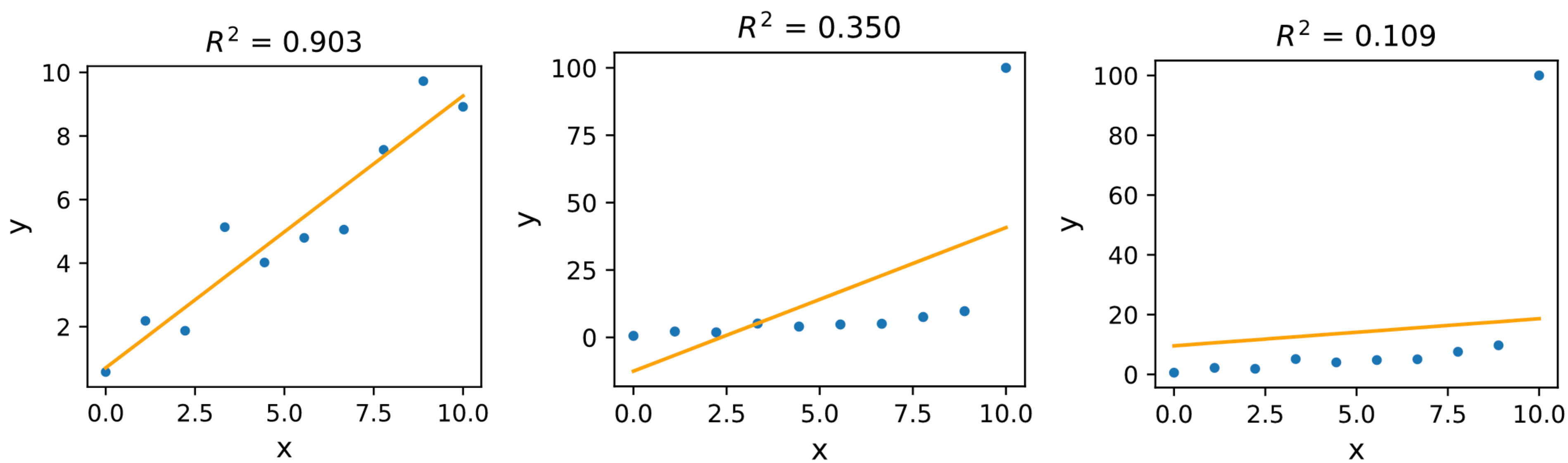
- How well our model performs compared to a “mean model”

$$R^2 = 1 - \frac{\text{Squared error}}{\text{Variation from mean}} = 1 - \frac{\sum_{i=1}^{n}(y_i - \boxed{\hat{y}_i})^2}{\sum_{i=1}^{n}(y_i - \boxed{\overline{y}})^2}$$

- Range of possible values: (−∞,1]
- Our model could be really bad, giving large negative numbers
- For OLS linear models, R^2 in [0,1]
- R^2 is default regressor metric for sklearn

Low R^2 doesn't always imply bad model

- Not best metric; here are 3 graphs with good, bad, decent fits
- Outliers can skew metrics that square deltas
- The 3rd has lowest R^2 but it's a way better model than 2nd



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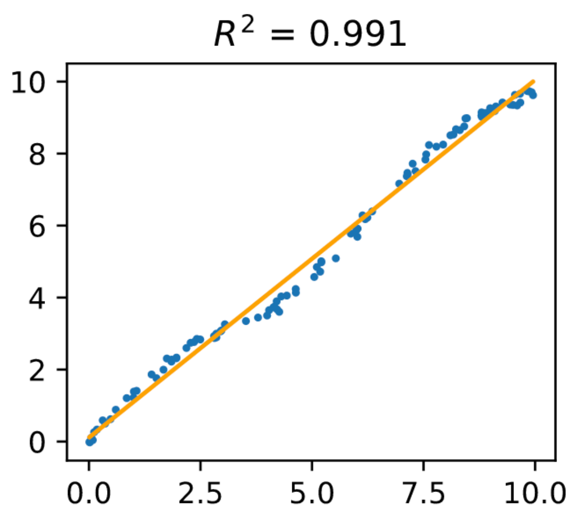
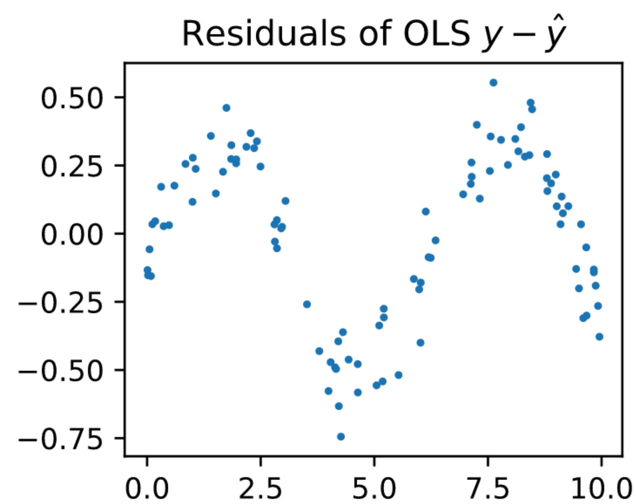
High R^2 doesn't always imply good model

- This linear model looks pretty good and has R^2 = 0.991
- But check the residual plot! Model doesn't capture nature of x,y





But, we want residuals to look like random noise!

See also https://statisticsbyjim.com/regression/interpret-r-squared-regression/

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Which metric should we use?

