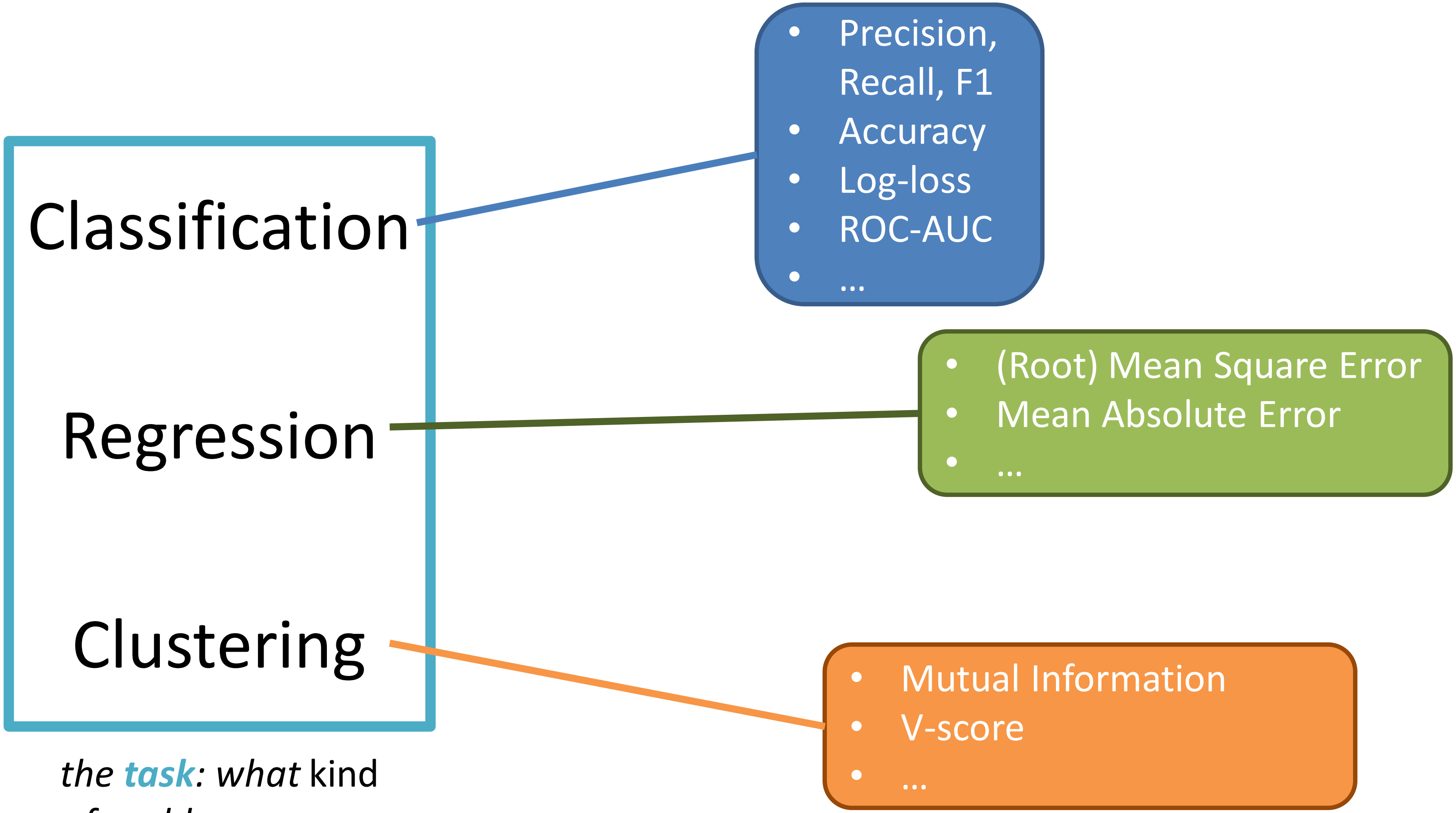
Experimental Setup,
Multi-class vs. Multi-label classification,
and
Evaluation

CMSC 678

UMBC

Central Question: How Well Are We Doing?



Classification

- Precision, Recall, F1
- Accuracy
- Log-loss
- ROC-AUC
- …

Regression

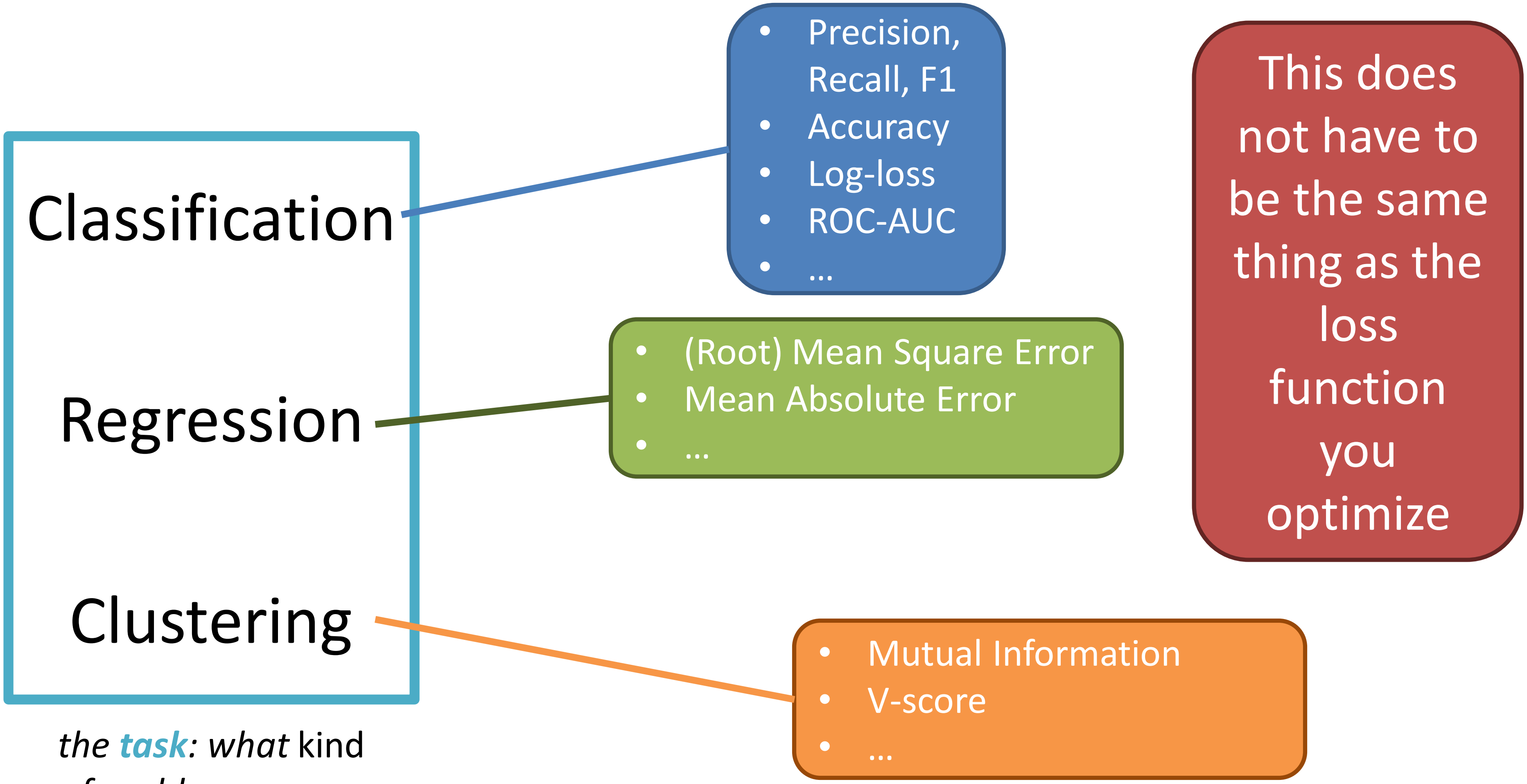
- (Root) Mean Square Error
- Mean Absolute Error
- …

Clustering

- Mutual Information
- V-score
- …

the ***task****: what* kind *of problem are you solving?*

Central Question: How Well Are We Doing?



Classification

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This does not have to be the same thing as the loss function you optimize

