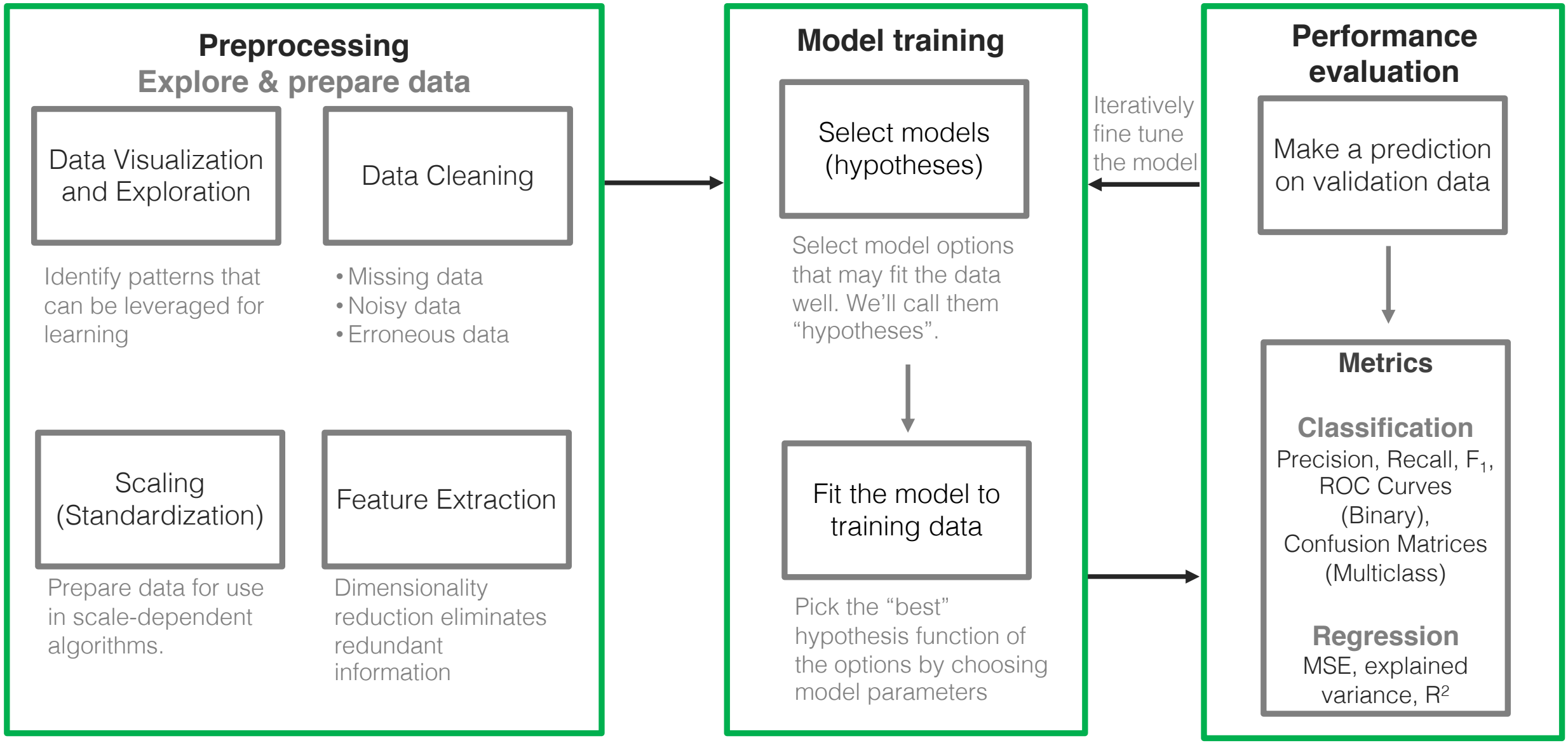
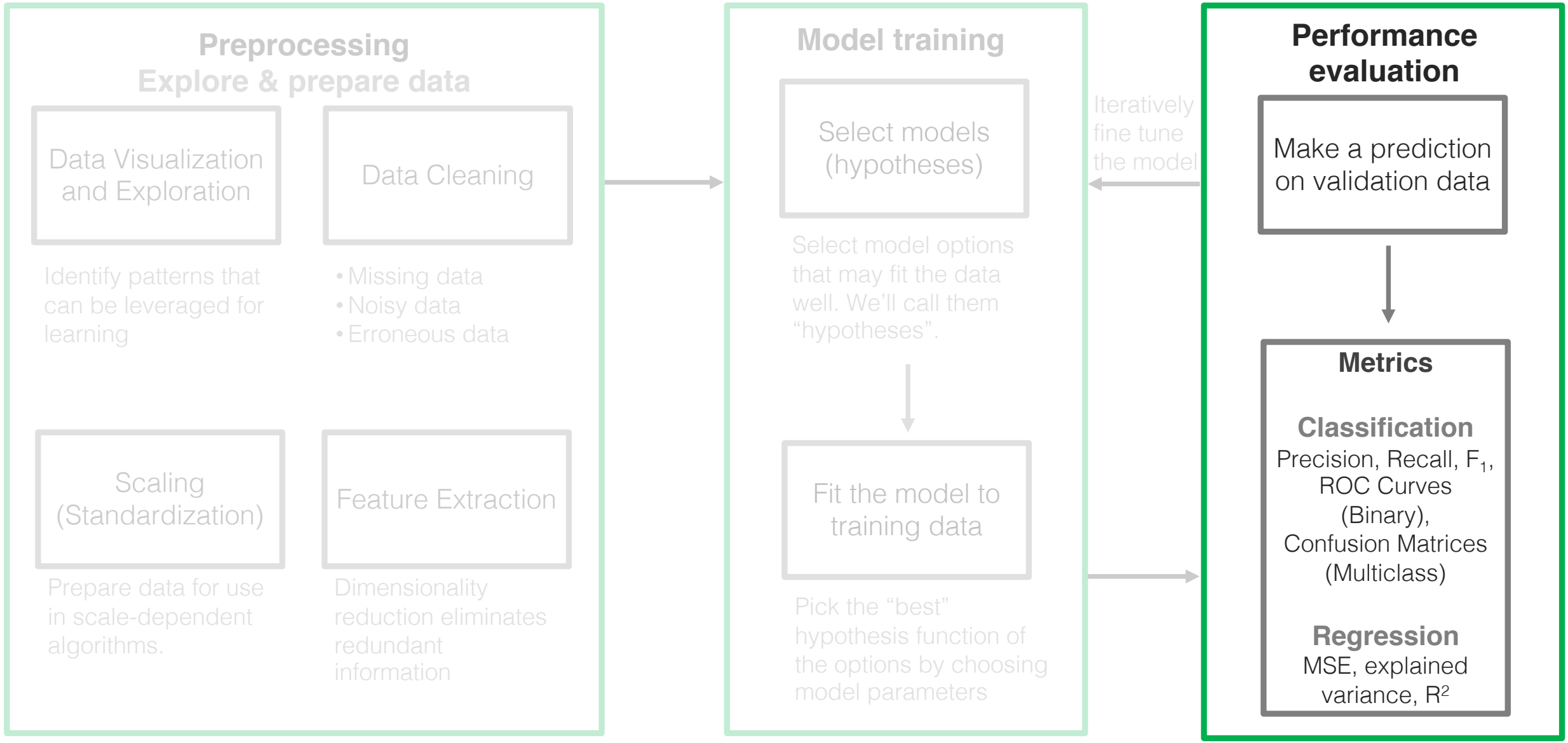
Evaluating Performance I

Lecture 06

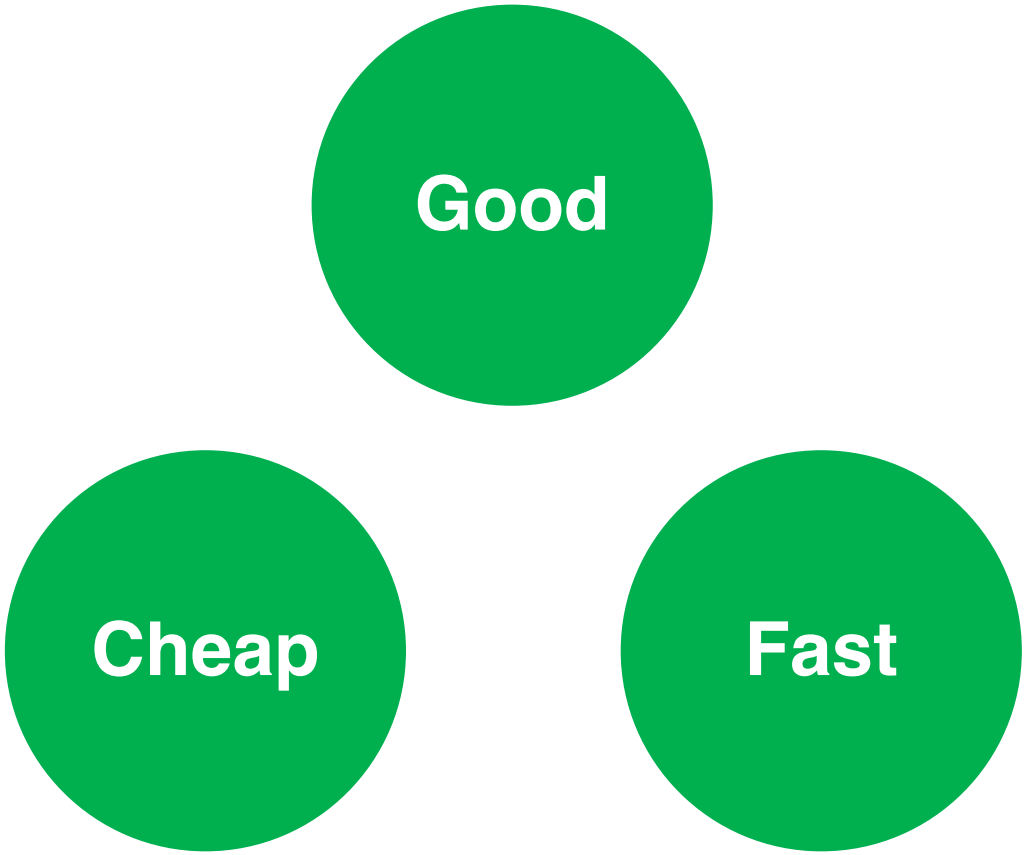
Supervised learning in practice



Supervised learning in practice



Choose 2



Modeling Considerations

Accuracy

Computational Efficiency

Interpretability

Accuracy

Supervised Learning Performance Evaluation

Regression

Classification

Binary

Receiver Operating Characteristic (ROC) curves

Multiclass

Confusion matrices

Common Metrics

- Mean squared error (MSE)
- Mean absolute error (MAE)
- R^2, coefficient of determination
- Adjusted R^2