- That depends what we care about for business reasons
- For prices, we usually care more about the percentage error than the absolute amount
- MAE \$500 for a \$1,000 apartment is 0.5x or 1.5x off and a big deal but \$500 error for a \$1 million apartment is a trivial difference
- For things like body temperature that will most likely all be within a small range, the mean absolute error (MAE) is a good and interpretable measure
- The percentage error can be interpretable but there are problems with it: asymmetry (see next slide)
- R^2, MSE and in general squaring errors yields metrics that are sensitive to big deltas from even a few test records

Symmetry in metrics

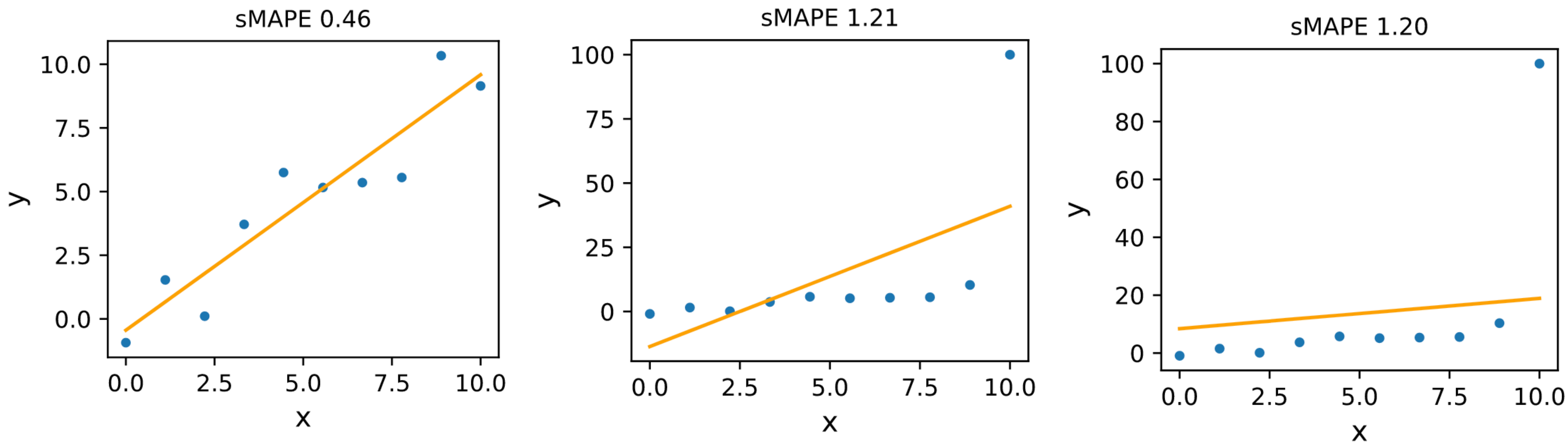
- Most metrics compute $y - \hat{y}$ but ratio $y/\hat{y}$ is often better
- But, most ratio-based metrics are asymmetric, which is bad!
  - If y=100, $\hat{y}$=0.01: MAPE = 0.9999
  - If y=0.01, $\hat{y}$=100: MAPE = 9999

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right|$$

- Try symmetric MAPE
  Range 0..2, unitless, symmetric,
  undefined when y=0 and $\hat{y}$ =0
  (have to work around those landmines)
  - If y=100, $\hat{y}$=0.01: sMAPE = 1.9996
  - If y=0.01, $\hat{y}$=100: sMAPE = 1.9996

$$sMAPE = \frac{1}{n}\sum_{i=1}^{n}\frac{|y_i - \hat{y}_i|}{\frac{1}{2}(|y_i| + |\hat{y}_i|)}$$

sMAPE in action



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Classifier losses/metrics

Common classifier metrics

(Ugh; much more complicated than for regressors)

- *TP* = true positive, *TN* = true negative
- *FP* = false positive, *FN* = false negative
- *Confusion matrix* for binary classification to right, but can have larger confusion matrices in general
- The matrices are clear but don't give single metric
- *Accuracy* = correct classification rate = (TN+TP)/n
- *Misclassification* rate is 1 – accuracy

		Predicted	
		F	**T**
Actual	**F**	TN	FP
	T	FN	TP

		Predicted	
		F	**T**
Actual	**F**	35	3
	T	1	75

(breast cancer RF)

See also https://en.wikipedia.org/wiki/Evaluation_of_binary_classifiers

True/False positive/negative **rates**

		Predicted	
		F	**T**
Actual	**F**	TN	FP
	T	FN	TP

- *True positive rate* is TP / num-positive (also called *recall*)
  Of the actually positive y, how many true positives in $\hat{y}$?
  - **TPR** = TP / true_y = TP / (TP + FN)
  - TP over sum of 2nd row in confusion matrix (num true-y is constant)
- *False positive rate* is FP / num-negative
  Of the actually false y, how many false positives in $\hat{y}$?
  - **FPR** = FP / false_y = FP / (FP + TN)
  - FP over sum of 1st row in confusion matrix (num false_y is constant)

Multi-class confusion matrix

- For C classes, we get C x C matrix
- Optimally, it's a diagonal matrix (correct classifications)
- Example; interest in NYC apartments (lo/med/hi); matrix indicates model is good at predicting low interest apts but not others (sometimes overall error is high but very low for some records)
- Should focus on features that are predictive of med/high to improve model

	predicted_low	predicted_medium	predicted_high
expected_low	3749	566	83
expected_medium	854	418	119
expected_high	189	174	141

More classifier metrics

(I like Precision/recall)

- Precision/recall typically used in binary classification, such as spam or cancer
- *Precision* = TP/(TP+FP) “of those predicted as positive, how many did we get right?”
- *Recall* = TP/true_y “of the positive samples, how many did we find (predict as positive)?”
- *F1* is harmonic mean of precision and recall; F1 = 2*(P*R)/(P+R), which gives equal importance to precision and recall

		Predicted	
		F	**T**
Actual	**F**	35	3
	T	1	75

precision= 75/(75+3)

		Predicted	
		F	**T**
Actual	**F**	35	3
	T	1	75

recall= 75/(75+1)