the ***task****: what* kind *of problem are you solving?*

Outline

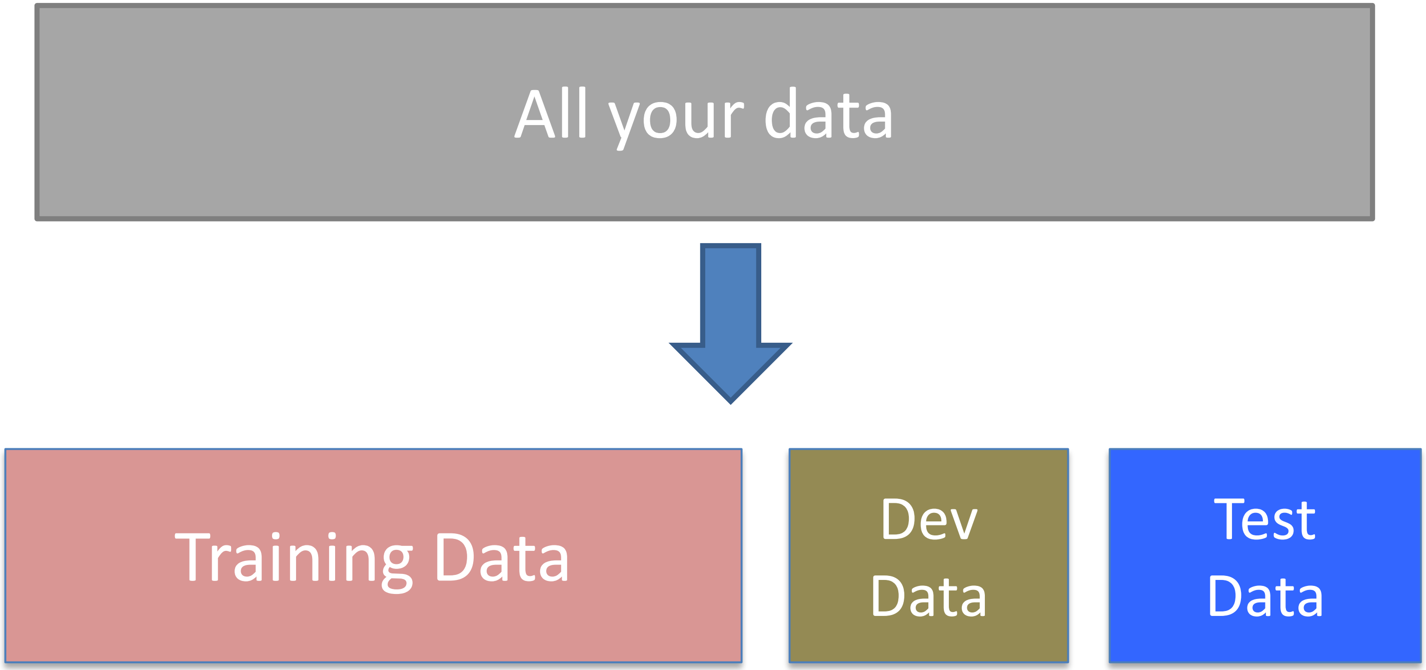
Experimental Design: Rule 1

Multi-class vs. Multi-label classification

Evaluation

- Regression Metrics
- Classification Metrics

Experimenting with Machine Learning Models



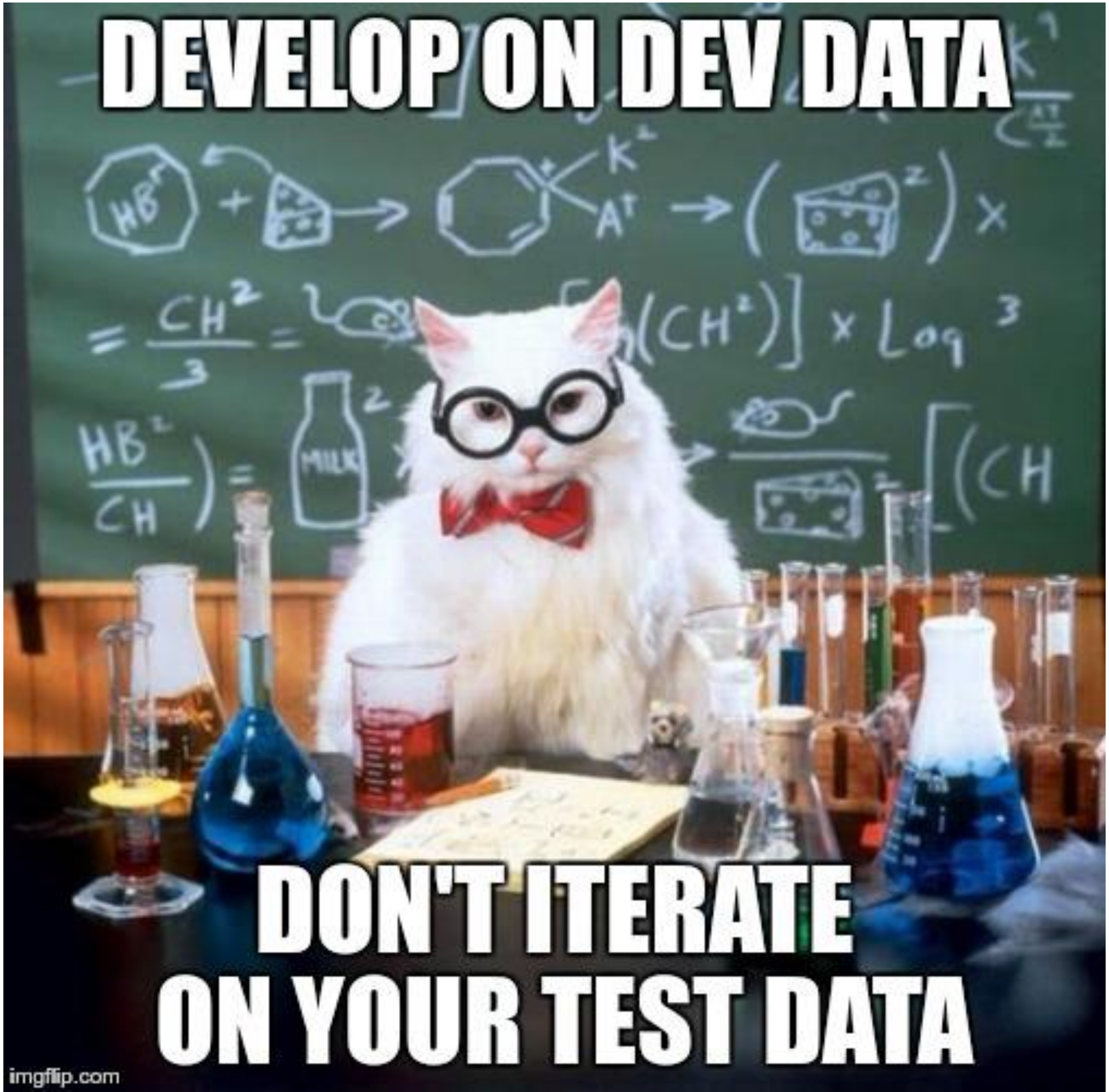
All your data

Training Data

Dev Data

Test Data

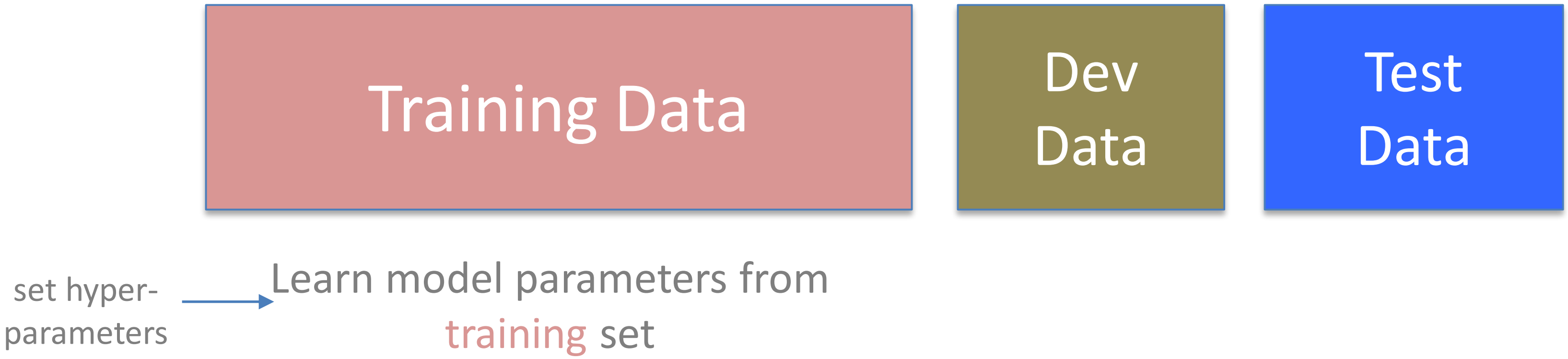
Rule #1


DEVELOP ON DEV DATA
DON'T ITERATE
ON YOUR TEST DATA
imgflip.com

Experimenting with Machine Learning Models

What is "correct?"

What is working "well?"



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set hyper-parameters → Learn model parameters from training set

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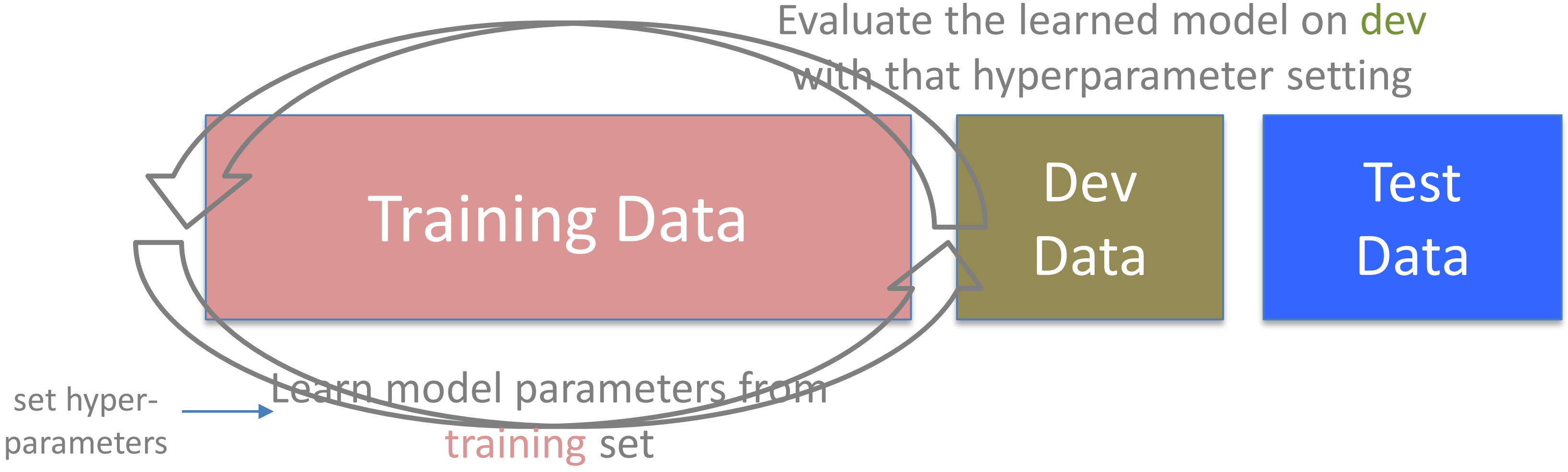

Evaluate the learned model on dev with that hyperparameter setting

Training Data

Dev Data

Test Data

set hyper-parameters

Learn model parameters from training set

Experimenting with Machine Learning Models

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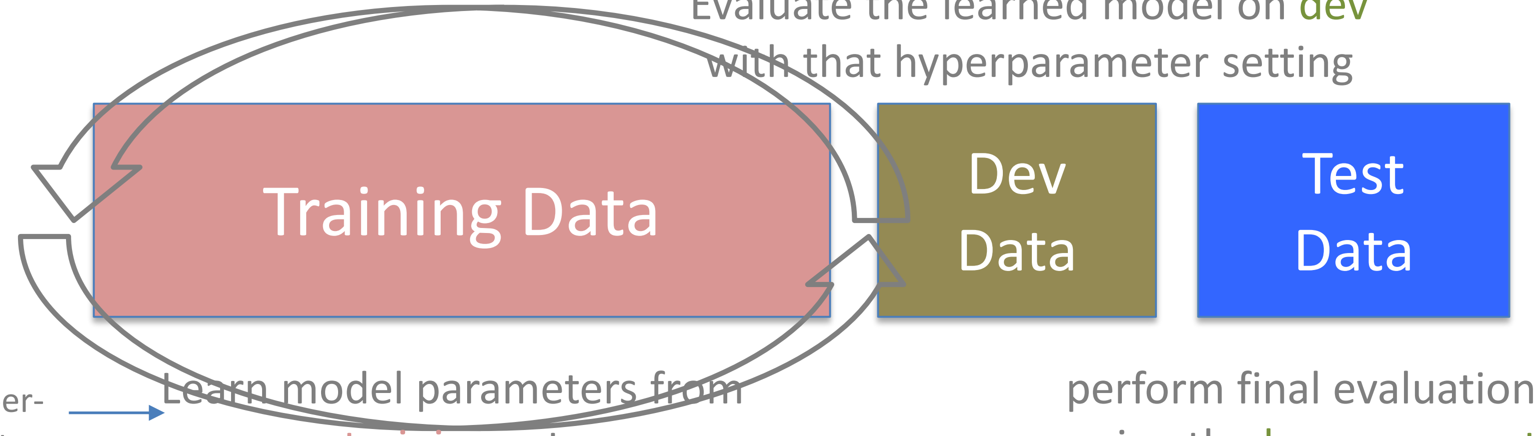