- Classification accuracy
- True positive rate
- False positive rate
- Precision
- F_1 Score
- Area under the ROC curve (AUC)

- Classification accuracy
- Micro-averaged F_1 Score
- Macro-averaged F_1 Score

Regression: Mean Squared Error

The mean squared error (MSE)

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

Absolute measure of performance

One of the most widely used loss / cost functions

Regression: Mean Absolute Error

The mean absolute error (MAE)

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

Absolute measure of performance

Regression: R^2 Coefficient of determination

Proportion of the response variable variation explained by the model

Residual sum of squares
(variation in the residuals)

$$SS_{res} = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Total sum of squares
(variation in the data)

$$SS_{tot} = \sum_{i=1}^{N} (y_i - \bar{y})^2$$

$$\bar{y} = \frac{1}{N} \sum_{i=1}^{N} y_i$$

R-squared

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

Relative measure of performance

Regression: Adjusted R^2

Problem: R^2 increases with more predictor variables

Adjusted R squared:

$$R^2_{adj} = 1 - (1 - R^2)\frac{N - 1}{N - p - 1}$$

Adjusts R squared to account for the number of predictor variables

This value is always less than or equal to the unadjusted R squared

Types of classification error

False Positive
(Type I error)

False Negative
(Type II error)

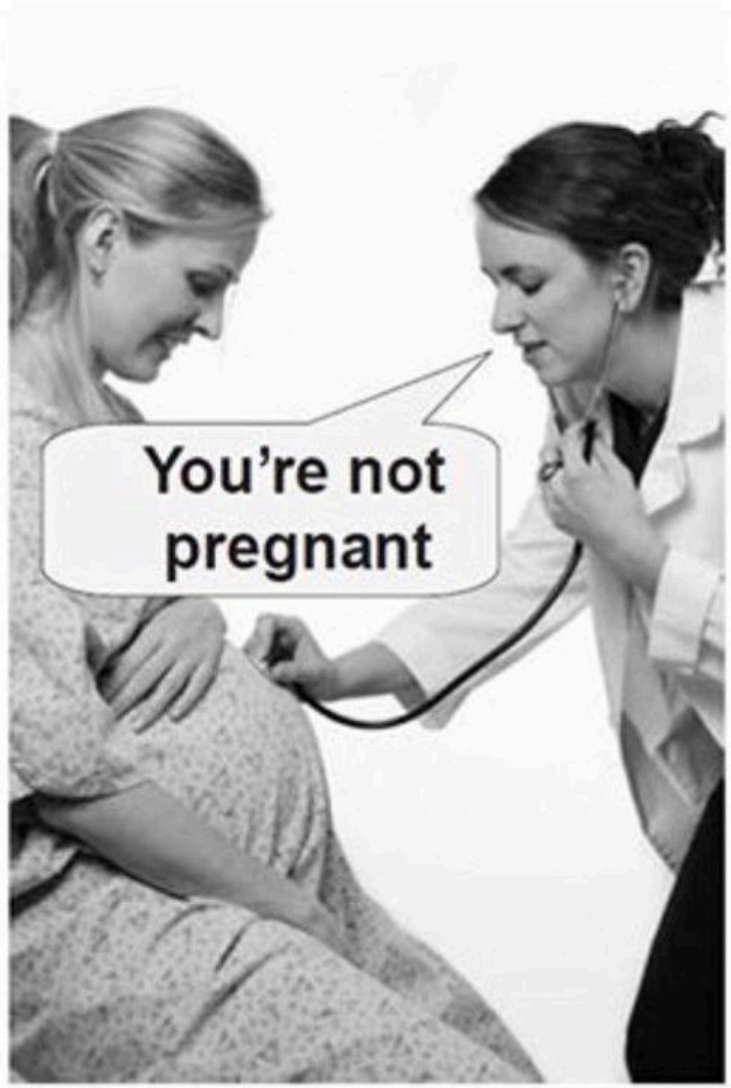
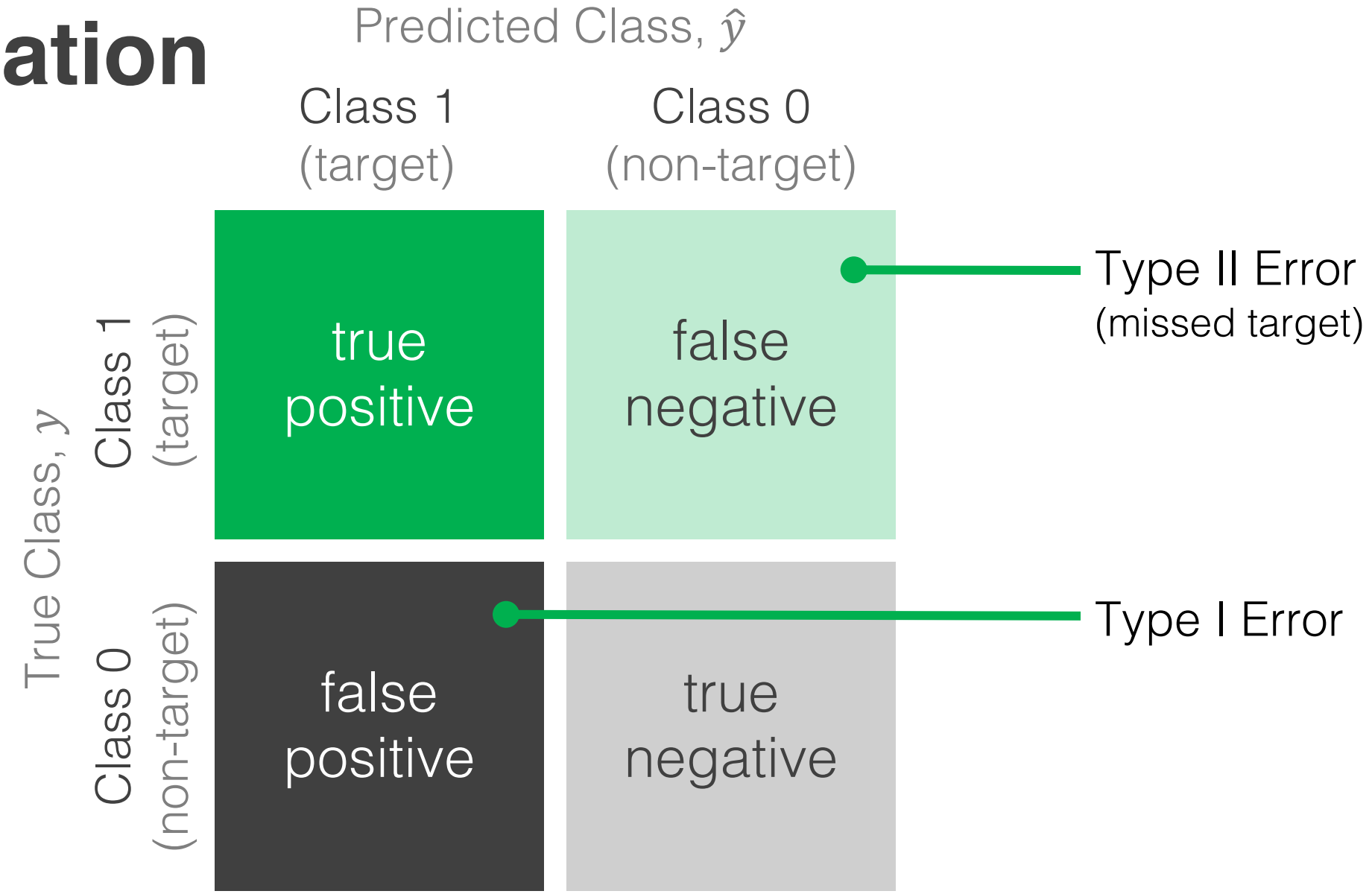
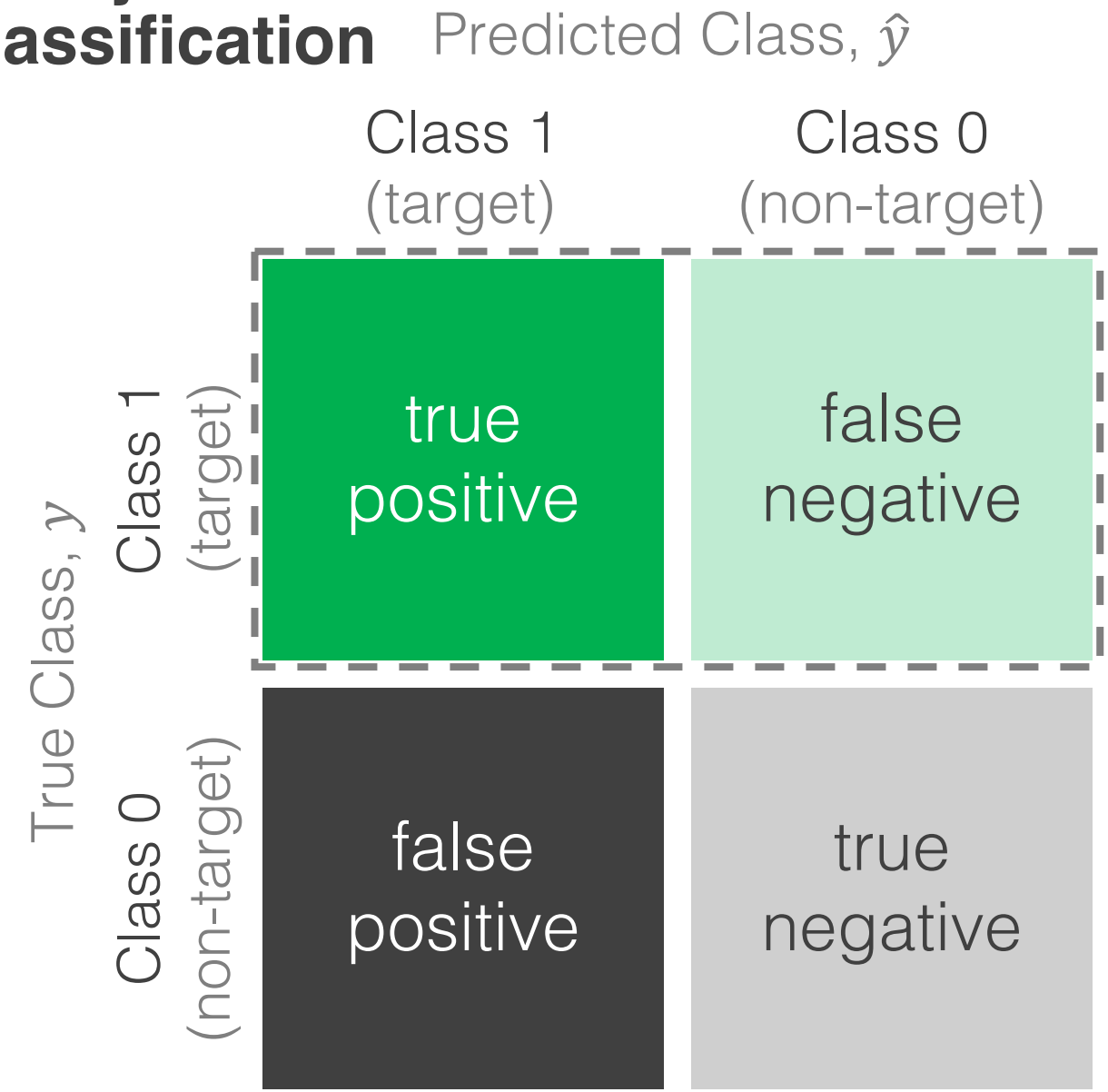