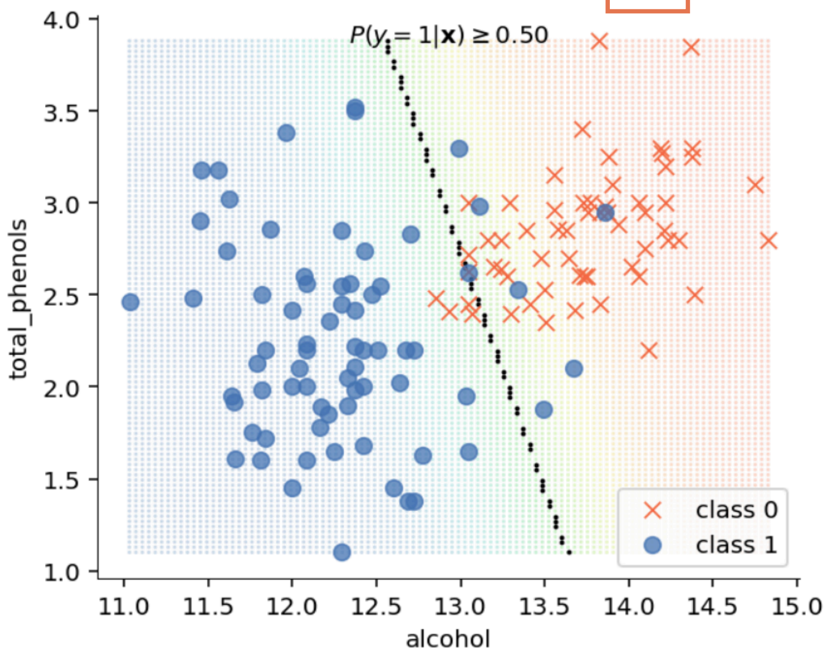
See also https://en.wikipedia.org/wiki/Precision_and_recall

ROC and PR curves

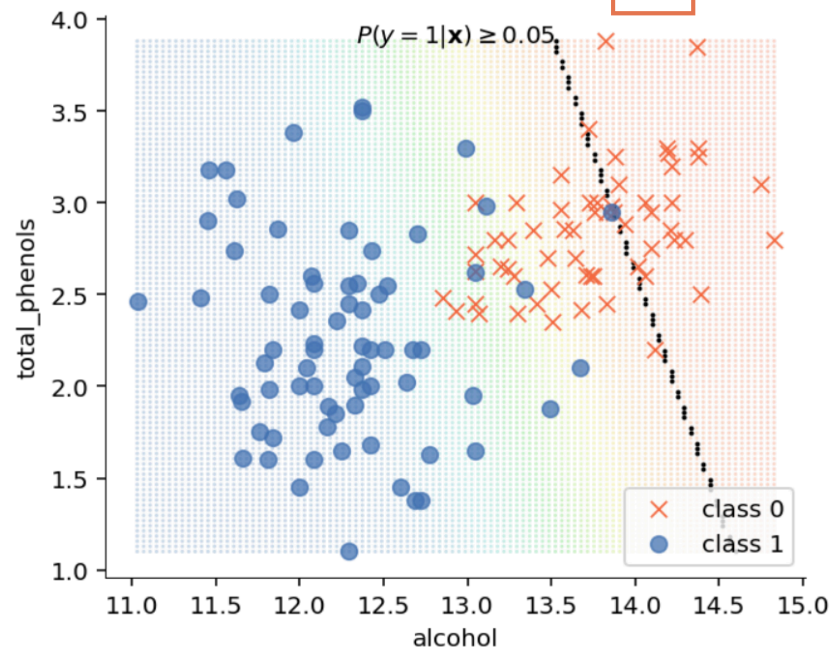
Classifier: $P(y = 1|\boldsymbol{x})$ and a threshold

- Different thresholds on the $P(y = 1|\boldsymbol{x})$ model output probabilities give different classifiers:

Accuracy 119/130=0.92
(threshold,precision,recall) = ($\boxed{0.50}$,0.941,0.901)



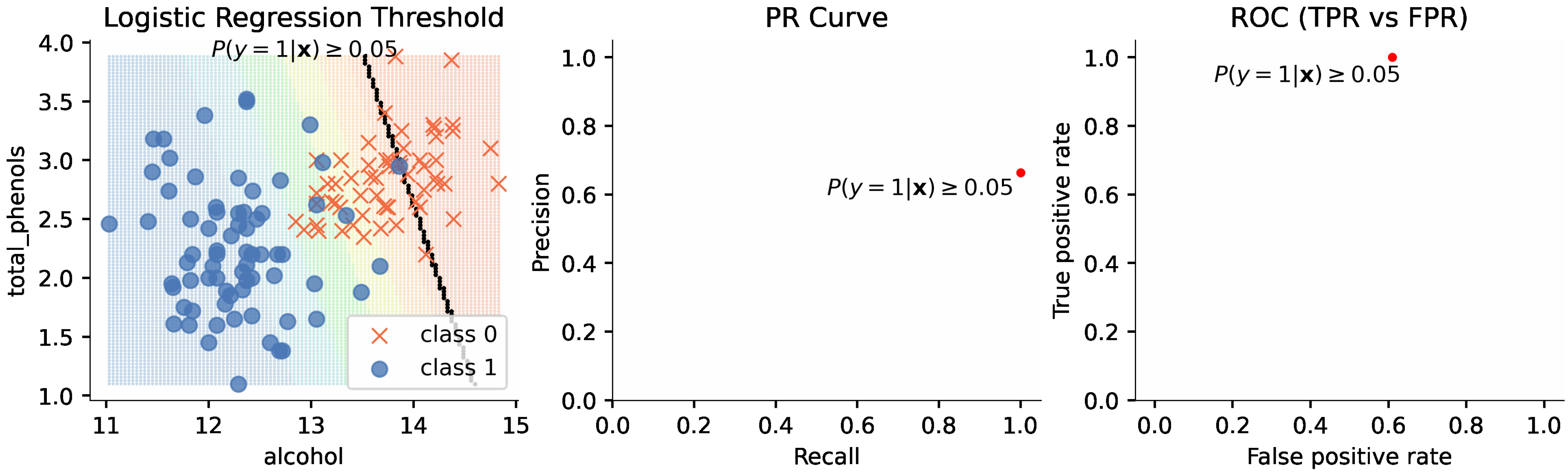
Accuracy 94/130=0.72
(threshold,precision,recall) = ($\boxed{0.05}$,0.664,1.000)



ROC == *receiver operator curve*
PR == *precision-recall*

Animated ROC or PR curves

- Shift $P(y = 1|\boldsymbol{x})$ threshold from 0.0 to 1.0, compute and plot (Precision, Recall) or (TPR/recall,FPR) coordinates for each classifier resulting from each threshold:



See https://github.com/parrt/msds621/blob/master/notebooks/assessment/PR-ROC-curves.ipynb