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perform final evaluation on test, using the hyperparameters that optimized dev performance and *retraining* the model

Experimenting with Machine Learning Models

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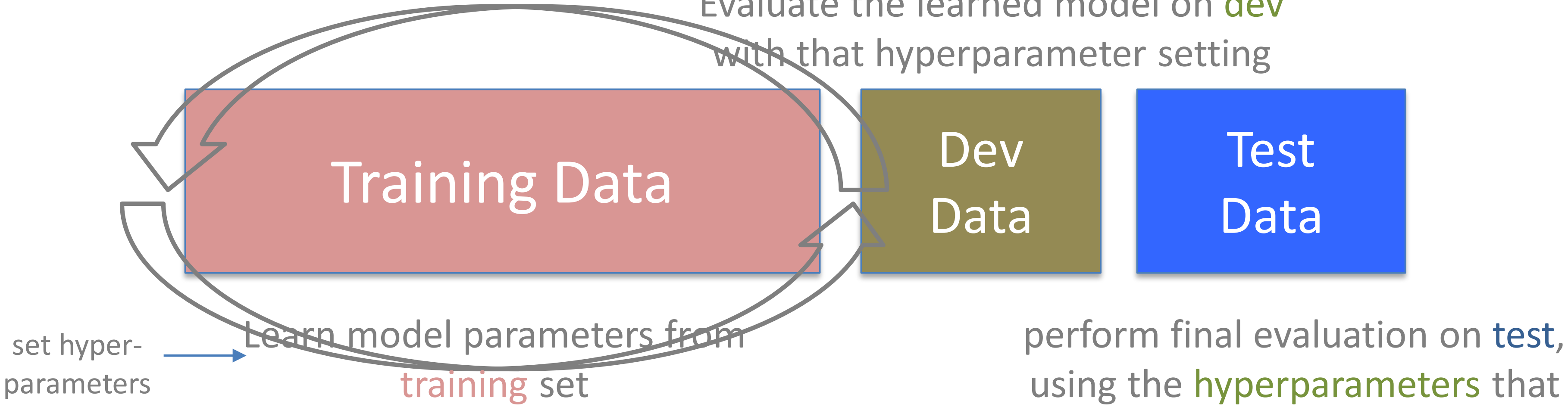

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perform final evaluation on test, using the hyperparameters that optimized dev performance and *retraining* the model

Rule 1: DO NOT ITERATE ON THE TEST DATA

On-board Exercise

Produce dev and test tables for a linear regression model with learned weights and set/fixed (non-learned) bias

Outline

Experimental Design: Rule 1

Multi-class vs. Multi-label classification

Evaluation

- Regression Metrics
- Classification Metrics

Multi-class Classification

Given input x, predict discrete label y

Multi-label Classification

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If $y \in \{0,1\}$ (or $y \in \{\text{True}, \text{False}\}$), then a binary classification task

Multi-label Classification

Multi-class Classification

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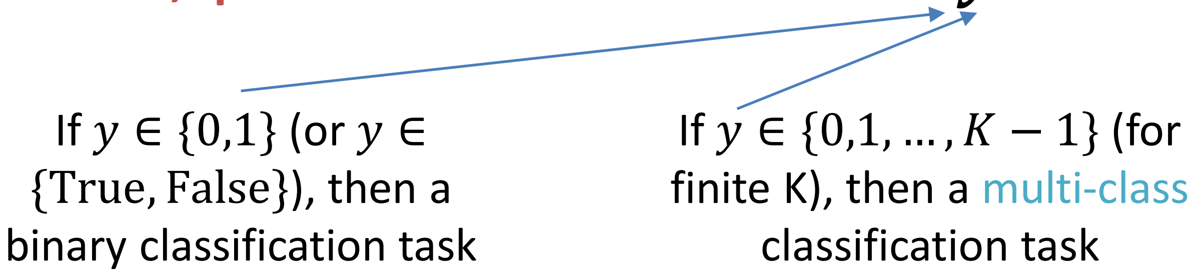

If $y \in \{0,1\}$ (or $y \in \{\text{True}, \text{False}\}$), then a binary classification task

If $y \in \{0,1, \ldots, K-1\}$ (for finite K), then a multi-class classification task

Q: What are some examples of multi-class classification?

Multi-label Classification

Multi-class Classification

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If $y \in \{0,1, \dots, K-1\}$ (for finite K), then a multi-class classification task

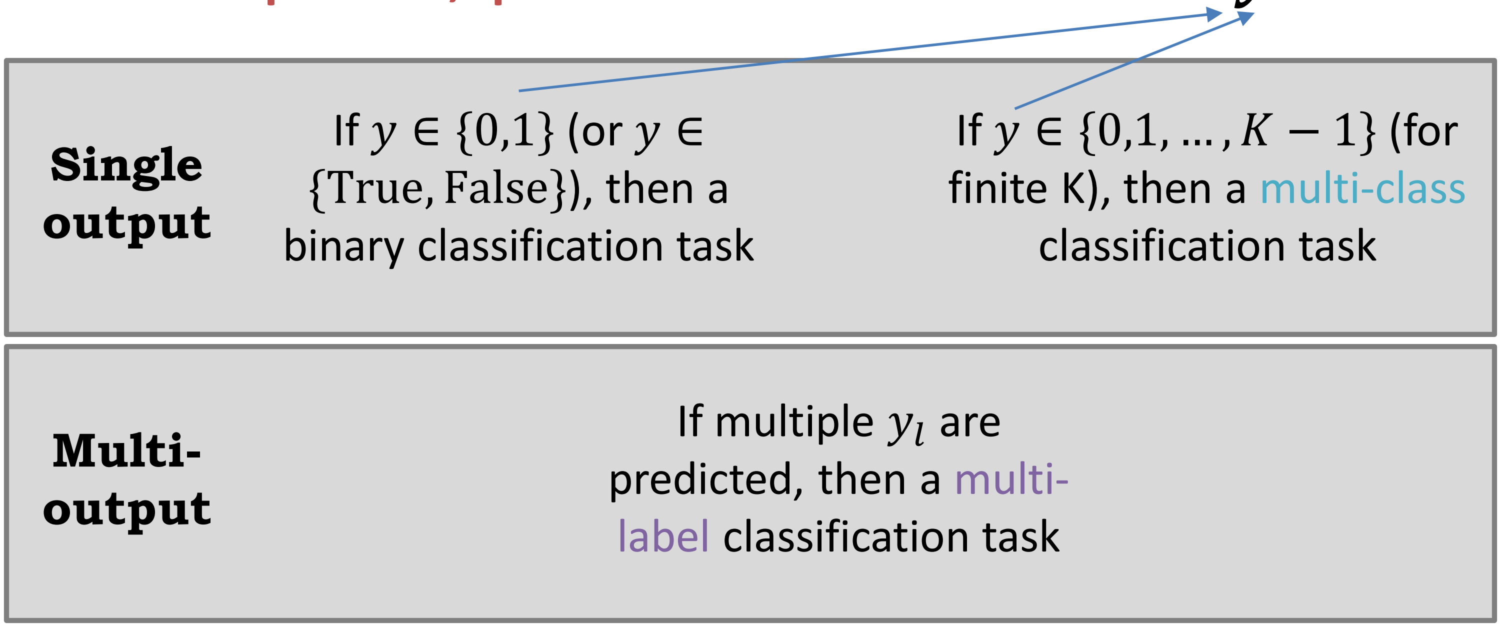
Q: What are some examples of multi-class classification?

A: Many possibilities. See A2, Q{1,2,4-7}

Multi-label Classification

Multi-class Classification

Given input x, predict discrete label y



Single output

If $y \in \{0,1\}$ (or $y \in \{\text{True}, \text{False}\}$), then a binary classification task

If $y \in \{0,1,\ldots,K-1\}$ (for finite K), then a multi-class classification task

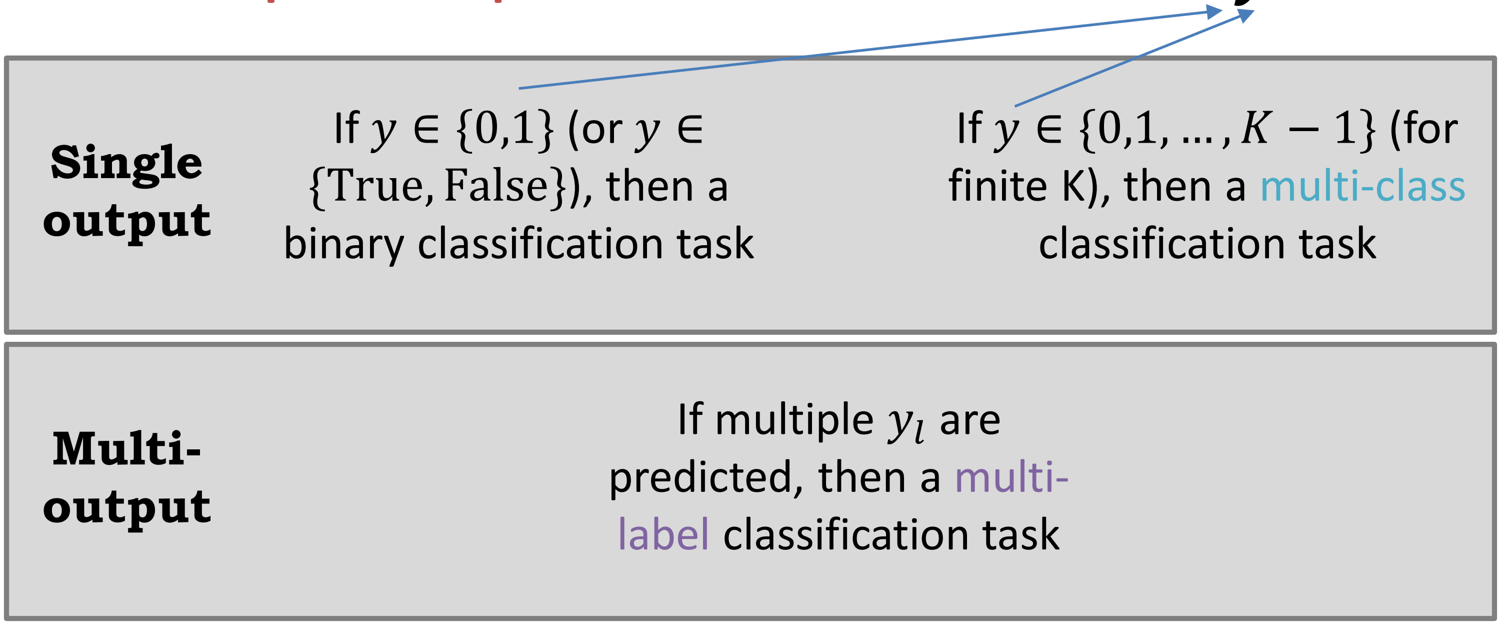
Multi-output

If multiple y_l are predicted, then a multi-label classification task

Multi-label Classification

Multi-class Classification

Given input x, predict discrete label y



Single output	If $y \in \{0,1\}$ (or $y \in \{\text{True}, \text{False}\}$), then a binary classification task	If $y \in \{0,1,\ldots,K-1\}$ (for finite K), then a multi-class classification task
Multi-output	If multiple y_l are predicted, then a multi-label classification task	