Image from: Ellis. *The Essential Guide to Effect Sizes*

Binary Classification



Binary Classification

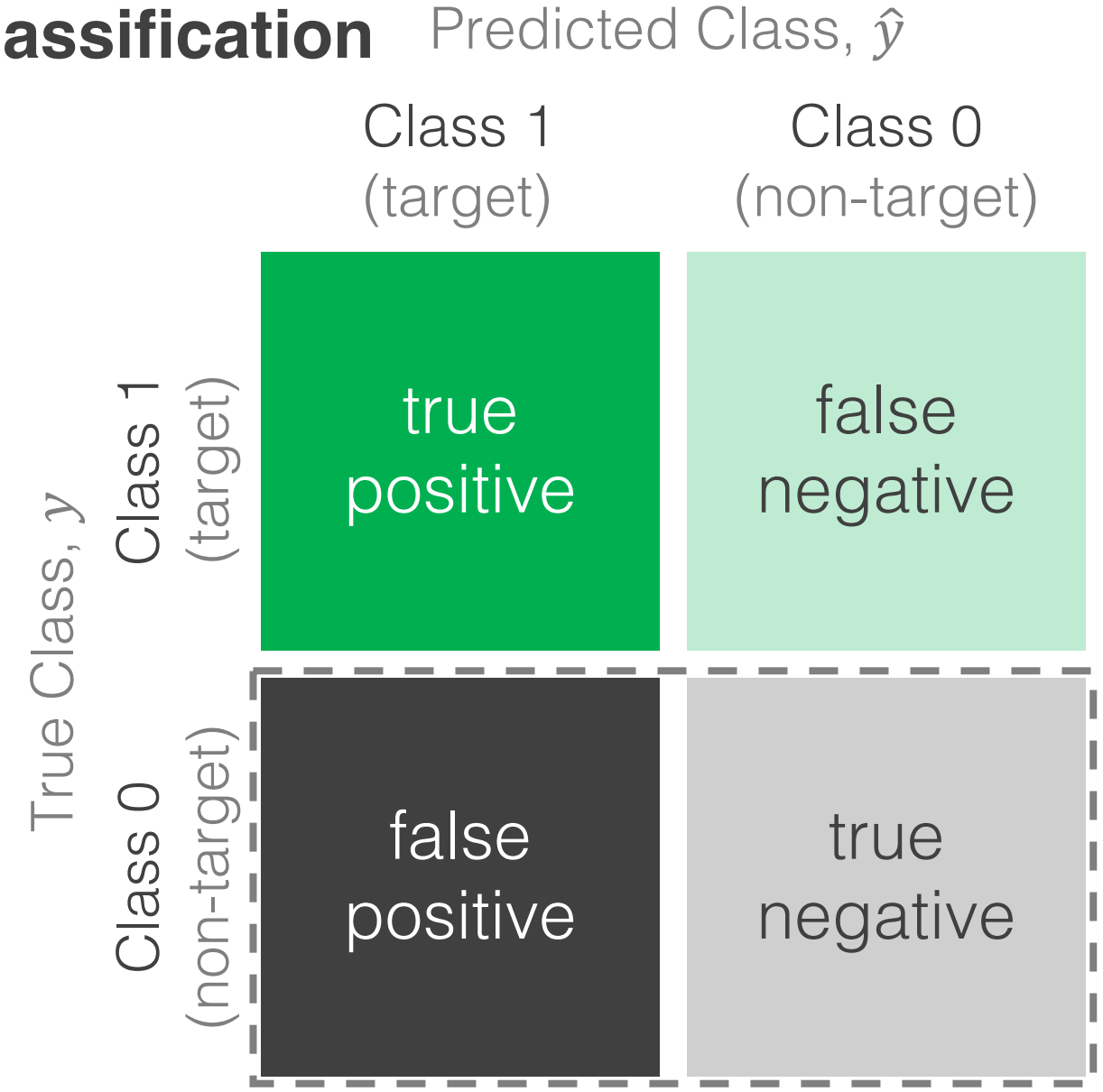


True positive rate
Probability of detection, p_D
Sensitivity
Recall

$$\frac{\text{true positive}}{\text{true positive} + \text{false negative}}$$

How many targets (Class 1) were correctly classified as targets?

Binary Classification

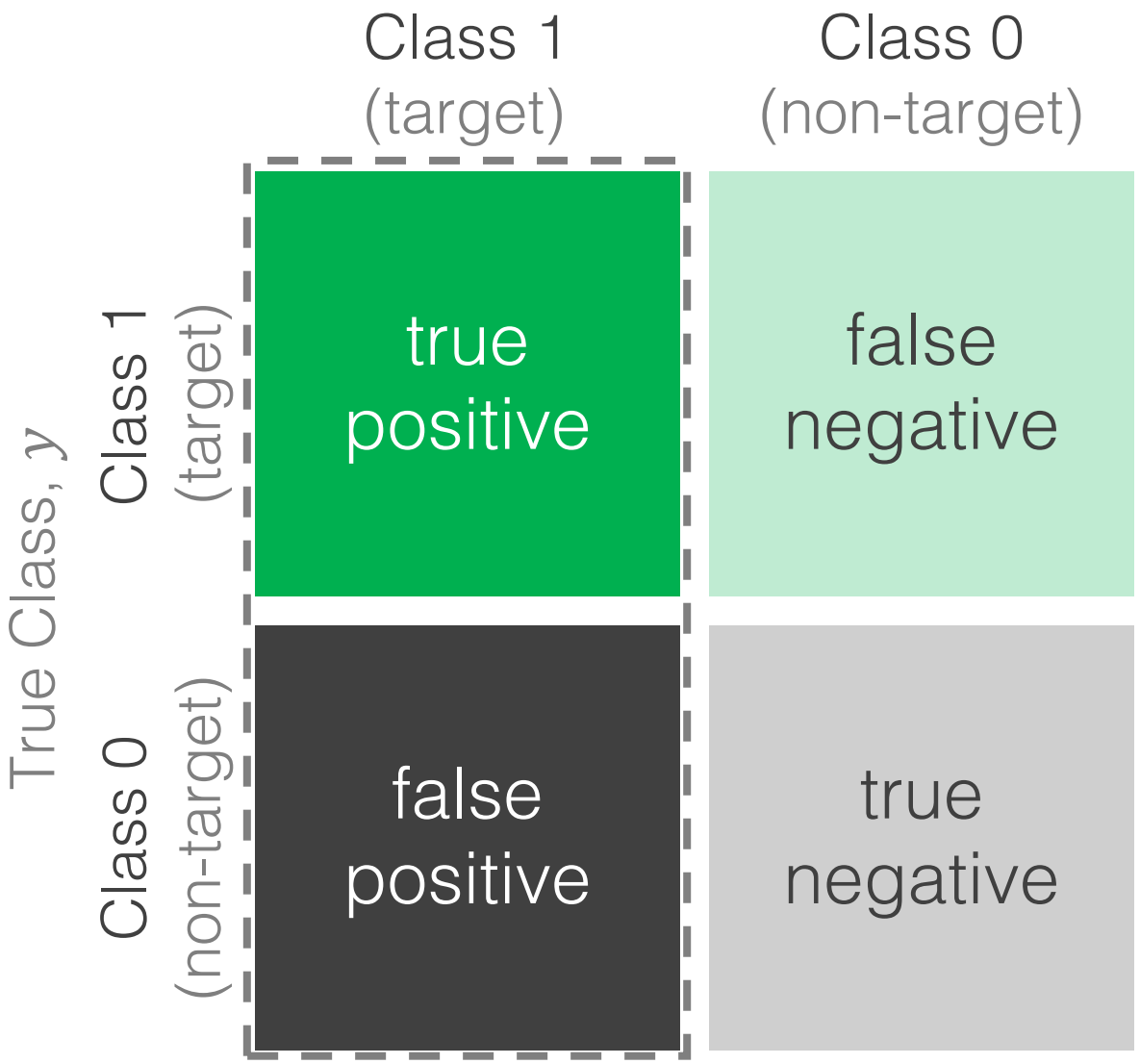


False positive rate
Probability of false alarm, p_{FA}

$$\frac{\text{false positive}}{\text{false positive} + \text{true negative}}$$

How many non-targets (Class 0) were incorrectly classified as targets?