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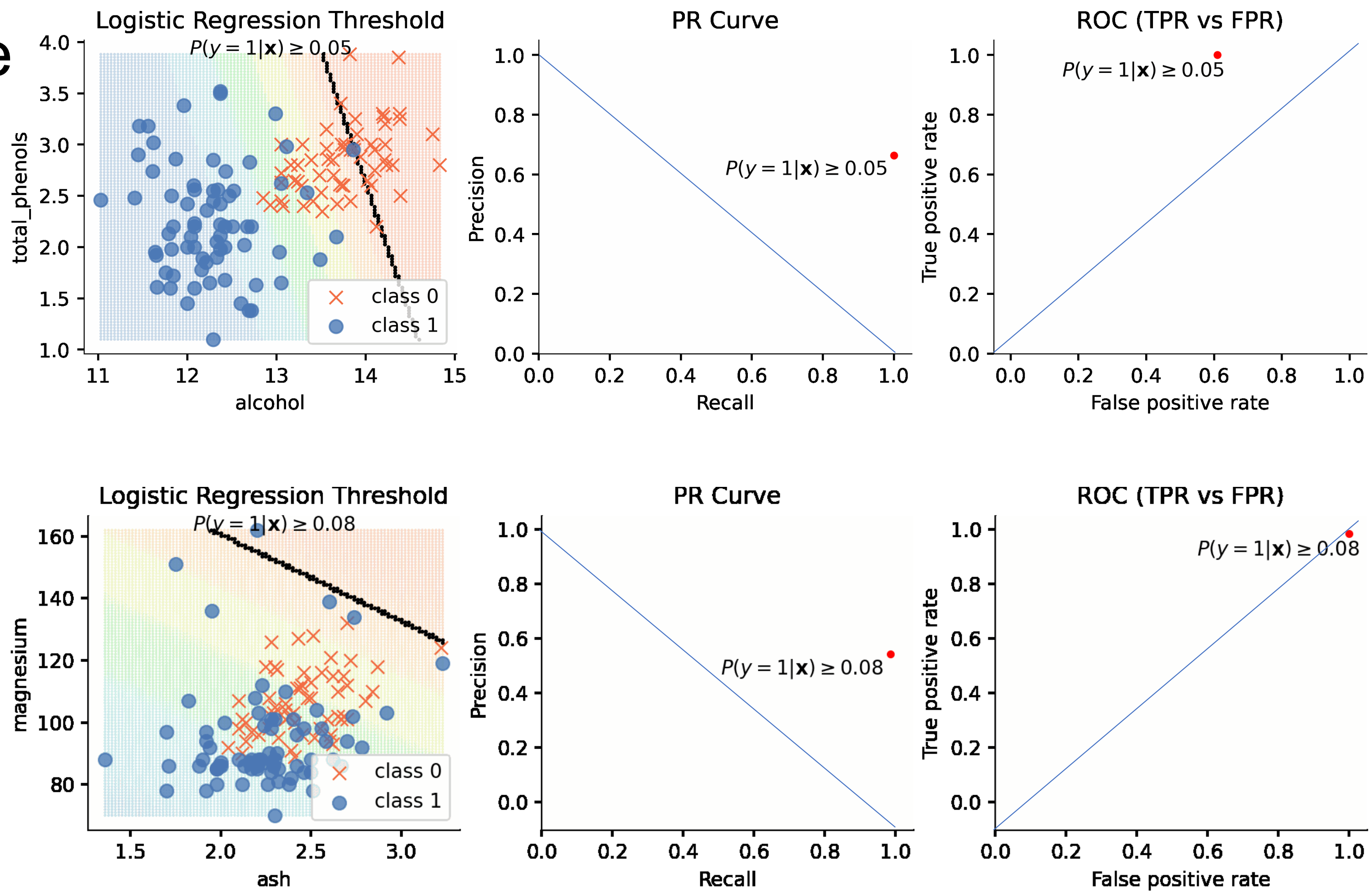
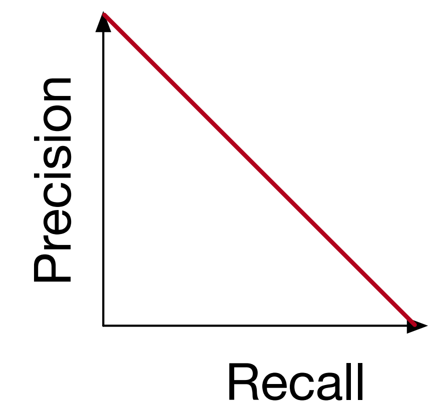
Compare with less predictive features

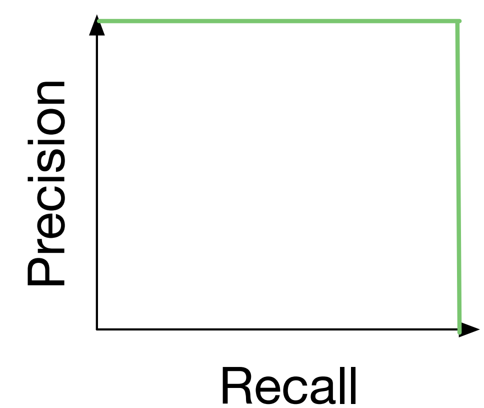
- Notice how the less predictive features yield a partition with much more overlap
- The curves for less well separated classes are much closer to the diagonal than for the good features



AUC precision-recall curve

- Goal: Conjure up scalar from curve using AUC (*area under the curve*)
- When distributions overlap exactly, moving threshold around gives -45 degree line, AUC=0.5
- When distributions are completely separate, AUC=1
- Any curve above 45° diagonal is better than overlapping distributions

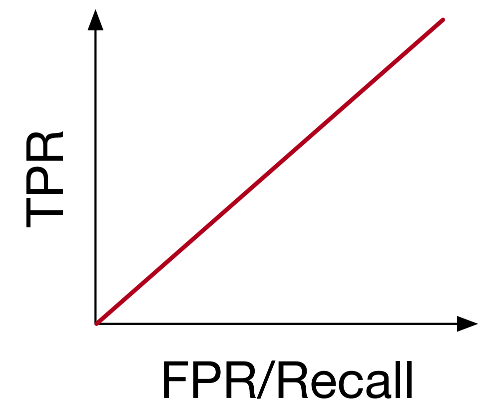


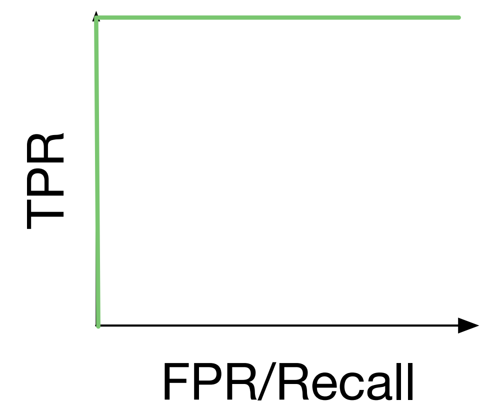


See also https://developers.google.com/machine-learning/crash-course/classification/roc-and-auc