Given input x, predict multiple discrete labels $y = (y_1, \ldots, y_L)$

Multi-label Classification

Multi-class Classification

Given input x, predict discrete label y

Single output	If $y \in \{0,1\}$ (or $y \in \{\text{True}, \text{False}\}$), then a binary classification task	If $y \in \{0,1,\ldots,K-1\}$ (for finite K), then a multi-class classification task
Multi-output	If multiple y_l are predicted, then a multi-label classification task	Each y_l could be binary or multi-class

Given input x, predict multiple discrete labels $y = (y_1, \ldots, y_L)$

Multi-label Classification

Multi-Label Classification…

Will not be a primary focus of this course

Many of the single output classification methods apply to multi-label classification

Predicting “in the wild” can be trickier

Evaluation can be trickier

We’ve only developed binary classifiers so far…

Option 1: Develop a multi-class version

Option 2: Build a one-vs-all (OvA) classifier

Option 3: Build an all-vs-all (AvA) classifier

(there can be others)

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Loss function may (or may not) need to be extended & the model structure may need to change (big or small)

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Loss function may (or may not) need to be extended & the model structure may need to change (big or small)

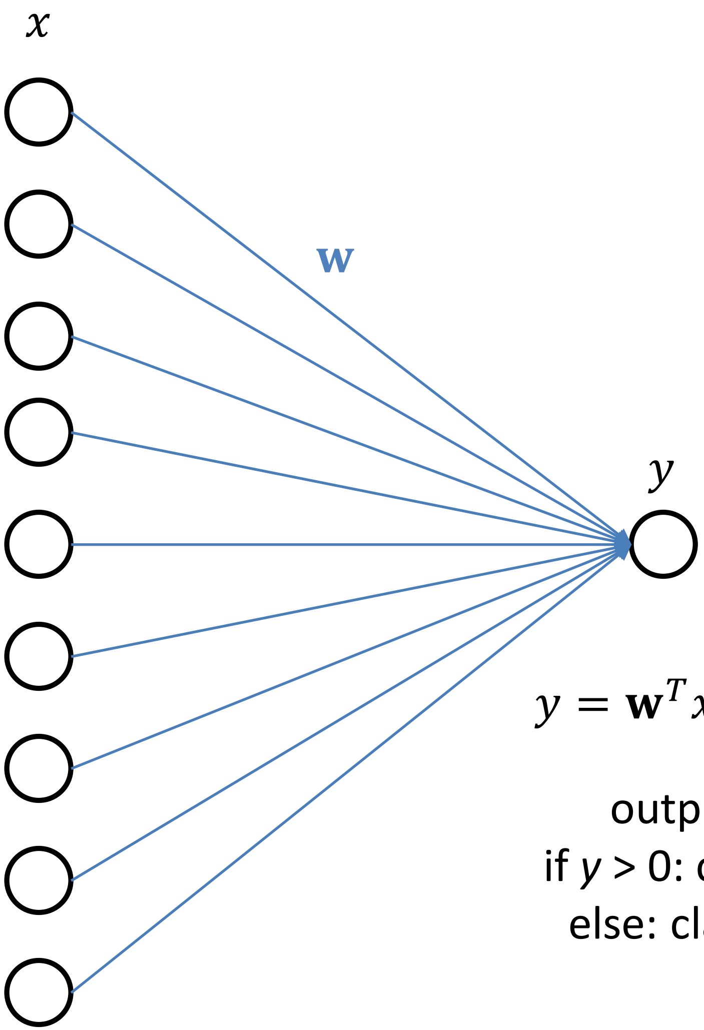
Common change:

instead of a single weight vector w, keep a weight vector $w^{(c)}$ for each class *c*

Compute class specific scores, e.g.,

$$\widehat{y_i^{(c)}} = \left(w^{(c)}\right)^T x + b^{(c)}$$

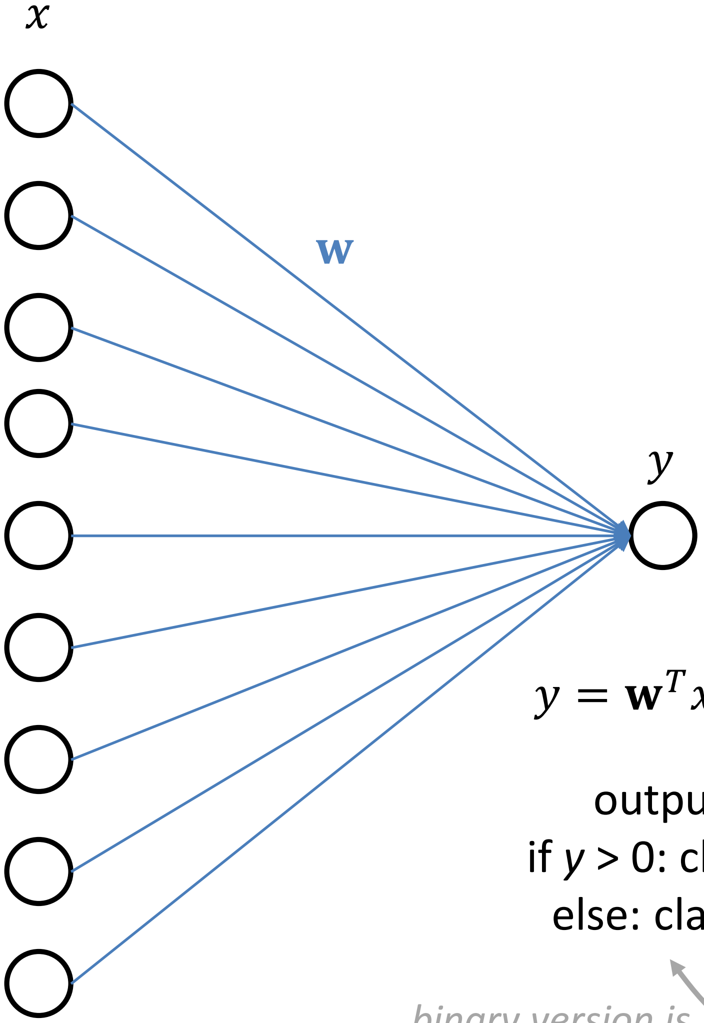
Multi-class Option 1: Linear Regression/Perceptron



$$y = \mathbf{w}^T x + b$$

output:
if $y > 0$: class 1
else: class 2

Multi-class Option 1: Linear Regression/Perceptron: A Per-Class View



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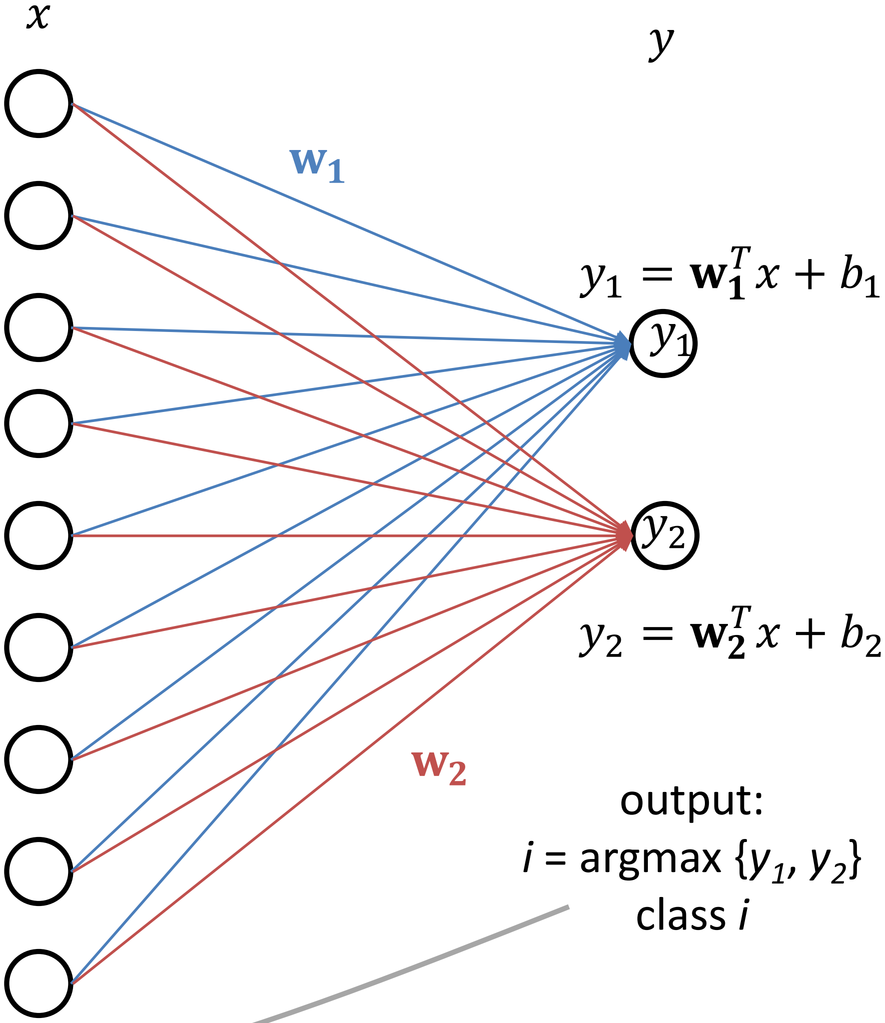