Binary Classification

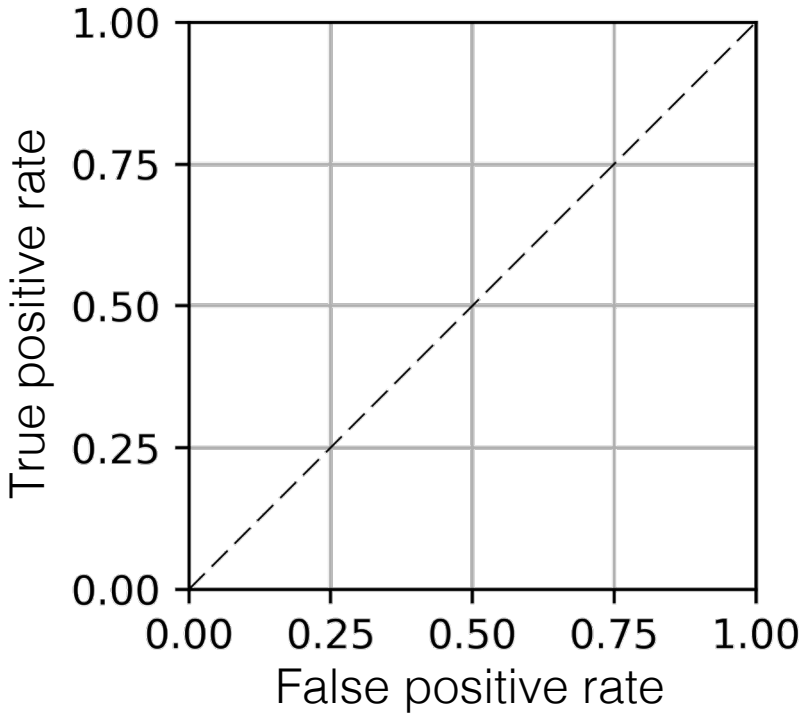


Precision

$$\frac{\text{true positive}}{\text{true positive} + \text{false positive}}$$

How many of the predicted targets are targets?

ROC Curves



Classifier decision rule:

$$\hat{y} = \begin{cases} 1, & \text{confidence score} > \text{thresh} \\ 0, & \text{confidence score} \leq \text{thresh} \end{cases}$$

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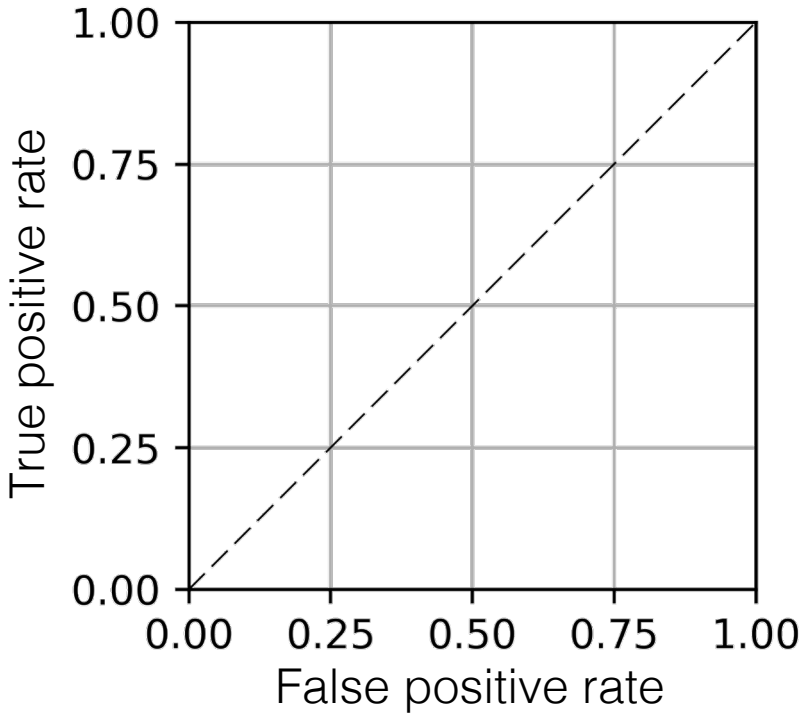
Estimate ($\hat{y}$)	True Class Label (y)	Classifier Confidence
?	1	1.40
?	1	0.95
?	0	0.80
?	1	0.60
?	0	-0.10

Threshold	# True Positives	True Positive Rate	# False Positives	False Positive Rate

ROC Curves



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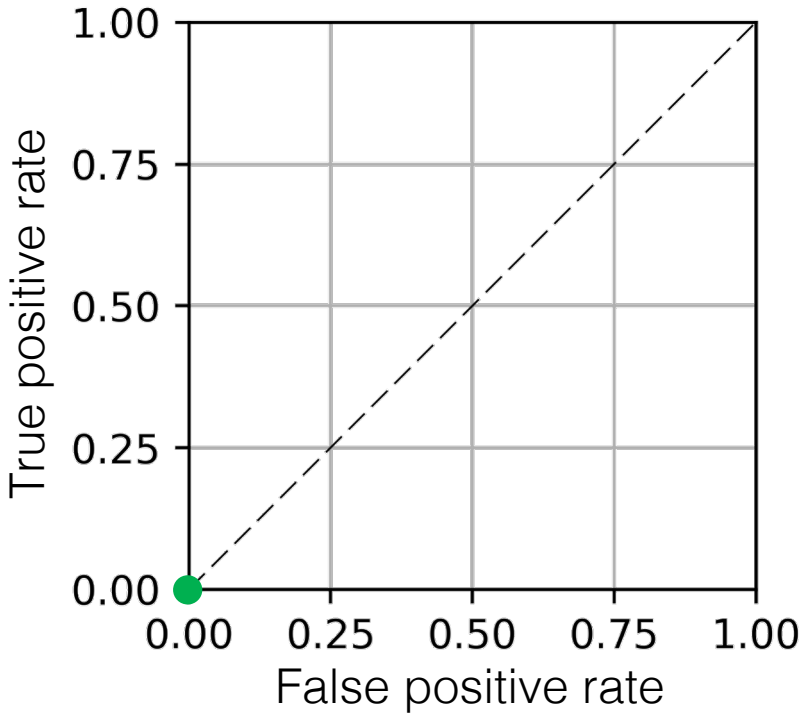
0	-0.10

Total Positives = 3

Total Negatives = 2

Threshold	# True Positives	True Positive Rate	# False Positives	False Positive Rate

ROC Curves



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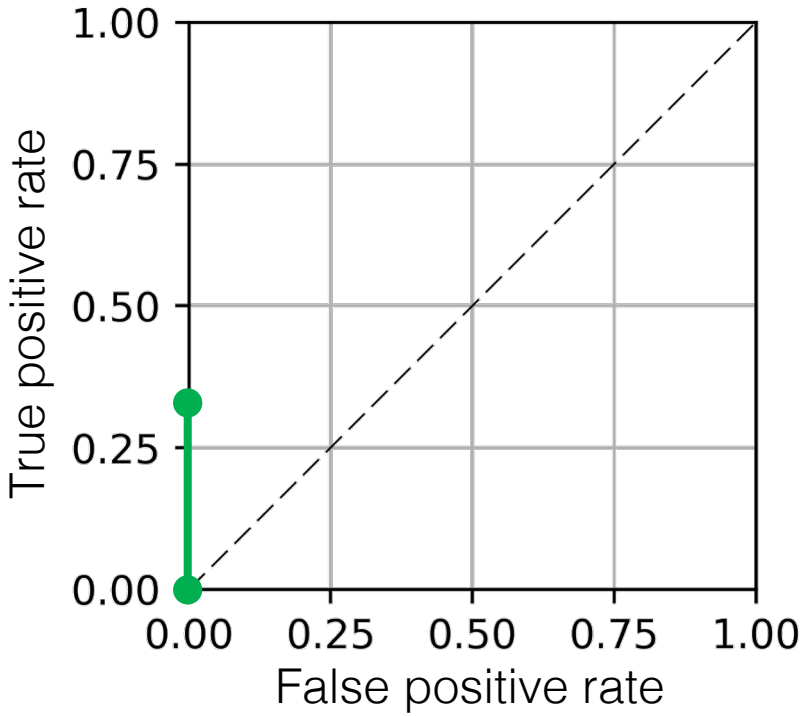
ROC Curves



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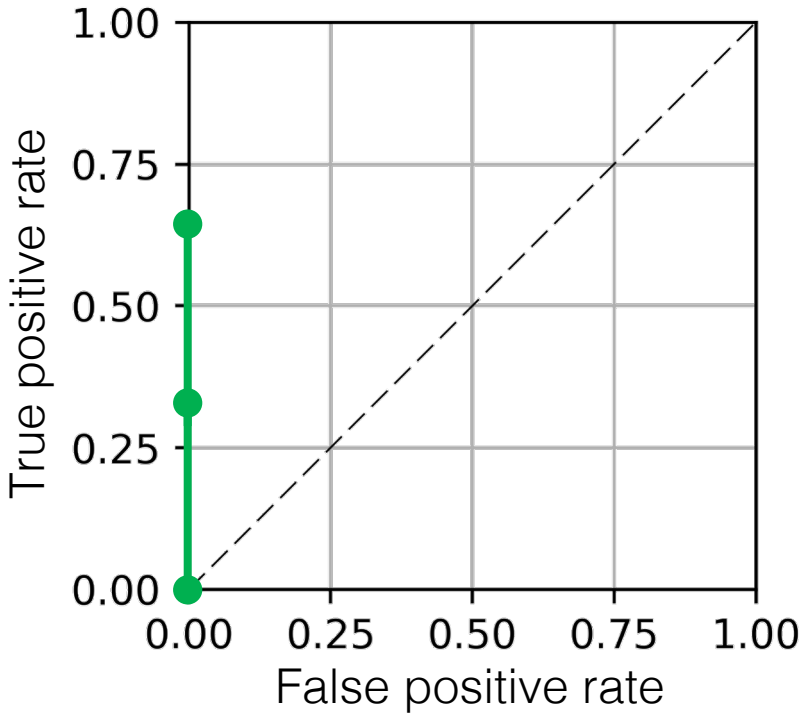
Threshold	# True Positives	True Positive Rate	# False Positives	False Positive Rate
∞	0	0	0	0
1.0	1	0.333	0	0