AUC ROC

- Goal: Conjure up scalar from curve using AUC (*area under the curve*)
- When distributions overlap exactly, moving threshold around gives 45 degree line, AUC=0.5
- When distributions are reversed, AUC = 0
- When distributions are completely separate, AUC=1
- Any curve above 45° diagonal is better than overlapping distributions

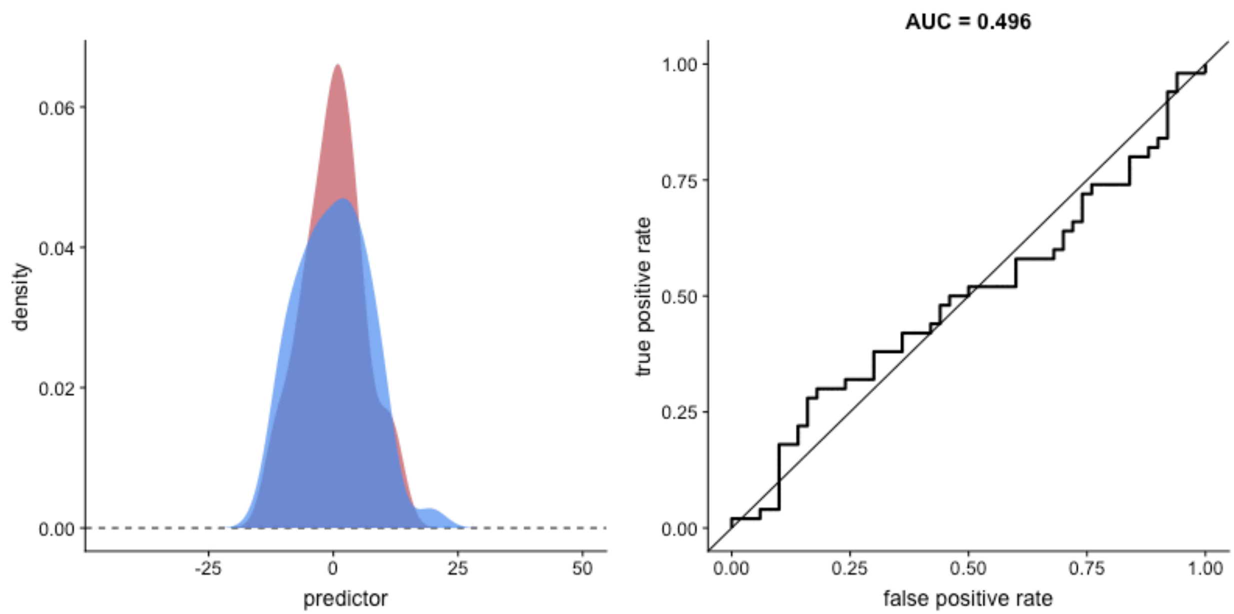




See also https://developers.google.com/machine-learning/crash-course/classification/roc-and-auc

Why ROC and PR curves?

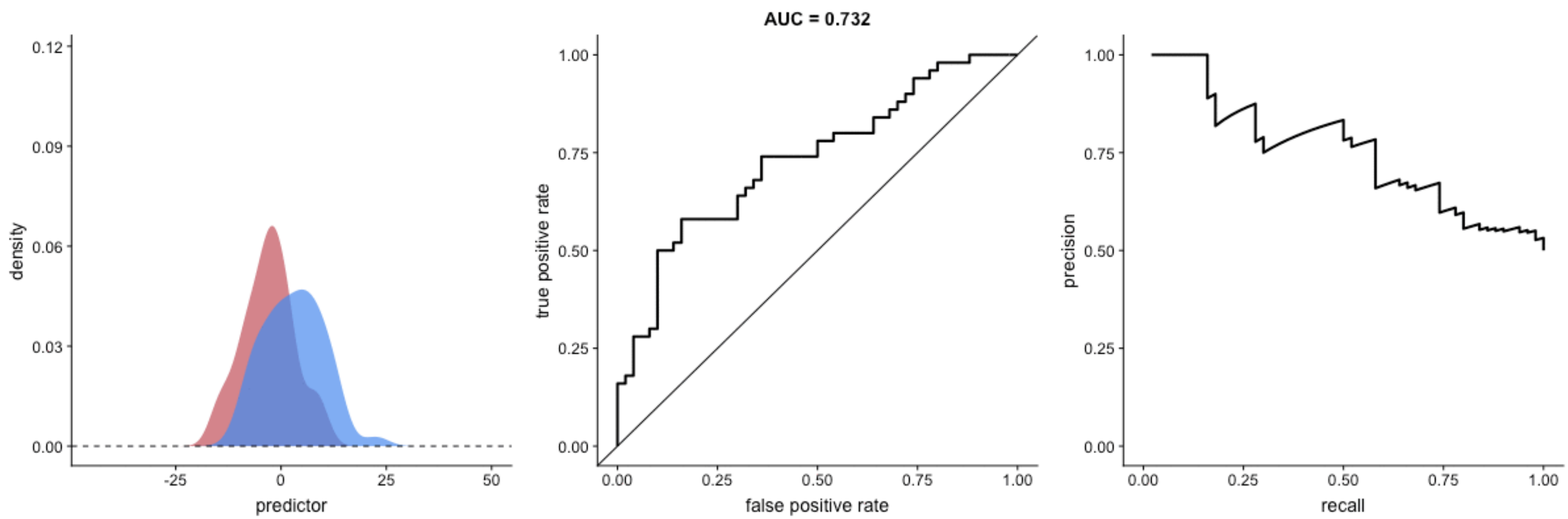
- Curves indicate quality of model
- More specifically, curves indicate how well/easily a model can separate class 0 from class 1 instances