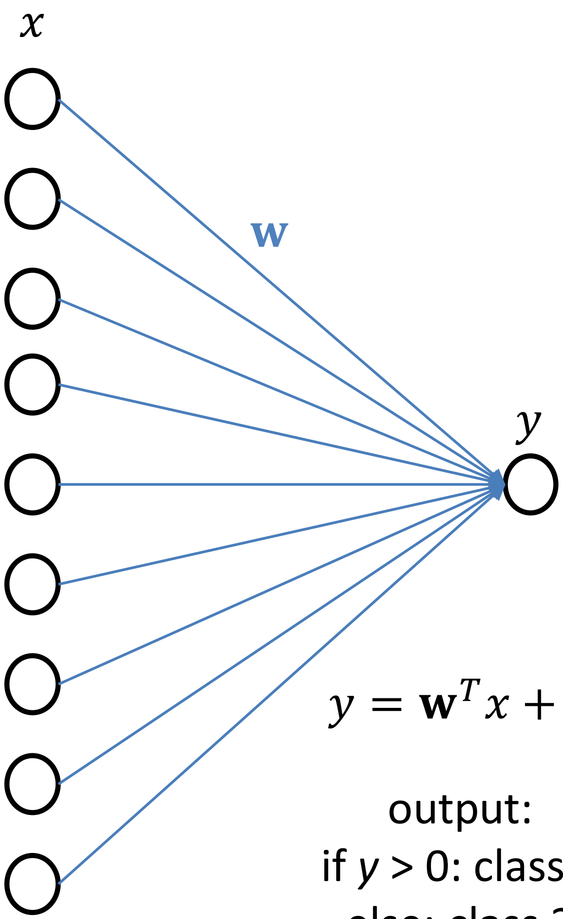
$$y_1 = \mathbf{w_1}^T x + b_1$$

$$y_2 = \mathbf{w_2}^T x + b_2$$

output:
i = argmax $\{y_1, y_2\}$
class i

binary version is special case

Multi-class Option 1: Linear Regression/Perceptron: A Per-Class View (alternative)



$$y = \mathbf{w}^T x + b$$

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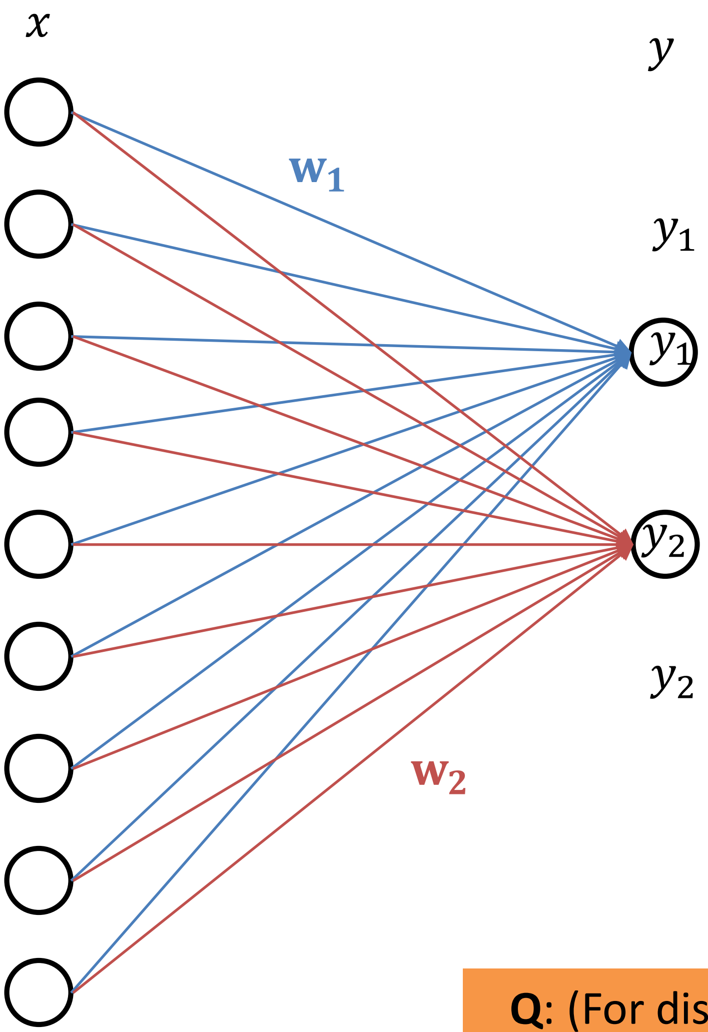

$$y_1 = [\boldsymbol{w_1}; \boldsymbol{w_2}]^{\boldsymbol{T}}[x; \mathbf{0}] + b_1$$

concatenation

$$y_2 = [\boldsymbol{w_1}; \boldsymbol{w_2}]^{\boldsymbol{T}}[\mathbf{0}; x] + b_2$$

output:
i = argmax $\{y_1, y_2\}$
class *i*

Q: (For discussion) Why does this work?

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With C classes:

Train C different binary classifiers $\gamma_c(x)$

$\gamma_c(x)$ predicts 1 if x is likely class c, 0 otherwise

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To test/predict a new instance *z*:

Get scores $s^c = \gamma_c(z)$

Output the max of these scores, $\hat{y} = \operatorname{argmax}_c s^c$

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To test/predict a new instance *z*:

Get scores or predictions $s^{c_1,c_2} = \gamma_{c_1,c_2}(z)$

Multiple options for final prediction:

(1) count # times a class *c* was predicted

(2) margin-based approach

We’ve only developed binary classifiers so far…

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Q: (to discuss)

Why might you want to use option 1 or options OvA/AvA?

What are the benefits of OvA vs. AvA?

We’ve only developed binary classifiers so far…

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(there can be others)

Q: (to discuss)

Why might you want to use option 1 or options OvA/AvA?

What are the benefits of OvA vs. AvA?

What if you start with a balanced dataset, e.g., 100 instances per class?

Outline

Experimental Design: Rule 1

Multi-class vs. Multi-label classification

Evaluation

- Regression Metrics
- Classification Metrics

Regression Metrics

(Root) Mean Square Error

$$RMSE = \sqrt{\frac{1}{N}\sum_{i}^{N}(y_i - \widehat{y_i})^2}$$

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Q: How can these reward/punish predictions differently?

Regression Metrics

(Root) Mean Square Error

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$$MAE = \frac{1}{N}\sum_{i}^{N}|y_i - \widehat{y_i}|$$

Q: How can these reward/punish predictions differently?

A: RMSE punishes outlier predictions more harshly

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Training Loss vs. Evaluation Score

In training, compute loss to update parameters

Sometimes loss is a computational compromise

- surrogate loss

The loss you use might not be as informative as you'd like

Binary classification: 90 of 100 training examples are +1, 10 of 100 are -1

Some Classification Metrics

Accuracy

Precision
Recall

AUC (Area Under Curve)

F1

Confusion Matrix

Classification Evaluation: the 2-by-2 contingency table

	Actually Correct	Actually Incorrect
Selected/ Guessed		
Not selected/ not guessed		

● ○

Classes/Choices

Classification Evaluation: the 2-by-2 contingency table

	Actually Correct	**Actually Incorrect**
Selected/ Guessed	True Positive ● *Correct* (TP) ● *Guessed*	
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● ○

Classes/Choices

Classification Evaluation: Accuracy, Precision, and Recall

Accuracy: % of items correct

$$\frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

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Classification Evaluation: Accuracy, Precision, and Recall

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Precision: % of selected items that are correct

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

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Recall: % of correct items that are selected

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Precision: % of selected items that are correct

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

Min: 0 ☹

Max: 1 😬

Recall: % of correct items that are selected

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

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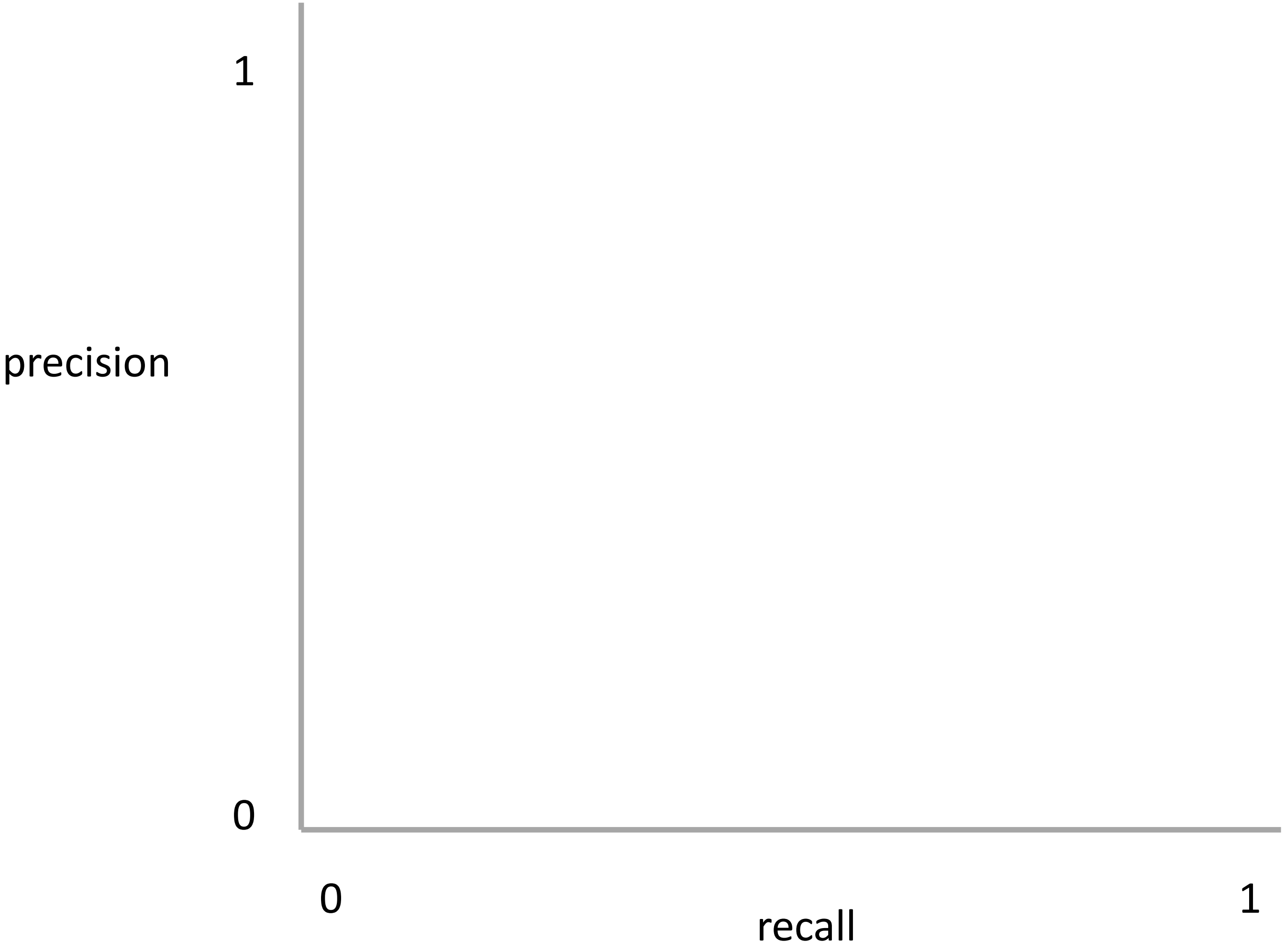
Precision and Recall Present a Tradeoff

Q: Where do you want your ideal model ?