ROC Curves



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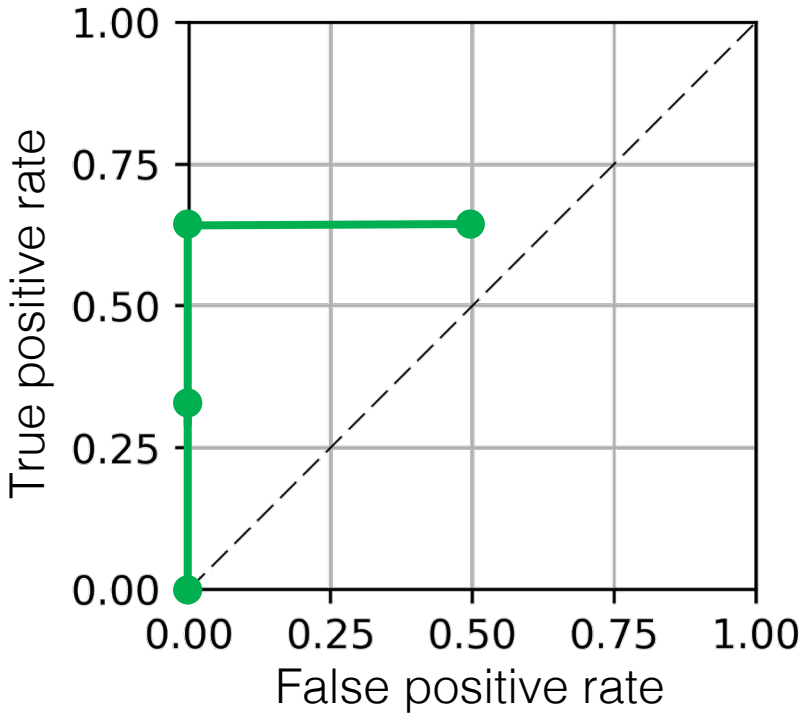
Threshold	# True Positives	True Positive Rate	# False Positives	False Positive Rate
∞	0	0	0	0
1.0	1	0.333	0	0
0.9	2	0.667	0	0

ROC Curves



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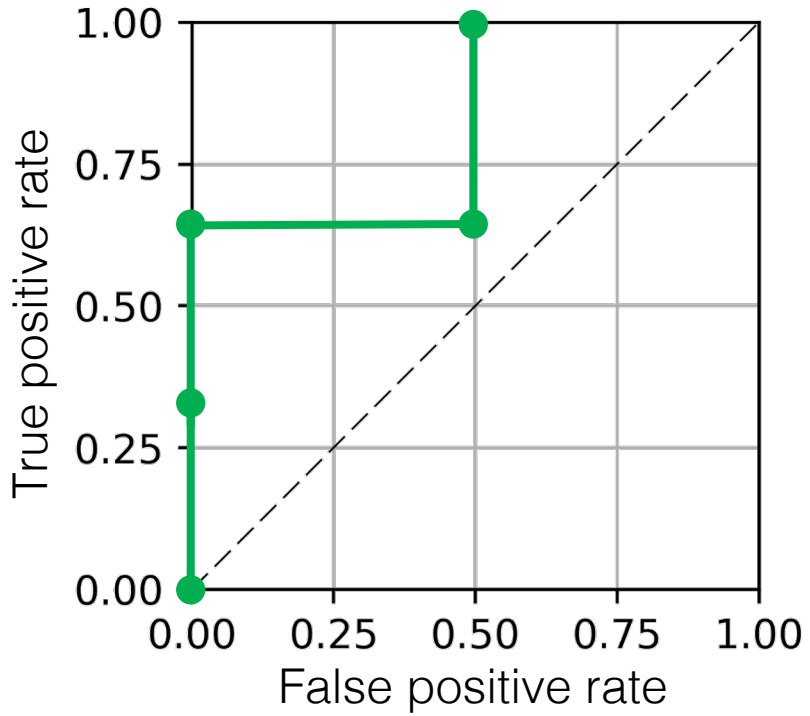
1.0	1	0.333	0	0
0.9	2	0.667	0	0
0.7	2	0.667	1	0.5

ROC Curves



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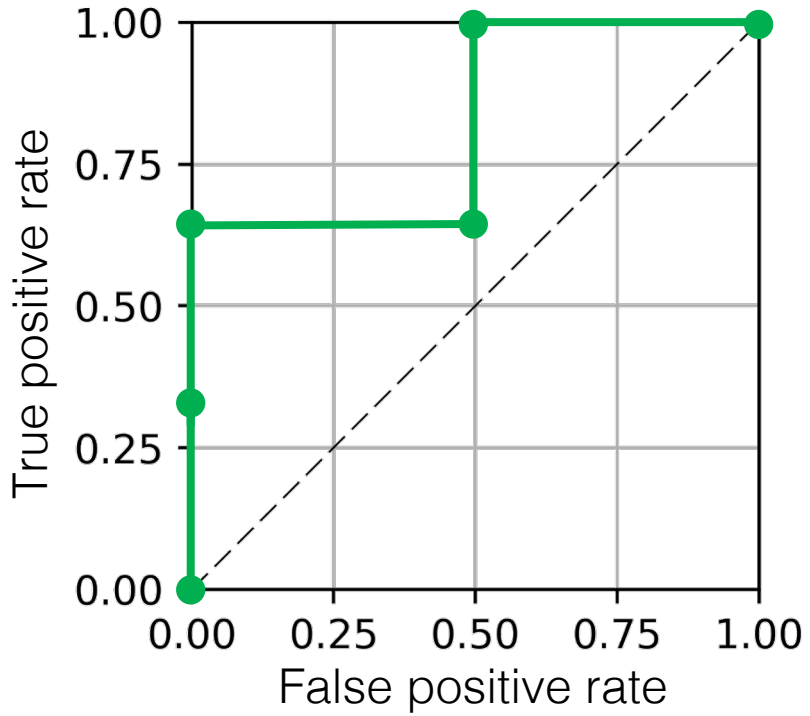
0.9	2	0.667	0	0
0.7	2	0.667	1	0.5
0.0	3	1	1	0.5

ROC Curves



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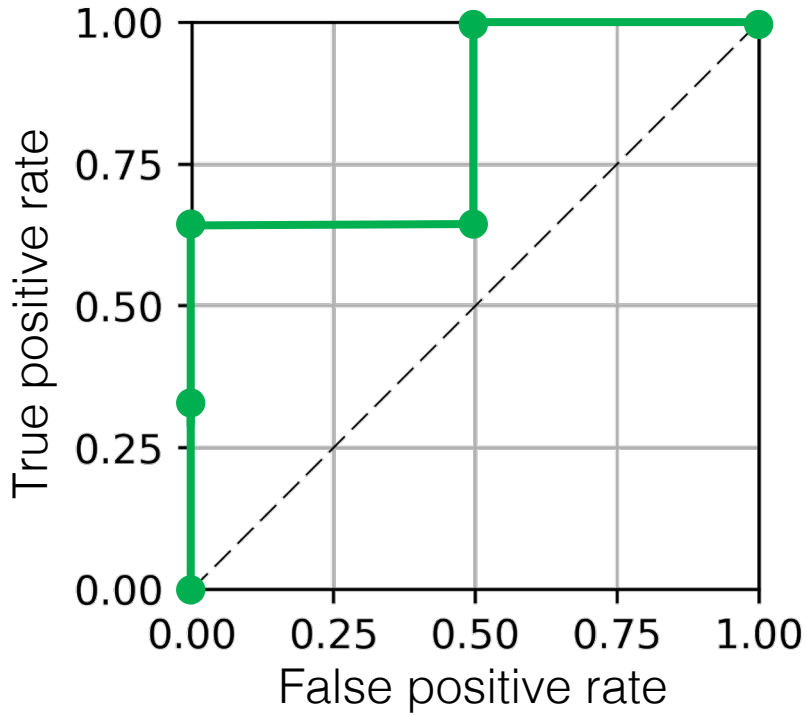
0.9	2	0.667	0	0
0.7	2	0.667	1	0.5
0.0	3	1	1	0.5
$-\infty$	3	1	2	1

ROC Curves



Classifier decision rule:

$$\hat{y} = \begin{cases} 1, & \text{confidence score} > \text{thresh} \\ 0, & \text{confidence score} \leq \text{thresh} \end{cases}$$

$$AUC = \left(\frac{2}{3}\right)\left(\frac{1}{2}\right) + (1)\left(\frac{1}{2}\right) = \frac{5}{6} \cong 0.833$$

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1	1	0.95
1	0	0.80
1	1	0.60
1	0	-0.10