Animation credits: https://github.com/dariyasydykova/open_projects/blob/master/ROC_animation/README.md

ROC vs Precision-Recall curve

- As variance tightens, with more overlap, ROC AUC goes up whereas PR goes down; ROC doesn't have good behavior



Animation credits: https://github.com/dariyasydykova/open_projects/blob/master/ROC_animation/README.md

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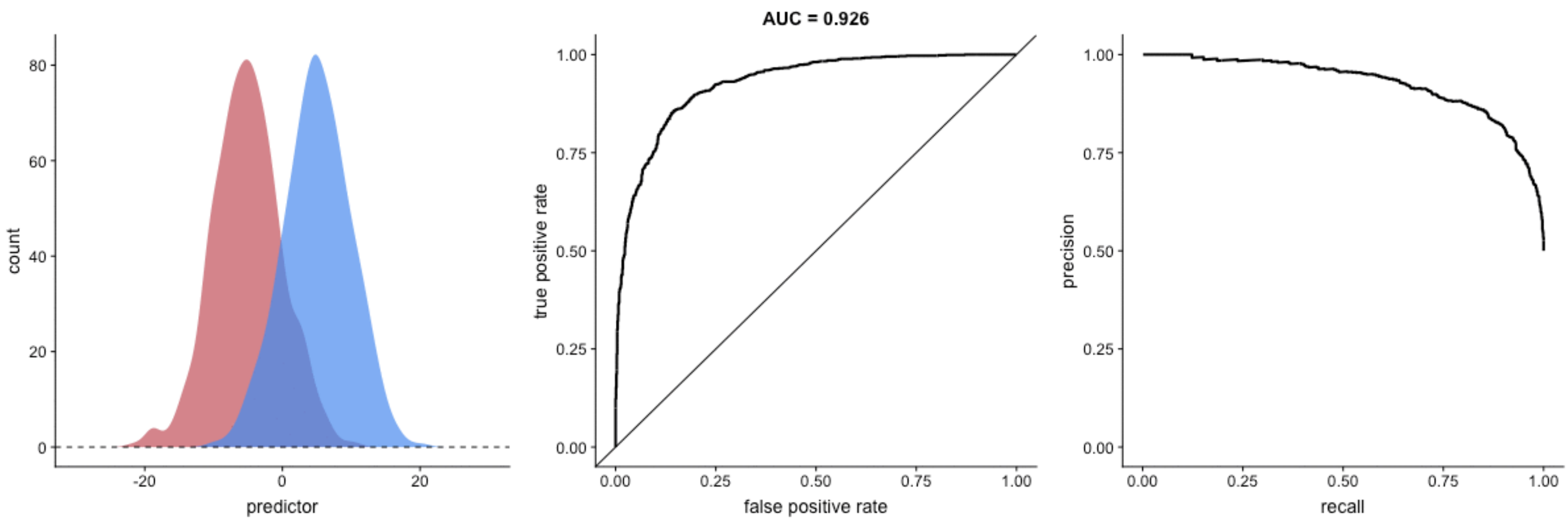
ROC vs PR curve: Imbalanced classes

- Spam, fraud detection problems are imbalanced; can't trust ROC!
- For same threshold/mean of distribution, only PR curve changes!
- In the end, I favor PR not ROC



Animation credits: https://github.com/dariyasydykova/open_projects/blob/master/ROC_animation/README.md

Upsampling minority class(es) in imbalanced data sets

Credit card data: https://www.kaggle.com/mlg-ulb/creditcardfraud

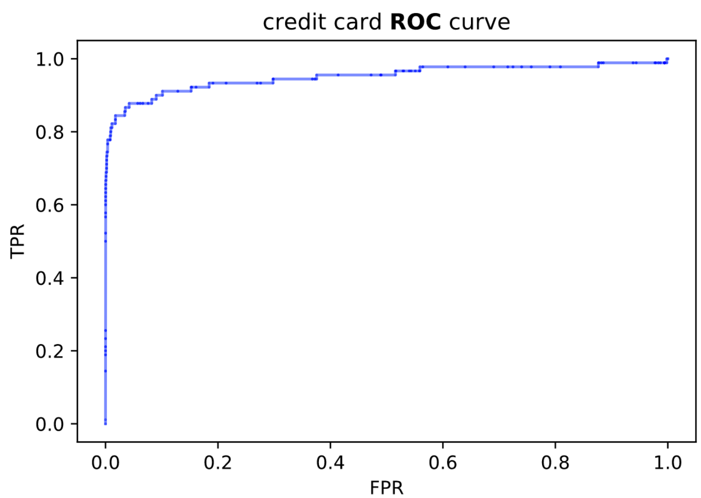
Naïve use of train_test_split() @ 20%

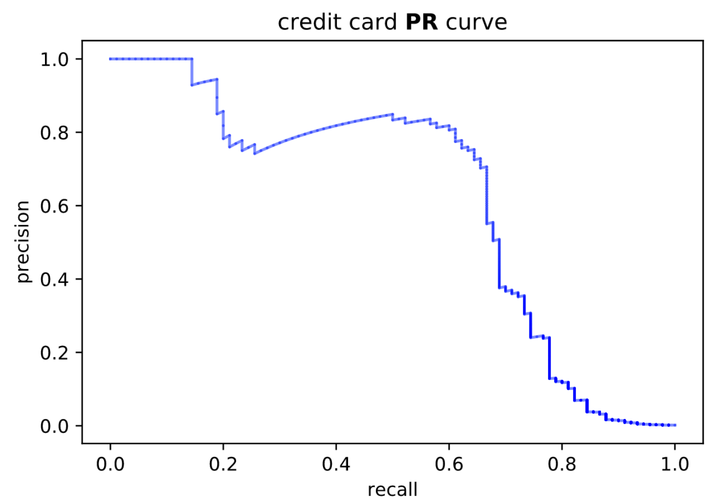
Imbalanced dataset: Kaggle credit card fraud

- Num anomalies 492/284807 = 0.17%
- L2 Regularized **LogisticRegression** model
  - bad → Accuracy 1.00, AUC ROC 0.93
  - good → F1 0.69, AUC PR 0.62

		predicted	
		F	**T**
actual	**F**	56840	16
	T	42	64

20% test set





Why is accuracy=1.0?
(That's rounded up)