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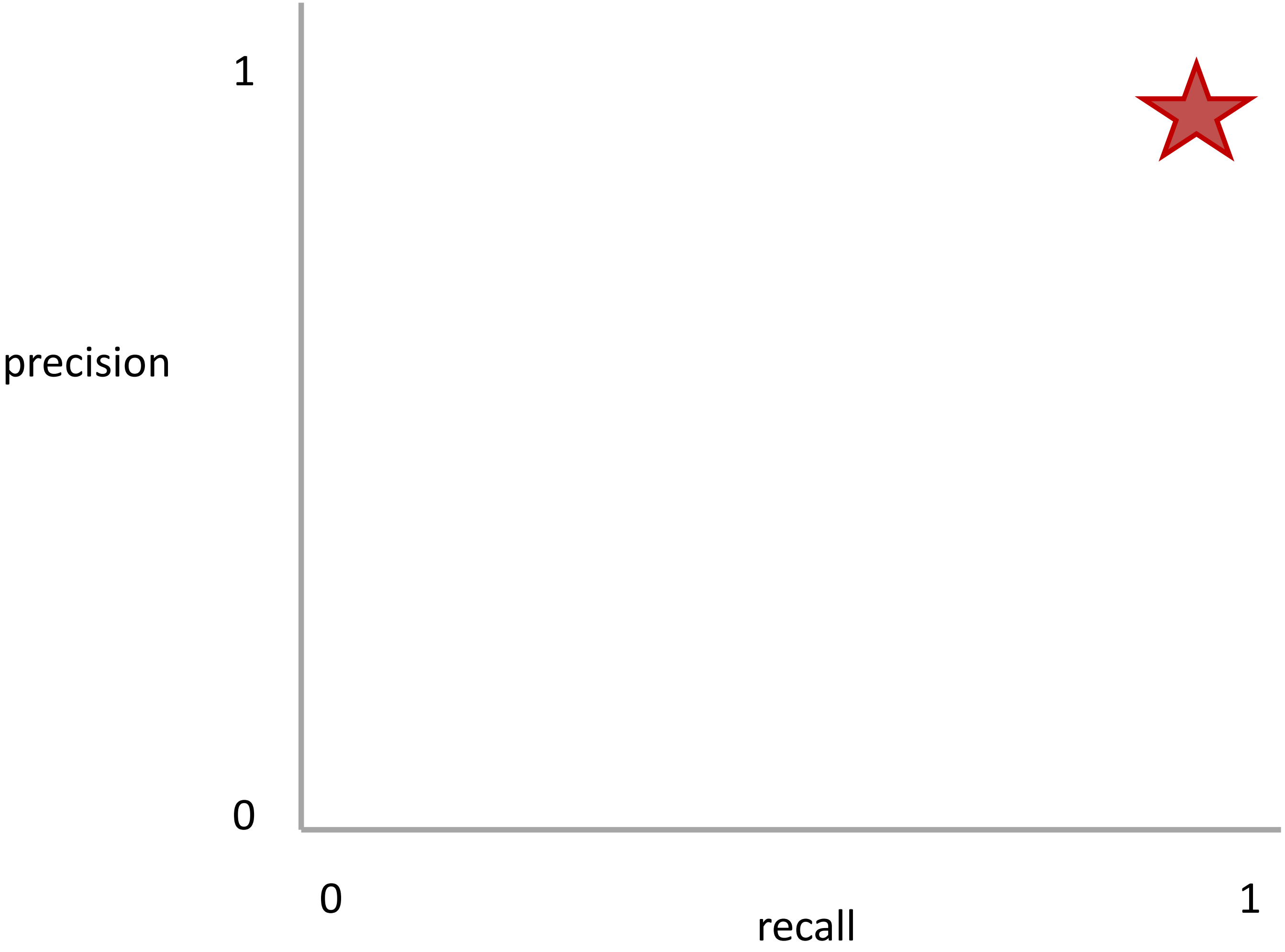
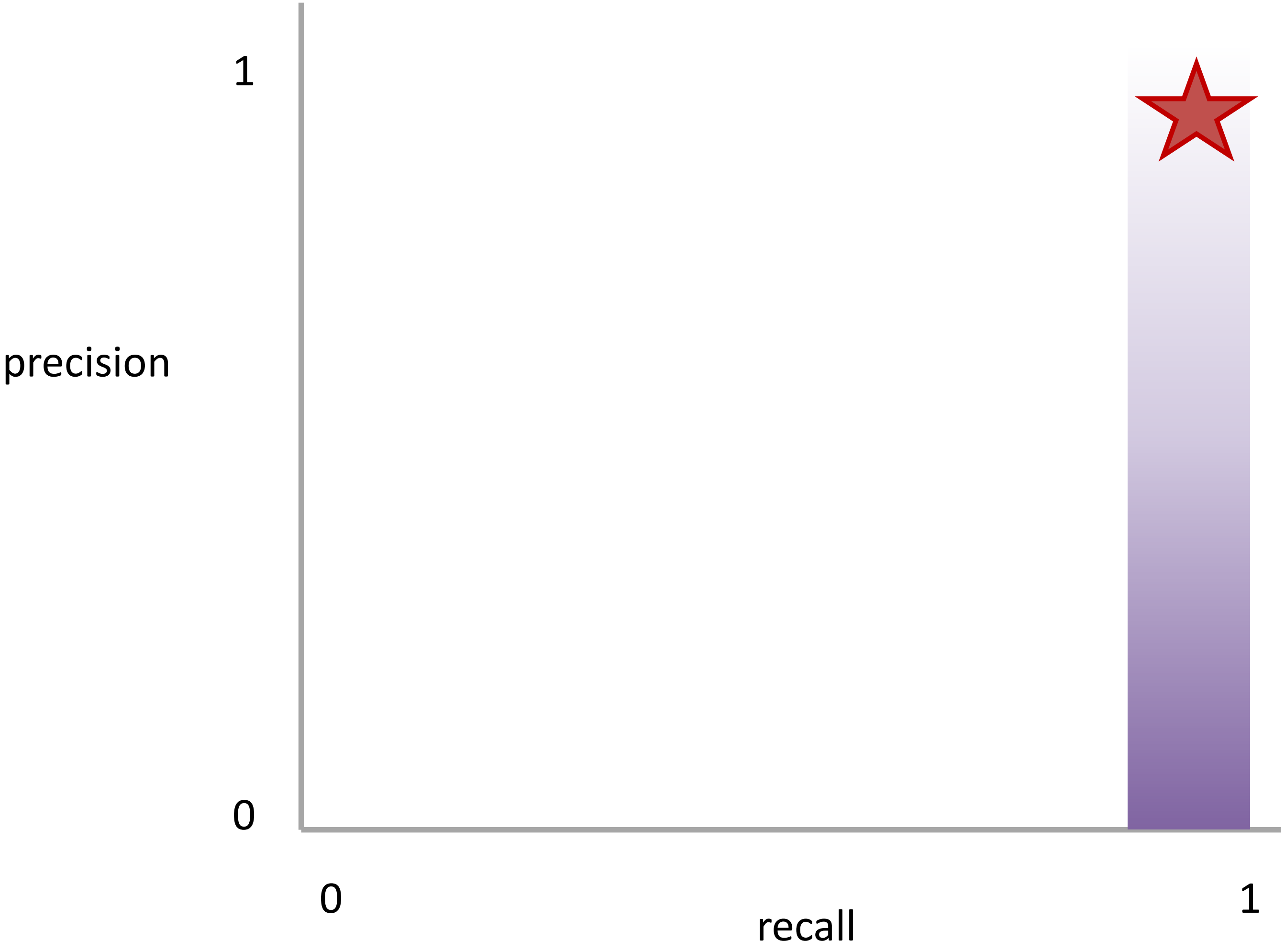


Q: Where do you want your ideal model ?

Q: You have a model that always identifies correct instances. Where on this graph is it?

Precision and Recall Present a Tradeoff



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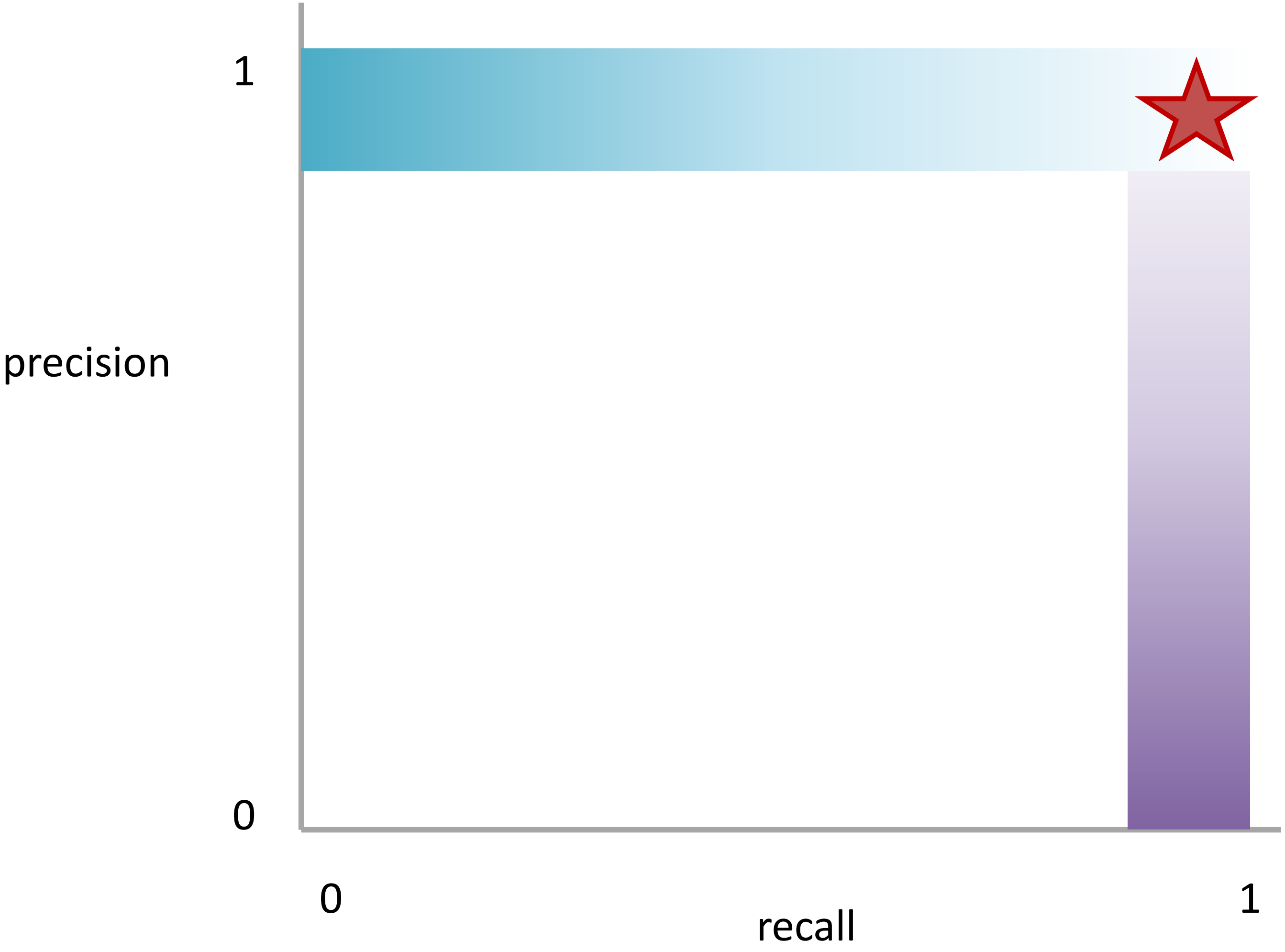