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0.9	2	0.667	0	0
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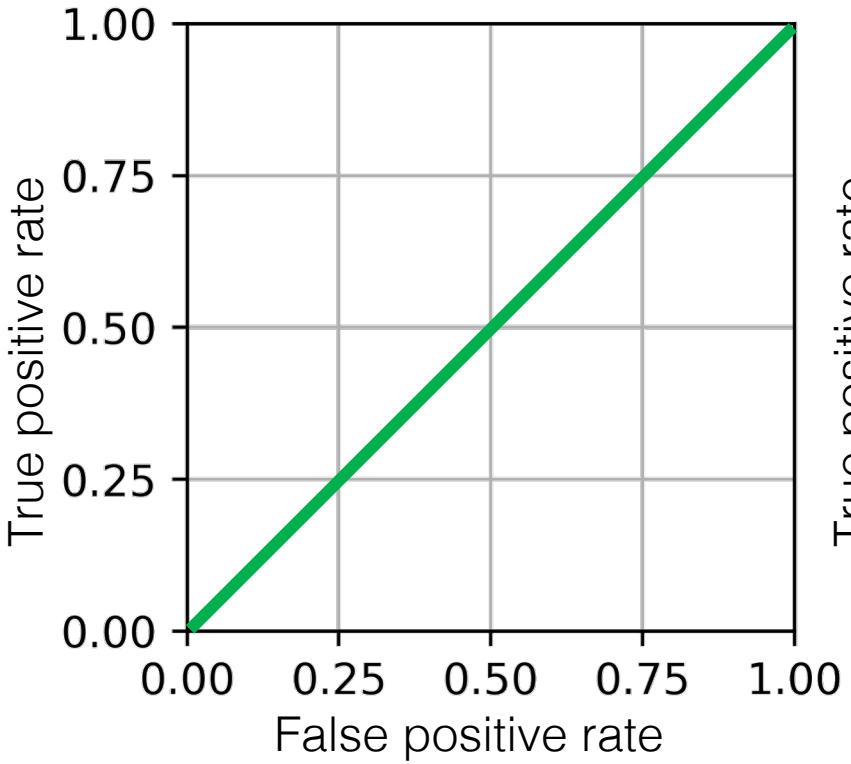
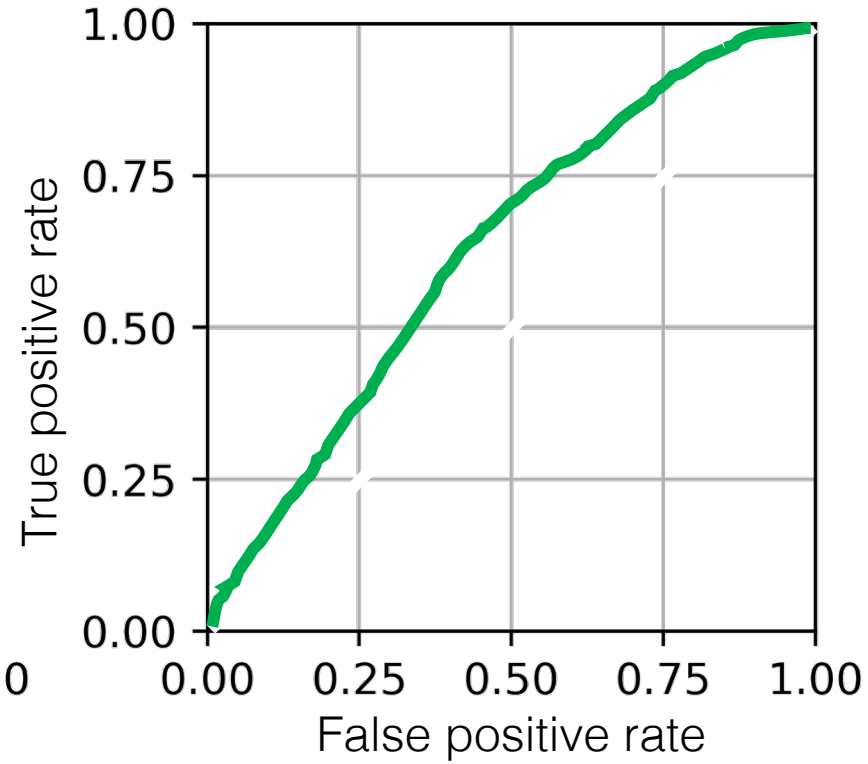
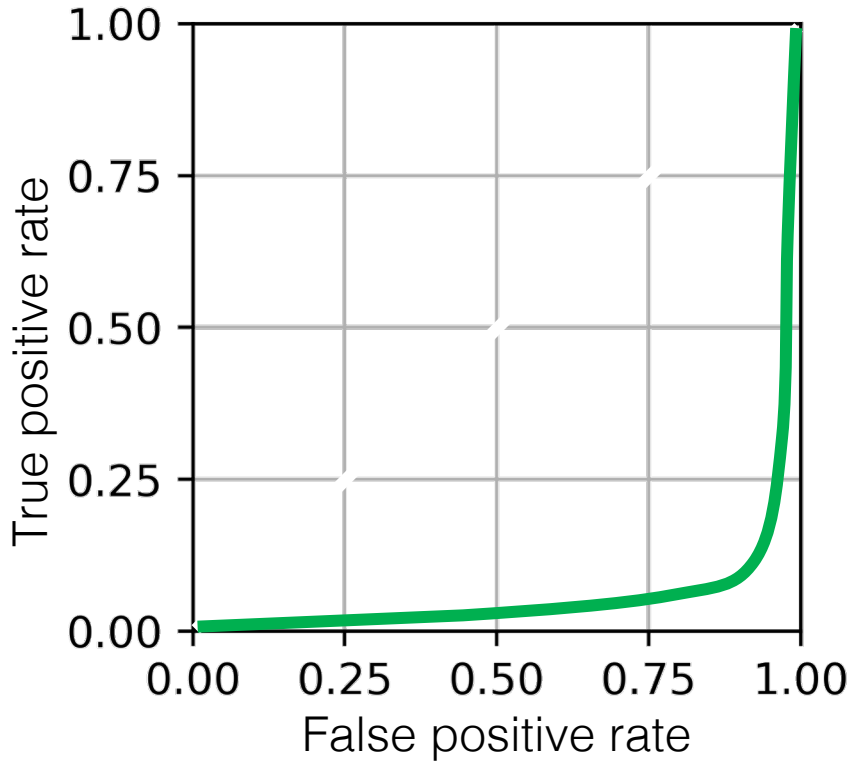
$-\infty$	3	1	2	1

ROC Curves: how do they compare?

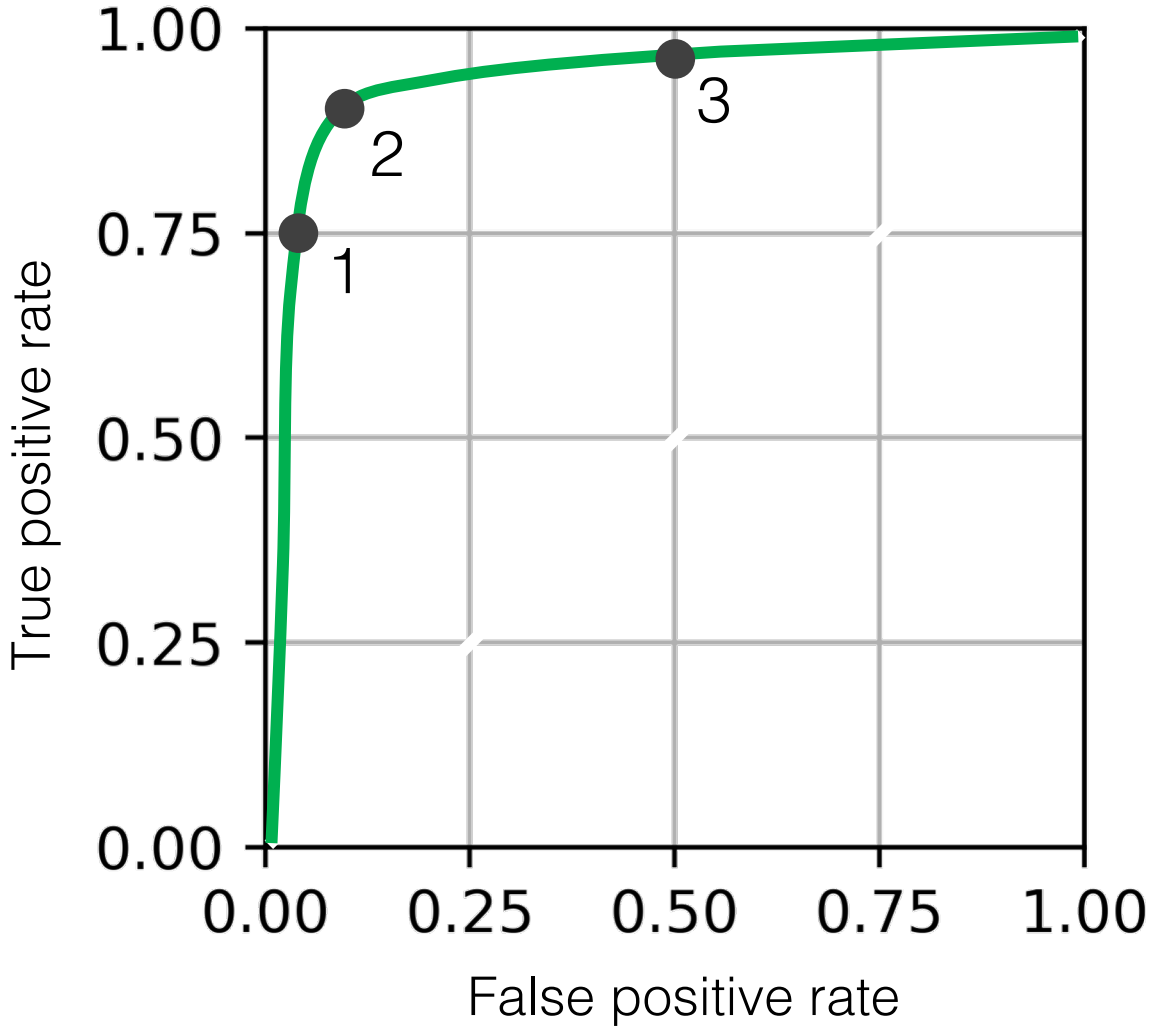






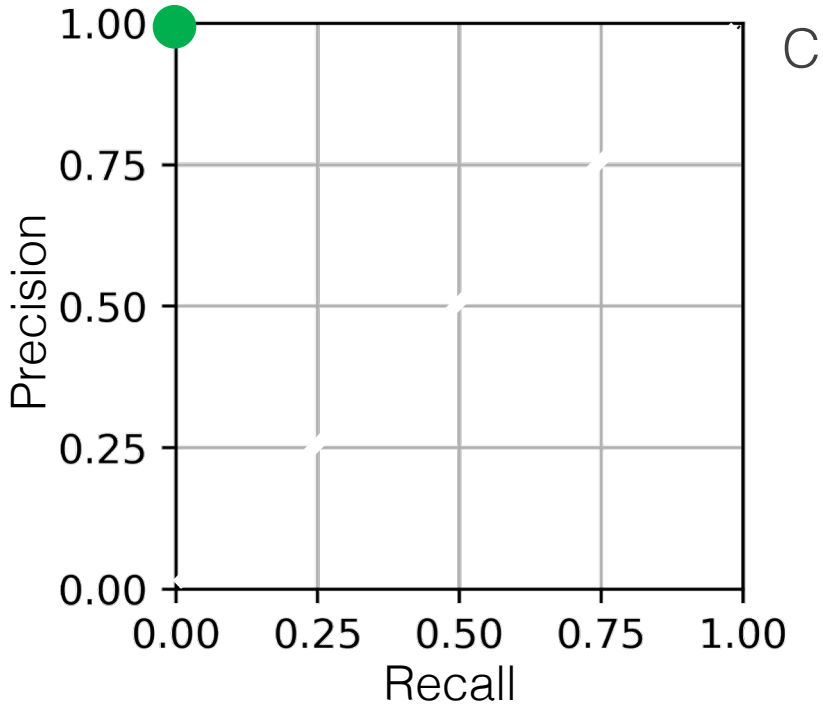
The model represented by this ROC curve is the most discriminative (but usually predicts incorrectly)

ROC Curves: where do we operate?



What does it mean to operate at a point on this curve?