See https://github.com/parrt/msds621/blob/master/notebooks/assessment/imbalanced.ipynb

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First: Proper split to ensure 20% minority class

- Must split out test set before modeling but get 20% from each class at original ratio of class 1 / class 0 (particularly important for small n)
- If num anomalies 492/284807 = 0.17%, then need:
  - TRAIN num fraud 393/227845 = 0.17%
  - TEST num fraud 99/56962 = 0.17%

- Accuracy 1.00, AUC ROC 0.93
- F1 0.70, AUC PR 0.65

	F	T
F	56848	15
T	37	62

```
df_good = df[df['Class']==0]
df_fraud = df[df['Class']==1]

df_train_good, df_test_good   = train_test_split(df_good, test_size=0.20)
df_train_fraud, df_test_fraud = train_test_split(df_fraud, test_size=0.20)

df_train = pd.concat([df_train_good, df_train_fraud], axis=0)
df_test  = pd.concat([df_test_good, df_test_fraud], axis=0)
```

Then: upsample minority in <u>training set</u>

- Upsampled TRAIN num fraud 3930/231382 = 1.70%
- TEST num fraud 99/56962 = 0.17%

```
df_good = df_train[df_train['Class']==0]
df_fraud = df_train[df_train['Class']==1]

df_fraud_balanced = df_fraud.sample(int(len(df_fraud)*10), replace=True)
df_train_upsampled = pd.concat([df_good, df_fraud_balanced], axis=0)
```

Do NOT upsamples before splitting out test set; you'll leak test data into training set!
Tweet/paper on how this can cause data leakage:
https://arxiv.org/abs/2001.06296
https://twitter.com/Gillesvdwiele/status/1219194600994283520

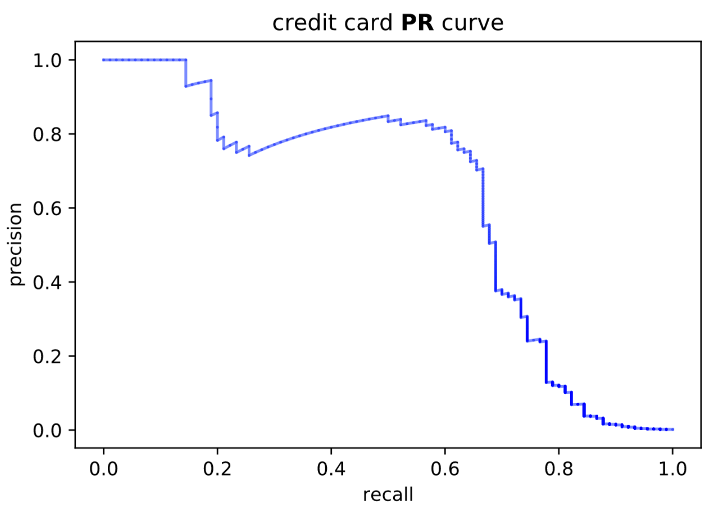
Upsampling fraud 10x in training data

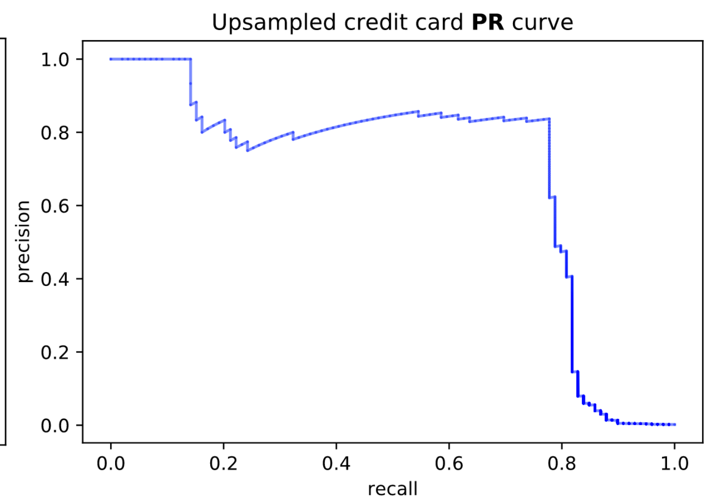
- We get improvement with upsampling for logistic regression, at least for this Kaggle credit card data set