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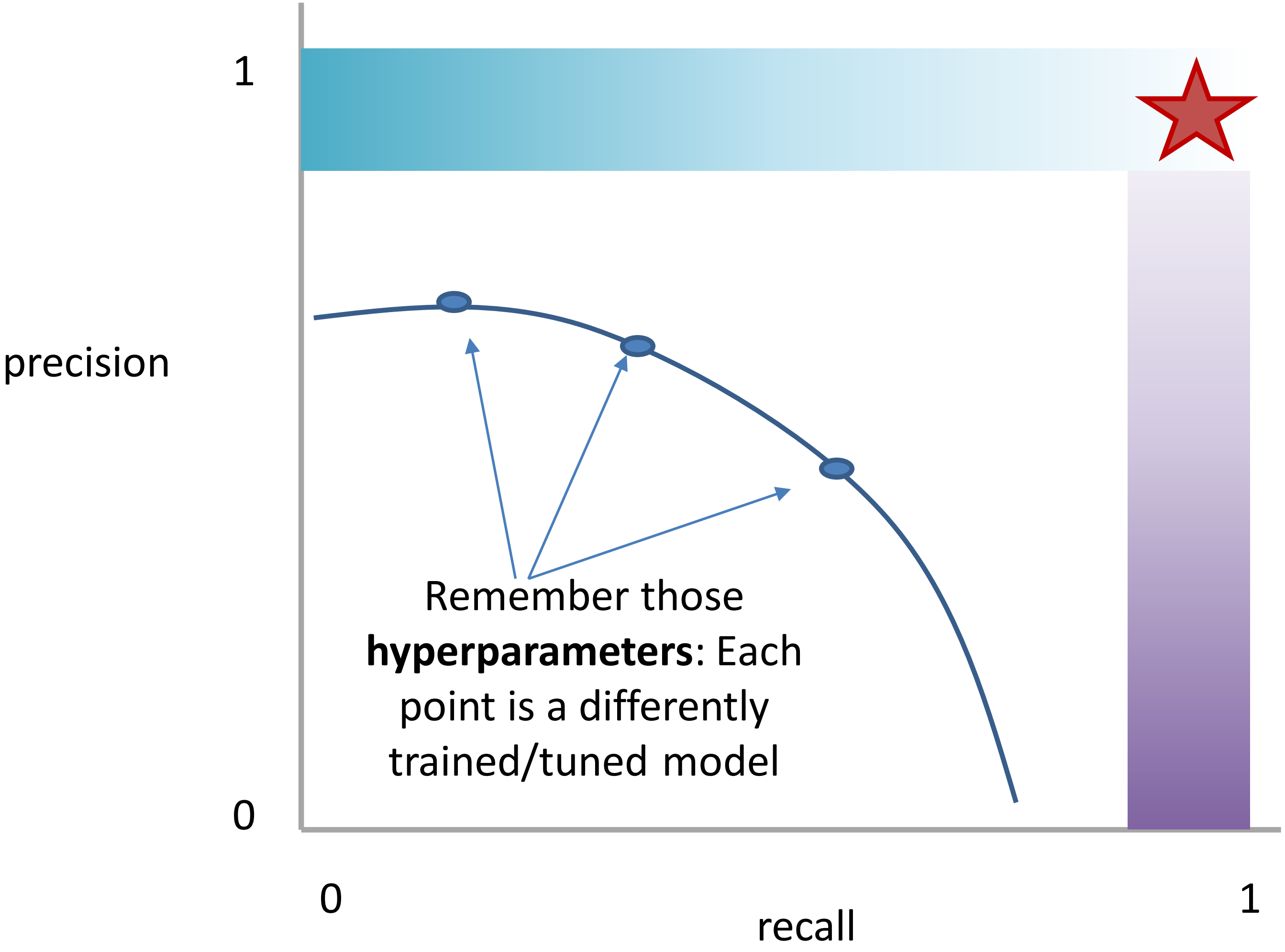

Remember those **hyperparameters**: Each point is a differently trained/tuned model

Q: Where do you want your ideal model ?

Q: You have a model that always identifies correct instances. Where on this graph is it?

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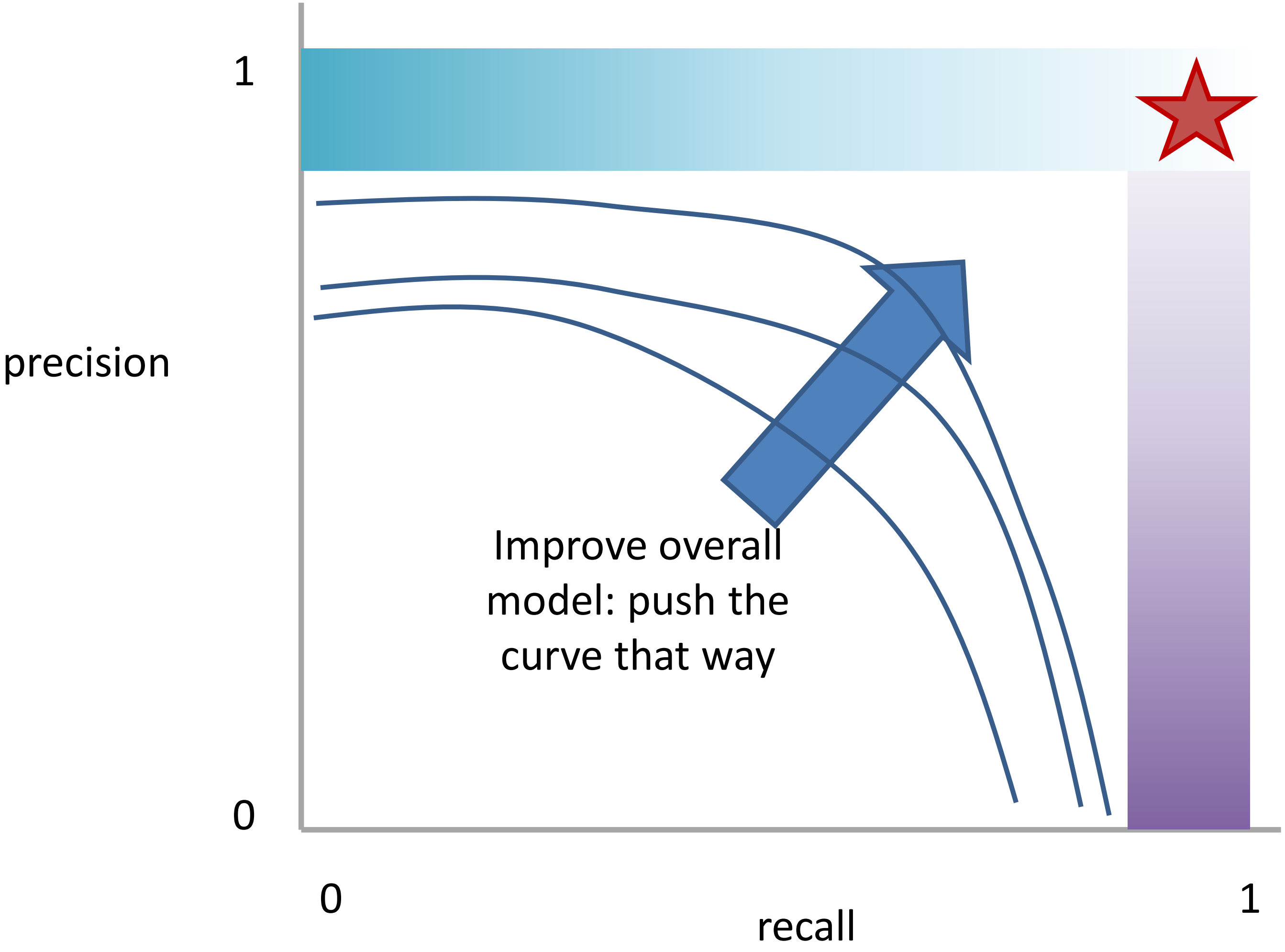
Idea: measure the tradeoff between precision and recall

Precision and Recall Present a Tradeoff



Improve overall model: push the curve that way

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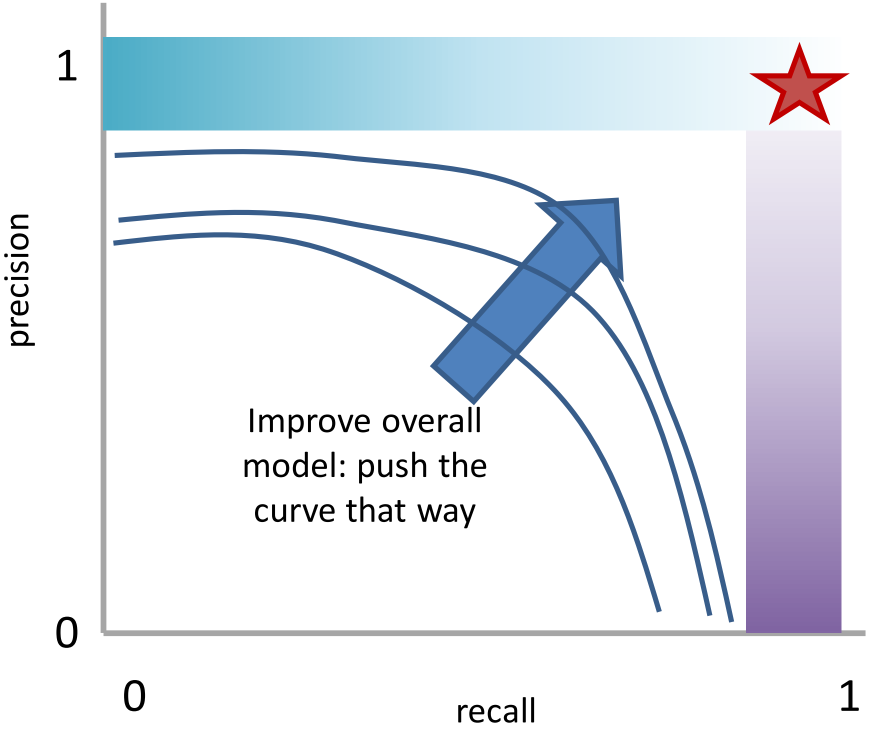
Idea: measure the tradeoff between precision and recall

Measure this Tradeoff: Area Under the Curve (AUC)