PR Curves



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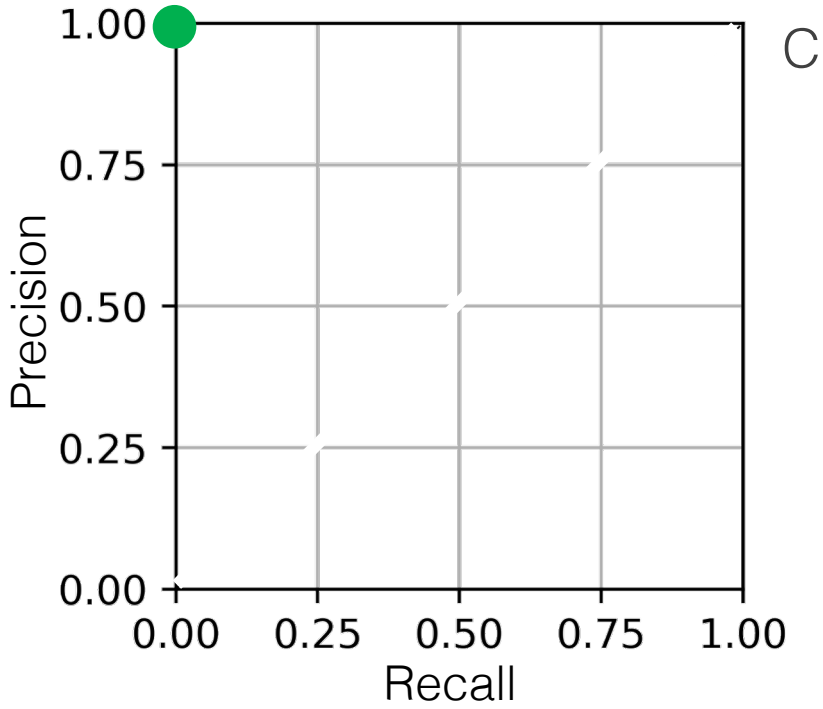
1	1.40
1	0.95
0	0.80
1	0.60
0	-0.10

Total Positives = 3 Total Negatives = 2

Threshold	# True Positives	Recall	# Predicted Positive	Precision

PR Curves



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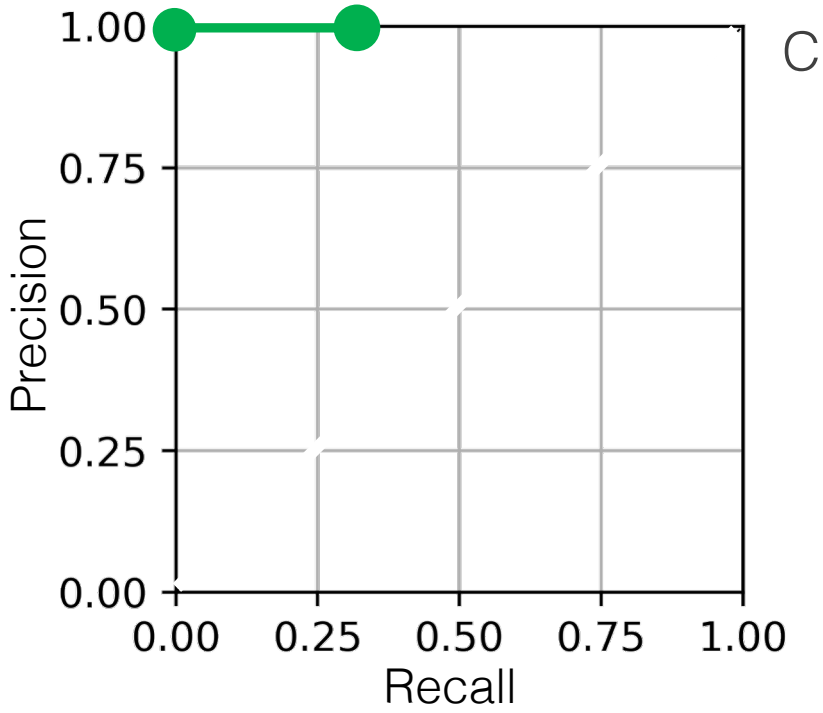
Total Positives = 3

Total Negatives = 2

Threshold	# True Positives	Recall	# Predicted Positive	Precision
∞	0	0	0	undefined

PR Curves



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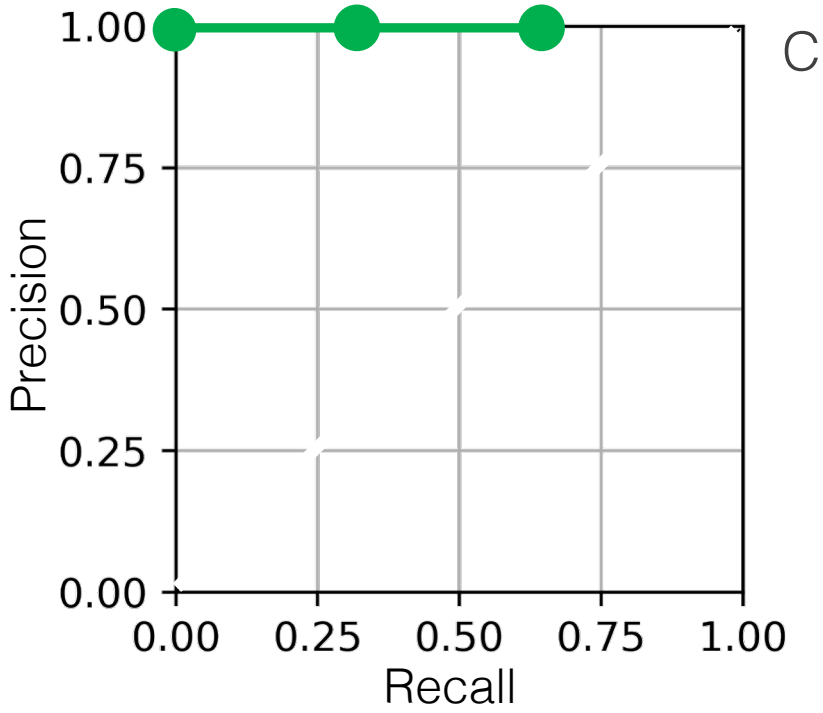

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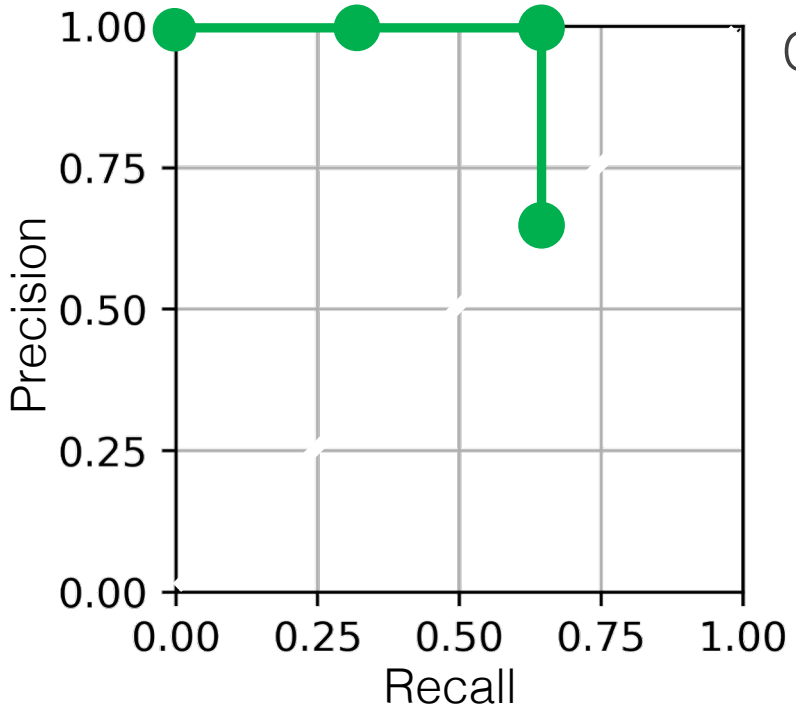
0.9	2	0.667	2	1

PR Curves



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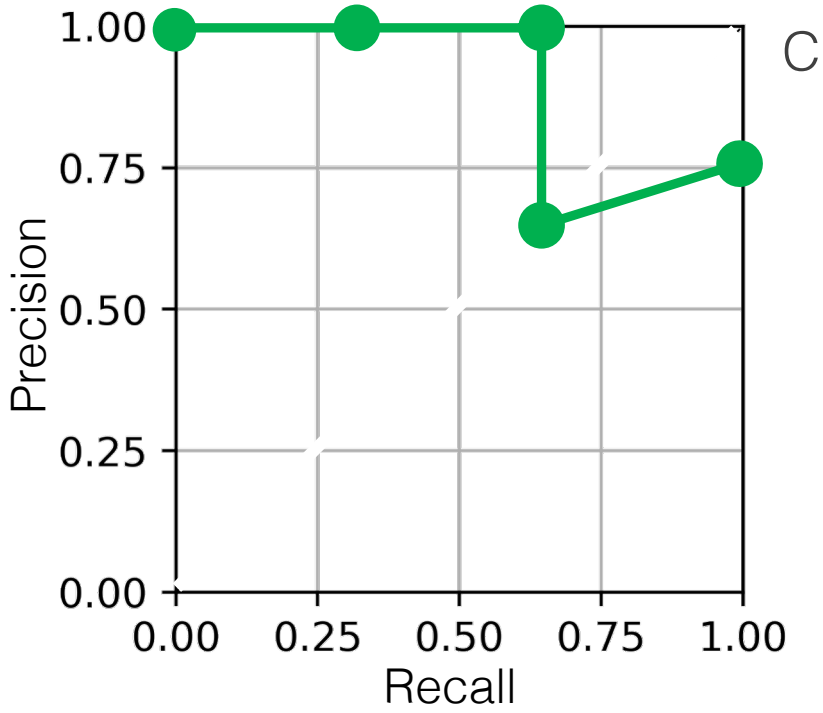
0.9	2	0.667	2	1
0.7	2	0.667	3	0.667