No upsampling

	F	T
F	56840	16
T	42	64

F1 0.69, AUC PR 0.62





- Accuracy 1.00, AUC ROC 0.95
- F1 0.73, AUC PR 0.70

predicted

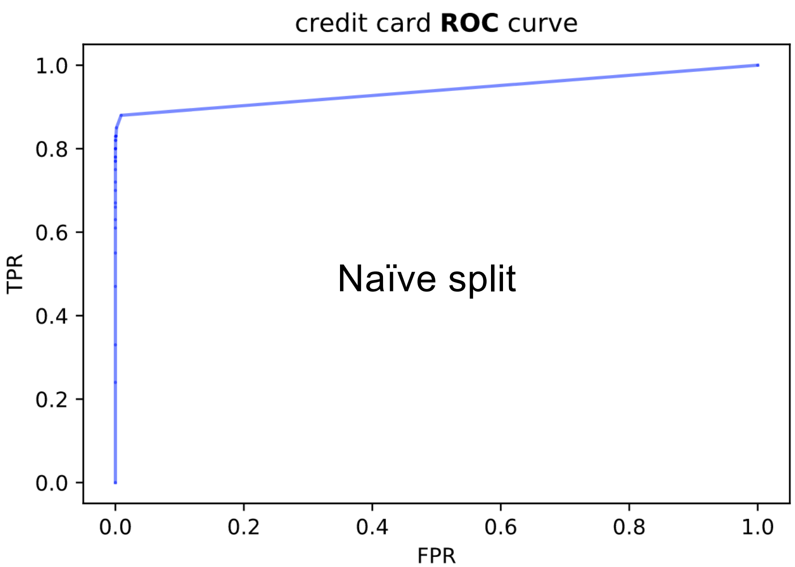
actual		F	T
	F	56827	36
	T	22	77

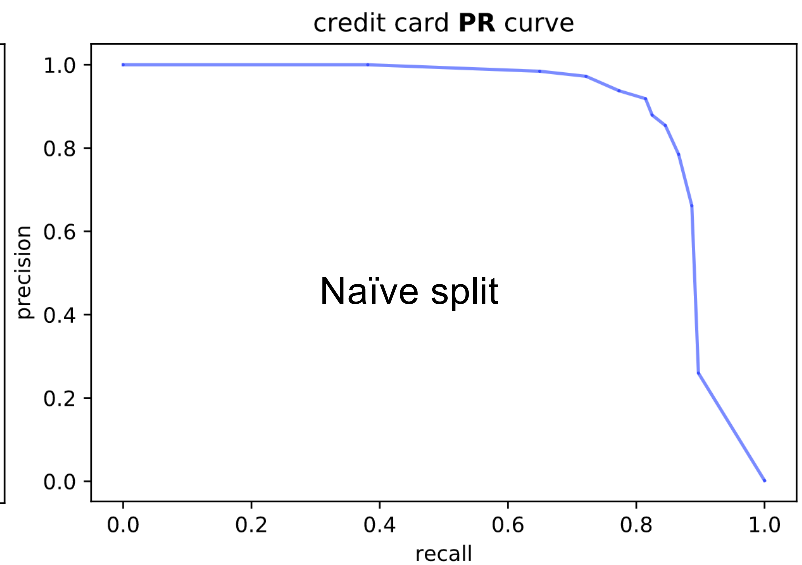
L2 Logistic Regression summary

- Naive split
  - F1 0.69, Accuracy 1.00
  - ROC 0.93, AUC PR 0.62
- Proper split (just making sure train/test balance is right can help)
  - F1 0.70, Accuracy 1.00
  - AUC ROC 0.93, AUC PR 0.65
- Upsample:
  - F1 0.73, Accuracy 1.00
  - AUC ROC 0.95, AUC PR 0.70
- (Varies depending on actual test set held out)

Credit card fraud with RF (10 trees)

- RFs do better than logistic: RF better at isolating minority samples
  - Naïve: ROC 0.92, AUC PR 0.84
  - Balanced split: AUC ROC 0.97, AUC PR 0.93
  - 10x upsampled training: AUC ROC 0.97, AUC PR 0.94 (doesn't really help)





	F	T
F	56860	3
T	13	86

Penalizing inappropriate confidence

- Terence's cousin went to the doctor with suspected skin cancer
- Doc was "100% positive mole was benign"
- 6 months later cousin loses most of her tricep / upper arm
- Doc's model was seriously flawed but not necessarily because of diagnosis
- The biggest mistake was the certainty of the incorrect diagnosis, as it allowed the cancer to spread
- Less certainty would've provided opportunities for more tests…
- Same concept of model assessment applies to ML models

Log loss (is both metric and loss function)

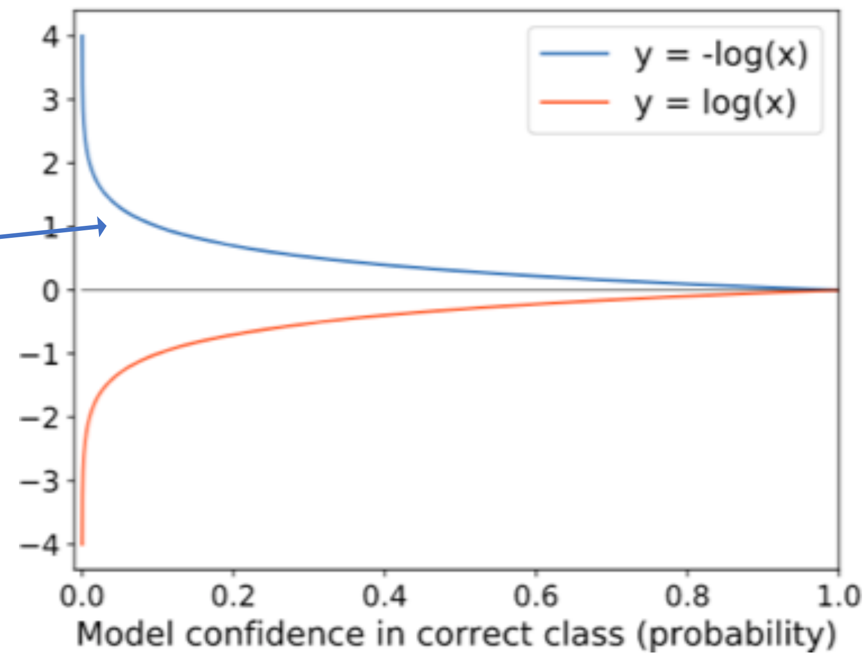
- Measures model performance when model gives probabilities, like logistic regression but RFs can give probabilities too
- Works for any number of classes; we'll do binary only
- Penalizes very confident misclassifications strongly
- Perfect score is 0 log loss, imperfection gives unbounded scores
- Let p be probability of true class, such as fraud or cancer; 1-p is then probability of false class, such as not fraud, not cancer
- Log loss is function of actual y and estimated p, not predicted class

Log loss continued

- Assume model gives us p (prob cancer) predicted from some $\boldsymbol{x}$
- Case 1: true y is cancer
  - If p=0.9, we are confident it's cancer and rightly so: loss should be low
  - If p=0.01, we are confident it's NOT cancer and wrongly so: **penalize** with high (i.e., bad) loss value
- Case 2: true y is benign (not cancer)
  - If p=0.9, we are confident it's cancer and wrongly so: **penalize**
  - If p=0.01, we are confident it's NOT cancer and rightly so: loss is low
- Let loss = *penalty*(p) if y =1 else *penalty*(1–p) if y=0
  where *penalty*(p) should be very high at low p (confident FP)

Log loss penalty

- loss = *penalty*(p) if y=1 else *penalty*(1– p)
- Let *penalty*(p) = -log(p)



$$loss = \frac{1}{n}\sum_{i=1}^{n}\begin{cases} -\log(p_i) & y = 1 \\ -\log(1-p_i) & y = 0 \end{cases}$$

$$loss = -\frac{1}{n}\sum_{i=1}^{n} y_i \log(p) + (1-y_i)\log(1-p_i)$$

So log loss is average penalty where penalty is very high for confidence in wrong answer