AUC measures the area under this tradeoff curve

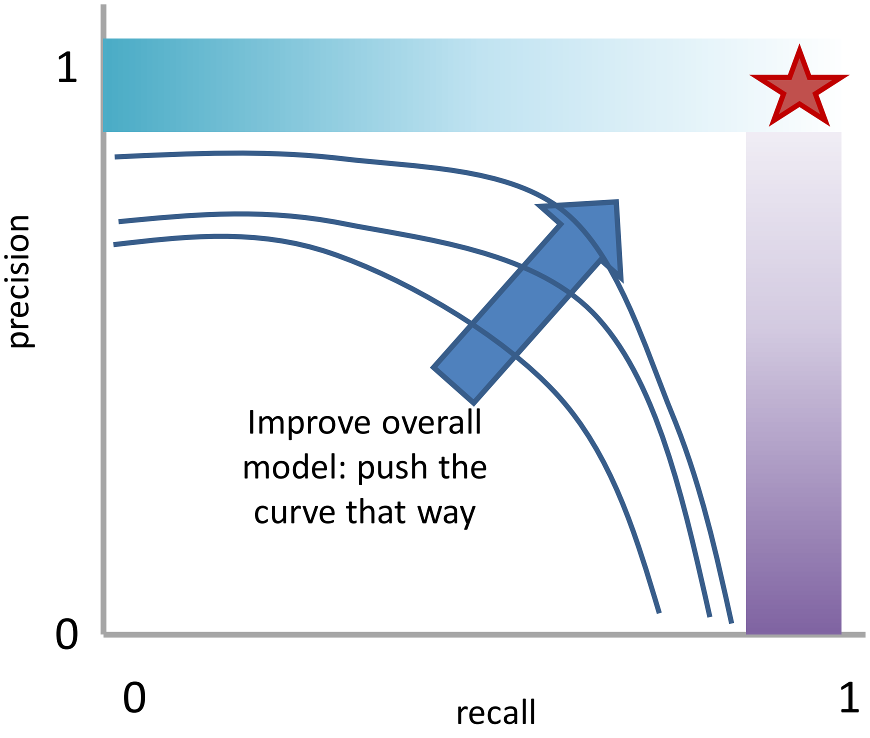


Improve overall model: push the curve that way

Min AUC: 0 ☹

Max AUC: 1 😁

Measure this Tradeoff: Area Under the Curve (AUC)



Min AUC: 0 ☹
Max AUC: 1 😁

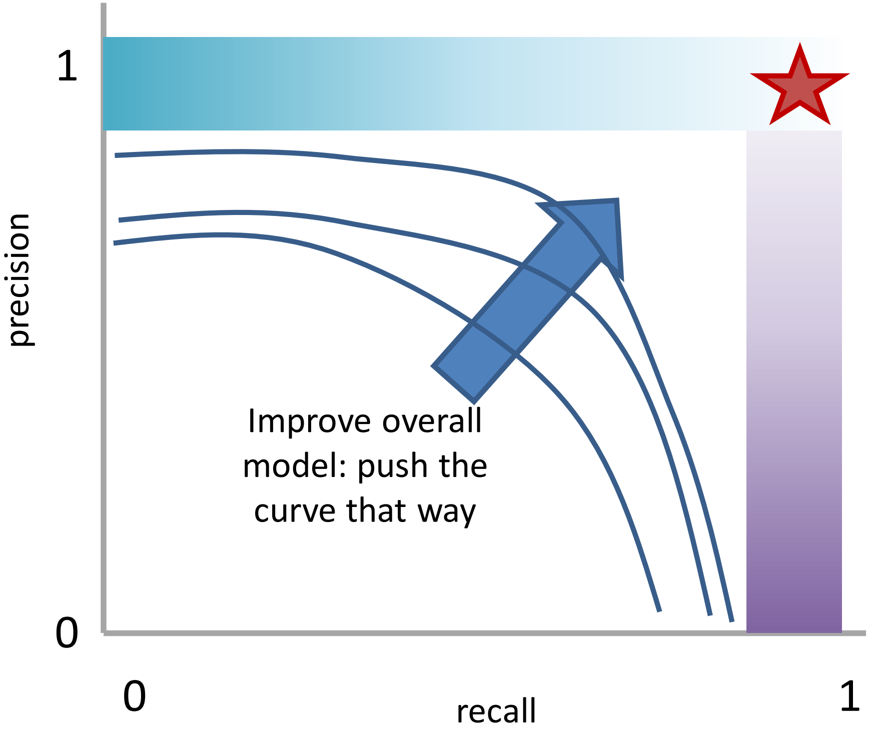
AUC measures the area under this tradeoff curve

1. Computing the curve

   You need true labels & predicted labels with some score/confidence estimate

   Threshold the scores and for each threshold compute precision and recall

Measure this Tradeoff: Area Under the Curve (AUC)



Improve overall model: push the curve that way

Min AUC: 0 ☹
Max AUC: 1 😁

AUC measures the area under this tradeoff curve

1. Computing the curve

   You need true labels & predicted labels with some score/confidence estimate

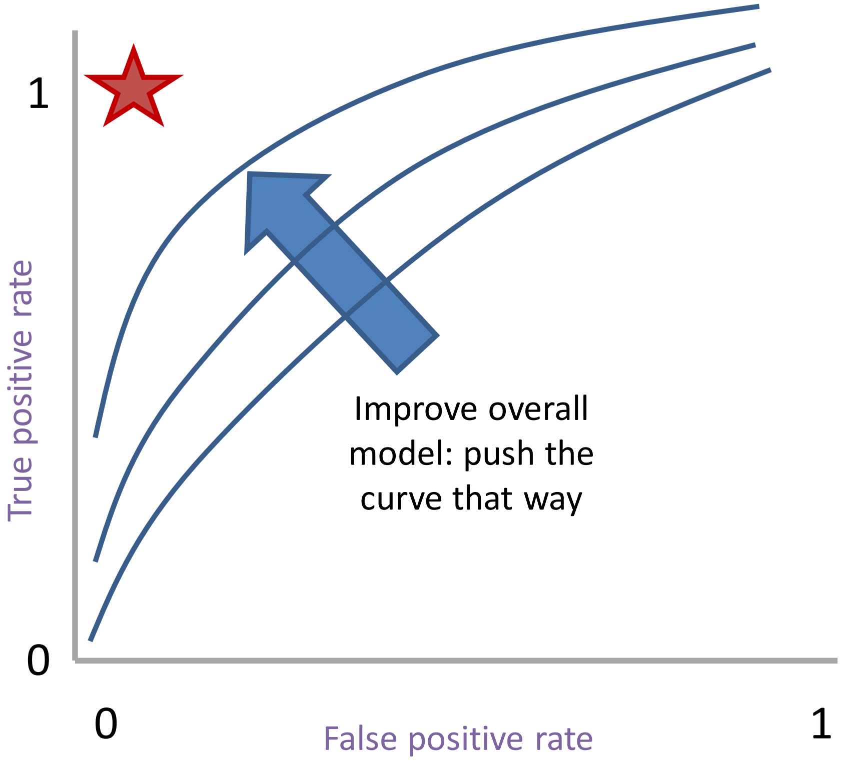
   Threshold the scores and for each threshold compute precision and recall

2. Finding the area

   How to implement: trapezoidal rule (& others)

In practice: external library like the sklearn.metrics module

Measure A Slightly Different Tradeoff: ROC-AUC



Min ROC-AUC: 0.5 ☹

Max ROC-AUC: 1 😁

AUC measures the area under this tradeoff curve

1. Computing the curve

   You need true labels & predicted labels with some score/confidence estimate

   Threshold the scores and for each threshold compute metrics

2. Finding the area

   How to implement: trapezoidal rule (& others)

In practice: external library like the sklearn.metrics module

Main variant: ROC-AUC

Same idea as before but with some flipped metrics

A combined measure: F

Weighted (harmonic) average of **P**recision & **R**ecall

$$F = \frac{1}{\alpha\frac{1}{P} + (1-\alpha)\frac{1}{R}}$$

A combined measure: F

Weighted (harmonic) average of **P**recision & **R**ecall

$$F = \frac{1}{\alpha \frac{1}{P} + (1 - \alpha) \frac{1}{R}} = \frac{(1 + \beta^2) \ * P \ * R}{(\beta^2 * P) + R}$$

algebra
(not important)

A combined measure: F

Weighted (harmonic) average of **P**recision & **R**ecall

$$F = \frac{(1+\beta^2) \ * P \ * R}{(\beta^2 * P) + R}$$

Balanced F1 measure: β=1

$$F_1 = \frac{2 \ * P \ * R}{P + R}$$

P/R/F in a Multi-class Setting: Micro- vs. Macro-Averaging

If we have more than one class, how do we combine multiple performance measures into one quantity?

Macroaveraging: Compute performance for each class, then average.

Microaveraging: Collect decisions for all classes, compute contingency table, evaluate.

P/R/F in a Multi-class Setting: Micro- vs. Macro-Averaging

Macroaveraging: Compute performance for each class, then average.

$$\text{macroprecision} = \sum_{c} \frac{\mathrm{TP_c}}{\mathrm{TP_c} + \mathrm{FP_c}} = \sum_{c} \text{precision}_{c}$$

Microaveraging: Collect decisions for all classes, compute contingency table, evaluate.

$$\text{microprecision} = \frac{\sum_{\mathrm{c}} \mathrm{TP_c}}{\sum_{\mathrm{c}} \mathrm{TP_c} + \sum_{\mathrm{c}} \mathrm{FP_c}}$$

P/R/F in a Multi-class Setting: Micro- vs. Macro-Averaging

Macroaveraging: Compute performance for each class, then average.

when to prefer the macroaverage?

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Microaveraging: Collect decisions for all classes, compute contingency table, evaluate.

when to prefer the microaverage?

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Micro- vs. Macro-Averaging: Example

Class 1

	Truth : yes	Truth : no
Classifier: yes	10	10
Classifier: no	10	970

Class 2

	Truth : yes	Truth : no
Classifier: yes	90	10
Classifier: no	10	890

Micro Ave. Table

	Truth : yes	Truth : no
Classifier: yes	100	20
Classifier: no	20	1860

Macroaveraged precision: (0.5 + 0.9)/2 = 0.7

Microaveraged precision: 100/120 = .83

Microaveraged score is dominated by score on frequent classes

Confusion Matrix: Generalizing the 2-by-2 contingency table

		Correct Value		
		●	○	▭
Guessed Value	●	#	#	#
	○	#	#	#
	▭	#	#	#

Confusion Matrix: Generalizing the 2-by-2 contingency table

		Correct Value		
		●	○	▭
Guessed Value	●	80	9	11
	○	7	86	7
	▭	2	8	9

Q: Is this a good result?

Confusion Matrix: Generalizing the 2-by-2 contingency table

		Correct Value		
		●	○	▭
Guessed Value	●	30	40	30
	○	25	30	50
	▭	30	35	35

Q: Is this a good result?

Confusion Matrix: Generalizing the 2-by-2 contingency table

		Correct Value		
		●	○	▭
Guessed Value	●	7	3	90
	○	4	8	88
	▭	3	7	90

Q: Is this a good result?

Some Classification Metrics

Accuracy

Precision
Recall

AUC (Area Under Curve)

F1

Confusion Matrix

Outline

Experimental Design: Rule 1

Multi-class vs. Multi-label classification

Evaluation

- Regression Metrics
- Classification Metrics