PR Curves



Classifier decision rule:

$$\hat{y} = \begin{cases} 1, \text{confidence score} > \text{thresh} \\ 0, \text{confidence score} \leq \text{thresh} \end{cases}$$

$$\frac{\text{true positive}}{\text{true positive} + \text{false negative}}$$

$$\frac{\text{true positive}}{\text{true positive} + \text{false positive}}$$

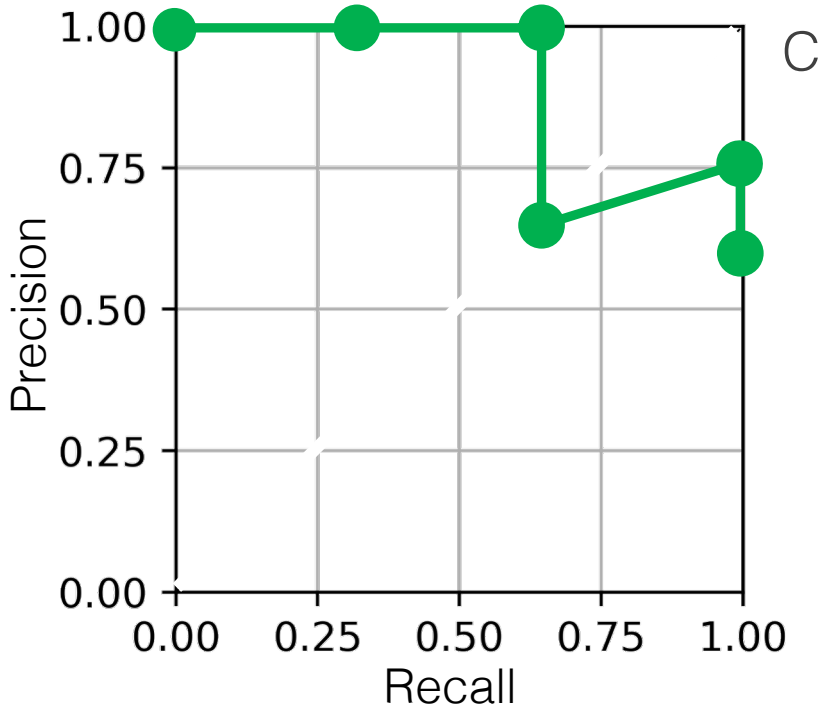
Estimate ($\hat{y}$)	True Class Label (y)	Classifier Confidence
1	1	1.40
1	1	0.95
1	0	0.80
1	1	0.60
0	0	-0.10

Total Positives = 3

Total Negatives = 2

Threshold	# True Positives	Recall	# Predicted Positive	Precision
∞	0	0	0	undefined
1.0	1	0.333	1	1
0.9	2	0.667	2	1
0.7	2	0.667	3	0.667
0.0	3	1	4	0.75

PR Curves



Classifier decision rule:

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0.7	2	0.667	3	0.667
0.0	3	1	4	0.75
$-\infty$	3	1	5	0.6

Be wary of overall accuracy as sole metric

Case study 1

i	y_i	$\hat{y}_i$
1	**1**	**1**
2	**1**	**1**
3	**1**	**1**
4	**1**	**1**
5	**1**	**1**
6	**1**	**1**
7	**1**	**0**
8	**0**	**1**
9	**0**	**0**
10	**0**	**0**
11	**0**	**0**
12	**0**	**0**
13	**0**	**0**
14	**0**	**0**
15	**0**	**0**

Overall classification accuracy = 13/15 = **0.87**

ROC Curves measure the tradeoff between…

A False positive rate = 1/8 = **0.13**

B True positive rate (Recall) = 6/7 = **0.86**

PR Curves measure the tradeoff between…

B True positive rate (Recall) = 6/7 = **0.86**

C Precision= 6/7 = **0.86**

A

$$\frac{\text{false positive}}{\text{false positive} + \text{true negative}}$$

B

$$\frac{\text{true positive}}{\text{true positive} + \text{false negative}}$$

C

$$\frac{\text{true positive}}{\text{true positive} + \text{false positive}}$$

Case study 2

i	y_i	$\hat{y}_i$
1	**1**	**1**
2	**1**	**1**
3	**1**	**0**
4	**1**	**0**
5	**0**	**0**
6	**0**	**0**
7	**0**	**0**
8	**0**	**0**
9	**0**	**0**
10	**0**	**0**
11	**0**	**0**
12	**0**	**0**
13	**0**	**0**
14	**0**	**0**
15	**0**	**0**

Overall classification accuracy = 13/15 = **0.87**

ROC Curves measure the tradeoff between…

A False positive rate = 0/11 = **0**

B True positive rate (Recall) = 2/4 = **0.5**

PR Curves measure the tradeoff between…

B True positive rate (Recall) = 2/4 = **0.5**

C Precision= 2/2 = **1**

A

$$\frac{\text{false positive}}{\text{false positive} + \text{true negative}}$$

B

$$\frac{\text{true positive}}{\text{true positive} + \text{false negative}}$$

C

$$\frac{\text{true positive}}{\text{true positive} + \text{false positive}}$$

Case study 3

i	y_i	$\hat{y}_i$
1	**1**	**1**
2	**1**	**1**
3	**1**	**1**
4	**1**	**1**
5	**1**	**1**
6	**1**	**1**
7	**1**	**1**
8	**1**	**1**
9	**1**	**1**
10	**1**	**1**
11	**1**	**1**
12	**1**	**1**
13	**1**	**1**
14	**0**	**1**
15	**0**	**1**

Overall classification accuracy = 13/15 = **0.87**

ROC Curves measure the tradeoff between…

A False positive rate = 2/2 = **1**

B True positive rate (Recall) = 13/13 = **1**

PR Curves measure the tradeoff between…

B True positive rate (Recall) = 13/13 = **1**

C Precision= 13/15 = **0.87**

A

$$\frac{\text{false positive}}{\text{false positive} + \text{true negative}}$$

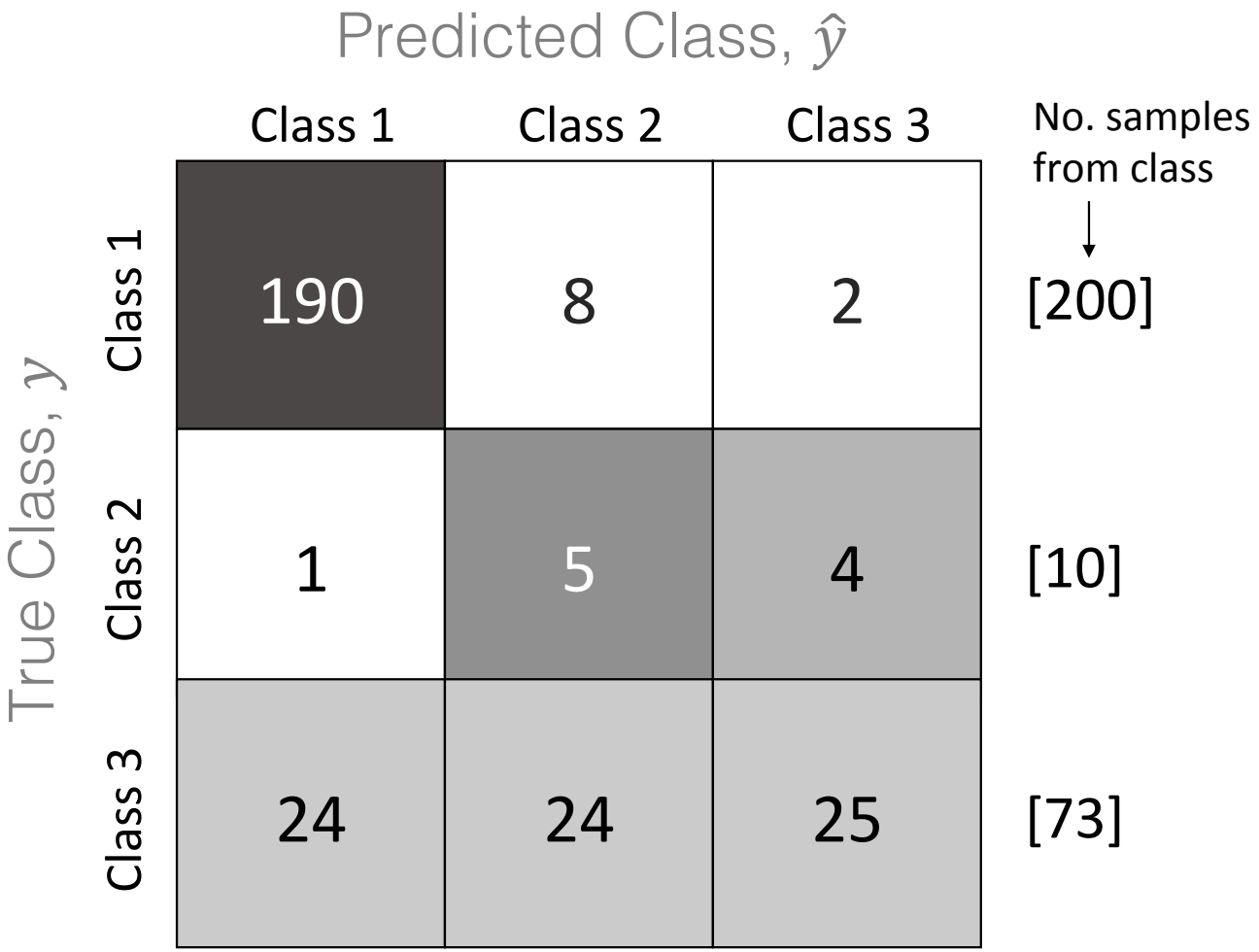
B

$$\frac{\text{true positive}}{\text{true positive} + \text{false negative}}$$

C

$$\frac{\text{true positive}}{\text{true positive} + \text{false positive}}$$

Multiclass Classification: Confusion Matrix



confusion matrix with number of samples

F_1-score

$$F_1 = 2\frac{1}{\frac{1}{\text{recall}} + \frac{1}{\text{precision}}}$$

Harmonic mean of precision and recall

$$= 2\frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

Generally:

$$F_\beta = (1 + \beta^2)\frac{\text{precision} \cdot \text{recall}}{\beta^2 \cdot \text{precision} + \text{recall}}$$

β controls the relative weight of precision/recall

Multiclass F_1

Micro-average: Calculate precision and recall metrics globally by counting the total true positives, false negatives, and false positives
(average for the whole dataset)

Macro-average: Use the average precision and recall for each class label
(average of class-averages)